



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 10:59 PM EDT

PDB ID : 1J5O / pdb_00001j5o
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

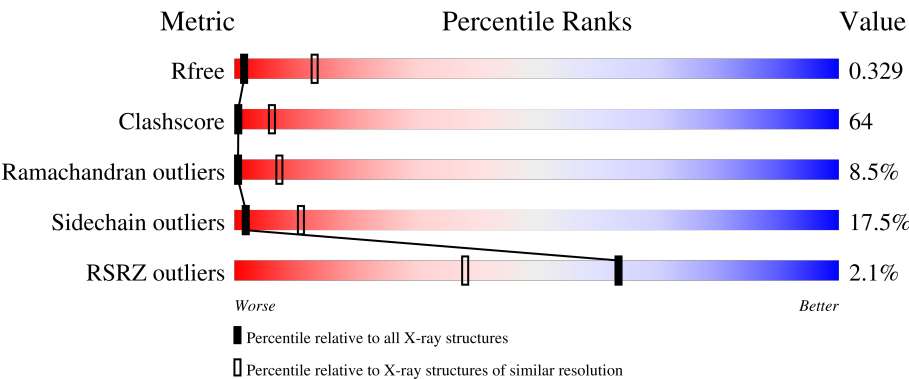
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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

Mol	Chain	Length	Quality of chain
1	T	19	
2	P	18	
3	A	558	
4	B	430	
5	L	214	

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Mol	Chain	Length	Quality of chain
6	H	220	24% 62% 14%

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 mutation	UNP P03366
A	280	SER	CYS	engineered mutation	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 mutation	UNP P03366
B	280	SER	CYS	engineered mutation	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			

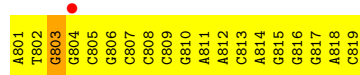
- Molecule 6 is a protein called ANTIBODY (HEAVY CHAIN).

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

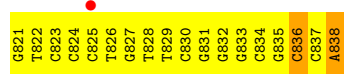
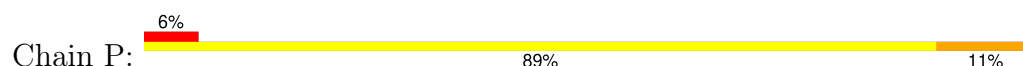
3 Residue-property plots

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

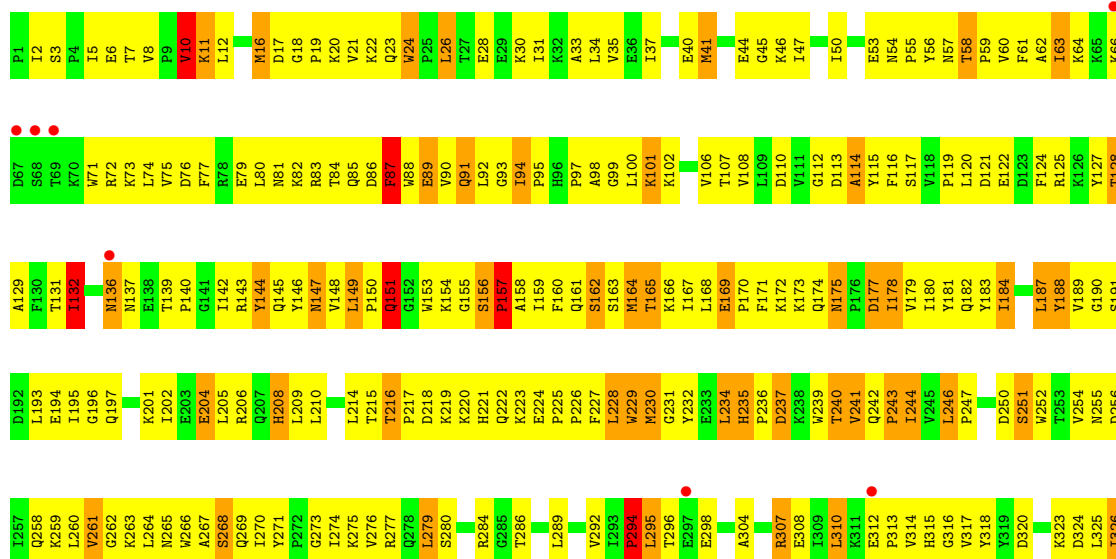
- Molecule 1: 5'-D(*AP*TP*GP*GP*CP*GP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*C)-3'

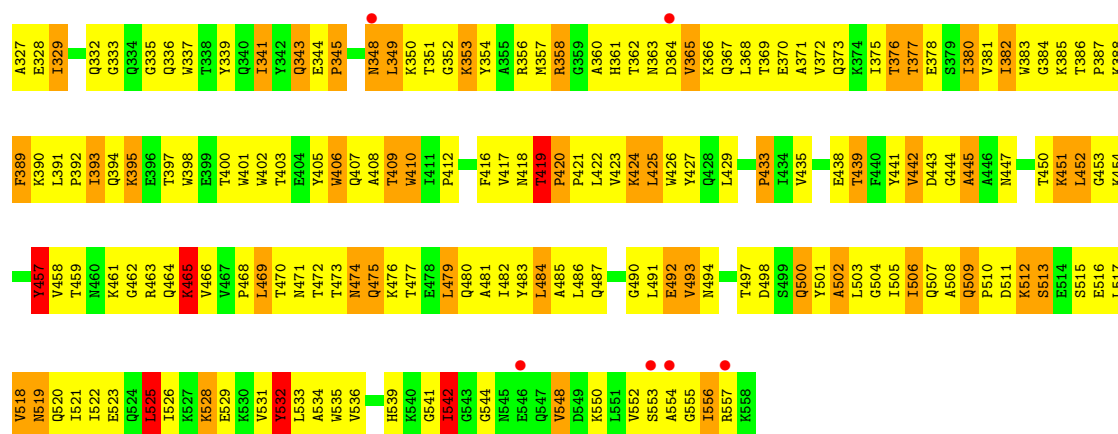


- Molecule 2: 5'-D(*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP*CP*CP*A)-3'

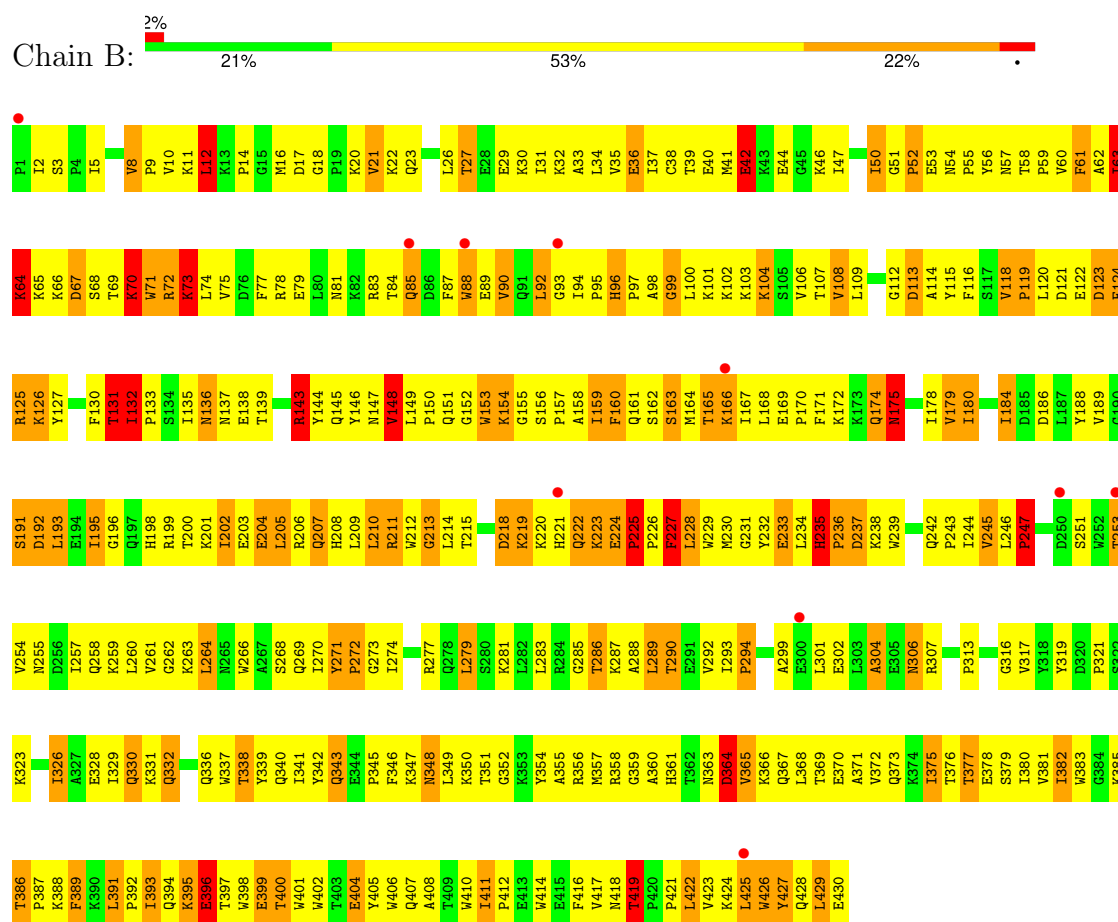


- Molecule 3: Reverse transcriptase

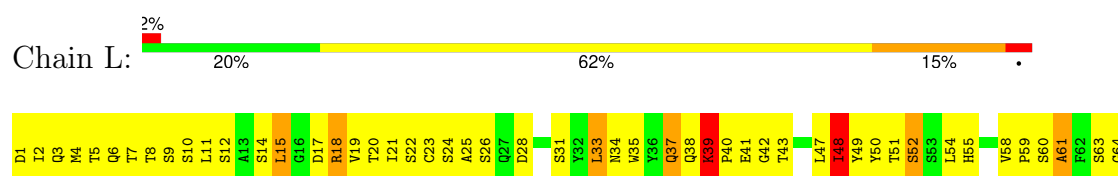




• Molecule 4: Reverse transcriptase

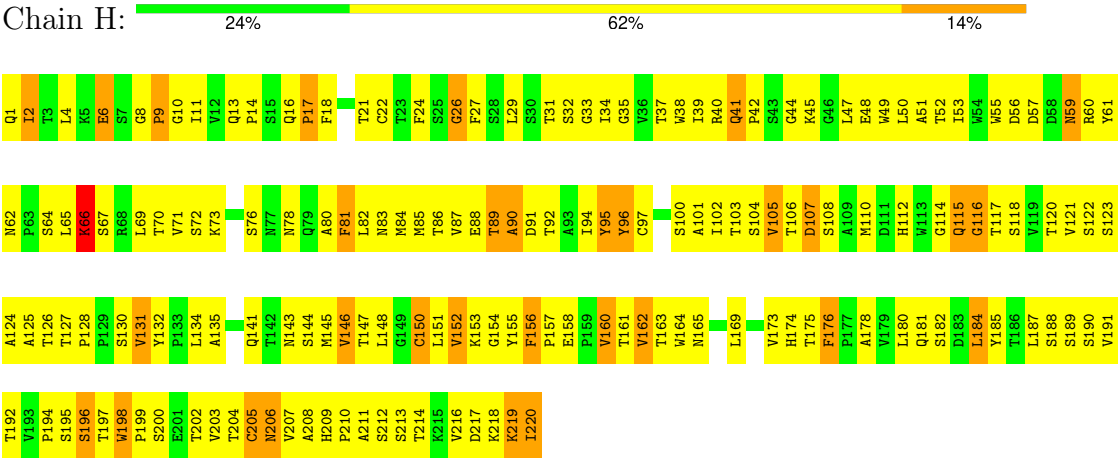


• Molecule 5: ANTIBODY (LIGHT CHAIN)





● 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 10.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	91.5 (10.00-3.50) 87.2 (10.00-3.50)	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	1272 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å ²)	98.8	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.049 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.39	0/439	0.75	1/676 (0.1%)
2	P	0.43	0/405	0.83	1/623 (0.2%)
3	A	0.67	0/4404	1.19	36/6017 (0.6%)
4	B	0.74	2/3510 (0.1%)	1.28	56/4784 (1.2%)
5	L	0.65	0/1654	1.29	28/2256 (1.2%)
6	H	0.74	0/1691	1.24	15/2320 (0.6%)
All	All	0.69	2/12103 (0.0%)	1.21	137/16676 (0.8%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	21	VAL	CA-CB	-5.99	1.47	1.54
4	B	225	PRO	CA-C	5.75	1.57	1.52

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	243	PRO	N-CA-CB	12.01	110.87	102.35
6	H	8	GLY	CA-C-N	10.58	130.40	119.19
6	H	8	GLY	C-N-CA	10.58	130.40	119.19
3	A	132	ILE	CA-C-N	9.72	129.54	120.21
3	A	132	ILE	C-N-CA	9.72	129.54	120.21
4	B	186	ASP	N-CA-C	9.29	124.72	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	79	GLU	CA-C-N	9.28	131.44	119.84
5	L	79	GLU	C-N-CA	9.28	131.44	119.84
4	B	338	THR	N-CA-C	8.40	122.77	109.50
3	A	320	ASP	CA-C-N	8.27	127.96	119.19
3	A	320	ASP	C-N-CA	8.27	127.96	119.19
4	B	235	HIS	CA-C-N	8.07	129.93	119.84
4	B	235	HIS	C-N-CA	8.07	129.93	119.84
3	A	344	GLU	CA-C-N	8.00	129.84	119.84
3	A	344	GLU	C-N-CA	8.00	129.84	119.84
4	B	391	LEU	N-CA-C	7.99	120.35	109.24
3	A	389	PHE	N-CA-C	7.89	122.10	108.76
4	B	247	PRO	N-CA-CB	7.76	111.39	103.25
6	H	197	THR	N-CA-C	7.67	120.38	111.02
4	B	419	THR	CA-C-N	7.66	128.27	120.38
4	B	419	THR	C-N-CA	7.66	128.27	120.38
4	B	389	PHE	N-CA-C	7.65	121.41	108.02
5	L	94	PHE	CA-C-N	-7.54	110.41	119.84
5	L	94	PHE	C-N-CA	-7.54	110.41	119.84
3	A	525	LEU	N-CA-C	-7.48	103.13	111.28
3	A	343	GLN	N-CA-C	-7.42	104.75	113.88
4	B	343	GLN	N-CA-C	-7.42	103.31	113.18
5	L	202	THR	N-CA-C	-7.39	101.77	111.74
3	A	555	GLY	N-CA-C	-7.23	105.86	115.40
3	A	509	GLN	CA-C-N	7.13	127.39	119.90
3	A	509	GLN	C-N-CA	7.13	127.39	119.90
5	L	72	SER	N-CA-C	7.11	121.27	108.69
6	H	205	CYS	N-CA-C	-6.96	97.89	109.24
4	B	123	ASP	N-CA-C	6.94	118.54	110.97
5	L	48	ILE	N-CA-C	6.81	117.34	108.35
3	A	294	PRO	N-CA-CB	6.80	110.39	103.25
4	B	224	GLU	CA-C-N	-6.79	113.39	120.38
4	B	224	GLU	C-N-CA	-6.79	113.39	120.38
4	B	391	LEU	CA-C-N	6.78	128.31	119.84
4	B	391	LEU	C-N-CA	6.78	128.31	119.84
3	A	247	PRO	N-CA-CB	6.78	110.06	102.67
4	B	131	THR	N-CA-C	6.73	119.71	108.13
4	B	223	LYS	N-CA-C	6.71	117.13	108.34
5	L	78	LEU	N-CA-C	6.67	120.36	109.76
4	B	42	GLU	N-CA-C	-6.65	103.96	111.14
6	H	202	THR	N-CA-C	6.52	119.21	110.35
4	B	262	GLY	N-CA-C	-6.43	104.76	113.37
6	H	41	GLN	CA-C-N	6.39	127.82	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	41	GLN	C-N-CA	6.39	127.82	119.84
4	B	419	THR	N-CA-C	6.37	119.59	109.40
3	A	149	LEU	CA-C-N	6.37	126.58	119.90
3	A	149	LEU	C-N-CA	6.37	126.58	119.90
4	B	411	ILE	CA-C-N	6.33	126.28	120.21
4	B	411	ILE	C-N-CA	6.33	126.28	120.21
5	L	140	TYR	N-CA-C	6.32	123.77	109.81
3	A	187	LEU	N-CA-C	6.28	119.01	108.02
5	L	39	LYS	CA-C-N	6.27	125.96	119.82
5	L	39	LYS	C-N-CA	6.27	125.96	119.82
3	A	542	ILE	N-CA-C	6.24	117.10	108.12
5	L	140	TYR	CA-C-N	-6.24	113.53	119.76
5	L	140	TYR	C-N-CA	-6.24	113.53	119.76
4	B	304	ALA	N-CA-C	-6.21	105.70	113.28
4	B	313	PRO	N-CA-CB	6.18	109.74	103.25
1	T	803	DG	N9-C1'-C2'	-6.15	104.27	113.50
5	L	5	THR	N-CA-C	6.07	119.44	108.69
5	L	142	LYS	N-CA-C	-6.07	103.83	111.11
4	B	277	ARG	N-CA-C	6.06	118.38	111.11
4	B	159	ILE	N-CA-C	6.05	116.24	110.74
5	L	41	GLU	N-CA-C	-5.97	106.24	112.93
3	A	216	THR	CA-C-N	5.96	125.97	119.89
3	A	216	THR	C-N-CA	5.96	125.97	119.89
3	A	451	LYS	N-CA-C	-5.94	104.69	113.72
4	B	96	HIS	CA-C-N	5.91	128.23	120.25
4	B	96	HIS	C-N-CA	5.91	128.23	120.25
4	B	61	PHE	N-CA-C	5.88	117.46	108.52
3	A	457	TYR	N-CA-C	5.85	116.27	108.38
3	A	28	GLU	N-CA-C	5.85	117.34	110.97
5	L	22	SER	N-CA-C	5.82	117.78	108.41
3	A	74	LEU	N-CA-C	5.81	119.42	110.42
4	B	386	THR	CA-C-N	5.80	125.70	119.85
4	B	386	THR	C-N-CA	5.80	125.70	119.85
5	L	82	ASP	N-CA-C	5.76	120.15	113.18
4	B	118	VAL	CA-C-N	5.75	127.03	119.84
4	B	118	VAL	C-N-CA	5.75	127.03	119.84
5	L	137	ASN	N-CA-C	5.75	118.44	109.52
4	B	165	THR	N-CA-C	5.73	117.22	110.97
4	B	71	TRP	N-CA-C	-5.71	103.11	110.19
3	A	136	ASN	N-CA-C	5.66	122.85	110.80
2	P	838	DA	C2'-C3'-O3'	5.64	119.97	111.50
4	B	143	ARG	N-CA-C	5.64	119.00	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	ALA	N-CA-C	-5.61	105.06	111.07
3	A	519	ASN	N-CA-C	-5.61	105.24	111.36
4	B	417	VAL	N-CA-C	5.60	115.61	107.88
5	L	21	ILE	N-CA-C	5.59	115.94	108.11
5	L	93	LYS	N-CA-C	-5.55	100.75	109.25
3	A	292	VAL	N-CA-C	5.55	114.80	106.42
6	H	123	SER	N-CA-C	-5.52	104.96	110.97
3	A	532	TYR	N-CA-C	-5.52	100.55	108.60
4	B	125	ARG	N-CA-C	5.51	117.72	111.11
5	L	89	GLN	N-CA-C	5.51	118.07	108.76
6	H	131	VAL	N-CA-C	5.47	116.11	108.89
4	B	227	PHE	N-CA-C	5.45	122.40	110.80
5	L	99	GLY	N-CA-C	-5.41	105.35	112.82
4	B	73	LYS	N-CA-C	-5.39	101.75	110.32
4	B	225	PRO	CB-CA-C	5.36	117.45	110.92
6	H	146	VAL	N-CA-C	5.36	116.38	108.45
4	B	293	ILE	CA-C-N	5.34	126.51	119.84
4	B	293	ILE	C-N-CA	5.34	126.51	119.84
4	B	224	GLU	N-CA-C	5.33	121.59	109.81
3	A	45	GLY	N-CA-C	-5.32	107.77	115.27
3	A	87	PHE	N-CA-C	-5.32	101.45	109.85
3	A	178	ILE	N-CA-C	-5.30	102.23	109.55
3	A	151	GLN	N-CA-C	5.26	122.00	110.80
4	B	246	LEU	CA-C-N	5.24	126.39	119.84
4	B	246	LEU	C-N-CA	5.24	126.39	119.84
3	A	169	GLU	N-CA-C	5.24	121.39	109.81
5	L	63	SER	N-CA-C	5.24	117.96	109.06
3	A	102	LYS	N-CA-C	5.23	117.97	109.24
4	B	375	ILE	N-CA-C	-5.22	105.52	110.42
4	B	132	ILE	CA-C-N	5.21	126.36	119.84
4	B	132	ILE	C-N-CA	5.21	126.36	119.84
4	B	51	GLY	CA-C-N	5.21	126.36	119.84
4	B	51	GLY	C-N-CA	5.21	126.36	119.84
5	L	105	GLU	N-CA-C	5.20	117.57	110.55
4	B	354	TYR	N-CA-C	-5.19	100.71	108.96
4	B	225	PRO	N-CA-C	5.19	117.03	110.70
6	H	135	ALA	CA-C-N	5.16	124.66	119.19
6	H	135	ALA	C-N-CA	5.16	124.66	119.19
3	A	229	TRP	N-CA-C	5.16	116.83	108.26
6	H	198	TRP	N-CA-C	5.15	119.17	112.17
6	H	154	GLY	N-CA-C	5.15	123.52	115.08
5	L	24	SER	N-CA-C	5.14	117.44	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	9	PRO	N-CA-C	5.11	120.26	113.57
4	B	180	ILE	N-CA-C	5.09	115.99	108.45
4	B	204	GLU	N-CA-C	-5.09	105.42	110.97
5	L	193	THR	N-CA-C	5.04	117.34	109.52
5	L	7	THR	N-CA-C	5.00	117.12	111.02

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	56	0
2	P	363	0	204	102	0
3	A	4292	0	4127	509	0
4	B	3411	0	3300	470	0
5	L	1616	0	1517	177	0
6	H	1648	0	1602	191	0
All	All	11720	0	10962	1443	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 64.

All (1443) 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
4:B:230:MET:HE2	6:H:104:SER:HA	1.28	1.12
2:P:831:DG:H2''	2:P:832:DG:H5'	1.17	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	1.19	1.06
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
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	1.05	0.99
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
4:B:16:MET:HE3	4:B:83:ARG:HA	1.50	0.94
4:B:50:ILE:HD12	4:B:145:GLN:HG3	1.47	0.94
6:H:61:TYR:CE2	6:H:70:THR:HA	2.01	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:H	3:A:101:LYS:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OP1	2:P:828:DT:H4'	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
4:B:22:LYS:HZ3	4:B:23:GLN:N	1.72	0.86
4:B:266:TRP:CD1	4:B:269:GLN:HE22	1.93	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
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
3:A:294:PRO:C	3:A:296:THR:H	1.84	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
4:B:292:VAL:C	4:B:294:PRO:HD3	2.02	0.85
3:A:16:MET:HE3	3:A:16:MET:H	1.42	0.84
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
5:L:1:ASP:H3	5:L:93:LYS:HD2	1.42	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
3:A:329:ILE:HG22	3:A:339:TYR:HB3	1.61	0.82
4:B:402:TRP:HH2	4:B:411:ILE:HD13	1.44	0.82
2:P:828:DT:H2'	2:P:829:DT:H71	1.60	0.82
4:B:274:ILE:HA	4:B:306:ASN:HD21	1.45	0.82
4:B:22:LYS:HZ3	4:B:23:GLN:H	1.24	0.81
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
5:L:48:ILE:HG22	5:L:54:LEU:HA	1.60	0.81
6:H:62:ASN:HD22	6:H:65:LEU:HG	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:120:LEU:HD12	3:A:121:ASP:H	1.46	0.81
3:A:486:LEU:HB3	3:A:528:LYS:HZ1	1.45	0.80
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
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
3:A:327:ALA:HB2	3:A:341:ILE:HG23	1.62	0.79
4:B:153:TRP:O	4:B:157:PRO:HD2	1.82	0.79
3:A:122:GLU:HA	3:A:125:ARG:HD2	1.65	0.79
2:P:827:DG:H2''	2:P:828:DT:O5'	1.83	0.79
2:P:838:DA:H1'	3:A:184:ILE:HD12	1.62	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:P:837:DC:H4'	3:A:230:MET:HE2	1.66	0.76
3:A:482:ILE:HG22	3:A:486:LEU:HD11	1.68	0.76
4:B:103:LYS:NZ	4:B:192:ASP:H	1.83	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
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
5:L:144:ILE:HG12	5:L:145:ASN:N	2.02	0.74
6:H:49:TRP:CZ2	6:H:51:ALA:HA	2.23	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
6:H:147:THR:C	6:H:148:LEU:HD22	2.14	0.73
3:A:175:ASN:HB2	3:A:178:ILE:HD13	1.69	0.73
5:L:161:ASN:HB3	5:L:177:SER:CA	2.18	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
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
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:509:GLN:N	3:A:510:PRO:HD3	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:479:LEU:HD13	3:A:502:ALA:CB	2.20	0.71
3:A:542:ILE:HD12	3:A:542:ILE:H	1.53	0.71
4:B:161:GLN:O	4:B:165:THR:HG23	1.90	0.71
5:L:3:GLN:HE21	5:L:3:GLN:HA	1.54	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
4:B:425:LEU:C	4:B:427:TYR:H	1.98	0.71
1:T:803:DG:H5'	1:T:803:DG:H8	1.55	0.71
2:P:829:DT:H2''	2:P:830:DC:O4'	1.90	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
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
3:A:450:THR:O	3:A:452:LEU:HD23	1.91	0.70
5:L:110:ASP:HA	5:L:140:TYR:HB2	1.73	0.70
4:B:166:LYS:O	4:B:169:GLU:HB3	1.91	0.70
6:H:16:GLN:O	6:H:87:VAL:HG23	1.92	0.70
4:B:14:PRO:O	4:B:16:MET:HG2	1.92	0.70
4:B:424:LYS:C	4:B:426:TRP:H	2.00	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
3:A:155:GLY:C	3:A:159:ILE:HG12	2.18	0.69
3:A:435:VAL:HG22	4:B:290:THR:HG23	1.75	0.69
6:H:92:THR:OG1	6:H:120:THR:HA	1.91	0.69
2:P:833:DG:C2'	2:P:834:DC:OP2	2.39	0.69
3:A:329:ILE:H	3:A:329:ILE:HD13	1.55	0.69
5:L:198:HIS:HB3	5:L:200:THR:HG23	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:29:GLU:HG2	4:B:71:TRP:CH2	2.28	0.69
5:L:147:ALA:HB3	5:L:195:ALA:HB3	1.72	0.69
1:T:801:DA:C2'	1:T:802:DT:H71	2.23	0.69
2:P:824:DC:C1'	3:A:475:GLN:HE22	2.05	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
6:H:40:ARG:HH11	6:H:91:ASP:HA	1.56	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:79:GLU:O	3:A:83:ARG:HG3	1.93	0.69
3:A:501:TYR:O	3:A:505:ILE:HG13	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
4:B:83:ARG:HG2	4:B:83:ARG:HH11	1.56	0.68
4:B:106:VAL:HG13	4:B:234:LEU:HB3	1.76	0.68
5:L:136:LEU:HD12	5:L:175:MET:HG2	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
4:B:218:ASP:C	4:B:219:LYS:HD3	2.19	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
4:B:400:THR:HG1	4:B:401:TRP:CD1	2.12	0.67
1:T:803:DG:H8	1:T:803:DG:C5'	2.06	0.67
3:A:101:LYS:H	3:A:101:LYS:CD	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:215:THR:C	3:A:217:PRO:HD3	2.19	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
3:A:156:SER:HB2	3:A:157:PRO:HD3	1.75	0.67
3:A:454:LYS:HG2	3:A:468:PRO:HB3	1.74	0.67
3:A:500:GLN:O	3:A:503:LEU:HB3	1.95	0.67
6:H:62:ASN:ND2	6:H:65:LEU:HG	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:162:VAL:HA	6:H:206:ASN:O	1.94	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
3:A:324:ASP:O	3:A:343:GLN:HG2	1.95	0.66
4:B:244:ILE:CB	4:B:426:TRP:HE1	2.08	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
6:H:219:LYS:HD2	6:H:219:LYS:C	2.21	0.65
2:P:837:DC:C2'	2:P:838:DA:H5'	2.26	0.65
4:B:328:GLU:C	4:B:329:ILE:HD12	2.21	0.65
5:L:6:GLN:HE22	5:L:87:TYR:HA	1.61	0.65
5:L:120:PRO:HG3	5:L:132:VAL:HG22	1.78	0.65
3:A:92:LEU:O	3:A:92:LEU:HG	1.94	0.65
4:B:319:TYR:CE2	4:B:321:PRO:HG3	2.31	0.65
3:A:400:THR:HA	3:A:403:THR:OG1	1.96	0.65
4:B:60:VAL:HA	4:B:74:LEU:O	1.95	0.65
4:B:236:PRO:HG2	4:B:237:ASP:H	1.62	0.65
6:H:163:THR:H	6:H:206:ASN:HD21	1.44	0.65
4:B:55:PRO:HG2	4:B:56:TYR:HD2	1.59	0.65
4:B:104:LYS:HB2	4:B:192:ASP:HA	1.79	0.65
4:B:47:ILE:CG2	4:B:144:TYR:HB3	2.27	0.65
2:P:825:DC:C6	2:P:826:DT:H72	2.32	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
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
6:H:198:TRP:HD1	6:H:203:VAL:HG23	1.62	0.64
3:A:325:LEU:HB3	3:A:387:PRO:HB3	1.79	0.64
4:B:423:VAL:HG12	4:B:428:GLN:HA	1.79	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
4:B:372:VAL:HG12	4:B:389:PHE:CE2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:348:ASN:HD22	3:A:349:LEU:H	1.45	0.64
4:B:103:LYS:HZ3	4:B:192:ASP:N	1.88	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:5:ILE:HD12	3:A:6:GLU:H	1.62	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
4:B:195:ILE:HD11	4:B:199:ARG:HE	1.63	0.64
4:B:180:ILE:HG12	4:B:189:VAL:HG22	1.80	0.64
4:B:373:GLN:NE2	4:B:406:TRP:HA	2.12	0.64
3:A:154:LYS:O	3:A:157:PRO:HD2	1.98	0.64
4:B:30:LYS:HZ3	4:B:61:PHE:HD1	1.45	0.64
4:B:423:VAL:C	4:B:425:LEU:H	2.04	0.64
3:A:26:LEU:HD11	3:A:61:PHE:HA	1.80	0.63
4:B:50:ILE:HD13	4:B:50:ILE:N	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
3:A:94:ILE:HB	3:A:95:PRO:HD2	1.79	0.63
5:L:48:ILE:HD11	5:L:73:LEU:HD13	1.80	0.63
5:L:130:ALA:HB3	5:L:181:LEU:O	1.99	0.63
3:A:542:ILE:HD12	3:A:542:ILE:N	2.13	0.63
4:B:195:ILE:HG23	4:B:196:GLY:H	1.62	0.63
4:B:258:GLN:O	4:B:261:VAL:HG12	1.98	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
3:A:132:ILE:HG23	3:A:142:ILE:HB	1.81	0.63
3:A:254:VAL:HG22	3:A:289:LEU:O	1.98	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: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
5:L:197:THR:HG23	5:L:204:PRO:HA	1.80	0.62
4:B:425:LEU:O	4:B:427:TYR:N	2.32	0.62
5:L:141:PRO:HD2	5:L:198:HIS:CE1	2.33	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
6:H:61:TYR:HE2	6:H:70:THR:CA	2.02	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:815:DG:C2'	1:T:816:DG:C8	2.81	0.62
3:A:486:LEU:HB3	3:A:528:LYS:NZ	2.14	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
4:B:174:GLN:O	4:B:175:ASN:HB3	1.99	0.62
3:A:31:ILE:O	3:A:35:VAL:HG23	1.99	0.62
3:A:129:ALA:HA	3:A:145:GLN:HA	1.82	0.62
4:B:395:LYS:HG3	4:B:416:PHE:CE1	2.34	0.62
4:B:402:TRP:CH2	4:B:411:ILE:HD13	2.30	0.62
3:A:461:LYS:O	3:A:463:ARG:N	2.30	0.62
6:H:165:ASN:HB2	6:H:169:LEU:CD1	2.29	0.62
2:P:838:DA:H4'	3:A:183:TYR:CD2	2.35	0.62
4:B:98:ALA:C	4:B:100:LEU:N	2.57	0.62
3:A:362:THR:HG22	3:A:366:LYS:NZ	2.15	0.61
4:B:166:LYS:O	4:B:170:PRO:HD3	1.99	0.61
6:H:37:THR:HG23	6:H:52:THR:OG1	2.00	0.61
6:H:148:LEU:HB2	6:H:191:VAL:HG23	1.82	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:96:HIS:NE2	4:B:100:LEU:HD23	2.15	0.61
4:B:106:VAL:HG12	4:B:234:LEU:O	2.00	0.61
4:B:328:GLU:HB2	4:B:340:GLN:NE2	2.16	0.61
4:B:387:PRO:HG2	4:B:389:PHE:HE1	1.59	0.61
4:B:422:LEU:O	4:B:425:LEU:HD22	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
3:A:165:THR:HG23	3:A:182:GLN:HE22	1.65	0.61
5:L:6:GLN:NE2	5:L:88:CYS:H	1.99	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:242:GLN:N	3:A:243:PRO:HD2	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:148:TRP:CE3	5:L:179:LEU:HD22	2.35	0.61
5:L:150:ILE:HG23	5:L:191:SER:O	2.00	0.61
6:H:39:ILE:HG23	6:H:48:GLU:O	2.00	0.61
3:A:53:GLU:O	3:A:55:PRO:HD3	2.00	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
4:B:135:ILE:HG13	4:B:135:ILE:O	2.00	0.61
6:H:165:ASN:HD21	6:H:203:VAL:HA	1.64	0.61
4:B:191:SER:H	4:B:198:HIS:CE1	2.18	0.60
1:T:804:DG:H5'	1:T:804:DG:H8	1.65	0.60
5:L:52:SER:HA	5:L:64:GLY:HA3	1.82	0.60
4:B:395:LYS:HG3	4:B:416:PHE:HE1	1.64	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
3:A:64:LYS:HG2	3:A:72:ARG:H	1.65	0.60
3:A:119:PRO:HA	3:A:148:VAL:HG12	1.81	0.60
4:B:326:ILE:HG13	4:B:342:TYR:O	2.02	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
5:L:14:SER:O	5:L:78:LEU:HD12	2.01	0.60
5:L:94:PHE:O	5:L:96:TRP:N	2.33	0.60
6:H:161:THR:OG1	6:H:208:ALA:HB3	2.01	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
3:A:372:VAL:HA	3:A:375:ILE:HD12	1.84	0.60
4:B:47:ILE:HG21	4:B:144:TYR:HD2	1.67	0.60
4:B:171:PHE:CD1	4:B:205:LEU:HG	2.37	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:260:LEU:O	4:B:263:LYS:HB3	2.02	0.60
4:B:375:ILE:O	4:B:378:GLU:HB3	2.01	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:H	3:A:279:LEU:CD1	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:188:TYR:HE2	3:A:234:LEU:HD11	1.66	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:50:ILE:HG22	3:A:145:GLN:HG2	1.84	0.59
3:A:329:ILE:HD11	3:A:392:PRO:HD2	1.85	0.59
4:B:202:ILE:HG22	4:B:203:GLU:N	2.17	0.59
5:L:3:GLN:HB3	5:L:26:SER:OG	2.02	0.59
5:L:141:PRO:HD2	5:L:198:HIS:NE2	2.17	0.59
5:L:169:LYS:HZ2	5:L:169:LYS:N	2.00	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
5:L:148:TRP:O	5:L:155:ALA:HA	2.02	0.59
3:A:202:ILE:O	3:A:205:LEU:HB3	2.03	0.59
5:L:11:LEU:HD11	5:L:19:VAL:HG11	1.84	0.59
6:H:161:THR:O	6:H:208:ALA:N	2.33	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
3:A:474:ASN:HD22	3:A:474:ASN:H	1.50	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
6:H:164:TRP:HA	6:H:204:THR:O	2.03	0.59
4:B:106:VAL:O	4:B:234:LEU:HB3	2.03	0.59
4:B:301:LEU:HG	4:B:302:GLU:OE2	2.03	0.59
4:B:336:GLN:HA	4:B:355:ALA:HA	1.83	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
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
4:B:98:ALA:O	4:B:100:LEU:N	2.36	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:101:LYS:HG2	2.04	0.58
3:A:450:THR:C	3:A:452:LEU:H	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:234:LEU:HD23	3:A:318:TYR:OH	2.04	0.58
5:L:35:TRP:HB2	5:L:48:ILE:CG1	2.33	0.58
1:T:805:DC:H2''	1:T:806:DG:C8	2.39	0.58
3:A:201:LYS:O	3:A:204:GLU:HB3	2.02	0.58
4:B:143:ARG:C	4:B:144:TYR:HD1	2.11	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
3:A:442:VAL:HG12	3:A:443:ASP:N	2.18	0.58
4:B:73:LYS:CD	4:B:151:GLN:HE21	2.17	0.58
4:B:207:GLN:O	4:B:210:LEU:HB2	2.04	0.58
3:A:270:ILE:HD12	3:A:314:VAL:HG23	1.85	0.58
3:A:398:TRP:HH2	3:A:409:THR:HG22	1.68	0.58
4:B:195:ILE:CD1	4:B:199:ARG:HE	2.16	0.58
5:L:20:THR:HG23	5:L:74:THR:OG1	2.03	0.58
3:A:358:ARG:HH12	4:B:394:GLN:HG3	1.69	0.58
3:A:441:TYR:CE2	3:A:544:GLY:N	2.72	0.58
3:A:506:ILE:HD13	3:A:506:ILE:N	2.19	0.58
3:A:532:TYR:CD2	3:A:533:LEU: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:22:LYS:HZ3	4:B:23:GLN:CA	2.17	0.57
3:A:168:LEU:O	3:A:172:LYS:HG3	2.05	0.57
4:B:369:THR:OG1	4:B:370:GLU:N	2.37	0.57
6:H:72:SER:OG	6:H:81:PHE:HD1	1.87	0.57
3:A:210:LEU:HA	3:A:214:LEU:O	2.03	0.57
3:A:377:THR:O	3:A:381:VAL:HG23	2.04	0.57
4:B:357:MET:HB3	4:B:361:HIS:HE1	1.69	0.57
5:L:3:GLN:HA	5:L:3:GLN:NE2	2.19	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
5:L:120:PRO:HB2	5:L:125:LEU:HD21	1.86	0.57
5:L:186:TYR:HA	5:L:192:TYR:OH	2.03	0.57
1:T:801:DA:H2''	1:T:802:DT:C5	2.39	0.57
4:B:64:LYS:NZ	4:B:64:LYS:HB3	2.20	0.57
4:B:418:ASN:CG	4:B:419:THR:N	2.63	0.57
4:B:429:LEU:HD12	4:B:429:LEU:H	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:98:ALA:HB1	3:A:383:TRP:HZ2	1.70	0.57
3:A:246:LEU:HD11	3:A:307:ARG:HE	1.70	0.57
6:H:84:MET:C	6:H:85:MET:HE3	2.30	0.57
1:T:803:DG:C5'	1:T:803:DG:C8	2.88	0.57
3:A:531:VAL:HG12	3:A:532:TYR:N	2.19	0.57
4:B:191:SER:OG	4:B:193:LEU:HG	2.04	0.57
2:P:823:DC:C3'	2:P:824:DC:H5''	2.33	0.57
3:A:62:ALA:CA	3:A:73:LYS:HA	2.30	0.57
4:B:27:THR:HG23	4:B:30:LYS:HG3	1.87	0.57
6:H:17:PRO:HB3	6:H:85:MET:HG3	1.85	0.57
3:A:516:GLU:O	3:A:520:GLN:HG3	2.05	0.56
4:B:22:LYS:NZ	4:B:23:GLN:H	2.00	0.56
4:B:34:LEU:HD23	4:B:132:ILE:HG12	1.86	0.56
4:B:163:SER:O	4:B:167:ILE:HG13	2.05	0.56
2:P:823:DC:C2	2:P:824:DC:C6	2.93	0.56
3:A:241:VAL:C	3:A:243:PRO:HD2	2.31	0.56
3:A:294:PRO:C	3:A:296:THR:N	2.53	0.56
4:B:254:VAL:CG2	4:B:289:LEU:HA	2.35	0.56
4:B:342:TYR:HA	4:B:349:LEU:CD1	2.35	0.56
5:L:15:LEU:HA	5:L:78:LEU:HB2	1.87	0.56
5:L:137:ASN:CA	5:L:174:SER:HB3	2.29	0.56
6:H:143:ASN:OD1	6:H:144:SER:N	2.38	0.56
4:B:180:ILE:HA	4:B:188:TYR:O	2.05	0.56
4:B:329:ILE:HD12	4:B:329:ILE:N	2.20	0.56
6:H:95:TYR:CD1	6:H:95:TYR:N	2.70	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
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:163:THR:N	6:H:206:ASN:HD21	2.04	0.56
3:A:46:LYS:HD3	3:A:116:PHE:HD2	1.69	0.56
4:B:212:TRP:CD1	4:B:213:GLY:N	2.73	0.56
4:B:369:THR:HG22	4:B:398:TRP:CH2	2.40	0.56
6:H:169:LEU:N	6:H:169:LEU:HD12	2.21	0.56
3:A:519:ASN:HA	3:A:522:ILE:HD12	1.85	0.56
3:A:554:ALA:C	3:A:556:ILE:H	2.14	0.56
4:B:113:ASP:O	4:B:116:PHE:HB2	2.06	0.56
4:B:393:ILE:HD11	4:B:397:THR:CG2	2.34	0.56
4:B:406:TRP:HZ2	4:B:410:TRP:O	1.88	0.56
3:A:425:LEU:HD12	3:A:425:LEU:H	1.71	0.56
6:H:27:PHE:CD2	6:H:34:ILE:HG21	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:444:GLY:O	3:A:445:ALA:HB2	2.06	0.56
4:B:30:LYS:NZ	4:B:61:PHE:HD1	2.04	0.56
3:A:110:ASP:O	3:A:217:PRO:HD2	2.06	0.56
3:A:470:THR:HG22	3:A:471:ASN:N	2.21	0.56
4:B:402:TRP:HH2	4:B:411:ILE:CD1	2.16	0.56
4:B:423:VAL:C	4:B:425:LEU:N	2.61	0.56
6:H:33:GLY:O	6:H:101:ALA:HA	2.06	0.56
1:T:802:DT:H2''	1:T:803:DG:OP2	2.05	0.56
3:A:394:GLN:HG2	3:A:416:PHE:CE1	2.40	0.56
4:B:75:VAL:HG11	4:B:77:PHE:CZ	2.41	0.56
4:B:101:LYS:HE3	4:B:102:LYS:HE3	1.88	0.56
3:A:155:GLY:C	3:A:157:PRO:HD2	2.32	0.55
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:94:ILE:HG13	3:A:95:PRO:O	2.06	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
4:B:146:TYR:CD2	4:B:150:PRO:HA	2.40	0.55
6:H:83:ASN:HB3	6:H:85:MET:HE1	1.88	0.55
3:A:101:LYS:HD2	3:A:101:LYS:N	2.12	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:113:PRO:HB3	5:L:139:PHE:CD2	2.42	0.55
5:L:150:ILE:O	5:L:151:ASP:C	2.49	0.55
6:H:92:THR:HG23	6:H:92:THR:O	2.07	0.55
3:A:255:ASN:HA	3:A:258:GLN:HE21	1.72	0.55
3:A:441:TYR:HE2	3:A:544:GLY:N	2.05	0.55
3:A:491:LEU:H	3:A:491:LEU:HD23	1.72	0.55
4:B:115:TYR:OH	4:B:157:PRO:HB3	2.06	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
5:L:166:GLN:HE21	5:L:171:SER:HB3	1.71	0.55
3:A:532:TYR:CD2	3:A:532:TYR:C	2.84	0.55
4:B:155:GLY:O	4:B:158:ALA:HB3	2.06	0.55
4:B:171:PHE:CZ	4:B:201:LYS:HD2	2.41	0.55
5:L:50:TYR:CE2	6:H:106:THR:HB	2.42	0.55
6:H:31:THR:HB	6:H:34:ILE:CG1	2.35	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
6:H:218:LYS:HE2	6:H:219:LYS:HZ1	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:L:198:HIS:C	5:L:200:THR:H	2.13	0.55
6:H:27:PHE:HD2	6:H:34:ILE:HG21	1.72	0.55
3:A:469:LEU:HD12	3:A:469:LEU:N	2.22	0.55
4:B:81:ASN:O	4:B:154:LYS:HE3	2.07	0.55
5:L:34:ASN:OD1	5:L:49:TYR:HA	2.07	0.55
5:L:75:ILE:N	5:L:75:ILE:HD12	2.21	0.55
3:A:242:GLN:C	3:A:244:ILE:H	2.15	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
6:H:53:ILE:HD12	6:H:80:ALA:HB1	1.89	0.55
3:A:178:ILE:N	3:A:178:ILE:HD12	2.22	0.54
4:B:228:LEU:HD23	4:B:232:TYR:HE1	1.70	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
1:T:810:DG:C6	1:T:811:DA:N6	2.75	0.54
3:A:63:ILE:HG23	3:A:63:ILE:O	2.06	0.54
3:A:261:VAL:HG13	3:A:276:VAL:CG1	2.35	0.54
4:B:107:THR:HG22	4:B:108:VAL:H	1.72	0.54
4:B:130:PHE:CZ	4:B:144:TYR:HB2	2.42	0.54
5:L:51:THR:CG2	5:L:71:TYR:HD2	2.20	0.54
4:B:16:MET:HB3	4:B:83:ARG:HD2	1.89	0.54
4:B:32:LYS:O	4:B:35:VAL:HB	2.08	0.54
4:B:230:MET:CE	6:H:104:SER:HA	2.20	0.54
4:B:393:ILE:HD12	4:B:394:GLN:OE1	2.08	0.54
5:L:2:ILE:HD12	5:L:2:ILE:N	2.22	0.54
5:L:35:TRP:CZ3	5:L:88:CYS:HB2	2.42	0.54
6:H:132:TYR:HD2	6:H:151:LEU:HD23	1.73	0.54
3:A:99:GLY:HA2	3:A:383:TRP:NE1	2.22	0.54
3:A:219:LYS:HD2	3:A:219:LYS:N	2.22	0.54
4:B:330:GLN:HB2	4:B:338:THR:OG1	2.07	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:246:LEU:N	3:A:246:LEU:HD23	2.22	0.54
3:A:317:VAL:HG22	3:A:318:TYR:H	1.72	0.54
4:B:23:GLN:NE2	4:B:26:LEU:HD11	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:33:ALA:O	4:B:37:ILE:HG22	2.07	0.54
6:H:59:ASN:OD1	6:H:61:TYR:HE1	1.91	0.54
6:H:69:LEU:HD11	6:H:82:LEU:HD21	1.89	0.54
6:H:146:VAL:C	6:H:192:THR:HG23	2.33	0.54
3:A:380:ILE:O	3:A:384:GLY:N	2.39	0.54
4:B:68:SER:OG	4:B:219:LYS:NZ	2.38	0.54
4:B:195:ILE:HD11	4:B:233:GLU:HG3	1.90	0.54
5:L:186:TYR:HE2	5:L:213:GLU:O	1.90	0.54
2:P:830:DC:C4	2:P:831:DG:O6	2.61	0.53
3:A:377:THR:O	3:A:380:ILE:HB	2.08	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:41:MET:HB2	3:A:47:ILE:HD11	1.90	0.53
3:A:225:PRO:HA	3:A:236:PRO:HD3	1.91	0.53
4:B:22:LYS:CD	4:B:23:GLN:H	2.21	0.53
4:B:47:ILE:HG21	4:B:144:TYR:HB3	1.91	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
3:A:24:TRP:NE1	3:A:61:PHE:CZ	2.76	0.53
4:B:21:VAL:HG12	4:B:22:LYS:N	2.23	0.53
4:B:376:THR:O	4:B:380:ILE:HG13	2.09	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:10:VAL:HG21	3:A:153:TRP:CZ2	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
4:B:64:LYS:HG3	4:B:71:TRP:CE2	2.43	0.53
6:H:2:ILE:CG2	6:H:26:GLY:HA3	2.37	0.53
6:H:94:ILE:HA	6:H:117:THR:O	2.07	0.53
3:A:169:GLU:O	3:A:172:LYS:HB2	2.09	0.53
4:B:62:ALA:C	4:B:63:ILE:HG22	2.34	0.53
4:B:271:TYR:CD1	4:B:271:TYR:N	2.76	0.53
2:P:825:DC:C4	2:P:826:DT:C4	2.97	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
5:L:79:GLU:O	5:L:81:GLU:N	2.41	0.53
6:H:125:ALA:O	6:H:127:THR:HG23	2.09	0.53
6:H:128:PRO:HA	6:H:212:SER:OG	2.09	0.53
3:A:357:MET:HE3	3:A:357:MET:HA	1.90	0.53
4:B:98:ALA:C	4:B:100:LEU:H	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:833:DG:C2	2:P:834:DC:C2	2.97	0.53
3:A:50:ILE:HD12	3:A:54:ASN:HB2	1.91	0.53
3:A:505:ILE:O	3:A:510:PRO:HG2	2.08	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
5:L:167:ASP:C	5:L:169:LYS:H	2.17	0.53
6:H:42:PRO:HB2	6:H:45:LYS:HB2	1.90	0.53
4:B:235:HIS:ND1	4:B:235:HIS:N	2.56	0.53
4:B:357:MET:HB3	4:B:361:HIS:CE1	2.43	0.53
3:A:254:VAL:HG21	3:A:289:LEU:HA	1.91	0.52
4:B:224:GLU:HA	4:B:227:PHE:HE2	1.73	0.52
4:B:254:VAL:HB	4:B:289:LEU:CA	2.35	0.52
3:A:378:GLU:O	3:A:382:ILE:HG12	2.09	0.52
4:B:41:MET:HE2	4:B:47:ILE:HG12	1.90	0.52
4:B:229:TRP:HA	4:B:232:TYR:CD1	2.44	0.52
6:H:195:SER:O	6:H:196:SER:C	2.50	0.52
2:P:824:DC:H2''	2:P:825:DC:O5'	2.09	0.52
3:A:11:LYS:O	3:A:85:GLN:HG2	2.09	0.52
3:A:153:TRP:CE3	3:A:155:GLY:HA3	2.45	0.52
4:B:254:VAL:O	4:B:258:GLN:HB2	2.08	0.52
4:B:328:GLU:HB2	4:B:340:GLN:HE21	1.73	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
6:H:148:LEU:N	6:H:191:VAL:O	2.37	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
4:B:203:GLU:O	4:B:206:ARG:HB2	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
4:B:425:LEU:C	4:B:427:TYR:N	2.67	0.52
6:H:160:VAL:HG13	6:H:160:VAL:O	2.10	0.52
3:A:167:ILE:HD12	3:A:167:ILE:N	2.25	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: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
5:L:193:THR:HG22	5:L:194:CYS:N	2.23	0.52
3:A:435:VAL:HA	4:B:290:THR:HG23	1.90	0.52
3:A:459:THR:HG21	3:A:463:ARG:HB3	1.91	0.52
3:A:533:LEU:HD12	3:A:534:ALA:N	2.25	0.52
4:B:47:ILE:HG21	4:B:144:TYR:CD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:178:ILE:HG22	4:B:179:VAL:N	2.25	0.52
5:L:149:ALA:HB1	5:L:153:SER:HA	1.91	0.52
6:H:65:LEU:O	6:H:66:LYS:C	2.52	0.52
6:H:104:SER:OG	6:H:105:VAL:N	2.41	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:307:ARG:HG3	3:A:307:ARG:NH1	2.25	0.52
3:A:465:LYS:HZ2	3:A:465:LYS:HB2	1.75	0.52
4:B:73:LYS:HD3	4:B:146:TYR:OH	2.10	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
6:H:66:LYS:HD3	6:H:67:SER:N	2.24	0.52
6:H:94:ILE:HG22	6:H:96:TYR:CE1	2.45	0.52
4:B:369:THR:HA	4:B:398:TRP:HH2	1.75	0.51
6:H:165:ASN:HD22	6:H:169:LEU:HD11	1.75	0.51
4:B:178:ILE:HD11	4:B:201:LYS:HG2	1.93	0.51
4:B:424:LYS:C	4:B:426:TRP:N	2.69	0.51
5:L:191:SER:HB2	5:L:210:ASN:OD1	2.11	0.51
3:A:86:ASP:O	4:B:55:PRO:HB3	2.10	0.51
3:A:153:TRP:CH2	3:A:155:GLY:HA3	2.45	0.51
3:A:337:TRP:HE1	3:A:367:GLN:HB3	1.75	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
4:B:395:LYS:O	4:B:396:GLU:C	2.53	0.51
6:H:2:ILE:HG22	6:H:26:GLY:CA	2.40	0.51
3:A:24:TRP:CD1	3:A:24:TRP:H	2.27	0.51
3:A:170:PRO:O	3:A:174:GLN:HG2	2.09	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
5:L:39:LYS:CG	5:L:40:PRO:HD2	2.40	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
3:A:193:LEU:HD13	3:A:197:GLN:HG3	1.93	0.51
3:A:317:VAL:HG22	3:A:318:TYR:N	2.25	0.51
3:A:328:GLU:HB3	3:A:390:LYS:HB2	1.92	0.51
3:A:403:THR:O	3:A:406:TRP:HZ3	1.93	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
5:L:116:SER:O	5:L:134:CYS:HA	2.10	0.51
6:H:160:VAL:HG23	6:H:208:ALA:O	2.10	0.51
3:A:556:ILE:HG12	3:A:557:ARG:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:134:CYS:SG	5:L:136:LEU:HD21	2.50	0.51
3:A:270:ILE:HA	3:A:351:THR:HG23	1.93	0.51
3:A:326:ILE:HD12	3:A:326:ILE:N	2.26	0.51
3:A:408:ALA:HA	4:B:364:ASP:OD2	2.11	0.51
3:A:438:GLU:OE1	3:A:463:ARG:NH2	2.43	0.51
3:A:523:GLU:HA	3:A:526:ILE:HB	1.91	0.51
4:B:287:LYS:HG3	4:B:288:ALA:H	1.75	0.51
6:H:1:GLN:HG2	6:H:2:ILE:CD1	2.40	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:113:ASP:OD1	3:A:116:PHE:HB2	2.11	0.51
3:A:395:LYS:N	3:A:395:LYS:HD2	2.26	0.51
3:A:459:THR:HG22	3:A:463:ARG:HB3	1.91	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
3:A:120:LEU:HD21	3:A:128:THR:HG21	1.92	0.50
3:A:120:LEU:N	3:A:148:VAL:HA	2.26	0.50
3:A:128:THR:OG1	3:A:146:TYR:HB2	2.11	0.50
3:A:453:GLY:O	3:A:468:PRO:HA	2.11	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
4:B:178:ILE:HG12	4:B:191:SER:HB2	1.93	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
6:H:53:ILE:HG21	6:H:73:LYS:HG2	1.91	0.50
6:H:132:TYR:CD2	6:H:151:LEU:HD23	2.46	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
1:T:812:DA:C4	1:T:813:DC:C5	2.99	0.50
3:A:47:ILE:HG22	3:A:145:GLN:O	2.11	0.50
3:A:337:TRP:CH2	3:A:368:LEU:HB2	2.46	0.50
3:A:419:THR:OG1	3:A:420:PRO:HD3	2.11	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
4:B:328:GLU:OE2	4:B:430:GLU:HG2	2.11	0.50
6:H:207:VAL:HG12	6:H:208:ALA:N	2.25	0.50
1:T:809:DC:H2''	1:T:810:DG:O5'	2.11	0.50
1:T:818:DA:C2	2:P:822:DT:O2	2.60	0.50
2:P:834:DC:OP2	2:P:834:DC:H2'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:194:GLU:O	3:A:197:GLN:N	2.45	0.50
4:B:332:GLN:OE1	4:B:424:LYS:HA	2.12	0.50
5:L:1:ASP:CA	5:L:95:PRO:HB2	2.42	0.50
6:H:206:ASN:ND2	6:H:206:ASN:O	2.45	0.50
2:P:831:DG:C4	2:P:832:DG:C8	3.00	0.50
3:A:354:TYR:CZ	3:A:356:ARG:HB3	2.46	0.50
3:A:523:GLU:O	3:A:526:ILE:HB	2.11	0.50
4:B:30:LYS:HG2	4:B:62:ALA:HB3	1.93	0.50
4:B:127:TYR:N	4:B:127:TYR:CD2	2.75	0.50
4:B:223:LYS:HE2	6:H:60:ARG:HH22	1.76	0.50
6:H:72:SER:HG	6:H:81:PHE:HD1	1.59	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:255:ASN:HA	3:A:258:GLN:NE2	2.26	0.50
3:A:438:GLU:HG2	3:A:461:LYS:CE	2.42	0.50
4:B:104:LYS:HD3	4:B:192:ASP:OD1	2.12	0.50
4:B:208:HIS:ND1	4:B:208:HIS:C	2.69	0.50
6:H:84:MET:O	6:H:85:MET:HE3	2.11	0.50
6:H:175:THR:HG23	6:H:189:SER:HB2	1.94	0.50
3:A:182:GLN:HA	3:A:187:LEU:HD23	1.93	0.49
3:A:329:ILE:HG22	3:A:339:TYR:CB	2.37	0.49
3:A:433:PRO:HB2	3:A:494:ASN:HD21	1.76	0.49
3:A:491:LEU:O	3:A:529:GLU:HB3	2.11	0.49
4:B:67:ASP:HA	4:B:221:HIS:HB2	1.94	0.49
3:A:170:PRO:O	3:A:173:LYS:HB2	2.12	0.49
4:B:386:THR:CG2	4:B:412:PRO:HB3	2.42	0.49
5:L:48:ILE:CG2	5:L:54:LEU:HA	2.37	0.49
6:H:94:ILE:HG22	6:H:116:GLY:HA3	1.93	0.49
6:H:198:TRP:HZ2	6:H:220:ILE:HG12	1.77	0.49
1:T:805:DC:H2''	1:T:806:DG:H8	1.77	0.49
3:A:139:THR:HB	3:A:140:PRO:HD3	1.95	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
6:H:95:TYR:N	6:H:95:TYR:HD1	2.10	0.49
1:T:802:DT:O5'	1:T:802:DT:H6	1.95	0.49
3:A:83:ARG:HG2	3:A:83:ARG:HH11	1.78	0.49
3:A:171:PHE:CE2	3:A:205:LEU:HD13	2.47	0.49
3:A:382:ILE:HB	3:A:383:TRP:CE3	2.47	0.49
3:A:392:PRO:O	3:A:393:ILE:HB	2.13	0.49
4:B:78:ARG:CZ	4:B:411:ILE:HG22	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:115:TYR:CE1	4:B:156:SER:HB3	2.47	0.49
4:B:348:ASN:HD21	4:B:429:LEU:HB3	1.76	0.49
5:L:9:SER:O	5:L:102:THR:HA	2.12	0.49
6:H:6:GLU:CD	6:H:6:GLU:H	2.20	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
3:A:450:THR:C	3:A:452:LEU:N	2.71	0.49
4:B:153:TRP:CH2	4:B:155:GLY:HA3	2.48	0.49
5:L:170:ASP:O	5:L:172:THR:HG23	2.12	0.49
5:L:190:ASN:HA	5:L:212:ASN:OD1	2.11	0.49
6:H:147:THR:HA	6:H:191:VAL:O	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
4:B:369:THR:O	4:B:370:GLU:C	2.56	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:269:GLN:O	3:A:350:LYS:HG2	2.11	0.49
3:A:348:ASN:HD22	3:A:349:LEU:N	2.10	0.49
1:T:810:DG:C2'	1:T:811:DA:C8	2.91	0.49
2:P:832:DG:C2	2:P:833:DG:O6	2.65	0.49
2:P:833:DG:O5'	2:P:833:DG:H2'	2.12	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
5:L:35:TRP:HB2	5:L:48:ILE:HG13	1.94	0.49
6:H:2:ILE:HD11	6:H:112:HIS:NE2	2.28	0.49
6:H:49:TRP:HZ3	6:H:62:ASN:HA	1.78	0.49
3:A:7:THR:HG21	3:A:121:ASP:HA	1.94	0.49
3:A:329:ILE:CD1	3:A:391:LEU:HA	2.42	0.49
4:B:3:SER:OG	4:B:5:ILE:HG13	2.13	0.49
4:B:112:GLY:O	4:B:114:ALA:N	2.46	0.49
4:B:236:PRO:O	4:B:237:ASP:C	2.56	0.49
6:H:176:PHE:HD1	6:H:188:SER:O	1.95	0.49
3:A:277:ARG:HA	3:A:280:SER:HB2	1.94	0.49
3:A:295:LEU:O	3:A:298:GLU:N	2.46	0.49
4:B:58:THR:CG2	4:B:59:PRO:HD2	2.43	0.49
4:B:164:MET:HA	4:B:167:ILE:HD12	1.94	0.49
4:B:201:LYS:O	4:B:204:GLU:HB2	2.13	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:420:PRO:O	3:A:422:LEU:N	2.46	0.48
3:A:442:VAL:HG12	3:A:481:ALA:HB1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:73:LYS:HA	6:H:80:ALA:HA	1.95	0.48
3:A:46:LYS:HD3	3:A:116:PHE:CD2	2.48	0.48
3:A:154:LYS:C	3:A:157:PRO:HD2	2.38	0.48
3:A:408:ALA:O	4:B:393:ILE:HD12	2.12	0.48
4:B:178:ILE:CD1	4:B:201:LYS:HG2	2.44	0.48
6:H:27:PHE:H	6:H:27:PHE:HD1	1.60	0.48
2:P:831:DG:N1	2:P:832:DG:C6	2.80	0.48
2:P:831:DG:C2	2:P:832:DG:C4	3.01	0.48
3:A:484:LEU:O	3:A:487:GLN:N	2.46	0.48
3:A:522:ILE:O	3:A:526:ILE:HG13	2.14	0.48
4:B:368:LEU:HD11	4:B:391:LEU:CD2	2.43	0.48
4:B:83:ARG:HG2	4:B:83:ARG:NH1	2.26	0.48
4:B:359:GLY:C	4:B:361:HIS:H	2.21	0.48
5:L:49:TYR:CD2	5:L:49:TYR:N	2.82	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:34:LEU:HG	4:B:132:ILE:HD11	1.95	0.48
4:B:79:GLU:CD	4:B:83:ARG:HH12	2.21	0.48
4:B:122:GLU:HA	4:B:125:ARG:HE	1.79	0.48
4:B:254:VAL:HG21	4:B:289:LEU:HA	1.94	0.48
5:L:118:PHE:HA	5:L:119:PRO:HD3	1.72	0.48
6:H:9:PRO:C	6:H:11:ILE:H	2.21	0.48
6:H:91:ASP:O	6:H:95:TYR:OH	2.28	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:98:ALA:HB1	3:A:383:TRP:CZ2	2.47	0.48
3:A:112:GLY:HA3	3:A:217:PRO:HG2	1.95	0.48
6:H:114:GLY:O	6:H:115:GLN:C	2.57	0.48
2:P:831:DG:C2	2:P:832:DG:C5	3.01	0.48
3:A:16:MET:H	3:A:16:MET:CE	2.21	0.48
3:A:146:TYR:CE2	3:A:150:PRO:HA	2.49	0.48
3:A:271:TYR:CE1	3:A:314:VAL:HG22	2.49	0.48
4:B:224:GLU:CD	5:L:96:TRP:HZ2	2.22	0.48
4:B:388:LYS:HD3	4:B:388:LYS:N	2.29	0.48
5:L:6:GLN:OE1	5:L:101:GLY:HA2	2.14	0.48
6:H:34:ILE:HG22	6:H:35:GLY:H	1.77	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:88:TRP:CH2	4:B:21:VAL:O	2.66	0.48
3:A:242:GLN:O	3:A:244:ILE:N	2.47	0.48
3:A:325:LEU:HB3	3:A:387:PRO:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:459:THR:HG21	3:A:463:ARG:HE	1.79	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
6:H:89:THR:O	6:H:90:ALA:C	2.57	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:194:GLU:O	3:A:196:GLY:N	2.47	0.47
3:A:277:ARG:CZ	3:A:336:GLN:HG2	2.44	0.47
3:A:362:THR:HG22	3:A:366:LYS:HZ3	1.79	0.47
3:A:465:LYS:HG3	3:A:466:VAL:N	2.29	0.47
4:B:339:TYR:CZ	4:B:352:GLY:HA3	2.49	0.47
5:L:51:THR:HG22	5:L:51:THR:O	2.13	0.47
4:B:88:TRP:HE1	4:B:92:LEU:HD22	1.78	0.47
4:B:125:ARG:C	4:B:127:TYR:N	2.72	0.47
6:H:173:VAL:HG12	6:H:174:HIS:N	2.29	0.47
4:B:376:THR:O	4:B:377:THR:C	2.56	0.47
2:P:831:DG:C6	2:P:832:DG:O6	2.68	0.47
3:A:24:TRP:CD1	3:A:24:TRP:N	2.81	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
3:A:366:LYS:O	3:A:369:THR:HB	2.14	0.47
3:A:498:ASP:HA	3:A:536:VAL:O	2.14	0.47
4:B:120:LEU:HB3	4:B:147:ASN:O	2.14	0.47
4:B:223:LYS:HG2	4:B:224:GLU:H	1.79	0.47
6:H:163:THR:CA	6:H:206:ASN:HD21	2.28	0.47
3:A:161:GLN:O	3:A:162:SER:C	2.57	0.47
3:A:353:LYS:HD3	3:A:353:LYS:C	2.40	0.47
4:B:68:SER:HG	4:B:219:LYS:HB2	1.80	0.47
4:B:123:ASP:O	4:B:125:ARG:N	2.47	0.47
4:B:402:TRP:CZ2	4:B:414:TRP:HH2	2.32	0.47
3:A:420:PRO:CB	3:A:421:PRO:HD2	2.42	0.47
4:B:229:TRP:HA	4:B:232:TYR:CG	2.50	0.47
6:H:131:VAL:HA	6:H:151:LEU:O	2.14	0.47
1:T:804:DG:H5'	1:T:804:DG:C8	2.48	0.47
3:A:20:LYS:CG	3:A:56:TYR:HD2	2.28	0.47
3:A:218:ASP:C	3:A:220:LYS:H	2.22	0.47
3:A:461:LYS:C	3:A:463:ARG:H	2.21	0.47
3:A:503:LEU:CD1	3:A:535:TRP:HB2	2.45	0.47
3:A:550:LYS:HA	3:A:553:SER:O	2.15	0.47
4:B:50:ILE:CD1	4:B:145:GLN:HG3	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:73:LYS:HD3	4:B:151:GLN:HE21	1.77	0.47
4:B:88:TRP:CD1	4:B:89:GLU:N	2.83	0.47
4:B:193:LEU:N	4:B:193:LEU:HD23	2.29	0.47
4:B:328:GLU:CD	4:B:430:GLU:HG2	2.40	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
3:A:333:GLY:H	3:A:336:GLN:CB	1.94	0.47
3:A:354:TYR:OH	3:A:356:ARG:HB3	2.15	0.47
3:A:536:VAL:HG12	3:A:542:ILE:HD13	1.97	0.47
3:A:122:GLU:O	3:A:125:ARG:HB2	2.15	0.47
3:A:508:ALA:O	3:A:509:GLN: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
4:B:406:TRP:NE1	4:B:408:ALA:H	2.13	0.47
6:H:11:ILE:HG12	6:H:120:THR:OG1	2.15	0.47
4:B:107:THR:HG22	4:B:108:VAL:N	2.29	0.47
4:B:121:ASP:O	4:B:125:ARG:HG3	2.14	0.47
4:B:225:PRO:HB2	4:B:226:PRO:HD3	1.96	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
6:H:96:TYR:CD1	6:H:96:TYR:N	2.84	0.47
6:H:155:TYR:CE1	6:H:185:TYR:HB2	2.49	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
4:B:115:TYR:HB3	4:B:149:LEU:CB	2.42	0.46
4:B:258:GLN:O	4:B:259:LYS:C	2.58	0.46
4:B:266:TRP:CZ2	4:B:423:VAL:HG22	2.51	0.46
6:H:104:SER:HB3	6:H:107:ASP:OD2	2.16	0.46
6:H:148:LEU:HD22	6:H:148:LEU:N	2.30	0.46
6:H:164:TRP:HB2	6:H:169:LEU:HB2	1.97	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
5:L:98:PHE:CD2	6:H:47:LEU:HB3	2.51	0.46
2:P:822:DT:C2'	2:P:823:DC:H5	2.27	0.46
3:A:81:ASN:OD1	3:A:154:LYS:HG2	2.15	0.46
3:A:294:PRO:O	3:A:296:THR:N	2.48	0.46
3:A:420:PRO:O	3:A:422:LEU:HD23	2.15	0.46
4:B:115:TYR:HE1	4:B:156:SER:C	2.23	0.46
4:B:254:VAL:HG22	4:B:294:PRO:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:391:LEU:HD23	4:B:392:PRO:HD2	1.97	0.46
5:L:167:ASP:C	5:L:169:LYS:N	2.73	0.46
3:A:47:ILE:HD12	3:A:144:TYR:CD2	2.50	0.46
3:A:376:THR:O	3:A:377:THR:C	2.58	0.46
3:A:395:LYS:HE2	3:A:416:PHE:HB2	1.97	0.46
2:P:825:DC:C4	2:P:826:DT:O4	2.68	0.46
3:A:150:PRO:HG2	3:A:153:TRP:CB	2.46	0.46
3:A:171:PHE:HB2	3:A:208:HIS:HD2	1.80	0.46
4:B:106:VAL:N	4:B:234:LEU:O	2.45	0.46
4:B:131:THR:HG23	4:B:143:ARG:HG2	1.96	0.46
4:B:162:SER:OG	4:B:163:SER:N	2.45	0.46
4:B:191:SER:CB	4:B:193:LEU:HG	2.45	0.46
4:B:289:LEU:C	4:B:289:LEU:HD12	2.40	0.46
1:T:803:DG:C2	1:T:804:DG:C5	3.04	0.46
3:A:385:LYS:HG2	3:A:386:THR:N	2.31	0.46
3:A:420:PRO:HB2	3:A:421:PRO:CD	2.44	0.46
4:B:23:GLN:HE21	4:B:26:LEU:HD11	1.81	0.46
4:B:224:GLU:O	4:B:227:PHE:CE2	2.68	0.46
4:B:404:GLU:HB2	4:B:405:TYR:CE2	2.50	0.46
6:H:88:GLU:O	6:H:89:THR:C	2.58	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
4:B:153:TRP:O	4:B:154:LYS:C	2.58	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:231:GLY:O	3:A:241:VAL:HG12	2.16	0.46
3:A:276:VAL:HG12	3:A:280:SER:OG	2.16	0.46
3:A:439:THR:HA	3:A:494:ASN:HB2	1.98	0.46
4:B:367:GLN:O	4:B:371:ALA:N	2.44	0.46
5:L:120:PRO:CB	5:L:125:LEU:HD21	2.45	0.46
3:A:8:VAL:O	3:A:121:ASP:HB2	2.16	0.46
4:B:122:GLU:HA	4:B:125:ARG:NE	2.31	0.46
4:B:160:PHE:HD2	4:B:164:MET:HB2	1.81	0.46
6:H:61:TYR:OH	6:H:71:VAL:HG22	2.16	0.46
4:B:69:THR:CG2	4:B:70:LYS:N	2.79	0.46
4:B:118:VAL:O	4:B:148:VAL:HG12	2.15	0.46
5:L:160:LEU:O	5:L:178:THR:N	2.46	0.46
6:H:37:THR:O	6:H:97:CYS:HA	2.15	0.46
1:T:805:DC:H5''	3:A:93:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:188:TYR:CD1	3:A:188:TYR:C	2.94	0.45
4:B:113:ASP:O	4:B:114:ALA:C	2.59	0.45
4:B:212:TRP:CD1	4:B:213:GLY:H	2.34	0.45
4:B:272:PRO:HG2	4:B:273:GLY:H	1.80	0.45
3:A:439:THR:O	3:A:439:THR:OG1	2.31	0.45
4:B:350:LYS:HG2	4:B:351:THR:N	2.31	0.45
4:B:365:VAL:O	4:B:366:LYS:C	2.58	0.45
5:L:167:ASP:O	5:L:169:LYS:N	2.49	0.45
5:L:193:THR:HG23	5:L:208:SER:OG	2.15	0.45
3:A:427:TYR:HE1	3:A:522:ILE:HG23	1.81	0.45
3:A:483:TYR:O	3:A:486:LEU:HB2	2.17	0.45
3:A:542:ILE:N	3:A:542:ILE:CD1	2.77	0.45
4:B:31:ILE:O	4:B:32:LYS:C	2.59	0.45
5:L:10:SER:CB	5:L:103:LYS:HB2	2.44	0.45
5:L:12:SER:HB3	5:L:105:GLU:CG	2.44	0.45
5:L:31:SER:HB2	5:L:50:TYR:HE1	1.80	0.45
3:A:163:SER:O	3:A:167:ILE:HD13	2.16	0.45
3:A:188:TYR:HE2	3:A:234:LEU:CD1	2.28	0.45
3:A:390:LYS:HB3	3:A:417:VAL:HG21	1.98	0.45
4:B:46:LYS:C	4:B:147:ASN:HD22	2.24	0.45
3:A:101:LYS:NZ	3:A:181:TYR:OH	2.49	0.45
3:A:470:THR:O	3:A:471:ASN:HB2	2.15	0.45
4:B:52:PRO:O	4:B:54:ASN:N	2.50	0.45
4:B:170:PRO:O	4:B:174:GLN:HB2	2.17	0.45
4:B:404:GLU:HB2	4:B:405:TYR:CD2	2.52	0.45
5:L:28:ASP:HA	5:L:68:GLY:O	2.16	0.45
5:L:98:PHE:HD2	6:H:47:LEU:O	2.00	0.45
6:H:39:ILE:HD11	6:H:110:MET:HE2	1.99	0.45
3:A:155:GLY:O	3:A:156:SER:C	2.59	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
3:A:522:ILE:HG22	3:A:526:ILE:HD11	1.99	0.45
4:B:260:LEU:C	4:B:260:LEU:HD23	2.42	0.45
4:B:377:THR:O	4:B:381:VAL:HG23	2.17	0.45
6:H:95:TYR:HD1	6:H:95:TYR:H	1.65	0.45
1:T:815:DG:C2	1:T:816:DG:C6	3.05	0.45
4:B:29:GLU:CG	4:B:71:TRP:HH2	2.27	0.45
5:L:17:ASP:O	5:L:78:LEU:HG	2.16	0.45
5:L:33:LEU:HA	5:L:89:GLN:O	2.17	0.45
6:H:145:MET:SD	6:H:194:PRO:HA	2.56	0.45
3:A:107:THR:HG23	3:A:221:HIS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:88:TRP:CD1	4:B:92:LEU:HD22	2.52	0.45
4:B:368:LEU:HD11	4:B:391:LEU:HD22	1.99	0.45
4:B:385:LYS:N	4:B:385:LYS:CD	2.76	0.45
6:H:92:THR:HG1	6:H:120:THR:HA	1.78	0.45
3:A:206:ARG:CG	3:A:216:THR:HG21	2.44	0.45
3:A:267:ALA:HB1	3:A:271:TYR:HD2	1.81	0.45
3:A:354:TYR:CD1	3:A:371:ALA:HA	2.52	0.45
3:A:361:HIS:CD2	3:A:505:ILE:HG23	2.52	0.45
3:A:473:THR:C	3:A:477:THR:HG23	2.42	0.45
3:A:486:LEU:HD22	3:A:528:LYS:NZ	2.32	0.45
4:B:195:ILE:HG13	4:B:199:ARG:HE	1.81	0.45
2:P:833:DG:C4	2:P:834:DC:C5	3.05	0.45
3:A:425:LEU:HD12	3:A:425:LEU:N	2.31	0.45
4:B:113:ASP:O	4:B:116:PHE:N	2.47	0.45
4:B:376:THR:O	4:B:379:SER:N	2.50	0.45
5:L:139:PHE:CE2	5:L:174:SER:HA	2.52	0.45
5:L:142:LYS:O	5:L:142:LYS:HE2	2.17	0.45
4:B:66:LYS:O	4:B:67:ASP:HB3	2.16	0.44
4:B:378:GLU:O	4:B:382:ILE:HG12	2.17	0.44
5:L:108:ARG:HB3	5:L:140:TYR:CD1	2.52	0.44
1:T:811:DA:H1'	1:T:812:DA:O5'	2.17	0.44
1:T:815:DG:N3	1:T:816:DG:C5	2.84	0.44
2:P:825:DC:H2'	2:P:826:DT:C7	2.47	0.44
3:A:116:PHE:HZ	3:A:151:GLN:OE1	1.99	0.44
3:A:146:TYR:HE2	3:A:150:PRO:HA	1.81	0.44
3:A:402:TRP:HE3	4:B:331:LYS:NZ	2.15	0.44
4:B:88:TRP:HD1	4:B:89:GLU:HG3	1.83	0.44
4:B:221:HIS:O	4:B:222:GLN:HG3	2.17	0.44
4:B:224:GLU:O	4:B:227:PHE:CZ	2.70	0.44
5:L:108:ARG:HB3	5:L:140:TYR:CE1	2.53	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
3:A:88:TRP:CD1	3:A:89:GLU:O	2.70	0.44
3:A:235:HIS:C	3:A:237:ASP:H	2.24	0.44
3:A:533:LEU:HD12	3:A:534:ALA:H	1.83	0.44
4:B:175:ASN:CG	4:B:175:ASN:O	2.61	0.44
4:B:212:TRP:O	4:B:213:GLY:C	2.59	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
4:B:326:ILE:O	4:B:341:ILE:HA	2.16	0.44
4:B:363:ASN:O	4:B:364:ASP:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:369:THR:O	4:B:372:VAL:HG22	2.17	0.44
5:L:84:ALA:O	5:L:86:TYR:CD1	2.70	0.44
3:A:115:TYR:C	3:A:117:SER:H	2.25	0.44
3:A:470:THR:CG2	3:A:471:ASN:N	2.81	0.44
4:B:271:TYR:HD1	4:B:271:TYR:H	1.65	0.44
6:H:155:TYR:CE2	6:H:160:VAL:HG11	2.53	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
3:A:50:ILE:CG2	3:A:145:GLN:HG2	2.47	0.44
3:A:492:GLU:O	3:A:493:VAL:HB	2.18	0.44
4:B:71:TRP:H	4:B:71:TRP:CD1	2.34	0.44
4:B:363:ASN:OD1	4:B:363:ASN:C	2.59	0.44
5:L:18:ARG:HA	5:L:76:SER:O	2.17	0.44
5:L:122:SER:O	5:L:126:THR:HG23	2.17	0.44
6:H:38:TRP:CZ3	6:H:97:CYS:HB3	2.52	0.44
6:H:96:TYR:N	6:H:96:TYR:HD1	2.16	0.44
6:H:121:VAL:O	6:H:122:SER:HB2	2.17	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
4:B:41:MET:HE3	4:B:116:PHE:CZ	2.53	0.44
4:B:74:LEU:HA	4:B:74:LEU:HD23	1.59	0.44
4:B:161:GLN:CD	4:B:165:THR:HG21	2.42	0.44
4:B:222:GLN:HA	4:B:229:TRP:CD1	2.52	0.44
6:H:66:LYS:O	6:H:66:LYS:NZ	2.48	0.44
6:H:132:TYR:HE2	6:H:153:LYS:HD3	1.82	0.44
1:T:814:DA:H2''	1:T:815:DG:C8	2.53	0.44
2:P:822:DT:H2'	2:P:823:DC:H5	1.83	0.44
3:A:79:GLU:O	3:A:82:LYS:HB3	2.18	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
4:B:120:LEU:O	4:B:121:ASP:C	2.60	0.44
4:B:130:PHE:O	4:B:143:ARG:HB3	2.18	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:27:PHE:CD1	6:H:27:PHE:N	2.80	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
3:A:504:GLY:O	3:A:505:ILE:C	2.61	0.44
4:B:12:LEU:HA	4:B:85:GLN:H	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:406:TRP:CG	4:B:407:GLN:N	2.85	0.44
6:H:17:PRO:HB2	6:H:85:MET:HE2	1.98	0.44
1:T:818:DA:H2''	1:T:819:DC:C5	2.53	0.44
2:P:838:DA:C4'	3:A:183:TYR:CE2	3.00	0.44
3:A:463:ARG:O	3:A:464:GLN:HG3	2.18	0.44
4:B:93:GLY:C	4:B:94:ILE:HG13	2.43	0.44
4:B:330:GLN:HE22	4:B:340:GLN:CD	2.25	0.44
4:B:345:PRO:C	4:B:347:LYS:H	2.26	0.44
6:H:78:ASN:N	6:H:78:ASN:OD1	2.51	0.44
6:H:81:PHE:CD1	6:H:81:PHE:N	2.86	0.44
3:A:201:LYS:O	3:A:202:ILE:C	2.61	0.43
3:A:368:LEU:HD21	3:A:391:LEU:HB3	2.00	0.43
3:A:521:ILE:O	3:A:525:LEU:HD22	2.18	0.43
2:P:827:DG:C2'	2:P:828:DT:O5'	2.57	0.43
3:A:208:HIS:ND1	3:A:208:HIS:C	2.75	0.43
3:A:406:TRP:HA	4:B:331:LYS:HD3	1.99	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:103:LYS:NZ	4:B:192:ASP:N	2.57	0.43
4:B:191:SER:C	4:B:193:LEU:H	2.25	0.43
4:B:395:LYS:O	4:B:397:THR:N	2.51	0.43
5:L:10:SER:HB3	5:L:103:LYS:HD3	1.99	0.43
5:L:81:GLU:H	5:L:81:GLU:CD	2.25	0.43
6:H:209:HIS:CE1	6:H:212:SER:H	2.36	0.43
1:T:808:DC:P	3:A:353:LYS:HZ2	2.41	0.43
2:P:832:DG:C2	2:P:833:DG:C6	3.06	0.43
3:A:2:ILE:CG2	3:A:3:SER:N	2.80	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:72:ARG:HG3	4:B:72:ARG:HH11	1.83	0.43
4:B:135:ILE:O	4:B:137:ASN:N	2.52	0.43
4:B:152:GLY:HA2	4:B:184:ILE:HG22	1.99	0.43
5:L:38:GLN:HG3	5:L:43:THR:O	2.18	0.43
3:A:5:ILE:HD11	3:A:166:LYS:HZ2	1.83	0.43
3:A:171:PHE:CE2	3:A:205:LEU:HB2	2.53	0.43
3:A:348:ASN:ND2	3:A:349:LEU:H	2.15	0.43
3:A:453:GLY:O	3:A:469:LEU:N	2.42	0.43
4:B:77:PHE:C	4:B:81:ASN:HD22	2.23	0.43
4:B:104:LYS:HB2	4:B:192:ASP:CA	2.48	0.43
6:H:6:GLU:HG3	6:H:97:CYS:SG	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:255:ASN:O	3:A:259:LYS:N	2.48	0.43
3:A:262:GLY:HA2	3:A:265:ASN:HB2	2.01	0.43
3:A:427:TYR:CE1	3:A:522:ILE:HG23	2.53	0.43
3:A:482:ILE:HG22	3:A:486:LEU:CD1	2.44	0.43
5:L:23:CYS:HB2	5:L:35:TRP:CZ2	2.54	0.43
5:L:61:ALA:O	5:L:75:ILE:HA	2.17	0.43
3:A:175:ASN:CB	3:A:178:ILE:HD13	2.46	0.43
3:A:239:TRP:CD1	3:A:316:GLY:O	2.71	0.43
3:A:408:ALA:HB2	4:B:337:TRP:HH2	1.82	0.43
3:A:463:ARG:CG	3:A:464:GLN:N	2.82	0.43
4:B:126:LYS:HG3	4:B:127:TYR:CD2	2.54	0.43
4:B:260:LEU:HD21	4:B:264:LEU:HD23	2.00	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
4:B:125:ARG:C	4:B:127:TYR:H	2.26	0.43
4:B:152:GLY:HA2	4:B:184:ILE:CG2	2.48	0.43
5:L:2:ILE:HD12	5:L:2:ILE:H	1.83	0.43
5:L:160:LEU:O	5:L:177:SER:HA	2.19	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
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
3:A:219:LYS:N	3:A:219:LYS:CD	2.82	0.43
3:A:500:GLN:OE1	4:B:421:PRO:HD2	2.19	0.43
4:B:130:PHE:N	4:B:130:PHE:CD1	2.87	0.43
4:B:163:SER:HA	4:B:166:LYS:CE	2.49	0.43
4:B:326:ILE:HD12	4:B:342:TYR:CE1	2.54	0.43
5:L:115:VAL:HG13	5:L:136:LEU:HD22	2.01	0.43
5:L:211:ALA:HB1	5:L:213:GLU:OE1	2.18	0.43
6:H:29:LEU:HD23	6:H:29:LEU:HA	1.74	0.43
6:H:146:VAL:O	6:H:192:THR:HG23	2.19	0.43
6:H:158:GLU:HA	6:H:185:TYR:CD2	2.52	0.43
6:H:176:PHE:CD1	6:H:176:PHE:N	2.86	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
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
3:A:486:LEU:HD22	3:A:528:LYS:HZ3	1.84	0.43
3:A:512:LYS:O	3:A:513:SER:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:L:166:GLN:NE2	5:L:171:SER:HB3	2.32	0.43
3:A:153:TRP:O	3:A:154:LYS:C	2.62	0.42
3:A:502:ALA:O	3:A:503:LEU:C	2.62	0.42
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
3:A:262:GLY:O	3:A:263:LYS:C	2.61	0.42
3:A:277:ARG:HH12	3:A:335:GLY:C	2.25	0.42
3:A:393:ILE:HG13	3:A:423:VAL:O	2.19	0.42
3:A:443:ASP:HB2	3:A:548:VAL:HG11	2.01	0.42
3:A:484:LEU:O	3:A:485:ALA:C	2.62	0.42
4:B:148:VAL:HB	4:B:149:LEU:H	1.52	0.42
6:H:14:PRO:HG3	6:H:121:VAL:CG1	2.36	0.42
6:H:210:PRO:HG2	6:H:211:ALA:H	1.83	0.42
3:A:179:VAL:O	3:A:189:VAL:HA	2.19	0.42
3:A:277:ARG:NH1	3:A:336:GLN:HG2	2.34	0.42
3:A:380:ILE:HD13	3:A:380:ILE:HA	1.83	0.42
3:A:410:TRP:CD2	4:B:363:ASN:ND2	2.87	0.42
3:A:424:LYS:HE2	3:A:426:TRP:CE3	2.54	0.42
3:A:458:VAL:HA	3:A:464:GLN:HA	2.00	0.42
3:A:463:ARG:C	3:A:464:GLN:HG3	2.44	0.42
4:B:21:VAL:CG1	4:B:22:LYS:N	2.81	0.42
4:B:104:LYS:H	4:B:192:ASP:HA	1.84	0.42
2:P:835:DG:H2''	2:P:836:DC:OP2	2.19	0.42
3:A:30:LYS:O	3:A:31:ILE:C	2.62	0.42
3:A:222:GLN:O	3:A:224:GLU:N	2.52	0.42
3:A:277:ARG:HH22	3:A:333:GLY:C	2.28	0.42
4:B:93:GLY:C	4:B:95:PRO:HD3	2.44	0.42
4:B:231:GLY:O	4:B:232:TYR:C	2.62	0.42
5:L:31:SER:HB2	5:L:50:TYR:CE1	2.55	0.42
5:L:84:ALA:O	5:L:86:TYR:HD1	2.03	0.42
6:H:32:SER:O	6:H:55:TRP:NE1	2.52	0.42
6:H:198:TRP:C	6:H:200:SER:N	2.75	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: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
3:A:114:ALA:O	3:A:117:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:279:LEU:N	3:A:279:LEU:CD1	2.79	0.42
3:A:491:LEU:O	3:A:492:GLU:HG3	2.20	0.42
4:B:245:VAL:CB	4:B:427:TYR:CE1	3.00	0.42
2:P:831:DG:C4	2:P:832:DG:C5	3.08	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
3:A:325:LEU:C	3:A:326:ILE:HG13	2.45	0.42
3:A:401:TRP:CZ2	3:A:405:TYR:CD2	3.07	0.42
3:A:459:THR:HG23	3:A:461:LYS:HB2	2.02	0.42
4:B:72:ARG:HH11	4:B:72:ARG:CG	2.33	0.42
4:B:126:LYS:HG3	4:B:127:TYR:CE2	2.55	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
5:L:113:PRO:HB3	5:L:139:PHE:HD2	1.83	0.42
5:L:179:LEU:HD12	5:L:179:LEU:HA	1.70	0.42
6:H:66:LYS:C	6:H:66:LYS:HD3	2.44	0.42
1:T:803:DG:C2'	1:T:804:DG:H5''	2.43	0.42
2:P:835:DG:H1'	2:P:836:DC:O5'	2.19	0.42
3:A:64:LYS:HG2	3:A:72:ARG:N	2.33	0.42
3:A:410:TRP:CE3	4:B:363:ASN:ND2	2.88	0.42
3:A:523:GLU:HA	3:A:526:ILE:CD1	2.44	0.42
4:B:73:LYS:HD2	4:B:151:GLN:NE2	2.35	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
5:L:166:GLN:HB2	5:L:173:TYR:OH	2.20	0.42
6:H:87:VAL:HG13	6:H:91:ASP:HB2	2.01	0.42
3:A:64:LYS:HG2	3:A:71:TRP:HA	2.00	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
3:A:264:LEU:O	3:A:265:ASN:C	2.62	0.42
3:A:368:LEU:O	3:A:369:THR:C	2.63	0.42
3:A:377:THR:O	3:A:378:GLU:C	2.61	0.42
6:H:61:TYR:HB2	6:H:66:LYS:HB2	2.02	0.42
2:P:829:DT:H2'	2:P:830:DC:C6	2.53	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
6:H:198:TRP:HB3	6:H:199:PRO:HD3	2.01	0.42
2:P:827:DG:P	3:A:360:ALA:H	2.43	0.42
4:B:253:THR:HB	4:B:292:VAL:O	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:203:SER:HA	5:L:204:PRO:HD3	1.64	0.42
6:H:152:VAL:N	6:H:187:LEU:O	2.39	0.42
6:H:162:VAL:HB	6:H:207:VAL:HG22	2.02	0.42
1:T:805:DC:C5'	3:A:93:GLY:HA2	2.50	0.41
3:A:221:HIS:NE2	3:A:228:LEU:HB3	2.35	0.41
3:A:254:VAL:CG2	3:A:289:LEU:HA	2.50	0.41
3:A:261:VAL:O	3:A:264:LEU:HB2	2.20	0.41
3:A:450:THR:O	3:A:451:LYS:HB2	2.20	0.41
3:A:474:ASN:HD22	3:A:474:ASN:N	2.16	0.41
4:B:180:ILE:CG1	4:B:189:VAL:HG22	2.48	0.41
5:L:81:GLU:N	5:L:81:GLU:CD	2.78	0.41
1:T:816:DG:H1	2:P:824:DC:H42	1.68	0.41
2:P:833:DG:C2'	2:P:833:DG:O5'	2.67	0.41
3:A:60:VAL:HG22	3:A:61:PHE:N	2.35	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
3:A:519:ASN:HA	3:A:522:ILE:CD1	2.50	0.41
4:B:94:ILE:N	4:B:95:PRO:HD3	2.34	0.41
4:B:224:GLU:OE2	5:L:96:TRP:HZ2	2.03	0.41
5:L:19:VAL:HG12	5:L:20:THR:N	2.35	0.41
1:T:804:DG:N2	1:T:805:DC:O2	2.53	0.41
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
3:A:329:ILE:HD13	3:A:329:ILE:N	2.26	0.41
4:B:387:PRO:HG2	4:B:389:PHE:CZ	2.54	0.41
6:H:2:ILE:HD11	6:H:112:HIS:CD2	2.55	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
3:A:61:PHE:N	3:A:61:PHE:CD1	2.87	0.41
3:A:149:LEU:HA	3:A:150:PRO:HD2	1.79	0.41
3:A:193:LEU:O	3:A:194:GLU:C	2.62	0.41
3:A:426:TRP:CE3	3:A:426:TRP:HA	2.56	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
4:B:326:ILE:O	4:B:341:ILE:HG23	2.20	0.41
5:L:35:TRP:CH2	5:L:88:CYS:HB2	2.56	0.41
3:A:312:GLU:HA	3:A:313:PRO:HD3	1.83	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
3:A:517:LEU:O	3:A:520:GLN:HB2	2.19	0.41
4:B:202:ILE:CG2	4:B:203:GLU:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:55:HIS:O	5:L:58:VAL:HG23	2.20	0.41
5:L:106:ILE:HG22	5:L:107:LYS:N	2.35	0.41
6:H:181:GLN:N	6:H:184:LEU:O	2.53	0.41
3:A:10:VAL:HG23	3:A:87:PHE:HE2	1.85	0.41
3:A:167:ILE:N	3:A:167:ILE:CD1	2.83	0.41
3:A:371:ALA:O	3:A:375:ILE:HG13	2.21	0.41
3:A:457:TYR:N	3:A:457:TYR:CD2	2.88	0.41
4:B:97:PRO:HG2	4:B:100:LEU:HD22	2.02	0.41
4:B:124:PHE:CZ	4:B:153:TRP:CZ2	3.09	0.41
4:B:266:TRP:CZ2	4:B:346:PHE:HE2	2.38	0.41
4:B:371:ALA:O	4:B:372:VAL:C	2.64	0.41
5:L:193:THR:CG2	5:L:194:CYS:N	2.83	0.41
6:H:141:GLN:OE1	6:H:199:PRO:HG2	2.20	0.41
6:H:176:PHE:O	6:H:187:LEU:HG	2.20	0.41
4:B:96:HIS:CE1	4:B:382:ILE:O	2.73	0.41
4:B:223:LYS:CE	6:H:60:ARG:HH22	2.33	0.41
4:B:258:GLN:NE2	4:B:283:LEU:HD21	2.35	0.41
5:L:204:PRO:O	5:L:206:VAL:HG23	2.20	0.41
3:A:60:VAL:C	3:A:61:PHE:CD1	2.99	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
3:A:522:ILE:O	3:A:525:LEU:HB2	2.20	0.41
4:B:8:VAL:HA	4:B:9:PRO:HD3	1.80	0.41
4:B:30:LYS:O	4:B:31:ILE:C	2.62	0.41
1:T:802:DT:C2'	1:T:803:DG:OP2	2.69	0.41
3:A:119:PRO:HA	3:A:148:VAL:HA	2.03	0.41
3:A:159:ILE:O	3:A:160:PHE:C	2.64	0.41
3:A:171:PHE:HB2	3:A:208:HIS:CD2	2.54	0.41
3:A:325:LEU:HD11	3:A:383:TRP:CE3	2.56	0.41
4:B:16:MET:C	4:B:18:GLY:H	2.27	0.41
4:B:50:ILE:HD11	4:B:144:TYR:C	2.46	0.41
4:B:61:PHE:O	4:B:74:LEU:HB2	2.20	0.41
4:B:89:GLU:HA	4:B:92:LEU:CD2	2.51	0.41
4:B:123:ASP:C	4:B:125:ARG:H	2.28	0.41
4:B:123:ASP:C	4:B:125:ARG:N	2.78	0.41
4:B:205:LEU:HD23	4:B:205:LEU:O	2.21	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
4:B:406:TRP:O	4:B:407:GLN:OE1	2.39	0.41
5:L:198:HIS:C	5:L:200:THR:N	2.73	0.41
6:H:39:ILE:HD11	6:H:110:MET:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:158:ALA:O	3:A:159:ILE:C	2.63	0.41
3:A:307:ARG:NH1	3:A:307:ARG:CG	2.84	0.41
3:A:376:THR:HB	3:A:377:THR:H	1.73	0.41
3:A:454:LYS:CA	3:A:468:PRO:HA	2.39	0.41
4:B:31:ILE:C	4:B:35:VAL:HG23	2.44	0.41
4:B:88:TRP:O	4:B:92:LEU:HB3	2.21	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
4:B:281:LYS:C	4:B:283:LEU:N	2.77	0.41
6:H:41:GLN:HA	6:H:42:PRO:HD3	1.67	0.41
3:A:75:VAL:HG12	3:A:76:ASP:N	2.35	0.40
3:A:372:VAL:HG13	3:A:389:PHE:CZ	2.56	0.40
4:B:112:GLY:O	4:B:113:ASP:C	2.64	0.40
4:B:288:ALA:O	4:B:292:VAL:CB	2.69	0.40
5:L:205:ILE:H	5:L:205:ILE:CD1	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:324:ASP:N	3:A:343:GLN:HE21	2.19	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
6:H:66:LYS:O	6:H:67:SER:C	2.65	0.40
3:A:209:LEU:O	3:A:214:LEU:HB2	2.20	0.40
3:A:250:ASP:O	3:A:251:SER:C	2.64	0.40
3:A:427:TYR:CE2	3:A:525:LEU:HD23	2.57	0.40
4:B:12:LEU:HA	4:B:84:THR:HA	2.03	0.40
4:B:135:ILE:C	4:B:137:ASN:H	2.29	0.40
4:B:161:GLN:O	4:B:162:SER:C	2.64	0.40
4:B:222:GLN:HE21	4:B:222:GLN:HB2	1.62	0.40
5:L:2:ILE:HD11	5:L:93:LYS:CB	2.49	0.40
6:H:155:TYR:CD1	6:H:155:TYR:C	2.99	0.40
2:P:834:DC:C2	2:P:835:DG:N7	2.89	0.40
3:A:131:THR:HA	3:A:142:ILE:O	2.21	0.40
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
4:B:236:PRO:HA	4:B:239:TRP:CE2	2.56	0.40
5:L:58:VAL:HA	5:L:59:PRO:HD3	1.91	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:64:LYS:HB2	4:B:71:TRP:CZ3	2.56	0.40
4:B:135:ILE:C	4:B:137:ASN:N	2.79	0.40
4:B:207:GLN:O	4:B:211:ARG:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:11:LEU:N	5:L:11:LEU:HD23	2.36	0.40
5:L:19:VAL:C	5:L:74:THR:HG23	2.47	0.40
5:L:39:LYS:O	5:L:42:GLY:N	2.54	0.40
5:L:84:ALA:O	5:L:104:LEU:HB3	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	9
4	B	428/430 (100%)	284 (66%)	96 (22%)	48 (11%)	0	5
5	L	212/214 (99%)	162 (76%)	35 (16%)	15 (7%)	1	10
6	H	218/220 (99%)	160 (73%)	42 (19%)	16 (7%)	1	9
All	All	1414/1422 (99%)	1000 (71%)	294 (21%)	120 (8%)	0	7

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	63	ILE
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	354 (82%)	80 (18%)	1	9
4	B	350/392 (89%)	282 (81%)	68 (19%)	1	8
5	L	182/182 (100%)	149 (82%)	33 (18%)	2	10
6	H	191/191 (100%)	169 (88%)	22 (12%)	5	24
All	All	1157/1263 (92%)	954 (82%)	203 (18%)	2	11

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	10	VAL
3	A	11	LYS
3	A	16	MET
3	A	22	LYS
3	A	24	TRP
3	A	26	LEU
3	A	41	MET
3	A	58	THR
3	A	87	PHE
3	A	89	GLU
3	A	94	ILE
3	A	101	LYS
3	A	132	ILE
3	A	147	ASN
3	A	151	GLN
3	A	157	PRO
3	A	162	SER
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	235	HIS
3	A	237	ASP
3	A	240	THR
3	A	241	VAL
3	A	246	LEU
3	A	256	ASP
3	A	268	SER
3	A	279	LEU
3	A	286	THR
3	A	307	ARG
3	A	308	GLU
3	A	310	LEU
3	A	326	ILE
3	A	329	ILE
3	A	341	ILE
3	A	345	PRO

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Mol	Chain	Res	Type
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	380	ILE
3	A	382	ILE
3	A	395	LYS
3	A	406	TRP
3	A	409	THR
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	442	VAL
3	A	452	LEU
3	A	457	TYR
3	A	465	LYS
3	A	469	LEU
3	A	474	ASN
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
3	A	548	VAL
3	A	556	ILE
4	B	2	ILE
4	B	8	VAL
4	B	11	LYS
4	B	12	LEU

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Mol	Chain	Res	Type
4	B	27	THR
4	B	36	GLU
4	B	40	GLU
4	B	42	GLU
4	B	44	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	132	ILE
4	B	143	ARG
4	B	148	VAL
4	B	154	LYS
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	200	THR
4	B	202	ILE
4	B	205	LEU
4	B	207	GLN
4	B	210	LEU
4	B	211	ARG
4	B	218	ASP
4	B	219	LYS
4	B	222	GLN
4	B	228	LEU

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Mol	Chain	Res	Type
4	B	233	GLU
4	B	235	HIS
4	B	253	THR
4	B	264	LEU
4	B	271	TYR
4	B	279	LEU
4	B	289	LEU
4	B	290	THR
4	B	306	ASN
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	393	ILE
4	B	396	GLU
4	B	419	THR
4	B	422	LEU
4	B	425	LEU
4	B	427	TYR
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	60	SER
5	L	75	ILE
5	L	77	ASN
5	L	90	GLN
5	L	91	TYR
5	L	97	THR
5	L	104	LEU
5	L	110	ASP
5	L	136	LEU
5	L	137	ASN
5	L	142	LYS
5	L	144	ILE
5	L	161	ASN

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Mol	Chain	Res	Type
5	L	165	ASP
5	L	168	SER
5	L	169	LYS
5	L	174	SER
5	L	175	MET
5	L	176	SER
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	81	PHE
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	152	VAL
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
6	H	220	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	147	ASN
3	A	175	ASN
3	A	182	GLN

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Mol	Chain	Res	Type
3	A	198	HIS
3	A	208	HIS
3	A	258	GLN
3	A	269	GLN
3	A	343	GLN
3	A	348	ASN
3	A	407	GLN
3	A	474	ASN
3	A	475	GLN
3	A	480	GLN
3	A	494	ASN
3	A	520	GLN
4	B	85	GLN
4	B	136	ASN
4	B	151	GLN
4	B	207	GLN
4	B	221	HIS
4	B	222	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
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	T	19/19 (100%)	1.38	1 (5%) 32 18	59, 76, 94, 96	0
2	P	18/18 (100%)	0.91	1 (5%) 30 17	61, 74, 86, 87	0
3	A	558/558 (100%)	0.04	13 (2%) 61 37	11, 52, 75, 92	0
4	B	430/430 (100%)	-0.05	10 (2%) 61 37	6, 32, 75, 93	0
5	L	214/214 (100%)	0.06	5 (2%) 61 37	17, 44, 66, 76	0
6	H	220/220 (100%)	-0.19	0 100 100	14, 33, 57, 68	0
All	All	1459/1459 (100%)	0.01	30 (2%) 63 38	6, 43, 75, 96	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	297	GLU	6.0
3	A	67	ASP	4.8
4	B	85	GLN	3.4
5	L	158	GLY	3.3
3	A	69	THR	3.2
4	B	425	LEU	3.0
4	B	250	ASP	3.0
3	A	554	ALA	2.9
3	A	68	SER	2.8
3	A	66	LYS	2.7
5	L	69	THR	2.7
5	L	212	ASN	2.6
3	A	136	ASN	2.6
3	A	553	SER	2.6
5	L	153	SER	2.5
1	T	804	DG	2.5
3	A	557	ARG	2.4
4	B	88	TRP	2.4
4	B	300	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
3	A	348	ASN	2.4
4	B	93	GLY	2.4
4	B	1	PRO	2.3
3	A	312	GLU	2.3
3	A	546	GLU	2.3
2	P	825	DC	2.2
4	B	166	LYS	2.2
4	B	221	HIS	2.1
4	B	253	THR	2.0
5	L	185	GLU	2.0
3	A	364	ASP	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 oligosaccharides 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.