



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:28 AM UTC

PDB ID : 4TW1 / pdb_00004tw1
Title : Crystal structure of the octameric pore complex of the Staphylococcus aureus
Bi-component Toxin LukGH
Authors : Logan, D.T.; Hakansson, M.; Saline, M.; Kimbung, R.; Badarau, A.; Rouha,
H.; Nagy, E.
Deposited on : 2014-06-29
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

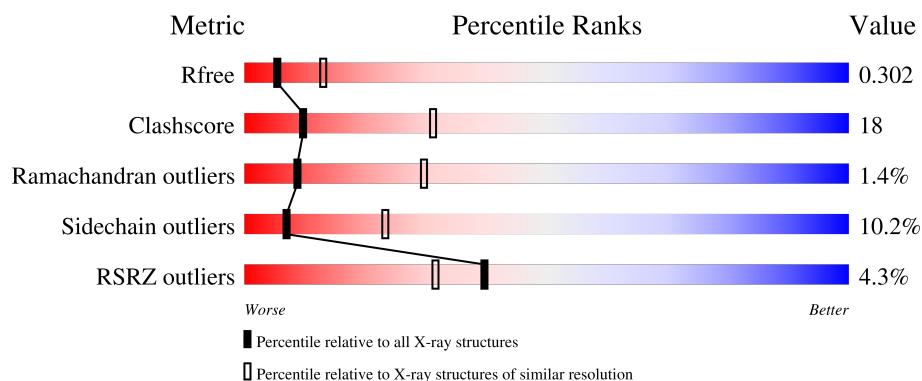
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	311	7% 55% 28% 7% 10%
1	C	311	6% 52% 34% • 10%
1	E	311	6% 56% 32% 5% • 7%
1	G	311	6% 59% 30% • 7%
1	I	311	6% 58% 30% 5% 7%

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Mol	Chain	Length	Quality of chain
1	K	311	
1	M	311	
1	O	311	
2	B	324	
2	D	324	
2	F	324	
2	H	324	
2	J	324	
2	L	324	
2	N	324	
2	P	324	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 37620 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 Possible leukocidin subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2289	1433	399	452	5			
1	C	281	Total	C	N	O	S	0	0	0
			2281	1425	398	453	5			
1	E	290	Total	C	N	O	S	0	0	0
			2356	1475	412	464	5			
1	G	290	Total	C	N	O	S	0	0	0
			2356	1475	412	464	5			
1	I	290	Total	C	N	O	S	0	0	0
			2356	1475	412	464	5			
1	K	281	Total	C	N	O	S	0	0	0
			2293	1438	398	452	5			
1	M	287	Total	C	N	O	S	0	0	0
			2332	1460	408	459	5			
1	O	283	Total	C	N	O	S	0	0	0
			2305	1447	400	453	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP A8Z4S0
A	0	LEU	-	expression tag	UNP A8Z4S0
C	-1	SER	-	expression tag	UNP A8Z4S0
C	0	LEU	-	expression tag	UNP A8Z4S0
E	-1	SER	-	expression tag	UNP A8Z4S0
E	0	LEU	-	expression tag	UNP A8Z4S0
G	-1	SER	-	expression tag	UNP A8Z4S0
G	0	LEU	-	expression tag	UNP A8Z4S0
I	-1	SER	-	expression tag	UNP A8Z4S0
I	0	LEU	-	expression tag	UNP A8Z4S0
K	-1	SER	-	expression tag	UNP A8Z4S0
K	0	LEU	-	expression tag	UNP A8Z4S0
M	-1	SER	-	expression tag	UNP A8Z4S0

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Chain	Residue	Modelled	Actual	Comment	Reference
M	0	LEU	-	expression tag	UNP A8Z4S0
O	-1	SER	-	expression tag	UNP A8Z4S0
O	0	LEU	-	expression tag	UNP A8Z4S0

- Molecule 2 is a protein called Possible leukocidin subunit.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	282	Total	C	N	O	0	0	0
			2320	1462	405	453			
2	D	289	Total	C	N	O	0	0	0
			2373	1496	413	464			
2	F	284	Total	C	N	O	0	0	0
			2340	1477	407	456			
2	H	288	Total	C	N	O	0	0	0
			2366	1492	412	462			
2	J	288	Total	C	N	O	0	0	0
			2366	1492	412	462			
2	L	288	Total	C	N	O	0	0	0
			2366	1492	412	462			
2	N	288	Total	C	N	O	0	0	0
			2366	1492	412	462			
2	P	286	Total	C	N	O	0	0	0
			2350	1482	409	459			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		
3	B	15	Total	O	0	0
			15	15		
3	C	11	Total	O	0	0
			11	11		
3	D	8	Total	O	0	0
			8	8		
3	E	11	Total	O	0	0
			11	11		
3	F	17	Total	O	0	0
			17	17		
3	G	13	Total	O	0	0
			13	13		
3	H	18	Total	O	0	0
			18	18		

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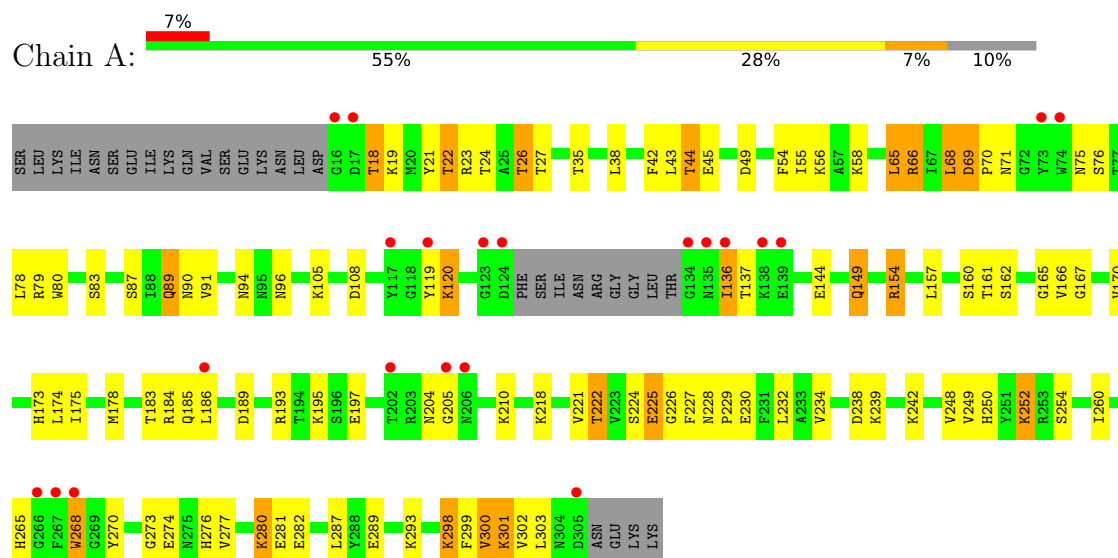
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	10	Total	O	0	0
			10	10		
3	J	17	Total	O	0	0
			17	17		
3	K	12	Total	O	0	0
			12	12		
3	L	16	Total	O	0	0
			16	16		
3	M	11	Total	O	0	0
			11	11		
3	N	9	Total	O	0	0
			9	9		
3	O	11	Total	O	0	0
			11	11		
3	P	17	Total	O	0	0
			17	17		

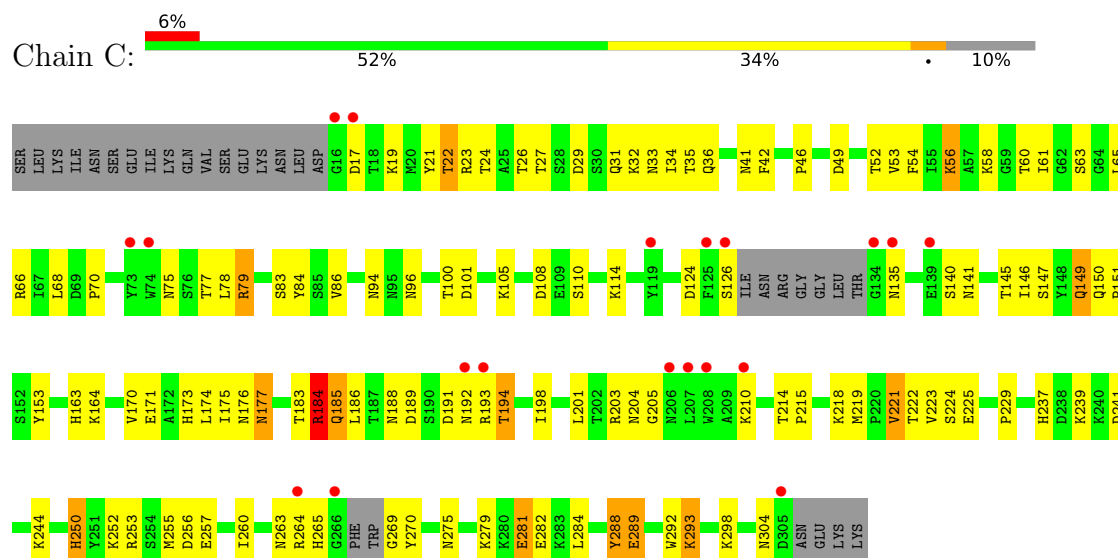
3 Residue-property plots

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: Possible leukocidin subunit

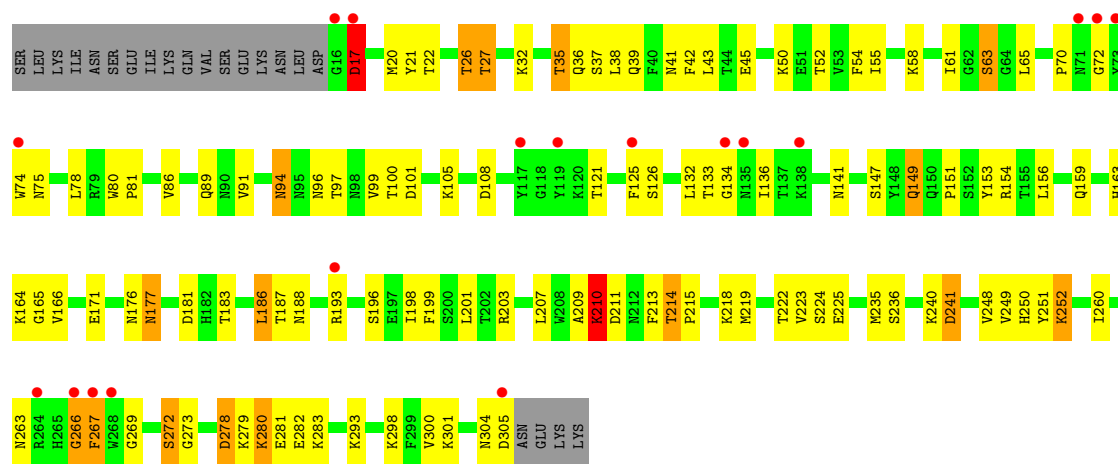


• Molecule 1: Possible leukocidin subunit

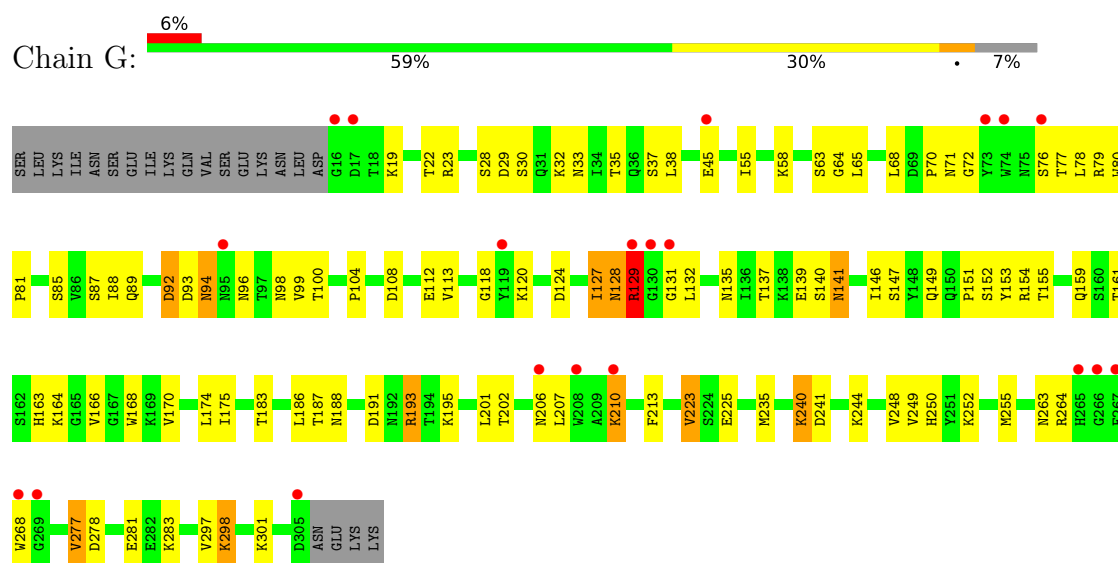


• Molecule 1: Possible leukocidin subunit

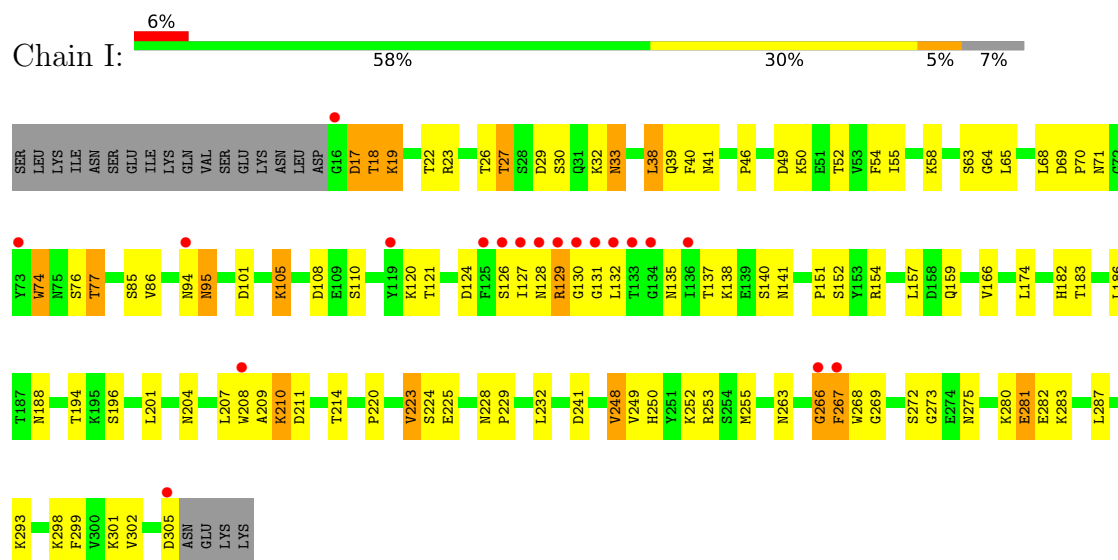




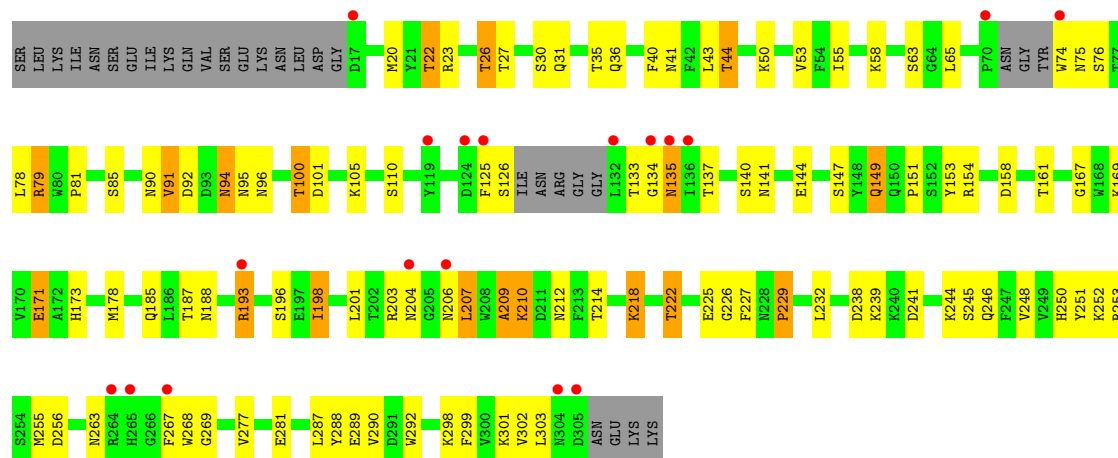
• Molecule 1: Possible leukocidin subunit



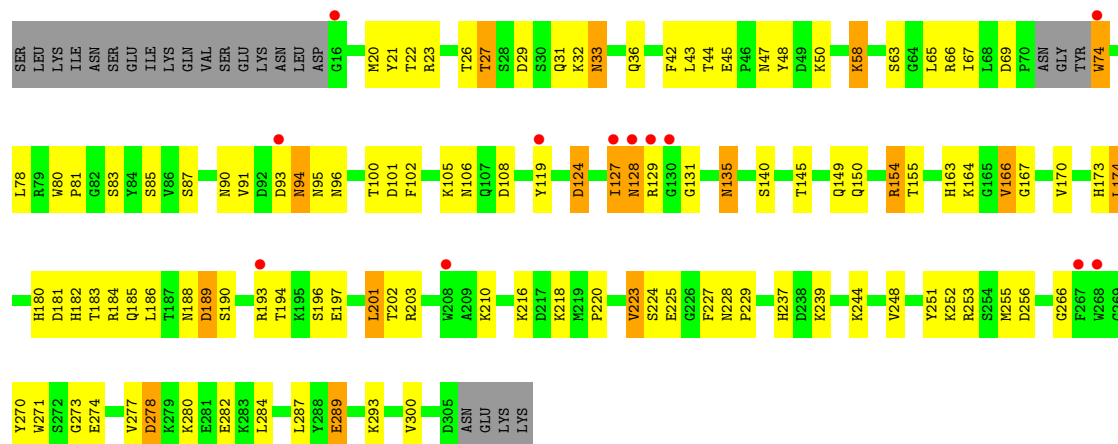
• Molecule 1: Possible leukocidin subunit



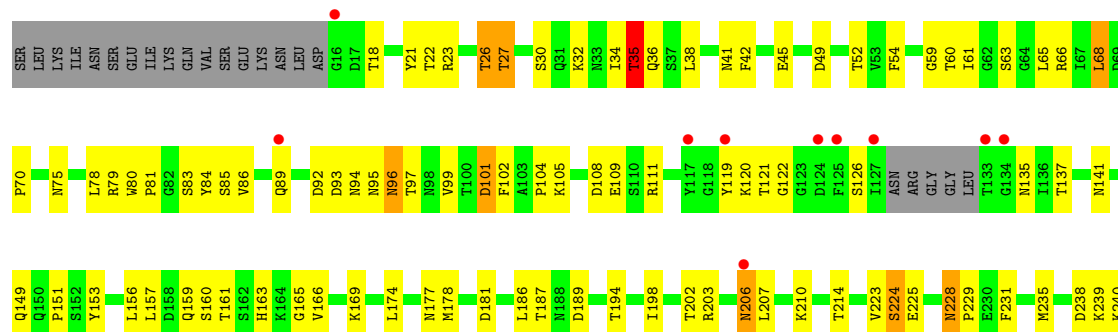
• Molecule 1: Possible leukocidin subunit



• Molecule 1: Possible leukocidin subunit

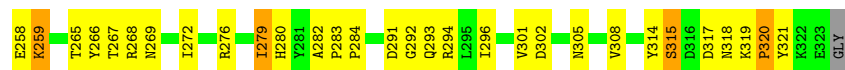
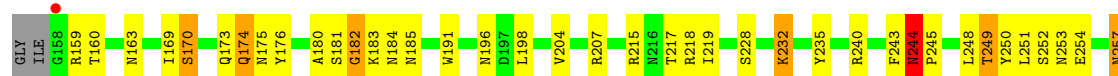
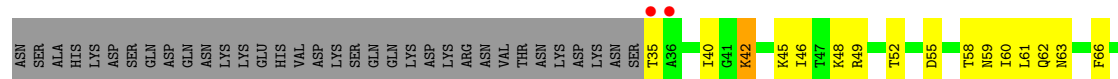


• Molecule 1: Possible leukocidin subunit

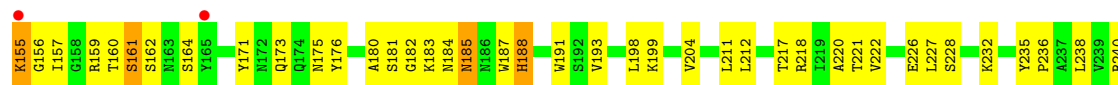
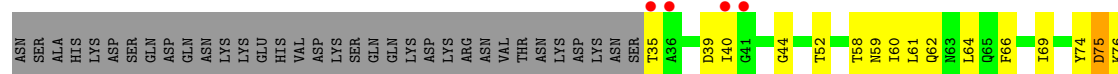




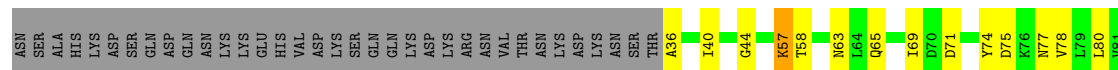
• Molecule 2: Possible leukocidin subunit

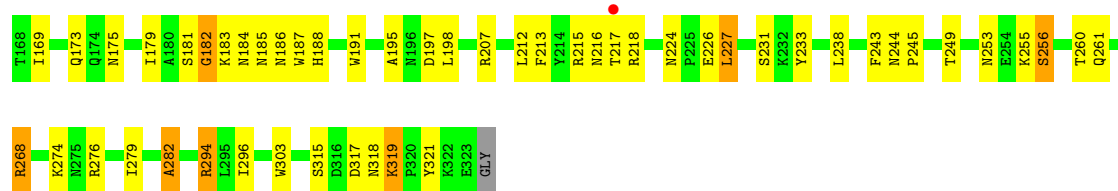


• Molecule 2: Possible leukocidin subunit

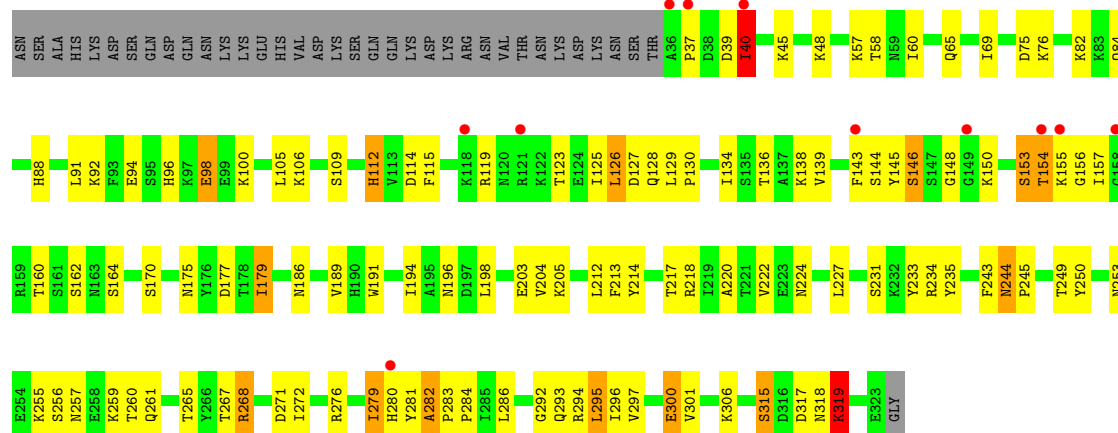


• Molecule 2: Possible leukocidin subunit

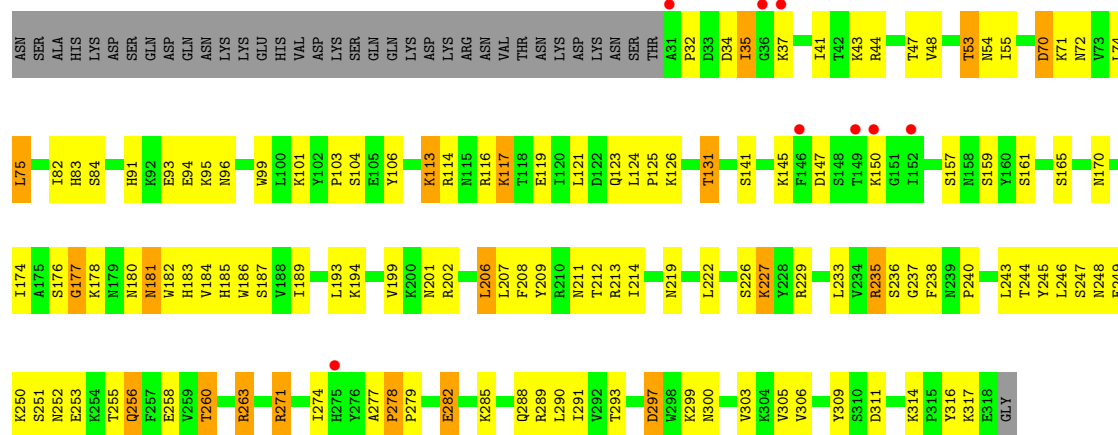




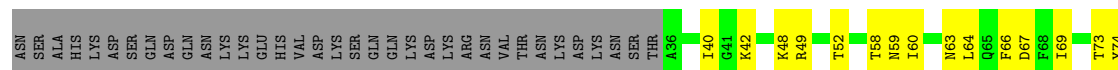
• Molecule 2: Possible leukocidin subunit

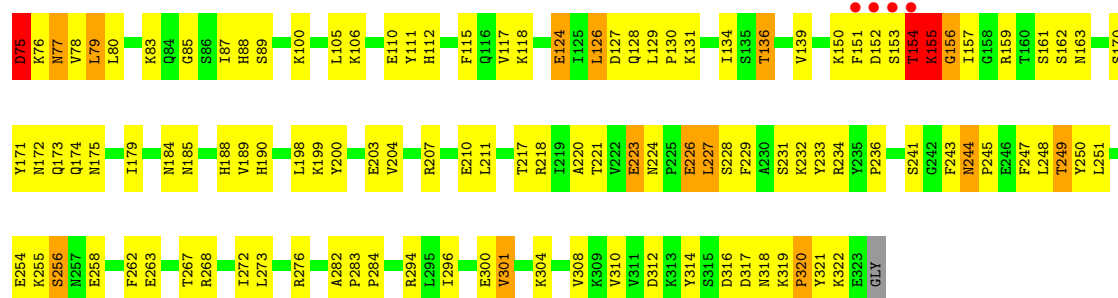


• Molecule 2: Possible leukocidin subunit

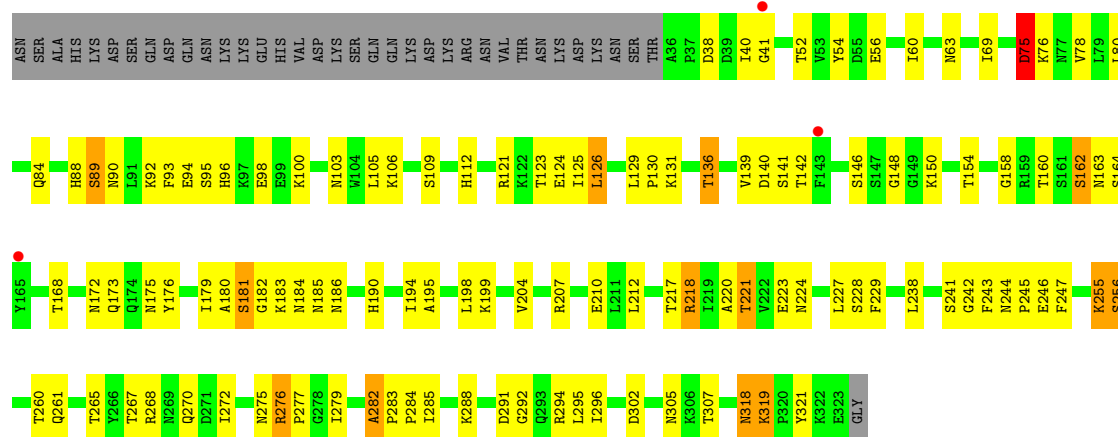


• Molecule 2: Possible leukocidin subunit

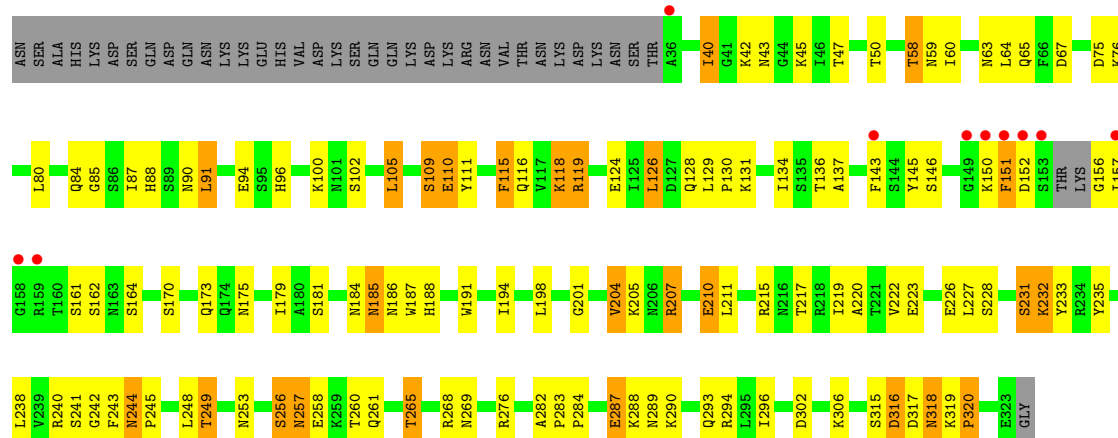




• Molecule 2: Possible leukocidin subunit



• Molecule 2: Possible leukocidin subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.50Å 198.56Å 179.53Å 90.00° 103.26° 90.00°	Depositor
Resolution (Å)	48.00 – 2.80 48.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (48.00-2.80) 96.3 (48.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.238 , 0.292 0.248 , 0.302	Depositor DCC
R_{free} test set	2207 reflections (0.97%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	37620	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% 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	0.90	0/2345	1.17	8/3170 (0.3%)
1	C	0.87	0/2334	1.11	2/3152 (0.1%)
1	E	0.88	0/2414	1.14	7/3264 (0.2%)
1	G	0.89	0/2414	1.14	8/3264 (0.2%)
1	I	0.89	1/2414 (0.0%)	1.16	7/3264 (0.2%)
1	K	0.90	0/2348	1.19	8/3173 (0.3%)
1	M	0.91	0/2388	1.14	5/3227 (0.2%)
1	O	0.92	1/2362 (0.0%)	1.16	8/3193 (0.3%)
2	B	0.92	1/2371 (0.0%)	1.21	10/3202 (0.3%)
2	D	0.92	1/2426 (0.0%)	1.18	12/3277 (0.4%)
2	F	0.87	0/2392	1.21	16/3230 (0.5%)
2	H	0.92	1/2419 (0.0%)	1.17	9/3267 (0.3%)
2	J	0.93	1/2419 (0.0%)	1.22	10/3267 (0.3%)
2	L	0.97	1/2419 (0.0%)	1.18	13/3267 (0.4%)
2	N	0.90	1/2419 (0.0%)	1.18	14/3267 (0.4%)
2	P	0.90	0/2402	1.20	7/3243 (0.2%)
All	All	0.91	8/38286 (0.0%)	1.17	144/51727 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	G	0	2
1	I	0	1
1	K	0	1
2	F	0	1
2	L	0	2
2	N	0	1
2	P	0	1
All	All	0	10

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	44	GLY	N-CA	6.70	1.51	1.45
2	N	185	ASN	CA-C	-6.30	1.44	1.53
2	B	185	ASN	CA-C	-5.69	1.45	1.52
2	H	257	ASN	CA-C	-5.38	1.46	1.53
2	L	79	LEU	CA-C	-5.33	1.46	1.52
2	J	180	ASN	CA-C	-5.15	1.45	1.53
1	I	301	LYS	CA-C	-5.09	1.46	1.52
1	O	206	ASN	CA-CB	5.01	1.59	1.52

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	GLU	N-CA-C	8.16	119.95	111.14
2	H	156	GLY	N-CA-C	7.74	124.99	112.61
1	A	80	TRP	N-CA-C	7.50	114.97	108.22
1	K	100	THR	N-CA-C	-7.26	104.28	113.43
1	A	228	ASN	CA-C-N	-7.25	113.21	120.31
1	A	228	ASN	C-N-CA	-7.25	113.21	120.31
2	L	244	ASN	CA-C-N	7.24	127.28	119.90
2	L	244	ASN	C-N-CA	7.24	127.28	119.90
2	J	278	PRO	CA-C-N	7.11	127.07	120.03
2	J	278	PRO	C-N-CA	7.11	127.07	120.03
2	D	44	GLY	N-CA-C	6.95	119.09	112.08
1	G	131	GLY	N-CA-C	6.88	123.00	112.81
2	P	42	LYS	N-CA-C	6.82	119.73	111.82
1	G	129	ARG	N-CA-C	-6.78	98.21	109.46
2	L	155	LYS	N-CA-C	-6.61	105.61	113.21
2	B	235	TYR	CA-C-N	6.60	126.96	119.83
2	B	235	TYR	C-N-CA	6.60	126.96	119.83
2	D	180	ALA	N-CA-C	-6.58	100.74	110.48
2	F	158	GLY	N-CA-C	6.57	124.99	112.51
1	C	192	ASN	N-CA-C	6.53	119.49	110.35
2	N	148	GLY	N-CA-C	6.47	121.86	110.80
1	K	207	LEU	N-CA-C	-6.45	100.67	109.95
2	H	194	ILE	N-CA-C	6.41	117.08	108.11
1	O	207	LEU	N-CA-C	-6.35	99.93	109.96
1	I	18	THR	N-CA-C	6.34	118.05	110.19
2	B	42	LYS	N-CA-C	6.29	118.66	111.11
1	I	95	ASN	N-CA-C	6.27	124.15	110.80
2	N	176	TYR	N-CA-C	6.25	119.32	108.76
2	F	282	ALA	CA-C-N	-6.25	113.94	120.38
2	F	282	ALA	C-N-CA	-6.25	113.94	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	209	ALA	N-CA-C	-6.24	104.17	110.97
1	K	141	ASN	N-CA-C	6.22	118.52	108.32
2	D	296	ILE	N-CA-C	6.21	115.66	106.85
2	B	180	ALA	N-CA-C	-6.20	101.76	110.50
2	P	194	ILE	N-CA-C	6.18	117.11	107.28
2	F	44	GLY	N-CA-C	6.16	117.81	111.95
2	D	74	TYR	CA-C-N	6.15	128.52	120.28
2	D	74	TYR	C-N-CA	6.15	128.52	120.28
2	P	265	THR	N-CA-C	6.10	118.89	108.02
2	N	75	ASP	CB-CA-C	-6.05	100.39	110.68
2	J	101	LYS	N-CA-C	6.00	117.00	108.54
1	M	278	ASP	N-CA-C	5.97	119.66	111.54
2	L	301	VAL	CB-CA-C	-5.96	103.05	111.21
2	P	257	ASN	N-CA-C	-5.94	99.05	108.73
2	N	41	GLY	N-CA-C	5.93	121.00	113.24
2	J	303	VAL	N-CA-C	5.90	116.58	107.78
1	G	278	ASP	N-CA-C	5.87	119.45	111.17
1	O	18	THR	N-CA-C	-5.84	101.87	110.52
2	F	74	TYR	CA-C-N	5.83	128.37	120.38
2	F	74	TYR	C-N-CA	5.83	128.37	120.38
2	L	74	TYR	CA-C-N	5.83	128.09	120.28
2	L	74	TYR	C-N-CA	5.83	128.09	120.28
2	F	319	LYS	CA-C-N	-5.81	113.80	119.78
2	F	319	LYS	C-N-CA	-5.81	113.80	119.78
2	L	310	VAL	N-CA-C	-5.81	101.31	109.21
1	E	61	ILE	CB-CA-C	-5.80	102.59	110.42
2	L	312	ASP	N-CA-C	5.79	117.20	108.46
2	J	229	ARG	N-CA-CB	-5.78	101.78	110.73
1	K	204	ASN	N-CA-C	5.76	120.69	113.43
2	N	244	ASN	CA-C-N	-5.73	114.07	119.85
2	N	244	ASN	C-N-CA	-5.73	114.07	119.85
1	A	265	HIS	N-CA-C	5.72	117.97	108.13
2	F	120	ASN	N-CA-C	-5.71	100.48	109.50
2	B	117	VAL	N-CA-C	-5.70	102.23	109.58
1	C	141	ASN	N-CA-C	5.68	116.78	108.14
2	N	158	GLY	N-CA-C	5.68	119.44	111.14
2	J	174	ILE	N-CA-C	5.68	116.04	107.80
1	G	207	LEU	N-CA-C	-5.66	101.02	109.96
2	N	180	ALA	N-CA-C	-5.60	102.19	110.48
2	N	181	SER	N-CA-C	5.60	117.81	109.25
1	I	223	VAL	CB-CA-C	-5.59	104.72	112.04
1	K	292	TRP	N-CA-C	5.58	118.29	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	141	ASN	N-CA-C	5.55	117.53	108.76
1	E	17	ASP	CA-C-N	5.55	129.65	120.94
1	E	17	ASP	C-N-CA	5.55	129.65	120.94
2	B	244	ASN	CA-C-N	5.54	126.02	120.14
2	B	244	ASN	C-N-CA	5.54	126.02	120.14
2	N	282	ALA	CA-C-N	-5.54	114.68	120.38
2	N	282	ALA	C-N-CA	-5.54	114.68	120.38
2	H	319	LYS	CA-C-N	-5.53	114.07	119.76
2	H	319	LYS	C-N-CA	-5.53	114.07	119.76
2	L	73	THR	CB-CA-C	-5.52	101.39	110.72
2	F	164	SER	N-CA-C	5.50	117.39	108.26
1	E	39	GLN	N-CA-C	5.50	117.39	108.26
2	J	305	VAL	N-CA-C	-5.48	100.53	108.87
2	J	180	ASN	CB-CA-C	-5.46	102.01	112.43
2	D	275	ASN	N-CA-C	5.46	118.33	109.06
1	G	141	ASN	N-CA-C	5.42	117.50	108.99
1	O	228	ASN	CB-CA-C	-5.42	103.30	110.34
2	L	172	ASN	N-CA-C	5.40	118.05	109.24
2	H	282	ALA	CA-C-N	-5.40	115.72	119.66
2	H	282	ALA	C-N-CA	-5.40	115.72	119.66
1	M	135	ASN	N-CA-C	5.40	117.28	109.07
2	B	176	TYR	N-CA-C	5.39	118.19	109.40
2	L	117	VAL	N-CA-C	-5.36	102.66	109.58
2	N	185	ASN	CB-CA-C	-5.36	101.35	112.44
1	O	35	THR	CB-CA-C	5.35	118.38	110.14
2	D	188	HIS	N-CA-C	5.35	116.91	107.61
2	N	255	LYS	N-CA-C	-5.34	103.29	110.24
1	I	27	THR	N-CA-C	5.31	117.03	108.32
1	A	162	SER	CB-CA-C	-5.31	106.86	114.87
1	I	17	ASP	N-CA-C	5.30	120.76	113.97
2	P	223	GLU	N-CA-C	-5.30	105.55	112.23
1	G	301	LYS	N-CA-C	-5.30	100.38	108.76
2	D	122	LYS	N-CA-C	-5.28	106.81	113.20
1	E	72	GLY	N-CA-C	5.26	118.39	111.03
2	F	75	ASP	N-CA-C	5.25	117.68	111.33
2	D	282	ALA	CA-C-N	-5.25	114.98	120.38
2	D	282	ALA	C-N-CA	-5.25	114.98	120.38
1	A	161	THR	N-CA-C	-5.24	102.63	110.23
1	A	160	SER	N-CA-C	-5.24	106.57	113.17
2	H	40	ILE	N-CA-C	5.23	116.70	111.00
1	O	224	SER	N-CA-C	5.23	117.72	111.71
1	G	223	VAL	N-CA-C	-5.22	107.32	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	270	TYR	N-CA-C	5.19	116.96	109.07
1	O	84	TYR	N-CA-C	-5.19	101.65	109.85
2	N	172	ASN	N-CA-C	5.18	118.26	109.76
2	F	279	ILE	N-CA-C	5.18	119.45	112.98
2	D	75	ASP	CB-CA-C	-5.17	102.21	110.79
2	H	112	HIS	N-CA-C	5.16	117.81	109.40
2	F	71	ASP	CA-C-N	-5.16	114.35	119.56
2	F	71	ASP	C-N-CA	-5.16	114.35	119.56
1	M	271	TRP	N-CA-C	5.15	117.10	107.99
1	O	101	ASP	N-CA-C	5.14	115.83	108.74
2	J	41	ILE	CB-CA-C	-5.13	104.55	110.91
2	J	260	THR	N-CA-C	5.13	115.78	107.32
2	P	58	THR	CB-CA-C	-5.09	101.58	110.09
2	D	136	THR	CB-CA-C	-5.09	98.87	110.07
2	F	57	LYS	N-CA-C	-5.09	105.42	110.97
2	F	294	ARG	N-CA-C	5.08	116.97	108.99
1	K	53	VAL	N-CA-C	5.08	115.29	107.77
2	H	315	SER	N-CA-C	5.07	116.89	109.24
2	B	107	TYR	CA-C-N	5.06	126.16	119.84
2	B	107	TYR	C-N-CA	5.06	126.16	119.84
1	K	74	TRP	CA-CB-CG	5.05	123.20	113.60
1	M	58	LYS	CB-CA-C	-5.05	109.79	117.07
1	I	130	GLY	N-CA-C	-5.05	108.64	115.36
1	G	248	VAL	N-CA-C	-5.05	101.21	108.48
1	E	278	ASP	N-CA-C	5.02	121.50	110.80
2	L	134	ILE	N-CA-C	-5.01	103.04	109.30
2	L	300	GLU	N-CA-C	5.01	116.79	108.02
2	P	185	ASN	CB-CA-C	-5.01	100.44	110.42
1	M	90	ASN	N-CA-C	-5.01	103.07	110.48
1	E	186	LEU	N-CA-C	5.01	117.12	111.11

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	94	ASN	Peptide
2	F	36	ALA	Peptide
1	G	128	ASN	Peptide
1	G	93	ASP	Peptide
1	I	94	ASN	Peptide
1	K	229	PRO	Peptide
2	L	156	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	L	75	ASP	Peptide
2	N	75	ASP	Peptide
2	P	256	SER	Peptide

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	2289	0	2171	74	0
1	C	2281	0	2165	83	0
1	E	2356	0	2240	79	0
1	G	2356	0	2240	65	0
1	I	2356	0	2240	85	0
1	K	2293	0	2181	70	0
1	M	2332	0	2221	94	0
1	O	2305	0	2193	79	0
2	B	2320	0	2268	109	0
2	D	2373	0	2321	110	0
2	F	2340	0	2285	96	0
2	H	2366	0	2314	94	0
2	J	2366	0	2314	99	0
2	L	2366	0	2314	108	0
2	N	2366	0	2314	101	0
2	P	2350	0	2293	101	0
3	A	9	0	0	2	0
3	B	15	0	0	4	0
3	C	11	0	0	0	0
3	D	8	0	0	1	0
3	E	11	0	0	2	0
3	F	17	0	0	2	0
3	G	13	0	0	1	0
3	H	18	0	0	1	0
3	I	10	0	0	0	0
3	J	17	0	0	2	0
3	K	12	0	0	1	0
3	L	16	0	0	1	0
3	M	11	0	0	1	0
3	N	9	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	11	0	0	0	0
3	P	17	0	0	3	0
All	All	37620	0	36074	1303	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 18.

All (1303) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:LYS:H	2:B:100:LYS:HD2	1.08	1.16
1:E:183:THR:HG21	3:E:409:HOH:O	1.47	1.13
2:F:88:HIS:HB3	1:G:159:GLN:HG2	1.32	1.12
2:B:170:SER:HB3	3:B:413:HOH:O	1.53	1.09
1:M:26:THR:HG23	2:N:186:ASN:HD22	1.16	1.09
2:L:75:ASP:HB3	2:L:76:LYS:HG3	1.33	1.08
2:H:294:ARG:HH21	2:H:319:LYS:HD3	1.11	1.07
2:D:287:GLU:OE1	2:D:290:LYS:HD3	1.56	1.03
2:B:80:LEU:HD11	2:B:248:LEU:HD23	1.40	1.03
2:N:224:ASN:HB3	2:N:227:LEU:HD12	1.35	1.03
2:B:100:LYS:HB2	2:B:276:ARG:NH2	1.72	1.02
2:P:88:HIS:O	2:P:268:ARG:NH1	1.92	1.02
2:F:100:LYS:HB3	2:F:276:ARG:NH1	1.74	1.02
2:L:80:LEU:HD11	2:L:248:LEU:CD2	1.90	1.01
2:P:207:ARG:HG2	2:P:207:ARG:HH11	1.23	1.00
1:K:253:ARG:HE	1:K:255:MET:HE2	1.27	0.98
2:J:70:ASP:HB3	2:J:71:LYS:HG3	1.43	0.97
1:O:177:ASN:HD21	1:O:214:THR:HG21	1.29	0.96
1:A:183:THR:HG21	3:A:409:HOH:O	1.63	0.96
2:L:175:ASN:HB2	1:M:108:ASP:OD1	1.65	0.96
1:K:149:GLN:NE2	1:K:149:GLN:HA	1.80	0.95
1:O:26:THR:HG23	2:P:186:ASN:HD22	1.31	0.95
1:C:101:ASP:OD1	1:C:105:LYS:NZ	1.98	0.95
2:B:58:THR:O	2:B:268:ARG:NH2	1.99	0.94
2:B:294:ARG:HH12	2:B:296:ILE:HD11	1.32	0.94
2:H:294:ARG:HH21	2:H:319:LYS:CD	1.81	0.94
1:M:244:LYS:HD3	1:M:289:GLU:OE2	1.67	0.93
2:J:53:THR:O	2:J:263:ARG:NH2	2.01	0.93
2:L:58:THR:O	2:L:268:ARG:NH2	2.01	0.93
1:M:26:THR:CG2	2:N:186:ASN:HD22	1.80	0.93
1:K:94:ASN:HD21	1:K:96:ASN:CG	1.75	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:SER:HB3	1:C:184:ARG:HH21	1.35	0.92
1:M:26:THR:HG23	2:N:186:ASN:ND2	1.85	0.92
2:B:88:HIS:O	2:B:268:ARG:NH1	2.02	0.92
2:D:316:ASP:OD2	2:D:319:LYS:HG3	1.69	0.92
2:N:75:ASP:HB3	2:N:76:LYS:HG3	1.51	0.92
2:H:58:THR:O	2:H:268:ARG:NH2	2.02	0.92
2:B:276:ARG:HH11	2:B:282:ALA:HB3	1.35	0.92
1:C:65:LEU:HD11	1:C:78:LEU:HD11	1.52	0.91
2:B:83:LYS:NZ	2:B:249:THR:HG23	1.83	0.91
2:L:106:LYS:HG2	2:L:272:ILE:HG12	1.49	0.91
2:B:100:LYS:H	2:B:100:LYS:CD	1.79	0.91
2:P:75:ASP:HB3	2:P:76:LYS:HG3	1.53	0.90
2:J:186:TRP:HH2	2:J:244:THR:CG2	1.85	0.90
2:L:80:LEU:HD11	2:L:248:LEU:HD23	1.52	0.89
1:O:35:THR:HG21	2:P:184:ASN:O	1.72	0.89
2:F:294:ARG:HH11	2:F:296:ILE:HD11	1.36	0.88
2:J:186:TRP:HH2	2:J:244:THR:HG22	1.38	0.88
1:K:44:THR:HG22	1:K:44:THR:O	1.71	0.88
2:H:88:HIS:O	2:H:268:ARG:NH1	2.06	0.88
2:B:83:LYS:HZ1	2:B:249:THR:HG23	1.36	0.88
2:B:75:ASP:HB3	2:B:76:LYS:HG3	1.56	0.88
2:D:260:THR:HG22	2:D:261:GLN:H	1.40	0.87
2:L:40:ILE:HG21	2:L:126:LEU:HD23	1.54	0.87
1:I:68:LEU:HD12	1:I:77:THR:CG2	2.05	0.87
2:B:294:ARG:HE	2:B:319:LYS:HE3	1.41	0.86
1:K:22:THR:O	1:K:23:ARG:HD3	1.75	0.86
1:C:68:LEU:HD12	1:C:77:THR:HG22	1.56	0.86
2:L:294:ARG:NH1	2:L:296:ILE:HD11	1.90	0.85
1:I:22:THR:O	1:I:23:ARG:HD3	1.77	0.85
2:L:319:LYS:O	2:L:320:PRO:O	1.93	0.84
2:H:92:LYS:HE3	2:H:94:GLU:OE2	1.77	0.84
1:I:64:GLY:HA3	1:I:255:MET:HE1	1.58	0.84
1:C:70:PRO:O	1:C:210:LYS:HG3	1.77	0.84
2:D:58:THR:O	2:D:268:ARG:NH2	2.10	0.84
1:G:70:PRO:O	1:G:210:LYS:HE2	1.78	0.84
1:C:22:THR:O	1:C:23:ARG:HD3	1.77	0.84
1:O:79:ARG:HG2	1:O:255:MET:HE3	1.58	0.84
2:B:122:LYS:HB2	2:B:257:ASN:ND2	1.92	0.84
1:E:26:THR:HG23	2:F:186:ASN:HD22	1.43	0.84
2:J:53:THR:HG22	2:J:288:GLN:HB3	1.60	0.83
2:P:40:ILE:HG21	2:P:126:LEU:HD23	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:THR:HG22	1:A:45:GLU:HA	1.60	0.83
1:E:65:LEU:HD11	1:E:78:LEU:HD11	1.58	0.83
2:F:58:THR:O	2:F:268:ARG:NH2	2.12	0.83
1:I:70:PRO:O	1:I:210:LYS:HB2	1.79	0.83
2:P:294:ARG:HH11	2:P:296:ILE:HD11	1.43	0.82
1:O:228:ASN:OD1	2:P:131:LYS:HB3	1.79	0.82
2:L:80:LEU:HD11	2:L:248:LEU:HD22	1.61	0.81
2:B:100:LYS:HD2	2:B:100:LYS:N	1.93	0.81
2:D:80:LEU:HD11	2:D:248:LEU:HD22	1.63	0.81
1:A:26:THR:OG1	2:B:124:GLU:OE1	1.98	0.81
2:D:260:THR:HG22	2:D:261:GLN:N	1.97	0.80
1:M:22:THR:O	1:M:23:ARG:HD3	1.80	0.80
2:F:127:ASP:OD1	2:F:131:LYS:HE3	1.81	0.80
1:I:18:THR:HG22	1:I:19:LYS:N	1.97	0.80
2:P:191:TRP:HH2	2:P:249:THR:HG22	1.47	0.80
2:B:259:LYS:HE2	2:B:302:ASP:HB2	1.64	0.80
2:D:144:SER:HB2	2:D:164:SER:HB2	1.64	0.80
2:N:40:ILE:HG21	2:N:126:LEU:HD23	1.64	0.80
2:L:294:ARG:HH12	2:L:296:ILE:HD11	1.46	0.79
2:F:255:LYS:O	2:F:256:SER:HB3	1.82	0.79
2:H:96:HIS:HB3	2:H:98:GLU:OE2	1.82	0.79
2:B:100:LYS:CB	2:B:276:ARG:HH21	1.96	0.79
1:C:65:LEU:CD1	1:C:78:LEU:HD11	2.13	0.79
1:I:253:ARG:HE	1:I:255:MET:HE2	1.48	0.79
2:F:40:ILE:HG21	2:F:126:LEU:HD23	1.63	0.79
2:F:294:ARG:NH1	2:F:296:ILE:HD11	1.98	0.78
2:H:294:ARG:NH2	2:H:319:LYS:HD3	1.95	0.78
2:D:106:LYS:HG2	2:D:272:ILE:HG12	1.66	0.78
2:D:211:LEU:N	2:D:211:LEU:HD12	1.98	0.77
1:C:263:ASN:HD22	1:C:270:TYR:HE1	1.33	0.77
1:A:19:LYS:HE2	1:A:21:TYR:CZ	2.20	0.77
2:B:276:ARG:HH11	2:B:282:ALA:CB	1.96	0.77
2:D:154:THR:HG22	2:D:155:LYS:HG2	1.67	0.77
1:O:149:GLN:HG3	2:P:136:THR:HG21	1.67	0.77
2:P:58:THR:O	2:P:268:ARG:NH2	2.19	0.76
1:K:126:SER:OG	1:K:133:THR:HB	1.86	0.76
1:A:35:THR:HB	3:B:414:HOH:O	1.85	0.76
2:N:294:ARG:CZ	2:N:319:LYS:HD3	2.15	0.76
2:H:217:THR:HG21	2:H:220:ALA:HB2	1.68	0.76
2:L:75:ASP:CB	2:L:76:LYS:HG3	2.15	0.76
1:E:38:LEU:HD21	1:E:249:VAL:HG21	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:157:ILE:HG22	2:F:158:GLY:H	1.49	0.76
1:A:298:LYS:HG2	1:A:299:PHE:O	1.86	0.75
2:F:294:ARG:HH21	2:F:319:LYS:HG2	1.51	0.75
1:M:173:HIS:CE1	1:M:174:LEU:HD12	2.21	0.75
2:B:100:LYS:HB2	2:B:276:ARG:HH21	1.48	0.75
2:F:175:ASN:HB2	1:G:108:ASP:OD1	1.86	0.75
2:F:77:ASN:HB2	2:F:253:ASN:HB3	1.68	0.75
1:A:38:LEU:HD21	1:A:249:VAL:HG21	1.67	0.74
1:C:68:LEU:HD12	1:C:77:THR:CG2	2.17	0.74
2:N:276:ARG:HB2	2:N:276:ARG:HH11	1.51	0.74
1:G:64:GLY:HA3	1:G:255:MET:HE1	1.68	0.74
2:L:87:ILE:HG21	2:L:111:TYR:HD1	1.53	0.74
2:N:243:PHE:CE2	2:N:245:PRO:HB3	2.22	0.74
1:I:266:GLY:O	1:I:267:PHE:HB2	1.88	0.74
2:H:144:SER:HB2	2:H:164:SER:OG	1.87	0.74
2:N:75:ASP:CB	2:N:76:LYS:HG3	2.18	0.74
1:O:178:MET:HE2	1:O:203:ARG:HH21	1.52	0.74
2:L:162:SER:C	2:L:163:ASN:HD22	1.95	0.73
1:O:177:ASN:HD21	1:O:214:THR:CG2	2.01	0.73
2:J:147:ASP:HB3	2:J:150:LYS:HB2	1.70	0.73
1:I:101:ASP:OD1	1:I:105:LYS:NZ	2.20	0.73
1:K:149:GLN:NE2	1:K:149:GLN:CA	2.50	0.73
1:A:49:ASP:O	1:A:239:LYS:HD2	1.87	0.73
2:H:128:GLN:N	2:H:128:GLN:OE1	2.22	0.73
1:G:29:ASP:CG	1:G:32:LYS:HG2	2.13	0.73
1:I:68:LEU:HD12	1:I:77:THR:HG21	1.70	0.73
1:I:68:LEU:HD12	1:I:77:THR:HG22	1.71	0.73
1:O:177:ASN:ND2	1:O:214:THR:HG21	2.04	0.73
2:D:191:TRP:HH2	2:D:249:THR:HG22	1.54	0.72
1:M:65:LEU:HD22	1:M:224:SER:HA	1.70	0.72
1:O:65:LEU:HD22	1:O:224:SER:HA	1.71	0.72
1:G:240:LYS:HG3	1:G:241:ASP:N	2.03	0.72
2:L:221:THR:HG22	2:L:227:LEU:HD13	1.71	0.72
1:A:183:THR:CG2	3:A:409:HOH:O	2.29	0.72
1:I:74:TRP:HA	1:I:74:TRP:CE3	2.25	0.72
1:G:22:THR:O	1:G:23:ARG:HD3	1.89	0.72
2:L:75:ASP:HB3	2:L:76:LYS:CG	2.18	0.72
1:A:21:TYR:HB2	1:A:42:PHE:HB2	1.72	0.72
1:O:49:ASP:O	1:O:239:LYS:HD2	1.89	0.72
1:O:66:ARG:NH1	1:O:68:LEU:HD23	2.04	0.72
2:P:243:PHE:C	2:P:244:ASN:HD22	1.97	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:SER:HB3	1:C:184:ARG:NH2	2.05	0.71
1:I:151:PRO:HB3	2:J:131:THR:HG23	1.70	0.71
1:K:301:LYS:HG2	1:K:302:VAL:O	1.89	0.71
1:K:154:ARG:HD3	1:K:173:HIS:CD2	2.26	0.71
1:M:74:TRP:CE3	1:M:74:TRP:HA	2.23	0.71
2:P:243:PHE:CE2	2:P:245:PRO:HB3	2.25	0.71
1:C:214:THR:O	1:C:219:MET:HE3	1.91	0.71
2:H:75:ASP:CB	2:H:76:LYS:HG3	2.20	0.71
1:C:24:THR:HG21	2:D:126:LEU:HD11	1.71	0.71
1:A:280:LYS:NZ	1:A:282:GLU:HG2	2.06	0.71
1:A:94:ASN:ND2	1:A:96:ASN:OD1	2.23	0.70
2:F:159:ARG:HD2	1:M:127:ILE:HG12	1.72	0.70
2:P:294:ARG:NH1	2:P:296:ILE:HD11	2.06	0.70
2:B:319:LYS:O	2:B:320:PRO:O	2.09	0.70
1:C:281:GLU:CG	1:C:281:GLU:O	2.38	0.70
2:B:276:ARG:NH1	2:B:282:ALA:CB	2.54	0.70
2:F:100:LYS:HB3	2:F:276:ARG:HH12	1.52	0.70
1:I:65:LEU:HD22	1:I:224:SER:HA	1.73	0.70
2:F:88:HIS:CB	1:G:159:GLN:HG2	2.18	0.70
2:D:212:LEU:HD23	2:D:273:LEU:HD11	1.73	0.70
2:H:260:THR:HG22	2:H:261:GLN:H	1.56	0.70
1:O:63:SER:HB3	1:O:225:GLU:C	2.17	0.70
2:D:101:ASN:OD1	2:D:276:ARG:HB2	1.92	0.69
1:K:253:ARG:HE	1:K:255:MET:CE	2.01	0.69
1:O:151:PRO:HB2	1:O:153:TYR:O	1.92	0.69
1:I:55:ILE:O	1:I:232:LEU:HD12	1.92	0.69
1:M:101:ASP:OD1	1:M:105:LYS:NZ	2.21	0.69
1:E:63:SER:HB3	1:E:225:GLU:C	2.18	0.69
1:K:101:ASP:OD1	1:K:105:LYS:NZ	2.21	0.69
1:E:32:LYS:HE2	1:E:282:GLU:OE1	1.92	0.69
1:K:94:ASN:ND2	1:K:96:ASN:CG	2.49	0.69
2:B:100:LYS:CB	2:B:276:ARG:NH2	2.50	0.68
2:H:75:ASP:HB3	2:H:76:LYS:HG3	1.72	0.68
1:A:22:THR:O	1:A:23:ARG:HD3	1.93	0.68
1:M:33:ASN:HD21	2:N:183:LYS:HE3	1.55	0.68
1:E:20:MET:HE2	1:E:43:LEU:HD13	1.73	0.68
2:B:294:ARG:NH1	2:B:296:ILE:HD11	2.08	0.68
2:P:232:LYS:O	2:P:240:ARG:HD3	1.94	0.68
1:A:56:LYS:HE2	1:A:230:GLU:OE2	1.94	0.68
1:E:26:THR:CG2	2:F:186:ASN:HD22	2.06	0.68
2:B:112:HIS:HB2	2:B:267:THR:HB	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:186:TRP:CH2	2:J:244:THR:HG22	2.26	0.67
1:M:183:THR:HG22	1:M:188:ASN:OD1	1.95	0.67
1:C:185:GLN:HG2	1:C:189:ASP:H	1.59	0.67
1:C:281:GLU:O	1:C:281:GLU:HG3	1.92	0.67
1:G:80:TRP:HB2	1:G:81:PRO:HD2	1.75	0.67
1:K:92:ASP:OD2	1:K:245:SER:HB3	1.94	0.67
1:I:18:THR:HG22	1:I:19:LYS:H	1.60	0.67
2:B:80:LEU:HD22	2:B:250:TYR:CE1	2.30	0.67
2:J:219:ASN:HB3	2:J:222:LEU:HD12	1.76	0.67
2:F:148:GLY:N	2:F:160:THR:O	2.24	0.67
1:I:74:TRP:HA	1:I:74:TRP:HE3	1.60	0.67
2:J:117:LYS:HE3	2:J:252:ASN:HB2	1.76	0.67
2:N:88:HIS:HB3	1:O:159:GLN:HG2	1.76	0.66
2:L:224:ASN:ND2	2:L:227:LEU:HD12	2.10	0.66
1:M:22:THR:HG21	2:N:40:ILE:CD1	2.25	0.66
2:F:181:SER:O	2:F:184:ASN:ND2	2.28	0.66
1:I:182:HIS:HA	1:I:188:ASN:OD1	1.95	0.66
1:K:44:THR:O	1:K:44:THR:CG2	2.41	0.66
2:D:75:ASP:HB3	2:D:76:LYS:HG3	1.77	0.66
1:E:65:LEU:CD1	1:E:78:LEU:HD11	2.26	0.66
2:L:221:THR:OG1	2:L:223:GLU:HG2	1.96	0.66
1:C:244:LYS:HE3	1:C:289:GLU:OE2	1.95	0.66
1:M:32:LYS:O	1:M:33:ASN:HB2	1.94	0.66
2:D:80:LEU:CD1	2:D:248:LEU:HD22	2.26	0.66
2:N:243:PHE:HE2	2:N:245:PRO:HB3	1.61	0.66
2:B:45:LYS:O	2:B:69:ILE:HA	1.97	0.65
1:E:300:VAL:HG12	1:E:301:LYS:HG2	1.76	0.65
2:J:186:TRP:CH2	2:J:244:THR:CG2	2.75	0.65
1:O:41:ASN:HB2	1:O:54:PHE:HB2	1.78	0.65
1:O:66:ARG:HH12	1:O:68:LEU:HD23	1.60	0.65
2:P:100:LYS:CB	2:P:276:ARG:HH21	2.09	0.65
2:F:136:THR:HG22	2:F:137:ALA:H	1.62	0.65
1:K:193:ARG:NH2	3:K:407:HOH:O	2.29	0.65
1:M:26:THR:HG21	2:N:124:GLU:HB3	1.78	0.65
1:K:94:ASN:ND2	1:K:96:ASN:H	1.94	0.65
2:F:233:TYR:OH	1:G:277:VAL:HG11	1.96	0.65
2:P:84:GLN:HA	2:P:245:PRO:O	1.96	0.65
2:F:317:ASP:CG	2:F:318:ASN:H	2.04	0.65
2:H:203:GLU:OE1	2:H:234:ARG:NH2	2.29	0.65
2:P:143:PHE:HE2	2:P:145:TYR:HD2	1.45	0.65
1:M:74:TRP:HA	1:M:74:TRP:HE3	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:260:THR:CG2	2:D:261:GLN:H	2.09	0.64
1:K:92:ASP:HB3	1:K:94:ASN:HB2	1.79	0.64
2:D:175:ASN:HB2	1:E:108:ASP:OD1	1.97	0.64
1:E:263:ASN:O	1:E:269:GLY:HA3	1.97	0.64
1:C:150:GLN:HG2	1:C:150:GLN:O	1.95	0.64
2:B:48:LYS:O	2:B:49:ARG:HD3	1.97	0.64
1:E:37:SER:HB3	1:E:58:LYS:HB3	1.79	0.64
1:K:94:ASN:HD22	1:K:96:ASN:H	1.44	0.64
1:K:65:LEU:HD11	1:K:78:LEU:HD11	1.79	0.64
1:O:27:THR:HG22	1:O:36:GLN:HB2	1.79	0.64
2:J:293:THR:HG22	2:J:306:VAL:HG23	1.78	0.63
2:F:88:HIS:O	2:F:268:ARG:NH1	2.30	0.63
1:M:96:ASN:O	1:M:237:HIS:HA	1.98	0.63
2:B:302:ASP:OD2	2:B:305:ASN:HB2	1.97	0.63
1:C:34:ILE:HG21	1:C:284:LEU:HB3	1.81	0.63
2:H:243:PHE:C	2:H:244:ASN:HD22	2.07	0.63
1:O:26:THR:HG23	2:P:186:ASN:ND2	2.11	0.63
2:D:316:ASP:OD2	2:D:319:LYS:CG	2.44	0.63
1:G:70:PRO:HA	1:G:210:LYS:HG3	1.79	0.63
1:I:225:GLU:HG3	2:J:177:GLY:H	1.63	0.63
2:L:63:ASN:OD1	2:L:85:GLY:HA2	1.98	0.63
2:B:59:ASN:HB3	2:B:90:ASN:HD21	1.62	0.63
2:H:153:SER:O	2:H:154:THR:C	2.42	0.63
1:M:220:PRO:HG2	1:M:223:VAL:HG12	1.80	0.63
1:O:259:LYS:HE2	1:O:261:ASP:OD2	1.99	0.63
1:E:248:VAL:HG12	1:E:250:HIS:NE2	2.13	0.63
1:G:94:ASN:OD1	1:G:96:ASN:N	2.30	0.63
1:O:122:GLY:HA3	1:O:137:THR:OG1	1.99	0.62
1:C:253:ARG:HE	1:C:255:MET:HE2	1.64	0.62
2:L:87:ILE:HG21	2:L:111:TYR:CD1	2.34	0.62
2:D:154:THR:HG22	2:D:155:LYS:CG	2.28	0.62
2:F:181:SER:C	2:F:183:LYS:H	2.07	0.62
2:H:244:ASN:HD22	2:H:244:ASN:N	1.98	0.62
2:H:255:LYS:O	2:H:256:SER:CB	2.48	0.62
1:E:22:THR:HG23	1:E:41:ASN:OD1	2.00	0.62
2:F:217:THR:HB	1:G:191:ASP:OD1	1.99	0.62
2:H:243:PHE:CE2	2:H:245:PRO:HB3	2.35	0.62
2:N:198:LEU:O	2:N:204:VAL:HA	1.98	0.62
1:I:18:THR:CG2	1:I:19:LYS:N	2.63	0.61
1:O:99:VAL:HA	1:O:235:MET:HG2	1.82	0.61
2:B:83:LYS:HZ2	2:B:249:THR:HG23	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:38:LEU:HD21	1:O:249:VAL:HG21	1.81	0.61
1:C:184:ARG:HD3	1:C:256:ASP:OD2	1.99	0.61
1:E:225:GLU:HG2	2:F:179:ILE:CG2	2.30	0.61
2:F:215:ARG:HE	2:F:217:THR:CG2	2.14	0.61
1:O:137:THR:HG22	2:P:150:LYS:CG	2.30	0.61
2:P:80:LEU:HD11	2:P:248:LEU:HD23	1.82	0.61
1:G:225:GLU:HG3	2:H:179:ILE:CG2	2.31	0.61
2:J:83:HIS:O	2:J:263:ARG:NH1	2.33	0.61
1:E:186:LEU:HD23	1:E:187:THR:HG23	1.81	0.61
2:D:298:THR:HG22	2:D:311:VAL:CG2	2.31	0.61
1:K:35:THR:HG21	2:L:184:ASN:O	2.01	0.61
1:K:263:ASN:O	1:K:269:GLY:HA3	2.01	0.61
2:L:258:GLU:OE1	2:L:304:LYS:HG3	2.00	0.61
1:E:183:THR:HG22	1:E:188:ASN:OD1	1.99	0.61
2:L:276:ARG:HH11	2:L:282:ALA:CB	2.14	0.61
1:G:63:SER:HB3	1:G:225:GLU:C	2.25	0.61
1:O:32:LYS:HG2	1:O:282:GLU:OE1	2.00	0.61
2:D:127:ASP:OD1	2:D:131:LYS:HE3	2.01	0.61
2:J:297:ASP:OD2	2:J:300:ASN:ND2	2.34	0.61
1:A:83:SER:HB2	1:A:254:SER:HB3	1.83	0.60
2:D:255:LYS:O	2:D:256:SER:HB3	2.00	0.60
1:O:35:THR:CG2	2:P:184:ASN:O	2.48	0.60
2:D:255:LYS:O	2:D:256:SER:CB	2.49	0.60
2:N:276:ARG:HH11	2:N:276:ARG:CB	2.14	0.60
2:H:191:TRP:HH2	2:H:249:THR:HG23	1.66	0.60
1:O:174:LEU:HD22	1:O:181:ASP:HB3	1.84	0.60
1:C:149:GLN:HG3	2:D:136:THR:HG21	1.83	0.60
2:D:287:GLU:OE1	2:D:290:LYS:CD	2.42	0.60
1:I:86:VAL:HA	1:I:250:HIS:O	2.02	0.60
2:P:75:ASP:CB	2:P:76:LYS:HG3	2.30	0.60
1:A:173:HIS:ND1	1:A:174:LEU:HG	2.17	0.60
2:H:231:SER:OG	2:H:233:TYR:CD2	2.55	0.60
2:L:87:ILE:CG2	2:L:111:TYR:CD1	2.84	0.60
2:L:127:ASP:OD1	2:L:131:LYS:NZ	2.34	0.60
1:M:33:ASN:ND2	2:N:183:LYS:HE3	2.17	0.60
1:O:300:VAL:HG12	1:O:301:LYS:HB3	1.82	0.60
2:P:100:LYS:HB3	2:P:276:ARG:NH2	2.17	0.60
1:E:201:LEU:HD13	1:E:215:PRO:HD3	1.83	0.60
2:N:103:ASN:ND2	2:N:277:PRO:HG3	2.17	0.60
1:A:55:ILE:O	1:A:232:LEU:HD12	2.02	0.60
1:M:23:ARG:HD2	2:N:75:ASP:OD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:63:SER:HB3	1:M:225:GLU:C	2.26	0.60
1:O:149:GLN:HG3	2:P:136:THR:CG2	2.30	0.60
2:F:40:ILE:CG2	2:F:126:LEU:HD23	2.32	0.60
1:A:70:PRO:O	1:A:210:LYS:HD2	2.02	0.60
2:D:112:HIS:HB2	2:D:267:THR:HB	1.84	0.60
2:J:271:ARG:NH1	2:J:277:ALA:CB	2.65	0.60
2:P:243:PHE:HE2	2:P:245:PRO:HB3	1.66	0.60
2:J:271:ARG:HH11	2:J:271:ARG:HB2	1.68	0.59
1:C:185:GLN:HG3	1:C:188:ASN:N	2.17	0.59
2:J:43:LYS:O	2:J:44:ARG:NH1	2.34	0.59
2:N:318:ASN:ND2	3:N:408:HOH:O	2.34	0.59
1:O:96:ASN:HB3	1:O:238:ASP:HB2	1.83	0.59
2:P:91:LEU:CD1	2:P:105:LEU:HD21	2.32	0.59
1:M:174:LEU:CD2	1:M:181:ASP:HB3	2.32	0.59
3:D:406:HOH:O	1:E:50:LYS:HE3	2.02	0.59
2:J:32:PRO:HD2	3:J:412:HOH:O	2.03	0.59
1:M:32:LYS:HG2	1:M:282:GLU:OE2	2.02	0.59
1:M:196:SER:O	1:M:273:GLY:HA3	2.02	0.59
1:K:206:ASN:HB2	1:K:268:TRP:CH2	2.38	0.58
2:B:175:ASN:HB3	2:B:198:LEU:HD23	1.84	0.58
1:C:22:THR:C	1:C:23:ARG:HD3	2.28	0.58
2:H:191:TRP:HH2	2:H:249:THR:CG2	2.17	0.58
2:L:128:GLN:OE1	2:L:128:GLN:N	2.36	0.58
1:I:50:LYS:HE2	3:P:402:HOH:O	2.04	0.58
1:M:174:LEU:HD22	1:M:181:ASP:HB3	1.85	0.58
2:B:294:ARG:NE	2:B:319:LYS:HE3	2.15	0.58
2:D:198:LEU:O	2:D:204:VAL:HA	2.03	0.58
2:D:232:LYS:HD2	2:D:240:ARG:NH1	2.18	0.58
2:H:231:SER:OG	2:H:233:TYR:HD2	1.87	0.58
2:H:260:THR:HG22	2:H:261:GLN:N	2.19	0.58
1:C:21:TYR:HB2	1:C:42:PHE:HB2	1.86	0.58
2:H:84:GLN:HA	2:H:245:PRO:O	2.04	0.58
1:K:196:SER:OG	1:K:198:ILE:HG22	2.03	0.58
1:A:280:LYS:HZ3	1:A:282:GLU:HG2	1.67	0.58
2:B:294:ARG:HH21	2:B:319:LYS:CE	2.16	0.58
2:H:198:LEU:O	2:H:204:VAL:HA	2.04	0.58
1:M:280:LYS:NZ	1:M:282:GLU:OE1	2.36	0.58
2:N:224:ASN:HB3	2:N:227:LEU:CD1	2.23	0.57
2:F:157:ILE:HG22	2:F:158:GLY:N	2.16	0.57
1:K:90:ASN:OD1	1:K:91:VAL:N	2.37	0.57
2:P:116:GLN:HG2	2:P:188:HIS:HD2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:PRO:HB2	1:E:153:TYR:O	2.03	0.57
2:L:87:ILE:CG2	2:L:111:TYR:HD1	2.15	0.57
2:B:122:LYS:HB2	2:B:257:ASN:HD22	1.68	0.57
2:F:104:TRP:CD1	2:F:274:LYS:HG2	2.40	0.57
1:K:151:PRO:HB3	2:L:136:THR:HG23	1.85	0.57
1:M:58:LYS:HA	1:M:229:PRO:O	2.04	0.57
1:A:287:LEU:HD23	1:A:300:VAL:HG11	1.87	0.57
1:C:27:THR:HG22	1:C:36:GLN:HB2	1.87	0.57
1:O:161:THR:HG23	1:O:166:VAL:HA	1.87	0.57
1:A:69:ASP:C	1:A:71:ASN:H	2.11	0.57
1:C:151:PRO:HB2	1:C:153:TYR:O	2.04	0.57
1:I:18:THR:CG2	1:I:19:LYS:H	2.16	0.57
2:P:143:PHE:CE2	2:P:145:TYR:HD2	2.23	0.57
1:K:63:SER:HB2	1:K:81:PRO:HG3	1.87	0.57
1:C:26:THR:HG22	2:D:124:GLU:OE1	2.05	0.57
1:G:206:ASN:HB2	1:G:268:TRP:CH2	2.40	0.57
1:O:135:ASN:HB2	2:P:151:PHE:O	2.03	0.57
2:D:62:GLN:HG2	2:D:266:TYR:CZ	2.39	0.57
2:P:63:ASN:OD1	2:P:85:GLY:HA2	2.05	0.57
1:G:137:THR:HG22	2:H:150:LYS:HG3	1.86	0.56
1:A:44:THR:HG22	1:A:44:THR:O	2.04	0.56
2:B:191:TRP:HH2	2:B:249:THR:HG22	1.71	0.56
2:D:183:LYS:O	2:D:185:ASN:ND2	2.37	0.56
2:F:276:ARG:HE	2:F:282:ALA:CB	2.18	0.56
1:G:128:ASN:HB3	1:G:129:ARG:O	2.05	0.56
2:H:276:ARG:HE	2:H:282:ALA:HB2	1.70	0.56
2:L:64:LEU:HB3	2:L:66:PHE:CE2	2.40	0.56
2:N:198:LEU:HD12	2:N:212:LEU:HD11	1.87	0.56
1:C:29:ASP:OD1	1:C:31:GLN:N	2.37	0.56
1:E:89:GLN:HG3	1:E:165:GLY:HA3	1.86	0.56
1:G:65:LEU:HD11	1:G:78:LEU:HD11	1.87	0.56
1:I:201:LEU:HD13	1:I:214:THR:HA	1.86	0.56
2:J:176:SER:HB2	2:J:185:HIS:HB3	1.87	0.56
2:L:224:ASN:HD22	2:L:227:LEU:HD12	1.69	0.56
1:M:65:LEU:CD1	1:M:78:LEU:HD11	2.35	0.56
2:P:207:ARG:HH11	2:P:207:ARG:CG	2.07	0.56
2:F:276:ARG:HE	2:F:282:ALA:HB2	1.70	0.56
1:I:26:THR:HG21	2:J:119:GLU:HB3	1.86	0.56
1:O:241:ASP:C	1:O:241:ASP:OD1	2.47	0.56
1:K:151:PRO:HB2	1:K:153:TYR:O	2.06	0.56
2:P:260:THR:HG22	2:P:261:GLN:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:32:LYS:O	1:I:33:ASN:HB2	2.05	0.56
2:B:215:ARG:CZ	2:B:217:THR:HG21	2.36	0.56
1:E:26:THR:HG23	2:F:186:ASN:ND2	2.16	0.56
1:G:64:GLY:HA3	1:G:255:MET:CE	2.35	0.56
2:H:276:ARG:HE	2:H:282:ALA:CB	2.19	0.56
1:M:135:ASN:ND2	2:N:150:LYS:HE2	2.20	0.56
1:A:94:ASN:C	1:A:94:ASN:OD1	2.48	0.56
1:A:248:VAL:HG12	1:A:250:HIS:CD2	2.40	0.56
1:I:253:ARG:HE	1:I:255:MET:CE	2.18	0.56
1:I:299:PHE:HZ	1:I:302:VAL:HG23	1.71	0.56
2:J:93:GLU:HG2	2:J:94:GLU:N	2.21	0.56
1:M:182:HIS:HA	1:M:188:ASN:ND2	2.21	0.56
2:P:100:LYS:HB3	2:P:276:ARG:HH21	1.70	0.56
2:P:207:ARG:HG2	2:P:207:ARG:NH1	2.03	0.56
2:D:127:ASP:OD1	2:D:131:LYS:CE	2.53	0.56
2:F:255:LYS:O	2:F:256:SER:CB	2.54	0.56
1:G:29:ASP:OD1	1:G:32:LYS:HG2	2.06	0.56
1:I:64:GLY:HA3	1:I:255:MET:CE	2.32	0.56
2:J:233:LEU:HA	2:J:237:GLY:O	2.04	0.56
1:K:134:GLY:O	1:K:135:ASN:HB3	2.05	0.56
1:M:22:THR:HG21	2:N:40:ILE:HD12	1.88	0.56
2:N:255:LYS:O	2:N:256:SER:CB	2.54	0.56
1:M:182:HIS:HA	1:M:188:ASN:HD21	1.71	0.55
2:F:233:TYR:O	1:G:154:ARG:NH2	2.38	0.55
1:A:44:THR:O	1:A:44:THR:CG2	2.54	0.55
2:P:110:GLU:OE2	2:P:207:ARG:NH2	2.39	0.55
2:P:287:GLU:OE1	2:P:290:LYS:HD3	2.06	0.55
2:B:106:LYS:HE2	2:B:272:ILE:HD11	1.87	0.55
2:F:57:LYS:NZ	2:F:315:SER:HB2	2.20	0.55
2:P:205:LYS:HE3	2:P:211:LEU:HB3	1.88	0.55
1:A:225:GLU:CG	2:B:182:GLY:H	2.19	0.55
1:C:22:THR:HG21	2:D:40:ILE:CD1	2.36	0.55
1:C:185:GLN:CG	1:C:189:ASP:H	2.20	0.55
1:G:132:LEU:HB2	2:L:161:SER:HB3	1.88	0.55
1:I:268:TRP:CG	1:I:269:GLY:H	2.24	0.55
2:L:184:ASN:OD1	2:L:189:VAL:HA	2.06	0.55
2:J:250:LYS:O	2:J:251:SER:OG	2.22	0.55
2:P:91:LEU:HD12	2:P:105:LEU:HD21	1.89	0.55
1:E:27:THR:HG22	1:E:36:GLN:HB2	1.89	0.55
1:E:132:LEU:HD12	1:I:268:TRP:CD1	2.42	0.55
1:I:248:VAL:HG23	1:I:287:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:181:SER:O	2:P:184:ASN:ND2	2.40	0.55
2:F:123:THR:OG1	2:F:253:ASN:OD1	2.23	0.55
1:I:183:THR:HG22	1:I:188:ASN:ND2	2.22	0.55
1:K:149:GLN:CA	1:K:149:GLN:HE21	2.18	0.55
2:L:319:LYS:C	2:L:320:PRO:O	2.50	0.55
2:P:100:LYS:HB2	2:P:276:ARG:HH21	1.71	0.55
2:D:211:LEU:N	2:D:211:LEU:CD1	2.69	0.55
1:E:225:GLU:HG2	2:F:179:ILE:HG23	1.88	0.55
2:N:291:ASP:OD1	2:N:318:ASN:ND2	2.39	0.55
2:P:319:LYS:O	2:P:320:PRO:O	2.24	0.55
2:F:88:HIS:HB3	1:G:159:GLN:CG	2.23	0.55
2:F:233:TYR:HE2	3:F:410:HOH:O	1.89	0.55
1:M:194:THR:HG21	1:M:203:ARG:HE	1.71	0.55
2:D:83:LYS:NZ	2:D:249:THR:HG23	2.22	0.54
1:E:101:ASP:OD1	1:E:105:LYS:NZ	2.35	0.54
1:E:225:GLU:OE2	2:F:182:GLY:N	2.25	0.54
2:F:136:THR:HG22	2:F:137:ALA:N	2.22	0.54
1:G:225:GLU:HG3	2:H:179:ILE:HG22	1.87	0.54
2:L:276:ARG:HH11	2:L:282:ALA:HB3	1.71	0.54
1:O:137:THR:HG22	2:P:150:LYS:HG2	1.87	0.54
1:A:105:LYS:NZ	2:H:84:GLN:OE1	2.40	0.54
2:D:265:THR:O	2:D:265:THR:HG22	2.06	0.54
2:L:59:ASN:C	2:L:60:ILE:HG13	2.32	0.54
2:B:207:ARG:O	2:B:207:ARG:HG2	1.98	0.54
2:F:215:ARG:NE	2:F:217:THR:HG21	2.23	0.54
2:F:215:ARG:NE	2:F:217:THR:CG2	2.71	0.54
1:I:129:ARG:NH1	1:I:129:ARG:HA	2.22	0.54
2:J:184:VAL:HG21	2:J:244:THR:HG21	1.90	0.54
2:J:193:LEU:O	2:J:199:VAL:HA	2.07	0.54
2:L:231:SER:OG	2:L:233:TYR:CD2	2.61	0.54
1:M:27:THR:HG23	1:M:284:LEU:HD21	1.89	0.54
2:N:60:ILE:HG22	2:N:295:LEU:HD23	1.88	0.54
2:N:106:LYS:HG2	2:N:272:ILE:HG12	1.88	0.54
1:E:252:LYS:HG3	1:E:283:LYS:HB2	1.88	0.54
1:I:196:SER:O	1:I:273:GLY:HA3	2.07	0.54
1:A:89:GLN:HG3	1:A:165:GLY:HA3	1.90	0.54
1:I:120:LYS:HG2	2:P:164:SER:HB3	1.89	0.54
1:C:22:THR:HG23	1:C:41:ASN:OD1	2.07	0.54
2:F:84:GLN:HA	2:F:245:PRO:O	2.07	0.54
1:I:26:THR:HG21	2:J:119:GLU:CG	2.38	0.54
2:P:100:LYS:CB	2:P:276:ARG:NH2	2.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ARG:HD3	1:A:173:HIS:CD2	2.43	0.54
2:D:76:LYS:HB3	2:D:253:ASN:O	2.08	0.54
2:D:88:HIS:O	2:D:268:ARG:NH1	2.40	0.54
1:I:225:GLU:CG	2:J:177:GLY:H	2.20	0.54
1:M:26:THR:HG22	2:N:124:GLU:OE1	2.08	0.54
1:O:101:ASP:O	1:O:102:PHE:HB3	2.06	0.54
2:B:126:LEU:HD11	2:B:252:SER:HB3	1.90	0.54
2:H:123:THR:HG23	2:H:253:ASN:HB2	1.88	0.54
2:J:289:ARG:NH2	2:J:314:LYS:HE2	2.22	0.54
2:L:87:ILE:HG22	2:L:111:TYR:CE1	2.43	0.54
2:F:100:LYS:HB3	2:F:276:ARG:HH11	1.66	0.54
2:H:281:TYR:C	2:H:281:TYR:CD2	2.86	0.54
2:P:269:ASN:HD22	2:P:289:ASN:CG	2.15	0.54
2:B:175:ASN:HB2	1:C:108:ASP:OD1	2.08	0.53
2:D:64:LEU:HB3	2:D:66:PHE:CE2	2.43	0.53
1:A:19:LYS:HE2	1:A:21:TYR:CE1	2.43	0.53
2:F:127:ASP:OD1	2:F:131:LYS:CE	2.56	0.53
1:G:63:SER:HB3	1:G:225:GLU:O	2.08	0.53
2:L:221:THR:CG2	2:L:227:LEU:HD13	2.38	0.53
1:M:154:ARG:HD3	1:M:173:HIS:CD2	2.43	0.53
2:N:90:ASN:ND2	2:N:268:ARG:NH2	2.56	0.53
2:N:90:ASN:HD22	2:N:268:ARG:NH2	2.06	0.53
1:E:35:THR:HG21	2:F:184:ASN:O	2.08	0.53
1:I:108:ASP:OD1	2:P:175:ASN:HB2	2.08	0.53
1:E:154:ARG:HG2	1:E:156:LEU:HD21	1.91	0.53
1:G:255:MET:HE2	3:G:401:HOH:O	2.07	0.53
1:A:189:ASP:OD2	2:H:234:ARG:NH1	2.41	0.53
1:M:45:GLU:HB3	1:M:47:ASN:OD1	2.08	0.53
1:M:201:LEU:HD23	1:M:202:THR:HG23	1.89	0.53
2:P:115:PHE:CD2	2:P:115:PHE:C	2.85	0.53
2:D:298:THR:HG22	2:D:311:VAL:HG23	1.90	0.53
2:B:218:ARG:HD2	2:B:279:ILE:O	2.09	0.53
1:C:150:GLN:O	1:C:150:GLN:CG	2.56	0.53
1:G:124:ASP:HB3	1:G:135:ASN:HB3	1.90	0.53
2:J:293:THR:HG22	2:J:306:VAL:CG2	2.39	0.53
1:M:93:ASP:OD1	1:M:94:ASN:N	2.42	0.53
2:N:95:SER:O	2:N:96:HIS:CD2	2.62	0.53
2:B:100:LYS:HB3	2:B:276:ARG:HH21	1.73	0.53
2:L:83:LYS:NZ	2:L:249:THR:CG2	2.72	0.53
2:N:238:LEU:HA	2:N:242:GLY:O	2.09	0.53
2:P:136:THR:HG22	2:P:137:ALA:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:60:ILE:HG22	2:D:295:LEU:HD23	1.90	0.52
1:E:252:LYS:NZ	1:E:281:GLU:OE1	2.36	0.52
2:H:76:LYS:HB3	2:H:253:ASN:O	2.09	0.52
2:H:268:ARG:O	2:H:292:GLY:HA2	2.09	0.52
1:O:186:LEU:HG	1:O:274:GLU:HG3	1.91	0.52
2:B:181:SER:O	2:B:184:ASN:ND2	2.42	0.52
1:C:185:GLN:HG2	1:C:189:ASP:N	2.24	0.52
2:F:260:THR:HG22	2:F:261:GLN:N	2.24	0.52
2:L:129:LEU:HA	2:L:130:PRO:C	2.35	0.52
1:E:80:TRP:HB2	1:E:81:PRO:HD2	1.92	0.52
1:I:39:GLN:HE22	2:J:34:ASP:HA	1.74	0.52
2:J:235:ARG:NH2	1:K:171:GLU:OE2	2.41	0.52
1:O:59:GLY:O	1:O:229:PRO:HD2	2.09	0.52
2:P:50:THR:HG22	2:P:65:GLN:HG3	1.91	0.52
1:A:58:LYS:O	1:A:229:PRO:HG2	2.09	0.52
2:D:243:PHE:C	2:D:244:ASN:HD22	2.18	0.52
2:F:212:LEU:HG	2:F:213:PHE:CD2	2.45	0.52
2:P:59:ASN:C	2:P:60:ILE:HG13	2.34	0.52
2:D:40:ILE:HG21	2:D:126:LEU:HD23	1.91	0.52
1:E:99:VAL:HA	1:E:235:MET:HG2	1.91	0.52
1:K:253:ARG:NE	1:K:255:MET:HE2	2.10	0.52
1:M:80:TRP:HB2	1:M:81:PRO:HD2	1.90	0.52
2:B:120:ASN:ND2	2:B:257:ASN:OD1	2.31	0.52
2:F:40:ILE:HG21	2:F:126:LEU:CD2	2.38	0.52
2:N:321:TYR:CD2	2:N:321:TYR:C	2.87	0.52
2:P:67:ASP:HB2	2:P:80:LEU:HB3	1.92	0.52
2:B:279:ILE:HG13	2:B:280:HIS:N	2.24	0.52
1:E:147:SER:HA	2:F:139:VAL:O	2.09	0.52
1:G:118:GLY:HA3	1:G:141:ASN:OD1	2.09	0.52
3:J:414:HOH:O	1:K:105:LYS:HE2	2.09	0.52
2:P:319:LYS:C	2:P:320:PRO:O	2.53	0.52
2:F:109:SER:HB2	2:F:110:GLU:HG3	1.91	0.52
2:F:157:ILE:HG13	1:G:127:ILE:O	2.10	0.52
2:H:294:ARG:HE	2:H:319:LYS:HB3	1.75	0.52
1:C:257:GLU:HG3	1:C:279:LYS:HB2	1.91	0.52
2:D:235:TYR:HB2	2:D:240:ARG:HB2	1.92	0.52
2:H:75:ASP:HB2	2:H:76:LYS:HG3	1.90	0.52
2:H:153:SER:O	2:H:155:LYS:N	2.43	0.52
2:J:71:LYS:HB3	2:J:248:ASN:O	2.10	0.52
1:A:225:GLU:HG3	2:B:182:GLY:H	1.74	0.51
2:B:129:LEU:HA	2:B:130:PRO:C	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:181:SER:C	2:F:183:LYS:N	2.68	0.51
1:K:147:SER:HA	2:L:139:VAL:O	2.09	0.51
1:K:248:VAL:CG1	1:K:250:HIS:NE2	2.73	0.51
2:F:69:ILE:O	2:F:78:VAL:HB	2.10	0.51
1:G:92:ASP:HB2	1:G:94:ASN:HB3	1.92	0.51
2:H:231:SER:HG	2:H:233:TYR:HD2	1.58	0.51
2:J:91:HIS:CD2	2:J:99:TRP:CE3	2.98	0.51
2:J:187:SER:CB	2:J:189:ILE:HD11	2.41	0.51
2:J:206:LEU:HD12	2:J:279:PRO:HG2	1.92	0.51
2:B:215:ARG:NE	2:B:217:THR:CG2	2.74	0.51
2:D:161:SER:O	2:D:162:SER:HB3	2.11	0.51
2:D:243:PHE:HE2	2:D:245:PRO:HB3	1.73	0.51
2:L:83:LYS:NZ	2:L:249:THR:HG23	2.25	0.51
1:O:101:ASP:OD1	1:O:105:LYS:NZ	2.43	0.51
1:C:65:LEU:HD22	1:C:224:SER:HA	1.92	0.51
2:F:187:TRP:CE3	2:F:188:HIS:HB2	2.45	0.51
1:I:29:ASP:OD2	1:I:32:LYS:HB2	2.11	0.51
1:K:96:ASN:HB3	1:K:238:ASP:HB3	1.91	0.51
2:P:265:THR:HG23	2:P:296:ILE:HG12	1.92	0.51
2:H:91:LEU:HD11	2:H:105:LEU:HD21	1.91	0.51
2:N:221:THR:OG1	2:N:223:GLU:OE1	2.28	0.51
1:O:137:THR:HG22	2:P:150:LYS:HG3	1.92	0.51
1:G:113:VAL:HG22	1:G:146:ILE:HG22	1.93	0.51
2:J:121:LEU:HD21	2:J:247:SER:HB3	1.93	0.51
2:P:317:ASP:CG	2:P:318:ASN:H	2.19	0.51
1:E:78:LEU:HB2	1:E:213:PHE:CE1	2.46	0.51
1:G:65:LEU:CD1	1:G:78:LEU:HD11	2.41	0.51
2:H:148:GLY:O	2:H:160:THR:HG22	2.11	0.51
2:L:154:THR:C	2:L:156:GLY:H	2.19	0.51
2:P:238:LEU:HA	2:P:242:GLY:O	2.09	0.51
2:D:64:LEU:HB3	2:D:66:PHE:HE2	1.76	0.51
2:D:103:ASN:ND2	2:D:277:PRO:HG3	2.26	0.51
2:D:243:PHE:CE2	2:D:245:PRO:HB3	2.45	0.51
2:J:170:ASN:HB3	2:J:193:LEU:HD23	1.91	0.51
2:P:204:VAL:O	2:P:205:LYS:HG3	2.11	0.51
1:A:18:THR:CG2	1:A:45:GLU:HA	2.36	0.51
2:D:176:TYR:CD2	2:D:193:VAL:HG12	2.45	0.51
2:H:125:ILE:HB	2:H:186:ASN:HA	1.92	0.51
1:K:36:GLN:OE1	1:K:288:TYR:OH	2.21	0.51
2:L:77:ASN:HD21	2:L:255:LYS:HG2	1.76	0.51
2:F:215:ARG:HE	2:F:217:THR:HG21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:60:ILE:HG22	2:H:295:LEU:HD23	1.94	0.50
2:P:185:ASN:HB2	2:P:187:TRP:H	1.76	0.50
1:C:29:ASP:OD1	1:C:29:ASP:C	2.53	0.50
1:K:206:ASN:HB2	1:K:268:TRP:HH2	1.75	0.50
1:A:75:ASN:HA	1:A:260:ILE:O	2.10	0.50
1:G:28:SER:OG	1:G:35:THR:HG23	2.12	0.50
2:H:259:LYS:HD3	2:H:300:GLU:OE2	2.12	0.50
1:K:36:GLN:HG2	1:K:251:TYR:CD1	2.46	0.50
1:K:248:VAL:HG12	1:K:250:HIS:CD2	2.47	0.50
2:L:77:ASN:ND2	2:L:255:LYS:HG2	2.26	0.50
1:M:184:ARG:HD3	1:M:256:ASP:OD2	2.11	0.50
2:B:84:GLN:HA	2:B:245:PRO:O	2.10	0.50
2:B:160:THR:HG22	1:C:124:ASP:OD1	2.11	0.50
1:G:22:THR:HG21	2:H:40:ILE:HD13	1.93	0.50
1:I:22:THR:C	1:I:23:ARG:HD3	2.36	0.50
2:J:74:LEU:HG	2:J:75:LEU:N	2.25	0.50
2:L:198:LEU:O	2:L:204:VAL:HA	2.11	0.50
2:F:100:LYS:CB	2:F:276:ARG:HH12	2.23	0.50
1:I:137:THR:HG22	2:J:145:LYS:HG2	1.93	0.50
2:J:249:GLU:C	2:J:250:LYS:O	2.51	0.50
2:J:316:TYR:C	2:J:316:TYR:CD2	2.89	0.50
1:M:67:ILE:HG22	1:M:69:ASP:H	1.77	0.50
1:M:287:LEU:HD23	1:M:300:VAL:HB	1.92	0.50
1:A:221:VAL:HG13	1:A:222:THR:N	2.26	0.50
1:C:219:MET:HB3	1:C:223:VAL:HG13	1.91	0.50
2:D:181:SER:HB3	2:D:184:ASN:OD1	2.12	0.50
1:E:196:SER:O	1:E:273:GLY:HA3	2.11	0.50
1:M:21:TYR:HB2	1:M:42:PHE:HB2	1.94	0.50
2:N:229:PHE:CE1	2:N:275:ASN:ND2	2.75	0.50
1:C:201:LEU:HD13	1:C:215:PRO:HD3	1.93	0.50
1:C:265:HIS:O	1:C:269:GLY:N	2.45	0.50
1:M:277:VAL:HG12	1:M:278:ASP:OD2	2.11	0.50
2:B:62:GLN:HG2	2:B:266:TYR:CE2	2.47	0.50
2:B:321:TYR:C	2:B:321:TYR:CD2	2.90	0.50
1:C:66:ARG:HH21	1:C:68:LEU:HD23	1.77	0.50
1:A:170:VAL:HG21	1:A:227:PHE:CZ	2.47	0.50
2:B:80:LEU:HD22	2:B:250:TYR:HE1	1.75	0.50
2:D:83:LYS:HZ1	2:D:249:THR:HG23	1.76	0.50
2:J:124:LEU:HA	2:J:125:PRO:C	2.37	0.50
1:K:137:THR:HG22	2:L:150:LYS:HG3	1.94	0.50
2:L:199:LYS:O	2:L:236:PRO:HD3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:321:TYR:C	2:L:321:TYR:CD2	2.89	0.50
2:N:217:THR:HG21	2:N:220:ALA:HB2	1.93	0.50
1:O:92:ASP:OD1	1:O:245:SER:HA	2.12	0.50
2:B:232:LYS:HG3	2:B:240:ARG:NH1	2.27	0.49
1:E:176:ASN:O	1:E:177:ASN:HB2	2.12	0.49
1:E:183:THR:CG2	3:E:409:HOH:O	2.23	0.49
1:M:186:LEU:CD1	1:M:274:GLU:HG2	2.42	0.49
1:G:92:ASP:CB	1:G:94:ASN:HB3	2.42	0.49
2:L:64:LEU:HB3	2:L:66:PHE:HE2	1.75	0.49
2:P:231:SER:C	2:P:233:TYR:H	2.20	0.49
1:C:35:THR:HG21	2:D:184:ASN:O	2.12	0.49
2:B:66:PHE:CD2	2:B:308:VAL:HG21	2.48	0.49
2:B:215:ARG:HG2	2:B:217:THR:HG23	1.94	0.49
2:F:173:GLN:HE22	2:F:197:ASP:HB2	1.78	0.49
2:F:216:ASN:OD1	2:F:218:ARG:NH2	2.42	0.49
2:J:187:SER:HB3	2:J:189:ILE:HD11	1.93	0.49
1:K:63:SER:O	1:K:255:MET:HE1	2.13	0.49
1:K:225:GLU:HG2	2:L:179:ILE:CG2	2.43	0.49
2:L:48:LYS:HE3	1:M:48:TYR:CD2	2.48	0.49
1:A:149:GLN:HG3	2:B:136:THR:HG21	1.94	0.49
2:F:159:ARG:HH11	1:M:127:ILE:HD13	1.77	0.49
1:I:186:LEU:HA	1:I:275:ASN:O	2.12	0.49
1:M:44:THR:O	1:M:44:THR:HG22	2.12	0.49
2:N:218:ARG:HD2	2:N:279:ILE:O	2.12	0.49
2:N:255:LYS:O	2:N:256:SER:HB3	2.13	0.49
1:A:69:ASP:C	1:A:71:ASN:N	2.71	0.49
2:B:122:LYS:HB2	2:B:257:ASN:HD21	1.75	0.49
2:F:238:LEU:HD21	2:F:243:PHE:HD1	1.78	0.49
2:H:105:LEU:HD23	2:H:106:LYS:N	2.28	0.49
1:O:252:LYS:HG2	1:O:253:ARG:N	2.27	0.49
2:P:191:TRP:HH2	2:P:249:THR:CG2	2.22	0.49
2:D:222:VAL:HG22	2:D:277:PRO:HG2	1.94	0.49
2:H:127:ASP:O	2:H:250:TYR:N	2.38	0.49
1:I:49:ASP:OD1	1:I:50:LYS:HG3	2.12	0.49
2:L:255:LYS:O	2:L:256:SER:CB	2.60	0.49
2:N:112:HIS:HB2	2:N:267:THR:HB	1.95	0.49
2:J:212:THR:HG21	2:J:222:LEU:O	2.12	0.49
2:L:87:ILE:HG22	2:L:111:TYR:HE1	1.77	0.49
2:H:57:LYS:NZ	2:H:315:SER:HB2	2.28	0.48
2:H:112:HIS:HB2	2:H:267:THR:HB	1.95	0.48
2:N:181:SER:HB2	2:N:190:HIS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PRO:O	1:A:210:LYS:CD	2.61	0.48
2:B:110:GLU:HB2	2:B:269:ASN:HB2	1.95	0.48
2:D:129:LEU:HD12	2:D:250:TYR:HE2	1.78	0.48
2:D:148:GLY:O	2:D:159:ARG:HG3	2.13	0.48
1:E:201:LEU:HD13	1:E:214:THR:HA	1.95	0.48
2:F:215:ARG:HE	2:F:217:THR:HG23	1.77	0.48
2:H:129:LEU:HA	2:H:130:PRO:C	2.38	0.48
2:N:282:ALA:O	2:N:283:PRO:C	2.55	0.48
1:O:206:ASN:HB2	1:O:268:TRP:CH2	2.48	0.48
2:H:212:LEU:C	2:H:214:TYR:H	2.21	0.48
1:M:228:ASN:HB3	2:N:131:LYS:HD3	1.94	0.48
2:B:40:ILE:HG21	2:B:126:LEU:CD1	2.44	0.48
2:D:191:TRP:HH2	2:D:249:THR:CG2	2.25	0.48
2:D:240:ARG:NH2	1:E:171:GLU:OE2	2.45	0.48
1:E:209:ALA:O	1:E:211:ASP:N	2.46	0.48
2:L:118:LYS:HE3	2:L:263:GLU:OE2	2.12	0.48
1:M:127:ILE:HD12	1:M:127:ILE:N	2.28	0.48
2:N:95:SER:O	2:N:96:HIS:HD2	1.94	0.48
2:P:185:ASN:HB2	2:P:188:HIS:H	1.78	0.48
1:A:270:TYR:CD1	1:A:270:TYR:C	2.91	0.48
2:D:97:LYS:H	2:D:97:LYS:HG2	1.40	0.48
2:J:72:ASN:HB2	2:J:248:ASN:HB3	1.94	0.48
2:B:215:ARG:NE	2:B:217:THR:HG23	2.29	0.48
1:C:63:SER:HB3	1:C:225:GLU:C	2.38	0.48
2:D:52:THR:HG23	2:D:61:LEU:HD11	1.95	0.48
2:J:289:ARG:HG2	2:J:311:ASP:HB3	1.96	0.48
1:K:81:PRO:O	1:K:153:TYR:OH	2.31	0.48
2:F:157:ILE:CG2	2:F:158:GLY:N	2.77	0.48
2:J:289:ARG:NH1	2:J:291:ILE:HD11	2.28	0.48
1:M:29:ASP:OD1	1:M:29:ASP:C	2.56	0.48
2:B:99:GLU:HB2	2:B:100:LYS:HD2	1.95	0.48
1:C:163:HIS:NE2	1:C:164:LYS:HG3	2.29	0.48
2:F:294:ARG:NH2	2:F:319:LYS:HG2	2.25	0.48
2:L:88:HIS:O	2:L:268:ARG:NH1	2.46	0.48
2:L:200:TYR:HE1	2:L:203:GLU:OE1	1.95	0.48
2:N:207:ARG:NH2	2:N:288:LYS:HG3	2.27	0.48
1:O:79:ARG:CG	1:O:255:MET:HE3	2.36	0.48
1:E:21:TYR:HB2	1:E:42:PHE:HB2	1.96	0.48
2:D:171:TYR:N	2:D:171:TYR:CD2	2.81	0.47
2:D:267:THR:HG21	2:D:321:TYR:HB2	1.96	0.47
2:H:82:LYS:HB2	3:H:418:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:29:ASP:CG	1:I:32:LYS:HB2	2.39	0.47
1:I:71:ASN:HD22	1:I:208:TRP:HZ3	1.59	0.47
2:J:84:SER:O	2:J:263:ARG:HD3	2.14	0.47
2:J:176:SER:C	2:J:178:LYS:H	2.22	0.47
1:O:178:MET:HE1	1:O:203:ARG:HB2	1.96	0.47
2:P:198:LEU:O	2:P:204:VAL:HA	2.13	0.47
2:P:226:GLU:OE1	2:P:232:LYS:HE2	2.14	0.47
2:D:244:ASN:HD22	2:D:244:ASN:N	2.12	0.47
1:I:186:LEU:HD12	1:I:275:ASN:O	2.15	0.47
2:J:260:THR:HG23	2:J:291:ILE:HG12	1.96	0.47
2:L:156:GLY:O	2:L:157:ILE:HD13	2.14	0.47
2:N:181:SER:HB3	2:N:184:ASN:OD1	2.14	0.47
2:N:181:SER:C	2:N:183:LYS:H	2.22	0.47
1:C:32:LYS:HG2	1:C:282:GLU:OE1	2.15	0.47
1:I:76:SER:HB2	1:I:209:ALA:CB	2.44	0.47
2:J:141:SER:HB3	2:J:157:SER:OG	2.13	0.47
2:N:270:GLN:OE1	2:N:291:ASP:HB3	2.14	0.47
1:O:34:ILE:HG21	1:O:284:LEU:HB3	1.96	0.47
2:P:215:ARG:HB3	2:P:228:SER:O	2.14	0.47
2:P:276:ARG:HD2	2:P:282:ALA:HB2	1.95	0.47
2:D:232:LYS:O	2:D:240:ARG:HD3	2.14	0.47
1:E:149:GLN:HG3	2:F:136:THR:HG21	1.96	0.47
2:H:58:THR:HG22	2:H:293:GLN:HB3	1.97	0.47
2:H:295:LEU:HD11	2:H:297:VAL:CG2	2.44	0.47
1:K:246:GLN:HB3	1:K:287:LEU:HD11	1.96	0.47
1:O:141:ASN:HB3	2:P:146:SER:CB	2.44	0.47
2:F:321:TYR:C	2:F:321:TYR:CD2	2.92	0.47
1:G:149:GLN:HE22	2:H:138:LYS:HB2	1.80	0.47
1:I:280:LYS:HG3	1:I:281:GLU:N	2.30	0.47
1:M:65:LEU:HD11	1:M:78:LEU:HD11	1.96	0.47
2:N:88:HIS:ND1	1:O:159:GLN:HA	2.30	0.47
2:N:195:ALA:HB1	2:N:198:LEU:HD21	1.96	0.47
2:N:305:ASN:O	2:N:307:THR:HG23	2.14	0.47
2:F:77:ASN:HB3	2:F:303:TRP:CE3	2.49	0.47
1:I:22:THR:HG21	2:J:35:ILE:HD12	1.96	0.47
2:L:231:SER:OG	2:L:233:TYR:HD2	1.96	0.47
2:N:173:GLN:HG2	1:O:111:ARG:NH2	2.30	0.47
1:A:248:VAL:HG22	1:A:287:LEU:HD12	1.97	0.47
1:A:280:LYS:HG3	1:A:281:GLU:N	2.29	0.47
2:B:244:ASN:HB3	3:B:412:HOH:O	2.13	0.47
1:C:33:ASN:ND2	2:D:183:LYS:HG2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:VAL:HG11	2:D:132:ASN:OD1	2.15	0.47
2:D:93:PHE:HA	2:D:104:TRP:O	2.14	0.47
1:E:17:ASP:OD1	1:E:17:ASP:N	2.47	0.47
1:E:181:ASP:OD2	2:F:167:LYS:NZ	2.48	0.47
2:H:153:SER:OG	2:H:154:THR:N	2.37	0.47
2:H:204:VAL:O	2:H:205:LYS:HG3	2.15	0.47
2:H:283:PRO:HA	2:H:284:PRO:HD3	1.74	0.47
1:I:252:LYS:HG3	1:I:283:LYS:HB2	1.95	0.47
1:K:227:PHE:CE2	1:K:229:PRO:HA	2.50	0.47
2:L:78:VAL:HG12	2:L:79:LEU:N	2.29	0.47
1:M:220:PRO:HG2	1:M:223:VAL:CG1	2.44	0.47
2:N:175:ASN:ND2	1:O:109:GLU:OE1	2.47	0.47
2:P:294:ARG:HH21	2:P:319:LYS:HG3	1.80	0.47
1:E:54:PHE:C	1:E:55:ILE:HG13	2.39	0.47
1:G:163:HIS:CD2	1:G:164:LYS:HG3	2.50	0.47
2:P:302:ASP:OD1	2:P:302:ASP:C	2.58	0.47
2:B:128:GLN:HA	2:B:248:LEU:O	2.15	0.47
1:C:219:MET:HB3	1:C:223:VAL:CG1	2.45	0.47
1:I:17:ASP:OD2	1:I:46:PRO:HB3	2.14	0.47
2:L:115:PHE:CZ	2:L:262:PHE:CD1	3.03	0.47
1:C:176:ASN:O	1:C:177:ASN:HB2	2.15	0.47
1:K:26:THR:CG2	2:L:124:GLU:OE1	2.62	0.47
2:D:321:TYR:C	2:D:321:TYR:CD2	2.93	0.46
1:I:26:THR:HG21	2:J:119:GLU:CB	2.44	0.46
1:I:225:GLU:HG3	2:J:177:GLY:N	2.29	0.46
2:J:255:THR:HG22	2:J:256:GLN:N	2.30	0.46
2:D:81:VAL:HG12	2:D:83:LYS:HZ2	1.81	0.46
1:I:154:ARG:NH1	2:P:235:TYR:O	2.47	0.46
1:O:186:LEU:HD23	1:O:187:THR:HG23	1.98	0.46
1:C:26:THR:HG21	2:D:124:GLU:HB3	1.97	0.46
1:C:75:ASN:HA	1:C:260:ILE:O	2.14	0.46
1:K:22:THR:C	1:K:23:ARG:HD3	2.38	0.46
2:N:69:ILE:HB	2:N:78:VAL:HB	1.97	0.46
1:G:55:ILE:HG21	1:G:88:ILE:HG21	1.97	0.46
1:G:297:VAL:HG12	1:G:298:LYS:N	2.30	0.46
2:L:59:ASN:O	2:L:60:ILE:HG13	2.16	0.46
2:L:244:ASN:HA	2:L:245:PRO:HD2	1.58	0.46
1:A:69:ASP:O	1:A:71:ASN:N	2.49	0.46
1:A:274:GLU:HG2	1:A:276:HIS:CE1	2.51	0.46
2:N:265:THR:HG23	2:N:296:ILE:HG12	1.97	0.46
2:D:260:THR:CG2	2:D:261:GLN:N	2.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:294:ARG:HH11	2:H:296:ILE:HD11	1.80	0.46
2:N:163:ASN:O	1:O:120:LYS:HA	2.15	0.46
1:A:120:LYS:HG3	2:H:164:SER:HB3	1.97	0.46
1:C:270:TYR:CD1	1:C:270:TYR:C	2.93	0.46
1:E:36:GLN:HG2	1:E:251:TYR:CD1	2.49	0.46
1:G:147:SER:HA	2:H:139:VAL:O	2.16	0.46
1:G:250:HIS:N	1:G:250:HIS:CD2	2.83	0.46
1:I:41:ASN:HB2	1:I:54:PHE:HB2	1.97	0.46
1:K:268:TRP:HA	1:K:268:TRP:CE3	2.49	0.46
2:L:267:THR:HG23	2:L:294:ARG:HB3	1.98	0.46
2:L:276:ARG:NH1	2:L:282:ALA:CB	2.78	0.46
1:M:135:ASN:HD22	2:N:150:LYS:HE2	1.81	0.46
2:N:302:ASP:OD1	2:N:302:ASP:C	2.59	0.46
2:B:55:ASP:CG	2:B:315:SER:OG	2.58	0.46
1:E:94:ASN:OD1	1:E:96:ASN:CG	2.59	0.46
1:G:161:THR:HG23	1:G:166:VAL:HA	1.98	0.46
1:I:58:LYS:HA	1:I:229:PRO:O	2.16	0.46
2:L:69:ILE:HB	2:L:78:VAL:HB	1.97	0.46
2:L:100:LYS:HB3	2:L:276:ARG:NH2	2.31	0.46
2:P:211:LEU:HD23	2:P:211:LEU:HA	1.68	0.46
1:A:119:TYR:O	2:H:164:SER:HA	2.16	0.46
1:C:17:ASP:HB3	1:C:46:PRO:HG3	1.98	0.46
1:E:63:SER:HB2	1:E:223:VAL:O	2.16	0.46
1:G:37:SER:O	1:G:38:LEU:HD12	2.16	0.46
1:G:206:ASN:HB2	1:G:268:TRP:HH2	1.80	0.46
2:L:185:ASN:HB2	2:L:188:HIS:H	1.79	0.46
2:L:231:SER:HG	2:L:233:TYR:HD2	1.63	0.46
1:M:166:VAL:HG22	1:M:167:GLY:N	2.30	0.46
2:F:101:ASN:HB3	2:F:274:LYS:HB3	1.97	0.46
1:G:128:ASN:HB3	1:G:129:ARG:C	2.40	0.46
2:J:121:LEU:HD13	2:J:247:SER:H	1.81	0.46
2:J:291:ILE:HD12	2:J:309:TYR:CD2	2.51	0.46
2:L:159:ARG:HG3	2:L:159:ARG:HH11	1.81	0.46
2:N:268:ARG:O	2:N:292:GLY:HA2	2.16	0.46
1:C:56:LYS:HB2	1:C:56:LYS:HE3	1.37	0.45
1:E:209:ALA:C	1:E:211:ASP:N	2.74	0.45
1:K:169:LYS:NZ	1:K:171:GLU:OE2	2.49	0.45
2:L:173:GLN:HG3	2:L:174:GLN:N	2.31	0.45
2:L:317:ASP:OD1	2:L:318:ASN:N	2.44	0.45
1:O:94:ASN:OD1	1:O:95:ASN:N	2.49	0.45
2:P:244:ASN:HD22	2:P:244:ASN:N	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:98:GLU:O	2:N:98:GLU:HG2	2.16	0.45
1:A:108:ASP:OD1	2:H:175:ASN:HB2	2.15	0.45
2:D:80:LEU:HD13	2:D:250:TYR:CE1	2.52	0.45
2:H:40:ILE:HG21	2:H:126:LEU:HD23	1.98	0.45
1:K:55:ILE:O	1:K:232:LEU:HD12	2.16	0.45
1:M:26:THR:CG2	2:N:124:GLU:OE1	2.63	0.45
1:M:145:THR:OG1	2:N:142:THR:HG23	2.15	0.45
1:O:23:ARG:HD2	2:P:75:ASP:CG	2.42	0.45
1:C:163:HIS:CD2	1:C:164:LYS:HG3	2.52	0.45
2:J:123:GLN:N	2:J:123:GLN:OE1	2.50	0.45
1:K:20:MET:CE	1:K:41:ASN:HB3	2.47	0.45
1:M:197:GLU:OE2	1:M:203:ARG:NH2	2.49	0.45
2:N:179:ILE:HD12	2:N:194:ILE:HD12	1.98	0.45
1:C:58:LYS:HA	1:C:229:PRO:O	2.15	0.45
1:O:93:ASP:O	1:O:94:ASN:C	2.59	0.45
1:A:301:LYS:HG3	1:A:302:VAL:O	2.17	0.45
2:B:265:THR:HG23	2:B:296:ILE:HG12	1.98	0.45
1:I:26:THR:HG22	2:J:119:GLU:CD	2.41	0.45
2:L:207:ARG:HD3	2:L:207:ARG:C	2.41	0.45
1:M:150:GLN:HE21	1:M:174:LEU:HB3	1.81	0.45
1:A:70:PRO:O	1:A:210:LYS:HG3	2.17	0.45
2:B:181:SER:C	2:B:183:LYS:H	2.24	0.45
2:B:276:ARG:NH1	2:B:282:ALA:HB1	2.30	0.45
1:C:194:THR:HG21	1:C:203:ARG:HE	1.82	0.45
1:C:263:ASN:ND2	1:C:270:TYR:HE1	2.08	0.45
1:C:288:TYR:N	1:C:288:TYR:CD2	2.85	0.45
1:E:266:GLY:O	1:E:267:PHE:HB2	2.16	0.45
2:L:110:GLU:OE1	2:L:112:HIS:NE2	2.46	0.45
1:M:166:VAL:CG2	1:M:167:GLY:N	2.79	0.45
2:N:40:ILE:HG21	2:N:126:LEU:CD2	2.43	0.45
2:N:246:GLU:O	2:N:247:PHE:CD1	2.70	0.45
1:O:240:LYS:HB2	1:O:240:LYS:NZ	2.32	0.45
2:B:91:LEU:HD11	2:B:105:LEU:HD21	1.98	0.45
2:B:145:TYR:HB2	2:B:163:ASN:HB3	1.99	0.45
1:I:105:LYS:HE2	3:P:417:HOH:O	2.17	0.45
1:K:50:LYS:HA	1:K:239:LYS:HG3	1.98	0.45
2:L:40:ILE:HD12	2:L:40:ILE:HA	1.81	0.45
2:L:163:ASN:HD22	2:L:163:ASN:N	2.15	0.45
1:A:185:GLN:HG3	2:H:231:SER:HB2	1.99	0.45
1:A:195:LYS:HB2	1:A:273:GLY:O	2.17	0.45
2:B:181:SER:C	2:B:183:LYS:N	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:LYS:HD3	1:E:218:LYS:HA	1.79	0.45
2:F:173:GLN:NE2	2:F:197:ASP:HB2	2.32	0.45
1:G:252:LYS:HB2	1:G:283:LYS:HB2	1.98	0.45
2:H:189:VAL:HG21	2:H:249:THR:CG2	2.47	0.45
1:I:266:GLY:O	1:I:267:PHE:CB	2.63	0.45
2:J:291:ILE:HD12	2:J:309:TYR:HD2	1.82	0.45
2:L:226:GLU:OE2	2:L:232:LYS:HD3	2.17	0.45
1:M:20:MET:HG3	1:M:21:TYR:N	2.32	0.45
1:M:188:ASN:O	1:M:190:SER:N	2.50	0.45
1:M:270:TYR:C	1:M:270:TYR:CD1	2.95	0.45
1:A:268:TRP:HA	1:A:268:TRP:CE3	2.51	0.45
2:B:127:ASP:OD1	2:B:131:LYS:HE3	2.17	0.45
2:F:217:THR:CG2	1:G:191:ASP:OD1	2.65	0.45
2:H:114:ASP:HB3	2:H:265:THR:HB	1.99	0.45
2:H:146:SER:HB3	2:H:162:SER:OG	2.17	0.45
2:J:212:THR:O	2:J:213:ARG:NH1	2.50	0.45
2:L:48:LYS:HB3	1:M:48:TYR:HB2	1.97	0.45
2:D:187:TRP:CE3	2:D:188:HIS:HB2	2.52	0.44
2:D:238:LEU:HD21	2:D:243:PHE:HD1	1.81	0.44
2:D:294:ARG:NH1	2:D:296:ILE:HD11	2.32	0.44
1:E:70:PRO:O	1:E:210:LYS:HG3	2.18	0.44
1:G:183:THR:HG22	1:G:188:ASN:OD1	2.17	0.44
2:H:294:ARG:NH1	2:H:296:ILE:HD11	2.32	0.44
1:I:128:ASN:HA	2:P:156:GLY:HA3	1.98	0.44
2:J:250:LYS:O	2:J:251:SER:CB	2.63	0.44
2:L:283:PRO:HA	2:L:284:PRO:HD3	1.74	0.44
2:N:217:THR:CG2	2:N:220:ALA:HB2	2.46	0.44
2:N:276:ARG:HB2	2:N:276:ARG:NH1	2.25	0.44
1:G:210:LYS:HB3	1:G:210:LYS:HE3	1.81	0.44
2:H:143:PHE:CZ	2:H:145:TYR:HD2	2.35	0.44
1:I:64:GLY:CA	1:I:255:MET:HE1	2.38	0.44
2:J:54:ASN:C	2:J:55:ILE:HG13	2.42	0.44
1:M:163:HIS:CD2	1:M:164:LYS:HG3	2.52	0.44
2:B:173:GLN:HG2	2:B:174:GLN:N	2.33	0.44
2:B:319:LYS:C	2:B:320:PRO:O	2.60	0.44
2:D:162:SER:HA	1:E:121:THR:O	2.17	0.44
2:H:57:LYS:HZ2	2:H:315:SER:HB2	1.82	0.44
2:J:96:ASN:OD1	2:J:271:ARG:NH1	2.50	0.44
1:O:194:THR:O	1:O:272:SER:HA	2.17	0.44
1:O:225:GLU:HG2	2:P:179:ILE:CG2	2.46	0.44
2:B:66:PHE:CE2	2:B:308:VAL:HG11	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:151:PHE:CG	2:F:152:ASP:N	2.86	0.44
1:G:104:PRO:HD2	1:G:168:TRP:NE1	2.31	0.44
2:H:48:LYS:HG3	2:H:65:GLN:NE2	2.33	0.44
2:L:153:SER:C	2:L:155:LYS:H	2.26	0.44
1:M:50:LYS:C	1:M:239:LYS:HE3	2.42	0.44
1:M:149:GLN:HG3	2:N:136:THR:HG21	1.99	0.44
1:O:104:PRO:HD2	1:O:231:PHE:HD1	1.82	0.44
1:O:157:LEU:HD12	1:O:157:LEU:HA	1.83	0.44
2:P:253:ASN:HD21	2:P:257:ASN:HB3	1.82	0.44
2:B:291:ASP:OD1	2:B:292:GLY:N	2.45	0.44
2:D:84:GLN:HG2	2:D:246:GLU:HG3	2.00	0.44
1:E:209:ALA:O	1:E:210:LYS:C	2.60	0.44
2:F:181:SER:O	2:F:183:LYS:N	2.50	0.44
1:K:154:ARG:CD	1:K:173:HIS:CD2	2.99	0.44
2:L:171:TYR:N	2:L:171:TYR:CD2	2.85	0.44
1:O:153:TYR:HB2	2:P:134:ILE:HD13	1.99	0.44
2:B:40:ILE:HG21	2:B:126:LEU:HD12	2.00	0.44
2:B:91:LEU:CD1	2:B:105:LEU:HD21	2.48	0.44
2:J:314:LYS:HB3	2:J:314:LYS:HE3	1.72	0.44
2:L:105:LEU:HD23	2:L:106:LYS:N	2.32	0.44
1:M:124:ASP:OD1	1:M:124:ASP:N	2.50	0.44
1:O:68:LEU:O	1:O:70:PRO:HD3	2.18	0.44
1:C:19:LYS:HE3	1:C:21:TYR:CE1	2.53	0.44
2:D:62:GLN:HG2	2:D:266:TYR:CE1	2.52	0.44
2:D:103:ASN:HD21	2:D:277:PRO:HG3	1.82	0.44
2:F:224:ASN:HB3	2:F:227:LEU:HD12	1.99	0.44
1:G:58:LYS:NZ	2:H:39:ASP:CG	2.76	0.44
2:H:109:SER:HG	2:H:271:ASP:CG	2.25	0.44
2:H:189:VAL:HG21	2:H:249:THR:HG21	1.99	0.44
1:I:26:THR:HG21	2:J:119:GLU:HG2	1.99	0.44
2:J:91:HIS:CD2	2:J:99:TRP:CD2	3.06	0.44
2:N:54:TYR:HB3	1:O:163:HIS:ND1	2.33	0.44
2:N:84:GLN:HA	2:N:245:PRO:O	2.18	0.44
2:N:93:PHE:O	2:N:94:GLU:HG3	2.18	0.44
2:P:128:GLN:N	2:P:128:GLN:CD	2.76	0.44
1:A:222:THR:HA	1:A:226:GLY:O	2.18	0.44
2:B:258:GLU:C	2:B:259:LYS:HG2	2.43	0.44
1:C:145:THR:HA	2:D:141:SER:O	2.18	0.44
2:D:240:ARG:HH21	1:E:171:GLU:CD	2.26	0.44
1:E:74:TRP:HA	1:E:74:TRP:CE3	2.53	0.44
2:L:317:ASP:CG	2:L:318:ASN:N	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:217:THR:HG21	2:P:220:ALA:HB2	1.99	0.44
1:C:41:ASN:HB2	1:C:54:PHE:HB2	2.00	0.44
1:C:79:ARG:O	1:C:79:ARG:HG3	2.15	0.44
2:F:231:SER:C	2:F:233:TYR:H	2.25	0.44
1:G:80:TRP:HB2	1:G:81:PRO:CD	2.44	0.44
2:H:157:ILE:O	2:H:157:ILE:HG23	2.18	0.44
2:J:54:ASN:O	2:J:55:ILE:HG13	2.18	0.44
1:K:222:THR:HA	1:K:226:GLY:O	2.18	0.44
1:K:302:VAL:O	1:K:303:LEU:HD23	2.18	0.44
2:P:118:LYS:O	2:P:119:ARG:C	2.61	0.44
2:D:294:ARG:HE	2:D:319:LYS:HB3	1.82	0.43
1:E:248:VAL:CG1	1:E:250:HIS:NE2	2.81	0.43
2:J:238:PHE:CE2	2:J:240:PRO:HB3	2.53	0.43
1:K:253:ARG:NE	1:K:255:MET:CE	2.73	0.43
2:L:317:ASP:CG	2:L:318:ASN:H	2.25	0.43
1:M:36:GLN:HG2	1:M:251:TYR:CD1	2.53	0.43
1:M:65:LEU:HD12	1:M:78:LEU:HD11	1.98	0.43
2:B:283:PRO:HA	2:B:284:PRO:HD3	1.82	0.43
1:G:38:LEU:HD21	1:G:249:VAL:HG21	1.99	0.43
1:G:99:VAL:HG22	1:G:235:MET:HE2	2.00	0.43
2:H:218:ARG:HD2	2:H:279:ILE:O	2.19	0.43
2:H:317:ASP:CG	2:H:318:ASN:H	2.25	0.43
1:I:26:THR:CG2	2:J:119:GLU:HG2	2.49	0.43
1:I:38:LEU:HD21	1:I:249:VAL:HG21	2.00	0.43
1:K:185:GLN:OE1	1:K:188:ASN:N	2.51	0.43
1:M:22:THR:CG2	2:N:40:ILE:CD1	2.94	0.43
1:M:128:ASN:N	1:M:128:ASN:OD1	2.51	0.43
1:M:170:VAL:HG21	1:M:227:PHE:CZ	2.54	0.43
2:N:218:ARG:HA	2:N:218:ARG:HD3	1.56	0.43
1:O:65:LEU:CD1	1:O:78:LEU:HD11	2.48	0.43
1:O:65:LEU:HD12	1:O:78:LEU:HD11	2.00	0.43
2:P:118:LYS:HE2	2:P:118:LYS:HB3	1.72	0.43
2:D:290:LYS:O	2:D:290:LYS:HG3	2.17	0.43
2:F:195:ALA:HB1	2:F:198:LEU:HD21	2.00	0.43
2:F:224:ASN:HD22	2:F:227:LEU:HD12	1.83	0.43
2:H:45:LYS:O	2:H:69:ILE:HA	2.17	0.43
2:H:100:LYS:HG2	2:H:276:ARG:HH12	1.83	0.43
1:I:159:GLN:HE21	2:P:241:SER:HA	1.82	0.43
2:N:40:ILE:CG2	2:N:126:LEU:HD23	2.43	0.43
1:O:262:TRP:CZ2	1:O:269:GLY:HA3	2.53	0.43
1:A:218:LYS:NZ	2:B:196:ASN:OD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:GLN:HG3	1:C:188:ASN:H	1.82	0.43
2:F:93:PHE:CG	2:F:226:GLU:HG2	2.53	0.43
1:I:220:PRO:HG2	1:I:223:VAL:HG23	2.00	0.43
2:L:217:THR:CG2	2:L:220:ALA:HB2	2.48	0.43
2:N:92:LYS:HZ2	2:N:94:GLU:CD	2.25	0.43
2:N:92:LYS:HZ2	2:N:94:GLU:CG	2.31	0.43
2:N:92:LYS:NZ	2:N:94:GLU:OE2	2.42	0.43
1:E:198:ILE:HG23	1:E:199:PHE:N	2.34	0.43
2:J:277:ALA:O	2:J:278:PRO:C	2.61	0.43
1:M:188:ASN:O	1:M:189:ASP:C	2.61	0.43
2:P:231:SER:C	2:P:233:TYR:N	2.75	0.43
2:D:176:TYR:HD2	2:D:193:VAL:HG12	1.83	0.43
2:F:191:TRP:HH2	2:F:249:THR:CG2	2.32	0.43
1:G:193:ARG:H	1:G:193:ARG:HG3	1.30	0.43
2:L:211:LEU:HD23	2:L:211:LEU:HA	1.86	0.43
2:L:294:ARG:NH2	2:L:319:LYS:HD3	2.33	0.43
2:P:191:TRP:CH2	2:P:249:THR:HG22	2.39	0.43
2:P:256:SER:O	2:P:256:SER:OG	2.36	0.43
1:A:66:ARG:HH11	1:A:68:LEU:HA	1.83	0.43
1:C:173:HIS:CD2	1:C:174:LEU:HD12	2.53	0.43
1:C:218:LYS:HA	1:C:218:LYS:HD2	1.89	0.43
2:F:238:LEU:HD21	2:F:243:PHE:CD1	2.53	0.43
2:H:106:LYS:HG2	2:H:272:ILE:HG12	2.00	0.43
1:I:152:SER:HA	1:I:174:LEU:O	2.19	0.43
2:J:95:LYS:O	2:J:271:ARG:HG3	2.19	0.43
2:L:83:LYS:HB2	2:L:83:LYS:HE2	1.53	0.43
2:P:293:GLN:HA	2:P:316:ASP:O	2.19	0.43
1:A:79:ARG:HE	1:A:79:ARG:HB2	1.57	0.43
1:A:238:ASP:OD1	1:A:238:ASP:C	2.62	0.43
2:D:107:TYR:CE1	2:D:109:SER:HA	2.54	0.43
1:E:249:VAL:HG12	1:E:250:HIS:N	2.34	0.43
1:E:260:ILE:HA	1:E:272:SER:O	2.18	0.43
2:F:93:PHE:CD1	2:F:226:GLU:HG2	2.54	0.43
2:J:245:TYR:C	2:J:246:LEU:HG	2.43	0.43
2:J:271:ARG:HH11	2:J:277:ALA:HB3	1.83	0.43
2:J:282:GLU:OE1	2:J:285:LYS:HD2	2.19	0.43
2:J:309:TYR:OH	2:J:311:ASP:OD1	2.22	0.43
1:M:58:LYS:O	1:M:229:PRO:HG2	2.19	0.43
2:N:89:SER:HB3	2:N:241:SER:C	2.44	0.43
1:O:89:GLN:OE1	1:O:165:GLY:HA3	2.19	0.43
1:O:248:VAL:HG12	1:O:250:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:59:ASN:O	2:P:60:ILE:HG13	2.19	0.43
2:B:55:ASP:OD1	2:B:315:SER:OG	2.36	0.43
2:B:130:PRO:HA	3:B:403:HOH:O	2.19	0.43
2:B:243:PHE:CE2	2:B:245:PRO:HB3	2.54	0.43
1:C:26:THR:CG2	2:D:124:GLU:OE1	2.66	0.43
1:E:219:MET:HB2	1:E:224:SER:HB3	2.01	0.43
1:E:304:ASN:O	1:E:305:ASP:HB2	2.18	0.43
2:F:105:LEU:HD23	2:F:106:LYS:N	2.33	0.43
1:I:298:LYS:HG2	1:I:299:PHE:O	2.19	0.43
1:K:158:ASP:HB3	1:K:167:GLY:C	2.44	0.43
1:M:26:THR:HG22	2:N:124:GLU:CD	2.44	0.43
1:M:218:LYS:HD3	1:M:218:LYS:HA	1.74	0.43
1:O:153:TYR:HE1	1:O:223:VAL:HG23	1.84	0.43
2:B:317:ASP:OD1	2:B:318:ASN:N	2.40	0.43
1:C:241:ASP:C	1:C:241:ASP:OD1	2.61	0.43
1:E:163:HIS:CD2	1:E:164:LYS:HG3	2.54	0.43
2:H:255:LYS:O	2:H:256:SER:HB3	2.19	0.43
2:J:37:LYS:HD3	2:J:37:LYS:HA	1.65	0.43
1:M:184:ARG:CD	1:M:256:ASP:OD2	2.67	0.43
2:N:52:THR:HG23	2:N:63:ASN:HD22	1.83	0.43
2:P:260:THR:CG2	2:P:261:GLN:N	2.82	0.43
1:A:252:LYS:HE3	1:A:281:GLU:CD	2.44	0.42
2:D:85:GLY:O	2:D:245:PRO:HD2	2.19	0.42
2:D:199:LYS:O	2:D:236:PRO:HG3	2.19	0.42
1:E:65:LEU:HD22	1:E:224:SER:HA	2.00	0.42
1:E:75:ASN:HB2	1:E:260:ILE:O	2.19	0.42
1:E:241:ASP:OD1	1:E:241:ASP:C	2.61	0.42
1:G:201:LEU:HB2	1:G:213:PHE:O	2.19	0.42
2:H:109:SER:OG	2:H:271:ASP:CG	2.62	0.42
2:L:105:LEU:HB2	2:L:229:PHE:CZ	2.53	0.42
3:M:409:HOH:O	2:N:131:LYS:HE2	2.19	0.42
2:N:121:ARG:C	2:N:123:THR:H	2.27	0.42
2:P:94:GLU:OE2	2:P:96:HIS:NE2	2.51	0.42
2:P:116:GLN:HG2	2:P:188:HIS:CD2	2.51	0.42
1:E:20:MET:SD	1:E:41:ASN:HB3	2.59	0.42
2:F:231:SER:C	2:F:233:TYR:N	2.77	0.42
1:G:155:THR:OG1	1:G:170:VAL:HG22	2.19	0.42
2:H:293:GLN:NE2	2:H:317:ASP:OD1	2.47	0.42
2:J:311:ASP:OD2	2:J:314:LYS:HB2	2.18	0.42
1:K:20:MET:HE1	1:K:41:ASN:HB3	1.99	0.42
1:M:93:ASP:CG	1:M:94:ASN:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:253:ARG:HG3	1:M:255:MET:SD	2.59	0.42
1:A:157:LEU:HD12	1:A:157:LEU:HA	1.66	0.42
1:C:86:VAL:HA	1:C:250:HIS:O	2.19	0.42
1:C:252:LYS:HE3	1:C:281:GLU:OE1	2.20	0.42
2:D:75:ASP:CB	2:D:76:LYS:HG3	2.48	0.42
2:D:218:ARG:HD2	2:D:279:ILE:O	2.19	0.42
2:N:217:THR:O	2:N:218:ARG:NH1	2.52	0.42
1:A:65:LEU:HD12	1:A:78:LEU:HD11	2.00	0.42
1:C:153:TYR:HD2	1:C:170:VAL:HG12	1.84	0.42
2:D:84:GLN:HE21	2:D:246:GLU:HG3	1.85	0.42
1:E:86:VAL:HA	1:E:250:HIS:O	2.20	0.42
1:E:97:THR:HA	1:E:236:SER:O	2.19	0.42
2:F:84:GLN:HB3	2:F:85:GLY:H	1.68	0.42
2:L:218:ARG:HA	2:L:218:ARG:HD3	1.60	0.42
1:M:101:ASP:O	1:M:102:PHE:HB3	2.20	0.42
2:P:129:LEU:HA	2:P:130:PRO:C	2.44	0.42
2:D:106:LYS:HE3	2:D:272:ILE:HD11	2.01	0.42
2:D:129:LEU:HA	2:D:130:PRO:C	2.44	0.42
1:I:38:LEU:HD12	1:I:38:LEU:HA	1.85	0.42
1:M:26:THR:HG21	2:N:124:GLU:CB	2.47	0.42
1:M:293:LYS:HB3	1:M:293:LYS:HE2	1.86	0.42
1:A:154:ARG:NH1	2:H:235:TYR:O	2.44	0.42
2:H:294:ARG:NH2	2:H:319:LYS:CD	2.65	0.42
2:J:209:TYR:CE2	2:J:211:ASN:HA	2.54	0.42
2:P:283:PRO:HA	2:P:284:PRO:HD3	1.88	0.42
2:P:316:ASP:OD2	2:P:319:LYS:HG3	2.19	0.42
1:A:65:LEU:CD1	1:A:78:LEU:HD11	2.49	0.42
2:B:294:ARG:HH21	2:B:319:LYS:HE3	1.84	0.42
1:C:96:ASN:O	1:C:237:HIS:HA	2.20	0.42
2:F:294:ARG:HE	2:F:319:LYS:HB3	1.84	0.42
1:G:120:LYS:HE3	1:G:139:GLU:OE1	2.20	0.42
1:I:157:LEU:HA	1:I:157:LEU:HD12	1.84	0.42
1:I:194:THR:O	1:I:272:SER:HA	2.20	0.42
2:L:211:LEU:HD23	2:L:284:PRO:HG2	2.02	0.42
2:N:199:LYS:HD3	1:O:111:ARG:HD3	2.02	0.42
1:O:94:ASN:O	1:O:95:ASN:CB	2.68	0.42
2:P:40:ILE:HD12	2:P:40:ILE:HA	1.86	0.42
1:C:29:ASP:OD2	1:C:32:LYS:HE2	2.19	0.42
1:E:209:ALA:C	1:E:211:ASP:H	2.28	0.42
2:F:321:TYR:HB2	3:F:414:HOH:O	2.20	0.42
1:G:152:SER:HA	1:G:174:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:263:ASN:O	1:I:269:GLY:HA3	2.19	0.42
2:J:251:SER:H	2:J:299:LYS:HZ3	1.67	0.42
1:K:187:THR:HA	1:K:196:SER:HB2	2.02	0.42
2:L:48:LYS:O	2:L:49:ARG:HD3	2.18	0.42
2:L:63:ASN:C	2:L:64:LEU:HD12	2.44	0.42
2:L:67:ASP:O	2:L:79:LEU:HD12	2.20	0.42
2:N:130:PRO:HD2	2:N:247:PHE:CD1	2.55	0.42
2:N:164:SER:HA	1:O:119:TYR:O	2.19	0.42
1:O:80:TRP:CE3	1:O:81:PRO:O	2.72	0.42
1:A:300:VAL:HG12	1:A:301:LYS:HB3	2.01	0.42
1:I:40:PHE:HA	1:I:54:PHE:O	2.20	0.42
1:I:50:LYS:HE3	3:P:416:HOH:O	2.18	0.42
1:I:129:ARG:C	1:I:131:GLY:H	2.27	0.42
2:J:113:LYS:HA	2:J:113:LYS:HD3	1.40	0.42
1:A:90:ASN:C	1:A:90:ASN:OD1	2.62	0.42
2:F:63:ASN:OD1	2:F:85:GLY:HA2	2.20	0.42
2:F:260:THR:CG2	2:F:261:GLN:N	2.83	0.42
2:J:182:TRP:CE3	2:J:183:HIS:HB2	2.54	0.42
1:K:218:LYS:HD3	1:K:218:LYS:HA	1.60	0.42
2:L:151:PHE:CD2	2:L:152:ASP:N	2.88	0.42
2:H:271:ASP:OD2	2:H:286:LEU:HD11	2.20	0.41
1:I:49:ASP:OD1	1:I:50:LYS:N	2.53	0.41
2:J:227:LYS:HD2	2:J:235:ARG:NH1	2.35	0.41
2:L:87:ILE:CG2	2:L:111:TYR:CE1	3.03	0.41
1:M:22:THR:CG2	2:N:40:ILE:HD13	2.50	0.41
1:M:277:VAL:HG12	1:M:278:ASP:CG	2.45	0.41
2:N:162:SER:HA	1:O:121:THR:O	2.20	0.41
2:N:241:SER:HB2	1:O:156:LEU:HB3	2.01	0.41
1:A:144:GLU:O	2:B:142:THR:HA	2.21	0.41
2:B:63:ASN:HB2	2:B:85:GLY:N	2.35	0.41
2:D:218:ARG:HA	2:D:218:ARG:HD3	1.74	0.41
2:F:109:SER:C	2:F:110:GLU:CG	2.93	0.41
1:I:22:THR:HG23	1:I:41:ASN:OD1	2.20	0.41
2:J:176:SER:C	2:J:178:LYS:N	2.78	0.41
2:J:271:ARG:HH11	2:J:277:ALA:CB	2.32	0.41
1:K:43:LEU:HD12	1:K:44:THR:N	2.35	0.41
1:K:298:LYS:HG2	1:K:299:PHE:O	2.19	0.41
2:L:221:THR:HG23	2:L:224:ASN:H	1.85	0.41
1:M:225:GLU:HG2	2:N:179:ILE:CG2	2.50	0.41
2:N:198:LEU:HD12	2:N:212:LEU:CD1	2.48	0.41
1:I:129:ARG:HA	1:I:129:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:40:PHE:CD1	1:K:55:ILE:HG12	2.55	0.41
1:M:183:THR:HG23	1:M:185:GLN:H	1.85	0.41
2:N:175:ASN:HB2	1:O:108:ASP:OD1	2.20	0.41
1:O:60:THR:HG22	1:O:61:ILE:N	2.36	0.41
2:P:143:PHE:HE2	2:P:145:TYR:CD2	2.30	0.41
1:A:178:MET:CE	1:A:197:GLU:OE1	2.68	0.41
1:A:178:MET:HE2	1:A:197:GLU:OE1	2.20	0.41
2:B:170:SER:HB2	1:C:114:LYS:HG2	2.01	0.41
2:D:181:SER:C	2:D:183:LYS:N	2.77	0.41
2:D:298:THR:CG2	2:D:311:VAL:HG23	2.50	0.41
2:H:177:ASP:OD2	2:H:196:ASN:ND2	2.47	0.41
1:O:21:TYR:HB2	1:O:42:PHE:HB2	2.01	0.41
2:P:63:ASN:HB2	2:P:85:GLY:N	2.35	0.41
1:A:136:ILE:O	2:B:150:LYS:HB2	2.21	0.41
2:B:58:THR:HB	2:B:293:GLN:HB3	2.01	0.41
2:B:59:ASN:C	2:B:60:ILE:HG13	2.45	0.41
2:B:79:LEU:HD23	2:B:251:LEU:HD13	2.03	0.41
2:B:115:PHE:CD2	2:B:115:PHE:C	2.99	0.41
2:B:122:LYS:CB	2:B:257:ASN:HD22	2.32	0.41
2:B:123:THR:OG1	2:B:253:ASN:OD1	2.39	0.41
2:B:198:LEU:O	2:B:204:VAL:HA	2.19	0.41
2:F:159:ARG:NH1	1:M:127:ILE:HD13	2.35	0.41
1:G:98:ASN:O	1:G:235:MET:HA	2.20	0.41
2:P:87:ILE:HG21	2:P:111:TYR:HD1	1.86	0.41
1:C:186:LEU:HA	1:C:275:ASN:O	2.20	0.41
2:D:78:VAL:HG12	2:D:79:LEU:N	2.36	0.41
2:D:265:THR:OG1	2:D:296:ILE:HG12	2.21	0.41
2:H:145:TYR:HA	2:H:162:SER:O	2.20	0.41
1:I:120:LYS:HG2	2:P:164:SER:CB	2.50	0.41
1:I:228:ASN:OD1	2:J:126:LYS:HB3	2.20	0.41
2:J:201:ASN:O	2:J:202:ARG:C	2.63	0.41
1:K:201:LEU:HD13	1:K:214:THR:HA	2.02	0.41
2:B:217:THR:HG22	1:C:191:ASP:OD1	2.21	0.41
2:B:258:GLU:OE1	2:B:258:GLU:HA	2.19	0.41
1:C:49:ASP:O	1:C:239:LYS:HE3	2.20	0.41
2:D:59:ASN:O	2:D:60:ILE:HG13	2.21	0.41
2:D:69:ILE:HB	2:D:78:VAL:HB	2.02	0.41
2:D:150:LYS:O	2:D:157:ILE:HA	2.20	0.41
2:F:108:PRO:HG2	2:F:111:TYR:OH	2.20	0.41
2:F:137:ALA:HB1	2:F:169:ILE:HG23	2.01	0.41
1:G:68:LEU:HB2	1:G:77:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:187:THR:HG22	1:G:195:LYS:HB3	2.02	0.41
2:J:116:ARG:HD2	2:J:116:ARG:HA	1.93	0.41
2:L:200:TYR:HA	2:L:234:ARG:O	2.20	0.41
2:N:125:ILE:HB	2:N:186:ASN:HA	2.03	0.41
2:B:293:GLN:N	2:B:293:GLN:CD	2.79	0.41
1:I:26:THR:CG2	2:J:119:GLU:CG	2.99	0.41
2:J:207:LEU:HG	2:J:208:PHE:CD2	2.56	0.41
1:K:79:ARG:HA	1:K:256:ASP:O	2.21	0.41
1:K:207:LEU:HD12	1:K:212:ASN:HA	2.02	0.41
2:L:256:SER:H	2:L:304:LYS:HZ3	1.69	0.41
1:O:27:THR:HG23	1:O:284:LEU:HD21	2.03	0.41
1:A:225:GLU:HG3	2:B:182:GLY:N	2.36	0.41
1:A:268:TRP:HA	1:A:268:TRP:HE3	1.85	0.41
2:B:85:GLY:O	2:B:245:PRO:HD2	2.21	0.41
2:B:107:TYR:HB2	2:B:108:PRO:HD2	2.02	0.41
2:B:292:GLY:C	2:B:293:GLN:NE2	2.79	0.41
1:C:53:VAL:HG21	1:C:292:TRP:HH2	1.84	0.41
1:C:124:ASP:H	1:C:135:ASN:HB3	1.85	0.41
2:D:87:ILE:HD11	2:D:266:TYR:HB3	2.02	0.41
2:D:110:GLU:OE1	2:D:112:HIS:NE2	2.54	0.41
2:D:276:ARG:HA	2:D:277:PRO:HD3	1.93	0.41
2:F:57:LYS:HZ2	2:F:315:SER:HB2	1.85	0.41
1:G:151:PRO:HB2	1:G:153:TYR:O	2.21	0.41
2:H:217:THR:CG2	2:H:220:ALA:HB2	2.43	0.41
2:H:224:ASN:ND2	2:H:227:LEU:HG	2.36	0.41
2:J:82:ILE:CG2	2:J:106:TYR:HD1	2.34	0.41
2:J:84:SER:HA	2:J:103:PRO:HG3	2.02	0.41
2:L:80:LEU:HD13	2:L:250:TYR:CE1	2.56	0.41
2:L:314:TYR:CD2	2:L:314:TYR:C	2.99	0.41
1:M:119:TYR:CD1	1:M:119:TYR:C	2.99	0.41
2:N:140:ASP:HB2	2:N:168:THR:HB	2.03	0.41
2:N:283:PRO:HA	2:N:284:PRO:HD3	1.82	0.41
1:A:154:ARG:HD3	1:A:173:HIS:HD2	1.84	0.41
2:B:128:GLN:N	2:B:128:GLN:OE1	2.54	0.41
2:B:217:THR:O	2:B:218:ARG:HD3	2.21	0.41
1:C:204:ASN:O	1:C:205:GLY:C	2.63	0.41
1:C:293:LYS:HB3	1:C:293:LYS:HE2	1.77	0.41
2:D:217:THR:HG23	2:D:220:ALA:HB2	2.03	0.41
1:E:80:TRP:CE2	1:E:199:PHE:HE2	2.39	0.41
2:F:185:ASN:HB2	2:F:188:HIS:H	1.85	0.41
1:I:220:PRO:HG2	1:I:223:VAL:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:91:HIS:HD2	2:J:99:TRP:CD2	2.38	0.41
1:K:76:SER:N	1:K:209:ALA:HB1	2.36	0.41
1:K:178:MET:HB3	1:K:178:MET:HE2	1.74	0.41
2:P:59:ASN:HB3	2:P:90:ASN:HD21	1.86	0.41
1:E:125:PHE:HA	1:E:134:GLY:HA2	2.03	0.40
1:G:118:GLY:CA	1:G:141:ASN:OD1	2.68	0.40
1:I:69:ASP:OD1	1:I:69:ASP:N	2.50	0.40
1:I:248:VAL:CG1	1:I:250:HIS:NE2	2.84	0.40
2:J:123:GLN:HB2	2:J:244:THR:HG22	2.03	0.40
2:N:139:VAL:HA	2:N:168:THR:O	2.22	0.40
2:N:260:THR:HG22	2:N:261:GLN:N	2.36	0.40
1:C:61:ILE:HG21	1:C:84:TYR:HD1	1.86	0.40
2:D:118:LYS:HA	2:D:118:LYS:HD3	1.91	0.40
2:H:115:PHE:CD2	2:H:115:PHE:C	2.99	0.40
2:J:181:ASN:C	2:J:181:ASN:HD22	2.27	0.40
2:J:213:ARG:HA	2:J:213:ARG:HD3	1.96	0.40
2:L:63:ASN:O	2:L:64:LEU:HD12	2.21	0.40
2:P:109:SER:C	2:P:110:GLU:HG2	2.46	0.40
2:P:210:GLU:H	2:P:210:GLU:HG3	1.58	0.40
1:A:87:SER:HA	1:A:167:GLY:HA2	2.04	0.40
2:D:217:THR:HG21	2:D:227:LEU:O	2.22	0.40
1:E:279:LYS:O	1:E:280:LYS:HB2	2.21	0.40
2:B:314:TYR:CD2	2:B:314:TYR:C	3.00	0.40
2:D:88:HIS:CE1	1:E:159:GLN:HA	2.56	0.40
2:D:274:LYS:N	2:D:285:ILE:O	2.51	0.40
1:E:94:ASN:OD1	1:E:96:ASN:ND2	2.54	0.40
1:E:240:LYS:HB2	1:E:240:LYS:HE3	1.87	0.40
2:J:253:GLU:OE1	2:J:253:GLU:HA	2.21	0.40
2:L:130:PRO:HD2	2:L:247:PHE:HD1	1.86	0.40
2:L:231:SER:C	2:L:233:TYR:H	2.30	0.40
2:L:243:PHE:CZ	2:L:245:PRO:HA	2.57	0.40
1:M:180:HIS:HB2	1:M:182:HIS:CE1	2.56	0.40
2:N:181:SER:C	2:N:183:LYS:N	2.79	0.40
1:A:43:LEU:HD23	1:A:54:PHE:HE2	1.86	0.40
1:E:293:LYS:HB2	1:E:293:LYS:HZ3	1.87	0.40
2:J:289:ARG:HH11	2:J:291:ILE:HD11	1.85	0.40
1:K:149:GLN:HG3	2:L:136:THR:HG21	2.03	0.40
2:L:112:HIS:HB3	2:L:190:HIS:CE1	2.56	0.40
3:L:415:HOH:O	1:M:105:LYS:HE2	2.21	0.40
1:M:91:VAL:HG21	1:M:248:VAL:HG23	2.02	0.40
2:N:105:LEU:HB2	2:N:229:PHE:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:86:VAL:HA	1:O:250:HIS:O	2.22	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	277/311 (89%)	248 (90%)	28 (10%)	1 (0%)	30	60
1	C	275/311 (88%)	247 (90%)	25 (9%)	3 (1%)	11	36
1	E	288/311 (93%)	260 (90%)	22 (8%)	6 (2%)	5	20
1	G	288/311 (93%)	251 (87%)	33 (12%)	4 (1%)	9	30
1	I	288/311 (93%)	262 (91%)	21 (7%)	5 (2%)	7	25
1	K	275/311 (88%)	241 (88%)	29 (10%)	5 (2%)	6	23
1	M	283/311 (91%)	245 (87%)	31 (11%)	7 (2%)	4	16
1	O	279/311 (90%)	249 (89%)	25 (9%)	5 (2%)	6	23
2	B	278/324 (86%)	257 (92%)	19 (7%)	2 (1%)	18	47
2	D	287/324 (89%)	258 (90%)	25 (9%)	4 (1%)	9	30
2	F	280/324 (86%)	261 (93%)	17 (6%)	2 (1%)	18	47
2	H	286/324 (88%)	261 (91%)	20 (7%)	5 (2%)	7	25
2	J	286/324 (88%)	263 (92%)	20 (7%)	3 (1%)	12	38
2	L	286/324 (88%)	259 (91%)	24 (8%)	3 (1%)	12	38
2	N	286/324 (88%)	266 (93%)	17 (6%)	3 (1%)	12	38
2	P	282/324 (87%)	259 (92%)	17 (6%)	6 (2%)	5	20
All	All	4524/5080 (89%)	4087 (90%)	373 (8%)	64 (1%)	9	30

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	320	PRO
1	E	210	LYS
1	E	267	PHE
1	G	94	ASN
2	H	37	PRO
2	H	153	SER
2	H	154	THR
1	I	95	ASN
1	I	210	LYS
1	I	267	PHE
1	K	94	ASN
2	L	154	THR
2	L	320	PRO
1	M	131	GLY
2	P	318	ASN
2	P	320	PRO
1	C	94	ASN
1	C	184	ARG
2	D	256	SER
1	E	177	ASN
1	E	278	ASP
2	F	256	SER
2	J	70	ASP
2	J	227	LYS
1	K	135	ASN
1	K	210	LYS
1	M	33	ASN
1	M	94	ASN
1	M	189	ASP
1	M	210	LYS
2	N	256	SER
1	O	267	PHE
1	O	278	ASP
2	B	182	GLY
1	C	177	ASN
2	D	156	GLY
2	D	226	GLU
1	E	280	LYS
2	F	182	GLY
1	G	72	GLY
1	I	266	GLY
1	K	241	ASP
1	M	266	GLY

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Mol	Chain	Res	Type
1	O	189	ASP
1	E	266	GLY
2	H	213	PHE
1	I	33	ASN
2	J	177	GLY
2	P	119	ARG
2	P	152	ASP
2	D	182	GLY
1	G	33	ASN
1	G	186	LEU
2	H	119	ARG
2	L	316	ASP
1	M	216	LYS
2	N	182	GLY
2	N	318	ASN
2	P	232	LYS
1	A	205	GLY
1	K	267	PHE
1	O	277	VAL
2	P	201	GLY
1	O	198	ILE

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	255/283 (90%)	217 (85%)	38 (15%)	3	10
1	C	255/283 (90%)	225 (88%)	30 (12%)	5	17
1	E	262/283 (93%)	237 (90%)	25 (10%)	8	26
1	G	262/283 (93%)	235 (90%)	27 (10%)	7	23
1	I	262/283 (93%)	232 (88%)	30 (12%)	5	18
1	K	257/283 (91%)	225 (88%)	32 (12%)	4	15
1	M	260/283 (92%)	235 (90%)	25 (10%)	8	26
1	O	257/283 (91%)	231 (90%)	26 (10%)	7	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	261/301 (87%)	236 (90%)	25 (10%)	8	26
2	D	267/301 (89%)	246 (92%)	21 (8%)	11	35
2	F	263/301 (87%)	245 (93%)	18 (7%)	14	42
2	H	266/301 (88%)	248 (93%)	18 (7%)	14	42
2	J	266/301 (88%)	236 (89%)	30 (11%)	5	19
2	L	266/301 (88%)	241 (91%)	25 (9%)	8	27
2	N	266/301 (88%)	245 (92%)	21 (8%)	11	35
2	P	264/301 (88%)	229 (87%)	35 (13%)	4	14
All	All	4189/4672 (90%)	3763 (90%)	426 (10%)	7	23

All (426) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	THR
1	A	22	THR
1	A	24	THR
1	A	26	THR
1	A	27	THR
1	A	44	THR
1	A	65	LEU
1	A	66	ARG
1	A	68	LEU
1	A	69	ASP
1	A	76	SER
1	A	89	GLN
1	A	91	VAL
1	A	120	LYS
1	A	136	ILE
1	A	137	THR
1	A	149	GLN
1	A	154	ARG
1	A	166	VAL
1	A	175	ILE
1	A	184	ARG
1	A	186	LEU
1	A	193	ARG
1	A	204	ASN
1	A	222	THR
1	A	224	SER

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Mol	Chain	Res	Type
1	A	234	VAL
1	A	242	LYS
1	A	252	LYS
1	A	268	TRP
1	A	277	VAL
1	A	280	LYS
1	A	289	GLU
1	A	293	LYS
1	A	298	LYS
1	A	300	VAL
1	A	301	LYS
1	A	303	LEU
2	B	35	THR
2	B	42	LYS
2	B	46	ILE
2	B	52	THR
2	B	61	LEU
2	B	80	LEU
2	B	91	LEU
2	B	100	LYS
2	B	105	LEU
2	B	136	THR
2	B	159	ARG
2	B	169	ILE
2	B	170	SER
2	B	174	GLN
2	B	219	ILE
2	B	228	SER
2	B	232	LYS
2	B	244	ASN
2	B	249	THR
2	B	254	GLU
2	B	257	ASN
2	B	259	LYS
2	B	279	ILE
2	B	301	VAL
2	B	315	SER
1	C	22	THR
1	C	52	THR
1	C	56	LYS
1	C	60	THR
1	C	79	ARG

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Mol	Chain	Res	Type
1	C	100	THR
1	C	110	SER
1	C	126	SER
1	C	140	SER
1	C	146	ILE
1	C	147	SER
1	C	149	GLN
1	C	171	GLU
1	C	175	ILE
1	C	183	THR
1	C	184	ARG
1	C	185	GLN
1	C	193	ARG
1	C	194	THR
1	C	198	ILE
1	C	221	VAL
1	C	222	THR
1	C	250	HIS
1	C	264	ARG
1	C	281	GLU
1	C	288	TYR
1	C	289	GLU
1	C	293	LYS
1	C	298	LYS
1	C	304	ASN
2	D	35	THR
2	D	39	ASP
2	D	95	SER
2	D	97	LYS
2	D	118	LYS
2	D	126	LEU
2	D	135	SER
2	D	136	THR
2	D	155	LYS
2	D	160	THR
2	D	161	SER
2	D	173	GLN
2	D	185	ASN
2	D	221	THR
2	D	228	SER
2	D	244	ASN
2	D	254	GLU

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Mol	Chain	Res	Type
2	D	264	VAL
2	D	266	TYR
2	D	276	ARG
2	D	294	ARG
1	E	17	ASP
1	E	26	THR
1	E	27	THR
1	E	35	THR
1	E	45	GLU
1	E	52	THR
1	E	63	SER
1	E	91	VAL
1	E	100	THR
1	E	126	SER
1	E	133	THR
1	E	136	ILE
1	E	141	ASN
1	E	149	GLN
1	E	166	VAL
1	E	193	ARG
1	E	203	ARG
1	E	207	LEU
1	E	210	LYS
1	E	214	THR
1	E	222	THR
1	E	241	ASP
1	E	252	LYS
1	E	272	SER
1	E	298	LYS
2	F	65	GLN
2	F	80	LEU
2	F	82	LYS
2	F	91	LEU
2	F	109	SER
2	F	119	ARG
2	F	120	ASN
2	F	124	GLU
2	F	126	LEU
2	F	138	LYS
2	F	144	SER
2	F	146	SER
2	F	147	SER

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Mol	Chain	Res	Type
2	F	161	SER
2	F	207	ARG
2	F	227	LEU
2	F	244	ASN
2	F	268	ARG
1	G	19	LYS
1	G	30	SER
1	G	45	GLU
1	G	71	ASN
1	G	76	SER
1	G	79	ARG
1	G	85	SER
1	G	87	SER
1	G	89	GLN
1	G	92	ASP
1	G	100	THR
1	G	112	GLU
1	G	127	ILE
1	G	129	ARG
1	G	140	SER
1	G	175	ILE
1	G	193	ARG
1	G	202	THR
1	G	210	LYS
1	G	223	VAL
1	G	240	LYS
1	G	244	LYS
1	G	263	ASN
1	G	264	ARG
1	G	277	VAL
1	G	281	GLU
1	G	298	LYS
2	H	40	ILE
2	H	98	GLU
2	H	126	LEU
2	H	134	ILE
2	H	136	THR
2	H	146	SER
2	H	170	SER
2	H	179	ILE
2	H	222	VAL
2	H	244	ASN

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Mol	Chain	Res	Type
2	H	268	ARG
2	H	279	ILE
2	H	280	HIS
2	H	295	LEU
2	H	300	GLU
2	H	301	VAL
2	H	306	LYS
2	H	319	LYS
1	I	19	LYS
1	I	27	THR
1	I	30	SER
1	I	38	LEU
1	I	52	THR
1	I	63	SER
1	I	74	TRP
1	I	77	THR
1	I	85	SER
1	I	105	LYS
1	I	110	SER
1	I	121	THR
1	I	124	ASP
1	I	126	SER
1	I	127	ILE
1	I	129	ARG
1	I	132	LEU
1	I	135	ASN
1	I	138	LYS
1	I	140	SER
1	I	166	VAL
1	I	204	ASN
1	I	207	LEU
1	I	211	ASP
1	I	241	ASP
1	I	248	VAL
1	I	281	GLU
1	I	282	GLU
1	I	293	LYS
1	I	305	ASP
2	J	35	ILE
2	J	47	THR
2	J	48	VAL
2	J	53	THR

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Mol	Chain	Res	Type
2	J	75	LEU
2	J	104	SER
2	J	113	LYS
2	J	114	ARG
2	J	117	LYS
2	J	131	THR
2	J	159	SER
2	J	161	SER
2	J	165	SER
2	J	181	ASN
2	J	194	LYS
2	J	206	LEU
2	J	214	ILE
2	J	226	SER
2	J	235	ARG
2	J	236	SER
2	J	243	LEU
2	J	256	GLN
2	J	258	GLU
2	J	263	ARG
2	J	271	ARG
2	J	274	ILE
2	J	282	GLU
2	J	290	LEU
2	J	297	ASP
2	J	317	LYS
1	K	22	THR
1	K	26	THR
1	K	27	THR
1	K	30	SER
1	K	31	GLN
1	K	44	THR
1	K	58	LYS
1	K	75	ASN
1	K	79	ARG
1	K	85	SER
1	K	91	VAL
1	K	95	ASN
1	K	100	THR
1	K	110	SER
1	K	125	PHE
1	K	140	SER

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Mol	Chain	Res	Type
1	K	144	GLU
1	K	149	GLN
1	K	161	THR
1	K	171	GLU
1	K	193	ARG
1	K	198	ILE
1	K	203	ARG
1	K	210	LYS
1	K	218	LYS
1	K	222	THR
1	K	244	LYS
1	K	252	LYS
1	K	277	VAL
1	K	281	GLU
1	K	289	GLU
1	K	290	VAL
2	L	42	LYS
2	L	52	THR
2	L	75	ASP
2	L	77	ASN
2	L	89	SER
2	L	124	GLU
2	L	126	LEU
2	L	136	THR
2	L	154	THR
2	L	155	LYS
2	L	170	SER
2	L	210	GLU
2	L	223	GLU
2	L	226	GLU
2	L	227	LEU
2	L	228	SER
2	L	241	SER
2	L	249	THR
2	L	251	LEU
2	L	254	GLU
2	L	256	SER
2	L	273	LEU
2	L	301	VAL
2	L	308	VAL
2	L	322	LYS
1	M	27	THR

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Mol	Chain	Res	Type
1	M	31	GLN
1	M	43	LEU
1	M	66	ARG
1	M	74	TRP
1	M	83	SER
1	M	85	SER
1	M	87	SER
1	M	95	ASN
1	M	100	THR
1	M	106	ASN
1	M	124	ASP
1	M	127	ILE
1	M	128	ASN
1	M	129	ARG
1	M	140	SER
1	M	154	ARG
1	M	155	THR
1	M	166	VAL
1	M	174	LEU
1	M	193	ARG
1	M	201	LEU
1	M	223	VAL
1	M	252	LYS
1	M	289	GLU
2	N	38	ASP
2	N	56	GLU
2	N	80	LEU
2	N	89	SER
2	N	100	LYS
2	N	109	SER
2	N	126	LEU
2	N	129	LEU
2	N	136	THR
2	N	141	SER
2	N	146	SER
2	N	154	THR
2	N	160	THR
2	N	162	SER
2	N	210	GLU
2	N	218	ARG
2	N	221	THR
2	N	228	SER

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Mol	Chain	Res	Type
2	N	276	ARG
2	N	285	ILE
2	N	319	LYS
1	O	22	THR
1	O	26	THR
1	O	27	THR
1	O	30	SER
1	O	35	THR
1	O	45	GLU
1	O	52	THR
1	O	68	LEU
1	O	75	ASN
1	O	83	SER
1	O	85	SER
1	O	96	ASN
1	O	97	THR
1	O	126	SER
1	O	160	SER
1	O	169	LYS
1	O	202	THR
1	O	210	LYS
1	O	261	ASP
1	O	268	TRP
1	O	274	GLU
1	O	281	GLU
1	O	287	LEU
1	O	290	VAL
1	O	293	LYS
1	O	300	VAL
2	P	40	ILE
2	P	43	ASN
2	P	45	LYS
2	P	47	THR
2	P	64	LEU
2	P	91	LEU
2	P	102	SER
2	P	105	LEU
2	P	109	SER
2	P	110	GLU
2	P	115	PHE
2	P	118	LYS
2	P	124	GLU

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Mol	Chain	Res	Type
2	P	126	LEU
2	P	151	PHE
2	P	157	ILE
2	P	161	SER
2	P	162	SER
2	P	170	SER
2	P	173	GLN
2	P	204	VAL
2	P	207	ARG
2	P	210	GLU
2	P	219	ILE
2	P	222	VAL
2	P	227	LEU
2	P	231	SER
2	P	244	ASN
2	P	249	THR
2	P	258	GLU
2	P	287	GLU
2	P	288	LYS
2	P	306	LYS
2	P	315	SER
2	P	316	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	150	GLN
1	A	204	ASN
1	A	263	ASN
1	A	296	ASN
2	B	63	ASN
2	B	77	ASN
2	B	103	ASN
2	B	132	ASN
2	B	172	ASN
2	B	224	ASN
2	B	269	ASN
1	C	96	ASN
1	C	176	ASN
1	C	182	HIS
1	C	204	ASN

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Mol	Chain	Res	Type
1	C	263	ASN
2	D	84	GLN
2	D	128	GLN
2	D	185	ASN
2	D	244	ASN
1	E	71	ASN
1	E	141	ASN
2	F	43	ASN
2	F	65	GLN
2	F	77	ASN
2	F	103	ASN
2	F	173	GLN
2	F	224	ASN
2	F	253	ASN
2	F	257	ASN
2	F	318	ASN
1	G	75	ASN
1	G	149	GLN
1	G	159	GLN
1	G	180	HIS
1	G	265	HIS
2	H	120	ASN
2	H	208	ASN
2	H	224	ASN
2	H	244	ASN
1	I	39	GLN
1	I	41	ASN
1	I	71	ASN
1	I	96	ASN
1	I	159	GLN
1	I	188	ASN
1	I	206	ASN
1	I	263	ASN
2	J	111	GLN
2	J	180	ASN
1	K	89	GLN
1	K	94	ASN
1	K	135	ASN
1	K	173	HIS
1	K	237	HIS
2	L	163	ASN
2	L	208	ASN

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Mol	Chain	Res	Type
2	L	224	ASN
2	L	269	ASN
2	L	289	ASN
1	M	33	ASN
1	M	96	ASN
1	M	98	ASN
1	M	173	HIS
1	M	204	ASN
2	N	63	ASN
2	N	65	GLN
2	N	116	GLN
2	N	173	GLN
2	N	261	GLN
2	N	318	ASN
1	O	95	ASN
1	O	159	GLN
1	O	173	HIS
1	O	177	ASN
1	O	263	ASN
1	O	295	HIS
2	P	77	ASN
2	P	163	ASN
2	P	172	ASN
2	P	186	ASN
2	P	188	HIS
2	P	224	ASN
2	P	244	ASN
2	P	253	ASN
2	P	269	ASN
2	P	275	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	281/311 (90%)	0.37	21 (7%) 20 15	17, 32, 79, 101	0
1	C	281/311 (90%)	0.46	19 (6%) 23 17	16, 37, 77, 101	0
1	E	290/311 (93%)	0.48	18 (6%) 26 20	17, 37, 72, 100	0
1	G	290/311 (93%)	0.37	20 (6%) 23 16	13, 34, 75, 101	0
1	I	290/311 (93%)	0.22	19 (6%) 24 18	13, 30, 81, 123	0
1	K	281/311 (90%)	0.31	18 (6%) 25 18	17, 33, 70, 98	0
1	M	287/311 (92%)	0.19	12 (4%) 40 32	13, 31, 67, 98	0
1	O	283/311 (90%)	0.23	13 (4%) 37 29	17, 32, 77, 98	0
2	B	282/324 (87%)	0.17	7 (2%) 58 48	16, 31, 58, 95	0
2	D	289/324 (89%)	0.30	8 (2%) 55 45	18, 33, 61, 97	0
2	F	284/324 (87%)	0.14	7 (2%) 58 48	14, 31, 57, 104	0
2	H	288/324 (88%)	0.14	11 (3%) 44 35	15, 28, 62, 86	0
2	J	288/324 (88%)	0.13	8 (2%) 55 45	16, 29, 58, 98	0
2	L	288/324 (88%)	0.03	4 (1%) 73 64	14, 27, 52, 110	0
2	N	288/324 (88%)	0.08	3 (1%) 79 72	15, 29, 55, 76	0
2	P	286/324 (88%)	0.09	10 (3%) 47 38	16, 29, 62, 108	0
All	All	4576/5080 (90%)	0.23	198 (4%) 40 31	13, 31, 69, 123	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	267	PHE	6.7
2	P	150	LYS	6.4
1	I	125	PHE	5.7
1	I	267	PHE	5.6
2	D	151	PHE	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	267	PHE	5.4
1	M	267	PHE	5.4
1	E	267	PHE	5.3
2	F	151	PHE	5.3
1	K	267	PHE	5.3
1	I	73	TYR	5.0
1	I	119	TYR	5.0
1	C	206	ASN	4.9
2	D	35	THR	4.9
1	C	266	GLY	4.8
2	F	152	ASP	4.8
1	I	132	LEU	4.8
1	K	125	PHE	4.7
2	P	151	PHE	4.7
1	G	206	ASN	4.6
1	I	134	GLY	4.6
2	B	158	GLY	4.6
1	A	119	TYR	4.5
1	I	130	GLY	4.5
1	O	267	PHE	4.5
1	E	73	TYR	4.4
2	F	145	TYR	4.4
2	B	35	THR	4.4
1	A	74	TRP	4.3
1	E	268	TRP	4.3
1	G	74	TRP	4.3
2	B	150	LYS	4.2
2	P	149	GLY	4.2
2	L	154	THR	4.2
2	J	146	PHE	4.1
1	C	74	TRP	4.1
2	D	36	ALA	4.1
1	I	131	GLY	4.0
1	A	134	GLY	4.0
2	H	154	THR	4.0
1	K	119	TYR	3.8
1	K	206	ASN	3.7
1	C	134	GLY	3.7
1	I	305	ASP	3.7
1	I	94	ASN	3.7
1	I	127	ILE	3.7
1	K	132	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	16	GLY	3.6
1	A	268	TRP	3.6
1	G	129	ARG	3.6
1	C	125	PHE	3.6
1	A	205	GLY	3.6
1	M	74	TRP	3.6
1	A	135	ASN	3.6
1	G	210	LYS	3.5
1	C	16	GLY	3.5
2	D	41	GLY	3.5
1	G	17	ASP	3.5
1	O	206	ASN	3.5
1	M	16	GLY	3.4
1	K	134	GLY	3.4
1	G	73	TYR	3.4
1	A	138	LYS	3.4
2	J	149	THR	3.3
1	A	124	ASP	3.3
1	E	17	ASP	3.3
1	K	305	ASP	3.3
1	G	119	TYR	3.3
1	O	127	ILE	3.3
1	A	305	ASP	3.3
1	E	119	TYR	3.3
1	A	206	ASN	3.3
2	D	145	TYR	3.2
2	L	153	SER	3.2
2	N	165	TYR	3.2
1	A	139	GLU	3.2
1	I	126	SER	3.2
1	E	193	ARG	3.2
2	H	280	HIS	3.2
2	J	275	HIS	3.2
1	I	208	TRP	3.2
1	O	119	TYR	3.1
1	C	126	SER	3.1
2	B	149	GLY	3.1
1	G	268	TRP	3.1
1	C	119	TYR	3.1
1	K	135	ASN	3.1
1	A	17	ASP	3.0
1	O	266	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
2	J	36	GLY	3.0
1	A	16	GLY	3.0
1	I	16	GLY	3.0
1	O	133	THR	3.0
1	K	74	TRP	3.0
1	G	305	ASP	3.0
1	C	17	ASP	3.0
1	M	128	ASN	3.0
1	E	138	LYS	2.9
2	P	36	ALA	2.9
1	C	264	ARG	2.9
1	A	136	ILE	2.9
1	E	125	PHE	2.9
1	E	16	GLY	2.9
1	C	208	TRP	2.8
1	A	73	TYR	2.8
1	M	129	ARG	2.8
2	J	150	LYS	2.8
1	K	304	ASN	2.8
2	F	160	THR	2.8
1	K	70	PRO	2.8
2	P	153	SER	2.8
2	H	149	GLY	2.8
1	M	119	TYR	2.7
1	O	268	TRP	2.7
2	B	145	TYR	2.7
1	M	130	GLY	2.7
1	M	193	ARG	2.7
1	M	208	TRP	2.6
2	F	100	LYS	2.6
2	H	143	PHE	2.6
2	J	37	LYS	2.6
1	M	268	TRP	2.6
2	B	148	GLY	2.6
2	F	217	THR	2.6
1	E	266	GLY	2.5
1	G	130	GLY	2.5
1	I	266	GLY	2.5
2	H	36	ALA	2.5
1	O	134	GLY	2.5
1	O	89	GLN	2.5
1	G	269	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	121	ARG	2.5
1	M	93	ASP	2.4
2	F	157	ILE	2.4
1	E	117	TYR	2.4
1	I	129	ARG	2.4
1	G	208	TRP	2.4
1	G	95	ASN	2.4
1	K	136	ILE	2.4
1	C	139	GLU	2.4
1	I	136	ILE	2.4
2	J	152	ILE	2.4
1	C	135	ASN	2.4
1	O	125	PHE	2.4
2	P	157	ILE	2.4
1	I	128	ASN	2.3
1	K	124	ASP	2.3
1	C	207	LEU	2.3
2	D	40	ILE	2.3
1	E	134	GLY	2.3
2	B	36	ALA	2.3
2	N	41	GLY	2.3
1	C	305	ASP	2.3
2	H	158	GLY	2.3
1	K	265	HIS	2.3
1	O	16	GLY	2.3
1	C	192	ASN	2.2
1	E	135	ASN	2.2
2	N	143	PHE	2.2
1	G	45	GLU	2.2
2	H	118	LYS	2.2
1	C	193	ARG	2.2
1	K	17	ASP	2.2
1	K	264	ARG	2.2
2	P	152	ASP	2.2
1	A	266	GLY	2.2
1	E	72	GLY	2.2
2	P	143	PHE	2.2
1	A	186	LEU	2.2
2	H	155	LYS	2.2
2	H	37	PRO	2.2
1	G	76	SER	2.2
2	D	155	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	J	31	ALA	2.2
2	P	159	ARG	2.2
1	E	74	TRP	2.2
1	E	264	ARG	2.1
1	K	204	ASN	2.1
1	C	210	LYS	2.1
1	A	123	GLY	2.1
1	I	133	THR	2.1
2	P	158	GLY	2.1
1	C	73	TYR	2.1
1	M	127	ILE	2.1
2	H	40	ILE	2.1
1	G	265	HIS	2.1
1	E	305	ASP	2.1
1	O	124	ASP	2.1
1	K	193	ARG	2.1
1	G	266	GLY	2.1
1	A	117	TYR	2.1
2	D	165	TYR	2.1
1	G	131	GLY	2.0
1	E	71	ASN	2.0
2	L	151	PHE	2.0
1	A	202	THR	2.0
2	L	152	ASP	2.0
1	O	117	TYR	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.