



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2020 – 03:40 PM BST

PDB ID : 7CE1
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.14.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.2

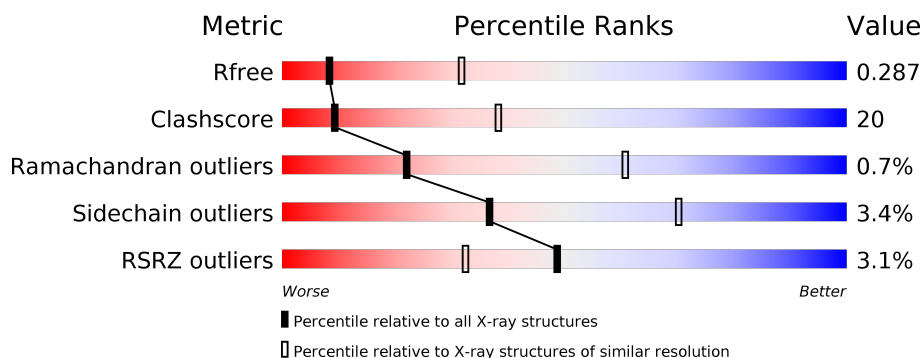
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (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 on 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	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>28%</div> <div>• •</div> </div> </div>
1	B	341	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>28%</div> <div>• •</div> </div> </div>
1	C	341	<div> <div></div> <div> <div></div> <div>72%</div> <div>24%</div> <div>• •</div> </div> </div>
1	D	341	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>31%</div> <div>• •</div> </div> </div>
1	G	341	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>• •</div> </div> </div>
1	H	341	<div> <div></div> <div> <div></div> <div>72%</div> <div>24%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	K	341	
1	L	341	
1	O	341	
1	P	341	
1	S	341	
1	T	341	
2	a	18	
2	b	18	
2	c	18	
2	d	18	
2	g	18	
2	h	18	
2	k	18	
2	l	18	
2	o	18	
2	p	18	
2	s	18	
2	t	18	

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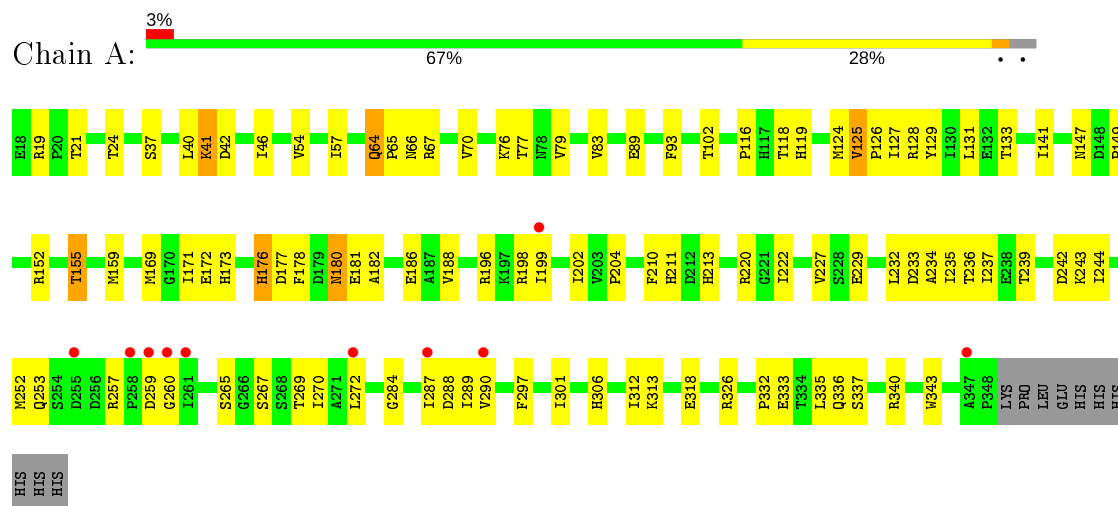
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	6	Total 6	O 6	0	0
3	D	2	Total 2	O 2	0	0
3	c	1	Total 1	O 1	0	0
3	d	1	Total 1	O 1	0	0
3	G	2	Total 2	O 2	0	0
3	H	1	Total 1	O 1	0	0
3	K	2	Total 2	O 2	0	0
3	L	2	Total 2	O 2	0	0
3	O	1	Total 1	O 1	0	0
3	P	1	Total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

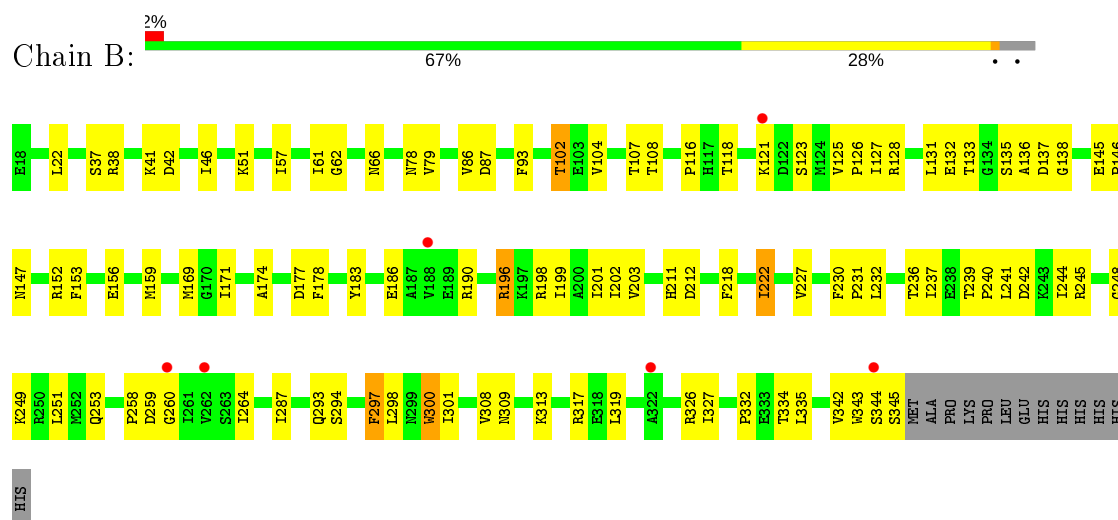
3 Residue-property plots [i](#)

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

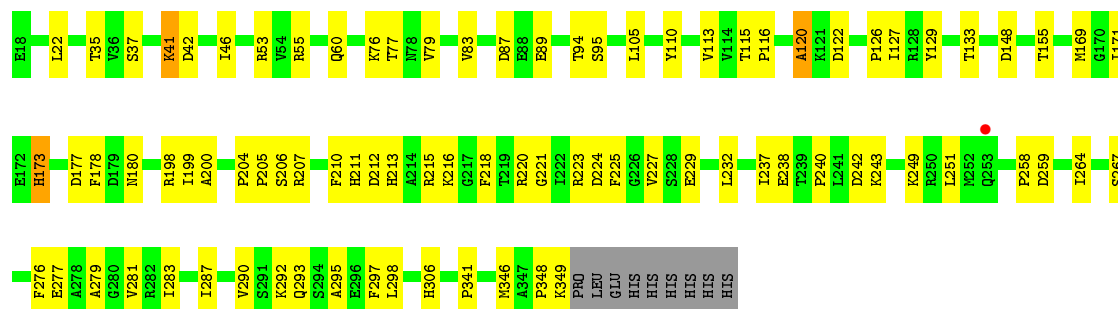


• Molecule 1: LacI-type transcription factor

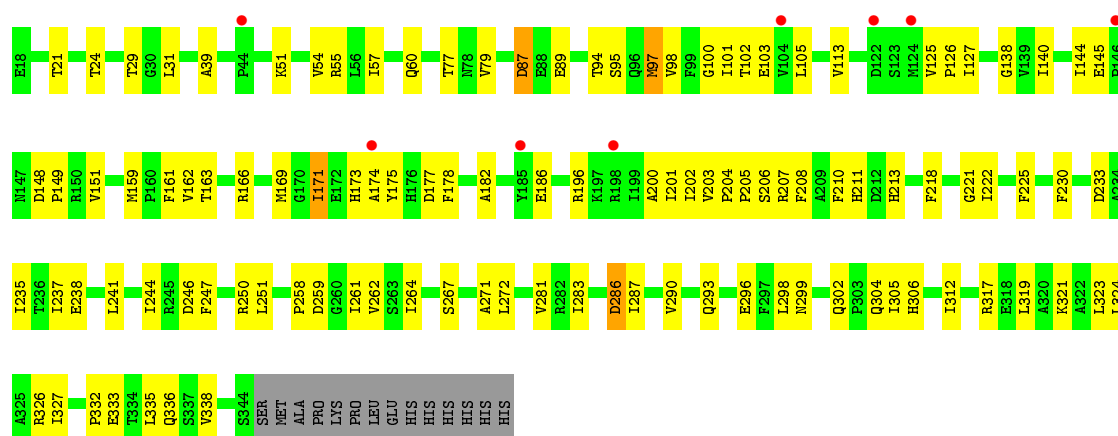


• Molecule 1: LacI-type transcription factor

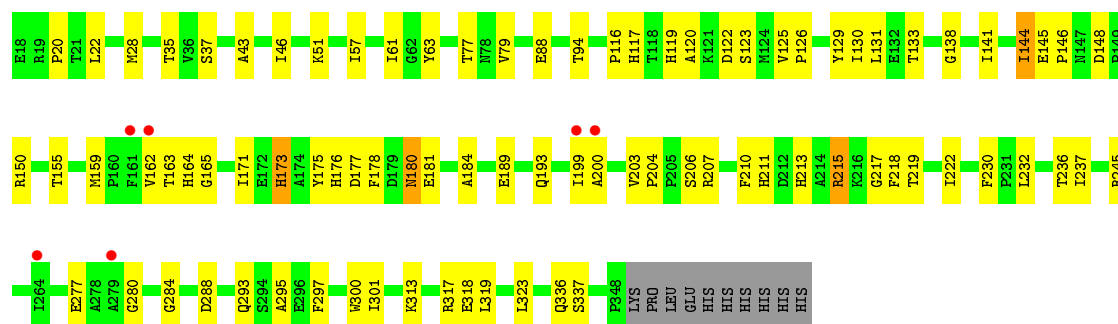
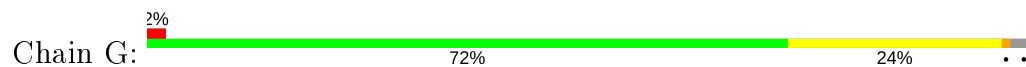




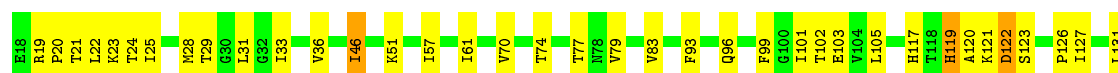
• Molecule 1: LacI-type transcription factor

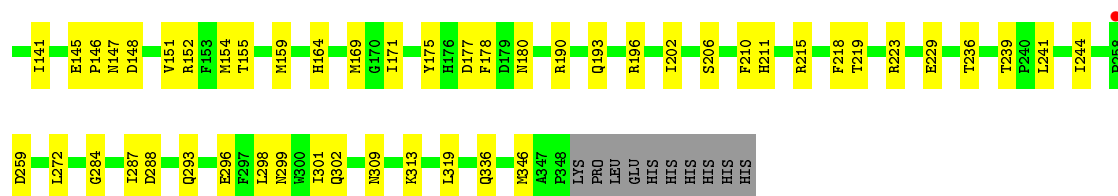


• Molecule 1: LacI-type transcription factor

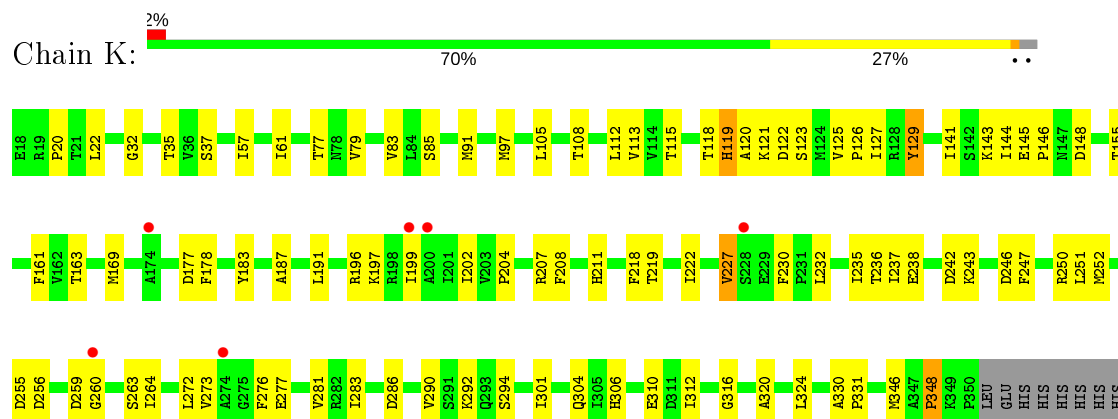


• Molecule 1: LacI-type transcription factor

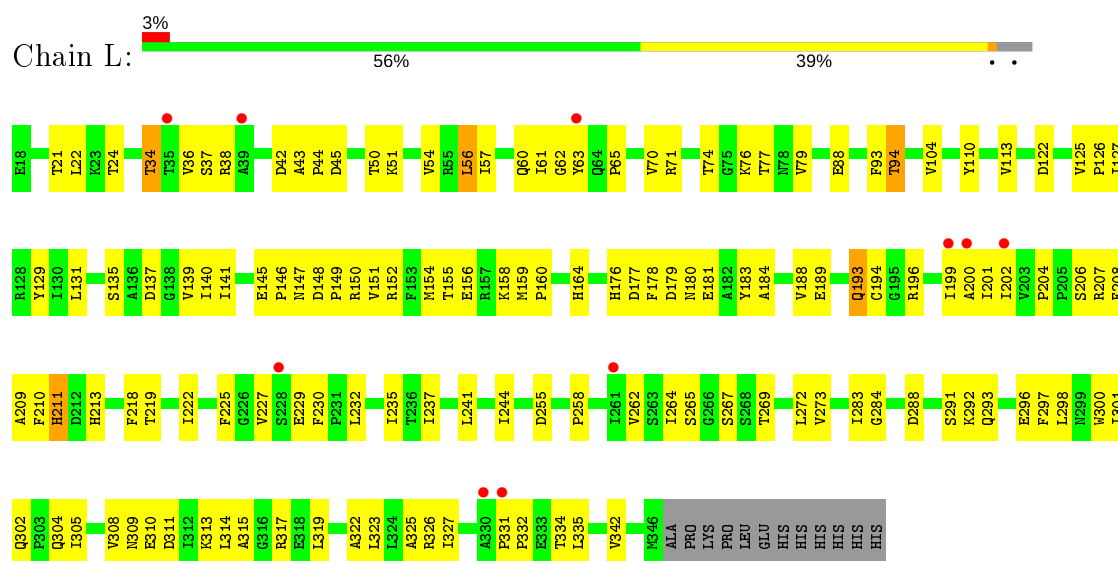




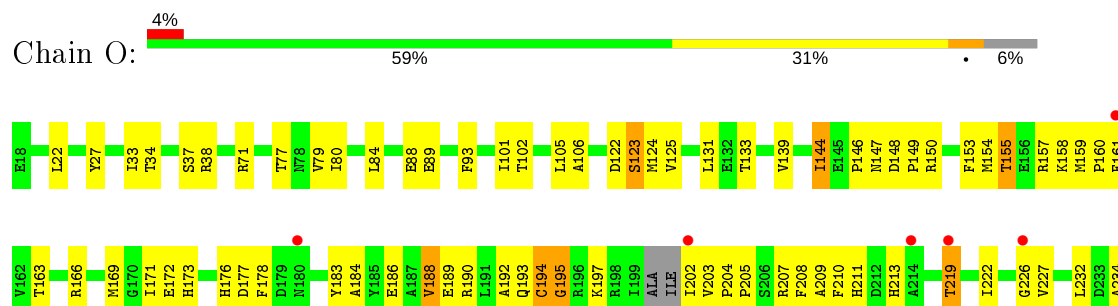
• Molecule 1: LacI-type transcription factor

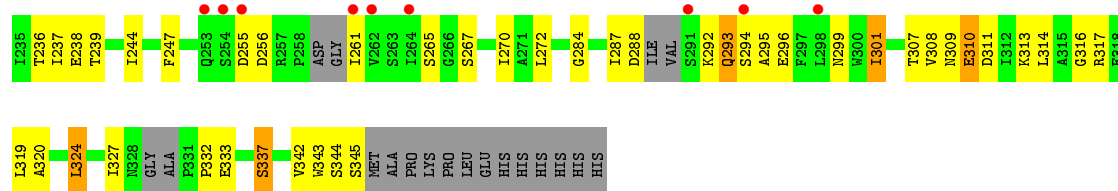


• Molecule 1: LacI-type transcription factor

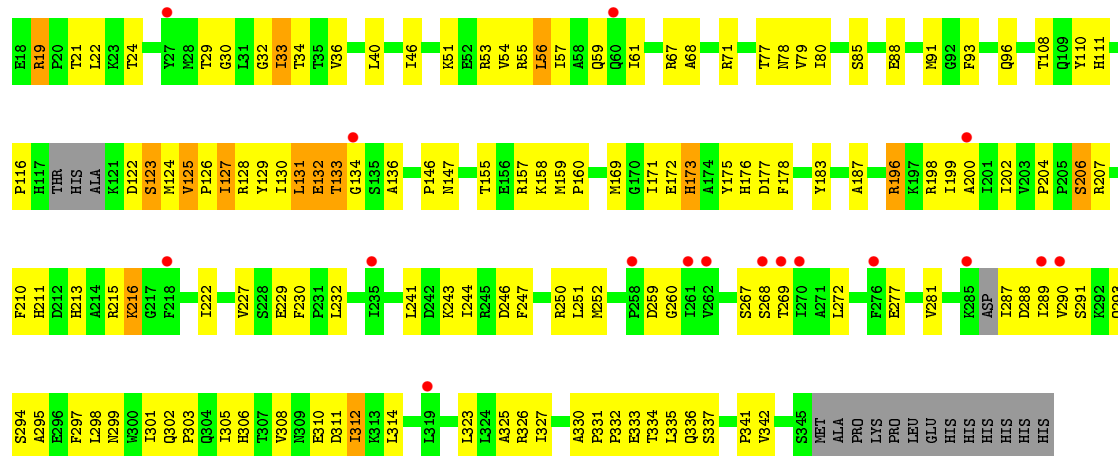


• Molecule 1: LacI-type transcription factor

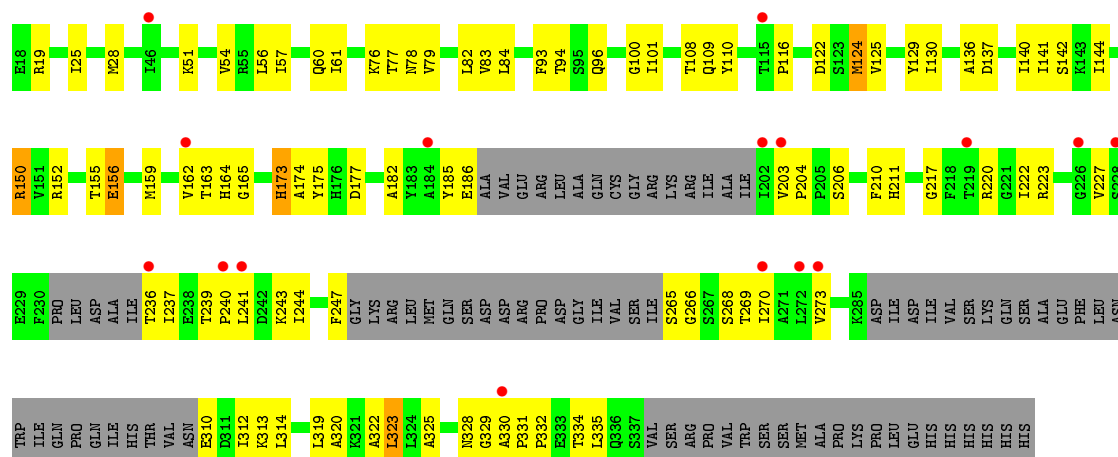




• Molecule 1: LacI-type transcription factor

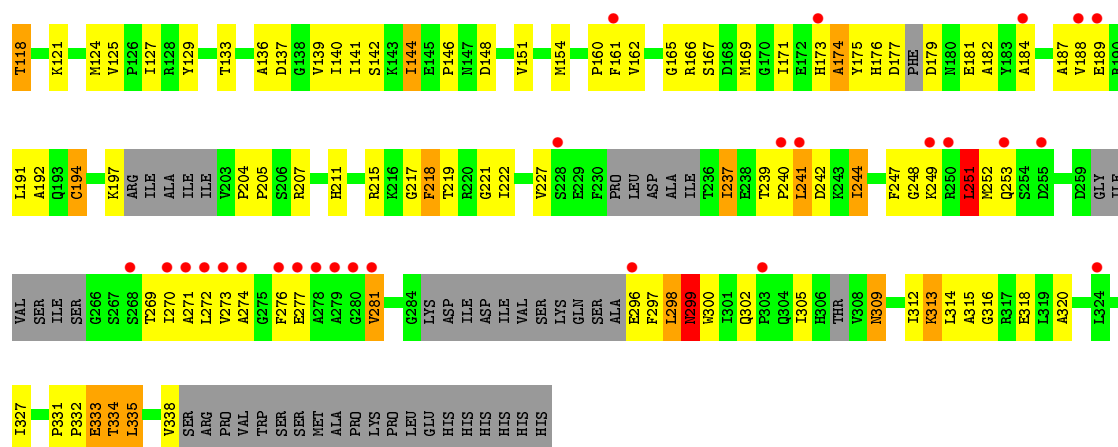


• Molecule 1: LacI-type transcription factor



• Molecule 1: LacI-type transcription factor





- Molecule 2: promoter DNA

Chain a: 72% 28%



- Molecule 2: promoter DNA

Chain b: 89% 11%



- Molecule 2: promoter DNA

Chain c: 94% 6%



- Molecule 2: promoter DNA

Chain d: 6% 94% 6%




- Molecule 2: promoter DNA

Chain g: 94% 6%




- Molecule 2: promoter DNA

Chain h:  89% 6% 6%



- Molecule 2: promoter DNA

Chain k:  83% 11% 6%



- Molecule 2: promoter DNA

Chain l:  94% 6%




- Molecule 2: promoter DNA

Chain o:  94% 6%



- Molecule 2: promoter DNA

Chain p:  89% 6% 6%



- Molecule 2: promoter DNA

Chain s:  78% 22%



- Molecule 2: promoter DNA

Chain t:  72% 6% 22%



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) 100.0 (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 0.241 , 0.287	Depositor DCC
R_{free} test set	5591 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)	0.30 , 90.7	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	0.41	0/2552	0.74	0/3471
1	B	0.41	0/2476	0.77	2/3374 (0.1%)
1	C	0.34	0/2584	0.69	0/3509
1	D	0.40	0/2471	0.75	2/3371 (0.1%)
1	G	0.36	0/2504	0.76	1/3412 (0.0%)
1	H	0.31	0/2574	0.67	0/3496
1	K	0.40	0/2510	0.76	1/3425 (0.0%)
1	L	0.38	0/2482	0.76	2/3385 (0.1%)
1	O	0.40	0/2285	0.77	3/3126 (0.1%)
1	P	0.44	0/2414	0.80	3/3293 (0.1%)
1	S	0.45	0/1796	0.86	2/2458 (0.1%)
1	T	0.50	0/2024	0.95	4/2770 (0.1%)
2	a	0.98	2/413 (0.5%)	1.03	4/635 (0.6%)
2	b	0.90	2/413 (0.5%)	0.94	0/635
2	c	0.77	0/413	1.06	1/635 (0.2%)
2	d	0.64	0/413	1.02	1/635 (0.2%)
2	g	0.74	0/391	1.05	0/601
2	h	0.70	0/391	1.04	1/601 (0.2%)
2	k	0.68	0/391	1.05	2/601 (0.3%)
2	l	0.75	0/391	1.03	0/601
2	o	0.80	1/413 (0.2%)	1.08	1/635 (0.2%)
2	p	0.73	0/391	0.98	1/601 (0.2%)
2	s	0.75	0/317	1.03	0/486
2	t	0.71	0/318	1.01	1/488 (0.2%)
All	All	0.47	5/33327 (0.0%)	0.82	32/46244 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	a	12	DT	O3'-P	-6.39	1.53	1.61
2	a	4	DC	O3'-P	-5.82	1.54	1.61
2	o	5	DT	O3'-P	5.19	1.67	1.61
2	b	4	DC	O3'-P	-5.18	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	12	DT	O3'-P	-5.17	1.54	1.61

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	56	LEU	CA-CB-CG	9.06	136.13	115.30
2	t	4	DC	O5'-P-OP2	-7.97	98.53	105.70
2	o	5	DT	P-O3'-C3'	7.66	128.89	119.70
2	a	3	DT	P-O3'-C3'	6.25	127.20	119.70
1	L	56	LEU	CA-CB-CG	-6.16	101.13	115.30
1	O	324	LEU	CA-CB-CG	6.13	129.41	115.30
1	P	232	LEU	CA-CB-CG	6.08	129.29	115.30
1	S	314	LEU	CA-CB-CG	5.99	129.07	115.30
1	T	189	GLU	CA-CB-CG	5.98	126.55	113.40
2	p	5	DT	O4'-C1'-N1	-5.86	103.89	108.00
1	L	34	THR	N-CA-CB	5.83	121.38	110.30
1	O	310	GLU	CA-CB-CG	5.71	125.97	113.40
1	T	298	LEU	N-CA-C	5.70	126.40	111.00
2	c	5	DT	O4'-C1'-N1	5.65	111.95	108.00
1	T	87	ASP	CB-CG-OD1	5.58	123.32	118.30
1	T	251	LEU	CA-CB-CG	5.54	128.03	115.30
2	k	4	DC	C1'-O4'-C4'	-5.50	104.60	110.10
1	S	323	LEU	CB-CG-CD1	-5.49	101.67	111.00
2	a	5	DT	P-O3'-C3'	5.46	126.25	119.70
2	h	6	DG	O4'-C1'-N9	-5.45	104.18	108.00
1	K	304	GLN	CA-CB-CG	-5.45	101.41	113.40
1	B	319	LEU	CA-CB-CG	5.41	127.73	115.30
2	a	4	DC	C1'-O4'-C4'	-5.40	104.70	110.10
1	O	195	GLY	N-CA-C	5.38	126.55	113.10
1	P	77	THR	CA-CB-CG2	-5.36	104.90	112.40
2	d	1	DT	O4'-C1'-N1	5.26	111.68	108.00
1	G	215	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	B	62	GLY	N-CA-C	-5.13	100.28	113.10
2	k	5	DT	P-O3'-C3'	5.11	125.83	119.70
1	D	319	LEU	CA-CB-CG	5.09	127.00	115.30
1	D	87	ASP	CB-CG-OD1	5.05	122.85	118.30
2	a	11	DG	P-O3'-C3'	5.05	125.76	119.70

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	78	0
1	B	2431	0	2372	74	0
1	C	2534	0	2518	59	0
1	D	2424	0	2345	111	0
1	G	2456	0	2391	60	0
1	H	2525	0	2512	55	0
1	K	2460	0	2386	85	0
1	L	2435	0	2346	119	0
1	O	2250	0	2082	119	0
1	P	2369	0	2283	114	0
1	S	1770	0	1641	89	0
1	T	1997	0	1822	170	0
2	a	369	0	204	0	0
2	b	369	0	204	0	0
2	c	369	0	204	0	0
2	d	369	0	204	0	0
2	g	349	0	192	0	0
2	h	349	0	192	0	0
2	k	349	0	192	0	0
2	l	349	0	192	0	0
2	o	369	0	204	0	0
2	p	349	0	192	0	0
2	s	284	0	159	0	0
2	t	285	0	159	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	d	1	0	0	0	0
All	All	32340	0	29462	1091	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 20.

All (1091) 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:T:83:VAL:HG23	1:T:141:ILE:HD13	1.11	1.08
1:D:148:ASP:HB3	1:D:151:VAL:HG21	1.35	1.08
1:O:202:ILE:HD11	1:O:272:LEU:CD1	1.87	1.04
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:HH11	1:S:150:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:O	1:T:241:LEU:HD23	1.79	0.82
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:ALA:HA	1:D:335:LEU:HD12	1.62	0.79
1:O:301:ILE:CG1	1:P:302:GLN:HE21	1.96	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: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
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:HD12	1:D:105:LEU:N	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:O:203:VAL:HG22	1:O:204:PRO:N	2.02	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:B:147:ASN:HA	1:B:169:MET:HG2	1.69	0.74
1:P:323:LEU:HD12	1:P:323:LEU:O	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
1:T:222:ILE:HG12	1:T:227:VAL:HG22	1.69	0.74
1:K:283:ILE:N	1:K:283:ILE:HD12	2.03	0.73
1:P:290:VAL:HG22	1:P:306:HIS:HB2	1.70	0.73
1:P:51:LYS:O	1:P:55:ARG:HG2	1.88	0.73
1:T:333:GLU:C	1:T:335:LEU:HD22	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B:344:SER:OG	1:B:345:SER:N	2.22	0.72
1:D:148:ASP:CB	1:D:151:VAL:HG21	2.18	0.72
1:K:283:ILE:H	1:K:283:ILE:HD12	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: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:296:GLU:HA	1:T:309:ASN:HD22	1.54	0.71
1:O:261:ILE:N	1:O:288:ASP:O	2.24	0.71
1:T:139:VAL:HB	1:T:154:MET:HE1	1.72	0.71
1:D:290:VAL:HG22	1:D:306:HIS:HB2	1.72	0.71
1:D:174:ALA:HB2	1:D:335:LEU:CD1	2.21	0.71
1:K:232:LEU:HD21	1:K:247:PHE:HZ	1.56	0.70
1:T:241:LEU:HG	1:T:244:ILE:HD12	1.74	0.70
1:T:51:LYS:HA	1:T:54:VAL:HG21	1.71	0.70
1:K:218:PHE:O	1:K:222:ILE:HG23	1.92	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:HD13	1:T:335:LEU:N	2.06	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:T:56:LEU:HD12	1:T:56:LEU:C	2.12	0.69
1:P:131:LEU:O	1:P:131:LEU:HD13	1.93	0.69
1:S:108:THR:OG1	1:S:109:GLN:N	2.25	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:C:37:SER:O	1:C:41:LYS:HG3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:H	1:A:259:ASP:HB2	1.58	0.69
1:B:79:VAL:HG13	1:B:136:ALA:HA	1.75	0.69
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
1:D:51:LYS:O	1:D:55:ARG:HG3	1.95	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: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: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:K:199:ILE:CD1	1:K:218:PHE:HZ	2.08	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:177:ASP:OD1	1:L:178:PHE:N	2.29	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
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:215:ARG:NH2	1:C:229:GLU:OE2	2.30	0.64
1:C:200:ALA:HB1	1:C:232:LEU:HD23	1.79	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:C	1:K:199:ILE:HD12	2.18	0.63
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:189:GLU:HA	1:L:225:PHE:CE2	2.35	0.62
1:K:301:ILE:HG21	1:L:301:ILE:HG23	1.81	0.62
1:O:204:PRO:HA	1:O:237:ILE:CG1	2.28	0.62
1:L:139:VAL:HB	1:L:154:MET:HE1	1.81	0.62
1:O:139:VAL:HB	1:O:154:MET:HE1	1.81	0.62
1:S:83:VAL:HG21	1:S:141:ILE:CD1	2.27	0.62
1:B:199:ILE:O	1:B:230:PHE:N	2.31	0.62
1:T:117:HIS:CE1	1:T:118:THR:HG23	2.34	0.62
1:C:148:ASP:H	1:C:169:MET:HE1	1.62	0.62
1:L:131:LEU:HD11	1:L:159:MET:HB2	1.81	0.62
1:D:148:ASP:CG	1:D:151:VAL:HG23	2.18	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: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:H	1:C:283:ILE:HD12	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: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:T:298:LEU:C	1:T:300:TRP:H	2.04	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:S:94:THR:HG1	1:T:95:SER:HB3	1.65	0.61
1:C:116:PRO:HG3	1:D:102:THR:HG21	1.83	0.61
1:P:222:ILE:HB	1:P:227:VAL:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:S:150:ARG:NH1	1:S:150:ARG:HG2	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: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: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
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: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:HG3	1:S:159:MET:O	2.03	0.59
1:L:122:ASP:O	1:L:125:VAL:HG12	2.03	0.59
1:L:193:GLN:N	1:L:193:GLN:OE1	2.34	0.59
1:L:230:PHE:HB3	1:L:258:PRO:HB3	1.85	0.59
1:H:61:ILE:HG13	1:S:60:GLN:HB3	1.84	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: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:HD12	1:O:33:ILE:H	1.67	0.59
1:H:25:ILE:HA	1:H:28:MET:HE2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:219:THR:O	1:K:222:ILE:HG13	2.02	0.58
1:L:34:THR:HG22	1:L:34:THR:O	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:D:218:PHE:CZ	1:D:222:ILE:HD11	2.38	0.58
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:K:118:THR:HG23	1:K:119:HIS:ND1	2.18	0.57
1:L:145:GLU:HG2	1:L:208:PHE:CE1	2.39	0.57
1:K:264:ILE:O	1:K:292:LYS:NZ	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:T:51:LYS:C	1:T:54:VAL:HG23	2.24	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:D:105:LEU:HD12	1:D:105:LEU:H	1.70	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
1:C:346:MET:SD	1:C:346:MET:N	2.78	0.56
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: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:H:127:ILE:HG23	1:H:154:MET:HE3	1.88	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:G:141:ILE:HD11	1:G:163:THR:HG22	1.87	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: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
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:C:148:ASP:H	1:C:169:MET:CE	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:108:THR:HG21	1:S:110:TYR:HD2	1.70	0.55
1:P:131:LEU:C	1:P:133:THR:H	2.07	0.55
1:B:147:ASN:HA	1:B:169:MET:CG	2.34	0.55
1:K:246:ASP:OD1	1:K:247:PHE:HB2	2.05	0.55
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:HH11	1:G:245:ARG:HG3	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
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: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:K:199:ILE:O	1:K:199:ILE:HD12	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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:145:GLU:OE2	1:K:207:ARG:HG2	2.08	0.54
1:D:127:ILE:N	1:D:127:ILE:HD12	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:T:51:LYS:C	1:T:54:VAL:CG2	2.77	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:G:144:ILE:CD1	1:G:144:ILE:H	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:CD1	1:P:129:TYR:O	2.61	0.53
1:A:67:ARG:HH11	1:A:67:ARG:HG2	1.74	0.53
1:B:196:ARG:N	1:B:196:ARG:HD2	2.23	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:C:173:HIS:HD1	1:C:173:HIS:C	2.11	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:D:293:GLN:OE1	1:D:296:GLU:HA	2.09	0.53
1:C:94:THR:HB	1:D:95:SER:HB3	1.90	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
1:H:145:GLU:HB3	1:H:146:PRO:HD2	1.91	0.53
1:P:269:THR:HG21	1:P:291:SER:OG	2.09	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:B:121:LYS:C	1:B:123:SER:H	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:169:MET:HE3	1:B:171:ILE:HD12	1.92	0.52
1:B:211:HIS:HD2	1:B:212:ASP:OD1	1.92	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:L:43:ALA:HB1	1:L:44:PRO:HD2	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:205:PRO:HD3	1:T:237:ILE:CG1	2.40	0.52
1:T:57:ILE:HD11	1:T:61:ILE:HG23	1.91	0.52
1:H:121:LYS:C	1:H:123:SER:H	2.09	0.52
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:D:204:PRO:HD3	1:D:264:ILE:HG21	1.92	0.51
1:S:185:TYR:HE1	1:S:220:ARG:H	1.56	0.51
1:S:100:GLY:HA3	1:S:313:LYS:O	2.10	0.51
1:A:176:HIS:C	1:A:176:HIS:ND1	2.62	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:D:201:ILE:HD12	1:D:262:VAL:O	2.11	0.51
1:T:29:THR:OG1	1:T:31:LEU:HD13	2.10	0.51
1:T:335:LEU:HD13	1:T:335:LEU:H	1.75	0.51
1:H:96:GLN:HB3	1:H:313:LYS:HB2	1.92	0.51
1:O:192:ALA:O	1:O:193:GLN:C	2.49	0.51
1:S:76:LYS:HD2	1:S:137:ASP:OD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:148:ASP:H	1:K:169:MET:HE3	1.75	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:D:105:LEU:CD1	1:D:105:LEU:N	2.73	0.51
1:G:148:ASP:OD1	1:G:150:ARG:HG2	2.11	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:187:ALA:O	1:T:191:LEU:HG	2.12	0.50
1:T:99:PHE:HA	1:T:102:THR:HG22	1.93	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
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:T:85:SER:OG	1:T:87:ASP:OD1	2.21	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:T:298:LEU:C	1:T:300:TRP:N	2.65	0.50
1:G:173:HIS:N	1:G:173:HIS:ND1	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:A:124:MET:HE1	1:A:149:PRO:HB2	1.93	0.50
1:L:211:HIS:CD2	1:L:211:HIS:C	2.84	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: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:T:333:GLU:N	1:T:333:GLU:CD	2.64	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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
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:HG13	1:T:144:ILE:O	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:G:28:MET:HE3	1:G:57:ILE:HD11	1.95	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: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:269:THR:HG21	1:L:291:SER:OG	2.12	0.49
1:L:77:THR:O	1:L:79:VAL:HG23	2.13	0.49
1:T:176:HIS:C	1:T:176:HIS:CD2	2.86	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:CD2	1:T:335:LEU:H	1.98	0.49
1:A:126:PRO:HG2	1:A:127:ILE:HD12	1.95	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:D:103:GLU:OE1	1:D:103:GLU:HA	2.12	0.48
1:P:67:ARG:NH1	1:P:111:HIS:ND1	2.60	0.48
1:S:25:ILE:HA	1:S:28:MET:HE3	1.95	0.48
1:B:236:THR:O	1:B:239:THR:OG1	2.24	0.48
1:L:273:VAL:HG21	1:L:305:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:S:185:TYR:N	1:S:217:GLY:O	2.46	0.48
1:S:94:THR:OG1	1:T:95:SER:CB	2.49	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:H:121:LYS:C	1:H:123:SER:N	2.67	0.48
1:P:172:GLU:CB	1:P:333:GLU:HG3	2.43	0.48
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:K:242:ASP:OD1	1:K:243:LYS:N	2.46	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: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
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:B:203:VAL:O	1:B:236:THR:OG1	2.20	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
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:D:138:GLY:HA2	1:D:159:MET:HE3	1.95	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:O	1:A:118:THR:HG22	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:O:192:ALA:C	1:O:194:CYS:N	2.63	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
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:HH11	1:T:207:ARG:HG2	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:235:ILE:HD11	1:D:247:PHE:HB3	1.95	0.47
1:D:77:THR:O	1:D:79:VAL:HG23	2.14	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:O:192:ALA:C	1:O:195:GLY:H	2.18	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:D:221:GLY:O	1:D:225:PHE:HD1	1.97	0.47
1:G:22:LEU:HD11	1:G:63:TYR:OH	2.15	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
1:B:198:ARG:O	1:B:260:GLY:N	2.42	0.47
1:D:237:ILE:HG13	1:D:238:GLU:N	2.29	0.47
1:H:147:ASN:HA	1:H:169:MET:HG2	1.97	0.47
1:L:38:ARG:HG3	1:L:38:ARG:NH2	2.30	0.47
1:S:206:SER:HA	1:S:211:HIS:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ARG:O	1:B:41:LYS:O	2.33	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:K:301:ILE:O	1:K:301:ILE:HG12	2.15	0.47
1:L:204:PRO:HG2	1:L:211:HIS:HA	1.97	0.47
1:L:21:THR:O	1:L:24:THR:OG1	2.25	0.47
1:L:255:ASP:N	1:L:255:ASP:OD1	2.47	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: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:L:293:GLN:CD	1:L:296:GLU:HA	2.35	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
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
1:K:121:LYS:C	1:K:123:SER:H	2.19	0.46
1:P:131:LEU:HD12	1:P:157:ARG:HD3	1.97	0.46
1:P:204:PRO:HG3	1:P:210:PHE:CE2	2.51	0.46
1:P:196:ARG:HD2	1:P:288:ASP:H	1.80	0.46
1:A:125:VAL:HG22	1:A:126:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:GLY:O	1:C:225:PHE:HD2	1.99	0.46
1:O:88:GLU:OE1	1:O:89:GLU:N	2.49	0.46
1:P:158:LYS:HD2	1:P:158:LYS:C	2.36	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: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: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:204:PRO:O	1:D:211:HIS:HD2	1.98	0.46
1:D:54:VAL:HA	1:D:57:ILE:HG22	1.98	0.46
1:H:119:HIS:CE1	1:H:122:ASP:H	2.34	0.46
1:H:83:VAL:HG22	1:H:141:ILE:HG22	1.98	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:G:300:TRP:C	1:G:301:ILE:HD13	2.35	0.46
1:L:38:ARG:HG3	1:L:38:ARG:HH21	1.80	0.46
1:P:331:PRO:HA	1:P:332:PRO:HD3	1.82	0.46
1:K:146:PRO:O	1:K:169:MET:HG2	2.16	0.46
1:T:242:ASP:N	1:T:242:ASP:OD1	2.49	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:284:GLY:N	1:O:287:ILE:O	2.49	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ALA:HB1	1:D:54:VAL:HG21	1.98	0.45
1:T:176:HIS:NE2	1:T:315:ALA:HB1	2.32	0.45
1:A:83:VAL:CG2	1:A:141:ILE:HG22	2.45	0.45
1:A:64:GLN:HA	1:A:65:PRO:HD3	1.79	0.45
1:C:22:LEU:HD13	1:C:37:SER:HB2	1.98	0.45
1:K:199:ILE:HD11	1:K:218:PHE:HZ	1.68	0.45
1:K:77:THR:O	1:K:79:VAL:HG23	2.17	0.45
1:S:241:LEU:HA	1:S:244:ILE:HG13	1.99	0.45
1:G:138:GLY:HA3	1:G:323:LEU:HD21	1.97	0.45
1:S:239:THR:HG22	1:S:240:PRO:O	2.15	0.45
1:A:152:ARG:CZ	1:A:152:ARG:HB2	2.47	0.45
1:A:188:VAL:CG1	1:A:199:ILE:HG21	2.46	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: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:S:173:HIS:C	1:S:173:HIS:HD1	2.19	0.45
1:S:96:GLN:O	1:S:313:LYS:HA	2.16	0.45
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: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:P:196:ARG:HD3	1:P:287:ILE:HA	1.98	0.45
1:S:152:ARG:HA	1:S:155:THR:CG2	2.47	0.45
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:124:MET:CE	1:S:150:ARG:HA	2.47	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
1:K:273:VAL:O	1:K:277:GLU:N	2.51	0.44
1:K:32:GLY:O	1:K:35:THR:OG1	2.25	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: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
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
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:218:PHE:CZ	1:L:229:GLU:HG3	2.52	0.44
1:L:201:ILE:HD12	1:L:262:VAL:O	2.18	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:L:293:GLN:OE1	1:L:298:LEU:N	2.33	0.44
1:P:241:LEU:HD22	1:P:268:SER:HA	1.99	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:295:ALA:O	1:G:297:PHE:HD1	2.00	0.43
1:G:77:THR:O	1:G:79:VAL:HG23	2.18	0.43
1:K:126:PRO:HG2	1:K:127:ILE:HD12	2.00	0.43
1:K:191:LEU:HD23	1:K:260:GLY:HA3	2.00	0.43
1:L:325:ALA:HB3	1:L:335:LEU:HD21	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:O:173:HIS:HA	1:O:332:PRO:HB3	2.01	0.43
1:O:186:GLU:C	1:O:189:GLU:HB3	2.38	0.43
1:P:85:SER:O	1:P:88:GLU:OE2	2.36	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:B:259:ASP:C	1:B:287:ILE:HD12	2.38	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:O:155:THR:HG23	1:O:161:PHE:CE1	2.53	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:K:199:ILE:C	1:K:199:ILE:CD1	2.85	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:A:126:PRO:O	1:A:129:TYR:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:VAL:HA	1:A:57:ILE:HG22	2.01	0.43
1:H:120:ALA:O	1:H:123:SER:HB3	2.18	0.43
1:H:57:ILE:O	1:H:61:ILE:HG22	2.18	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:198:ARG:O	1:A:260:GLY:N	2.51	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: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
1:S:237:ILE:HD12	1:S:237:ILE:H	1.84	0.43
1:A:269:THR:O	1:A:272:LEU:HG	2.18	0.43
1:A:102:THR:CB	1:B:116:PRO:HG3	2.49	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
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:HA	1:A:335:LEU:HD23	1.78	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:B:169:MET:CE	1:B:171:ILE:HD12	2.49	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:L:176:HIS:HB3	1:L:319:LEU:CD1	2.48	0.42
1:K:301:ILE:HD12	1:L:301:ILE:HG23	2.01	0.42
1:O:301:ILE:HA	1:O:301:ILE:HD12	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: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
1:S:310:GLU:HG2	1:S:312:ILE:CG2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:VAL:O	1:D:102:THR:HG23	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
1:D:233:ASP:OD2	1:P:216:LYS:HE3	2.19	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:196:ARG:CD	1:P:288:ASP:H	2.33	0.42
1:P:80:ILE:HD12	1:P:323:LEU:HD23	2.00	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:L:313:LYS:HB3	1:L:313:LYS:HE2	1.72	0.42
1:L:54:VAL:HA	1:L:57:ILE:CG2	2.50	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
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:331:PRO:HA	1:S:332:PRO:HD3	1.92	0.42
1:S:330:ALA:HB3	1:S:335:LEU:HD11	2.00	0.42
1:S:57:ILE:O	1:S:61:ILE:HG12	2.20	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
1:G:141:ILE:HD12	1:G:150:ARG:HD2	2.01	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:152:ARG:HB2	1:H:169:MET:HE1	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:174:ALA:HB2	1:S:335:LEU:HB2	2.01	0.42
1:T:117:HIS:CD2	1:T:125:VAL:HG13	2.55	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
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: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:D:103:GLU:CG	1:D:317:ARG:HH11	2.20	0.41
1:H:164:HIS:HB2	1:H:319:LEU:HD21	2.02	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:CD1	1:T:161:PHE:N	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:126:PRO:O	1:L:129:TYR:HB3	2.20	0.41
1:L:135:SER:OG	1:L:135:SER:O	2.37	0.41
1:L:61:ILE:HG23	1:L:63:TYR:N	2.35	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
1:O:293:GLN:O	1:O:309:ASN:HA	2.20	0.41
1:P:243:LYS:O	1:P:247:PHE:N	2.47	0.41
1:P:91:MET:H	1:P:267:SER:HB3	1.85	0.41
1:O:301:ILE:CD1	1:P:302:GLN:HE21	2.34	0.41
1:S:83:VAL:O	1:S:84:LEU:HG	2.20	0.41
1:T:239:THR:HA	1:T:240:PRO:HD3	1.85	0.41
1:T:29:THR:HG23	1:T:31:LEU:HB2	2.02	0.41
1:T:302:GLN:HB2	1:T:305:ILE:HD12	2.01	0.41
1:D:321:LYS:HB2	1:D:321:LYS:HE2	1.74	0.41
1:D:39:ALA:CB	1:D:54:VAL:HG21	2.50	0.41
1:G:165:GLY:HA2	1:G:177:ASP:HB2	2.02	0.41
1:G:43:ALA:O	1:G:51:LYS:NZ	2.37	0.41
1:O:154:MET:HB3	1:O:154:MET:HE2	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:124:MET:HE1	1:S:150:ARG:HA	2.03	0.41
1:A:210:PHE:H	1:A:210:PHE:HD1	1.68	0.41
1:A:40:LEU:HA	1:A:40:LEU:HD23	1.80	0.41
1:K:144:ILE:HG13	1:K:163:THR:HB	2.02	0.41
1:L:77:THR:N	1:L:137:ASP:OD2	2.50	0.41
1:S:222:ILE:HG13	1:S:223:ARG:N	2.35	0.41
1:D:105:LEU:CD1	1:D:105:LEU:H	2.33	0.41
1:D:251:LEU:HD21	1:D:258:PRO:CD	2.37	0.41
1:S:335:LEU:H	1:S:335:LEU:HD12	1.85	0.41
1:A:198:ARG:C	1:A:199:ILE:HD13	2.41	0.41
1:B:138:GLY:HA3	1:B:327:ILE:HD11	2.02	0.41
1:C:205:PRO:HG2	1:C:238:GLU:OE1	2.20	0.41
1:C:283:ILE:N	1:C:283:ILE:HD12	2.34	0.41
1:C:293:GLN:HG2	1:C:295:ALA:O	2.21	0.41
1:C:349:LYS:CG	1:C:349:LYS:O	2.69	0.41
1:D:205:PRO:HG3	1:D:238:GLU:CD	2.40	0.41
1:G:277:GLU:C	1:G:280:GLY:H	2.23	0.41
1:K:148:ASP:N	1:K:169:MET:HE3	2.36	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:198:ARG:H	1:P:259:ASP:CB	2.33	0.41
1:P:96:GLN:HB2	1:P:312:ILE:HD11	2.02	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:B:126:PRO:HG2	1:B:127:ILE:HD12	2.02	0.41
1:B:245:ARG:O	1:B:248:GLY:N	2.53	0.41
1:O:333:GLU:H	1:O:333:GLU:CD	2.24	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
1:H:29:THR:HB	1:H:31:LEU:HB2	2.03	0.41
1:K:281:VAL:HG12	1:K:286:ASP:HB2	2.01	0.41
1:K:112:LEU:O	1:L:113:VAL:HA	2.20	0.41
1:L:283:ILE:HG22	1:L:304:GLN:CG	2.51	0.41
1:L:70:VAL:O	1:L:74:THR:HG22	2.20	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
1:C:120:ALA:HB1	1:C:207:ARG:NH1	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:293:GLN:NE2	1:B:298:LEU:HB2	2.37	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:122:ASP:CB	1:S:125:VAL:HG23	2.51	0.40
1:S:25:ILE:HA	1:S:28:MET:CE	2.51	0.40
1:T:338:VAL:O	1:T:338:VAL:HG13	2.21	0.40
1:B:334:THR:HB	1:B:335:LEU:HD23	2.04	0.40
1:B:46:ILE:O	1:B:51:LYS:HE3	2.22	0.40
1:B:42:ASP:OD1	1:B:51:LYS:NZ	2.54	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
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: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:H	1:O:237:ILE:HG13	1.73	0.40
1:O:344:SER:O	1:O:345:SER:OG	2.35	0.40
1:P:327:ILE:HA	1:P:327:ILE:HD13	1.81	0.40
1:T:99:PHE:HB2	1:T:313:LYS:HZ1	1.86	0.40
1:A:270:ILE:HD11	1:A:297:PHE:CE2	2.56	0.40
1:C:295:ALA:O	1:C:297:PHE:N	2.55	0.40
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:CG	1:P:124:MET:O	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	329/341 (96%)	315 (96%)	12 (4%)	2 (1%)	25	64
1	B	326/341 (96%)	314 (96%)	11 (3%)	1 (0%)	41	74
1	C	330/341 (97%)	315 (96%)	11 (3%)	4 (1%)	13	49
1	D	325/341 (95%)	314 (97%)	10 (3%)	1 (0%)	41	74
1	G	329/341 (96%)	315 (96%)	14 (4%)	0	100	100
1	H	329/341 (96%)	319 (97%)	7 (2%)	3 (1%)	17	56
1	K	331/341 (97%)	315 (95%)	15 (4%)	1 (0%)	41	74
1	L	327/341 (96%)	318 (97%)	8 (2%)	1 (0%)	41	74
1	O	310/341 (91%)	295 (95%)	14 (4%)	1 (0%)	41	74
1	P	318/341 (93%)	302 (95%)	12 (4%)	4 (1%)	12	47
1	S	249/341 (73%)	241 (97%)	6 (2%)	2 (1%)	19	58
1	T	278/341 (82%)	258 (93%)	12 (4%)	8 (3%)	4	28
All	All	3781/4092 (92%)	3621 (96%)	132 (4%)	28 (1%)	22	61

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

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Mol	Chain	Res	Type
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%)	250 (95%)	12 (5%)	27	63
1	B	249/287 (87%)	240 (96%)	9 (4%)	35	69
1	C	267/287 (93%)	261 (98%)	6 (2%)	52	79
1	D	245/287 (85%)	237 (97%)	8 (3%)	38	71
1	G	253/287 (88%)	249 (98%)	4 (2%)	62	84
1	H	266/287 (93%)	263 (99%)	3 (1%)	73	88
1	K	251/287 (88%)	248 (99%)	3 (1%)	71	88
1	L	246/287 (86%)	242 (98%)	4 (2%)	62	84
1	O	215/287 (75%)	205 (95%)	10 (5%)	26	62
1	P	238/287 (83%)	223 (94%)	15 (6%)	18	52
1	S	160/287 (56%)	154 (96%)	6 (4%)	33	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T	183/287 (64%)	166 (91%)	17 (9%)	9	33
All	All	2835/3444 (82%)	2738 (97%)	97 (3%)	37	70

All (97) 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	76	LYS
1	A	125	VAL
1	A	155	THR
1	A	173	HIS
1	A	176	HIS
1	A	180	ASN
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	196	ARG
1	B	222	ILE
1	B	242	ASP
1	B	297	PHE
1	B	300	TRP
1	C	41	LYS
1	C	55	ARG
1	C	60	GLN
1	C	87	ASP
1	C	173	HIS
1	C	277	GLU
1	D	60	GLN
1	D	87	ASP
1	D	97	MET
1	D	171	ILE
1	D	173	HIS
1	D	207	ARG
1	D	286	ASP
1	D	299	ASN
1	G	144	ILE

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Mol	Chain	Res	Type
1	G	173	HIS
1	G	180	ASN
1	G	318	GLU
1	H	46	ILE
1	H	119	HIS
1	H	223	ARG
1	K	119	HIS
1	K	129	TYR
1	K	227	VAL
1	L	45	ASP
1	L	94	THR
1	L	193	GLN
1	L	211	HIS
1	O	84	LEU
1	O	144	ILE
1	O	155	THR
1	O	188	VAL
1	O	194	CYS
1	O	219	THR
1	O	293	GLN
1	O	301	ILE
1	O	311	ASP
1	O	337	SER
1	P	19	ARG
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	173	HIS
1	P	196	ARG
1	P	206	SER
1	P	216	LYS
1	P	277	GLU
1	P	294	SER
1	P	312	ILE
1	P	336	GLN
1	S	124	MET
1	S	150	ARG
1	S	156	GLU
1	S	162	VAL

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Mol	Chain	Res	Type
1	S	173	HIS
1	S	210	PHE
1	T	54	VAL
1	T	56	LEU
1	T	78	ASN
1	T	96	GLN
1	T	144	ILE
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	313	LYS
1	T	333	GLU
1	T	335	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	HIS
1	A	180	ASN
1	B	293	GLN
1	B	309	ASN
1	C	180	ASN
1	D	173	HIS
1	D	211	HIS
1	D	293	GLN
1	H	299	ASN
1	O	293	GLN
1	O	328	ASN
1	P	173	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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	331/341 (97%)	0.12	10 (3%) 50 34	55, 99, 149, 231	0
1	B	328/341 (96%)	0.06	6 (1%) 68 55	49, 112, 181, 255	0
1	C	332/341 (97%)	-0.03	1 (0%) 94 92	45, 81, 125, 178	0
1	D	327/341 (95%)	0.09	8 (2%) 59 44	59, 109, 168, 236	0
1	G	331/341 (97%)	0.14	6 (1%) 68 55	46, 113, 175, 244	0
1	H	331/341 (97%)	-0.02	1 (0%) 94 92	41, 84, 139, 227	0
1	K	333/341 (97%)	0.10	6 (1%) 68 55	61, 110, 169, 238	0
1	L	329/341 (96%)	0.22	10 (3%) 50 34	66, 118, 178, 233	0
1	O	320/341 (93%)	0.28	15 (4%) 31 19	85, 143, 198, 244	0
1	P	324/341 (95%)	0.23	17 (5%) 27 15	79, 141, 191, 224	0
1	S	259/341 (75%)	0.32	16 (6%) 20 11	74, 145, 210, 255	0
1	T	292/341 (85%)	0.47	28 (9%) 8 4	84, 156, 216, 272	0
2	a	18/18 (100%)	-0.30	0 100 100	61, 77, 104, 107	0
2	b	18/18 (100%)	-0.32	0 100 100	58, 77, 102, 128	0
2	c	18/18 (100%)	-0.27	0 100 100	76, 104, 141, 159	0
2	d	18/18 (100%)	-0.11	1 (5%) 24 13	71, 105, 177, 220	0
2	g	17/18 (94%)	-0.38	0 100 100	54, 85, 118, 141	0
2	h	17/18 (94%)	-0.43	0 100 100	64, 78, 111, 119	0
2	k	17/18 (94%)	-0.21	0 100 100	96, 132, 196, 200	0
2	l	17/18 (94%)	-0.26	0 100 100	90, 121, 214, 226	0
2	o	18/18 (100%)	-0.30	0 100 100	111, 124, 168, 172	0
2	p	17/18 (94%)	-0.49	0 100 100	102, 123, 178, 190	0
2	s	14/18 (77%)	-0.33	0 100 100	110, 144, 153, 191	0
2	t	14/18 (77%)	-0.36	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%)	0.14	125 (3%)	49	32	41, 116, 188, 272	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	180	ASN	5.1
1	T	271	ALA	5.0
1	P	285	LYS	4.8
1	T	270	ILE	4.7
1	S	272	LEU	4.6
1	B	260	GLY	4.5
1	A	290	VAL	4.5
1	T	296	GLU	4.5
1	S	219	THR	4.3
1	T	188	VAL	4.3
1	T	279	ALA	4.2
1	O	202	ILE	4.1
1	S	228	SER	4.1
1	G	199	ILE	4.1
1	O	261	ILE	3.9
2	d	1	DT	3.8
1	B	188	VAL	3.7
1	T	274	ALA	3.7
1	P	261	ILE	3.7
1	T	273	VAL	3.7
1	S	240	PRO	3.6
1	T	280	GLY	3.6
1	O	264	ILE	3.6
1	T	278	ALA	3.5
1	O	298	LEU	3.5
1	G	161	PHE	3.4
1	K	200	ALA	3.4
1	T	173	HIS	3.4
1	B	344	SER	3.4
1	A	260	GLY	3.2
1	O	291	SER	3.2
1	T	228	SER	3.2
1	L	63	TYR	3.2
1	O	226	GLY	3.1
1	G	200	ALA	3.1
1	K	199	ILE	3.1
1	O	253	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	124	MET	3.0
1	L	200	ALA	3.0
1	D	44	PRO	2.9
1	P	200	ALA	2.9
1	K	174	ALA	2.9
1	T	281	VAL	2.8
1	P	268	SER	2.8
1	O	219	THR	2.8
1	A	261	ILE	2.8
1	D	198	ARG	2.7
1	P	134	GLY	2.7
1	O	254	SER	2.7
1	P	258	PRO	2.7
1	T	241	LEU	2.7
1	L	228	SER	2.7
1	B	262	VAL	2.6
1	L	199	ILE	2.6
1	S	202	ILE	2.6
1	T	303	PRO	2.6
1	T	161	PHE	2.6
1	T	272	LEU	2.6
1	K	260	GLY	2.6
1	T	277	GLU	2.6
1	O	214	ALA	2.5
1	S	241	LEU	2.5
1	P	235	ILE	2.5
1	G	279	ALA	2.5
1	O	294	SER	2.5
1	S	273	VAL	2.5
1	D	104	VAL	2.4
1	S	203	VAL	2.4
1	P	276	PHE	2.4
1	P	60	GLN	2.4
1	T	324	LEU	2.4
1	A	258	PRO	2.4
1	O	161	PHE	2.4
1	G	264	ILE	2.4
1	S	236	THR	2.4
1	P	218	PHE	2.3
1	A	347	ALA	2.3
1	T	276	PHE	2.3
1	H	258	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	T	255	ASP	2.3
1	A	287	ILE	2.3
1	S	184	ALA	2.3
1	S	226	GLY	2.3
1	A	259	ASP	2.3
1	L	39	ALA	2.3
1	T	189	GLU	2.3
1	A	199	ILE	2.3
1	D	122	ASP	2.2
1	L	35	THR	2.2
1	T	249	LYS	2.2
1	G	162	VAL	2.2
1	O	255	ASP	2.2
1	P	289	ILE	2.2
1	K	274	ALA	2.2
1	P	27	TYR	2.2
1	B	121	LYS	2.2
1	T	250	ARG	2.2
1	T	184	ALA	2.2
1	S	46	ILE	2.2
1	S	162	VAL	2.1
1	L	331	PRO	2.1
1	P	269	THR	2.1
1	T	36	VAL	2.1
1	L	202	ILE	2.1
1	P	270	ILE	2.1
1	T	268	SER	2.1
1	C	253	GLN	2.1
1	P	319	LEU	2.1
1	A	255	ASP	2.1
1	L	330	ALA	2.1
1	B	322	ALA	2.1
1	P	262	VAL	2.1
1	P	290	VAL	2.1
1	A	272	LEU	2.1
1	O	262	VAL	2.0
1	D	146	PRO	2.0
1	L	261	ILE	2.0
1	S	115	THR	2.0
1	S	270	ILE	2.0
1	S	330	ALA	2.0
1	T	240	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	185	TYR	2.0
1	K	228	SER	2.0
1	D	174	ALA	2.0
1	T	253	GLN	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 monosaccharides 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.