



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:11 PM GMT

PDB ID : 1J5O
Title : CRYSTAL STRUCTURE OF MET184ILE MUTANT OF HIV-1 REVERSE TRANSCRIPTASE IN COMPLEX WITH DOUBLE STRANDED DNA TEMPLATE-PRIMER
Authors : Sarafianos, S.G.; Das, K.; Arnold, E.
Deposited on : 2002-05-24
Resolution : 3.50 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

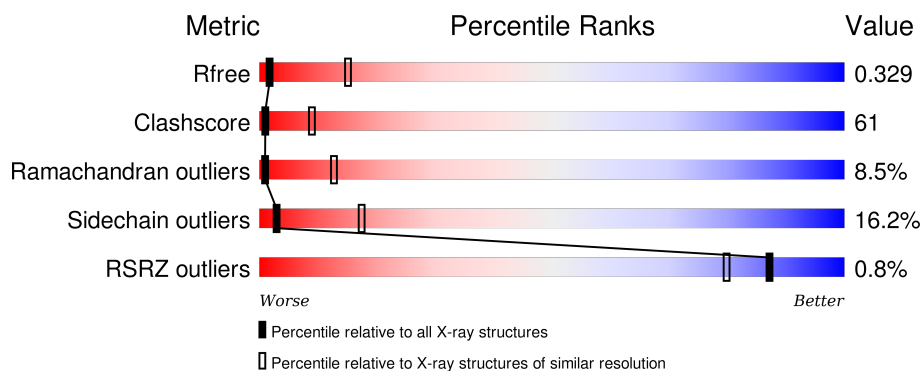
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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

Mol	Chain	Length	Quality of chain
1	T	19	<div> <div>11%</div> <div>5% 95%</div> </div>
2	P	18	<div> <div>6%</div> <div>89% 11%</div> </div>
3	A	558	<div> <div>28% 56% 14%</div> </div>
4	B	430	<div> <div>% 25% 56% 17%</div> </div>
5	L	214	<div> <div>% 25% 59% 15%</div> </div>

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Mol	Chain	Length	Quality of chain
6	H	220	 A horizontal bar chart showing the quality of chain H. The bar is divided into three segments: green (27%), yellow (61%), and orange (11%). The percentages are labeled below the bar.

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11720 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 DNA chain called 5'-D(*AP*TP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	19	Total	C	N	O	P	0	0	0
			390	184	80	108	18			

- Molecule 2 is a DNA chain called 5'-D(*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP*CP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	18	Total	C	N	O	P	0	0	0
			363	173	64	109	17			

- Molecule 3 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	558	Total	C	N	O	S	0	0	0
			4292	2778	713	795	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	ILE	MET	ENGINEERED	UNP P03366
A	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 4 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	430	Total	C	N	O	S	0	0	0
			3411	2217	568	620	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	184	ILE	MET	ENGINEERED	UNP P03366
B	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 5 is a protein called ANTIBODY (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	214	Total	C	N	O	S	0	0	0
			1616	1010	256	343	7			

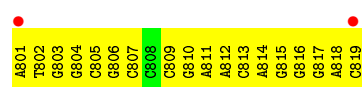
- Molecule 6 is a protein called ANTIBODY (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	220	Total	C	N	O	S	0	0	0
			1648	1037	270	333	8			

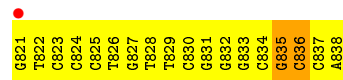
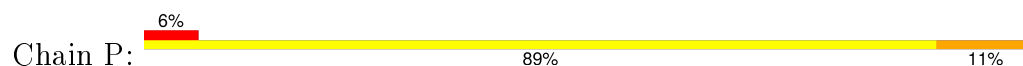
3 Residue-property plots

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

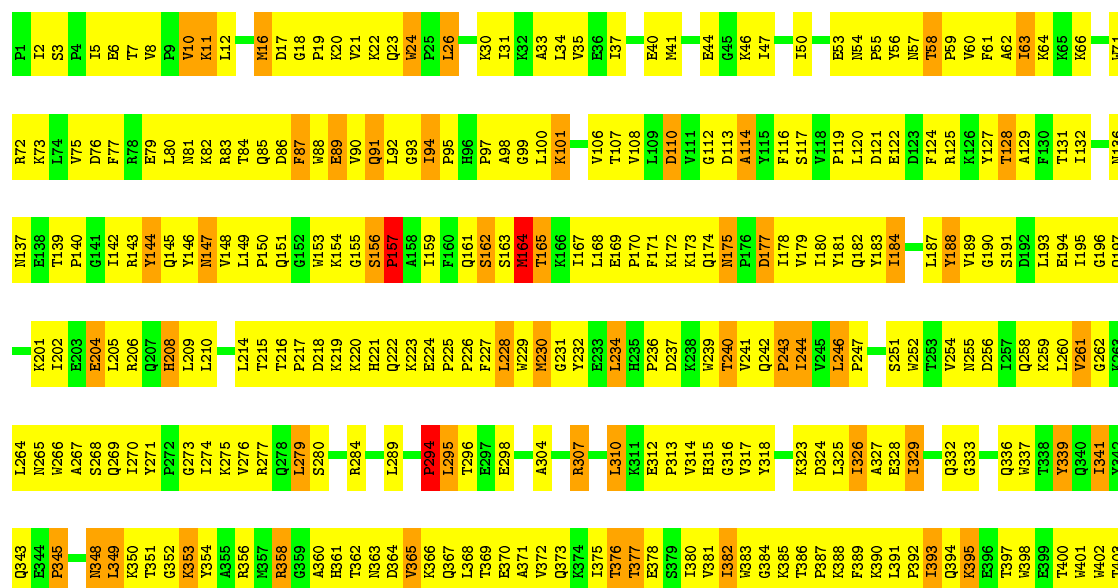
- Molecule 1: 5'-D(*AP*TP*GP*GP*CP*GP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*C)-3'

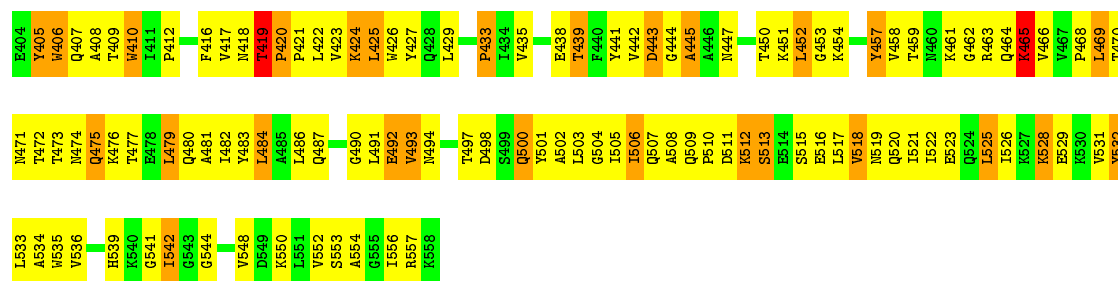


- Molecule 2: 5'-D(*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP*CP*CP*A)-3'

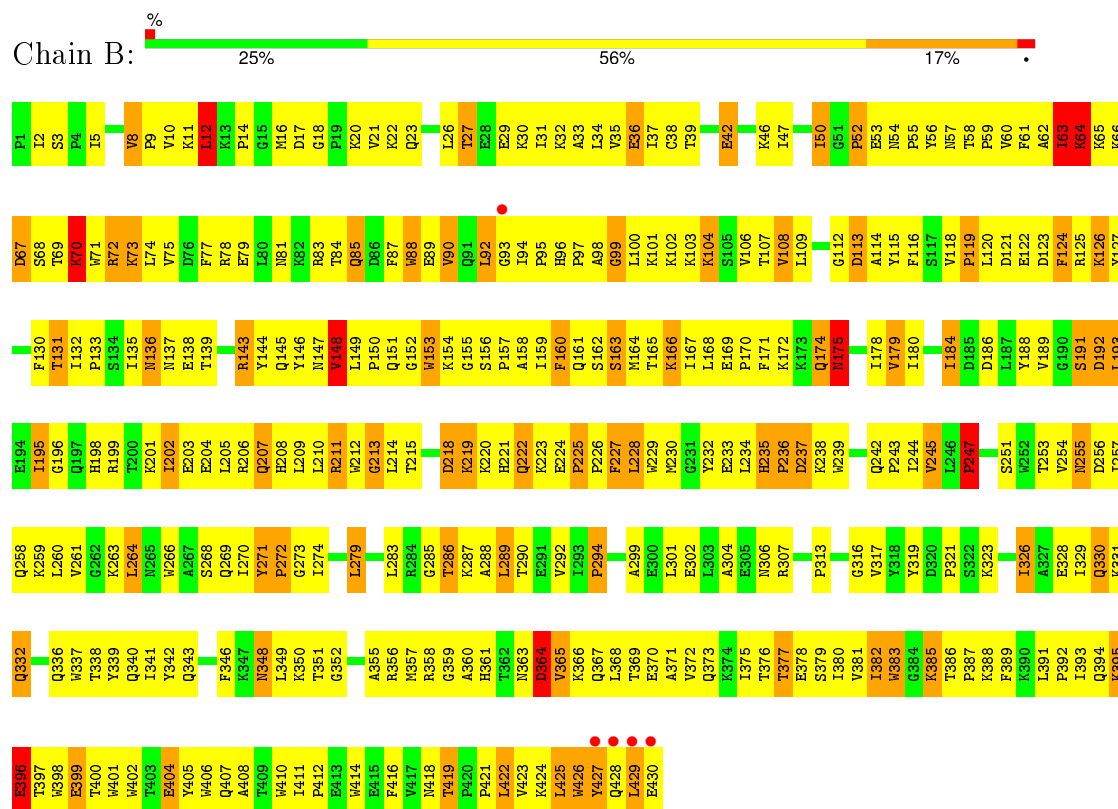


- Molecule 3: Reverse transcriptase

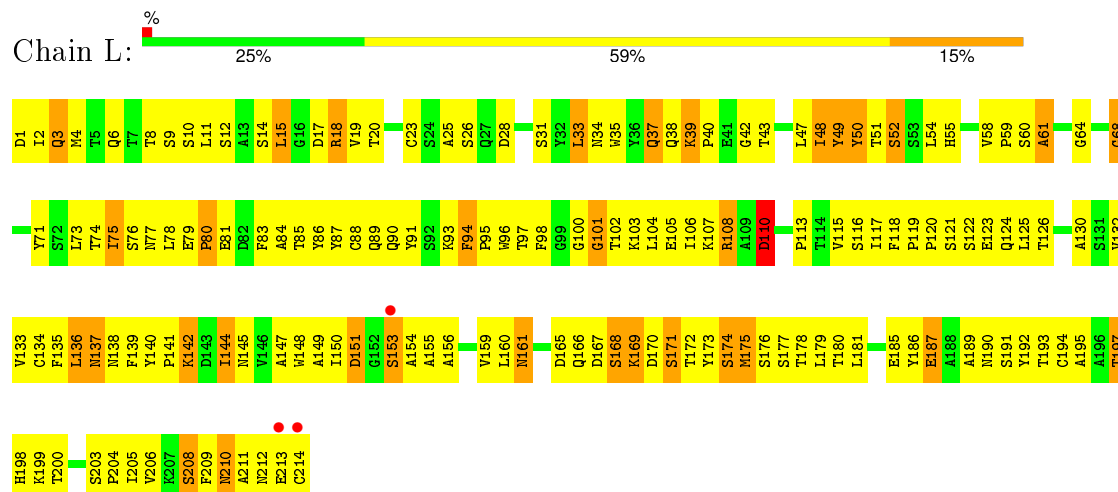




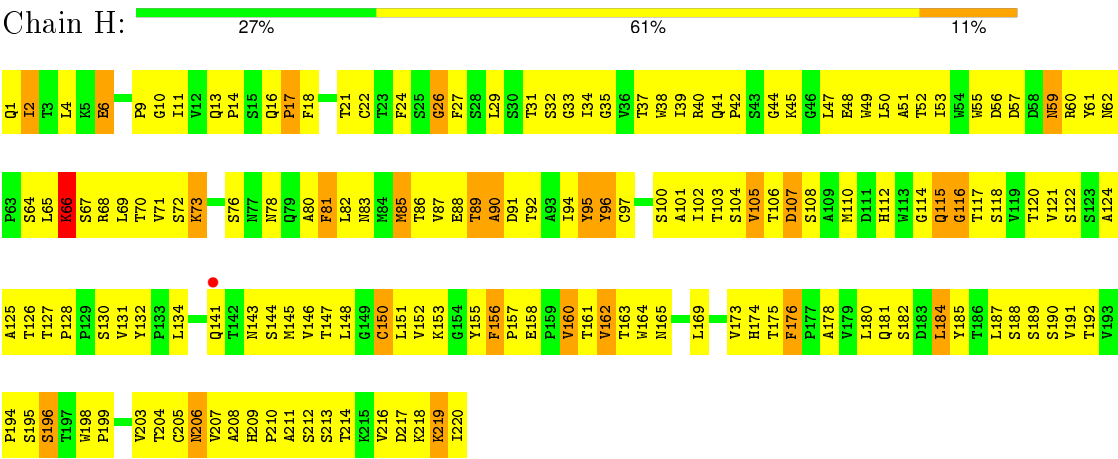
• Molecule 4: Reverse transcriptase



• Molecule 5: ANTIBODY (LIGHT CHAIN)



● Molecule 6: ANTIBODY (HEAVY CHAIN)



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	169.18Å 169.18Å 221.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.50 39.97 – 3.50	Depositor EDS
% Data completeness (in resolution range)	91.5 (10.00-3.50) 91.4 (39.97-3.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.48Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.262 , 0.338 0.259 , 0.329	Depositor DCC
R_{free} test set	1219 reflections (3.04%)	DCC
Wilson B-factor (Å ²)	98.8	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 114.3	EDS
Estimated twinning fraction	0.049 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 42000 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	11720	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	T	0.55	0/439	0.76	0/676
2	P	0.56	1/405 (0.2%)	0.81	0/623
3	A	0.56	0/4404	0.78	2/6017 (0.0%)
4	B	0.63	0/3510	0.84	4/4784 (0.1%)
5	L	0.54	0/1654	0.85	0/2256
6	H	0.58	0/1691	0.85	0/2320
All	All	0.58	1/12103 (0.0%)	0.82	6/16676 (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
2	P	0	1
3	A	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	835	DG	O3'-P	-5.99	1.53	1.61

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	247	PRO	N-CA-CB	6.75	111.39	103.30
4	B	243	PRO	N-CA-CB	6.31	110.87	103.30
3	A	294	PRO	N-CA-CB	5.91	110.39	103.30
3	A	247	PRO	N-CA-CB	5.63	110.06	103.30
4	B	313	PRO	N-CA-CB	5.37	109.74	103.30
4	B	186	ASP	N-CA-C	5.08	124.72	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	144	TYR	Sidechain
2	P	836	DC	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	390	0	212	55	0
2	P	363	0	204	103	0
3	A	4292	0	4127	482	0
4	B	3411	0	3300	446	0
5	L	1616	0	1517	174	0
6	H	1648	0	1602	184	0
All	All	11720	0	10962	1380	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 61.

All (1380) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:822:DT:H2''	2:P:823:DC:C6	1.75	1.22
1:T:803:DG:H2''	1:T:804:DG:C5'	1.77	1.14
2:P:831:DG:H2''	2:P:832:DG:H5'	1.17	1.11
3:A:20:LYS:HA	3:A:57:ASN:H	1.15	1.10
3:A:333:GLY:H	3:A:336:GLN:HB2	0.99	1.09
6:H:61:TYR:HE2	6:H:70:THR:HA	1.17	1.08
2:P:823:DC:H2''	2:P:824:DC:C5'	1.84	1.07
2:P:823:DC:H2''	2:P:824:DC:H5''	1.07	1.07
4:B:103:LYS:HZ2	4:B:191:SER:HA	1.20	1.05
3:A:106:VAL:HB	3:A:227:PHE:HE2	1.17	1.05
2:P:823:DC:C2'	2:P:824:DC:H5''	1.85	1.04
2:P:825:DC:H2''	2:P:826:DT:H5'	1.04	1.03
2:P:825:DC:H2''	2:P:826:DT:C5'	1.87	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:803:DG:H2''	1:T:804:DG:H5'	1.38	1.03
3:A:20:LYS:HG2	3:A:56:TYR:HA	1.42	1.02
2:P:833:DG:H2''	2:P:834:DC:OP2	1.56	1.01
4:B:103:LYS:HZ3	4:B:192:ASP:H	1.04	1.00
5:L:33:LEU:HD21	5:L:88:CYS:SG	2.03	0.98
1:T:815:DG:H2''	1:T:816:DG:C8	1.99	0.97
4:B:60:VAL:HG12	4:B:75:VAL:HG22	1.46	0.96
2:P:825:DC:C2'	2:P:826:DT:H5'	1.96	0.95
3:A:333:GLY:N	3:A:336:GLN:HB2	1.80	0.95
5:L:137:ASN:HA	5:L:174:SER:HB3	1.49	0.95
1:T:817:DG:H2''	1:T:818:DA:H5'	1.49	0.94
3:A:279:LEU:HD12	3:A:279:LEU:H	1.31	0.94
6:H:61:TYR:CE2	6:H:70:THR:HA	2.01	0.94
4:B:50:ILE:HD12	4:B:145:GLN:HG3	1.47	0.94
2:P:821:DG:H2'	2:P:822:DT:H71	1.47	0.94
2:P:831:DG:C2'	2:P:832:DG:H5'	1.99	0.93
5:L:161:ASN:HB3	5:L:177:SER:HA	1.50	0.93
5:L:15:LEU:HD21	5:L:80:PRO:HD3	1.52	0.92
6:H:40:ARG:NH1	6:H:91:ASP:HA	1.83	0.91
3:A:101:LYS:HD2	3:A:101:LYS:H	1.33	0.91
2:P:822:DT:H2''	2:P:823:DC:H6	1.28	0.91
6:H:195:SER:O	6:H:199:PRO:HD2	1.71	0.91
1:T:801:DA:H2''	1:T:802:DT:C7	2.00	0.91
3:A:458:VAL:HG12	3:A:459:THR:H	1.33	0.90
5:L:144:ILE:HG12	5:L:145:ASN:H	1.35	0.90
4:B:342:TYR:HB3	4:B:348:ASN:HA	1.54	0.90
6:H:14:PRO:HG3	6:H:121:VAL:HG12	1.54	0.89
1:T:810:DG:H2''	1:T:811:DA:C8	2.07	0.89
6:H:163:THR:H	6:H:206:ASN:ND2	1.70	0.89
3:A:178:ILE:HA	3:A:191:SER:HB3	1.51	0.89
3:A:454:LYS:HA	3:A:468:PRO:HA	1.54	0.89
1:T:811:DA:H2''	1:T:812:DA:OP2	1.70	0.88
3:A:106:VAL:HB	3:A:227:PHE:CE2	2.09	0.88
3:A:62:ALA:HA	3:A:73:LYS:HA	1.54	0.88
1:T:812:DA:H2''	1:T:813:DC:OP2	1.72	0.88
4:B:268:SER:HA	4:B:274:ILE:HG13	1.53	0.88
2:P:828:DT:H4'	2:P:828:DT:OP1	1.72	0.87
2:P:837:DC:H2''	2:P:838:DA:O5'	1.74	0.87
2:P:822:DT:H2''	2:P:823:DC:C5	2.10	0.86
2:P:837:DC:H2''	2:P:838:DA:C5'	2.04	0.86
4:B:372:VAL:HG12	4:B:389:PHE:CD2	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:103:THR:HB	6:H:107:ASP:HB2	1.58	0.86
1:T:801:DA:H2''	1:T:802:DT:H71	1.56	0.86
5:L:110:ASP:HA	5:L:140:TYR:CB	2.06	0.86
1:T:810:DG:H2''	1:T:811:DA:H8	1.41	0.85
4:B:10:VAL:HG22	4:B:87:PHE:HZ	1.37	0.85
4:B:387:PRO:HG2	4:B:389:PHE:CE1	2.10	0.85
2:P:821:DG:H2'	2:P:822:DT:C7	2.06	0.85
4:B:55:PRO:HG2	4:B:56:TYR:CD2	2.12	0.85
3:A:450:THR:HB	3:A:452:LEU:HG	1.57	0.84
3:A:277:ARG:HH12	3:A:336:GLN:N	1.75	0.83
4:B:254:VAL:HB	4:B:289:LEU:HA	1.59	0.83
4:B:219:LYS:N	4:B:219:LYS:HZ2	1.77	0.83
2:P:830:DC:C2'	2:P:831:DG:C8	2.62	0.83
3:A:34:LEU:HA	3:A:37:ILE:HD12	1.60	0.82
5:L:47:LEU:HA	5:L:58:VAL:HG21	1.60	0.82
4:B:402:TRP:HH2	4:B:411:ILE:HD13	1.44	0.82
3:A:329:ILE:HG22	3:A:339:TYR:HB3	1.61	0.82
4:B:274:ILE:HA	4:B:306:ASN:HD21	1.45	0.82
4:B:219:LYS:HZ2	4:B:219:LYS:H	1.28	0.81
2:P:821:DG:C2'	2:P:822:DT:H71	2.10	0.81
6:H:62:ASN:HD22	6:H:65:LEU:HG	1.44	0.81
5:L:48:ILE:HG22	5:L:54:LEU:HA	1.60	0.81
3:A:458:VAL:HG22	3:A:464:GLN:HG2	1.63	0.81
2:P:833:DG:H1'	2:P:834:DC:H5'	1.63	0.81
3:A:294:PRO:C	3:A:296:THR:H	1.84	0.81
3:A:120:LEU:HD12	3:A:121:ASP:H	1.46	0.81
4:B:146:TYR:CE2	4:B:150:PRO:HA	2.15	0.80
5:L:205:ILE:H	5:L:205:ILE:HD12	1.44	0.80
4:B:292:VAL:C	4:B:294:PRO:HD3	2.02	0.80
3:A:483:TYR:HA	3:A:486:LEU:HD12	1.63	0.80
3:A:479:LEU:HD13	3:A:502:ALA:HB1	1.62	0.79
2:P:830:DC:H2'	2:P:831:DG:C8	2.17	0.79
4:B:153:TRP:O	4:B:157:PRO:HD2	1.82	0.79
3:A:327:ALA:HB2	3:A:341:ILE:HG23	1.62	0.79
3:A:122:GLU:HA	3:A:125:ARG:HD2	1.65	0.79
2:P:838:DA:H1'	3:A:184:ILE:HD12	1.62	0.79
2:P:827:DG:H2''	2:P:828:DT:O5'	1.83	0.79
6:H:40:ARG:HB2	6:H:50:LEU:HD11	1.63	0.79
2:P:829:DT:H2''	2:P:830:DC:C6	2.18	0.79
4:B:270:ILE:HB	4:B:271:TYR:HD1	1.48	0.79
4:B:292:VAL:O	4:B:294:PRO:HD3	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:156:PHE:HB3	6:H:157:PRO:HD3	1.64	0.79
6:H:62:ASN:HD21	6:H:64:SER:HB3	1.47	0.79
4:B:254:VAL:CB	4:B:289:LEU:HA	2.12	0.78
2:P:824:DC:H1'	3:A:475:GLN:HE22	1.47	0.78
3:A:457:TYR:CE2	3:A:465:LYS:HB3	2.19	0.78
3:A:501:TYR:CE1	3:A:505:ILE:HD11	2.19	0.78
4:B:10:VAL:HG22	4:B:87:PHE:CZ	2.18	0.78
4:B:31:ILE:O	4:B:35:VAL:HG23	1.84	0.78
1:T:803:DG:H2''	1:T:804:DG:H5''	1.64	0.78
3:A:501:TYR:CZ	3:A:505:ILE:HD11	2.18	0.78
3:A:261:VAL:HG13	3:A:276:VAL:HG11	1.67	0.77
6:H:92:THR:HB	6:H:121:VAL:HG23	1.66	0.77
3:A:542:ILE:HG22	4:B:283:LEU:HD23	1.66	0.77
4:B:103:LYS:NZ	4:B:191:SER:HA	1.99	0.77
4:B:270:ILE:HB	4:B:271:TYR:CD1	2.20	0.77
4:B:369:THR:HG22	4:B:398:TRP:CZ3	2.20	0.77
4:B:22:LYS:HZ3	4:B:23:GLN:N	1.83	0.77
3:A:518:VAL:O	3:A:522:ILE:HG13	1.85	0.77
4:B:373:GLN:HE22	4:B:406:TRP:HA	1.49	0.77
2:P:837:DC:H4'	3:A:230:MET:HE2	1.65	0.77
5:L:175:MET:HG3	5:L:176:SER:N	1.99	0.76
5:L:51:THR:HG21	5:L:71:TYR:HD2	1.49	0.76
4:B:209:LEU:HB3	4:B:215:THR:HB	1.66	0.76
6:H:187:LEU:HD23	6:H:188:SER:N	2.01	0.76
1:T:804:DG:H2''	1:T:805:DC:O5'	1.84	0.76
2:P:822:DT:C2'	2:P:823:DC:C5	2.68	0.76
3:A:20:LYS:HA	3:A:57:ASN:N	1.98	0.76
4:B:271:TYR:HB2	4:B:274:ILE:HD11	1.68	0.76
4:B:103:LYS:NZ	4:B:192:ASP:H	1.83	0.76
3:A:482:ILE:HG22	3:A:486:LEU:HD11	1.68	0.76
6:H:2:ILE:HG22	6:H:26:GLY:HA3	1.69	0.75
3:A:435:VAL:HA	4:B:290:THR:CG2	2.17	0.75
2:P:830:DC:H2''	2:P:831:DG:C8	2.21	0.75
4:B:67:ASP:HB2	4:B:220:LYS:HA	1.67	0.75
3:A:164:MET:O	3:A:168:LEU:HD23	1.87	0.75
1:T:812:DA:H1'	1:T:813:DC:O5'	1.86	0.74
4:B:47:ILE:HG23	4:B:145:GLN:O	1.86	0.74
4:B:88:TRP:NE1	4:B:92:LEU:HD22	2.01	0.74
3:A:206:ARG:HG2	3:A:216:THR:HG21	1.70	0.74
6:H:165:ASN:HB2	6:H:169:LEU:HD13	1.68	0.74
3:A:260:LEU:O	3:A:264:LEU:HG	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:37:GLN:HB3	5:L:47:LEU:HD11	1.70	0.74
4:B:138:GLU:HG2	4:B:139:THR:HG23	1.69	0.74
6:H:49:TRP:CZ2	6:H:51:ALA:HA	2.23	0.74
5:L:144:ILE:HG12	5:L:145:ASN:N	2.02	0.74
3:A:407:GLN:HE21	4:B:393:ILE:HA	1.53	0.74
3:A:447:ASN:HB3	3:A:450:THR:HG23	1.68	0.73
5:L:161:ASN:HB3	5:L:177:SER:CA	2.18	0.73
3:A:175:ASN:HB2	3:A:178:ILE:HD13	1.69	0.73
4:B:115:TYR:HB3	4:B:149:LEU:HB2	1.71	0.73
3:A:304:ALA:HA	3:A:307:ARG:HB2	1.69	0.73
4:B:68:SER:OG	4:B:219:LYS:HB2	1.89	0.73
6:H:182:SER:O	6:H:184:LEU:HD12	1.88	0.73
3:A:523:GLU:HA	3:A:526:ILE:HD12	1.71	0.73
3:A:153:TRP:CZ3	3:A:155:GLY:HA3	2.24	0.73
5:L:1:ASP:H3	5:L:93:LYS:HD2	1.54	0.73
3:A:224:GLU:HB3	3:A:225:PRO:HD3	1.70	0.72
4:B:225:PRO:HB2	4:B:226:PRO:CD	2.19	0.72
3:A:442:VAL:HG12	3:A:443:ASP:H	1.54	0.72
3:A:509:GLN:N	3:A:510:PRO:HD3	2.04	0.72
2:P:837:DC:H2''	2:P:838:DA:H5'	1.71	0.72
2:P:837:DC:H4'	3:A:230:MET:CE	2.18	0.72
3:A:407:GLN:NE2	4:B:393:ILE:HA	2.05	0.72
3:A:23:GLN:OE1	3:A:59:PRO:HA	1.89	0.72
4:B:385:LYS:HD2	4:B:385:LYS:N	2.04	0.72
3:A:542:ILE:H	3:A:542:ILE:HD12	1.53	0.71
3:A:479:LEU:HD13	3:A:502:ALA:CB	2.20	0.71
5:L:3:GLN:HA	5:L:3:GLN:HE21	1.54	0.71
4:B:161:GLN:O	4:B:165:THR:HG23	1.90	0.71
4:B:230:MET:CE	6:H:104:SER:HA	2.20	0.71
3:A:87:PHE:CE1	3:A:155:GLY:HA2	2.25	0.71
3:A:420:PRO:HB2	3:A:421:PRO:HD2	1.73	0.71
2:P:829:DT:H2''	2:P:830:DC:O4'	1.90	0.71
1:T:803:DG:H5'	1:T:803:DG:H8	1.55	0.71
4:B:239:TRP:CZ3	4:B:378:GLU:HG3	2.25	0.71
3:A:90:VAL:O	3:A:91:GLN:HG2	1.90	0.71
3:A:457:TYR:HE2	3:A:465:LYS:HB3	1.55	0.71
3:A:472:THR:HA	3:A:476:LYS:HD2	1.73	0.71
2:P:838:DA:H4'	3:A:183:TYR:CE2	2.26	0.71
4:B:368:LEU:O	4:B:371:ALA:HB3	1.91	0.71
5:L:51:THR:HG21	5:L:71:TYR:CD2	2.25	0.71
3:A:215:THR:O	3:A:217:PRO:HD3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:826:DT:H2''	2:P:827:DG:C8	2.26	0.70
3:A:181:TYR:HE1	4:B:136:ASN:HD22	1.38	0.70
5:L:19:VAL:O	5:L:74:THR:HG23	1.91	0.70
3:A:458:VAL:HG12	3:A:459:THR:N	2.06	0.70
4:B:329:ILE:HA	4:B:338:THR:O	1.90	0.70
5:L:110:ASP:HA	5:L:140:TYR:HB2	1.73	0.70
3:A:450:THR:O	3:A:452:LEU:HD23	1.91	0.70
6:H:16:GLN:O	6:H:87:VAL:HG23	1.92	0.70
4:B:166:LYS:O	4:B:169:GLU:HB3	1.91	0.70
4:B:14:PRO:O	4:B:16:MET:HG2	1.92	0.70
4:B:366:LYS:O	4:B:370:GLU:HG3	1.92	0.70
4:B:421:PRO:O	4:B:425:LEU:HD13	1.91	0.70
2:P:830:DC:H2'	2:P:831:DG:N7	2.07	0.69
4:B:274:ILE:HA	4:B:306:ASN:ND2	2.06	0.69
6:H:178:ALA:HB2	6:H:187:LEU:HB2	1.73	0.69
6:H:92:THR:OG1	6:H:120:THR:HA	1.91	0.69
3:A:435:VAL:HG22	4:B:290:THR:HG23	1.75	0.69
2:P:833:DG:C2'	2:P:834:DC:OP2	2.39	0.69
5:L:198:HIS:HB3	5:L:200:THR:HG23	1.74	0.69
3:A:329:ILE:HD13	3:A:329:ILE:H	1.55	0.69
3:A:33:ALA:O	3:A:37:ILE:HG13	1.91	0.69
5:L:1:ASP:N	5:L:93:LYS:HD2	2.07	0.69
5:L:147:ALA:HB3	5:L:195:ALA:HB3	1.72	0.69
4:B:29:GLU:HG2	4:B:71:TRP:CH2	2.28	0.69
2:P:824:DC:C1'	3:A:475:GLN:HE22	2.05	0.69
1:T:801:DA:C2'	1:T:802:DT:H71	2.23	0.69
6:H:40:ARG:HH11	6:H:91:ASP:HA	1.56	0.69
3:A:438:GLU:HG2	3:A:461:LYS:HE3	1.75	0.69
4:B:365:VAL:O	4:B:369:THR:HG23	1.92	0.69
3:A:435:VAL:HA	4:B:290:THR:HG21	1.74	0.69
4:B:29:GLU:HG2	4:B:71:TRP:HH2	1.56	0.69
2:P:829:DT:C2'	2:P:830:DC:C6	2.76	0.69
3:A:501:TYR:O	3:A:505:ILE:HG13	1.93	0.69
3:A:79:GLU:O	3:A:83:ARG:HG3	1.93	0.69
5:L:12:SER:HB3	5:L:105:GLU:HG3	1.75	0.69
4:B:224:GLU:HA	4:B:227:PHE:CE2	2.27	0.69
3:A:120:LEU:HD12	3:A:121:ASP:N	2.07	0.69
6:H:147:THR:C	6:H:148:LEU:HD22	2.14	0.69
4:B:83:ARG:HH11	4:B:83:ARG:HG2	1.56	0.68
4:B:22:LYS:HZ3	4:B:23:GLN:H	1.38	0.68
5:L:136:LEU:HD12	5:L:175:MET:HG2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:106:VAL:HG13	4:B:234:LEU:HB3	1.76	0.68
3:A:548:VAL:O	3:A:552:VAL:HG23	1.94	0.68
5:L:23:CYS:HB2	5:L:35:TRP:CH2	2.28	0.68
4:B:63:ILE:HG12	4:B:63:ILE:O	1.92	0.68
4:B:393:ILE:HD11	4:B:397:THR:HG21	1.75	0.68
5:L:83:PHE:HA	5:L:104:LEU:HG	1.76	0.68
1:T:818:DA:H2	2:P:822:DT:O2	1.75	0.68
4:B:257:ILE:HG13	4:B:258:GLN:N	2.09	0.68
6:H:31:THR:HB	6:H:34:ILE:HG13	1.75	0.68
4:B:331:LYS:O	4:B:331:LYS:HG2	1.93	0.68
1:T:803:DG:C5'	1:T:803:DG:H8	2.06	0.67
3:A:101:LYS:CD	3:A:101:LYS:H	2.04	0.67
6:H:1:GLN:HG2	6:H:2:ILE:HD13	1.76	0.67
1:T:815:DG:H2''	1:T:816:DG:H8	1.56	0.67
6:H:143:ASN:ND2	6:H:145:MET:HB2	2.09	0.67
3:A:307:ARG:HG3	3:A:307:ARG:HH11	1.58	0.67
4:B:125:ARG:HD3	4:B:147:ASN:HA	1.76	0.67
4:B:425:LEU:C	4:B:427:TYR:H	1.98	0.67
6:H:62:ASN:ND2	6:H:65:LEU:HG	2.09	0.67
6:H:162:VAL:HA	6:H:206:ASN:O	1.94	0.67
3:A:454:LYS:HG2	3:A:468:PRO:HB3	1.74	0.67
3:A:156:SER:HB2	3:A:157:PRO:HD3	1.75	0.67
3:A:500:GLN:O	3:A:503:LEU:HB3	1.95	0.67
6:H:212:SER:O	6:H:214:THR:HG23	1.96	0.67
3:A:473:THR:O	3:A:477:THR:HG23	1.95	0.66
4:B:244:ILE:CB	4:B:426:TRP:HE1	2.08	0.66
3:A:324:ASP:O	3:A:343:GLN:HG2	1.95	0.66
5:L:110:ASP:HA	5:L:140:TYR:HB3	1.77	0.66
5:L:140:TYR:HB3	5:L:141:PRO:HD3	1.78	0.66
6:H:89:THR:O	6:H:92:THR:HG22	1.94	0.66
2:P:830:DC:H4'	2:P:830:DC:OP1	1.95	0.66
2:P:824:DC:H1'	3:A:475:GLN:NE2	2.11	0.66
2:P:831:DG:C6	2:P:832:DG:C6	2.84	0.66
3:A:40:GLU:O	3:A:44:GLU:HG3	1.96	0.66
3:A:19:PRO:HG3	3:A:80:LEU:HD23	1.78	0.66
4:B:206:ARG:NH2	4:B:219:LYS:HG3	2.11	0.66
4:B:60:VAL:CG1	4:B:75:VAL:HG22	2.23	0.65
5:L:192:TYR:HB2	5:L:209:PHE:CE2	2.29	0.65
2:P:837:DC:C2'	2:P:838:DA:H5'	2.26	0.65
5:L:6:GLN:HE22	5:L:87:TYR:HA	1.61	0.65
4:B:424:LYS:C	4:B:426:TRP:H	2.00	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:120:PRO:HG3	5:L:132:VAL:HG22	1.78	0.65
4:B:319:TYR:CE2	4:B:321:PRO:HG3	2.31	0.65
3:A:92:LEU:HG	3:A:92:LEU:O	1.94	0.65
4:B:60:VAL:HA	4:B:74:LEU:O	1.95	0.65
6:H:163:THR:H	6:H:206:ASN:HD21	1.44	0.65
4:B:236:PRO:HG2	4:B:237:ASP:H	1.62	0.65
3:A:400:THR:HA	3:A:403:THR:OG1	1.96	0.65
4:B:103:LYS:HZ3	4:B:192:ASP:N	1.87	0.65
4:B:104:LYS:HB2	4:B:192:ASP:HA	1.79	0.65
4:B:55:PRO:HG2	4:B:56:TYR:HD2	1.59	0.65
4:B:47:ILE:CG2	4:B:144:TYR:HB3	2.27	0.65
3:A:155:GLY:C	3:A:159:ILE:HG12	2.18	0.65
2:P:825:DC:C6	2:P:826:DT:H72	2.32	0.64
5:L:33:LEU:HD11	5:L:88:CYS:SG	2.36	0.64
5:L:107:LYS:HD2	5:L:140:TYR:OH	1.97	0.64
3:A:337:TRP:NE1	3:A:367:GLN:HB3	2.12	0.64
4:B:164:MET:SD	4:B:168:LEU:HD11	2.37	0.64
6:H:198:TRP:HD1	6:H:203:VAL:HG23	1.62	0.64
4:B:423:VAL:HG12	4:B:428:GLN:HA	1.79	0.64
3:A:325:LEU:HB3	3:A:387:PRO:HB3	1.79	0.64
4:B:372:VAL:HG12	4:B:389:PHE:CE2	2.32	0.64
3:A:146:TYR:CD2	3:A:150:PRO:HB3	2.32	0.64
3:A:225:PRO:HB2	3:A:226:PRO:HD3	1.78	0.64
3:A:348:ASN:HD22	3:A:349:LEU:H	1.45	0.64
4:B:118:VAL:HG13	4:B:119:PRO:HD2	1.77	0.64
4:B:212:TRP:O	4:B:214:LEU:N	2.31	0.64
3:A:12:LEU:HD23	3:A:124:PHE:HE1	1.61	0.64
3:A:332:GLN:HB3	3:A:336:GLN:HB3	1.79	0.64
3:A:393:ILE:HG12	3:A:397:THR:OG1	1.98	0.64
3:A:5:ILE:HD12	3:A:6:GLU:H	1.62	0.64
4:B:195:ILE:HD11	4:B:199:ARG:HE	1.63	0.64
4:B:373:GLN:NE2	4:B:406:TRP:HA	2.12	0.64
4:B:180:ILE:HG12	4:B:189:VAL:HG22	1.80	0.64
3:A:154:LYS:O	3:A:157:PRO:HD2	1.98	0.64
3:A:26:LEU:HD11	3:A:61:PHE:HA	1.80	0.63
4:B:50:ILE:N	4:B:50:ILE:HD13	2.14	0.63
5:L:1:ASP:HA	5:L:95:PRO:HB2	1.80	0.63
3:A:459:THR:CG2	3:A:463:ARG:HB3	2.28	0.63
2:P:838:DA:H1'	3:A:184:ILE:CD1	2.28	0.63
5:L:48:ILE:HD11	5:L:73:LEU:HD13	1.80	0.63
4:B:218:ASP:C	4:B:219:LYS:HD3	2.19	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:130:ALA:HB3	5:L:181:LEU:O	1.99	0.63
3:A:94:ILE:HB	3:A:95:PRO:HD2	1.79	0.63
3:A:542:ILE:HD12	3:A:542:ILE:N	2.13	0.63
4:B:30:LYS:HZ3	4:B:61:PHE:HD1	1.45	0.63
4:B:258:GLN:O	4:B:261:VAL:HG12	1.98	0.63
4:B:195:ILE:HG23	4:B:196:GLY:H	1.62	0.63
3:A:150:PRO:HG2	3:A:153:TRP:HB3	1.79	0.63
4:B:34:LEU:O	4:B:38:CYS:HB2	1.98	0.63
2:P:822:DT:C2'	2:P:823:DC:C6	2.67	0.63
4:B:39:THR:O	4:B:42:GLU:HB3	1.98	0.63
4:B:195:ILE:O	4:B:199:ARG:HG3	1.98	0.63
3:A:254:VAL:HG22	3:A:289:LEU:O	1.98	0.63
3:A:132:ILE:HG23	3:A:142:ILE:HB	1.81	0.63
4:B:230:MET:HE2	6:H:104:SER:HA	1.80	0.62
3:A:326:ILE:HG23	3:A:388:LYS:HB2	1.80	0.62
1:T:803:DG:H5'	1:T:803:DG:C8	2.34	0.62
5:L:159:VAL:HG12	5:L:161:ASN:OD1	2.00	0.62
3:A:486:LEU:HB3	3:A:528:LYS:NZ	2.14	0.62
5:L:197:THR:HG23	5:L:204:PRO:HA	1.80	0.62
5:L:141:PRO:HD2	5:L:198:HIS:CE1	2.33	0.62
4:B:425:LEU:O	4:B:427:TYR:N	2.32	0.62
6:H:61:TYR:HE2	6:H:70:THR:CA	2.02	0.62
3:A:179:VAL:N	3:A:190:GLY:O	2.32	0.62
3:A:240:THR:HG23	3:A:315:HIS:HA	1.80	0.62
1:T:815:DG:C2'	1:T:816:DG:C8	2.81	0.62
6:H:49:TRP:CE2	6:H:51:ALA:HA	2.35	0.62
6:H:132:TYR:HB2	6:H:151:LEU:HB3	1.81	0.62
2:P:831:DG:C4	2:P:832:DG:N7	2.68	0.62
3:A:277:ARG:HH12	3:A:336:GLN:H	1.46	0.62
3:A:215:THR:C	3:A:217:PRO:HD3	2.19	0.62
4:B:174:GLN:O	4:B:175:ASN:HB3	1.99	0.62
4:B:395:LYS:HG3	4:B:416:PHE:CE1	2.34	0.62
3:A:129:ALA:HA	3:A:145:GLN:HA	1.82	0.62
3:A:31:ILE:O	3:A:35:VAL:HG23	1.99	0.62
4:B:402:TRP:CH2	4:B:411:ILE:HD13	2.30	0.62
6:H:165:ASN:HB2	6:H:169:LEU:CD1	2.29	0.62
3:A:461:LYS:O	3:A:463:ARG:N	2.30	0.62
2:P:838:DA:H4'	3:A:183:TYR:CD2	2.35	0.62
4:B:166:LYS:O	4:B:170:PRO:HD3	1.99	0.61
6:H:148:LEU:HB2	6:H:191:VAL:HG23	1.82	0.61
3:A:362:THR:HG22	3:A:366:LYS:NZ	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:37:THR:HG23	6:H:52:THR:OG1	2.00	0.61
1:T:801:DA:C2'	1:T:802:DT:C7	2.77	0.61
3:A:279:LEU:HD12	3:A:279:LEU:N	2.10	0.61
4:B:387:PRO:HG2	4:B:389:PHE:HE1	1.59	0.61
3:A:294:PRO:C	3:A:296:THR:N	2.53	0.61
4:B:96:HIS:NE2	4:B:100:LEU:HD23	2.15	0.61
4:B:328:GLU:HB2	4:B:340:GLN:NE2	2.16	0.61
4:B:422:LEU:O	4:B:425:LEU:HD22	2.00	0.61
4:B:106:VAL:HG12	4:B:234:LEU:O	2.00	0.61
6:H:130:SER:HB3	6:H:153:LYS:O	1.99	0.61
4:B:421:PRO:HA	4:B:424:LYS:CB	2.31	0.61
5:L:4:MET:SD	5:L:25:ALA:HA	2.40	0.61
3:A:12:LEU:HD11	3:A:127:TYR:CZ	2.35	0.61
3:A:155:GLY:O	3:A:159:ILE:HG12	2.01	0.61
3:A:21:VAL:N	3:A:57:ASN:O	2.33	0.61
6:H:40:ARG:HH12	6:H:91:ASP:HA	1.63	0.61
6:H:146:VAL:O	6:H:192:THR:HA	2.00	0.61
5:L:169:LYS:HZ2	5:L:169:LYS:N	1.97	0.61
5:L:6:GLN:NE2	5:L:88:CYS:H	1.99	0.61
3:A:165:THR:HG23	3:A:182:GLN:HE22	1.65	0.61
6:H:10:GLY:HA2	6:H:118:SER:O	2.00	0.61
5:L:10:SER:HB3	5:L:103:LYS:HB2	1.80	0.61
3:A:363:ASN:OD1	3:A:365:VAL:HG23	2.00	0.61
5:L:89:GLN:HG3	5:L:98:PHE:CE1	2.35	0.61
6:H:39:ILE:HG23	6:H:48:GLU:O	2.00	0.61
5:L:150:ILE:HG23	5:L:191:SER:O	2.00	0.61
5:L:148:TRP:CE3	5:L:179:LEU:HD22	2.35	0.61
3:A:242:GLN:N	3:A:243:PRO:HD2	2.14	0.61
3:A:377:THR:HG22	3:A:378:GLU:N	2.16	0.61
5:L:150:ILE:HG21	5:L:189:ALA:HB1	1.83	0.61
3:A:53:GLU:O	3:A:55:PRO:HD3	2.00	0.61
6:H:165:ASN:HD21	6:H:203:VAL:HA	1.64	0.61
4:B:135:ILE:O	4:B:135:ILE:HG13	2.00	0.61
4:B:191:SER:H	4:B:198:HIS:CE1	2.18	0.60
4:B:328:GLU:C	4:B:329:ILE:HD12	2.21	0.60
6:H:219:LYS:HD2	6:H:219:LYS:C	2.21	0.60
1:T:804:DG:H8	1:T:804:DG:H5'	1.65	0.60
5:L:52:SER:HA	5:L:64:GLY:HA3	1.82	0.60
6:H:62:ASN:HD22	6:H:65:LEU:CG	2.13	0.60
6:H:162:VAL:HB	6:H:207:VAL:HA	1.82	0.60
4:B:395:LYS:HG3	4:B:416:PHE:HE1	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:326:ILE:HG13	4:B:342:TYR:O	2.02	0.60
3:A:119:PRO:HA	3:A:148:VAL:HG12	1.81	0.60
3:A:64:LYS:HG2	3:A:72:ARG:H	1.65	0.60
5:L:14:SER:O	5:L:78:LEU:HD12	2.01	0.60
4:B:167:ILE:O	4:B:170:PRO:HD2	2.01	0.60
4:B:323:LYS:HB2	4:B:343:GLN:NE2	2.17	0.60
6:H:161:THR:OG1	6:H:208:ALA:HB3	2.01	0.60
5:L:94:PHE:O	5:L:96:TRP:N	2.33	0.60
3:A:509:GLN:H	3:A:510:PRO:HD3	1.66	0.60
4:B:245:VAL:CB	4:B:427:TYR:HE1	2.15	0.60
5:L:105:GLU:HB2	5:L:166:GLN:OE1	2.01	0.60
4:B:171:PHE:CD1	4:B:205:LEU:HG	2.37	0.60
4:B:47:ILE:HG21	4:B:144:TYR:HD2	1.67	0.60
3:A:372:VAL:HA	3:A:375:ILE:HD12	1.84	0.60
5:L:12:SER:HA	5:L:105:GLU:O	2.01	0.60
4:B:285:GLY:O	4:B:287:LYS:N	2.34	0.60
4:B:319:TYR:CZ	4:B:383:TRP:HB3	2.37	0.60
4:B:36:GLU:O	4:B:39:THR:HG22	2.02	0.60
4:B:255:ASN:HB2	4:B:289:LEU:HD13	1.83	0.60
4:B:375:ILE:O	4:B:378:GLU:HB3	2.01	0.60
4:B:260:LEU:O	4:B:263:LYS:HB3	2.02	0.60
3:A:80:LEU:O	3:A:83:ARG:N	2.35	0.59
3:A:261:VAL:HA	3:A:264:LEU:HD12	1.82	0.59
3:A:279:LEU:CD1	3:A:279:LEU:H	2.07	0.59
4:B:230:MET:HE1	6:H:104:SER:HA	1.83	0.59
6:H:2:ILE:HD11	6:H:112:HIS:CE1	2.36	0.59
6:H:143:ASN:HD21	6:H:145:MET:HB2	1.65	0.59
3:A:122:GLU:HA	3:A:125:ARG:CD	2.31	0.59
4:B:58:THR:HG23	4:B:59:PRO:HD2	1.83	0.59
4:B:89:GLU:HA	4:B:92:LEU:HD23	1.84	0.59
3:A:188:TYR:HE2	3:A:234:LEU:HD11	1.66	0.59
5:L:141:PRO:HD2	5:L:198:HIS:NE2	2.17	0.59
4:B:202:ILE:HG22	4:B:203:GLU:N	2.17	0.59
3:A:329:ILE:HD11	3:A:392:PRO:HD2	1.85	0.59
5:L:3:GLN:HB3	5:L:26:SER:OG	2.02	0.59
3:A:50:ILE:HG22	3:A:145:GLN:HG2	1.84	0.59
1:T:806:DG:H2"	1:T:807:DC:OP2	2.02	0.59
4:B:50:ILE:HG21	4:B:145:GLN:OE1	2.02	0.59
4:B:423:VAL:C	4:B:425:LEU:H	2.04	0.59
5:L:148:TRP:O	5:L:155:ALA:HA	2.02	0.59
6:H:161:THR:O	6:H:208:ALA:N	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:11:LEU:HD11	5:L:19:VAL:HG11	1.84	0.59
3:A:202:ILE:O	3:A:205:LEU:HB3	2.03	0.59
2:P:828:DT:H2"	2:P:829:DT:O5'	2.03	0.59
3:A:453:GLY:O	3:A:469:LEU:HD12	2.02	0.59
4:B:266:TRP:HA	4:B:269:GLN:NE2	2.17	0.59
5:L:31:SER:O	5:L:50:TYR:HD1	1.85	0.59
3:A:472:THR:CA	3:A:476:LYS:HD2	2.33	0.59
6:H:164:TRP:HA	6:H:204:THR:O	2.03	0.59
4:B:125:ARG:O	4:B:127:TYR:N	2.36	0.59
6:H:24:PHE:CZ	6:H:78:ASN:HA	2.37	0.59
3:A:474:ASN:H	3:A:474:ASN:HD22	1.50	0.59
4:B:342:TYR:HA	4:B:349:LEU:HD13	1.83	0.59
4:B:399:GLU:O	4:B:401:TRP:N	2.36	0.59
4:B:106:VAL:O	4:B:234:LEU:HB3	2.03	0.59
4:B:336:GLN:HA	4:B:355:ALA:HA	1.83	0.59
4:B:301:LEU:HG	4:B:302:GLU:OE2	2.03	0.59
2:P:833:DG:N2	2:P:834:DC:C2	2.70	0.59
5:L:37:GLN:O	5:L:37:GLN:HG3	2.01	0.59
3:A:121:ASP:O	3:A:125:ARG:HG3	2.03	0.58
3:A:427:TYR:OH	3:A:510:PRO:HD2	2.02	0.58
5:L:6:GLN:HB2	5:L:100:GLY:O	2.03	0.58
6:H:18:PHE:CD2	6:H:87:VAL:HG21	2.38	0.58
4:B:98:ALA:O	4:B:100:LEU:N	2.36	0.58
4:B:98:ALA:O	4:B:101:LYS:HG2	2.04	0.58
3:A:402:TRP:HE3	4:B:331:LYS:HZ1	1.51	0.58
4:B:103:LYS:HA	4:B:192:ASP:OD2	2.03	0.58
4:B:395:LYS:HA	4:B:416:PHE:CE1	2.39	0.58
5:L:39:LYS:HG3	5:L:40:PRO:HD2	1.86	0.58
5:L:35:TRP:HB2	5:L:48:ILE:CG1	2.33	0.58
3:A:234:LEU:HD23	3:A:318:TYR:OH	2.04	0.58
1:T:805:DC:H2"	1:T:806:DG:C8	2.39	0.58
4:B:22:LYS:NZ	4:B:23:GLN:H	2.00	0.58
3:A:201:LYS:O	3:A:204:GLU:HB3	2.02	0.58
3:A:277:ARG:HB3	3:A:336:GLN:NE2	2.19	0.58
3:A:373:GLN:OE1	4:B:397:THR:HA	2.02	0.58
4:B:73:LYS:CD	4:B:151:GLN:HE21	2.17	0.58
3:A:442:VAL:HG12	3:A:443:ASP:N	2.18	0.58
4:B:207:GLN:O	4:B:210:LEU:HB2	2.04	0.58
5:L:20:THR:HG23	5:L:74:THR:OG1	2.03	0.58
4:B:195:ILE:CD1	4:B:199:ARG:HE	2.16	0.58
3:A:270:ILE:HD12	3:A:314:VAL:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:398:TRP:HH2	3:A:409:THR:HG22	1.68	0.58
3:A:506:ILE:N	3:A:506:ILE:HD13	2.19	0.58
3:A:358:ARG:HH12	4:B:394:GLN:HG3	1.69	0.58
3:A:532:TYR:CD2	3:A:533:LEU:N	2.72	0.58
3:A:441:TYR:CE2	3:A:544:GLY:N	2.72	0.58
4:B:247:PRO:CB	4:B:307:ARG:HH22	2.17	0.58
1:T:815:DG:H2''	1:T:816:DG:N7	2.18	0.57
4:B:369:THR:OG1	4:B:370:GLU:N	2.37	0.57
3:A:168:LEU:O	3:A:172:LYS:HG3	2.05	0.57
6:H:72:SER:OG	6:H:81:PHE:HD1	1.87	0.57
5:L:3:GLN:NE2	5:L:3:GLN:HA	2.19	0.57
4:B:96:HIS:HE2	4:B:100:LEU:HD23	1.70	0.57
3:A:377:THR:O	3:A:381:VAL:HG23	2.04	0.57
3:A:210:LEU:HA	3:A:214:LEU:O	2.03	0.57
4:B:357:MET:HB3	4:B:361:HIS:HE1	1.69	0.57
2:P:836:DC:H2''	2:P:837:DC:O5'	2.04	0.57
3:A:339:TYR:CD2	3:A:375:ILE:HG12	2.40	0.57
3:A:486:LEU:HB3	3:A:528:LYS:HZ1	1.69	0.57
5:L:186:TYR:HA	5:L:192:TYR:OH	2.03	0.57
5:L:120:PRO:HB2	5:L:125:LEU:HD21	1.86	0.57
1:T:801:DA:H2''	1:T:802:DT:C5	2.39	0.57
4:B:429:LEU:HD12	4:B:429:LEU:H	1.70	0.57
4:B:64:LYS:HB3	4:B:64:LYS:NZ	2.20	0.57
2:P:825:DC:C2'	2:P:826:DT:C5'	2.71	0.57
4:B:118:VAL:CG1	4:B:119:PRO:HD2	2.33	0.57
4:B:266:TRP:HA	4:B:269:GLN:HE21	1.69	0.57
5:L:117:ILE:HD12	5:L:194:CYS:HB2	1.87	0.57
6:H:218:LYS:HE2	6:H:219:LYS:NZ	2.20	0.57
3:A:246:LEU:HD11	3:A:307:ARG:HE	1.70	0.57
4:B:98:ALA:C	4:B:100:LEU:N	2.57	0.57
3:A:98:ALA:HB1	3:A:383:TRP:HZ2	1.70	0.57
1:T:803:DG:C5'	1:T:803:DG:C8	2.88	0.57
4:B:191:SER:OG	4:B:193:LEU:HG	2.04	0.57
3:A:531:VAL:HG12	3:A:532:TYR:N	2.19	0.57
2:P:823:DC:C3'	2:P:824:DC:H5''	2.33	0.57
4:B:27:THR:HG23	4:B:30:LYS:HG3	1.87	0.57
3:A:62:ALA:CA	3:A:73:LYS:HA	2.30	0.57
6:H:17:PRO:HB3	6:H:85:MET:HG3	1.85	0.57
4:B:163:SER:O	4:B:167:ILE:HG13	2.05	0.56
4:B:34:LEU:HD23	4:B:132:ILE:HG12	1.86	0.56
3:A:516:GLU:O	3:A:520:GLN:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:823:DC:C2	2:P:824:DC:C6	2.93	0.56
5:L:137:ASN:CA	5:L:174:SER:HB3	2.29	0.56
5:L:15:LEU:HA	5:L:78:LEU:HB2	1.87	0.56
4:B:342:TYR:HA	4:B:349:LEU:CD1	2.35	0.56
4:B:254:VAL:CG2	4:B:289:LEU:HA	2.35	0.56
6:H:143:ASN:OD1	6:H:144:SER:N	2.38	0.56
6:H:95:TYR:N	6:H:95:TYR:CD1	2.70	0.56
4:B:329:ILE:N	4:B:329:ILE:HD12	2.20	0.56
4:B:180:ILE:HA	4:B:188:TYR:O	2.05	0.56
3:A:106:VAL:HG12	3:A:107:THR:N	2.21	0.56
4:B:47:ILE:CD1	4:B:146:TYR:HA	2.36	0.56
6:H:163:THR:N	6:H:206:ASN:HD21	2.04	0.56
4:B:406:TRP:CZ2	4:B:410:TRP:O	2.58	0.56
5:L:2:ILE:HD11	5:L:93:LYS:HB3	1.86	0.56
6:H:169:LEU:N	6:H:169:LEU:HD12	2.21	0.56
4:B:369:THR:HG22	4:B:398:TRP:CH2	2.40	0.56
4:B:212:TRP:CD1	4:B:213:GLY:N	2.73	0.56
3:A:46:LYS:HD3	3:A:116:PHE:HD2	1.69	0.56
3:A:519:ASN:HA	3:A:522:ILE:HD12	1.85	0.56
4:B:406:TRP:HZ2	4:B:410:TRP:O	1.88	0.56
4:B:393:ILE:HD11	4:B:397:THR:CG2	2.34	0.56
4:B:113:ASP:O	4:B:116:PHE:HB2	2.06	0.56
6:H:218:LYS:HE2	6:H:219:LYS:HZ1	1.71	0.56
6:H:27:PHE:CD2	6:H:34:ILE:HG21	2.41	0.56
3:A:425:LEU:HD12	3:A:425:LEU:H	1.71	0.56
4:B:30:LYS:NZ	4:B:61:PHE:HD1	2.04	0.56
3:A:444:GLY:O	3:A:445:ALA:HB2	2.06	0.56
4:B:402:TRP:HH2	4:B:411:ILE:CD1	2.16	0.56
3:A:110:ASP:O	3:A:217:PRO:HD2	2.06	0.56
6:H:33:GLY:O	6:H:101:ALA:HA	2.06	0.56
3:A:470:THR:HG22	3:A:471:ASN:N	2.21	0.56
1:T:802:DT:H2"	1:T:803:DG:OP2	2.05	0.56
4:B:75:VAL:HG11	4:B:77:PHE:CZ	2.41	0.56
3:A:394:GLN:HG2	3:A:416:PHE:CE1	2.40	0.56
4:B:101:LYS:HE3	4:B:102:LYS:HE3	1.88	0.56
3:A:363:ASN:HA	3:A:511:ASP:H	1.68	0.55
3:A:515:SER:O	3:A:519:ASN:HB2	2.06	0.55
4:B:163:SER:HA	4:B:166:LYS:HE2	1.88	0.55
3:A:363:ASN:HB3	3:A:509:GLN:O	2.06	0.55
4:B:393:ILE:HG13	4:B:394:GLN:N	2.21	0.55
3:A:94:ILE:HG13	3:A:95:PRO:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:146:TYR:CD2	4:B:150:PRO:HA	2.40	0.55
5:L:113:PRO:HB3	5:L:139:PHE:CD2	2.42	0.55
3:A:101:LYS:N	3:A:101:LYS:HD2	2.12	0.55
6:H:92:THR:O	6:H:92:THR:HG23	2.07	0.55
3:A:171:PHE:CZ	3:A:205:LEU:HB2	2.42	0.55
5:L:85:THR:HA	5:L:102:THR:O	2.05	0.55
5:L:23:CYS:HB2	5:L:35:TRP:HH2	1.71	0.55
5:L:34:ASN:N	5:L:89:GLN:O	2.38	0.55
4:B:115:TYR:OH	4:B:157:PRO:HB3	2.06	0.55
5:L:166:GLN:HE21	5:L:171:SER:HB3	1.71	0.55
3:A:441:TYR:HE2	3:A:544:GLY:N	2.05	0.55
3:A:491:LEU:HD23	3:A:491:LEU:H	1.72	0.55
3:A:255:ASN:HA	3:A:258:GLN:HE21	1.72	0.55
4:B:171:PHE:CZ	4:B:201:LYS:HD2	2.41	0.55
4:B:155:GLY:O	4:B:158:ALA:HB3	2.06	0.55
6:H:31:THR:HB	6:H:34:ILE:CG1	2.35	0.55
5:L:50:TYR:CE2	6:H:106:THR:HB	2.42	0.55
6:H:32:SER:O	6:H:55:TRP:CE2	2.60	0.55
4:B:191:SER:H	4:B:198:HIS:HE1	1.54	0.55
2:P:823:DC:C2	2:P:824:DC:C5	2.94	0.55
3:A:180:ILE:CG2	3:A:187:LEU:HD22	2.36	0.55
6:H:27:PHE:HD2	6:H:34:ILE:HG21	1.72	0.55
5:L:34:ASN:OD1	5:L:49:TYR:HA	2.07	0.55
3:A:469:LEU:N	3:A:469:LEU:HD12	2.22	0.55
4:B:81:ASN:O	4:B:154:LYS:HE3	2.07	0.55
5:L:75:ILE:HD12	5:L:75:ILE:N	2.21	0.55
3:A:458:VAL:CG1	3:A:459:THR:H	2.13	0.55
4:B:16:MET:O	4:B:18:GLY:N	2.36	0.55
5:L:135:PHE:CE2	6:H:190:SER:HB3	2.42	0.55
4:B:423:VAL:C	4:B:425:LEU:N	2.61	0.55
6:H:53:ILE:HD12	6:H:80:ALA:HB1	1.89	0.55
4:B:228:LEU:HD23	4:B:232:TYR:HE1	1.70	0.54
3:A:178:ILE:N	3:A:178:ILE:HD12	2.22	0.54
5:L:107:LYS:HA	5:L:140:TYR:OH	2.07	0.54
5:L:187:GLU:HA	5:L:212:ASN:HB3	1.88	0.54
3:A:261:VAL:HG13	3:A:276:VAL:CG1	2.35	0.54
4:B:130:PHE:CZ	4:B:144:TYR:HB2	2.42	0.54
1:T:810:DG:C6	1:T:811:DA:N6	2.75	0.54
5:L:51:THR:CG2	5:L:71:TYR:HD2	2.20	0.54
3:A:63:ILE:HG23	3:A:63:ILE:O	2.06	0.54
4:B:107:THR:HG22	4:B:108:VAL:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:35:TRP:CZ3	5:L:88:CYS:HB2	2.42	0.54
4:B:16:MET:HB3	4:B:83:ARG:HD2	1.89	0.54
3:A:450:THR:C	3:A:452:LEU:H	2.11	0.54
4:B:32:LYS:O	4:B:35:VAL:HB	2.08	0.54
4:B:393:ILE:HD12	4:B:394:GLN:OE1	2.08	0.54
5:L:2:ILE:N	5:L:2:ILE:HD12	2.22	0.54
6:H:132:TYR:HD2	6:H:151:LEU:HD23	1.73	0.54
4:B:330:GLN:HB2	4:B:338:THR:OG1	2.07	0.54
3:A:99:GLY:HA2	3:A:383:TRP:NE1	2.22	0.54
3:A:219:LYS:N	3:A:219:LYS:HD2	2.22	0.54
4:B:115:TYR:CD1	4:B:156:SER:HB3	2.43	0.54
4:B:195:ILE:HG23	4:B:196:GLY:N	2.23	0.54
4:B:304:ALA:HA	4:B:307:ARG:HG3	1.90	0.54
3:A:502:ALA:O	3:A:506:ILE:HG12	2.07	0.54
6:H:150:CYS:O	6:H:188:SER:HA	2.07	0.54
3:A:317:VAL:HG22	3:A:318:TYR:H	1.72	0.54
3:A:246:LEU:N	3:A:246:LEU:HD23	2.22	0.54
6:H:59:ASN:OD1	6:H:61:TYR:HE1	1.91	0.54
4:B:23:GLN:NE2	4:B:26:LEU:HD11	2.22	0.54
4:B:33:ALA:O	4:B:37:ILE:HG22	2.07	0.54
6:H:69:LEU:HD11	6:H:82:LEU:HD21	1.89	0.54
4:B:68:SER:OG	4:B:219:LYS:NZ	2.38	0.54
5:L:186:TYR:HE2	5:L:213:GLU:O	1.90	0.54
3:A:380:ILE:O	3:A:384:GLY:N	2.39	0.54
4:B:195:ILE:HD11	4:B:233:GLU:HG3	1.90	0.54
2:P:830:DC:C4	2:P:831:DG:O6	2.61	0.53
4:B:143:ARG:C	4:B:144:TYR:HD1	2.11	0.53
4:B:236:PRO:O	4:B:238:LYS:N	2.42	0.53
4:B:266:TRP:CD1	4:B:269:GLN:NE2	2.70	0.53
3:A:377:THR:O	3:A:380:ILE:HB	2.08	0.53
4:B:47:ILE:HG21	4:B:144:TYR:HB3	1.91	0.53
4:B:22:LYS:CD	4:B:23:GLN:H	2.21	0.53
3:A:225:PRO:HA	3:A:236:PRO:HD3	1.91	0.53
3:A:41:MET:HB2	3:A:47:ILE:HD11	1.90	0.53
5:L:75:ILE:HD12	5:L:75:ILE:H	1.74	0.53
5:L:149:ALA:HA	5:L:154:ALA:O	2.08	0.53
2:P:831:DG:C2'	2:P:832:DG:H8	2.20	0.53
4:B:21:VAL:HG12	4:B:22:LYS:N	2.23	0.53
4:B:394:GLN:O	4:B:397:THR:HB	2.08	0.53
6:H:34:ILE:HG22	6:H:35:GLY:N	2.24	0.53
3:A:24:TRP:NE1	3:A:61:PHE:CZ	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:376:THR:O	4:B:380:ILE:HG13	2.09	0.53
3:A:16:MET:CE	3:A:16:MET:H	2.21	0.53
3:A:10:VAL:HG21	3:A:153:TRP:CZ2	2.43	0.53
6:H:2:ILE:CG2	6:H:26:GLY:HA3	2.37	0.53
4:B:64:LYS:HG3	4:B:71:TRP:CE2	2.43	0.53
3:A:41:MET:O	3:A:44:GLU:HB2	2.08	0.53
3:A:97:PRO:HG3	3:A:232:TYR:CD2	2.43	0.53
6:H:94:ILE:HA	6:H:117:THR:O	2.07	0.53
4:B:271:TYR:N	4:B:271:TYR:CD1	2.76	0.53
3:A:169:GLU:O	3:A:172:LYS:HB2	2.09	0.53
6:H:17:PRO:HB2	6:H:85:MET:HE3	1.89	0.53
2:P:825:DC:C4	2:P:826:DT:C4	2.97	0.53
5:L:79:GLU:O	5:L:81:GLU:N	2.41	0.53
6:H:128:PRO:HA	6:H:212:SER:OG	2.09	0.53
3:A:171:PHE:CD2	3:A:205:LEU:HD13	2.43	0.53
3:A:271:TYR:CE2	3:A:310:LEU:HD23	2.44	0.53
6:H:125:ALA:O	6:H:127:THR:HG23	2.09	0.53
3:A:505:ILE:O	3:A:510:PRO:HG2	2.08	0.53
2:P:833:DG:C2	2:P:834:DC:C2	2.97	0.53
4:B:47:ILE:HD13	4:B:146:TYR:HA	1.90	0.53
4:B:92:LEU:O	4:B:95:PRO:HG3	2.09	0.53
3:A:50:ILE:HD12	3:A:54:ASN:HB2	1.91	0.53
6:H:42:PRO:HB2	6:H:45:LYS:HB2	1.90	0.53
4:B:357:MET:HB3	4:B:361:HIS:CE1	2.43	0.53
4:B:235:HIS:ND1	4:B:235:HIS:N	2.56	0.53
4:B:254:VAL:HB	4:B:289:LEU:CA	2.35	0.52
4:B:224:GLU:HA	4:B:227:PHE:HE2	1.73	0.52
3:A:254:VAL:HG21	3:A:289:LEU:HA	1.91	0.52
3:A:378:GLU:O	3:A:382:ILE:HG12	2.09	0.52
4:B:229:TRP:HA	4:B:232:TYR:CD1	2.44	0.52
4:B:418:ASN:CG	4:B:419:THR:N	2.63	0.52
2:P:824:DC:H2''	2:P:825:DC:O5'	2.09	0.52
4:B:254:VAL:O	4:B:258:GLN:HB2	2.08	0.52
3:A:153:TRP:CE3	3:A:155:GLY:HA3	2.45	0.52
4:B:328:GLU:HB2	4:B:340:GLN:HE21	1.73	0.52
6:H:148:LEU:N	6:H:191:VAL:O	2.37	0.52
5:L:39:LYS:HB3	5:L:43:THR:OG1	2.09	0.52
6:H:72:SER:OG	6:H:81:PHE:CD1	2.62	0.52
3:A:11:LYS:O	3:A:85:GLN:HG2	2.09	0.52
2:P:830:DC:C2'	2:P:831:DG:H8	2.17	0.52
3:A:107:THR:HG22	3:A:108:VAL:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:203:GLU:O	4:B:206:ARG:HB2	2.10	0.52
6:H:160:VAL:HG13	6:H:160:VAL:O	2.10	0.52
3:A:87:PHE:HE1	3:A:155:GLY:HA2	1.73	0.52
3:A:482:ILE:O	3:A:486:LEU:HG	2.10	0.52
5:L:15:LEU:HD23	5:L:78:LEU:O	2.10	0.52
5:L:37:GLN:HG2	5:L:47:LEU:HD21	1.92	0.52
3:A:329:ILE:HD11	3:A:391:LEU:HA	1.92	0.52
4:B:406:TRP:CZ2	4:B:408:ALA:HB3	2.44	0.52
5:L:193:THR:HG22	5:L:194:CYS:N	2.23	0.52
3:A:167:ILE:N	3:A:167:ILE:HD12	2.25	0.52
4:B:178:ILE:HG22	4:B:179:VAL:N	2.25	0.52
4:B:47:ILE:HG21	4:B:144:TYR:CD2	2.44	0.52
3:A:459:THR:HG21	3:A:463:ARG:HB3	1.91	0.52
6:H:104:SER:OG	6:H:105:VAL:N	2.41	0.52
3:A:435:VAL:HA	4:B:290:THR:HG23	1.90	0.52
6:H:156:PHE:CB	6:H:157:PRO:HD3	2.37	0.52
6:H:173:VAL:HG22	6:H:191:VAL:HG12	1.92	0.52
3:A:533:LEU:HD12	3:A:534:ALA:N	2.25	0.52
5:L:149:ALA:HB1	5:L:153:SER:HA	1.91	0.52
2:P:828:DT:C6	2:P:829:DT:H72	2.45	0.52
6:H:66:LYS:HD3	6:H:67:SER:N	2.24	0.52
4:B:73:LYS:HD3	4:B:146:TYR:OH	2.10	0.52
3:A:465:LYS:HZ2	3:A:465:LYS:HB2	1.75	0.52
3:A:307:ARG:HG3	3:A:307:ARG:NH1	2.25	0.52
4:B:96:HIS:NE2	4:B:382:ILE:O	2.43	0.52
4:B:195:ILE:CG1	4:B:199:ARG:HE	2.23	0.52
3:A:241:VAL:C	3:A:243:PRO:HD2	2.31	0.52
6:H:94:ILE:HG22	6:H:96:TYR:CE1	2.45	0.52
6:H:165:ASN:HD22	6:H:169:LEU:HD11	1.75	0.51
4:B:369:THR:HA	4:B:398:TRP:HH2	1.75	0.51
4:B:178:ILE:HD11	4:B:201:LYS:HG2	1.93	0.51
5:L:191:SER:HB2	5:L:210:ASN:OD1	2.11	0.51
3:A:554:ALA:C	3:A:556:ILE:H	2.14	0.51
3:A:86:ASP:O	4:B:55:PRO:HB3	2.10	0.51
3:A:337:TRP:HE1	3:A:367:GLN:HB3	1.75	0.51
3:A:153:TRP:CH2	3:A:155:GLY:HA3	2.45	0.51
6:H:2:ILE:HG22	6:H:26:GLY:CA	2.40	0.51
4:B:101:LYS:HG3	4:B:102:LYS:HG3	1.92	0.51
4:B:160:PHE:CD2	4:B:164:MET:HB2	2.45	0.51
3:A:332:GLN:HB3	3:A:336:GLN:CB	2.39	0.51
3:A:447:ASN:HB3	3:A:450:THR:CG2	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:39:LYS:CG	5:L:40:PRO:HD2	2.40	0.51
3:A:170:PRO:O	3:A:174:GLN:HG2	2.09	0.51
3:A:277:ARG:HB3	3:A:336:GLN:HE21	1.75	0.51
5:L:33:LEU:CD2	5:L:88:CYS:SG	2.89	0.51
6:H:160:VAL:HG23	6:H:208:ALA:O	2.10	0.51
4:B:16:MET:HE2	4:B:83:ARG:HA	1.92	0.51
5:L:116:SER:O	5:L:134:CYS:HA	2.10	0.51
3:A:317:VAL:HG22	3:A:318:TYR:N	2.25	0.51
4:B:93:GLY:HA3	4:B:161:GLN:HG3	1.92	0.51
4:B:163:SER:O	4:B:166:LYS:HG3	2.11	0.51
3:A:403:THR:O	3:A:406:TRP:HZ3	1.93	0.51
3:A:193:LEU:HD13	3:A:197:GLN:HG3	1.93	0.51
3:A:328:GLU:HB3	3:A:390:LYS:HB2	1.92	0.51
5:L:134:CYS:SG	5:L:136:LEU:HD21	2.50	0.51
3:A:556:ILE:HG12	3:A:557:ARG:N	2.26	0.51
3:A:523:GLU:HA	3:A:526:ILE:HB	1.91	0.51
3:A:438:GLU:OE1	3:A:463:ARG:NH2	2.43	0.51
4:B:287:LYS:HG3	4:B:288:ALA:H	1.75	0.51
3:A:155:GLY:C	3:A:157:PRO:HD2	2.32	0.51
6:H:1:GLN:HG2	6:H:2:ILE:CD1	2.40	0.51
3:A:408:ALA:HA	4:B:364:ASP:OD2	2.11	0.51
3:A:326:ILE:N	3:A:326:ILE:HD12	2.26	0.51
3:A:270:ILE:HA	3:A:351:THR:HG23	1.93	0.51
6:H:165:ASN:ND2	6:H:203:VAL:HA	2.25	0.51
2:P:829:DT:C2	2:P:830:DC:C2	2.99	0.51
2:P:829:DT:O2	2:P:830:DC:C2	2.64	0.51
3:A:459:THR:HG22	3:A:463:ARG:HB3	1.91	0.51
4:B:16:MET:CE	4:B:83:ARG:HA	2.41	0.51
3:A:395:LYS:HD2	3:A:395:LYS:N	2.26	0.51
3:A:113:ASP:OD1	3:A:116:PHE:HB2	2.11	0.51
4:B:279:LEU:HD23	4:B:299:ALA:HB1	1.93	0.51
2:P:830:DC:C2'	2:P:831:DG:N7	2.73	0.50
4:B:178:ILE:HG12	4:B:191:SER:HB2	1.93	0.50
3:A:453:GLY:O	3:A:468:PRO:HA	2.11	0.50
4:B:206:ARG:HH22	4:B:219:LYS:HG3	1.75	0.50
4:B:402:TRP:CE2	4:B:414:TRP:HH2	2.28	0.50
3:A:120:LEU:HD21	3:A:128:THR:HG21	1.92	0.50
3:A:128:THR:OG1	3:A:146:TYR:HB2	2.11	0.50
3:A:120:LEU:N	3:A:148:VAL:HA	2.26	0.50
3:A:473:THR:H	3:A:476:LYS:HB2	1.76	0.50
4:B:160:PHE:CD2	4:B:160:PHE:O	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:132:TYR:CD2	6:H:151:LEU:HD23	2.46	0.50
5:L:150:ILE:O	5:L:151:ASP:C	2.49	0.50
6:H:53:ILE:HG21	6:H:73:LYS:HG2	1.91	0.50
3:A:323:LYS:HB3	3:A:343:GLN:NE2	2.27	0.50
2:P:825:DC:N3	2:P:826:DT:C4	2.79	0.50
3:A:88:TRP:CZ3	4:B:57:ASN:HB3	2.47	0.50
3:A:532:TYR:C	3:A:532:TYR:CD2	2.84	0.50
1:T:812:DA:C4	1:T:813:DC:C5	2.99	0.50
6:H:207:VAL:HG12	6:H:208:ALA:N	2.25	0.50
3:A:337:TRP:CH2	3:A:368:LEU:HB2	2.46	0.50
3:A:480:GLN:HE22	3:A:483:TYR:HD2	1.59	0.50
4:B:23:GLN:OE1	4:B:59:PRO:HA	2.12	0.50
3:A:419:THR:OG1	3:A:420:PRO:HD3	2.11	0.50
4:B:328:GLU:OE2	4:B:430:GLU:HG2	2.11	0.50
3:A:47:ILE:HG22	3:A:145:GLN:O	2.11	0.50
2:P:834:DC:OP2	2:P:834:DC:H2'	2.12	0.50
1:T:818:DA:C2	2:P:822:DT:O2	2.60	0.50
1:T:809:DC:H2''	1:T:810:DG:O5'	2.11	0.50
6:H:206:ASN:O	6:H:206:ASN:ND2	2.45	0.50
5:L:198:HIS:C	5:L:200:THR:H	2.13	0.50
5:L:1:ASP:CA	5:L:95:PRO:HB2	2.42	0.50
4:B:332:GLN:OE1	4:B:424:LYS:HA	2.12	0.50
3:A:194:GLU:O	3:A:197:GLN:N	2.45	0.50
3:A:523:GLU:O	3:A:526:ILE:HB	2.11	0.50
2:P:831:DG:C4	2:P:832:DG:C8	3.00	0.50
4:B:30:LYS:HG2	4:B:62:ALA:HB3	1.93	0.50
3:A:354:TYR:CZ	3:A:356:ARG:HB3	2.46	0.50
4:B:223:LYS:HE2	6:H:60:ARG:HH22	1.76	0.50
4:B:127:TYR:N	4:B:127:TYR:CD2	2.75	0.50
5:L:133:VAL:HG11	6:H:134:LEU:HD13	1.93	0.50
6:H:22:CYS:HB2	6:H:38:TRP:CH2	2.46	0.50
3:A:242:GLN:C	3:A:244:ILE:H	2.15	0.50
4:B:104:LYS:HD3	4:B:192:ASP:OD1	2.12	0.50
3:A:438:GLU:HG2	3:A:461:LYS:CE	2.42	0.50
3:A:255:ASN:HA	3:A:258:GLN:NE2	2.26	0.50
6:H:175:THR:HG23	6:H:189:SER:HB2	1.94	0.50
4:B:67:ASP:HA	4:B:221:HIS:HB2	1.94	0.49
3:A:433:PRO:HB2	3:A:494:ASN:HD21	1.76	0.49
3:A:329:ILE:HG22	3:A:339:TYR:CB	2.37	0.49
3:A:182:GLN:HA	3:A:187:LEU:HD23	1.93	0.49
3:A:491:LEU:O	3:A:529:GLU:HB3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:48:ILE:CG2	5:L:54:LEU:HA	2.37	0.49
6:H:198:TRP:HZ2	6:H:220:ILE:HG12	1.77	0.49
4:B:386:THR:CG2	4:B:412:PRO:HB3	2.42	0.49
6:H:94:ILE:HG22	6:H:116:GLY:HA3	1.93	0.49
3:A:170:PRO:O	3:A:173:LYS:HB2	2.12	0.49
1:T:805:DC:H2''	1:T:806:DG:H8	1.77	0.49
6:H:95:TYR:N	6:H:95:TYR:HD1	2.10	0.49
3:A:354:TYR:OH	3:A:370:GLU:HB3	2.12	0.49
3:A:480:GLN:NE2	3:A:483:TYR:HB3	2.27	0.49
4:B:90:VAL:O	4:B:94:ILE:N	2.45	0.49
3:A:139:THR:HB	3:A:140:PRO:HD3	1.95	0.49
1:T:802:DT:O5'	1:T:802:DT:H6	1.95	0.49
3:A:83:ARG:HH11	3:A:83:ARG:HG2	1.78	0.49
4:B:348:ASN:HD21	4:B:429:LEU:HB3	1.76	0.49
4:B:78:ARG:CZ	4:B:411:ILE:HG22	2.42	0.49
3:A:392:PRO:O	3:A:393:ILE:HB	2.13	0.49
4:B:115:TYR:CE1	4:B:156:SER:HB3	2.47	0.49
3:A:382:ILE:HB	3:A:383:TRP:CE3	2.47	0.49
3:A:171:PHE:CE2	3:A:205:LEU:HD13	2.47	0.49
5:L:9:SER:O	5:L:102:THR:HA	2.12	0.49
6:H:56:ASP:O	6:H:57:ASP:HB3	2.12	0.49
3:A:394:GLN:O	3:A:397:THR:OG1	2.30	0.49
4:B:153:TRP:CH2	4:B:155:GLY:HA3	2.48	0.49
6:H:147:THR:HA	6:H:191:VAL:O	2.12	0.49
5:L:190:ASN:HA	5:L:212:ASN:OD1	2.11	0.49
5:L:170:ASP:O	5:L:172:THR:HG23	2.12	0.49
4:B:225:PRO:HB2	4:B:226:PRO:HD2	1.94	0.49
4:B:266:TRP:CH2	4:B:423:VAL:HG22	2.47	0.49
6:H:148:LEU:HB2	6:H:191:VAL:CG2	2.43	0.49
1:T:815:DG:N2	1:T:816:DG:C2	2.81	0.49
3:A:348:ASN:HD22	3:A:349:LEU:N	2.10	0.49
3:A:269:GLN:O	3:A:350:LYS:HG2	2.11	0.49
2:P:833:DG:O5'	2:P:833:DG:H2'	2.12	0.49
2:P:832:DG:C2	2:P:833:DG:O6	2.65	0.49
6:H:49:TRP:HZ3	6:H:62:ASN:HA	1.78	0.49
5:L:35:TRP:HB2	5:L:48:ILE:HG13	1.94	0.49
1:T:810:DG:C2'	1:T:811:DA:C8	2.91	0.49
6:H:2:ILE:HD11	6:H:112:HIS:NE2	2.28	0.49
3:A:5:ILE:HD12	3:A:6:GLU:N	2.28	0.49
3:A:131:THR:HG23	3:A:143:ARG:HD2	1.93	0.49
3:A:329:ILE:CD1	3:A:391:LEU:HA	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:7:THR:HG21	3:A:121:ASP:HA	1.94	0.49
6:H:176:PHE:HD1	6:H:188:SER:O	1.95	0.49
4:B:112:GLY:O	4:B:114:ALA:N	2.46	0.49
4:B:3:SER:OG	4:B:5:ILE:HG13	2.13	0.49
3:A:277:ARG:HA	3:A:280:SER:HB2	1.94	0.49
4:B:201:LYS:O	4:B:204:GLU:HB2	2.13	0.49
4:B:58:THR:CG2	4:B:59:PRO:HD2	2.43	0.49
4:B:162:SER:OG	4:B:163:SER:N	2.45	0.49
4:B:164:MET:HA	4:B:167:ILE:HD12	1.94	0.49
6:H:146:VAL:C	6:H:192:THR:HG23	2.33	0.49
3:A:295:LEU:O	3:A:298:GLU:N	2.46	0.49
2:P:837:DC:C1'	2:P:838:DA:H5'	2.43	0.48
3:A:106:VAL:HG12	3:A:107:THR:H	1.76	0.48
3:A:442:VAL:HG12	3:A:481:ALA:HB1	1.95	0.48
3:A:420:PRO:O	3:A:422:LEU:N	2.46	0.48
6:H:73:LYS:HA	6:H:80:ALA:HA	1.95	0.48
4:B:178:ILE:CD1	4:B:201:LYS:HG2	2.44	0.48
3:A:408:ALA:O	4:B:393:ILE:HD12	2.12	0.48
6:H:27:PHE:HD1	6:H:27:PHE:H	1.60	0.48
3:A:46:LYS:HD3	3:A:116:PHE:CD2	2.48	0.48
3:A:522:ILE:O	3:A:526:ILE:HG13	2.14	0.48
2:P:831:DG:C2	2:P:832:DG:C4	3.01	0.48
2:P:831:DG:N1	2:P:832:DG:C6	2.80	0.48
4:B:368:LEU:HD11	4:B:391:LEU:CD2	2.43	0.48
3:A:484:LEU:O	3:A:487:GLN:N	2.46	0.48
5:L:49:TYR:CD2	5:L:49:TYR:N	2.82	0.48
4:B:62:ALA:C	4:B:63:ILE:HG22	2.34	0.48
4:B:83:ARG:NH1	4:B:83:ARG:HG2	2.26	0.48
5:L:133:VAL:HG22	5:L:134:CYS:N	2.28	0.48
2:P:837:DC:H1'	2:P:838:DA:H5'	1.96	0.48
4:B:254:VAL:HG21	4:B:289:LEU:HA	1.94	0.48
4:B:98:ALA:C	4:B:100:LEU:H	2.16	0.48
4:B:122:GLU:HA	4:B:125:ARG:HE	1.79	0.48
4:B:34:LEU:HG	4:B:132:ILE:HD11	1.95	0.48
5:L:118:PHE:HA	5:L:119:PRO:HD3	1.72	0.48
2:P:821:DG:C2'	2:P:822:DT:C7	2.81	0.48
2:P:831:DG:C2'	2:P:832:DG:C8	2.97	0.48
3:A:112:GLY:HA3	3:A:217:PRO:HG2	1.95	0.48
3:A:98:ALA:HB1	3:A:383:TRP:CZ2	2.47	0.48
6:H:72:SER:HG	6:H:81:PHE:HD1	1.61	0.48
2:P:831:DG:C2	2:P:832:DG:C5	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:167:ASP:C	5:L:169:LYS:H	2.17	0.48
5:L:6:GLN:OE1	5:L:101:GLY:HA2	2.14	0.48
3:A:146:TYR:CE2	3:A:150:PRO:HA	2.49	0.48
6:H:34:ILE:HG22	6:H:35:GLY:H	1.77	0.48
3:A:271:TYR:CE1	3:A:314:VAL:HG22	2.49	0.48
4:B:388:LYS:N	4:B:388:LYS:HD3	2.29	0.48
2:P:823:DC:C2'	2:P:824:DC:C5'	2.68	0.48
3:A:18:GLY:HA3	3:A:56:TYR:CD2	2.48	0.48
3:A:459:THR:HG21	3:A:463:ARG:HE	1.79	0.48
3:A:88:TRP:CH2	4:B:21:VAL:O	2.66	0.48
3:A:325:LEU:HB3	3:A:387:PRO:CB	2.43	0.48
3:A:242:GLN:O	3:A:244:ILE:N	2.47	0.48
5:L:115:VAL:HG13	5:L:136:LEU:CD2	2.44	0.48
5:L:124:GLN:HE21	6:H:153:LYS:NZ	2.11	0.48
6:H:37:THR:HG22	6:H:38:TRP:N	2.28	0.48
1:T:804:DG:H2''	1:T:805:DC:C5'	2.43	0.47
1:T:804:DG:C2	1:T:805:DC:N3	2.82	0.47
3:A:277:ARG:CZ	3:A:336:GLN:HG2	2.44	0.47
6:H:195:SER:O	6:H:196:SER:C	2.50	0.47
3:A:465:LYS:HG3	3:A:466:VAL:N	2.29	0.47
5:L:51:THR:O	5:L:51:THR:HG22	2.13	0.47
3:A:194:GLU:O	3:A:196:GLY:N	2.47	0.47
4:B:339:TYR:CZ	4:B:352:GLY:HA3	2.49	0.47
4:B:88:TRP:HE1	4:B:92:LEU:HD22	1.78	0.47
6:H:173:VAL:HG12	6:H:174:HIS:N	2.29	0.47
2:P:831:DG:C6	2:P:832:DG:O6	2.68	0.47
6:H:163:THR:CA	6:H:206:ASN:HD21	2.28	0.47
3:A:498:ASP:HA	3:A:536:VAL:O	2.14	0.47
3:A:229:TRP:CE3	3:A:234:LEU:HD12	2.48	0.47
3:A:304:ALA:O	3:A:307:ARG:HB2	2.15	0.47
4:B:223:LYS:HG2	4:B:224:GLU:H	1.79	0.47
4:B:120:LEU:HB3	4:B:147:ASN:O	2.14	0.47
3:A:24:TRP:CD1	3:A:24:TRP:N	2.81	0.47
3:A:366:LYS:O	3:A:369:THR:HB	2.14	0.47
4:B:68:SER:HG	4:B:219:LYS:HB2	1.80	0.47
4:B:402:TRP:CZ2	4:B:414:TRP:HH2	2.32	0.47
4:B:123:ASP:O	4:B:125:ARG:N	2.47	0.47
4:B:229:TRP:HA	4:B:232:TYR:CG	2.50	0.47
3:A:420:PRO:CB	3:A:421:PRO:HD2	2.42	0.47
6:H:131:VAL:HA	6:H:151:LEU:O	2.14	0.47
1:T:804:DG:C8	1:T:804:DG:H5'	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:20:LYS:CG	3:A:56:TYR:HD2	2.28	0.47
6:H:65:LEU:O	6:H:66:LYS:C	2.52	0.47
4:B:193:LEU:HD23	4:B:193:LEU:N	2.29	0.47
4:B:50:ILE:CD1	4:B:145:GLN:HG3	2.31	0.47
4:B:73:LYS:HD3	4:B:151:GLN:HE21	1.77	0.47
4:B:369:THR:O	4:B:372:VAL:CG2	2.62	0.47
5:L:198:HIS:O	5:L:200:THR:N	2.40	0.47
4:B:88:TRP:CD1	4:B:89:GLU:N	2.83	0.47
3:A:503:LEU:CD1	3:A:535:TRP:HB2	2.45	0.47
4:B:425:LEU:C	4:B:427:TYR:N	2.67	0.47
3:A:550:LYS:HA	3:A:553:SER:O	2.15	0.47
3:A:333:GLY:H	3:A:336:GLN:CB	1.94	0.47
3:A:536:VAL:HG12	3:A:542:ILE:HD13	1.97	0.47
3:A:354:TYR:OH	3:A:356:ARG:HB3	2.15	0.47
3:A:508:ALA:O	3:A:509:GLN:HB2	2.15	0.47
6:H:11:ILE:HG12	6:H:120:THR:OG1	2.15	0.47
3:A:122:GLU:O	3:A:125:ARG:HB2	2.15	0.47
4:B:22:LYS:HD2	4:B:23:GLN:H	1.80	0.47
4:B:169:GLU:O	4:B:172:LYS:HG3	2.15	0.47
6:H:155:TYR:CE1	6:H:185:TYR:HB2	2.49	0.47
4:B:365:VAL:O	4:B:368:LEU:N	2.48	0.47
5:L:116:SER:O	5:L:135:PHE:N	2.47	0.47
4:B:395:LYS:O	4:B:396:GLU:C	2.53	0.47
4:B:225:PRO:HB2	4:B:226:PRO:HD3	1.96	0.47
4:B:121:ASP:O	4:B:125:ARG:HG3	2.14	0.47
4:B:107:THR:HG22	4:B:108:VAL:N	2.29	0.47
6:H:96:TYR:N	6:H:96:TYR:CD1	2.84	0.47
2:P:823:DC:O2	2:P:824:DC:C6	2.67	0.46
2:P:826:DT:OP1	3:A:361:HIS:NE2	2.45	0.46
6:H:164:TRP:HB2	6:H:169:LEU:HB2	1.97	0.46
6:H:104:SER:HB3	6:H:107:ASP:OD2	2.16	0.46
4:B:115:TYR:HB3	4:B:149:LEU:CB	2.42	0.46
4:B:266:TRP:CZ2	4:B:423:VAL:HG22	2.51	0.46
6:H:148:LEU:HD22	6:H:148:LEU:N	2.30	0.46
5:L:98:PHE:CD2	6:H:47:LEU:HB3	2.51	0.46
3:A:88:TRP:HH2	4:B:21:VAL:O	1.99	0.46
3:A:408:ALA:HB2	4:B:337:TRP:CH2	2.50	0.46
3:A:410:TRP:CH2	3:A:412:PRO:HA	2.50	0.46
4:B:263:LYS:HE3	4:B:425:LEU:O	2.14	0.46
2:P:822:DT:C2'	2:P:823:DC:H5	2.27	0.46
4:B:391:LEU:HD23	4:B:392:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:254:VAL:HG22	4:B:294:PRO:HG2	1.97	0.46
3:A:294:PRO:O	3:A:296:THR:N	2.48	0.46
3:A:81:ASN:OD1	3:A:154:LYS:HG2	2.15	0.46
3:A:420:PRO:O	3:A:422:LEU:HD23	2.15	0.46
3:A:395:LYS:HE2	3:A:416:PHE:HB2	1.97	0.46
3:A:47:ILE:HD12	3:A:144:TYR:CD2	2.50	0.46
2:P:825:DC:C4	2:P:826:DT:O4	2.68	0.46
4:B:191:SER:CB	4:B:193:LEU:HG	2.45	0.46
4:B:131:THR:HG23	4:B:143:ARG:HG2	1.96	0.46
4:B:73:LYS:HZ2	4:B:146:TYR:HE1	1.62	0.46
6:H:92:THR:HG1	6:H:120:THR:HA	1.77	0.46
3:A:150:PRO:HG2	3:A:153:TRP:CB	2.46	0.46
4:B:106:VAL:N	4:B:234:LEU:O	2.45	0.46
3:A:171:PHE:HB2	3:A:208:HIS:HD2	1.80	0.46
1:T:803:DG:C2	1:T:804:DG:C5	3.04	0.46
4:B:23:GLN:HE21	4:B:26:LEU:HD11	1.81	0.46
3:A:420:PRO:HB2	3:A:421:PRO:CD	2.44	0.46
4:B:224:GLU:O	4:B:227:PHE:CE2	2.68	0.46
3:A:385:LYS:HG2	3:A:386:THR:N	2.31	0.46
4:B:404:GLU:HB2	4:B:405:TYR:CE2	2.50	0.46
2:P:833:DG:N3	2:P:834:DC:C6	2.83	0.46
3:A:261:VAL:HA	3:A:264:LEU:CD1	2.45	0.46
4:B:42:GLU:HA	4:B:47:ILE:O	2.16	0.46
5:L:195:ALA:HA	5:L:206:VAL:HG22	1.96	0.46
6:H:55:TRP:CG	6:H:56:ASP:N	2.84	0.46
2:P:835:DG:H2''	2:P:836:DC:O5'	2.16	0.46
3:A:276:VAL:HG12	3:A:280:SER:OG	2.16	0.46
4:B:367:GLN:O	4:B:371:ALA:N	2.44	0.46
3:A:439:THR:HA	3:A:494:ASN:HB2	1.98	0.46
5:L:120:PRO:CB	5:L:125:LEU:HD21	2.45	0.46
3:A:231:GLY:O	3:A:241:VAL:HG12	2.16	0.46
6:H:61:TYR:OH	6:H:71:VAL:HG22	2.16	0.46
3:A:8:VAL:O	3:A:121:ASP:HB2	2.16	0.46
4:B:160:PHE:HD2	4:B:164:MET:HB2	1.81	0.46
4:B:122:GLU:HA	4:B:125:ARG:NE	2.31	0.46
5:L:160:LEU:O	5:L:178:THR:N	2.46	0.46
4:B:118:VAL:O	4:B:148:VAL:HG12	2.15	0.46
6:H:37:THR:O	6:H:97:CYS:HA	2.15	0.46
4:B:69:THR:CG2	4:B:70:LYS:N	2.79	0.46
1:T:805:DC:H5''	3:A:93:GLY:HA2	1.98	0.45
4:B:272:PRO:HG2	4:B:273:GLY:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:439:THR:OG1	3:A:439:THR:O	2.31	0.45
5:L:193:THR:HG23	5:L:208:SER:OG	2.15	0.45
5:L:167:ASP:O	5:L:169:LYS:N	2.49	0.45
4:B:350:LYS:HG2	4:B:351:THR:N	2.31	0.45
3:A:427:TYR:HE1	3:A:522:ILE:HG23	1.81	0.45
3:A:542:ILE:CD1	3:A:542:ILE:N	2.77	0.45
3:A:483:TYR:O	3:A:486:LEU:HB2	2.17	0.45
5:L:12:SER:HB3	5:L:105:GLU:CG	2.44	0.45
5:L:10:SER:CB	5:L:103:LYS:HB2	2.44	0.45
5:L:31:SER:HB2	5:L:50:TYR:HE1	1.80	0.45
3:A:188:TYR:HE2	3:A:234:LEU:CD1	2.28	0.45
3:A:163:SER:O	3:A:167:ILE:HD13	2.16	0.45
3:A:390:LYS:HB3	3:A:417:VAL:HG21	1.98	0.45
5:L:98:PHE:HD2	6:H:47:LEU:O	2.00	0.45
3:A:101:LYS:NZ	3:A:181:TYR:OH	2.49	0.45
4:B:170:PRO:O	4:B:174:GLN:HB2	2.17	0.45
3:A:470:THR:O	3:A:471:ASN:HB2	2.15	0.45
4:B:404:GLU:HB2	4:B:405:TYR:CD2	2.52	0.45
4:B:52:PRO:O	4:B:54:ASN:N	2.50	0.45
5:L:28:ASP:HA	5:L:68:GLY:O	2.16	0.45
3:A:522:ILE:HG22	3:A:526:ILE:HD11	1.99	0.45
6:H:95:TYR:H	6:H:95:TYR:HD1	1.65	0.45
4:B:377:THR:O	4:B:381:VAL:HG23	2.17	0.45
3:A:266:TRP:O	3:A:269:GLN:HG3	2.17	0.45
3:A:274:ILE:CG2	3:A:275:LYS:N	2.79	0.45
1:T:815:DG:C2	1:T:816:DG:C6	3.05	0.45
5:L:33:LEU:HA	5:L:89:GLN:O	2.17	0.45
5:L:17:ASP:O	5:L:78:LEU:HG	2.16	0.45
4:B:29:GLU:CG	4:B:71:TRP:HH2	2.27	0.45
6:H:145:MET:SD	6:H:194:PRO:HA	2.56	0.45
4:B:208:HIS:ND1	4:B:208:HIS:C	2.69	0.45
3:A:107:THR:HG23	3:A:221:HIS:O	2.16	0.45
4:B:368:LEU:HD11	4:B:391:LEU:HD22	1.99	0.45
4:B:88:TRP:CD1	4:B:92:LEU:HD22	2.52	0.45
4:B:385:LYS:CD	4:B:385:LYS:N	2.76	0.45
3:A:361:HIS:CD2	3:A:505:ILE:HG23	2.52	0.45
3:A:354:TYR:CD1	3:A:371:ALA:HA	2.52	0.45
3:A:486:LEU:HD22	3:A:528:LYS:NZ	2.32	0.45
3:A:206:ARG:CG	3:A:216:THR:HG21	2.44	0.45
4:B:195:ILE:HG13	4:B:199:ARG:HE	1.81	0.45
3:A:267:ALA:HB1	3:A:271:TYR:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:833:DG:C4	2:P:834:DC:C5	3.05	0.45
5:L:139:PHE:CE2	5:L:174:SER:HA	2.52	0.45
4:B:113:ASP:O	4:B:116:PHE:N	2.47	0.45
6:H:6:GLU:CD	6:H:6:GLU:H	2.20	0.45
3:A:425:LEU:HD12	3:A:425:LEU:N	2.31	0.45
4:B:376:THR:O	4:B:379:SER:N	2.50	0.45
5:L:142:LYS:HE2	5:L:142:LYS:O	2.17	0.45
4:B:66:LYS:O	4:B:67:ASP:HB3	2.16	0.44
5:L:108:ARG:HB3	5:L:140:TYR:CD1	2.52	0.44
3:A:450:THR:C	3:A:452:LEU:N	2.71	0.44
4:B:378:GLU:O	4:B:382:ILE:HG12	2.17	0.44
2:P:825:DC:H2'	2:P:826:DT:C7	2.47	0.44
1:T:815:DG:N3	1:T:816:DG:C5	2.84	0.44
4:B:221:HIS:O	4:B:222:GLN:HG3	2.17	0.44
1:T:811:DA:H1'	1:T:812:DA:O5'	2.17	0.44
5:L:108:ARG:HB3	5:L:140:TYR:CE1	2.53	0.44
3:A:146:TYR:HE2	3:A:150:PRO:HA	1.81	0.44
4:B:88:TRP:HD1	4:B:89:GLU:HG3	1.83	0.44
4:B:224:GLU:O	4:B:227:PHE:CZ	2.70	0.44
3:A:116:PHE:HZ	3:A:151:GLN:OE1	1.99	0.44
6:H:69:LEU:HD12	6:H:83:ASN:O	2.17	0.44
1:T:818:DA:H1'	1:T:819:DC:C6	2.52	0.44
4:B:326:ILE:O	4:B:341:ILE:HA	2.16	0.44
4:B:369:THR:O	4:B:370:GLU:C	2.56	0.44
4:B:369:THR:O	4:B:372:VAL:HG22	2.17	0.44
3:A:88:TRP:CD1	3:A:89:GLU:O	2.70	0.44
5:L:84:ALA:O	5:L:86:TYR:CD1	2.70	0.44
3:A:533:LEU:HD12	3:A:534:ALA:H	1.83	0.44
4:B:279:LEU:CD2	4:B:299:ALA:HB1	2.47	0.44
4:B:286:THR:HG22	4:B:286:THR:O	2.17	0.44
6:H:155:TYR:CE2	6:H:160:VAL:HG11	2.53	0.44
4:B:271:TYR:H	4:B:271:TYR:HD1	1.65	0.44
3:A:470:THR:CG2	3:A:471:ASN:N	2.81	0.44
6:H:216:VAL:HG22	6:H:217:ASP:N	2.32	0.44
2:P:830:DC:H2''	2:P:831:DG:H8	1.76	0.44
6:H:121:VAL:O	6:H:122:SER:HB2	2.17	0.44
4:B:236:PRO:O	4:B:237:ASP:C	2.56	0.44
3:A:50:ILE:CG2	3:A:145:GLN:HG2	2.47	0.44
6:H:38:TRP:CZ3	6:H:97:CYS:HB3	2.52	0.44
3:A:492:GLU:O	3:A:493:VAL:HB	2.18	0.44
6:H:96:TYR:N	6:H:96:TYR:HD1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:122:SER:O	5:L:126:THR:HG23	2.17	0.44
5:L:18:ARG:HA	5:L:76:SER:O	2.17	0.44
4:B:222:GLN:HA	4:B:229:TRP:CD1	2.52	0.44
4:B:74:LEU:HA	4:B:74:LEU:HD23	1.59	0.44
4:B:79:GLU:CD	4:B:83:ARG:HH12	2.21	0.44
3:A:10:VAL:HG21	3:A:153:TRP:HZ2	1.80	0.44
4:B:22:LYS:NZ	4:B:23:GLN:O	2.51	0.44
6:H:132:TYR:HE2	6:H:153:LYS:HD3	1.82	0.44
2:P:822:DT:H2'	2:P:823:DC:H5	1.83	0.44
1:T:814:DA:H2''	1:T:815:DG:C8	2.53	0.44
3:A:79:GLU:O	3:A:82:LYS:HB3	2.18	0.44
4:B:130:PHE:O	4:B:143:ARG:HB3	2.18	0.44
4:B:230:MET:HE1	6:H:103:THR:O	2.16	0.44
3:A:87:PHE:CZ	3:A:155:GLY:HA2	2.53	0.44
3:A:418:ASN:O	3:A:419:THR:HG23	2.18	0.44
6:H:27:PHE:CD1	6:H:27:PHE:N	2.80	0.44
5:L:169:LYS:HD3	5:L:169:LYS:HA	1.65	0.44
6:H:21:THR:HG23	6:H:81:PHE:CD2	2.53	0.44
6:H:115:GLN:HG2	6:H:115:GLN:O	2.17	0.44
2:P:838:DA:C1'	3:A:184:ILE:HD12	2.40	0.44
4:B:257:ILE:HG13	4:B:258:GLN:H	1.79	0.44
4:B:289:LEU:HD12	4:B:290:THR:N	2.32	0.44
3:A:154:LYS:C	3:A:157:PRO:HD2	2.38	0.44
4:B:406:TRP:CG	4:B:407:GLN:N	2.85	0.44
4:B:12:LEU:HA	4:B:85:GLN:H	1.83	0.44
2:P:838:DA:C4'	3:A:183:TYR:CE2	3.00	0.44
1:T:818:DA:H2''	1:T:819:DC:C5	2.53	0.44
3:A:463:ARG:O	3:A:464:GLN:HG3	2.18	0.44
4:B:22:LYS:HZ1	4:B:23:GLN:HB3	1.83	0.44
6:H:78:ASN:OD1	6:H:78:ASN:N	2.51	0.44
6:H:81:PHE:N	6:H:81:PHE:CD1	2.86	0.44
3:A:521:ILE:O	3:A:525:LEU:HD22	2.18	0.43
3:A:368:LEU:HD21	3:A:391:LEU:HB3	2.00	0.43
4:B:359:GLY:C	4:B:361:HIS:H	2.21	0.43
2:P:827:DG:C2'	2:P:828:DT:O5'	2.57	0.43
4:B:103:LYS:NZ	4:B:192:ASP:N	2.57	0.43
6:H:9:PRO:C	6:H:11:ILE:H	2.21	0.43
4:B:18:GLY:HA3	4:B:56:TYR:CE1	2.53	0.43
4:B:78:ARG:NH1	4:B:412:PRO:O	2.51	0.43
4:B:395:LYS:O	4:B:397:THR:N	2.51	0.43
3:A:406:TRP:HA	4:B:331:LYS:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:209:HIS:CE1	6:H:212:SER:H	2.36	0.43
5:L:10:SER:HB3	5:L:103:LYS:HD3	1.99	0.43
2:P:832:DG:C2	2:P:833:DG:C6	3.06	0.43
3:A:20:LYS:HG2	3:A:56:TYR:HD2	1.83	0.43
3:A:339:TYR:CE1	3:A:352:GLY:CA	3.01	0.43
4:B:58:THR:HG22	4:B:59:PRO:N	2.32	0.43
4:B:135:ILE:O	4:B:137:ASN:N	2.52	0.43
5:L:38:GLN:HG3	5:L:43:THR:O	2.18	0.43
6:H:114:GLY:O	6:H:115:GLN:C	2.57	0.43
4:B:152:GLY:HA2	4:B:184:ILE:HG22	1.99	0.43
3:A:2:ILE:CG2	3:A:3:SER:N	2.80	0.43
4:B:72:ARG:HG3	4:B:72:ARG:HH11	1.83	0.43
4:B:104:LYS:HB2	4:B:192:ASP:CA	2.48	0.43
3:A:453:GLY:O	3:A:469:LEU:N	2.42	0.43
3:A:348:ASN:ND2	3:A:349:LEU:H	2.15	0.43
6:H:6:GLU:HG3	6:H:97:CYS:SG	2.58	0.43
3:A:171:PHE:CE2	3:A:205:LEU:HB2	2.53	0.43
3:A:427:TYR:CE1	3:A:522:ILE:HG23	2.53	0.43
5:L:23:CYS:HB2	5:L:35:TRP:CZ2	2.54	0.43
6:H:91:ASP:O	6:H:95:TYR:OH	2.28	0.43
3:A:482:ILE:HG22	3:A:486:LEU:CD1	2.44	0.43
3:A:182:GLN:HG2	4:B:139:THR:HG22	1.99	0.43
3:A:225:PRO:HB2	3:A:226:PRO:CD	2.47	0.43
4:B:224:GLU:CD	5:L:96:TRP:HZ2	2.22	0.43
3:A:255:ASN:O	3:A:259:LYS:N	2.48	0.43
5:L:61:ALA:O	5:L:75:ILE:HA	2.17	0.43
3:A:262:GLY:HA2	3:A:265:ASN:HB2	2.01	0.43
3:A:463:ARG:CG	3:A:464:GLN:N	2.82	0.43
3:A:175:ASN:CB	3:A:178:ILE:HD13	2.46	0.43
3:A:408:ALA:HB2	4:B:337:TRP:HH2	1.82	0.43
4:B:260:LEU:HD21	4:B:264:LEU:HD23	2.00	0.43
4:B:126:LYS:HG3	4:B:127:TYR:CD2	2.54	0.43
3:A:239:TRP:CD1	3:A:316:GLY:O	2.71	0.43
3:A:427:TYR:CZ	3:A:525:LEU:HD23	2.53	0.43
4:B:65:LYS:HE3	4:B:220:LYS:HE3	2.01	0.43
5:L:160:LEU:O	5:L:177:SER:HA	2.19	0.43
6:H:89:THR:O	6:H:90:ALA:C	2.57	0.43
5:L:2:ILE:HD12	5:L:2:ILE:H	1.83	0.43
4:B:152:GLY:HA2	4:B:184:ILE:CG2	2.48	0.43
4:B:78:ARG:CZ	4:B:411:ILE:CG2	2.96	0.43
5:L:193:THR:CG2	5:L:206:VAL:HG13	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:402:TRP:HE3	4:B:331:LYS:NZ	2.15	0.43
2:P:837:DC:C4'	3:A:230:MET:CE	2.93	0.43
3:A:19:PRO:CG	3:A:80:LEU:HD23	2.48	0.43
4:B:130:PHE:N	4:B:130:PHE:CD1	2.87	0.43
4:B:326:ILE:HD12	4:B:342:TYR:CE1	2.54	0.43
6:H:158:GLU:HA	6:H:185:TYR:CD2	2.52	0.43
5:L:115:VAL:HG13	5:L:136:LEU:HD22	2.01	0.43
6:H:176:PHE:CD1	6:H:176:PHE:N	2.86	0.43
4:B:163:SER:HA	4:B:166:LYS:CE	2.49	0.43
3:A:500:GLN:OE1	4:B:421:PRO:HD2	2.19	0.43
4:B:125:ARG:C	4:B:127:TYR:N	2.72	0.43
5:L:211:ALA:HB1	5:L:213:GLU:OE1	2.18	0.43
6:H:146:VAL:O	6:H:192:THR:HG23	2.19	0.43
3:A:219:LYS:N	3:A:219:LYS:CD	2.82	0.43
6:H:29:LEU:HD23	6:H:29:LEU:HA	1.74	0.43
3:A:56:TYR:CE1	3:A:127:TYR:CE1	3.07	0.43
3:A:57:ASN:OD1	3:A:58:THR:N	2.51	0.43
4:B:229:TRP:HA	4:B:232:TYR:CE1	2.53	0.43
5:L:80:PRO:HG2	5:L:81:GLU:OE2	2.19	0.43
3:A:354:TYR:CE2	3:A:356:ARG:HB3	2.54	0.43
3:A:443:ASP:HB2	3:A:548:VAL:CG1	2.49	0.43
5:L:166:GLN:NE2	5:L:171:SER:HB3	2.32	0.43
4:B:376:THR:O	4:B:377:THR:C	2.56	0.43
3:A:512:LYS:O	3:A:513:SER:HB2	2.19	0.43
4:B:63:ILE:O	4:B:65:LYS:N	2.52	0.42
4:B:114:ALA:HB1	4:B:160:PHE:CZ	2.53	0.42
5:L:124:GLN:HG3	6:H:132:TYR:CZ	2.53	0.42
3:A:17:ASP:O	3:A:83:ARG:HD3	2.19	0.42
6:H:14:PRO:HG3	6:H:121:VAL:CG1	2.36	0.42
3:A:393:ILE:HG13	3:A:423:VAL:O	2.19	0.42
4:B:148:VAL:HB	4:B:149:LEU:H	1.52	0.42
3:A:443:ASP:HB2	3:A:548:VAL:HG11	2.01	0.42
3:A:353:LYS:HD3	3:A:353:LYS:C	2.40	0.42
6:H:210:PRO:HG2	6:H:211:ALA:H	1.83	0.42
3:A:161:GLN:O	3:A:162:SER:C	2.57	0.42
3:A:277:ARG:NH1	3:A:336:GLN:HG2	2.34	0.42
4:B:104:LYS:H	4:B:192:ASP:HA	1.84	0.42
3:A:458:VAL:HA	3:A:464:GLN:HA	2.00	0.42
4:B:21:VAL:CG1	4:B:22:LYS:N	2.81	0.42
3:A:410:TRP:CD2	4:B:363:ASN:ND2	2.87	0.42
3:A:380:ILE:HD13	3:A:380:ILE:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:179:VAL:O	3:A:189:VAL:HA	2.19	0.42
3:A:424:LYS:HE2	3:A:426:TRP:CE3	2.54	0.42
2:P:835:DG:H2''	2:P:836:DC:OP2	2.19	0.42
3:A:222:GLN:O	3:A:224:GLU:N	2.52	0.42
5:L:84:ALA:O	5:L:86:TYR:HD1	2.03	0.42
5:L:31:SER:HB2	5:L:50:TYR:CE1	2.55	0.42
6:H:32:SER:O	6:H:55:TRP:NE1	2.52	0.42
1:T:818:DA:H2''	1:T:819:DC:C6	2.55	0.42
3:A:19:PRO:O	3:A:57:ASN:N	2.53	0.42
3:A:279:LEU:CD1	3:A:279:LEU:N	2.79	0.42
3:A:59:PRO:O	3:A:75:VAL:HG13	2.19	0.42
3:A:90:VAL:O	3:A:91:GLN:CG	2.63	0.42
4:B:328:GLU:CD	4:B:430:GLU:HG2	2.40	0.42
4:B:245:VAL:CB	4:B:427:TYR:CE1	3.00	0.42
3:A:491:LEU:O	3:A:492:GLU:HG3	2.20	0.42
3:A:114:ALA:O	3:A:117:SER:HB2	2.19	0.42
3:A:218:ASP:C	3:A:220:LYS:H	2.22	0.42
2:P:831:DG:C4	2:P:832:DG:C5	3.08	0.42
5:L:113:PRO:HB3	5:L:139:PHE:HD2	1.83	0.42
3:A:459:THR:HG23	3:A:461:LYS:HB2	2.02	0.42
4:B:161:GLN:NE2	4:B:165:THR:HG21	2.35	0.42
5:L:86:TYR:CE1	5:L:104:LEU:HD23	2.55	0.42
4:B:126:LYS:HG3	4:B:127:TYR:CE2	2.55	0.42
5:L:179:LEU:HA	5:L:179:LEU:HD12	1.70	0.42
3:A:84:THR:HG22	3:A:85:GLN:N	2.35	0.42
3:A:274:ILE:HG22	3:A:275:LYS:N	2.34	0.42
4:B:72:ARG:CG	4:B:72:ARG:HH11	2.33	0.42
3:A:401:TRP:CZ2	3:A:405:TYR:CD2	3.07	0.42
3:A:523:GLU:HA	3:A:526:ILE:CD1	2.44	0.42
2:P:835:DG:H1'	2:P:836:DC:O5'	2.19	0.42
1:T:803:DG:C2'	1:T:804:DG:H5''	2.43	0.42
4:B:73:LYS:HD2	4:B:151:GLN:NE2	2.35	0.42
6:H:87:VAL:HG13	6:H:91:ASP:HB2	2.01	0.42
4:B:202:ILE:HD13	4:B:202:ILE:HA	1.92	0.42
4:B:203:GLU:HA	4:B:206:ARG:HD3	2.02	0.42
3:A:410:TRP:CE3	4:B:363:ASN:ND2	2.88	0.42
5:L:166:GLN:HB2	5:L:173:TYR:OH	2.20	0.42
3:A:64:LYS:HG2	3:A:72:ARG:N	2.33	0.42
6:H:61:TYR:HB2	6:H:66:LYS:HB2	2.02	0.42
3:A:156:SER:HB2	3:A:157:PRO:CD	2.46	0.42
3:A:165:THR:HG23	3:A:182:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:64:LYS:HG2	3:A:71:TRP:HA	2.00	0.42
2:P:829:DT:H2'	2:P:830:DC:C6	2.53	0.42
6:H:198:TRP:HB3	6:H:199:PRO:HD3	2.01	0.42
4:B:258:GLN:O	4:B:259:LYS:C	2.58	0.42
3:A:473:THR:OG1	3:A:476:LYS:HG3	2.20	0.42
4:B:121:ASP:OD2	4:B:123:ASP:N	2.53	0.42
5:L:167:ASP:C	5:L:169:LYS:N	2.73	0.42
2:P:827:DG:P	3:A:360:ALA:H	2.43	0.42
2:P:828:DT:H2'	2:P:829:DT:C7	2.49	0.42
6:H:162:VAL:HB	6:H:207:VAL:HG22	2.02	0.42
4:B:289:LEU:HD12	4:B:289:LEU:C	2.40	0.42
4:B:253:THR:HB	4:B:292:VAL:O	2.19	0.42
4:B:115:TYR:HE1	4:B:156:SER:C	2.23	0.42
6:H:152:VAL:N	6:H:187:LEU:O	2.39	0.42
5:L:203:SER:HA	5:L:204:PRO:HD3	1.64	0.42
5:L:121:SER:O	5:L:125:LEU:HG	2.20	0.42
5:L:122:SER:OG	5:L:123:GLU:N	2.53	0.42
1:T:805:DC:C5'	3:A:93:GLY:HA2	2.50	0.41
3:A:261:VAL:O	3:A:264:LEU:HB2	2.20	0.41
3:A:221:HIS:NE2	3:A:228:LEU:HB3	2.35	0.41
3:A:450:THR:O	3:A:451:LYS:HB2	2.20	0.41
3:A:155:GLY:O	3:A:156:SER:C	2.59	0.41
4:B:22:LYS:HZ3	4:B:23:GLN:CA	2.33	0.41
4:B:180:ILE:CG1	4:B:189:VAL:HG22	2.48	0.41
3:A:254:VAL:CG2	3:A:289:LEU:HA	2.50	0.41
3:A:474:ASN:HD22	3:A:474:ASN:N	2.16	0.41
3:A:519:ASN:HA	3:A:522:ILE:CD1	2.50	0.41
2:P:833:DG:O5'	2:P:833:DG:C2'	2.67	0.41
1:T:816:DG:H1	2:P:824:DC:H42	1.68	0.41
4:B:94:ILE:N	4:B:95:PRO:HD3	2.34	0.41
3:A:180:ILE:HA	3:A:188:TYR:O	2.19	0.41
3:A:412:PRO:HD3	4:B:401:TRP:CZ2	2.56	0.41
5:L:19:VAL:HG12	5:L:20:THR:N	2.35	0.41
4:B:424:LYS:C	4:B:426:TRP:N	2.69	0.41
4:B:224:GLU:OE2	5:L:96:TRP:HZ2	2.03	0.41
3:A:376:THR:O	3:A:377:THR:C	2.58	0.41
3:A:60:VAL:HG22	3:A:61:PHE:N	2.35	0.41
1:T:804:DG:N2	1:T:805:DC:O2	2.53	0.41
4:B:387:PRO:HG2	4:B:389:PHE:CZ	2.54	0.41
3:A:329:ILE:HD13	3:A:329:ILE:N	2.26	0.41
6:H:2:ILE:HD11	6:H:112:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:97:PRO:O	3:A:100:LEU:HB3	2.20	0.41
3:A:139:THR:N	3:A:140:PRO:CD	2.84	0.41
1:T:803:DG:N3	1:T:804:DG:C8	2.88	0.41
3:A:12:LEU:HD11	3:A:127:TYR:CE1	2.55	0.41
5:L:35:TRP:CH2	5:L:88:CYS:HB2	2.56	0.41
4:B:326:ILE:O	4:B:341:ILE:HG23	2.20	0.41
6:H:88:GLU:O	6:H:89:THR:C	2.58	0.41
3:A:149:LEU:HA	3:A:150:PRO:HD2	1.79	0.41
4:B:97:PRO:O	4:B:100:LEU:HB3	2.20	0.41
4:B:223:LYS:HE2	6:H:60:ARG:NH2	2.35	0.41
3:A:61:PHE:N	3:A:61:PHE:CD1	2.87	0.41
3:A:426:TRP:CE3	3:A:426:TRP:HA	2.56	0.41
5:L:106:ILE:HG22	5:L:107:LYS:N	2.35	0.41
4:B:202:ILE:CG2	4:B:203:GLU:N	2.84	0.41
5:L:55:HIS:O	5:L:58:VAL:HG23	2.20	0.41
3:A:329:ILE:HD11	3:A:392:PRO:CD	2.50	0.41
3:A:339:TYR:CE1	3:A:352:GLY:N	2.88	0.41
4:B:153:TRP:O	4:B:154:LYS:C	2.58	0.41
6:H:181:GLN:N	6:H:184:LEU:O	2.53	0.41
3:A:377:THR:CG2	3:A:378:GLU:N	2.83	0.41
3:A:517:LEU:O	3:A:520:GLN:HB2	2.19	0.41
3:A:312:GLU:HA	3:A:313:PRO:HD3	1.83	0.41
6:H:141:GLN:OE1	6:H:199:PRO:HG2	2.20	0.41
5:L:198:HIS:C	5:L:200:THR:N	2.73	0.41
3:A:371:ALA:O	3:A:375:ILE:HG13	2.21	0.41
3:A:10:VAL:HG23	3:A:87:PHE:HE2	1.85	0.41
4:B:124:PHE:CZ	4:B:153:TRP:CZ2	3.09	0.41
3:A:457:TYR:CD2	3:A:457:TYR:N	2.88	0.41
6:H:176:PHE:O	6:H:187:LEU:HG	2.20	0.41
4:B:97:PRO:HG2	4:B:100:LEU:HD22	2.02	0.41
4:B:266:TRP:CZ2	4:B:346:PHE:HE2	2.38	0.41
5:L:193:THR:CG2	5:L:194:CYS:N	2.83	0.41
3:A:167:ILE:N	3:A:167:ILE:CD1	2.83	0.41
4:B:258:GLN:NE2	4:B:283:LEU:HD21	2.35	0.41
4:B:96:HIS:CE1	4:B:382:ILE:O	2.73	0.41
5:L:204:PRO:O	5:L:206:VAL:HG23	2.20	0.41
4:B:223:LYS:CE	6:H:60:ARG:HH22	2.33	0.41
3:A:522:ILE:O	3:A:525:LEU:HB2	2.20	0.41
3:A:125:ARG:NH2	3:A:147:ASN:O	2.54	0.41
3:A:503:LEU:HD23	3:A:504:GLY:N	2.36	0.41
4:B:8:VAL:HA	4:B:9:PRO:HD3	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:802:DT:C2'	1:T:803:DG:OP2	2.69	0.41
4:B:205:LEU:O	4:B:205:LEU:HD23	2.21	0.41
4:B:61:PHE:O	4:B:74:LEU:HB2	2.20	0.41
4:B:365:VAL:O	4:B:366:LYS:C	2.58	0.41
3:A:119:PRO:HA	3:A:148:VAL:HA	2.03	0.41
4:B:406:TRP:O	4:B:407:GLN:OE1	2.39	0.41
4:B:89:GLU:HA	4:B:92:LEU:CD2	2.51	0.41
3:A:188:TYR:C	3:A:188:TYR:CD1	2.94	0.41
4:B:113:ASP:O	4:B:114:ALA:C	2.59	0.41
4:B:227:PHE:CZ	6:H:108:SER:HB2	2.55	0.41
4:B:319:TYR:HE2	4:B:321:PRO:HG3	1.80	0.41
3:A:325:LEU:HD11	3:A:383:TRP:CE3	2.56	0.41
3:A:362:THR:HG22	3:A:366:LYS:HZ2	1.83	0.41
6:H:39:ILE:HD11	6:H:110:MET:CE	2.51	0.41
3:A:171:PHE:HB2	3:A:208:HIS:CD2	2.54	0.41
3:A:454:LYS:CA	3:A:468:PRO:HA	2.39	0.41
4:B:31:ILE:O	4:B:32:LYS:C	2.59	0.41
4:B:88:TRP:O	4:B:92:LEU:HB3	2.21	0.41
3:A:307:ARG:CG	3:A:307:ARG:NH1	2.84	0.41
4:B:99:GLY:HA2	4:B:102:LYS:HD2	2.03	0.41
4:B:224:GLU:OE1	6:H:102:ILE:HD11	2.21	0.41
3:A:376:THR:HB	3:A:377:THR:H	1.73	0.41
6:H:41:GLN:HA	6:H:42:PRO:HD3	1.67	0.41
4:B:288:ALA:O	4:B:292:VAL:CB	2.69	0.40
3:A:372:VAL:HG13	3:A:389:PHE:CZ	2.56	0.40
5:L:205:ILE:H	5:L:205:ILE:CD1	2.19	0.40
3:A:75:VAL:HG12	3:A:76:ASP:N	2.35	0.40
4:B:46:LYS:C	4:B:147:ASN:HD22	2.24	0.40
3:A:442:VAL:CG1	3:A:481:ALA:HB1	2.50	0.40
4:B:266:TRP:CA	4:B:269:GLN:HE21	2.34	0.40
3:A:324:ASP:N	3:A:343:GLN:HE21	2.19	0.40
3:A:60:VAL:CG2	3:A:61:PHE:N	2.83	0.40
3:A:265:ASN:O	3:A:268:SER:OG	2.39	0.40
3:A:427:TYR:CE2	3:A:525:LEU:HD23	2.57	0.40
4:B:222:GLN:HE21	4:B:222:GLN:HB2	1.62	0.40
3:A:461:LYS:C	3:A:463:ARG:H	2.21	0.40
5:L:2:ILE:HD11	5:L:93:LYS:CB	2.49	0.40
4:B:260:LEU:HD23	4:B:260:LEU:C	2.42	0.40
3:A:209:LEU:O	3:A:214:LEU:HB2	2.20	0.40
4:B:12:LEU:HA	4:B:84:THR:HA	2.03	0.40
2:P:834:DC:C2	2:P:835:DG:N7	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:260:LEU:HD11	3:A:264:LEU:HD21	2.03	0.40
3:A:433:PRO:CB	4:B:289:LEU:HD11	2.52	0.40
5:L:58:VAL:HA	5:L:59:PRO:HD3	1.91	0.40
4:B:22:LYS:NZ	4:B:23:GLN:N	2.60	0.40
4:B:236:PRO:HA	4:B:239:TRP:CE2	2.56	0.40
3:A:131:THR:HA	3:A:142:ILE:O	2.21	0.40
1:T:817:DG:H2''	1:T:818:DA:C5'	2.35	0.40
3:A:30:LYS:O	3:A:33:ALA:HB3	2.22	0.40
4:B:363:ASN:O	4:B:364:ASP:C	2.60	0.40
5:L:11:LEU:HD23	5:L:11:LEU:N	2.36	0.40
4:B:64:LYS:HB2	4:B:71:TRP:CZ3	2.56	0.40
5:L:84:ALA:O	5:L:104:LEU:HB3	2.21	0.40
5:L:39:LYS:O	5:L:42:GLY:N	2.54	0.40
4:B:207:GLN:O	4:B:211:ARG:HG2	2.21	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	
3	A	556/558 (100%)	394 (71%)	121 (22%)	41 (7%)	1	16
4	B	428/430 (100%)	284 (66%)	96 (22%)	48 (11%)	0	7
5	L	212/214 (99%)	162 (76%)	35 (16%)	15 (7%)	1	17
6	H	218/220 (99%)	160 (73%)	42 (19%)	16 (7%)	1	16
All	All	1414/1422 (99%)	1000 (71%)	294 (21%)	120 (8%)	1	13

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	63	ILE

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Mol	Chain	Res	Type
3	A	66	LYS
3	A	136	ASN
3	A	195	ILE
3	A	223	LYS
3	A	251	SER
3	A	273	GLY
3	A	294	PRO
3	A	345	PRO
3	A	358	ARG
4	B	12	LEU
4	B	63	ILE
4	B	85	GLN
4	B	213	GLY
4	B	225	PRO
4	B	227	PHE
4	B	237	ASP
4	B	242	GLN
4	B	247	PRO
4	B	286	THR
4	B	332	GLN
4	B	395	LYS
4	B	400	THR
5	L	80	PRO
5	L	110	ASP
5	L	153	SER
6	H	180	LEU
3	A	91	GLN
3	A	114	ALA
3	A	137	ASN
3	A	184	ILE
3	A	252	TRP
3	A	376	THR
3	A	393	ILE
3	A	462	GLY
3	A	465	LYS
3	A	493	VAL
3	A	513	SER
3	A	528	LYS
4	B	53	GLU
4	B	64	LYS
4	B	113	ASP
4	B	126	LYS

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Mol	Chain	Res	Type
4	B	245	VAL
4	B	251	SER
4	B	382	ILE
4	B	396	GLU
4	B	399	GLU
4	B	426	TRP
4	B	429	LEU
5	L	101	GLY
5	L	138	ASN
6	H	76	SER
6	H	89	THR
6	H	116	GLY
3	A	128	THR
3	A	284	ARG
3	A	295	LEU
3	A	419	THR
3	A	445	ALA
3	A	484	LEU
3	A	539	HIS
4	B	17	ASP
4	B	70	LYS
4	B	124	PHE
4	B	153	TRP
4	B	160	PHE
4	B	175	ASN
4	B	358	ARG
5	L	52	SER
5	L	61	ALA
5	L	151	ASP
5	L	156	ALA
5	L	168	SER
6	H	115	GLN
6	H	124	ALA
6	H	126	THR
3	A	77	PHE
3	A	243	PRO
3	A	244	ILE
4	B	99	GLY
4	B	119	PRO
4	B	136	ASN
4	B	184	ILE
4	B	272	PRO

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Mol	Chain	Res	Type
4	B	360	ALA
5	L	199	LYS
6	H	17	PRO
6	H	105	VAL
6	H	160	VAL
6	H	213	SER
3	A	164	MET
3	A	177	ASP
4	B	20	LYS
4	B	148	VAL
4	B	317	VAL
4	B	404	GLU
5	L	68	GLY
5	L	144	ILE
6	H	90	ALA
3	A	156	SER
3	A	157	PRO
3	A	433	PRO
4	B	195	ILE
4	B	316	GLY
4	B	364	ASP
5	L	171	SER
6	H	26	GLY
6	H	66	LYS
6	H	156	PHE
4	B	236	PRO
3	A	10	VAL
3	A	490	GLY
4	B	133	PRO
5	L	94	PHE
3	A	261	VAL
4	B	90	VAL
3	A	541	GLY
4	B	294	PRO
6	H	44	GLY

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	434/498 (87%)	364 (84%)	70 (16%)	3	18
4	B	350/392 (89%)	290 (83%)	60 (17%)	2	15
5	L	182/182 (100%)	148 (81%)	34 (19%)	2	11
6	H	191/191 (100%)	168 (88%)	23 (12%)	6	30
All	All	1157/1263 (92%)	970 (84%)	187 (16%)	3	17

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	11	LYS
3	A	16	MET
3	A	22	LYS
3	A	24	TRP
3	A	26	LEU
3	A	58	THR
3	A	87	PHE
3	A	89	GLU
3	A	94	ILE
3	A	101	LYS
3	A	110	ASP
3	A	147	ASN
3	A	157	PRO
3	A	162	SER
3	A	164	MET
3	A	165	THR
3	A	175	ASN
3	A	177	ASP
3	A	188	TYR
3	A	204	GLU
3	A	208	HIS
3	A	228	LEU
3	A	230	MET
3	A	234	LEU
3	A	237	ASP
3	A	240	THR
3	A	246	LEU
3	A	256	ASP
3	A	279	LEU
3	A	307	ARG
3	A	310	LEU

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Mol	Chain	Res	Type
3	A	326	ILE
3	A	329	ILE
3	A	339	TYR
3	A	341	ILE
3	A	345	PRO
3	A	348	ASN
3	A	349	LEU
3	A	353	LYS
3	A	364	ASP
3	A	365	VAL
3	A	377	THR
3	A	382	ILE
3	A	395	LYS
3	A	405	TYR
3	A	406	TRP
3	A	410	TRP
3	A	419	THR
3	A	420	PRO
3	A	424	LYS
3	A	425	LEU
3	A	429	LEU
3	A	439	THR
3	A	443	ASP
3	A	452	LEU
3	A	457	TYR
3	A	465	LYS
3	A	469	LEU
3	A	475	GLN
3	A	479	LEU
3	A	492	GLU
3	A	497	THR
3	A	500	GLN
3	A	506	ILE
3	A	507	GLN
3	A	512	LYS
3	A	518	VAL
3	A	525	LEU
3	A	532	TYR
3	A	542	ILE
4	B	2	ILE
4	B	8	VAL
4	B	11	LYS

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Mol	Chain	Res	Type
4	B	12	LEU
4	B	27	THR
4	B	36	GLU
4	B	42	GLU
4	B	50	ILE
4	B	52	PRO
4	B	63	ILE
4	B	64	LYS
4	B	67	ASP
4	B	70	LYS
4	B	72	ARG
4	B	73	LYS
4	B	88	TRP
4	B	92	LEU
4	B	104	LYS
4	B	108	VAL
4	B	109	LEU
4	B	131	THR
4	B	143	ARG
4	B	148	VAL
4	B	159	ILE
4	B	163	SER
4	B	166	LYS
4	B	174	GLN
4	B	175	ASN
4	B	179	VAL
4	B	191	SER
4	B	192	ASP
4	B	193	LEU
4	B	202	ILE
4	B	207	GLN
4	B	211	ARG
4	B	218	ASP
4	B	219	LYS
4	B	222	GLN
4	B	228	LEU
4	B	235	HIS
4	B	255	ASN
4	B	256	ASP
4	B	264	LEU
4	B	271	TYR
4	B	279	LEU

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Mol	Chain	Res	Type
4	B	289	LEU
4	B	326	ILE
4	B	330	GLN
4	B	348	ASN
4	B	356	ARG
4	B	364	ASP
4	B	365	VAL
4	B	377	THR
4	B	383	TRP
4	B	385	LYS
4	B	396	GLU
4	B	419	THR
4	B	422	LEU
4	B	425	LEU
4	B	427	TYR
5	L	3	GLN
5	L	8	THR
5	L	15	LEU
5	L	18	ARG
5	L	33	LEU
5	L	37	GLN
5	L	39	LYS
5	L	48	ILE
5	L	49	TYR
5	L	50	TYR
5	L	60	SER
5	L	75	ILE
5	L	77	ASN
5	L	90	GLN
5	L	91	TYR
5	L	97	THR
5	L	108	ARG
5	L	110	ASP
5	L	136	LEU
5	L	137	ASN
5	L	142	LYS
5	L	161	ASN
5	L	165	ASP
5	L	168	SER
5	L	169	LYS
5	L	174	SER
5	L	175	MET

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Mol	Chain	Res	Type
5	L	180	THR
5	L	185	GLU
5	L	187	GLU
5	L	197	THR
5	L	208	SER
5	L	210	ASN
5	L	214	CYS
6	H	2	ILE
6	H	4	LEU
6	H	6	GLU
6	H	13	GLN
6	H	59	ASN
6	H	66	LYS
6	H	68	ARG
6	H	73	LYS
6	H	81	PHE
6	H	85	MET
6	H	86	THR
6	H	95	TYR
6	H	96	TYR
6	H	100	SER
6	H	107	ASP
6	H	150	CYS
6	H	162	VAL
6	H	176	PHE
6	H	184	LEU
6	H	196	SER
6	H	205	CYS
6	H	206	ASN
6	H	219	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	147	ASN
3	A	175	ASN
3	A	182	GLN
3	A	198	HIS
3	A	258	GLN
3	A	269	GLN
3	A	330	GLN
3	A	348	ASN

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Mol	Chain	Res	Type
3	A	407	GLN
3	A	428	GLN
3	A	474	ASN
3	A	475	GLN
3	A	480	GLN
3	A	494	ASN
4	B	136	ASN
4	B	151	GLN
4	B	207	GLN
4	B	221	HIS
4	B	222	GLN
4	B	258	GLN
4	B	306	ASN
4	B	330	GLN
4	B	340	GLN
5	L	3	GLN
5	L	6	GLN
5	L	37	GLN
5	L	38	GLN
5	L	77	ASN
5	L	124	GLN
5	L	145	ASN
5	L	210	ASN
6	H	1	GLN
6	H	59	ASN
6	H	62	ASN
6	H	83	ASN
6	H	206	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	T	19/19 (100%)	0.58	2 (10%) 8 8	59, 76, 94, 96	0
2	P	18/18 (100%)	0.14	1 (5%) 28 22	61, 74, 86, 87	0
3	A	558/558 (100%)	-0.31	0 100 100	11, 52, 75, 92	0
4	B	430/430 (100%)	-0.42	5 (1%) 81 72	6, 32, 75, 93	0
5	L	214/214 (100%)	-0.32	3 (1%) 78 68	17, 44, 66, 76	0
6	H	220/220 (100%)	-0.44	1 (0%) 91 88	14, 33, 57, 68	0
All	All	1459/1459 (100%)	-0.35	12 (0%) 87 80	6, 43, 75, 96	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	L	214	CYS	5.9
4	B	429	LEU	5.6
1	T	801	DA	3.9
4	B	427	TYR	3.5
4	B	428	GLN	3.2
4	B	93	GLY	3.2
6	H	141	GLN	2.8
5	L	213	GLU	2.5
2	P	821	DG	2.4
1	T	819	DC	2.3
5	L	153	SER	2.1
4	B	430	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.