



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:50 PM UTC

PDB ID : 7CE1 / pdb_00007ce1
Title : Complex STRUCTURE OF TRANSCRIPTION FACTOR SghR with its COGNATE DNA
Authors : Ye, F.Z.; Wang, C.; Yan, X.F.; Zhang, L.H.; Gao, Y.G.
Deposited on : 2020-06-21
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

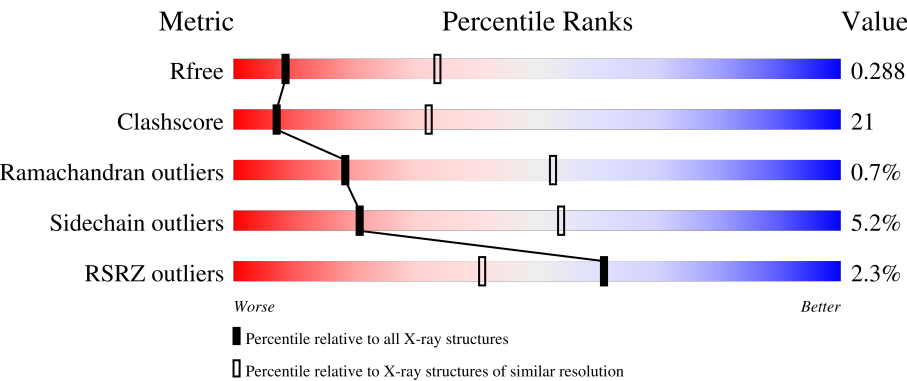
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A	341	
1	B	341	
1	C	341	
1	D	341	
1	G	341	

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Mol	Chain	Length	Quality of chain
1	H	341	 67% 27% 2% 4%
1	K	341	 64% 29% 5% 2%
1	L	341	 53% 39% 2% 6%
1	O	341	 55% 33% 6% 6%
1	P	341	 52% 36% 6% 5%
1	S	341	 45% 27% 4% 24%
1	T	341	 41% 35% 8% 14%
2	a	18	 28% 61% 11%
2	b	18	 67% 28% 6%
2	c	18	 39% 61%
2	d	18	 28% 72%
2	g	18	 39% 44% 11% 6%
2	h	18	 44% 50% 6%
2	k	18	 61% 22% 11% 6%
2	l	18	 28% 67% 6%
2	o	18	 33% 61% 6%
2	p	18	 44% 50% 6%
2	s	18	 39% 39% 22%
2	t	18	 33% 44% 22%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32340 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called LacI-type transcription factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2505	1576	443	476	10			
1	B	328	Total	C	N	O	S	0	0	0
			2431	1535	425	462	9			
1	C	332	Total	C	N	O	S	0	0	0
			2534	1602	445	477	10			
1	D	327	Total	C	N	O	S	0	0	0
			2424	1534	424	459	7			
1	G	331	Total	C	N	O	S	0	0	0
			2456	1554	423	469	10			
1	H	331	Total	C	N	O	S	0	0	0
			2525	1593	448	474	10			
1	K	333	Total	C	N	O	S	0	0	0
			2460	1560	426	465	9			
1	L	329	Total	C	N	O	S	0	0	0
			2435	1537	428	462	8			
1	O	320	Total	C	N	O	S	0	0	0
			2250	1420	381	441	8			
1	P	324	Total	C	N	O	S	0	0	0
			2369	1509	404	449	7			
1	S	259	Total	C	N	O	S	0	0	0
			1770	1123	303	339	5			
1	T	292	Total	C	N	O	S	0	0	0
			1997	1254	348	388	7			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	351	LEU	-	expression tag	UNP A0A2I4PGE9
A	352	GLU	-	expression tag	UNP A0A2I4PGE9
A	353	HIS	-	expression tag	UNP A0A2I4PGE9
A	354	HIS	-	expression tag	UNP A0A2I4PGE9
A	355	HIS	-	expression tag	UNP A0A2I4PGE9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	356	HIS	-	expression tag	UNP A0A2I4PGE9
A	357	HIS	-	expression tag	UNP A0A2I4PGE9
A	358	HIS	-	expression tag	UNP A0A2I4PGE9
B	351	LEU	-	expression tag	UNP A0A2I4PGE9
B	352	GLU	-	expression tag	UNP A0A2I4PGE9
B	353	HIS	-	expression tag	UNP A0A2I4PGE9
B	354	HIS	-	expression tag	UNP A0A2I4PGE9
B	355	HIS	-	expression tag	UNP A0A2I4PGE9
B	356	HIS	-	expression tag	UNP A0A2I4PGE9
B	357	HIS	-	expression tag	UNP A0A2I4PGE9
B	358	HIS	-	expression tag	UNP A0A2I4PGE9
C	351	LEU	-	expression tag	UNP A0A2I4PGE9
C	352	GLU	-	expression tag	UNP A0A2I4PGE9
C	353	HIS	-	expression tag	UNP A0A2I4PGE9
C	354	HIS	-	expression tag	UNP A0A2I4PGE9
C	355	HIS	-	expression tag	UNP A0A2I4PGE9
C	356	HIS	-	expression tag	UNP A0A2I4PGE9
C	357	HIS	-	expression tag	UNP A0A2I4PGE9
C	358	HIS	-	expression tag	UNP A0A2I4PGE9
D	351	LEU	-	expression tag	UNP A0A2I4PGE9
D	352	GLU	-	expression tag	UNP A0A2I4PGE9
D	353	HIS	-	expression tag	UNP A0A2I4PGE9
D	354	HIS	-	expression tag	UNP A0A2I4PGE9
D	355	HIS	-	expression tag	UNP A0A2I4PGE9
D	356	HIS	-	expression tag	UNP A0A2I4PGE9
D	357	HIS	-	expression tag	UNP A0A2I4PGE9
D	358	HIS	-	expression tag	UNP A0A2I4PGE9
G	351	LEU	-	expression tag	UNP A0A2I4PGE9
G	352	GLU	-	expression tag	UNP A0A2I4PGE9
G	353	HIS	-	expression tag	UNP A0A2I4PGE9
G	354	HIS	-	expression tag	UNP A0A2I4PGE9
G	355	HIS	-	expression tag	UNP A0A2I4PGE9
G	356	HIS	-	expression tag	UNP A0A2I4PGE9
G	357	HIS	-	expression tag	UNP A0A2I4PGE9
G	358	HIS	-	expression tag	UNP A0A2I4PGE9
H	351	LEU	-	expression tag	UNP A0A2I4PGE9
H	352	GLU	-	expression tag	UNP A0A2I4PGE9
H	353	HIS	-	expression tag	UNP A0A2I4PGE9
H	354	HIS	-	expression tag	UNP A0A2I4PGE9
H	355	HIS	-	expression tag	UNP A0A2I4PGE9
H	356	HIS	-	expression tag	UNP A0A2I4PGE9
H	357	HIS	-	expression tag	UNP A0A2I4PGE9

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Chain	Residue	Modelled	Actual	Comment	Reference
H	358	HIS	-	expression tag	UNP A0A2I4PGE9
K	351	LEU	-	expression tag	UNP A0A2I4PGE9
K	352	GLU	-	expression tag	UNP A0A2I4PGE9
K	353	HIS	-	expression tag	UNP A0A2I4PGE9
K	354	HIS	-	expression tag	UNP A0A2I4PGE9
K	355	HIS	-	expression tag	UNP A0A2I4PGE9
K	356	HIS	-	expression tag	UNP A0A2I4PGE9
K	357	HIS	-	expression tag	UNP A0A2I4PGE9
K	358	HIS	-	expression tag	UNP A0A2I4PGE9
L	351	LEU	-	expression tag	UNP A0A2I4PGE9
L	352	GLU	-	expression tag	UNP A0A2I4PGE9
L	353	HIS	-	expression tag	UNP A0A2I4PGE9
L	354	HIS	-	expression tag	UNP A0A2I4PGE9
L	355	HIS	-	expression tag	UNP A0A2I4PGE9
L	356	HIS	-	expression tag	UNP A0A2I4PGE9
L	357	HIS	-	expression tag	UNP A0A2I4PGE9
L	358	HIS	-	expression tag	UNP A0A2I4PGE9
O	351	LEU	-	expression tag	UNP A0A2I4PGE9
O	352	GLU	-	expression tag	UNP A0A2I4PGE9
O	353	HIS	-	expression tag	UNP A0A2I4PGE9
O	354	HIS	-	expression tag	UNP A0A2I4PGE9
O	355	HIS	-	expression tag	UNP A0A2I4PGE9
O	356	HIS	-	expression tag	UNP A0A2I4PGE9
O	357	HIS	-	expression tag	UNP A0A2I4PGE9
O	358	HIS	-	expression tag	UNP A0A2I4PGE9
P	351	LEU	-	expression tag	UNP A0A2I4PGE9
P	352	GLU	-	expression tag	UNP A0A2I4PGE9
P	353	HIS	-	expression tag	UNP A0A2I4PGE9
P	354	HIS	-	expression tag	UNP A0A2I4PGE9
P	355	HIS	-	expression tag	UNP A0A2I4PGE9
P	356	HIS	-	expression tag	UNP A0A2I4PGE9
P	357	HIS	-	expression tag	UNP A0A2I4PGE9
P	358	HIS	-	expression tag	UNP A0A2I4PGE9
S	351	LEU	-	expression tag	UNP A0A2I4PGE9
S	352	GLU	-	expression tag	UNP A0A2I4PGE9
S	353	HIS	-	expression tag	UNP A0A2I4PGE9
S	354	HIS	-	expression tag	UNP A0A2I4PGE9
S	355	HIS	-	expression tag	UNP A0A2I4PGE9
S	356	HIS	-	expression tag	UNP A0A2I4PGE9
S	357	HIS	-	expression tag	UNP A0A2I4PGE9
S	358	HIS	-	expression tag	UNP A0A2I4PGE9
T	351	LEU	-	expression tag	UNP A0A2I4PGE9

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Chain	Residue	Modelled	Actual	Comment	Reference
T	352	GLU	-	expression tag	UNP A0A2I4PGE9
T	353	HIS	-	expression tag	UNP A0A2I4PGE9
T	354	HIS	-	expression tag	UNP A0A2I4PGE9
T	355	HIS	-	expression tag	UNP A0A2I4PGE9
T	356	HIS	-	expression tag	UNP A0A2I4PGE9
T	357	HIS	-	expression tag	UNP A0A2I4PGE9
T	358	HIS	-	expression tag	UNP A0A2I4PGE9

- Molecule 2 is a DNA chain called promoter DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	a	18	Total	C	N	O	P	0	0	0
			369	176	67	108	18			
2	b	18	Total	C	N	O	P	0	0	0
			369	176	67	108	18			
2	c	18	Total	C	N	O	P	0	0	0
			369	176	67	108	18			
2	d	18	Total	C	N	O	P	0	0	0
			369	176	67	108	18			
2	g	17	Total	C	N	O	P	0	0	0
			349	166	65	101	17			
2	h	17	Total	C	N	O	P	0	0	0
			349	166	65	101	17			
2	k	17	Total	C	N	O	P	0	0	0
			349	166	65	101	17			
2	l	17	Total	C	N	O	P	0	0	0
			349	166	65	101	17			
2	o	18	Total	C	N	O	P	0	0	0
			369	176	67	108	18			
2	p	17	Total	C	N	O	P	0	0	0
			349	166	65	101	17			
2	s	14	Total	C	N	O	P	0	0	0
			284	136	50	84	14			
2	t	14	Total	C	N	O	P	0	0	0
			285	136	50	85	14			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	2	Total	O	0	0
			2	2		

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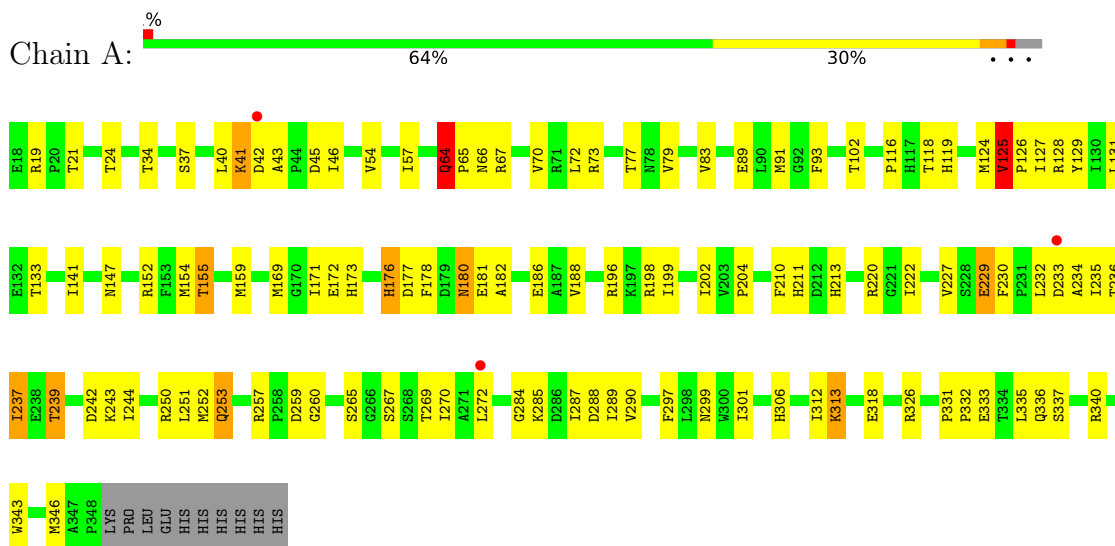
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	6	Total 6	O 6	0	0
3	D	2	Total 2	O 2	0	0
3	c	1	Total 1	O 1	0	0
3	d	1	Total 1	O 1	0	0
3	G	2	Total 2	O 2	0	0
3	H	1	Total 1	O 1	0	0
3	K	2	Total 2	O 2	0	0
3	L	2	Total 2	O 2	0	0
3	O	1	Total 1	O 1	0	0
3	P	1	Total 1	O 1	0	0
3	S	1	Total 1	O 1	0	0
3	T	1	Total 1	O 1	0	0

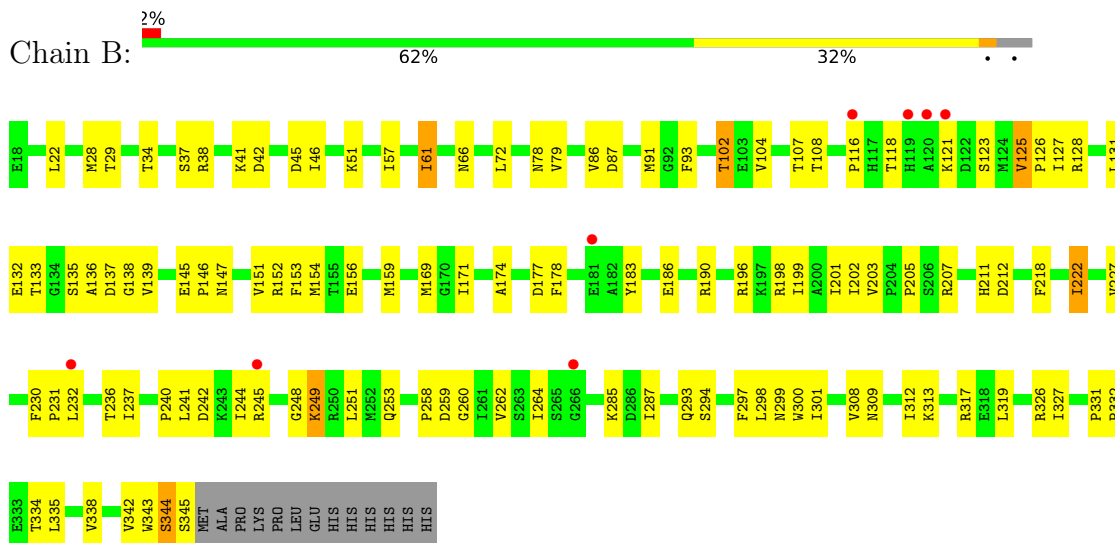
3 Residue-property plots

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

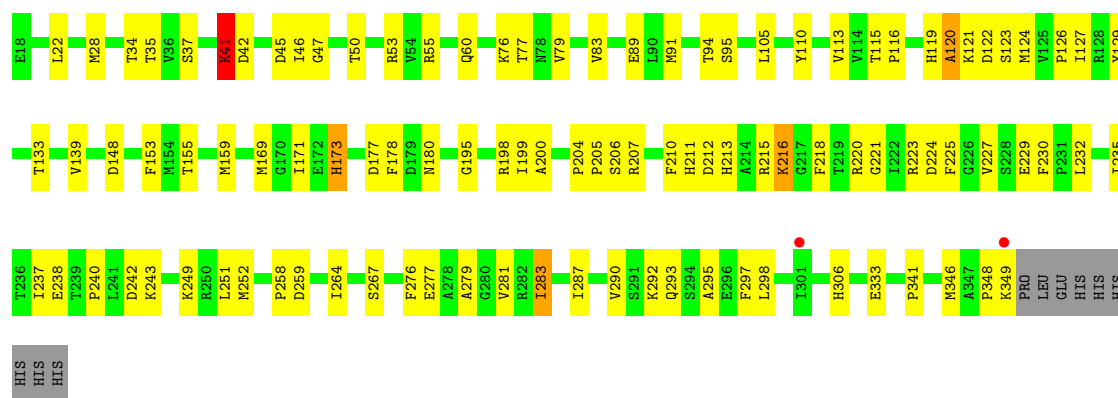


- Molecule 1: LacI-type transcription factor

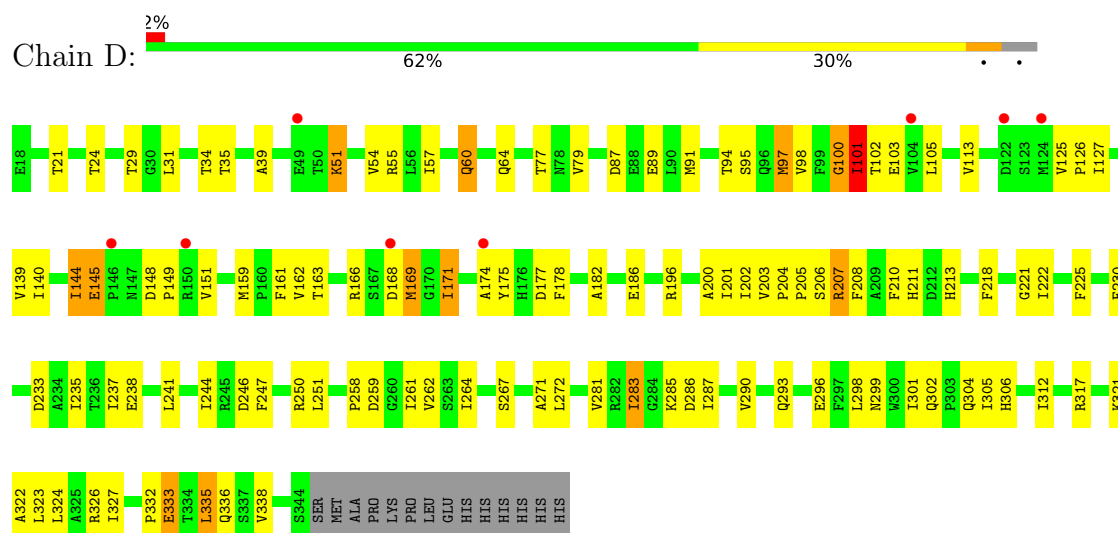


- Molecule 1: LacI-type transcription factor

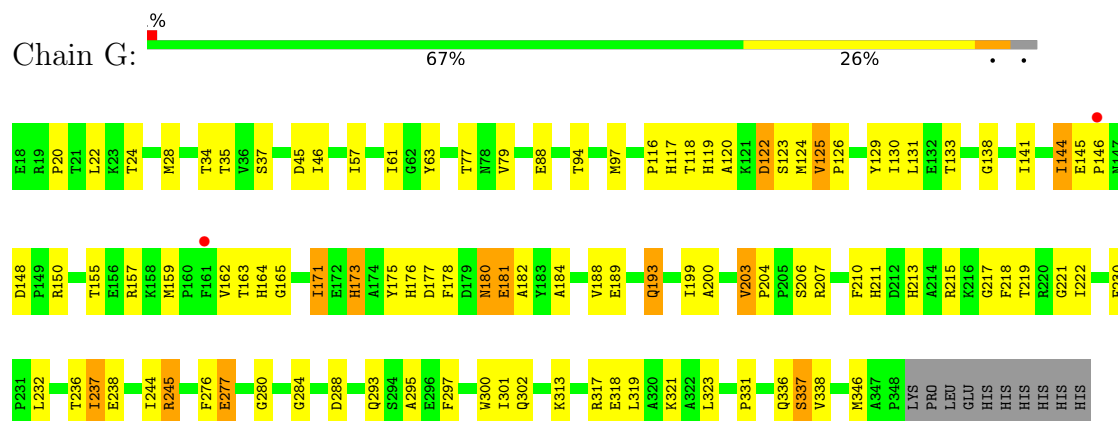




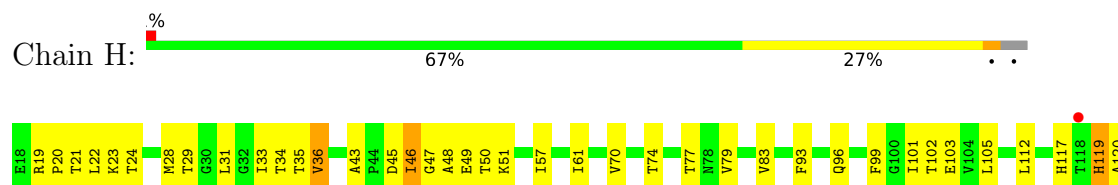
• Molecule 1: LacI-type transcription factor

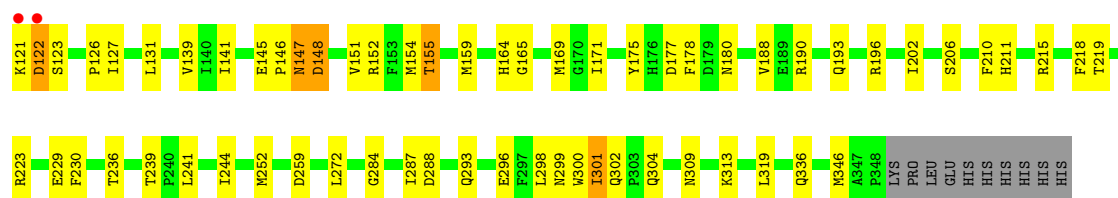


• Molecule 1: LacI-type transcription factor

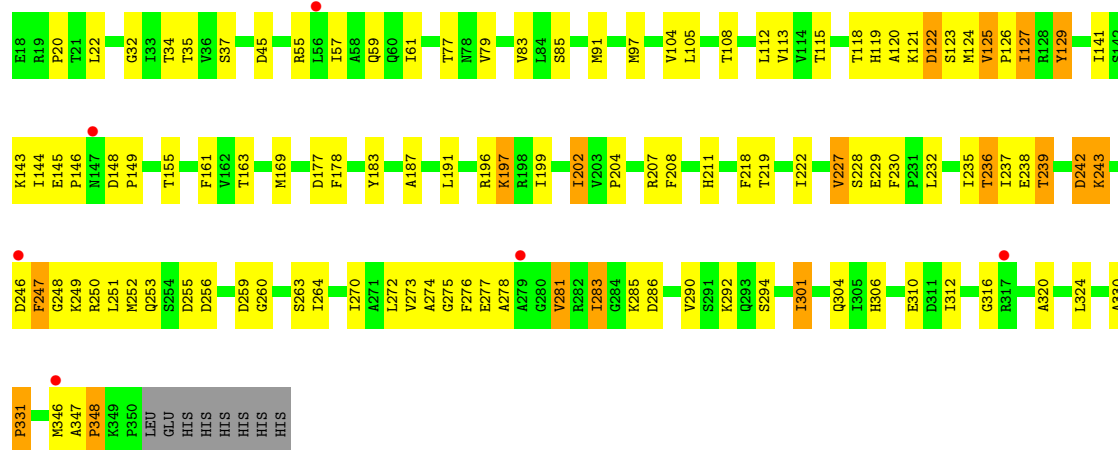


• Molecule 1: LacI-type transcription factor

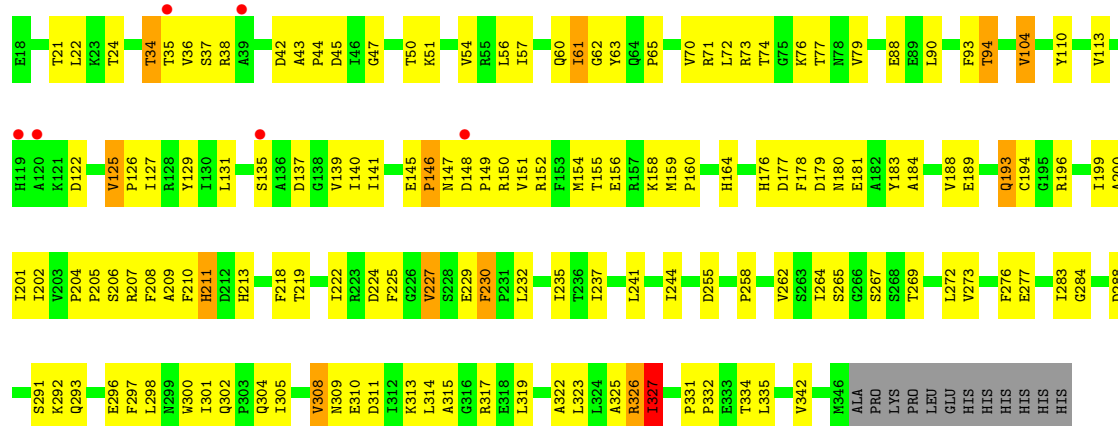




• Molecule 1: LacI-type transcription factor

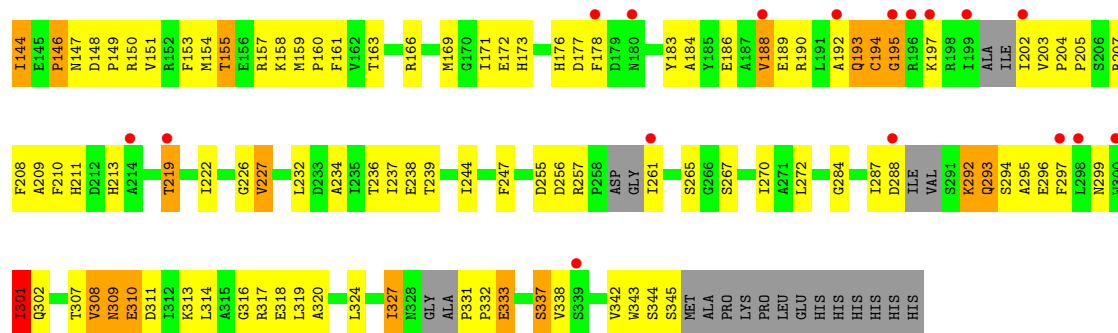


• Molecule 1: LacI-type transcription factor

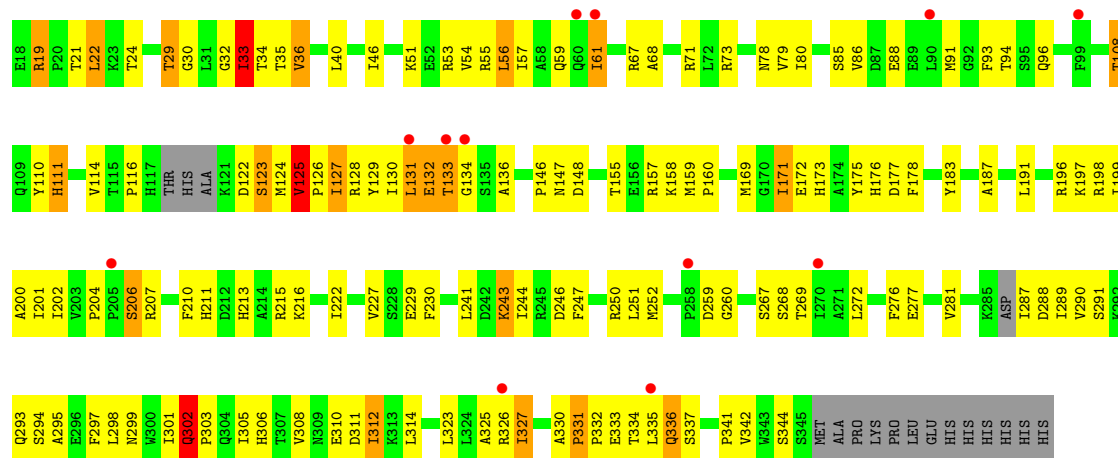


• Molecule 1: LacI-type transcription factor

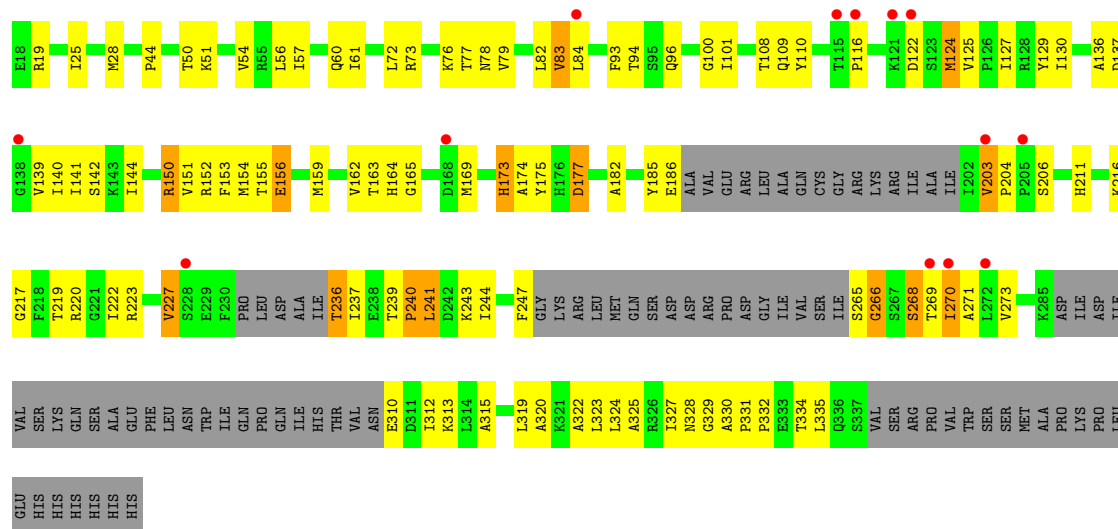
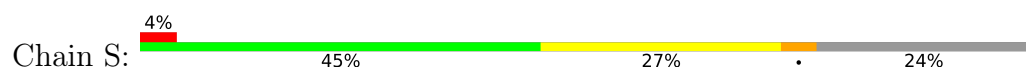




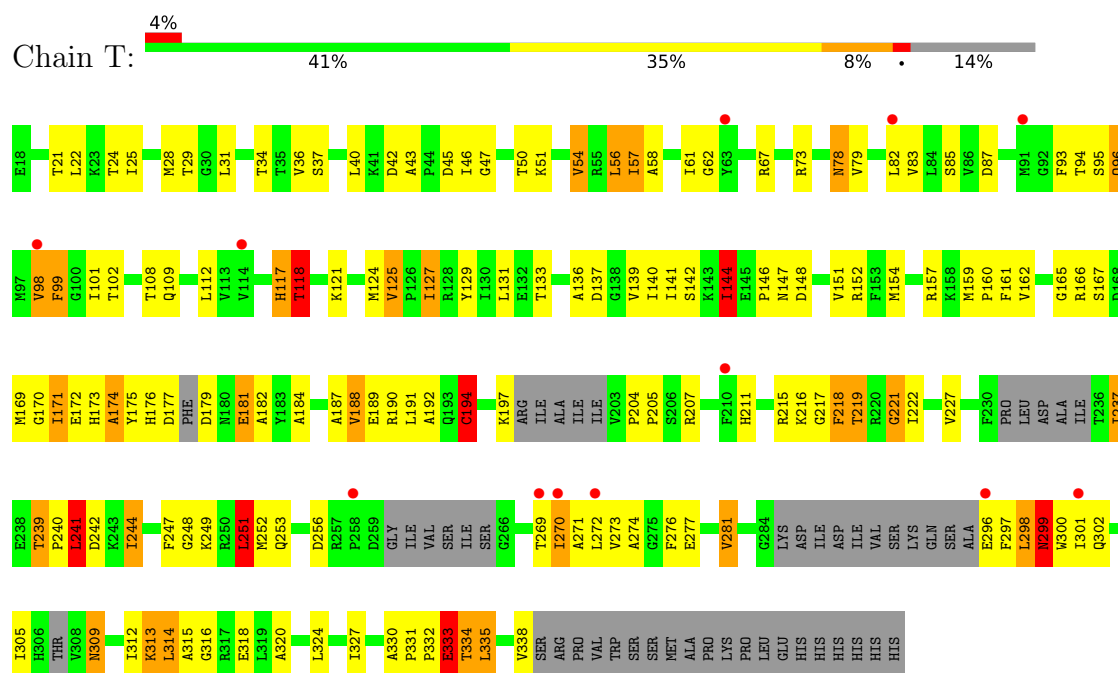
• Molecule 1: LacI-type transcription factor



• Molecule 1: LacI-type transcription factor



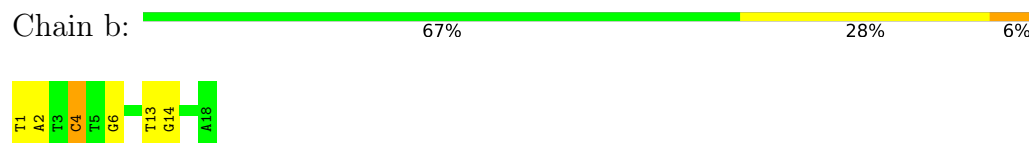
• Molecule 1: LacI-type transcription factor



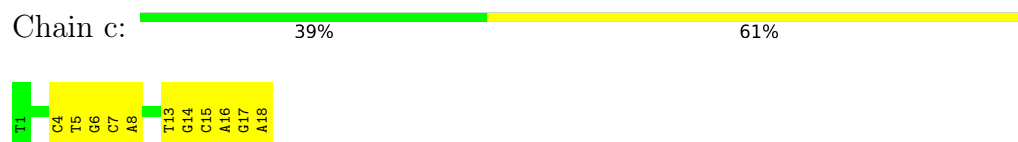
- Molecule 2: promoter DNA



- Molecule 2: promoter DNA



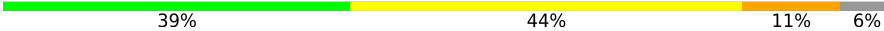
- Molecule 2: promoter DNA



- Molecule 2: promoter DNA



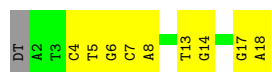
- Molecule 2: promoter DNA

Chain g:  39% 44% 11% 6%



• Molecule 2: promoter DNA

Chain h:  44% 50% 6%

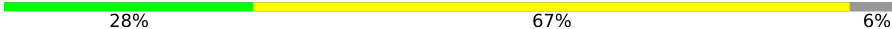


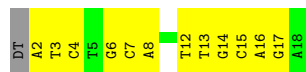
• Molecule 2: promoter DNA

Chain k:  61% 22% 11% 6%

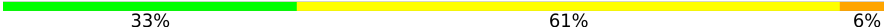


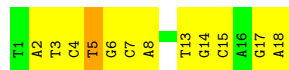
• Molecule 2: promoter DNA

Chain l:  28% 67% 6%



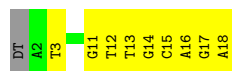
• Molecule 2: promoter DNA

Chain o:  33% 61% 6%



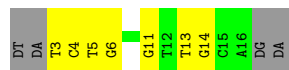
• Molecule 2: promoter DNA

Chain p:  44% 50% 6%

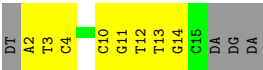
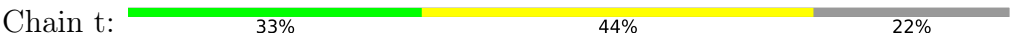


• Molecule 2: promoter DNA

Chain s:  39% 39% 22%



• Molecule 2: promoter DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.90Å 218.96Å 284.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 3.20 49.15 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.15-3.20) 99.9 (49.15-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.233 , 0.281 0.246 , 0.288	Depositor DCC
R_{free} test set	5593 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	98.6	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 89.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32340	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% 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	A	0.60	1/2552 (0.0%)	1.14	19/3471 (0.5%)
1	B	0.57	0/2476	1.12	9/3374 (0.3%)
1	C	0.46	0/2584	1.04	7/3509 (0.2%)
1	D	0.60	0/2471	1.17	16/3371 (0.5%)
1	G	0.52	1/2504 (0.0%)	1.14	17/3412 (0.5%)
1	H	0.45	0/2574	1.04	10/3496 (0.3%)
1	K	0.58	1/2510 (0.0%)	1.17	22/3425 (0.6%)
1	L	0.55	2/2482 (0.1%)	1.12	12/3385 (0.4%)
1	O	0.57	0/2285	1.21	22/3126 (0.7%)
1	P	0.61	0/2414	1.22	23/3293 (0.7%)
1	S	0.68	1/1796 (0.1%)	1.36	17/2458 (0.7%)
1	T	0.71	2/2024 (0.1%)	1.48	35/2770 (1.3%)
2	a	0.71	1/413 (0.2%)	0.91	1/635 (0.2%)
2	b	0.63	0/413	0.82	1/635 (0.2%)
2	c	0.37	0/413	0.66	0/635
2	d	0.31	0/413	0.62	0/635
2	g	0.45	0/391	0.88	3/601 (0.5%)
2	h	0.35	0/391	0.63	0/601
2	k	0.39	0/391	0.86	2/601 (0.3%)
2	l	0.35	0/391	0.67	0/601
2	o	0.47	0/413	0.75	1/635 (0.2%)
2	p	0.42	0/391	0.66	0/601
2	s	0.33	0/317	0.62	0/486
2	t	0.36	0/318	0.64	0/488
All	All	0.56	9/33327 (0.0%)	1.12	217/46244 (0.5%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	243	LYS	C-O	-5.97	1.16	1.24
1	S	271	ALA	CA-CB	-5.82	1.44	1.53
1	L	327	ILE	CA-CB	5.58	1.62	1.54
1	A	125	VAL	CA-CB	5.41	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	144	ILE	CA-CB	-5.30	1.47	1.54
1	G	125	VAL	CA-CB	5.29	1.57	1.53
1	L	125	VAL	CA-CB	5.29	1.57	1.53
1	T	333	GLU	N-CA	5.22	1.52	1.46
2	a	12	DT	O3'-P	-5.12	1.53	1.61

All (217) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	98	VAL	N-CA-C	13.65	123.52	110.42
1	H	300	TRP	N-CA-C	-10.53	99.89	111.36
1	S	203	VAL	CA-C-N	-9.28	110.83	120.38
1	S	203	VAL	C-N-CA	-9.28	110.83	120.38
1	S	266	GLY	N-CA-C	8.95	125.44	113.99
1	O	297	PHE	N-CA-C	-8.93	101.06	112.93
1	D	207	ARG	N-CA-C	8.72	121.88	111.33
1	D	169	MET	N-CA-C	-8.71	97.61	109.54
1	O	195	GLY	N-CA-C	8.51	126.55	114.64
1	O	301	ILE	N-CA-C	8.41	119.19	110.62
1	B	29	THR	N-CA-C	8.37	123.27	112.89
1	T	298	LEU	N-CA-C	8.36	126.40	113.28
1	O	310	GLU	CA-C-N	-8.24	112.13	122.84
1	O	310	GLU	C-N-CA	-8.24	112.13	122.84
1	C	50	THR	N-CA-C	-8.13	102.39	111.82
1	K	278	ALA	N-CA-C	-8.07	102.56	111.36
1	C	230	PHE	CA-C-N	-8.03	111.62	120.14
1	C	230	PHE	C-N-CA	-8.03	111.62	120.14
1	G	331	PRO	CA-C-N	8.03	128.47	119.32
1	G	331	PRO	C-N-CA	8.03	128.47	119.32
1	K	122	ASP	N-CA-C	-7.92	104.10	113.21
1	D	101	ILE	N-CA-C	7.90	117.96	110.53
1	K	104	VAL	N-CA-C	7.86	118.66	110.72
1	S	270	ILE	CA-C-N	7.77	131.01	120.44
1	S	270	ILE	C-N-CA	7.77	131.01	120.44
1	S	169	MET	N-CA-C	-7.76	103.96	113.50
1	T	241	LEU	N-CA-C	7.75	119.73	111.28
1	D	168	ASP	N-CA-C	7.73	120.34	107.20
1	G	302	GLN	CA-C-N	7.65	127.29	119.56
1	G	302	GLN	C-N-CA	7.65	127.29	119.56
1	B	125	VAL	CB-CA-C	-7.59	106.30	114.35
1	K	228	SER	N-CA-C	7.59	121.30	108.02
2	g	5	DT	C4'-C3'-O3'	7.50	121.25	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	ILE	N-CA-C	7.47	124.30	113.16
2	g	5	DT	C2'-C3'-O3'	7.46	122.70	111.50
1	S	271	ALA	N-CA-C	7.44	119.18	111.14
1	K	275	GLY	N-CA-C	-7.41	103.53	112.49
1	S	315	ALA	N-CA-C	-7.38	103.18	111.07
1	D	322	ALA	N-CA-C	-7.35	103.21	111.07
1	K	242	ASP	N-CA-C	-7.27	103.36	111.28
1	L	125	VAL	CA-C-N	-7.27	111.48	119.19
1	L	125	VAL	C-N-CA	-7.27	111.48	119.19
1	A	230	PHE	CA-C-N	-7.21	110.83	119.84
1	A	230	PHE	C-N-CA	-7.21	110.83	119.84
1	A	43	ALA	CA-C-N	7.20	126.83	119.19
1	A	43	ALA	C-N-CA	7.20	126.83	119.19
1	P	302	GLN	CA-C-N	7.16	127.00	119.05
1	P	302	GLN	C-N-CA	7.16	127.00	119.05
1	L	61	ILE	N-CA-C	7.13	120.99	111.44
1	S	219	THR	N-CA-C	7.04	119.99	111.82
1	G	125	VAL	CA-C-N	-7.02	111.20	118.85
1	G	125	VAL	C-N-CA	-7.02	111.20	118.85
1	P	276	PHE	N-CA-C	7.02	118.58	111.07
1	O	193	GLN	N-CA-C	-7.01	99.81	111.37
1	T	333	GLU	N-CA-C	6.99	121.81	113.28
1	T	157	ARG	N-CA-C	-6.98	104.75	113.20
1	D	145	GLU	CA-C-N	-6.97	111.13	119.84
1	D	145	GLU	C-N-CA	-6.97	111.13	119.84
1	T	108	THR	N-CA-C	-6.93	99.61	110.36
2	k	5	DT	C4'-C3'-O3'	6.92	120.39	110.00
1	B	331	PRO	CA-C-N	6.89	126.70	119.05
1	B	331	PRO	C-N-CA	6.89	126.70	119.05
1	A	331	PRO	CA-C-N	6.86	127.14	119.32
1	A	331	PRO	C-N-CA	6.86	127.14	119.32
1	T	219	THR	N-CA-C	-6.82	103.93	111.36
1	T	314	LEU	N-CA-C	-6.78	103.97	111.36
1	L	34	THR	N-CA-CB	6.74	121.38	110.40
1	K	274	ALA	N-CA-C	-6.72	103.96	111.28
1	S	268	SER	N-CA-C	-6.60	103.91	112.23
1	T	117	HIS	N-CA-C	6.60	119.18	108.76
1	P	29	THR	N-CA-C	6.58	121.05	112.89
1	T	270	ILE	N-CA-C	6.58	117.33	110.62
1	A	237	ILE	N-CA-C	6.58	117.27	110.36
1	G	203	VAL	N-CA-CB	-6.57	107.30	111.83
1	H	147	ASN	N-CA-C	6.51	120.14	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	148	ASP	CA-C-N	6.49	126.42	119.28
1	H	148	ASP	C-N-CA	6.49	126.42	119.28
1	T	152	ARG	N-CA-C	6.47	119.65	111.69
1	G	182	ALA	N-CA-C	-6.47	104.23	111.28
1	P	331	PRO	CA-C-N	6.47	126.23	119.05
1	P	331	PRO	C-N-CA	6.47	126.23	119.05
1	S	240	PRO	N-CA-C	-6.44	101.12	111.03
1	A	251	LEU	N-CA-C	-6.41	100.80	110.28
1	S	216	LYS	N-CA-C	-6.40	104.31	111.28
1	K	304	GLN	CA-CB-CG	-6.35	101.41	114.10
1	T	221	GLY	CA-C-N	-6.34	113.24	122.69
1	T	221	GLY	C-N-CA	-6.34	113.24	122.69
1	O	302	GLN	CA-C-N	6.34	125.97	119.56
1	O	302	GLN	C-N-CA	6.34	125.97	119.56
1	P	22	LEU	N-CA-C	-6.27	104.44	111.28
2	b	4	DC	C2'-C3'-O3'	-6.27	102.10	111.50
1	G	118	THR	N-CA-C	-6.24	105.82	113.50
1	T	189	GLU	CA-CB-CG	6.23	126.55	114.10
1	K	197	LYS	N-CA-C	6.20	118.12	111.36
1	A	64	GLN	CA-C-N	6.16	126.53	119.93
1	A	64	GLN	C-N-CA	6.16	126.53	119.93
1	D	100	GLY	N-CA-C	-6.14	105.36	112.73
1	D	285	LYS	N-CA-C	6.10	117.73	111.14
1	L	276	PHE	N-CA-C	6.07	117.69	111.14
1	C	41	LYS	N-CA-C	-6.06	97.84	108.20
1	K	125	VAL	CA-C-N	-6.05	112.78	119.19
1	K	125	VAL	C-N-CA	-6.05	112.78	119.19
1	O	90	LEU	N-CA-C	6.04	117.53	111.07
1	B	344	SER	N-CA-C	6.00	123.57	110.80
1	G	171	ILE	CA-C-N	-5.94	114.52	122.72
1	G	171	ILE	C-N-CA	-5.94	114.52	122.72
1	O	310	GLU	CA-CB-CG	5.94	125.97	114.10
1	D	144	ILE	N-CA-C	5.93	117.13	108.53
2	a	5	DT	C2'-C3'-O3'	5.89	120.34	111.50
1	D	168	ASP	CB-CA-C	-5.88	104.14	111.43
1	P	111	HIS	N-CA-CB	5.86	119.43	110.70
1	P	125	VAL	CB-CA-C	-5.86	108.14	114.35
1	T	256	ASP	N-CA-C	5.81	117.99	108.52
1	T	251	LEU	N-CA-C	-5.81	105.08	111.82
1	T	188	VAL	N-CA-C	5.80	119.21	111.44
2	o	5	DT	P-O3'-C3'	5.79	128.89	120.20
1	B	285	LYS	N-CA-C	5.76	117.36	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	324	LEU	N-CA-C	-5.76	104.91	111.07
1	T	190	ARG	N-CA-C	-5.76	104.97	112.23
1	H	165	GLY	N-CA-C	-5.74	105.77	111.85
1	P	94	THR	N-CA-C	5.73	118.47	111.82
1	L	104	VAL	CB-CA-C	-5.70	104.36	112.22
1	T	99	PHE	N-CA-C	-5.69	105.22	111.82
1	K	239	THR	CA-C-N	5.68	125.68	119.89
1	K	239	THR	C-N-CA	5.68	125.68	119.89
1	P	56	LEU	CA-CB-CG	5.67	136.13	116.30
1	P	197	LYS	N-CA-C	5.67	120.26	113.23
1	P	114	VAL	N-CA-C	5.64	116.61	108.48
1	L	146	PRO	N-CA-C	-5.64	105.41	113.47
2	g	4	DC	C2'-C3'-O3'	-5.63	103.06	111.50
1	P	201	ILE	N-CA-C	5.63	116.22	108.12
1	P	191	LEU	N-CA-C	5.58	117.44	111.36
1	T	125	VAL	CA-C-N	-5.56	113.30	119.19
1	T	125	VAL	C-N-CA	-5.56	113.30	119.19
1	G	276	PHE	N-CA-C	5.53	116.99	111.07
1	H	304	GLN	CA-CB-CG	-5.53	103.04	114.10
1	G	157	ARG	N-CA-C	5.53	117.61	110.65
1	D	301	ILE	N-CA-C	5.50	116.54	111.81
1	A	125	VAL	CA-C-N	-5.50	113.36	119.19
1	A	125	VAL	C-N-CA	-5.50	113.36	119.19
1	P	344	SER	N-CA-C	5.49	117.56	108.49
1	K	248	GLY	N-CA-C	-5.49	106.13	112.83
1	T	94	THR	N-CA-C	5.49	118.19	111.82
1	O	309	ASN	N-CA-C	5.48	117.45	108.52
2	k	7	DC	C4'-C3'-O3'	5.47	118.21	110.00
1	C	195	GLY	N-CA-C	-5.45	107.59	115.27
1	B	319	LEU	N-CA-C	-5.42	105.37	111.28
1	K	331	PRO	CA-C-N	5.42	125.06	119.05
1	K	331	PRO	C-N-CA	5.42	125.06	119.05
1	D	333	GLU	N-CA-C	5.40	117.17	111.28
1	H	230	PHE	CA-C-N	-5.39	115.03	120.31
1	H	230	PHE	C-N-CA	-5.39	115.03	120.31
1	A	313	LYS	N-CA-C	-5.39	106.21	112.89
1	K	127	ILE	N-CA-C	5.39	115.59	110.42
1	T	98	VAL	CB-CA-C	-5.37	105.09	111.97
1	K	229	GLU	N-CA-C	5.37	122.23	110.80
1	G	237	ILE	CB-CA-C	-5.36	105.10	111.97
1	T	171	ILE	N-CA-C	-5.36	100.67	108.17
1	L	326	ARG	N-CA-C	5.33	117.17	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	262	VAL	N-CA-C	5.33	115.63	108.17
1	S	151	VAL	N-CA-C	5.32	115.52	110.42
1	O	120	ALA	N-CA-C	-5.30	105.92	112.38
1	P	336	GLN	N-CA-C	-5.30	101.06	109.96
1	K	249	LYS	N-CA-C	5.29	119.66	112.04
1	P	19	ARG	CA-C-N	5.29	125.19	119.85
1	P	19	ARG	C-N-CA	5.29	125.19	119.85
1	O	41	LYS	N-CA-C	-5.28	102.67	110.48
1	T	239	THR	CA-C-N	5.28	125.44	119.90
1	T	239	THR	C-N-CA	5.28	125.44	119.90
1	A	239	THR	CA-C-N	5.26	125.25	119.89
1	A	239	THR	C-N-CA	5.26	125.25	119.89
1	G	122	ASP	N-CA-C	-5.26	105.10	112.25
1	S	327	ILE	N-CA-C	-5.26	105.41	110.72
1	T	118	THR	N-CA-C	5.25	121.98	110.80
1	D	60	GLN	N-CA-C	5.24	117.07	111.36
1	L	47	GLY	N-CA-C	-5.24	108.91	114.67
1	C	235	ILE	N-CA-C	5.24	117.40	108.86
1	S	177	ASP	N-CA-C	-5.24	101.34	109.14
1	O	146	PRO	CA-C-N	-5.23	115.44	122.86
1	O	146	PRO	C-N-CA	-5.23	115.44	122.86
1	O	308	VAL	CA-C-N	-5.22	115.74	123.05
1	O	308	VAL	C-N-CA	-5.22	115.74	123.05
1	T	216	LYS	N-CA-C	-5.22	105.59	111.28
1	P	148	ASP	CA-C-N	5.20	125.00	119.28
1	P	148	ASP	C-N-CA	5.20	125.00	119.28
1	A	229	GLU	N-CA-C	5.20	117.20	107.99
1	O	338	VAL	N-CA-C	5.20	115.61	108.12
1	H	48	ALA	N-CA-C	5.17	119.90	111.37
1	L	230	PHE	CA-C-N	-5.17	114.29	120.13
1	L	230	PHE	C-N-CA	-5.17	114.29	120.13
1	G	337	SER	N-CA-C	5.15	117.07	108.99
1	H	148	ASP	N-CA-C	5.12	116.14	109.64
1	G	181	GLU	CA-CB-CG	5.11	124.32	114.10
1	S	44	PRO	N-CA-C	-5.11	107.20	113.84
1	K	247	PHE	N-CA-C	-5.10	105.36	112.45
1	D	335	LEU	N-CA-C	5.09	116.83	111.28
1	A	250	ARG	CA-C-N	-5.09	113.65	120.87
1	A	250	ARG	C-N-CA	-5.09	113.65	120.87
1	P	61	ILE	N-CA-C	-5.08	105.44	112.50
1	T	170	GLY	CA-C-N	-5.08	116.90	123.19
1	T	170	GLY	C-N-CA	-5.08	116.90	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	77	THR	N-CA-C	-5.07	107.26	113.50
1	D	283	ILE	N-CA-C	-5.07	102.31	109.21
1	K	285	LYS	N-CA-C	5.06	116.60	111.14
1	K	59	GLN	CA-CB-CG	5.05	124.21	114.10
1	C	119	HIS	N-CA-C	5.05	116.74	108.76
1	T	330	ALA	CA-C-N	5.05	125.58	120.38
1	T	330	ALA	C-N-CA	5.05	125.58	120.38
1	P	171	ILE	N-CA-C	5.04	115.22	108.17
1	O	257	ARG	N-CA-C	-5.02	103.15	110.08
1	T	194	CYS	N-CA-C	5.02	117.64	111.82
1	O	331	PRO	CA-C-N	5.02	124.62	119.05
1	O	331	PRO	C-N-CA	5.02	124.62	119.05
1	T	108	THR	CA-C-N	-5.01	115.19	122.86
1	T	108	THR	C-N-CA	-5.01	115.19	122.86
1	L	90	LEU	N-CA-C	5.01	116.74	111.28
1	A	285	LYS	N-CA-C	5.00	116.55	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2505	0	2466	86	0
1	B	2431	0	2372	86	0
1	C	2534	0	2518	71	0
1	D	2424	0	2345	118	0
1	G	2456	0	2391	73	0
1	H	2525	0	2512	64	0
1	K	2460	0	2386	90	0
1	L	2435	0	2346	128	0
1	O	2250	0	2082	126	0
1	P	2369	0	2283	125	0
1	S	1770	0	1641	97	0
1	T	1997	0	1822	189	0
2	a	369	0	204	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	369	0	204	5	0
2	c	369	0	204	13	0
2	d	369	0	204	12	0
2	g	349	0	192	11	0
2	h	349	0	192	6	0
2	k	349	0	192	14	0
2	l	349	0	192	20	0
2	o	369	0	204	14	0
2	p	349	0	192	10	0
2	s	284	0	159	11	0
2	t	285	0	159	9	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	6	0	0	0	0
3	D	2	0	0	0	0
3	G	2	0	0	0	0
3	H	1	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
3	c	1	0	0	0	0
3	d	1	0	0	0	0
All	All	32340	0	29462	1284	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 21.

All (1284) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:83:VAL:CG2	1:T:141:ILE:HD13	1.48	1.39
1:D:148:ASP:HB3	1:D:151:VAL:CG2	1.64	1.25
1:T:241:LEU:CD1	1:T:271:ALA:HB3	1.71	1.20
1:T:83:VAL:HG23	1:T:141:ILE:CD1	1.79	1.11
1:O:202:ILE:HD11	1:O:272:LEU:HD11	1.24	1.10
1:D:148:ASP:HB3	1:D:151:VAL:HG21	1.35	1.08
1:T:83:VAL:HG23	1:T:141:ILE:HD13	1.11	1.08
1:O:202:ILE:HD11	1:O:272:LEU:CD1	1.87	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:51:LYS:O	1:T:54:VAL:HG23	1.55	1.04
1:D:148:ASP:HB3	1:D:151:VAL:HG23	1.38	1.04
1:T:241:LEU:HD22	1:T:271:ALA:HB1	1.39	1.03
1:T:332:PRO:O	1:T:335:LEU:HD21	1.55	1.03
1:O:301:ILE:HG13	1:P:302:GLN:NE2	1.71	1.03
1:D:326:ARG:HH22	1:D:332:PRO:HG3	1.27	1.00
1:D:326:ARG:NH2	1:D:332:PRO:HG3	1.75	1.00
1:H:299:ASN:HD22	1:H:346:MET:HB2	1.26	0.99
1:P:125:VAL:HG13	1:P:126:PRO:HD3	1.41	0.99
1:T:83:VAL:CG2	1:T:141:ILE:CD1	2.40	0.98
1:O:197:LYS:O	1:O:227:VAL:HG13	1.62	0.98
1:S:150:ARG:HG2	1:S:150:ARG:HH11	1.29	0.98
1:G:144:ILE:HD12	1:G:144:ILE:H	1.23	0.98
1:T:50:THR:O	1:T:54:VAL:HG22	1.62	0.97
1:T:83:VAL:HG21	1:T:141:ILE:HD13	1.44	0.97
1:T:241:LEU:CD2	1:T:271:ALA:HB3	1.94	0.97
1:S:93:PHE:O	1:S:312:ILE:HD11	1.64	0.96
1:T:241:LEU:CD2	1:T:271:ALA:CB	2.44	0.96
1:O:222:ILE:HG23	1:O:227:VAL:O	1.65	0.95
1:S:94:THR:OG1	1:T:95:SER:HB3	1.65	0.95
1:T:241:LEU:HD22	1:T:271:ALA:CB	1.98	0.93
1:T:51:LYS:HA	1:T:54:VAL:CG2	1.98	0.93
1:T:241:LEU:HD11	1:T:271:ALA:HB3	1.49	0.92
1:O:190:ARG:O	1:O:194:CYS:HB2	1.70	0.92
1:T:166:ARG:CB	1:T:175:TYR:CB	2.47	0.92
1:T:335:LEU:HD22	1:T:335:LEU:H	1.33	0.92
1:D:251:LEU:HD21	1:D:258:PRO:HD2	1.51	0.91
1:O:204:PRO:HG3	1:O:237:ILE:HG12	1.50	0.91
1:O:301:ILE:HG21	1:P:301:ILE:HG23	1.51	0.91
1:D:174:ALA:HB2	1:D:335:LEU:HD13	1.51	0.91
1:S:241:LEU:HD12	1:S:244:ILE:HD12	1.50	0.91
1:D:321:LYS:HA	1:D:324:LEU:HB2	1.53	0.90
1:P:125:VAL:HG13	1:P:126:PRO:CD	2.01	0.89
1:S:83:VAL:HG21	1:S:141:ILE:HD12	1.53	0.89
1:D:174:ALA:CB	1:D:335:LEU:HD13	2.03	0.89
1:O:202:ILE:CD1	1:O:272:LEU:HD11	2.00	0.89
1:D:148:ASP:CB	1:D:151:VAL:CG2	2.51	0.88
1:O:146:PRO:HD3	1:O:207:ARG:O	1.72	0.88
1:G:200:ALA:HB1	1:G:232:LEU:HD23	1.54	0.88
1:D:148:ASP:CB	1:D:151:VAL:HG23	2.03	0.88
1:T:174:ALA:HA	1:T:335:LEU:HG	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:304:GLN:O	1:L:304:GLN:NE2	2.07	0.87
1:O:202:ILE:CD1	1:O:272:LEU:CD1	2.53	0.86
1:H:145:GLU:HB2	1:H:148:ASP:HB3	1.55	0.86
1:T:269:THR:O	1:T:273:VAL:HG23	1.75	0.86
1:K:273:VAL:HA	1:K:276:PHE:HB2	1.57	0.85
1:T:22:LEU:HD21	1:T:37:SER:HB3	1.58	0.85
1:K:197:LYS:O	1:K:227:VAL:HG12	1.74	0.85
1:O:222:ILE:CG2	1:O:227:VAL:O	2.24	0.84
1:D:103:GLU:HG2	1:D:317:ARG:HH11	1.43	0.84
1:L:206:SER:HA	1:L:211:HIS:ND1	1.92	0.84
1:A:204:PRO:HG2	1:A:211:HIS:HA	1.60	0.84
1:L:180:ASN:HD22	1:L:210:PHE:HB2	1.41	0.83
1:S:116:PRO:HG3	1:T:102:THR:HG21	1.58	0.83
1:T:241:LEU:CD1	1:T:271:ALA:CB	2.55	0.83
1:O:204:PRO:HG2	1:O:210:PHE:CE2	2.14	0.83
1:K:199:ILE:HD11	1:K:218:PHE:CZ	2.14	0.82
1:T:241:LEU:HD23	1:T:241:LEU:O	1.79	0.82
1:K:347:ALA:O	2:p:18:DA:H2''	1.80	0.81
1:O:301:ILE:HG12	1:P:301:ILE:HG21	1.62	0.81
1:O:301:ILE:HG13	1:P:302:GLN:HE21	1.46	0.81
1:D:101:ILE:O	1:D:105:LEU:HD13	1.82	0.80
1:O:71:ARG:HG2	1:P:68:ALA:HB2	1.62	0.80
1:T:169:MET:HG3	1:T:171:ILE:HG12	1.62	0.80
2:a:1:DT:H2''	2:a:2:DA:H5'	1.63	0.79
1:T:241:LEU:HD13	1:T:271:ALA:CB	2.13	0.79
1:O:204:PRO:HA	1:O:237:ILE:HG13	1.64	0.79
1:D:174:ALA:HA	1:D:335:LEU:HD12	1.62	0.79
2:k:7:DC:N4	2:l:14:DG:N1	2.31	0.79
1:O:301:ILE:CG1	1:P:302:GLN:HE21	1.96	0.78
1:T:333:GLU:C	1:T:335:LEU:HD22	2.08	0.78
1:P:122:ASP:O	1:P:125:VAL:HG12	1.82	0.78
1:K:199:ILE:CD1	1:K:218:PHE:CZ	2.67	0.78
1:T:117:HIS:ND1	1:T:118:THR:HG23	1.99	0.77
1:C:113:VAL:HG12	1:D:113:VAL:HG12	1.66	0.77
1:P:93:PHE:HZ	1:P:295:ALA:HB3	1.49	0.77
1:G:129:TYR:CE1	1:G:133:THR:HG21	2.19	0.77
1:S:124:MET:HE3	1:S:150:ARG:HA	1.65	0.77
1:C:180:ASN:HD22	1:C:210:PHE:HB2	1.48	0.77
1:K:196:ARG:CB	1:K:259:ASP:OD2	2.33	0.77
1:P:325:ALA:HB3	1:P:335:LEU:HD13	1.65	0.76
1:S:142:SER:HA	1:S:164:HIS:HB3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:82:LEU:HD23	1:T:112:LEU:HD21	1.65	0.76
1:T:241:LEU:HD13	1:T:271:ALA:HB3	1.60	0.76
1:C:178:PHE:HD2	1:C:180:ASN:OD1	1.67	0.76
1:D:148:ASP:OD2	1:D:151:VAL:HG23	1.84	0.76
1:D:204:PRO:HA	1:D:237:ILE:HG12	1.68	0.76
1:D:105:LEU:N	1:D:105:LEU:HD12	2.01	0.76
1:P:128:ARG:O	1:P:132:GLU:HG2	1.85	0.76
1:T:299:ASN:OD1	1:T:299:ASN:N	2.18	0.76
1:P:146:PRO:HD3	1:P:207:ARG:O	1.85	0.75
1:B:293:GLN:NE2	1:B:298:LEU:H	1.83	0.75
1:L:222:ILE:HD12	1:L:227:VAL:HG13	1.67	0.75
1:P:127:ILE:HD12	1:P:127:ILE:O	1.87	0.75
1:O:301:ILE:CG1	1:P:302:GLN:NE2	2.49	0.75
1:A:131:LEU:HD11	1:A:159:MET:HB2	1.69	0.75
1:T:332:PRO:HB2	1:T:333:GLU:OE2	1.87	0.75
1:O:294:SER:HA	1:O:310:GLU:O	1.87	0.75
1:O:203:VAL:HG22	1:O:204:PRO:N	2.02	0.74
1:B:147:ASN:HA	1:B:169:MET:HG2	1.69	0.74
1:P:323:LEU:O	1:P:323:LEU:HD12	1.87	0.74
1:H:202:ILE:HD11	1:H:272:LEU:HD13	1.68	0.74
1:S:241:LEU:HD23	1:T:300:TRP:CH2	2.23	0.74
1:H:29:THR:HG22	1:H:31:LEU:HD13	1.69	0.74
2:k:7:DC:N4	2:l:14:DG:H1	1.85	0.74
1:T:222:ILE:HG12	1:T:227:VAL:HG22	1.69	0.74
1:O:139:VAL:HB	1:O:154:MET:HE1	1.70	0.74
1:B:28:MET:HE2	1:B:57:ILE:HD11	1.68	0.74
1:T:56:LEU:C	1:T:56:LEU:HD12	2.12	0.74
1:K:283:ILE:N	1:K:283:ILE:HD12	2.03	0.73
1:P:51:LYS:O	1:P:55:ARG:HG2	1.88	0.73
1:P:290:VAL:HG22	1:P:306:HIS:HB2	1.70	0.73
1:B:293:GLN:OE1	1:B:309:ASN:ND2	2.21	0.73
1:P:196:ARG:HD3	1:P:259:ASP:O	1.89	0.73
1:K:35:THR:HG21	2:l:4:DC:H3'	1.69	0.73
1:D:174:ALA:HA	1:D:335:LEU:CD1	2.17	0.73
1:D:103:GLU:HG2	1:D:317:ARG:NH1	2.03	0.73
2:k:5:DT:C6	2:l:17:DG:N2	2.56	0.73
1:T:241:LEU:CG	1:T:271:ALA:HB3	2.17	0.73
1:P:311:ASP:HB3	1:P:314:LEU:HD23	1.71	0.73
1:S:77:THR:O	1:S:79:VAL:N	2.22	0.73
1:L:200:ALA:HB1	1:L:232:LEU:HD23	1.69	0.72
1:G:145:GLU:HB3	1:G:146:PRO:CD	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:ASP:CB	1:D:151:VAL:HG21	2.18	0.72
1:K:283:ILE:HD12	1:K:283:ILE:H	1.55	0.72
1:L:194:CYS:SG	1:L:288:ASP:OD2	2.46	0.72
1:O:314:LEU:HA	1:O:317:ARG:HE	1.55	0.72
1:L:34:THR:HG23	1:L:37:SER:OG	1.88	0.72
1:P:29:THR:O	1:P:53:ARG:NH2	2.23	0.71
1:B:28:MET:HE3	1:G:57:ILE:HA	1.72	0.71
1:K:272:LEU:O	1:K:276:PHE:N	2.20	0.71
1:P:202:ILE:HD11	1:P:272:LEU:HD22	1.73	0.71
1:D:162:VAL:HA	1:D:174:ALA:HB3	1.73	0.71
1:T:131:LEU:HD22	1:T:159:MET:HE2	1.73	0.71
1:T:296:GLU:HA	1:T:309:ASN:HD22	1.54	0.71
1:B:344:SER:OG	1:B:345:SER:N	2.22	0.71
1:O:261:ILE:N	1:O:288:ASP:O	2.24	0.71
1:D:174:ALA:HB2	1:D:335:LEU:CD1	2.21	0.71
1:D:290:VAL:HG22	1:D:306:HIS:HB2	1.72	0.71
2:k:5:DT:H71	2:l:16:DA:N1	2.06	0.71
1:K:232:LEU:HD21	1:K:247:PHE:HZ	1.56	0.70
1:T:51:LYS:HA	1:T:54:VAL:HG21	1.71	0.70
1:T:241:LEU:HG	1:T:244:ILE:HD12	1.74	0.70
1:K:218:PHE:O	1:K:222:ILE:HG23	1.92	0.70
1:A:299:ASN:HB2	1:A:346:MET:HE3	1.73	0.70
1:T:335:LEU:HD22	1:T:335:LEU:N	2.06	0.70
1:D:103:GLU:HG2	1:D:317:ARG:HE	1.56	0.70
1:T:146:PRO:O	1:T:167:SER:HB2	1.91	0.70
1:H:121:LYS:O	1:H:123:SER:N	2.21	0.69
1:T:335:LEU:N	1:T:335:LEU:HD13	2.06	0.69
2:o:17:DG:H2''	2:o:18:DA:H5'	1.74	0.69
2:d:2:DA:H2''	2:d:3:DT:H5''	1.74	0.69
1:G:117:HIS:ND1	1:G:119:HIS:O	2.26	0.69
1:O:186:GLU:O	1:O:189:GLU:HB3	1.91	0.69
1:T:174:ALA:CA	1:T:335:LEU:HG	2.22	0.69
1:T:174:ALA:CB	1:T:335:LEU:HG	2.22	0.69
1:P:131:LEU:HD13	1:P:131:LEU:O	1.93	0.69
1:S:108:THR:OG1	1:S:109:GLN:N	2.25	0.69
1:C:37:SER:O	1:C:41:LYS:HG3	1.92	0.69
1:K:120:ALA:O	1:K:123:SER:HB3	1.93	0.69
1:L:76:LYS:NZ	1:L:110:TYR:OH	2.26	0.69
1:A:198:ARG:H	1:A:259:ASP:HB2	1.58	0.69
2:c:14:DG:H2''	2:c:15:DC:H5''	1.75	0.69
1:B:79:VAL:HG13	1:B:136:ALA:HA	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:152:ARG:HA	1:L:155:THR:OG1	1.92	0.68
1:P:124:MET:HG2	1:P:128:ARG:HG3	1.75	0.68
1:T:137:ASP:O	1:T:327:ILE:HD11	1.93	0.68
1:P:57:ILE:O	1:P:61:ILE:HG12	1.93	0.68
1:D:175:TYR:CZ	1:D:336:GLN:HG3	2.28	0.68
1:O:34:THR:O	1:O:38:ARG:HG2	1.94	0.68
1:T:51:LYS:O	1:T:54:VAL:CG2	2.36	0.68
1:T:57:ILE:HD12	1:T:57:ILE:O	1.93	0.68
2:k:5:DT:H71	2:l:16:DA:C2	2.29	0.68
1:D:51:LYS:O	1:D:55:ARG:HG3	1.95	0.67
1:K:199:ILE:C	1:K:199:ILE:HD12	2.18	0.67
1:P:21:THR:HG23	2:p:11:DG:H3'	1.75	0.67
1:T:51:LYS:CA	1:T:54:VAL:CG2	2.70	0.67
1:G:144:ILE:HD12	1:G:144:ILE:N	2.06	0.67
1:G:145:GLU:HB3	1:G:146:PRO:HD2	1.77	0.67
1:P:108:THR:HG22	1:P:110:TYR:H	1.58	0.67
1:K:232:LEU:HD21	1:K:247:PHE:CZ	2.28	0.67
1:S:150:ARG:HH11	1:S:150:ARG:CG	2.06	0.67
1:T:67:ARG:NH2	1:T:109:GLN:O	2.27	0.67
1:C:204:PRO:HA	1:C:237:ILE:HG12	1.77	0.67
1:D:97:MET:HB2	1:D:312:ILE:HG22	1.76	0.67
1:P:131:LEU:O	1:P:131:LEU:HD22	1.94	0.67
1:B:241:LEU:HA	1:B:244:ILE:CG2	2.25	0.67
1:D:148:ASP:CG	1:D:151:VAL:HG23	2.18	0.67
1:D:202:ILE:HD11	1:D:272:LEU:HD22	1.76	0.67
1:P:32:GLY:O	1:P:34:THR:N	2.28	0.67
1:T:101:ILE:HD11	1:T:112:LEU:HG	1.77	0.67
1:T:188:VAL:O	1:T:192:ALA:N	2.28	0.66
1:S:204:PRO:HG2	1:S:211:HIS:HA	1.76	0.66
1:L:145:GLU:HG2	1:L:208:PHE:HE1	1.58	0.66
1:L:146:PRO:HD3	1:L:207:ARG:O	1.94	0.66
1:C:264:ILE:O	1:C:292:LYS:HE2	1.95	0.66
1:D:139:VAL:HG23	1:D:159:MET:HE2	1.77	0.66
1:O:293:GLN:O	1:O:310:GLU:N	2.29	0.66
1:A:236:THR:HG22	1:A:239:THR:HG23	1.78	0.66
1:T:241:LEU:HD21	1:T:271:ALA:HB3	1.76	0.66
1:B:183:TYR:CE1	1:B:308:VAL:HG11	2.31	0.66
1:B:251:LEU:HD21	1:B:258:PRO:HD2	1.78	0.66
1:T:298:LEU:C	1:T:300:TRP:H	2.04	0.66
2:t:2:DA:H2''	2:t:3:DT:H5''	1.77	0.66
1:K:199:ILE:CD1	1:K:218:PHE:HZ	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:270:ILE:O	1:S:273:VAL:HG22	1.96	0.65
1:O:177:ASP:OD1	1:O:178:PHE:N	2.29	0.65
1:O:236:THR:HG22	1:O:238:GLU:H	1.61	0.65
1:T:148:ASP:HB3	1:T:151:VAL:HG23	1.78	0.65
1:B:241:LEU:HA	1:B:244:ILE:HG22	1.79	0.65
2:g:2:DA:H1'	2:g:3:DT:H5'	1.78	0.65
1:H:178:PHE:HD2	1:H:180:ASN:ND2	1.94	0.65
1:P:160:PRO:HG3	1:P:327:ILE:HD11	1.78	0.65
1:P:334:THR:HG23	1:P:335:LEU:HG	1.77	0.65
1:K:246:ASP:OD1	1:K:247:PHE:N	2.28	0.65
1:L:139:VAL:HB	1:L:154:MET:HE1	1.78	0.65
1:L:177:ASP:OD1	1:L:178:PHE:N	2.29	0.65
2:l:2:DA:H1'	2:l:3:DT:H5'	1.78	0.65
1:B:152:ARG:O	1:B:156:GLU:HG2	1.96	0.65
1:G:206:SER:HA	1:G:211:HIS:CG	2.32	0.65
1:A:237:ILE:HD12	1:A:265:SER:HB3	1.77	0.65
1:P:147:ASN:HA	1:P:169:MET:SD	2.36	0.65
2:o:2:DA:H2'	2:o:3:DT:H5'	1.79	0.65
1:T:204:PRO:HA	1:T:237:ILE:HD11	1.79	0.65
1:T:218:PHE:O	1:T:222:ILE:HG22	1.96	0.65
1:C:200:ALA:HB1	1:C:232:LEU:HD23	1.79	0.64
1:C:215:ARG:NH2	1:C:229:GLU:OE2	2.30	0.64
2:d:4:DC:H2'	2:d:5:DT:H71	1.78	0.64
1:D:174:ALA:CA	1:D:335:LEU:CD1	2.75	0.64
1:H:178:PHE:HD2	1:H:180:ASN:HD22	1.45	0.64
1:L:178:PHE:HD2	1:L:180:ASN:OD1	1.81	0.64
1:D:161:PHE:O	1:D:174:ALA:HB3	1.97	0.64
1:L:206:SER:CA	1:L:211:HIS:ND1	2.60	0.64
1:P:71:ARG:NH1	1:P:134:GLY:O	2.31	0.64
1:O:169:MET:SD	1:O:171:ILE:HD12	2.37	0.64
1:L:51:LYS:HA	1:L:54:VAL:HG22	1.80	0.64
1:O:133:THR:HA	1:P:19:ARG:HH22	1.63	0.64
1:T:174:ALA:HA	1:T:335:LEU:CG	2.28	0.64
1:L:308:VAL:HG23	1:L:342:VAL:O	1.98	0.64
1:L:334:THR:HG23	1:L:335:LEU:HG	1.79	0.64
1:K:199:ILE:CD1	1:K:218:PHE:CE1	2.80	0.63
1:L:218:PHE:O	1:L:222:ILE:HG22	1.98	0.63
1:L:241:LEU:HA	1:L:244:ILE:HG22	1.79	0.63
1:T:151:VAL:HG12	1:T:171:ILE:HD11	1.79	0.63
1:A:181:GLU:OE2	1:A:220:ARG:NH2	2.31	0.63
1:O:293:GLN:HE22	1:O:296:GLU:HA	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:VAL:HG23	1:C:159:MET:HE2	1.79	0.63
1:S:94:THR:HG1	1:T:95:SER:HB3	1.63	0.63
1:A:178:PHE:CD2	1:A:180:ASN:ND2	2.66	0.63
1:O:192:ALA:O	1:O:195:GLY:N	2.32	0.63
1:A:176:HIS:HB2	1:A:337:SER:OG	1.99	0.63
1:L:322:ALA:HA	1:L:335:LEU:HD22	1.81	0.63
2:k:5:DT:H6	2:l:17:DG:N2	1.97	0.63
1:P:34:THR:HG21	2:o:6:DG:H1	1.64	0.63
1:T:241:LEU:CD2	1:T:271:ALA:HB1	2.15	0.63
1:A:290:VAL:HG22	1:A:306:HIS:HB2	1.81	0.62
1:D:103:GLU:HG2	1:D:317:ARG:NE	2.14	0.62
1:O:123:SER:OG	1:O:124:MET:N	2.31	0.62
1:P:210:PHE:HA	1:P:213:HIS:ND1	2.14	0.62
1:T:222:ILE:HG13	1:T:222:ILE:O	1.99	0.62
1:T:241:LEU:HA	1:T:244:ILE:HG13	1.81	0.62
1:K:301:ILE:HG21	1:L:301:ILE:HG23	1.81	0.62
1:L:189:GLU:HA	1:L:225:PHE:CE2	2.35	0.62
1:O:204:PRO:HA	1:O:237:ILE:CG1	2.28	0.62
1:L:139:VAL:HG23	1:L:159:MET:HE2	1.81	0.62
1:S:83:VAL:HG21	1:S:141:ILE:CD1	2.27	0.62
1:B:139:VAL:HG23	1:B:159:MET:HE2	1.82	0.62
1:B:199:ILE:O	1:B:230:PHE:N	2.31	0.62
1:O:147:ASN:HA	1:O:169:MET:HE2	1.81	0.62
1:T:117:HIS:CE1	1:T:118:THR:HG23	2.34	0.62
2:a:4:DC:H2'	2:a:5:DT:H71	1.82	0.62
1:L:131:LEU:HD11	1:L:159:MET:HB2	1.81	0.62
1:O:101:ILE:HA	1:O:320:ALA:HB2	1.80	0.62
1:H:131:LEU:HD11	1:H:159:MET:HB2	1.82	0.61
1:T:51:LYS:C	1:T:54:VAL:HG23	2.24	0.61
2:o:18:DA:N7	2:p:3:DT:H72	2.14	0.61
1:T:139:VAL:HB	1:T:154:MET:HE1	1.82	0.61
1:T:217:GLY:O	1:T:221:GLY:N	2.33	0.61
1:O:204:PRO:CG	1:O:237:ILE:HG12	2.28	0.61
1:T:333:GLU:HA	1:T:335:LEU:CD2	2.30	0.61
1:B:177:ASP:OD1	1:B:178:PHE:N	2.34	0.61
1:C:283:ILE:HD12	1:C:283:ILE:H	1.64	0.61
1:D:177:ASP:OD1	1:D:178:PHE:N	2.33	0.61
1:O:204:PRO:HB3	1:O:205:PRO:HD2	1.83	0.61
1:D:148:ASP:OD2	1:D:151:VAL:CG2	2.49	0.61
1:D:196:ARG:HD2	1:D:259:ASP:HB2	1.81	0.61
1:H:47:GLY:N	2:g:4:DC:OP2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:241:LEU:HA	1:H:244:ILE:HG22	1.82	0.61
1:L:126:PRO:HG2	1:L:127:ILE:HD12	1.82	0.61
1:B:169:MET:HE3	1:B:171:ILE:HD12	1.82	0.61
1:L:158:LYS:O	1:L:160:PRO:HD3	2.01	0.61
1:O:316:GLY:HA2	1:O:319:LEU:HD12	1.83	0.61
1:T:241:LEU:HD21	1:T:271:ALA:CB	2.28	0.61
1:D:125:VAL:N	1:D:126:PRO:HD2	2.16	0.61
1:K:145:GLU:HB3	1:K:208:PHE:HA	1.83	0.61
1:O:147:ASN:CB	1:O:169:MET:HB3	2.30	0.61
1:T:222:ILE:HD11	1:T:227:VAL:HG13	1.82	0.61
1:B:128:ARG:O	1:B:132:GLU:HG3	2.01	0.61
1:K:247:PHE:CZ	1:K:251:LEU:HD11	2.36	0.61
1:O:301:ILE:HG12	1:P:301:ILE:CG2	2.31	0.61
1:S:77:THR:O	1:S:137:ASP:HB2	2.01	0.61
1:C:116:PRO:HG3	1:D:102:THR:HG21	1.83	0.61
2:a:2:DA:H1'	2:a:3:DT:H5'	1.81	0.60
1:P:222:ILE:HB	1:P:227:VAL:O	2.00	0.60
1:T:154:MET:HE3	1:T:159:MET:HE3	1.82	0.60
1:A:147:ASN:HA	1:A:169:MET:HG2	1.83	0.60
1:K:199:ILE:HD13	1:K:218:PHE:CE1	2.36	0.60
1:P:199:ILE:HD12	1:P:260:GLY:HA3	1.82	0.60
1:A:180:ASN:HD22	1:A:180:ASN:N	1.98	0.60
1:G:24:THR:HG22	1:G:28:MET:HE2	1.82	0.60
1:S:150:ARG:HG2	1:S:150:ARG:NH1	2.09	0.60
1:S:222:ILE:HB	1:S:227:VAL:O	2.00	0.60
1:T:169:MET:CG	1:T:171:ILE:HG12	2.30	0.60
1:L:219:THR:HA	1:L:222:ILE:HG22	1.84	0.60
1:A:176:HIS:HD2	1:A:318:GLU:HB2	1.67	0.60
1:D:174:ALA:CA	1:D:335:LEU:HD12	2.32	0.60
1:K:177:ASP:OD1	1:K:178:PHE:N	2.32	0.60
1:K:264:ILE:O	1:K:292:LYS:NZ	2.25	0.60
2:k:5:DT:C7	2:l:16:DA:N1	2.65	0.60
1:T:36:VAL:O	1:T:40:LEU:HD12	2.01	0.60
1:A:196:ARG:NH1	1:A:284:GLY:O	2.35	0.60
1:P:131:LEU:C	1:P:133:THR:H	2.07	0.60
1:S:156:GLU:HA	1:S:156:GLU:OE1	2.00	0.60
1:A:242:ASP:OD1	1:A:243:LYS:N	2.35	0.59
1:L:196:ARG:NH2	1:L:284:GLY:O	2.34	0.59
1:S:51:LYS:HA	1:S:54:VAL:HG22	1.83	0.59
1:B:201:ILE:HD12	1:B:218:PHE:CG	2.36	0.59
1:D:144:ILE:HG22	1:D:145:GLU:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:334:THR:HB	1:S:335:LEU:HD12	1.83	0.59
1:P:22:LEU:HD22	1:P:36:VAL:HG23	1.83	0.59
1:S:165:GLY:HA2	1:S:177:ASP:HB3	1.85	0.59
1:G:28:MET:HE3	1:G:57:ILE:HD11	1.85	0.59
1:G:177:ASP:OD1	1:G:178:PHE:N	2.31	0.59
1:O:308:VAL:HG23	1:O:342:VAL:O	2.02	0.59
1:S:159:MET:O	1:S:159:MET:HG3	2.03	0.59
1:H:61:ILE:HG13	1:S:60:GLN:HB3	1.84	0.59
1:L:122:ASP:O	1:L:125:VAL:HG12	2.03	0.59
1:L:193:GLN:OE1	1:L:193:GLN:N	2.34	0.59
1:L:230:PHE:HB3	1:L:258:PRO:HB3	1.85	0.59
1:T:21:THR:N	1:T:24:THR:OG1	2.23	0.59
1:D:175:TYR:CZ	1:D:336:GLN:CG	2.85	0.59
1:T:85:SER:OG	1:T:87:ASP:OD1	2.21	0.59
1:B:125:VAL:N	1:B:126:PRO:HD2	2.17	0.59
1:G:126:PRO:O	1:G:130:ILE:HG12	2.03	0.59
1:A:333:GLU:N	1:A:333:GLU:OE1	2.35	0.59
1:K:247:PHE:CE2	1:K:251:LEU:HD11	2.38	0.59
1:O:33:ILE:H	1:O:33:ILE:HD12	1.67	0.59
1:T:51:LYS:C	1:T:54:VAL:CG2	2.77	0.58
1:D:103:GLU:CG	1:D:317:ARG:HE	2.16	0.58
1:D:163:THR:N	1:D:174:ALA:O	2.33	0.58
1:H:190:ARG:HA	1:H:193:GLN:HG2	1.86	0.58
1:K:199:ILE:HD13	1:K:218:PHE:HE1	1.67	0.58
1:K:219:THR:O	1:K:222:ILE:HG13	2.02	0.58
1:L:34:THR:O	1:L:34:THR:HG22	2.02	0.58
1:T:96:GLN:O	1:T:313:LYS:HG2	2.04	0.58
1:O:294:SER:HA	1:O:310:GLU:HB3	1.85	0.58
1:S:129:TYR:OH	1:T:109:GLN:NE2	2.34	0.58
1:D:333:GLU:OE1	1:D:333:GLU:HA	2.03	0.58
1:P:177:ASP:OD1	1:P:178:PHE:N	2.36	0.58
1:P:301:ILE:HG22	1:P:302:GLN:HG2	1.86	0.58
1:S:182:ALA:O	1:S:186:GLU:HG3	2.03	0.58
1:A:93:PHE:O	1:A:312:ILE:HD11	2.02	0.58
1:H:299:ASN:ND2	1:H:346:MET:HB2	2.08	0.58
1:O:147:ASN:HB2	1:O:169:MET:HB3	1.85	0.58
1:S:325:ALA:O	1:S:329:GLY:N	2.35	0.58
1:A:253:GLN:N	1:A:253:GLN:OE1	2.37	0.58
1:B:128:ARG:HG2	1:B:153:PHE:CE2	2.39	0.58
1:C:173:HIS:C	1:C:173:HIS:HD1	2.11	0.58
1:D:218:PHE:CZ	1:D:222:ILE:HD11	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ILE:HG22	1:B:237:ILE:HG13	1.85	0.58
1:O:144:ILE:HD11	1:O:163:THR:HB	1.85	0.58
1:S:165:GLY:O	1:S:175:TYR:HB2	2.04	0.58
1:H:21:THR:HG23	1:H:24:THR:H	1.69	0.57
1:L:183:TYR:CE1	1:L:308:VAL:HG11	2.38	0.57
1:O:203:VAL:CG2	1:O:204:PRO:N	2.67	0.57
1:P:33:ILE:O	1:P:36:VAL:HG22	2.04	0.57
1:P:125:VAL:N	1:P:126:PRO:HD2	2.19	0.57
1:T:215:ARG:HG3	1:T:219:THR:HG23	1.86	0.57
1:P:308:VAL:HG23	1:P:342:VAL:O	2.04	0.57
1:S:152:ARG:HA	1:S:155:THR:HG22	1.85	0.57
1:C:155:THR:HG21	1:C:171:ILE:HG21	1.86	0.57
1:C:242:ASP:OD1	1:C:243:LYS:N	2.37	0.57
1:K:246:ASP:O	1:K:250:ARG:HG2	2.04	0.57
1:O:153:PHE:CE2	1:O:157:ARG:HG3	2.39	0.57
1:B:121:LYS:C	1:B:123:SER:H	2.13	0.57
1:K:118:THR:HG23	1:K:119:HIS:ND1	2.18	0.57
2:s:5:DT:H2'	2:s:6:DG:C2	2.40	0.57
1:L:145:GLU:HG2	1:L:208:PHE:CE1	2.39	0.57
1:P:183:TYR:O	1:P:187:ALA:N	2.38	0.57
1:T:140:ILE:HG23	1:T:162:VAL:HG13	1.86	0.57
1:A:199:ILE:HD12	1:A:260:GLY:HA3	1.85	0.57
1:C:349:LYS:O	1:C:349:LYS:HG2	2.05	0.57
1:D:169:MET:H	1:D:171:ILE:HG12	1.70	0.57
1:K:113:VAL:HG12	1:L:113:VAL:HG12	1.87	0.57
1:O:102:THR:O	1:O:106:ALA:N	2.37	0.57
1:O:133:THR:HA	1:P:19:ARG:NH2	2.20	0.57
1:P:325:ALA:CB	1:P:335:LEU:HD13	2.35	0.57
1:T:204:PRO:O	1:T:211:HIS:HD2	1.88	0.57
1:D:29:THR:HB	1:D:31:LEU:HD13	1.87	0.57
1:S:322:ALA:O	1:S:335:LEU:HD23	2.05	0.57
1:D:34:THR:HB	2:c:6:DG:H22	1.70	0.57
1:T:222:ILE:CG1	1:T:227:VAL:HG22	2.35	0.56
1:P:331:PRO:HG2	1:P:334:THR:HG22	1.87	0.56
1:T:188:VAL:HG21	1:T:222:ILE:HD13	1.87	0.56
1:C:148:ASP:H	1:C:169:MET:HE1	1.69	0.56
1:C:346:MET:SD	1:C:346:MET:N	2.78	0.56
1:D:105:LEU:HD12	1:D:105:LEU:H	1.70	0.56
1:H:121:LYS:C	1:H:123:SER:H	2.09	0.56
1:H:259:ASP:HA	1:H:287:ILE:HG22	1.85	0.56
1:K:236:THR:HG22	1:K:238:GLU:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:222:ILE:O	1:O:226:GLY:N	2.38	0.56
1:P:79:VAL:HG13	1:P:136:ALA:HA	1.87	0.56
1:P:215:ARG:NH2	1:P:229:GLU:OE2	2.38	0.56
1:C:290:VAL:HG22	1:C:306:HIS:HB2	1.87	0.56
1:O:172:GLU:HA	1:O:172:GLU:OE1	2.06	0.56
1:A:176:HIS:ND1	1:A:176:HIS:C	2.62	0.56
1:L:54:VAL:HA	1:L:57:ILE:HG22	1.87	0.56
1:O:71:ARG:HD2	1:O:77:THR:HA	1.86	0.56
1:T:204:PRO:HA	1:T:237:ILE:CD1	2.35	0.56
1:A:196:ARG:NH1	1:A:288:ASP:OD1	2.34	0.56
1:L:145:GLU:HB2	1:L:147:ASN:O	2.04	0.56
1:L:204:PRO:HB3	1:L:237:ILE:HD11	1.86	0.56
1:O:183:TYR:CE1	1:O:308:VAL:HG11	2.40	0.56
1:S:28:MET:HE3	1:S:57:ILE:HD11	1.87	0.56
1:T:167:SER:OG	1:T:169:MET:HE3	2.06	0.56
1:G:141:ILE:HD11	1:G:163:THR:HG22	1.87	0.56
1:H:35:THR:OG1	2:g:5:DT:OP2	2.23	0.56
1:P:21:THR:H	1:P:24:THR:HB	1.71	0.56
1:T:98:VAL:O	1:T:101:ILE:HG13	2.06	0.56
1:A:73:ARG:NH2	2:a:14:DG:O4'	2.38	0.56
1:D:174:ALA:CB	1:D:335:LEU:CD1	2.79	0.56
1:G:122:ASP:O	1:G:125:VAL:HG12	2.06	0.56
1:L:331:PRO:O	1:L:334:THR:HG22	2.05	0.56
2:t:12:DT:H2'	2:t:13:DT:C6	2.41	0.56
1:A:37:SER:O	1:A:41:LYS:HG3	2.05	0.56
1:H:284:GLY:HA2	1:H:288:ASP:OD1	2.06	0.56
1:K:283:ILE:H	1:K:283:ILE:CD1	2.19	0.56
1:S:124:MET:HE1	1:S:153:PHE:CB	2.36	0.56
1:C:148:ASP:H	1:C:169:MET:CE	2.19	0.56
1:L:35:THR:OG1	2:k:5:DT:OP2	2.22	0.56
1:O:192:ALA:O	1:O:193:GLN:C	2.49	0.56
1:P:67:ARG:CZ	1:P:111:HIS:ND1	2.69	0.56
1:B:237:ILE:HD11	1:B:264:ILE:HB	1.87	0.55
1:C:276:PHE:HB3	1:C:281:VAL:CG1	2.36	0.55
1:O:344:SER:OG	1:O:345:SER:N	2.39	0.55
1:P:46:ILE:O	1:P:51:LYS:HE3	2.06	0.55
1:S:108:THR:HG21	1:S:110:TYR:HD2	1.70	0.55
2:l:16:DA:H2'	2:l:17:DG:O4'	2.05	0.55
1:B:147:ASN:HA	1:B:169:MET:CG	2.34	0.55
2:a:17:DG:H2'	2:a:18:DA:C8	2.42	0.55
1:K:246:ASP:OD1	1:K:247:PHE:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:247:PHE:O	1:K:251:LEU:HG	2.06	0.55
1:O:313:LYS:O	1:O:317:ARG:HG2	2.05	0.55
1:T:191:LEU:HA	1:T:194:CYS:HB3	1.89	0.55
1:D:148:ASP:OD1	1:D:149:PRO:HD2	2.06	0.55
1:G:245:ARG:HG3	1:G:245:ARG:HH11	1.71	0.55
1:P:93:PHE:CZ	1:P:295:ALA:HB3	2.36	0.55
1:S:243:LYS:O	1:S:247:PHE:N	2.32	0.55
1:T:274:ALA:O	1:T:277:GLU:HB2	2.06	0.55
1:B:326:ARG:HB2	1:B:335:LEU:CD1	2.36	0.55
2:b:13:DT:H2"	2:b:14:DG:C8	2.42	0.55
1:A:270:ILE:HG22	1:B:300:TRP:HB3	1.87	0.55
1:C:129:TYR:O	1:C:133:THR:HG22	2.05	0.55
1:C:206:SER:HA	1:C:211:HIS:CG	2.41	0.55
1:G:215:ARG:O	1:G:219:THR:HG23	2.07	0.55
1:L:152:ARG:O	1:L:156:GLU:HG2	2.06	0.55
1:L:264:ILE:O	1:L:292:LYS:HD2	2.07	0.55
1:T:298:LEU:C	1:T:300:TRP:N	2.65	0.55
1:C:240:PRO:HB2	1:C:243:LYS:HG2	1.88	0.55
1:G:181:GLU:HB3	1:G:213:HIS:O	2.07	0.55
1:H:50:THR:OG1	2:g:4:DC:OP1	2.21	0.55
1:K:199:ILE:HD12	1:K:199:ILE:O	2.06	0.55
1:L:140:ILE:HG23	1:L:319:LEU:HD23	1.87	0.55
1:L:222:ILE:CD1	1:L:227:VAL:HG13	2.34	0.55
1:B:222:ILE:HG13	1:B:227:VAL:O	2.07	0.55
1:D:200:ALA:HB2	1:D:230:PHE:HB3	1.89	0.55
1:L:211:HIS:C	1:L:211:HIS:CD2	2.84	0.55
1:D:103:GLU:HG2	1:D:317:ARG:CZ	2.37	0.55
1:H:177:ASP:OD1	1:H:178:PHE:N	2.40	0.55
1:P:169:MET:HB2	1:P:171:ILE:CD1	2.37	0.55
1:A:155:THR:HG21	1:A:171:ILE:HG21	1.89	0.54
1:H:206:SER:HA	1:H:211:HIS:CG	2.42	0.54
1:K:197:LYS:O	1:K:227:VAL:CG1	2.50	0.54
1:L:73:ARG:NE	2:l:13:DT:O2	2.33	0.54
1:T:165:GLY:HA2	1:T:177:ASP:HB2	1.88	0.54
1:G:123:SER:OG	1:G:150:ARG:NH1	2.40	0.54
1:S:130:ILE:HG23	1:S:136:ALA:HB3	1.90	0.54
1:T:248:GLY:HA3	1:T:276:PHE:CE1	2.42	0.54
1:T:333:GLU:N	1:T:333:GLU:CD	2.64	0.54
1:D:174:ALA:CA	1:D:335:LEU:HD13	2.37	0.54
1:A:232:LEU:HD21	1:A:235:ILE:HG12	1.88	0.54
1:G:116:PRO:HG3	1:H:102:THR:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:301:ILE:CG1	1:P:301:ILE:CG2	2.86	0.54
1:H:180:ASN:OD1	1:H:210:PHE:HB2	2.08	0.54
1:K:145:GLU:OE2	1:K:207:ARG:HG2	2.08	0.54
1:T:22:LEU:HB2	2:t:12:DT:OP2	2.08	0.54
1:D:127:ILE:HD12	1:D:127:ILE:N	2.22	0.54
1:H:46:ILE:HD11	1:H:51:LYS:HB2	1.89	0.54
1:O:265:SER:OG	1:O:267:SER:OG	2.22	0.54
1:S:56:LEU:HD11	1:S:60:GLN:HE21	1.71	0.54
1:T:188:VAL:HA	1:T:191:LEU:HG	1.90	0.54
1:H:45:ASP:CG	2:g:4:DC:H41	2.16	0.54
1:O:255:ASP:OD1	1:O:256:ASP:N	2.41	0.54
1:T:161:PHE:CE2	1:T:173:HIS:CD2	2.95	0.54
1:P:298:LEU:HD21	1:P:305:ILE:HD12	1.89	0.53
1:T:176:HIS:C	1:T:176:HIS:CD2	2.86	0.53
1:G:144:ILE:H	1:G:144:ILE:CD1	2.00	0.53
1:L:22:LEU:HD23	1:L:36:VAL:HG12	1.90	0.53
1:O:183:TYR:HE1	1:O:308:VAL:HG11	1.72	0.53
1:P:129:TYR:O	1:P:129:TYR:CD1	2.61	0.53
1:A:67:ARG:HG2	1:A:67:ARG:HH11	1.74	0.53
1:B:196:ARG:HD2	1:B:196:ARG:N	2.23	0.53
2:g:13:DT:H2''	2:g:14:DG:C8	2.44	0.53
1:P:173:HIS:CD2	1:P:175:TYR:HD2	2.26	0.53
1:P:308:VAL:HG21	1:P:341:PRO:HB3	1.90	0.53
1:B:145:GLU:HB3	1:B:146:PRO:HD2	1.89	0.53
1:C:177:ASP:OD1	1:C:178:PHE:N	2.42	0.53
1:T:83:VAL:HG23	1:T:141:ILE:HD12	1.85	0.53
1:D:293:GLN:HE22	1:D:298:LEU:H	1.57	0.53
1:O:232:LEU:HD21	1:O:247:PHE:CZ	2.43	0.53
1:T:67:ARG:NH2	1:T:78:ASN:HB3	2.22	0.53
1:B:133:THR:HG22	1:B:133:THR:O	2.08	0.53
1:H:121:LYS:C	1:H:123:SER:N	2.67	0.53
1:C:94:THR:HB	1:D:95:SER:HB3	1.90	0.53
1:C:124:MET:HE1	1:C:153:PHE:HB2	1.91	0.53
1:D:293:GLN:OE1	1:D:296:GLU:HA	2.09	0.53
1:O:139:VAL:HG23	1:O:159:MET:HE2	1.89	0.53
1:K:45:ASP:O	2:l:3:DT:H2'	2.08	0.53
1:K:204:PRO:HA	1:K:237:ILE:HG12	1.91	0.53
1:O:122:ASP:O	1:O:125:VAL:HG23	2.08	0.53
1:B:218:PHE:O	1:B:222:ILE:HG22	2.08	0.53
2:b:1:DT:H6	2:b:1:DT:O5'	1.92	0.53
1:H:145:GLU:HB3	1:H:146:PRO:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:269:THR:HG21	1:P:291:SER:OG	2.09	0.53
1:S:50:THR:HG21	2:t:4:DC:OP2	2.08	0.53
1:T:99:PHE:O	1:T:102:THR:HG22	2.09	0.53
1:G:218:PHE:O	1:G:222:ILE:HG23	2.09	0.53
1:L:219:THR:HA	1:L:222:ILE:CG2	2.39	0.53
1:O:93:PHE:CE2	1:O:295:ALA:HB3	2.43	0.53
1:D:35:THR:HG22	2:c:5:DT:H71	1.91	0.52
1:L:50:THR:O	1:L:54:VAL:HG13	2.10	0.52
1:T:29:THR:HG23	1:T:31:LEU:H	1.74	0.52
1:K:202:ILE:HD11	1:K:263:SER:OG	2.09	0.52
1:L:178:PHE:CE2	1:L:292:LYS:HE2	2.45	0.52
1:S:320:ALA:O	1:S:323:LEU:HB3	2.10	0.52
1:B:249:LYS:O	1:B:253:GLN:HB2	2.10	0.52
1:G:200:ALA:HB2	1:G:230:PHE:HB3	1.92	0.52
1:K:124:MET:HE1	1:K:149:PRO:HB2	1.91	0.52
1:T:222:ILE:CD1	1:T:227:VAL:HG22	2.39	0.52
1:T:273:VAL:O	1:T:277:GLU:HG3	2.09	0.52
1:K:141:ILE:HD11	1:K:163:THR:HG22	1.91	0.52
2:k:5:DT:H3'	2:k:5:DT:O2	2.09	0.52
1:O:192:ALA:C	1:O:194:CYS:N	2.63	0.52
1:T:312:ILE:O	1:T:316:GLY:N	2.34	0.52
1:C:89:GLU:HG2	1:C:267:SER:OG	2.09	0.52
1:G:181:GLU:HA	1:G:184:ALA:HB3	1.91	0.52
1:H:61:ILE:HD11	1:S:60:GLN:OE1	2.09	0.52
1:S:54:VAL:HA	1:S:57:ILE:HG22	1.90	0.52
1:T:73:ARG:NH1	2:t:14:DG:O4'	2.43	0.52
1:B:211:HIS:HD2	1:B:212:ASP:OD1	1.92	0.52
1:O:192:ALA:C	1:O:195:GLY:H	2.18	0.52
1:S:73:ARG:NH1	2:s:14:DG:O4'	2.39	0.52
1:D:127:ILE:N	1:D:127:ILE:CD1	2.73	0.52
1:S:310:GLU:HG2	1:S:312:ILE:HG22	1.91	0.52
1:C:47:GLY:N	2:d:3:DT:H3'	2.25	0.52
1:L:43:ALA:HB1	1:L:44:PRO:HD2	1.91	0.52
1:O:28:MET:HE3	1:O:57:ILE:HD11	1.91	0.52
1:T:215:ARG:HE	1:T:219:THR:HG22	1.74	0.52
1:T:249:LYS:O	1:T:253:GLN:N	2.41	0.52
1:A:198:ARG:NH1	1:A:257:ARG:O	2.42	0.52
1:L:210:PHE:HA	1:L:213:HIS:ND1	2.24	0.52
1:T:57:ILE:HD11	1:T:61:ILE:HG23	1.91	0.52
1:T:205:PRO:HD3	1:T:237:ILE:CG1	2.40	0.52
1:A:45:ASP:OD1	2:b:4:DC:H5	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:188:VAL:HG11	1:L:222:ILE:HA	1.92	0.52
1:P:122:ASP:O	1:P:124:MET:N	2.42	0.52
1:T:176:HIS:HE2	1:T:315:ALA:HB1	1.75	0.52
1:D:204:PRO:HD3	1:D:264:ILE:HG21	1.92	0.51
1:S:100:GLY:HA3	1:S:313:LYS:O	2.10	0.51
1:S:185:TYR:HE1	1:S:220:ARG:H	1.56	0.51
1:C:178:PHE:CD2	1:C:180:ASN:OD1	2.56	0.51
1:O:148:ASP:OD2	1:O:150:ARG:NE	2.32	0.51
1:A:116:PRO:CD	1:B:102:THR:HG21	2.40	0.51
1:H:21:THR:H	1:H:24:THR:HB	1.75	0.51
1:K:243:LYS:O	1:K:246:ASP:OD1	2.29	0.51
1:L:293:GLN:CD	1:L:296:GLU:HA	2.35	0.51
1:D:201:ILE:HD12	1:D:262:VAL:O	2.11	0.51
1:G:300:TRP:C	1:G:301:ILE:HD13	2.35	0.51
1:P:158:LYS:HD2	1:P:158:LYS:C	2.36	0.51
2:t:13:DT:H2''	2:t:14:DG:C8	2.46	0.51
1:K:121:LYS:C	1:K:123:SER:H	2.19	0.51
1:T:29:THR:OG1	1:T:31:LEU:HD13	2.10	0.51
1:T:335:LEU:H	1:T:335:LEU:HD13	1.75	0.51
1:C:28:MET:HE2	1:O:56:LEU:HG	1.93	0.51
1:H:96:GLN:HB3	1:H:313:LYS:HB2	1.92	0.51
1:S:76:LYS:HD2	1:S:137:ASP:OD2	2.10	0.51
1:G:300:TRP:CH2	1:G:346:MET:HE1	2.46	0.51
1:K:148:ASP:H	1:K:169:MET:HE3	1.76	0.51
2:k:5:DT:H2''	2:k:6:DG:H5'	1.93	0.51
1:P:259:ASP:O	1:P:287:ILE:HG13	2.10	0.51
1:A:77:THR:O	1:A:79:VAL:HG23	2.10	0.51
1:C:252:MET:HE2	1:C:281:VAL:HG21	1.93	0.51
1:D:105:LEU:N	1:D:105:LEU:CD1	2.73	0.51
1:G:28:MET:HE1	1:G:61:ILE:HD13	1.91	0.51
1:G:148:ASP:OD1	1:G:150:ARG:HG2	2.11	0.51
1:L:22:LEU:HD12	2:l:12:DT:P	2.50	0.51
1:A:177:ASP:OD1	1:A:178:PHE:N	2.41	0.50
1:G:57:ILE:O	1:G:61:ILE:HG12	2.10	0.50
1:L:56:LEU:O	1:L:60:GLN:HB2	2.11	0.50
1:S:265:SER:O	1:S:269:THR:HG23	2.11	0.50
1:T:99:PHE:HA	1:T:102:THR:HG22	1.93	0.50
1:T:187:ALA:O	1:T:191:LEU:HG	2.12	0.50
1:A:66:ASN:O	1:A:70:VAL:HG23	2.11	0.50
1:B:293:GLN:HE22	1:B:298:LEU:H	1.58	0.50
1:C:95:SER:HB3	1:D:94:THR:HB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:346:MET:O	1:K:348:PRO:HD3	2.11	0.50
1:L:315:ALA:O	1:L:319:LEU:HD13	2.11	0.50
1:T:174:ALA:HA	1:T:335:LEU:CD2	2.41	0.50
1:L:160:PRO:HB3	1:L:326:ARG:HG3	1.92	0.50
1:P:246:ASP:O	1:P:250:ARG:HG3	2.11	0.50
1:A:210:PHE:HA	1:A:213:HIS:ND1	2.26	0.50
1:K:97:MET:HG3	1:K:316:GLY:HA2	1.94	0.50
1:S:269:THR:O	1:S:273:VAL:HG13	2.11	0.50
1:T:205:PRO:HD3	1:T:237:ILE:HG13	1.92	0.50
1:D:35:THR:HG22	2:c:5:DT:C7	2.41	0.50
1:G:173:HIS:ND1	1:G:173:HIS:N	2.60	0.50
1:L:176:HIS:HB3	1:L:319:LEU:HD12	1.94	0.50
1:O:22:LEU:HD13	1:O:37:SER:HB2	1.92	0.50
1:P:297:PHE:O	1:P:301:ILE:HD12	2.12	0.50
1:D:235:ILE:HD13	1:D:244:ILE:HG12	1.94	0.50
1:K:22:LEU:HD13	1:K:37:SER:HB2	1.94	0.50
1:H:77:THR:O	1:H:79:VAL:HG23	2.12	0.50
1:K:122:ASP:O	1:K:125:VAL:HG12	2.11	0.50
1:O:308:VAL:HA	1:O:343:TRP:HA	1.93	0.50
1:S:141:ILE:HD12	1:S:142:SER:H	1.76	0.50
1:T:29:THR:HG23	1:T:31:LEU:N	2.27	0.50
1:C:45:ASP:HB3	2:d:4:DC:H5	1.77	0.49
1:D:35:THR:HG21	2:c:4:DC:H3'	1.93	0.49
2:g:5:DT:H2'	2:g:6:DG:C2	2.47	0.49
1:L:34:THR:CG2	1:L:37:SER:OG	2.59	0.49
1:O:147:ASN:HB3	1:O:169:MET:HB3	1.93	0.49
1:G:20:PRO:HB3	1:G:61:ILE:HD12	1.94	0.49
1:P:289:ILE:HG23	1:P:305:ILE:HG12	1.94	0.49
1:S:173:HIS:HD1	1:S:173:HIS:C	2.19	0.49
1:B:131:LEU:HD11	1:B:159:MET:HB2	1.94	0.49
1:S:310:GLU:CG	1:S:312:ILE:HG22	2.43	0.49
1:T:147:ASN:HA	1:T:169:MET:HE2	1.94	0.49
1:A:182:ALA:O	1:A:186:GLU:HG3	2.13	0.49
1:B:313:LYS:O	1:B:317:ARG:HG3	2.12	0.49
2:h:17:DG:H2'	2:h:18:DA:C8	2.47	0.49
1:P:126:PRO:O	1:P:130:ILE:HG13	2.12	0.49
1:T:248:GLY:HA2	1:T:251:LEU:HD23	1.94	0.49
1:A:21:THR:H	1:A:24:THR:HB	1.77	0.49
1:K:91:MET:HG2	1:L:93:PHE:HE1	1.76	0.49
1:L:235:ILE:HG21	1:L:244:ILE:HG13	1.93	0.49
1:P:124:MET:HG3	1:P:127:ILE:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:126:PRO:O	1:P:129:TYR:HB3	2.11	0.49
1:P:241:LEU:HD23	1:P:244:ILE:HD12	1.93	0.49
1:T:144:ILE:O	1:T:144:ILE:HG13	2.12	0.49
1:T:331:PRO:HG2	1:T:334:THR:OG1	2.13	0.49
1:O:77:THR:O	1:O:79:VAL:HG23	2.11	0.49
1:C:155:THR:HG21	1:C:171:ILE:CG2	2.42	0.49
1:A:270:ILE:HD11	1:A:297:PHE:HE2	1.78	0.49
1:C:198:ARG:H	1:C:259:ASP:HB3	1.78	0.49
1:D:35:THR:CG2	2:c:5:DT:H71	2.42	0.49
1:G:204:PRO:HG3	1:G:210:PHE:CE1	2.48	0.49
1:L:265:SER:OG	1:L:267:SER:OG	2.31	0.49
1:D:182:ALA:O	1:D:186:GLU:HG3	2.11	0.49
1:H:175:TYR:CE2	1:H:336:GLN:HG2	2.48	0.49
1:L:77:THR:O	1:L:79:VAL:HG23	2.13	0.49
1:L:269:THR:HG21	1:L:291:SER:OG	2.12	0.49
1:T:179:ASP:HB3	1:T:182:ALA:HB3	1.95	0.49
1:T:222:ILE:HD11	1:T:227:VAL:H	1.78	0.49
1:T:297:PHE:H	1:T:309:ASN:ND2	2.10	0.49
1:T:335:LEU:H	1:T:335:LEU:CD2	1.98	0.49
1:A:126:PRO:HG2	1:A:127:ILE:HD12	1.95	0.49
1:B:139:VAL:HG11	1:B:154:MET:HE1	1.93	0.49
1:H:70:VAL:O	1:H:74:THR:HG22	2.13	0.49
1:K:252:MET:HG3	1:K:281:VAL:HG21	1.94	0.49
1:T:57:ILE:HD11	1:T:61:ILE:CG2	2.43	0.49
1:B:151:VAL:HB	1:B:169:MET:HE1	1.95	0.48
2:a:13:DT:H2''	2:a:14:DG:C8	2.47	0.48
1:D:103:GLU:OE1	1:D:103:GLU:HA	2.12	0.48
1:H:139:VAL:HG11	1:H:154:MET:HE1	1.95	0.48
1:P:67:ARG:NH1	1:P:111:HIS:ND1	2.60	0.48
2:p:12:DT:H2'	2:p:13:DT:C6	2.48	0.48
1:L:273:VAL:HG21	1:L:305:ILE:HD11	1.95	0.48
1:B:22:LEU:HD13	1:B:37:SER:HB2	1.95	0.48
1:G:210:PHE:HA	1:G:213:HIS:ND1	2.29	0.48
1:K:141:ILE:HG13	1:K:144:ILE:HD11	1.96	0.48
1:K:290:VAL:HG22	1:K:306:HIS:HB2	1.94	0.48
2:p:13:DT:H2''	2:p:14:DG:C8	2.48	0.48
1:S:94:THR:OG1	1:T:95:SER:CB	2.49	0.48
1:S:185:TYR:N	1:S:217:GLY:O	2.46	0.48
1:A:272:LEU:HD11	1:A:289:ILE:HD13	1.96	0.48
1:D:97:MET:O	1:D:101:ILE:HG13	2.14	0.48
1:P:172:GLU:CB	1:P:333:GLU:HG3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:116:PRO:HG3	1:T:102:THR:CG2	2.36	0.48
1:T:58:ALA:O	1:T:62:GLY:N	2.46	0.48
1:A:89:GLU:HG2	1:A:267:SER:OG	2.13	0.48
1:B:133:THR:CG2	1:B:135:SER:HB3	2.44	0.48
1:C:124:MET:HE1	1:C:153:PHE:CB	2.44	0.48
1:K:242:ASP:OD1	1:K:243:LYS:N	2.46	0.48
1:O:186:GLU:C	1:O:189:GLU:HB3	2.38	0.48
1:O:209:ALA:HB1	1:O:213:HIS:HE1	1.79	0.48
1:T:333:GLU:HA	1:T:335:LEU:HD21	1.95	0.48
1:A:176:HIS:CD2	1:A:318:GLU:HB2	2.48	0.48
1:D:210:PHE:HA	1:D:213:HIS:CD2	2.49	0.48
1:A:67:ARG:HG2	1:A:67:ARG:NH1	2.28	0.48
1:B:86:VAL:HG11	1:B:118:THR:HA	1.95	0.48
1:B:259:ASP:C	1:B:287:ILE:HD12	2.38	0.48
1:C:77:THR:O	1:C:79:VAL:HG23	2.14	0.48
1:G:313:LYS:HE2	1:G:317:ARG:HH21	1.79	0.48
1:L:61:ILE:N	1:L:62:GLY:HA2	2.28	0.48
1:A:19:ARG:NH1	1:B:133:THR:O	2.46	0.48
1:L:230:PHE:CB	1:L:258:PRO:HB3	2.43	0.48
1:O:176:HIS:HA	1:O:337:SER:O	2.14	0.48
2:o:18:DA:H2'	2:o:18:DA:N3	2.28	0.48
1:S:330:ALA:CB	1:S:335:LEU:HD11	2.43	0.48
1:S:335:LEU:HD12	1:S:335:LEU:N	2.28	0.48
1:T:99:PHE:HB2	1:T:313:LYS:HZ1	1.79	0.48
1:C:204:PRO:HG2	1:C:211:HIS:HA	1.94	0.48
1:B:201:ILE:HG12	1:B:203:VAL:HG13	1.94	0.48
1:G:162:VAL:HG11	1:G:319:LEU:O	2.14	0.48
2:h:4:DC:H2'	2:h:5:DT:H71	1.96	0.48
1:K:292:LYS:HE2	1:K:310:GLU:OE1	2.13	0.48
1:T:117:HIS:ND1	1:T:118:THR:N	2.62	0.48
1:T:241:LEU:HD23	1:T:241:LEU:C	2.39	0.48
2:d:13:DT:H2''	2:d:14:DG:C8	2.49	0.47
1:H:148:ASP:OD1	1:H:151:VAL:HG23	2.13	0.47
1:L:311:ASP:O	1:L:314:LEU:HG	2.14	0.47
1:S:140:ILE:HG21	1:S:319:LEU:HD13	1.96	0.47
1:T:184:ALA:HB3	1:T:217:GLY:HA3	1.95	0.47
1:A:118:THR:HG22	1:A:118:THR:O	2.13	0.47
1:A:180:ASN:ND2	1:A:180:ASN:N	2.62	0.47
1:B:186:GLU:HB3	1:B:343:TRP:CH2	2.49	0.47
1:B:203:VAL:O	1:B:236:THR:OG1	2.20	0.47
2:a:4:DC:H2''	2:a:5:DT:H5'	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:THR:O	1:D:24:THR:OG1	2.30	0.47
1:D:166:ARG:HH12	1:D:338:VAL:HG21	1.79	0.47
1:L:141:ILE:HD11	1:L:150:ARG:CZ	2.43	0.47
1:L:199:ILE:HD12	1:L:222:ILE:HD13	1.96	0.47
1:G:97:MET:HE3	1:G:319:LEU:HD13	1.94	0.47
1:K:199:ILE:CD1	1:K:199:ILE:C	2.85	0.47
1:L:45:ASP:O	2:k:3:DT:H2'	2.14	0.47
1:L:104:VAL:HG23	1:L:317:ARG:HG3	1.95	0.47
1:S:83:VAL:CG2	1:S:141:ILE:HA	2.44	0.47
1:T:222:ILE:CG1	1:T:227:VAL:H	2.27	0.47
2:a:2:DA:N3	2:a:2:DA:H2'	2.27	0.47
1:G:22:LEU:CD2	1:G:37:SER:HB2	2.44	0.47
1:H:99:PHE:O	1:H:103:GLU:HB2	2.14	0.47
1:O:270:ILE:HD11	1:P:301:ILE:HG13	1.95	0.47
1:P:325:ALA:CB	1:P:335:LEU:CD1	2.91	0.47
1:S:266:GLY:O	1:S:269:THR:OG1	2.31	0.47
1:T:207:ARG:HG2	1:T:207:ARG:HH11	1.79	0.47
1:T:269:THR:O	1:T:273:VAL:CG2	2.56	0.47
1:T:297:PHE:H	1:T:309:ASN:HD21	1.63	0.47
1:C:276:PHE:O	1:C:281:VAL:HG12	2.14	0.47
1:D:77:THR:O	1:D:79:VAL:HG23	2.14	0.47
1:D:235:ILE:HD11	1:D:247:PHE:HB3	1.95	0.47
1:K:199:ILE:HD11	1:K:218:PHE:CE1	2.46	0.47
1:L:297:PHE:O	1:L:300:TRP:HD1	1.96	0.47
1:C:76:LYS:NZ	1:C:110:TYR:OH	2.48	0.47
1:D:208:PHE:O	1:D:211:HIS:HB3	2.15	0.47
1:K:199:ILE:O	1:K:230:PHE:HB3	2.14	0.47
1:L:296:GLU:OE2	1:L:309:ASN:ND2	2.47	0.47
1:O:232:LEU:HD11	1:O:234:ALA:HB3	1.96	0.47
1:S:141:ILE:CG2	1:S:163:THR:HG22	2.44	0.47
1:T:179:ASP:OD1	1:T:181:GLU:HB2	2.13	0.47
1:B:198:ARG:O	1:B:260:GLY:N	2.42	0.47
1:D:221:GLY:O	1:D:225:PHE:HD1	1.97	0.47
1:D:237:ILE:HG13	1:D:238:GLU:N	2.29	0.47
1:G:22:LEU:HD11	1:G:63:TYR:OH	2.15	0.47
1:H:147:ASN:HA	1:H:169:MET:HG2	1.97	0.47
1:K:236:THR:O	1:K:239:THR:OG1	2.30	0.47
1:L:38:ARG:HG3	1:L:38:ARG:NH2	2.30	0.47
1:O:204:PRO:CB	1:O:205:PRO:HD2	2.45	0.47
1:O:293:GLN:NE2	1:O:295:ALA:O	2.47	0.47
1:P:176:HIS:HA	1:P:337:SER:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:206:SER:HA	1:S:211:HIS:CB	2.44	0.47
1:B:38:ARG:O	1:B:41:LYS:O	2.33	0.47
1:B:91:MET:HE3	1:B:297:PHE:HE2	1.79	0.47
1:H:83:VAL:CG2	1:H:141:ILE:HG22	2.45	0.47
1:H:236:THR:O	1:H:239:THR:HG22	2.15	0.47
1:L:21:THR:O	1:L:24:THR:OG1	2.25	0.47
1:L:204:PRO:HG2	1:L:211:HIS:HA	1.97	0.47
1:O:184:ALA:O	1:O:188:VAL:HG23	2.14	0.47
1:P:206:SER:HA	1:P:211:HIS:CG	2.50	0.47
1:T:57:ILE:O	1:T:61:ILE:HG12	2.14	0.47
1:A:127:ILE:HG12	1:A:154:MET:HE2	1.97	0.47
1:A:176:HIS:HA	1:A:337:SER:O	2.14	0.47
1:D:204:PRO:HG2	1:D:211:HIS:HA	1.96	0.47
1:D:293:GLN:HE22	1:D:298:LEU:HB2	1.80	0.47
1:G:176:HIS:HA	1:G:337:SER:O	2.14	0.47
1:K:320:ALA:O	1:K:324:LEU:HD13	2.14	0.47
1:O:131:LEU:HD11	1:O:159:MET:HB2	1.96	0.47
1:O:203:VAL:CG2	1:O:204:PRO:CD	2.92	0.47
1:O:267:SER:O	1:O:270:ILE:HG22	2.14	0.47
1:T:118:THR:OG1	1:T:121:LYS:O	2.27	0.47
1:B:104:VAL:HG21	1:B:317:ARG:O	2.14	0.47
1:G:131:LEU:HD21	1:G:159:MET:HB2	1.97	0.47
1:L:179:ASP:OD1	1:L:181:GLU:HB3	2.14	0.47
1:S:84:LEU:O	1:S:116:PRO:HA	2.15	0.47
1:T:248:GLY:HA3	1:T:276:PHE:HE1	1.79	0.47
1:C:35:THR:HG23	1:C:46:ILE:HD12	1.97	0.46
1:D:293:GLN:NE2	1:D:298:LEU:HB2	2.30	0.46
1:G:204:PRO:HG2	1:G:211:HIS:HB2	1.97	0.46
1:P:54:VAL:HA	1:P:57:ILE:HG22	1.97	0.46
1:S:82:LEU:HD11	1:S:140:ILE:HD12	1.95	0.46
1:A:232:LEU:HD12	1:A:234:ALA:H	1.81	0.46
2:c:14:DG:H2''	2:c:15:DC:C5'	2.45	0.46
1:H:296:GLU:CG	1:H:309:ASN:HD21	2.28	0.46
1:P:299:ASN:CB	1:P:303:PRO:HA	2.46	0.46
1:S:325:ALA:HA	1:S:328:ASN:HB2	1.97	0.46
1:B:78:ASN:N	1:B:137:ASP:OD2	2.48	0.46
1:D:166:ARG:HH12	1:D:338:VAL:CG2	2.28	0.46
2:c:13:DT:H2''	2:c:14:DG:C8	2.50	0.46
1:P:131:LEU:HD12	1:P:157:ARG:HD3	1.97	0.46
1:P:196:ARG:HD2	1:P:288:ASP:H	1.80	0.46
1:P:204:PRO:HG3	1:P:210:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:VAL:HG22	1:A:126:PRO:HD3	1.97	0.46
1:C:221:GLY:O	1:C:225:PHE:HD2	1.99	0.46
2:k:16:DA:H2''	2:k:17:DG:H5'	1.97	0.46
1:O:88:GLU:OE1	1:O:89:GLU:N	2.49	0.46
1:P:252:MET:HG3	1:P:281:VAL:HG21	1.98	0.46
1:T:241:LEU:HA	1:T:244:ILE:CD1	2.45	0.46
1:B:86:VAL:CG1	1:B:118:THR:HA	2.46	0.46
1:C:249:LYS:HA	1:C:279:ALA:HB2	1.96	0.46
1:D:205:PRO:HG3	1:D:238:GLU:CD	2.40	0.46
1:K:20:PRO:HB3	1:K:61:ILE:HD12	1.97	0.46
1:L:71:ARG:HH11	1:L:77:THR:HB	1.80	0.46
1:P:35:THR:HG23	2:o:5:DT:H73	1.96	0.46
1:T:34:THR:HG21	2:s:6:DG:H1	1.81	0.46
1:T:176:HIS:HE2	1:T:315:ALA:CB	2.28	0.46
1:T:241:LEU:HD13	1:T:271:ALA:HB2	1.96	0.46
1:P:247:PHE:CZ	1:P:251:LEU:HD21	2.51	0.46
1:T:314:LEU:O	1:T:318:GLU:HB2	2.15	0.46
1:A:326:ARG:NH2	1:A:332:PRO:HG3	2.30	0.46
1:D:54:VAL:HA	1:D:57:ILE:HG22	1.98	0.46
1:D:204:PRO:O	1:D:211:HIS:HD2	1.98	0.46
1:H:83:VAL:HG22	1:H:141:ILE:HG22	1.98	0.46
1:H:119:HIS:CE1	1:H:122:ASP:H	2.34	0.46
1:A:222:ILE:HG13	1:A:229:GLU:HB2	1.98	0.46
1:B:174:ALA:HB2	1:B:335:LEU:HD12	1.98	0.46
1:D:246:ASP:O	1:D:250:ARG:HG2	2.15	0.46
1:L:38:ARG:HG3	1:L:38:ARG:HH21	1.80	0.46
1:P:131:LEU:HD22	1:P:131:LEU:C	2.38	0.46
1:P:331:PRO:HA	1:P:332:PRO:HD3	1.82	0.46
2:c:5:DT:H2'	2:c:6:DG:C2	2.50	0.46
1:K:146:PRO:O	1:K:169:MET:HG2	2.16	0.46
1:S:25:ILE:HA	1:S:28:MET:HE2	1.97	0.46
1:T:242:ASP:OD1	1:T:242:ASP:N	2.49	0.46
2:t:2:DA:C2'	2:t:3:DT:H5''	2.46	0.46
1:A:198:ARG:C	1:A:199:ILE:HD13	2.41	0.46
1:C:89:GLU:HG2	1:C:267:SER:HG	1.80	0.46
1:K:301:ILE:CD1	1:L:301:ILE:HG23	2.46	0.46
1:O:97:MET:HE3	1:O:319:LEU:CD1	2.46	0.46
1:O:284:GLY:N	1:O:287:ILE:O	2.49	0.46
2:p:15:DC:H2''	2:p:16:DA:O4'	2.16	0.46
1:A:301:ILE:HG21	1:B:301:ILE:HG23	1.99	0.45
1:C:53:ARG:HD3	1:O:27:TYR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:105:LEU:O	1:K:108:THR:N	2.47	0.45
1:K:145:GLU:HB2	1:K:146:PRO:HD2	1.98	0.45
1:O:204:PRO:HG2	1:O:210:PHE:CZ	2.50	0.45
1:S:144:ILE:HD13	1:S:164:HIS:O	2.17	0.45
1:T:197:LYS:O	1:T:227:VAL:HG21	2.16	0.45
1:T:300:TRP:H	1:T:300:TRP:CD1	2.34	0.45
1:G:277:GLU:C	1:G:280:GLY:H	2.23	0.45
1:L:292:LYS:HD3	1:L:310:GLU:OE1	2.16	0.45
1:O:205:PRO:O	1:O:211:HIS:CB	2.63	0.45
1:P:78:ASN:HA	1:P:110:TYR:CD1	2.51	0.45
1:T:101:ILE:HG22	1:T:316:GLY:O	2.15	0.45
1:D:175:TYR:CE2	1:D:336:GLN:HG3	2.51	0.45
1:O:219:THR:HG22	1:O:222:ILE:HG13	1.98	0.45
1:O:333:GLU:CD	1:O:333:GLU:H	2.24	0.45
1:D:39:ALA:HB1	1:D:54:VAL:HG21	1.98	0.45
1:A:64:GLN:HA	1:A:65:PRO:HD3	1.79	0.45
1:A:83:VAL:CG2	1:A:141:ILE:HG22	2.45	0.45
2:a:12:DT:H2'	2:a:13:DT:C6	2.52	0.45
1:C:22:LEU:HD13	1:C:37:SER:HB2	1.98	0.45
1:K:77:THR:O	1:K:79:VAL:HG23	2.17	0.45
1:K:199:ILE:HD11	1:K:218:PHE:HZ	1.68	0.45
1:L:255:ASP:OD1	1:L:255:ASP:N	2.47	0.45
1:S:241:LEU:HA	1:S:244:ILE:HG13	1.99	0.45
2:s:4:DC:H2''	2:s:5:DT:H5'	1.98	0.45
1:G:138:GLY:HA3	1:G:323:LEU:HD21	1.97	0.45
1:O:73:ARG:NH2	2:o:14:DG:O4'	2.49	0.45
1:S:239:THR:HG22	1:S:240:PRO:O	2.15	0.45
1:A:152:ARG:HB2	1:A:152:ARG:CZ	2.47	0.45
1:A:188:VAL:CG1	1:A:199:ILE:HG21	2.46	0.45
2:d:4:DC:H2'	2:d:5:DT:C6	2.52	0.45
1:K:91:MET:HE2	1:L:297:PHE:HB2	1.99	0.45
1:L:202:ILE:HD11	1:L:272:LEU:HD22	1.97	0.45
1:P:67:ARG:CZ	1:P:111:HIS:CE1	3.00	0.45
1:A:239:THR:OG1	1:A:244:ILE:HD11	2.16	0.45
1:G:181:GLU:HB2	1:G:217:GLY:HA3	1.99	0.45
1:H:43:ALA:O	1:H:51:LYS:NZ	2.49	0.45
1:K:255:ASP:OD1	1:K:256:ASP:N	2.49	0.45
1:L:160:PRO:HB2	1:L:327:ILE:HG23	1.99	0.45
1:O:148:ASP:OD1	1:O:149:PRO:HD2	2.17	0.45
1:P:73:ARG:NH1	2:p:14:DG:O4'	2.50	0.45
1:S:96:GLN:O	1:S:313:LYS:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:188:VAL:HA	1:T:191:LEU:CG	2.47	0.45
1:A:188:VAL:HG12	1:A:199:ILE:HG21	1.98	0.45
1:B:251:LEU:HD21	1:B:258:PRO:CD	2.46	0.45
1:B:259:ASP:O	1:B:287:ILE:HD12	2.16	0.45
1:G:22:LEU:HD13	2:g:12:DT:P	2.56	0.45
1:S:203:VAL:O	1:S:236:THR:HA	2.16	0.45
1:A:222:ILE:HG23	1:A:227:VAL:O	2.16	0.45
1:C:215:ARG:HA	1:C:218:PHE:HB3	1.98	0.45
1:D:89:GLU:HG2	1:D:267:SER:OG	2.17	0.45
1:D:323:LEU:O	1:D:327:ILE:HG13	2.16	0.45
1:G:35:THR:HG23	1:G:46:ILE:HD12	1.97	0.45
1:K:85:SER:OG	1:K:143:LYS:HE3	2.17	0.45
1:L:206:SER:HB2	1:L:211:HIS:CE1	2.52	0.45
1:L:209:ALA:O	1:L:213:HIS:ND1	2.44	0.45
1:O:97:MET:HE3	1:O:319:LEU:HD13	1.99	0.45
1:P:196:ARG:HD3	1:P:287:ILE:HA	1.98	0.45
1:S:127:ILE:HD13	1:S:154:MET:HE3	1.98	0.45
1:S:152:ARG:HA	1:S:155:THR:CG2	2.47	0.45
1:D:35:THR:CG2	2:c:5:DT:C7	2.95	0.44
1:K:183:TYR:O	1:K:187:ALA:N	2.50	0.44
1:A:232:LEU:HD12	1:A:233:ASP:N	2.32	0.44
1:D:140:ILE:HG12	1:D:162:VAL:CG1	2.47	0.44
1:G:34:THR:HG21	2:h:6:DG:O6	2.17	0.44
1:H:218:PHE:HE2	1:H:229:GLU:CG	2.31	0.44
1:O:237:ILE:HD12	1:O:238:GLU:N	2.32	0.44
1:T:57:ILE:CD1	1:T:61:ILE:HG23	2.46	0.44
1:T:79:VAL:HG13	1:T:136:ALA:HA	1.99	0.44
1:A:196:ARG:HD2	1:A:259:ASP:O	2.17	0.44
1:D:233:ASP:OD1	1:D:233:ASP:N	2.47	0.44
1:D:281:VAL:HG13	1:D:286:ASP:HB2	1.99	0.44
2:d:15:DC:H2''	2:d:16:DA:O5'	2.18	0.44
1:K:32:GLY:O	1:K:35:THR:OG1	2.25	0.44
1:K:273:VAL:O	1:K:277:GLU:N	2.51	0.44
1:O:153:PHE:O	1:O:157:ARG:N	2.46	0.44
1:O:301:ILE:HG13	1:P:302:GLN:HE22	1.69	0.44
1:P:178:PHE:HB2	1:P:310:GLU:OE2	2.18	0.44
1:T:124:MET:O	1:T:127:ILE:HG22	2.17	0.44
1:T:299:ASN:O	1:T:302:GLN:C	2.60	0.44
1:A:202:ILE:HD11	1:A:272:LEU:HD22	2.00	0.44
1:B:297:PHE:CE1	1:B:298:LEU:HG	2.53	0.44
1:B:308:VAL:HG23	1:B:342:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:GLU:OE2	1:G:94:THR:HG21	2.17	0.44
1:O:144:ILE:O	1:O:208:PHE:HA	2.18	0.44
2:p:17:DG:H2''	2:p:18:DA:H5'	1.99	0.44
1:T:56:LEU:C	1:T:56:LEU:CD1	2.85	0.44
1:T:176:HIS:NE2	1:T:315:ALA:HB1	2.32	0.44
1:A:306:HIS:HB3	1:A:343:TRP:CZ3	2.51	0.44
1:C:211:HIS:HD2	1:C:212:ASP:OD1	2.00	0.44
1:C:293:GLN:OE1	1:C:298:LEU:N	2.45	0.44
1:L:178:PHE:CD2	1:L:180:ASN:OD1	2.67	0.44
1:C:105:LEU:HD22	1:C:110:TYR:HB2	1.99	0.44
1:G:203:VAL:HG22	1:G:211:HIS:ND1	2.33	0.44
1:L:201:ILE:HD12	1:L:262:VAL:O	2.18	0.44
1:L:218:PHE:CZ	1:L:229:GLU:HG3	2.52	0.44
1:P:198:ARG:C	1:P:199:ILE:HD13	2.42	0.44
1:T:47:GLY:N	2:s:3:DT:H3'	2.33	0.44
1:T:129:TYR:O	1:T:133:THR:HG22	2.18	0.44
1:T:141:ILE:HD12	1:T:142:SER:H	1.82	0.44
1:T:327:ILE:HD13	1:T:327:ILE:HA	1.83	0.44
1:H:23:LYS:HA	1:H:33:ILE:HG12	1.98	0.44
1:H:169:MET:HE2	1:H:171:ILE:HD12	1.99	0.44
1:L:293:GLN:OE1	1:L:298:LEU:N	2.33	0.44
2:l:7:DC:H2''	2:l:8:DA:O5'	2.18	0.44
1:P:241:LEU:HD22	1:P:268:SER:HA	1.99	0.44
1:S:73:ARG:HB2	2:s:11:DG:N2	2.33	0.44
1:S:204:PRO:CG	1:S:211:HIS:HA	2.46	0.44
1:S:220:ARG:HA	1:S:223:ARG:CB	2.48	0.44
1:A:91:MET:HE1	1:B:297:PHE:CD2	2.53	0.44
1:G:189:GLU:O	1:G:193:GLN:HB2	2.17	0.44
1:A:46:ILE:HD12	1:A:46:ILE:HG23	1.74	0.43
1:B:57:ILE:O	1:B:61:ILE:HG12	2.17	0.43
1:K:83:VAL:HA	1:K:115:THR:O	2.18	0.43
1:K:126:PRO:O	1:K:129:TYR:HB3	2.18	0.43
1:L:164:HIS:HB2	1:L:319:LEU:HD21	2.00	0.43
1:O:239:THR:HB	1:O:244:ILE:HD11	1.99	0.43
1:P:200:ALA:HB2	1:P:230:PHE:HB3	2.00	0.43
1:C:210:PHE:HA	1:C:213:HIS:ND1	2.33	0.43
1:C:223:ARG:HG3	1:C:224:ASP:N	2.33	0.43
1:G:45:ASP:HB3	2:h:4:DC:H5	1.83	0.43
1:G:77:THR:O	1:G:79:VAL:HG23	2.18	0.43
1:G:295:ALA:O	1:G:297:PHE:HD1	2.00	0.43
1:K:126:PRO:HG2	1:K:127:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:191:LEU:HD23	1:K:260:GLY:HA3	2.00	0.43
1:L:51:LYS:O	1:L:54:VAL:HG22	2.18	0.43
1:L:71:ARG:NH1	1:L:77:THR:HB	2.32	0.43
1:L:325:ALA:HB3	1:L:335:LEU:HD21	2.00	0.43
1:O:173:HIS:HA	1:O:332:PRO:HB3	2.01	0.43
1:P:85:SER:O	1:P:88:GLU:OE2	2.36	0.43
2:o:18:DA:N7	2:p:3:DT:C7	2.80	0.43
1:A:124:MET:HG2	1:A:128:ARG:HE	1.83	0.43
1:A:176:HIS:HD2	1:A:318:GLU:CB	2.29	0.43
1:D:210:PHE:HD1	1:D:210:PHE:H	1.66	0.43
1:H:117:HIS:HB3	1:H:126:PRO:HG3	2.00	0.43
1:S:140:ILE:HD13	1:S:319:LEU:CD1	2.48	0.43
1:T:137:ASP:O	1:T:160:PRO:HG2	2.18	0.43
1:T:197:LYS:O	1:T:227:VAL:CG2	2.67	0.43
1:T:215:ARG:O	1:T:219:THR:HG23	2.18	0.43
1:B:107:THR:HG23	1:B:108:THR:HG23	2.00	0.43
1:C:251:LEU:HD21	1:C:258:PRO:HG3	2.01	0.43
1:K:219:THR:HA	1:K:222:ILE:HG12	2.00	0.43
1:L:302:GLN:HB3	1:L:305:ILE:HG13	2.00	0.43
1:O:169:MET:HG3	1:O:171:ILE:HG13	2.00	0.43
1:O:210:PHE:HA	1:O:213:HIS:ND1	2.33	0.43
1:P:125:VAL:CG1	1:P:126:PRO:CD	2.85	0.43
1:T:204:PRO:O	1:T:211:HIS:CD2	2.69	0.43
1:B:240:PRO:O	1:B:244:ILE:HG22	2.19	0.43
1:C:178:PHE:CZ	1:C:341:PRO:HB3	2.54	0.43
1:G:124:MET:HE3	1:G:124:MET:HB3	1.90	0.43
1:O:155:THR:HG23	1:O:161:PHE:CE1	2.53	0.43
2:o:4:DC:H2''	2:o:5:DT:H5'	2.01	0.43
1:S:173:HIS:C	1:S:173:HIS:ND1	2.76	0.43
1:T:99:PHE:C	1:T:102:THR:HG22	2.43	0.43
1:A:172:GLU:OE1	1:A:336:GLN:NE2	2.50	0.43
1:B:128:ARG:HG2	1:B:153:PHE:HE2	1.82	0.43
1:G:22:LEU:HD23	1:G:37:SER:HB2	2.00	0.43
1:H:215:ARG:O	1:H:219:THR:HG23	2.18	0.43
1:L:331:PRO:HA	1:L:332:PRO:HD3	1.93	0.43
1:P:29:THR:N	1:P:30:GLY:HA2	2.33	0.43
1:P:36:VAL:O	1:P:40:LEU:HD13	2.19	0.43
1:P:127:ILE:HD12	1:P:127:ILE:C	2.42	0.43
1:T:172:GLU:CB	1:T:333:GLU:CD	2.91	0.43
2:t:10:DC:H5	2:t:11:DG:N7	2.16	0.43
1:A:54:VAL:HA	1:A:57:ILE:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:PRO:O	1:A:129:TYR:HB3	2.18	0.43
1:G:97:MET:HE3	1:G:319:LEU:CD1	2.49	0.43
1:H:57:ILE:O	1:H:61:ILE:HG22	2.18	0.43
1:H:120:ALA:O	1:H:123:SER:HB3	2.18	0.43
2:k:7:DC:N4	2:l:14:DG:C6	2.87	0.43
1:O:160:PRO:HG2	1:O:327:ILE:HG22	2.00	0.43
1:O:244:ILE:CG2	1:O:272:LEU:HG	2.49	0.43
1:T:24:THR:O	1:T:28:MET:HG3	2.18	0.43
1:T:298:LEU:O	1:T:300:TRP:N	2.52	0.43
1:A:124:MET:HE2	1:A:124:MET:HB2	1.69	0.43
1:A:198:ARG:O	1:A:260:GLY:N	2.51	0.43
1:A:306:HIS:C	1:A:343:TRP:HZ3	2.26	0.43
1:B:125:VAL:N	1:B:126:PRO:CD	2.82	0.43
1:D:204:PRO:HG3	1:D:210:PHE:CE2	2.52	0.43
1:G:146:PRO:HD3	1:G:207:ARG:O	2.19	0.43
1:K:204:PRO:HG2	1:K:211:HIS:HA	1.99	0.43
1:P:323:LEU:HD12	1:P:323:LEU:C	2.31	0.43
1:B:232:LEU:HD11	1:B:251:LEU:CD1	2.49	0.43
1:G:144:ILE:HD11	1:G:164:HIS:O	2.18	0.43
1:L:148:ASP:HA	1:L:149:PRO:HD2	1.82	0.43
2:l:2:DA:C1'	2:l:3:DT:H5'	2.46	0.43
2:l:15:DC:H2''	2:l:16:DA:O5'	2.18	0.43
1:S:237:ILE:HD12	1:S:237:ILE:H	1.84	0.43
1:A:102:THR:CB	1:B:116:PRO:HG3	2.49	0.43
1:A:269:THR:O	1:A:272:LEU:HG	2.18	0.43
1:B:121:LYS:C	1:B:123:SER:N	2.76	0.43
1:C:173:HIS:C	1:C:173:HIS:ND1	2.74	0.43
1:D:235:ILE:HD11	1:D:247:PHE:CB	2.49	0.43
1:D:283:ILE:HG22	1:D:304:GLN:HB2	2.00	0.43
2:d:1:DT:H2''	2:d:2:DA:O4'	2.18	0.43
1:O:147:ASN:OD1	1:O:147:ASN:O	2.37	0.43
1:P:159:MET:SD	1:P:160:PRO:HD2	2.59	0.43
1:S:237:ILE:HG13	1:S:268:SER:OG	2.18	0.43
1:A:335:LEU:HD23	1:A:335:LEU:HA	1.78	0.42
2:a:18:DA:N6	2:b:2:DA:N6	2.67	0.42
1:K:57:ILE:O	1:K:61:ILE:HG12	2.19	0.42
1:L:56:LEU:O	1:L:60:GLN:N	2.47	0.42
1:L:88:GLU:OE2	1:L:94:THR:HG21	2.19	0.42
1:O:101:ILE:O	1:O:105:LEU:HD13	2.18	0.42
1:O:190:ARG:O	1:O:194:CYS:CB	2.56	0.42
1:A:91:MET:HE1	1:B:297:PHE:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:MET:CE	1:B:171:ILE:HD12	2.49	0.42
2:d:17:DG:H2'	2:d:18:DA:C8	2.53	0.42
1:H:19:ARG:HA	1:H:20:PRO:HD3	1.95	0.42
1:K:219:THR:HA	1:K:222:ILE:CG1	2.50	0.42
1:K:301:ILE:HD12	1:L:301:ILE:HG23	2.01	0.42
1:L:176:HIS:HB3	1:L:319:LEU:CD1	2.48	0.42
1:O:301:ILE:HD12	1:O:301:ILE:HA	1.61	0.42
1:T:241:LEU:HA	1:T:244:ILE:CG1	2.46	0.42
1:B:196:ARG:HG3	1:B:259:ASP:O	2.18	0.42
1:H:152:ARG:HB2	1:H:169:MET:HE1	2.01	0.42
2:l:2:DA:C2'	2:l:3:DT:H5'	2.50	0.42
1:O:299:ASN:CB	1:O:307:THR:HG21	2.48	0.42
1:O:324:LEU:O	1:O:327:ILE:HG13	2.19	0.42
1:P:325:ALA:HB1	1:P:335:LEU:HD11	2.00	0.42
2:o:13:DT:H2''	2:o:14:DG:C8	2.53	0.42
1:S:310:GLU:HG2	1:S:312:ILE:CG2	2.48	0.42
1:B:72:LEU:O	2:a:10:DC:H1'	2.19	0.42
1:D:98:VAL:O	1:D:102:THR:HG23	2.19	0.42
1:D:233:ASP:OD2	1:P:216:LYS:HE3	2.19	0.42
1:G:180:ASN:OD1	1:G:210:PHE:HB2	2.19	0.42
1:G:204:PRO:HB3	1:G:237:ILE:HD12	2.02	0.42
1:G:293:GLN:HG3	1:G:295:ALA:O	2.19	0.42
1:K:202:ILE:HG22	1:K:235:ILE:HD11	2.01	0.42
1:O:292:LYS:HA	1:O:308:VAL:HG13	2.01	0.42
2:o:2:DA:N6	2:p:18:DA:C2	2.88	0.42
1:A:102:THR:HB	1:B:116:PRO:HG3	2.00	0.42
1:G:120:ALA:O	1:G:123:SER:HB2	2.19	0.42
1:G:199:ILE:O	1:G:230:PHE:N	2.52	0.42
1:O:80:ILE:HD12	1:O:105:LEU:HD21	2.00	0.42
1:P:80:ILE:HD12	1:P:323:LEU:HD23	2.00	0.42
1:P:196:ARG:CD	1:P:288:ASP:H	2.33	0.42
1:T:47:GLY:H	2:s:3:DT:H3'	1.83	0.42
1:T:215:ARG:HE	1:T:219:THR:CG2	2.32	0.42
1:T:244:ILE:O	1:T:247:PHE:HB3	2.19	0.42
1:D:125:VAL:N	1:D:126:PRO:CD	2.82	0.42
1:G:188:VAL:HG21	1:G:221:GLY:C	2.44	0.42
1:G:300:TRP:CZ2	1:G:346:MET:HE1	2.54	0.42
1:L:54:VAL:HA	1:L:57:ILE:CG2	2.50	0.42
1:L:313:LYS:HB3	1:L:313:LYS:HE2	1.72	0.42
1:B:241:LEU:CA	1:B:244:ILE:HG22	2.49	0.42
1:L:323:LEU:O	1:L:327:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:166:ARG:NH1	1:O:213:HIS:HD2	2.17	0.42
1:O:204:PRO:HB3	1:O:237:ILE:HD11	2.01	0.42
1:S:57:ILE:O	1:S:61:ILE:HG12	2.20	0.42
1:S:330:ALA:HB3	1:S:335:LEU:HD11	2.00	0.42
1:S:331:PRO:HA	1:S:332:PRO:HD3	1.92	0.42
1:A:236:THR:CG2	1:A:239:THR:HG23	2.46	0.42
1:L:265:SER:O	1:L:269:THR:HG23	2.19	0.42
1:L:317:ARG:HH21	1:L:317:ARG:HD2	1.69	0.42
1:B:332:PRO:O	1:B:335:LEU:HB2	2.19	0.42
1:C:259:ASP:O	1:C:287:ILE:HG13	2.20	0.42
2:c:16:DA:C6	2:c:17:DG:C6	3.08	0.42
1:G:141:ILE:HD12	1:G:150:ARG:HD2	2.01	0.42
1:H:34:THR:HB	2:g:6:DG:H22	1.85	0.42
1:L:22:LEU:HD12	2:l:12:DT:OP2	2.20	0.42
1:P:131:LEU:C	1:P:133:THR:N	2.76	0.42
1:S:322:ALA:O	1:S:325:ALA:HB3	2.19	0.42
1:T:87:ASP:OD1	1:T:87:ASP:O	2.38	0.42
1:T:99:PHE:CA	1:T:102:THR:HG22	2.49	0.42
1:D:261:ILE:HG13	1:D:287:ILE:HD11	2.02	0.42
1:H:155:THR:HG21	1:H:171:ILE:HG21	2.02	0.42
1:H:293:GLN:HB3	1:H:298:LEU:HD12	2.01	0.42
2:k:16:DA:H2'	2:k:17:DG:C8	2.55	0.42
1:O:28:MET:HE1	1:O:61:ILE:HD13	2.01	0.42
1:O:151:VAL:HB	1:O:169:MET:HE1	2.02	0.42
1:P:293:GLN:HE21	1:P:298:LEU:HB2	1.84	0.42
1:P:302:GLN:HA	1:P:303:PRO:HD2	1.78	0.42
1:S:122:ASP:CB	1:S:125:VAL:CG2	2.98	0.42
1:S:174:ALA:HB2	1:S:335:LEU:HB2	2.01	0.42
2:s:13:DT:H2''	2:s:14:DG:C8	2.55	0.42
1:P:131:LEU:HD23	1:P:159:MET:HE2	2.02	0.41
1:T:117:HIS:CD2	1:T:125:VAL:HG13	2.55	0.41
2:a:14:DG:H2''	2:a:15:DC:H5'	2.02	0.41
1:C:83:VAL:HA	1:C:115:THR:O	2.20	0.41
1:C:276:PHE:HB3	1:C:281:VAL:HG11	2.02	0.41
1:D:125:VAL:CG2	1:D:126:PRO:HD3	2.50	0.41
1:G:284:GLY:O	1:G:288:ASP:OD1	2.38	0.41
2:g:12:DT:H2'	2:g:13:DT:C6	2.56	0.41
1:L:206:SER:N	1:L:211:HIS:ND1	2.68	0.41
1:P:326:ARG:HA	1:P:330:ALA:HB3	2.02	0.41
1:S:72:LEU:HD23	2:t:10:DC:C2	2.55	0.41
1:D:103:GLU:CG	1:D:317:ARG:HH11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:ASP:O	1:D:287:ILE:HG13	2.20	0.41
1:D:302:GLN:HB3	1:D:305:ILE:HG13	2.02	0.41
1:G:165:GLY:HA2	1:G:177:ASP:CG	2.45	0.41
1:H:164:HIS:HB2	1:H:319:LEU:HD21	2.02	0.41
2:g:7:DC:H2''	2:g:8:DA:O5'	2.20	0.41
1:O:158:LYS:HD2	1:O:158:LYS:N	2.35	0.41
1:P:125:VAL:N	1:P:126:PRO:CD	2.83	0.41
1:S:150:ARG:CG	1:S:150:ARG:NH1	2.72	0.41
1:T:161:PHE:N	1:T:161:PHE:CD1	2.88	0.41
1:C:126:PRO:HG2	1:C:127:ILE:HD12	2.01	0.41
1:H:301:ILE:HG22	1:H:302:GLN:N	2.34	0.41
1:K:155:THR:HG23	1:K:161:PHE:CZ	2.54	0.41
1:L:61:ILE:HG23	1:L:63:TYR:N	2.35	0.41
1:L:126:PRO:O	1:L:129:TYR:HB3	2.20	0.41
1:L:135:SER:O	1:L:135:SER:OG	2.37	0.41
1:P:35:THR:HG21	2:o:4:DC:H3'	2.02	0.41
1:T:34:THR:OG1	2:s:6:DG:N2	2.28	0.41
1:A:237:ILE:HG23	1:A:265:SER:HB3	2.03	0.41
1:B:93:PHE:HD2	1:B:294:SER:HB2	1.85	0.41
1:D:100:GLY:O	1:D:317:ARG:HG2	2.20	0.41
1:D:241:LEU:HB3	1:D:271:ALA:HB2	2.03	0.41
1:G:236:THR:HG22	1:G:237:ILE:N	2.35	0.41
1:H:22:LEU:HD22	1:H:36:VAL:HG23	2.01	0.41
2:h:7:DC:H2''	2:h:8:DA:O5'	2.20	0.41
1:O:293:GLN:O	1:O:309:ASN:HA	2.20	0.41
1:O:301:ILE:CD1	1:P:302:GLN:HE21	2.34	0.41
1:P:91:MET:H	1:P:267:SER:HB3	1.85	0.41
1:P:243:LYS:O	1:P:247:PHE:N	2.47	0.41
1:S:83:VAL:O	1:S:84:LEU:HG	2.20	0.41
1:T:29:THR:HG23	1:T:31:LEU:HB2	2.02	0.41
1:T:239:THR:HA	1:T:240:PRO:HD3	1.85	0.41
1:T:302:GLN:HB2	1:T:305:ILE:HD12	2.01	0.41
1:D:39:ALA:CB	1:D:54:VAL:HG21	2.50	0.41
1:D:321:LYS:HB2	1:D:321:LYS:HE2	1.74	0.41
1:G:165:GLY:HA2	1:G:177:ASP:HB2	2.02	0.41
1:S:77:THR:C	1:S:79:VAL:N	2.77	0.41
1:A:40:LEU:HA	1:A:40:LEU:HD23	1.80	0.41
1:A:210:PHE:HD1	1:A:210:PHE:H	1.68	0.41
1:G:211:HIS:CD2	1:G:211:HIS:C	2.98	0.41
1:H:127:ILE:HG23	1:H:154:MET:HE3	2.03	0.41
1:K:144:ILE:HG13	1:K:163:THR:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:77:THR:N	1:L:137:ASP:OD2	2.50	0.41
2:o:14:DG:H2''	2:o:15:DC:O5'	2.20	0.41
1:S:222:ILE:HG13	1:S:223:ARG:N	2.35	0.41
1:T:34:THR:HG21	2:s:6:DG:N1	2.35	0.41
1:C:121:LYS:C	1:C:123:SER:H	2.29	0.41
1:D:105:LEU:H	1:D:105:LEU:CD1	2.33	0.41
1:D:251:LEU:HD21	1:D:258:PRO:CD	2.37	0.41
2:c:18:DA:H2	2:d:4:DC:C2	2.38	0.41
1:H:24:THR:HG22	1:H:28:MET:HE2	2.02	0.41
1:S:335:LEU:HD12	1:S:335:LEU:H	1.85	0.41
1:B:126:PRO:HG2	1:B:127:ILE:HD12	2.02	0.41
1:B:138:GLY:HA3	1:B:327:ILE:HD11	2.02	0.41
1:B:245:ARG:O	1:B:248:GLY:N	2.53	0.41
1:C:205:PRO:HG2	1:C:238:GLU:OE1	2.20	0.41
1:C:283:ILE:HD12	1:C:283:ILE:N	2.34	0.41
1:C:293:GLN:HG2	1:C:295:ALA:O	2.21	0.41
1:C:349:LYS:O	1:C:349:LYS:CG	2.69	0.41
1:K:294:SER:HB3	1:K:312:ILE:HG13	2.03	0.41
1:L:140:ILE:CG2	1:L:319:LEU:HD23	2.51	0.41
1:P:96:GLN:HB2	1:P:312:ILE:HD11	2.02	0.41
1:P:198:ARG:H	1:P:259:ASP:CB	2.33	0.41
1:T:222:ILE:HA	1:T:222:ILE:HD12	1.72	0.41
1:T:270:ILE:HD12	1:T:271:ALA:N	2.35	0.41
1:T:333:GLU:CA	1:T:335:LEU:CD2	2.99	0.41
1:A:129:TYR:HE1	1:A:133:THR:HG21	1.86	0.41
1:C:199:ILE:HG12	1:C:227:VAL:HG11	2.03	0.41
2:d:1:DT:H2''	2:d:2:DA:C5'	2.51	0.41
2:d:7:DC:H2''	2:d:8:DA:O5'	2.21	0.41
1:H:29:THR:HB	1:H:31:LEU:HB2	2.03	0.41
1:H:112:LEU:HD23	1:H:112:LEU:C	2.46	0.41
1:K:112:LEU:O	1:L:113:VAL:HA	2.20	0.41
1:K:281:VAL:HG12	1:K:286:ASP:HB2	2.01	0.41
1:L:70:VAL:O	1:L:74:THR:HG22	2.20	0.41
1:L:283:ILE:HG22	1:L:304:GLN:CG	2.51	0.41
1:S:241:LEU:HA	1:S:244:ILE:CG1	2.51	0.41
1:T:252:MET:HB3	1:T:281:VAL:HG11	2.02	0.41
1:T:313:LYS:HE3	1:T:313:LYS:HB3	1.72	0.41
2:a:14:DG:H1'	2:a:15:DC:H5'	2.03	0.40
1:C:91:MET:HE1	1:D:91:MET:HE1	2.02	0.40
1:C:120:ALA:HB1	1:C:207:ARG:NH1	2.36	0.40
1:K:34:THR:HG21	2:l:6:DG:O6	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:205:PRO:C	1:L:211:HIS:ND1	2.80	0.40
1:L:224:ASP:C	1:L:225:PHE:HD1	2.29	0.40
1:O:204:PRO:CA	1:O:237:ILE:CG1	2.97	0.40
1:S:83:VAL:HG22	1:S:140:ILE:O	2.21	0.40
1:S:101:ILE:HG12	1:S:320:ALA:HB2	2.03	0.40
1:T:101:ILE:HA	1:T:320:ALA:HB2	2.03	0.40
1:B:205:PRO:C	1:B:207:ARG:N	2.78	0.40
1:B:293:GLN:NE2	1:B:298:LEU:HB2	2.37	0.40
1:C:333:GLU:CD	1:C:333:GLU:H	2.29	0.40
1:D:162:VAL:CA	1:D:174:ALA:HB3	2.48	0.40
1:D:203:VAL:HG23	1:D:204:PRO:HD2	2.02	0.40
1:L:183:TYR:CD1	1:L:308:VAL:HG11	2.56	0.40
1:S:25:ILE:HA	1:S:28:MET:CE	2.51	0.40
1:S:122:ASP:CB	1:S:125:VAL:HG23	2.51	0.40
1:B:42:ASP:OD1	1:B:51:LYS:NZ	2.54	0.40
1:B:46:ILE:O	1:B:51:LYS:HE3	2.22	0.40
1:B:334:THR:HB	1:B:335:LEU:HD23	2.04	0.40
1:C:91:MET:HE2	1:C:297:PHE:CE2	2.57	0.40
1:D:203:VAL:CG2	1:D:204:PRO:HD2	2.51	0.40
1:G:175:TYR:H	1:G:336:GLN:HA	1.85	0.40
1:H:218:PHE:HE2	1:H:229:GLU:HG3	1.85	0.40
2:h:13:DT:H2''	2:h:14:DG:C8	2.56	0.40
1:K:330:ALA:HA	1:K:331:PRO:HD3	1.95	0.40
1:L:131:LEU:HD11	1:L:159:MET:CB	2.51	0.40
1:L:148:ASP:CB	1:L:151:VAL:HG23	2.51	0.40
1:L:184:ALA:O	1:L:188:VAL:HG23	2.22	0.40
1:P:56:LEU:HA	1:P:59:GLN:HB3	2.02	0.40
1:T:45:ASP:OD1	2:s:4:DC:H5	2.05	0.40
1:B:45:ASP:O	2:a:3:DT:H2'	2.21	0.40
2:a:14:DG:C2'	2:a:15:DC:H5'	2.51	0.40
1:C:216:LYS:O	1:C:220:ARG:HG3	2.22	0.40
1:H:101:ILE:O	1:H:105:LEU:HD13	2.21	0.40
1:L:189:GLU:HA	1:L:225:PHE:HE2	1.86	0.40
1:O:237:ILE:HG13	1:O:237:ILE:H	1.73	0.40
1:P:327:ILE:HD13	1:P:327:ILE:HA	1.81	0.40
2:o:7:DC:H2'	2:o:8:DA:C8	2.57	0.40
1:A:34:THR:HG21	2:b:6:DG:O6	2.21	0.40
1:A:270:ILE:HD11	1:A:297:PHE:CE2	2.56	0.40
1:B:34:THR:OG1	2:a:6:DG:N1	2.45	0.40
1:C:295:ALA:O	1:C:297:PHE:N	2.55	0.40
2:c:7:DC:H2''	2:c:8:DA:O5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:155:THR:HG21	1:G:171:ILE:HG12	2.04	0.40
1:L:63:TYR:OH	1:L:65:PRO:HA	2.22	0.40
1:O:203:VAL:HG22	1:O:204:PRO:CD	2.52	0.40
1:P:124:MET:O	1:P:124:MET:CG	2.69	0.40
1:P:206:SER:HA	1:P:211:HIS:CB	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	329/341 (96%)	315 (96%)	12 (4%)	2 (1%)	21	56
1	B	326/341 (96%)	314 (96%)	11 (3%)	1 (0%)	36	68
1	C	330/341 (97%)	315 (96%)	11 (3%)	4 (1%)	10	42
1	D	325/341 (95%)	314 (97%)	10 (3%)	1 (0%)	36	68
1	G	329/341 (96%)	315 (96%)	14 (4%)	0	100	100
1	H	329/341 (96%)	319 (97%)	7 (2%)	3 (1%)	14	47
1	K	331/341 (97%)	315 (95%)	15 (4%)	1 (0%)	36	68
1	L	327/341 (96%)	318 (97%)	8 (2%)	1 (0%)	36	68
1	O	310/341 (91%)	295 (95%)	14 (4%)	1 (0%)	36	68
1	P	318/341 (93%)	302 (95%)	12 (4%)	4 (1%)	9	40
1	S	249/341 (73%)	241 (97%)	6 (2%)	2 (1%)	16	50
1	T	278/341 (82%)	258 (93%)	12 (4%)	8 (3%)	3	24
All	All	3781/4092 (92%)	3621 (96%)	132 (4%)	28 (1%)	18	52

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	120	ALA
1	C	122	ASP
1	H	122	ASP
1	P	123	SER
1	S	78	ASN
1	A	119	HIS
1	A	252	MET
1	C	42	ASP
1	H	196	ARG
1	L	42	ASP
1	T	93	PHE
1	T	309	ASN
1	K	348	PRO
1	O	123	SER
1	P	33	ILE
1	P	132	GLU
1	S	19	ARG
1	T	118	THR
1	T	334	THR
1	T	42	ASP
1	T	174	ALA
1	D	206	SER
1	H	93	PHE
1	P	116	PRO
1	C	348	PRO
1	T	299	ASN
1	B	231	PRO
1	T	43	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	262/287 (91%)	249 (95%)	13 (5%)	22	55
1	B	249/287 (87%)	239 (96%)	10 (4%)	28	61
1	C	267/287 (93%)	259 (97%)	8 (3%)	36	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	245/287 (85%)	236 (96%)	9 (4%)	30	63
1	G	253/287 (88%)	242 (96%)	11 (4%)	26	59
1	H	266/287 (93%)	257 (97%)	9 (3%)	32	64
1	K	251/287 (88%)	241 (96%)	10 (4%)	28	61
1	L	246/287 (86%)	238 (97%)	8 (3%)	33	65
1	O	215/287 (75%)	199 (93%)	16 (7%)	13	43
1	P	238/287 (83%)	220 (92%)	18 (8%)	12	42
1	S	160/287 (56%)	150 (94%)	10 (6%)	16	48
1	T	183/287 (64%)	158 (86%)	25 (14%)	3	18
All	All	2835/3444 (82%)	2688 (95%)	147 (5%)	21	54

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	42	ASP
1	A	64	GLN
1	A	72	LEU
1	A	125	VAL
1	A	155	THR
1	A	173	HIS
1	A	176	HIS
1	A	180	ASN
1	A	253	GLN
1	A	287	ILE
1	A	313	LYS
1	A	340	ARG
1	B	66	ASN
1	B	87	ASP
1	B	102	THR
1	B	190	ARG
1	B	222	ILE
1	B	242	ASP
1	B	249	LYS
1	B	299	ASN
1	B	312	ILE
1	B	338	VAL
1	C	34	THR
1	C	41	LYS

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Mol	Chain	Res	Type
1	C	55	ARG
1	C	60	GLN
1	C	173	HIS
1	C	216	LYS
1	C	277	GLU
1	C	283	ILE
1	D	51	LYS
1	D	60	GLN
1	D	64	GLN
1	D	87	ASP
1	D	97	MET
1	D	101	ILE
1	D	171	ILE
1	D	207	ARG
1	D	299	ASN
1	G	144	ILE
1	G	173	HIS
1	G	180	ASN
1	G	193	GLN
1	G	238	GLU
1	G	244	ILE
1	G	245	ARG
1	G	277	GLU
1	G	318	GLU
1	G	321	LYS
1	G	338	VAL
1	H	36	VAL
1	H	46	ILE
1	H	49	GLU
1	H	119	HIS
1	H	155	THR
1	H	188	VAL
1	H	223	ARG
1	H	252	MET
1	H	301	ILE
1	K	55	ARG
1	K	129	TYR
1	K	202	ILE
1	K	227	VAL
1	K	236	THR
1	K	253	GLN
1	K	270	ILE

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Mol	Chain	Res	Type
1	K	281	VAL
1	K	283	ILE
1	K	301	ILE
1	L	72	LEU
1	L	94	THR
1	L	193	GLN
1	L	211	HIS
1	L	227	VAL
1	L	277	GLU
1	L	308	VAL
1	L	327	ILE
1	O	84	LEU
1	O	90	LEU
1	O	144	ILE
1	O	155	THR
1	O	188	VAL
1	O	194	CYS
1	O	219	THR
1	O	227	VAL
1	O	292	LYS
1	O	293	GLN
1	O	301	ILE
1	O	311	ASP
1	O	318	GLU
1	O	327	ILE
1	O	333	GLU
1	O	337	SER
1	P	33	ILE
1	P	36	VAL
1	P	86	VAL
1	P	108	THR
1	P	123	SER
1	P	125	VAL
1	P	127	ILE
1	P	131	LEU
1	P	133	THR
1	P	155	THR
1	P	206	SER
1	P	243	LYS
1	P	277	GLU
1	P	294	SER
1	P	302	GLN

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Mol	Chain	Res	Type
1	P	312	ILE
1	P	327	ILE
1	P	336	GLN
1	S	83	VAL
1	S	124	MET
1	S	139	VAL
1	S	150	ARG
1	S	156	GLU
1	S	162	VAL
1	S	173	HIS
1	S	227	VAL
1	S	236	THR
1	S	241	LEU
1	T	25	ILE
1	T	46	ILE
1	T	54	VAL
1	T	56	LEU
1	T	57	ILE
1	T	78	ASN
1	T	96	GLN
1	T	127	ILE
1	T	144	ILE
1	T	181	GLU
1	T	194	CYS
1	T	218	PHE
1	T	237	ILE
1	T	241	LEU
1	T	244	ILE
1	T	251	LEU
1	T	272	LEU
1	T	281	VAL
1	T	299	ASN
1	T	301	ILE
1	T	313	LYS
1	T	324	LEU
1	T	333	GLU
1	T	335	LEU
1	T	338	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	HIS
1	A	180	ASN
1	A	302	GLN
1	B	66	ASN
1	B	293	GLN
1	B	309	ASN
1	C	180	ASN
1	C	299	ASN
1	D	211	HIS
1	D	293	GLN
1	D	328	ASN
1	G	96	GLN
1	G	299	ASN
1	H	299	ASN
1	K	299	ASN
1	K	304	GLN
1	O	111	HIS
1	O	293	GLN
1	P	173	HIS
1	P	180	ASN
1	P	211	HIS
1	P	302	GLN
1	P	328	ASN
1	T	109	GLN
1	T	173	HIS
1	T	211	HIS
1	T	309	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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 ⓘ

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	A	331/341 (97%)	0.05	3 (0%) 81 64	55, 99, 149, 231	0
1	B	328/341 (96%)	0.19	8 (2%) 59 40	49, 112, 181, 255	0
1	C	332/341 (97%)	-0.23	2 (0%) 85 73	45, 81, 125, 178	0
1	D	327/341 (95%)	0.14	8 (2%) 59 40	59, 109, 168, 236	0
1	G	331/341 (97%)	0.15	2 (0%) 85 73	46, 113, 175, 244	0
1	H	331/341 (97%)	-0.11	3 (0%) 81 64	41, 84, 139, 227	0
1	K	333/341 (97%)	0.13	6 (1%) 67 48	61, 110, 169, 238	0
1	L	329/341 (96%)	0.32	6 (1%) 67 48	66, 118, 178, 233	0
1	O	320/341 (93%)	0.52	18 (5%) 30 19	85, 143, 198, 244	0
1	P	324/341 (95%)	0.47	12 (3%) 45 28	79, 141, 191, 224	0
1	S	259/341 (75%)	0.44	13 (5%) 34 22	74, 145, 210, 255	0
1	T	292/341 (85%)	0.49	12 (4%) 41 25	84, 156, 216, 272	0
2	a	18/18 (100%)	-0.29	0 100 100	61, 77, 104, 107	0
2	b	18/18 (100%)	-0.45	0 100 100	58, 77, 102, 128	0
2	c	18/18 (100%)	-0.34	0 100 100	76, 104, 141, 159	0
2	d	18/18 (100%)	-0.40	0 100 100	71, 105, 177, 220	0
2	g	17/18 (94%)	-0.45	0 100 100	54, 85, 118, 141	0
2	h	17/18 (94%)	-0.60	0 100 100	64, 78, 111, 119	0
2	k	17/18 (94%)	-0.00	0 100 100	96, 132, 196, 200	0
2	l	17/18 (94%)	0.03	0 100 100	90, 121, 214, 226	0
2	o	18/18 (100%)	-0.09	0 100 100	111, 124, 168, 172	0
2	p	17/18 (94%)	-0.14	0 100 100	102, 123, 178, 190	0
2	s	14/18 (77%)	0.25	0 100 100	110, 144, 153, 191	0
2	t	14/18 (77%)	-0.04	0 100 100	112, 128, 166, 185	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4040/4308 (93%)	0.18	93 (2%) 61 41	41, 116, 188, 272	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	124	MET	5.5
1	T	270	ILE	5.4
1	T	114	VAL	5.2
1	D	146	PRO	4.3
1	O	199	ILE	4.1
1	S	115	THR	4.1
1	O	288	ASP	3.9
1	D	122	ASP	3.9
1	T	63	TYR	3.8
1	O	196	ARG	3.6
1	D	104	VAL	3.5
1	T	91	MET	3.5
1	O	202	ILE	3.4
1	O	219	THR	3.4
1	O	188	VAL	3.2
1	K	246	ASP	3.1
1	T	296	GLU	3.1
1	K	56	LEU	3.0
1	B	245	ARG	3.0
1	O	298	LEU	3.0
1	B	232	LEU	2.9
1	T	272	LEU	2.9
1	T	301	ILE	2.9
1	L	119	HIS	2.8
1	T	82	LEU	2.8
1	P	99	PHE	2.8
1	D	174	ALA	2.8
1	B	119	HIS	2.7
1	P	134	GLY	2.7
1	S	272	LEU	2.7
1	D	168	ASP	2.7
1	L	148	ASP	2.7
1	O	115	THR	2.7
1	K	147	ASN	2.7
1	S	270	ILE	2.6
1	H	118	THR	2.6
1	S	121	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	122	ASP	2.6
1	O	180	ASN	2.6
1	D	150	ARG	2.6
1	O	300	TRP	2.5
1	T	258	PRO	2.5
1	B	121	LYS	2.5
1	A	42	ASP	2.5
1	S	269	THR	2.5
1	G	161	PHE	2.5
1	T	269	THR	2.4
1	C	349	LYS	2.4
1	A	272	LEU	2.4
1	O	178	PHE	2.4
1	L	135	SER	2.4
1	P	60	GLN	2.3
1	S	203	VAL	2.3
1	S	138	GLY	2.3
1	O	214	ALA	2.3
1	S	84	LEU	2.3
1	P	326	ARG	2.3
1	B	120	ALA	2.3
1	L	39	ALA	2.3
1	P	90	LEU	2.3
1	P	131	LEU	2.3
1	P	133	THR	2.3
1	O	197	LYS	2.3
1	B	181	GLU	2.2
1	T	98	VAL	2.2
1	G	146	PRO	2.2
1	O	261	ILE	2.2
1	O	297	PHE	2.2
1	T	210	PHE	2.2
1	P	270	ILE	2.2
1	P	335	LEU	2.1
1	O	195	GLY	2.1
1	P	205	PRO	2.1
1	S	116	PRO	2.1
1	C	301	ILE	2.1
1	K	346	MET	2.1
1	A	233	ASP	2.1
1	S	168	ASP	2.1
1	L	35	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	120	ALA	2.1
1	S	205	PRO	2.1
1	O	339	SER	2.1
1	S	228	SER	2.1
1	S	122	ASP	2.1
1	K	279	ALA	2.1
1	B	116	PRO	2.1
1	H	121	LYS	2.0
1	P	61	ILE	2.0
1	B	266	GLY	2.0
1	P	258	PRO	2.0
1	K	317	ARG	2.0
1	O	192	ALA	2.0
1	D	49	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 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.