



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:43 PM UTC

PDB ID : 4GUO / pdb_00004guo
Title : structure of p73 DNA binding domain complex with 12 bp DNA
Authors : Ethayathulla, A.S.; Viadiu, H.
Deposited on : 2012-08-29
Resolution : 3.19 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

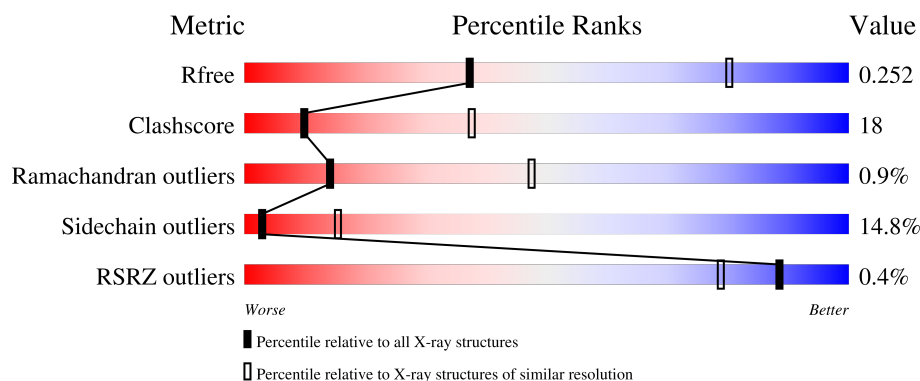
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	210	
1	B	210	
1	C	210	
1	D	210	
1	I	210	

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Mol	Chain	Length	Quality of chain
1	J	210	
1	K	210	
1	L	210	
2	E	12	
2	G	12	
2	M	12	
2	O	12	
3	F	12	
3	H	12	
3	N	12	
3	P	12	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14607 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 Tumor protein p73.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1571	982	283	295	11			
1	B	198	Total	C	N	O	S	0	0	0
			1553	975	279	288	11			
1	C	201	Total	C	N	O	S	0	0	0
			1586	993	285	297	11			
1	D	198	Total	C	N	O	S	0	0	0
			1551	971	279	290	11			
1	I	198	Total	C	N	O	S	0	0	0
			1556	973	280	292	11			
1	J	199	Total	C	N	O	S	0	0	0
			1561	976	281	293	11			
1	K	201	Total	C	N	O	S	0	0	0
			1576	988	282	295	11			
1	L	201	Total	C	N	O	S	0	0	0
			1581	991	284	295	11			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	MET	-	initiating methionine	UNP O15350
A	104	GLY	-	expression tag	UNP O15350
A	105	HIS	-	expression tag	UNP O15350
A	106	HIS	-	expression tag	UNP O15350
A	107	HIS	-	expression tag	UNP O15350
A	108	HIS	-	expression tag	UNP O15350
A	109	HIS	-	expression tag	UNP O15350
A	110	HIS	-	expression tag	UNP O15350
A	111	HIS	-	expression tag	UNP O15350
A	112	HIS	-	expression tag	UNP O15350
A	113	GLU	-	expression tag	UNP O15350
A	114	PHE	-	expression tag	UNP O15350
B	103	MET	-	initiating methionine	UNP O15350

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Chain	Residue	Modelled	Actual	Comment	Reference
B	104	GLY	-	expression tag	UNP O15350
B	105	HIS	-	expression tag	UNP O15350
B	106	HIS	-	expression tag	UNP O15350
B	107	HIS	-	expression tag	UNP O15350
B	108	HIS	-	expression tag	UNP O15350
B	109	HIS	-	expression tag	UNP O15350
B	110	HIS	-	expression tag	UNP O15350
B	111	HIS	-	expression tag	UNP O15350
B	112	HIS	-	expression tag	UNP O15350
B	113	GLU	-	expression tag	UNP O15350
B	114	PHE	-	expression tag	UNP O15350
C	103	MET	-	initiating methionine	UNP O15350
C	104	GLY	-	expression tag	UNP O15350
C	105	HIS	-	expression tag	UNP O15350
C	106	HIS	-	expression tag	UNP O15350
C	107	HIS	-	expression tag	UNP O15350
C	108	HIS	-	expression tag	UNP O15350
C	109	HIS	-	expression tag	UNP O15350
C	110	HIS	-	expression tag	UNP O15350
C	111	HIS	-	expression tag	UNP O15350
C	112	HIS	-	expression tag	UNP O15350
C	113	GLU	-	expression tag	UNP O15350
C	114	PHE	-	expression tag	UNP O15350
D	103	MET	-	initiating methionine	UNP O15350
D	104	GLY	-	expression tag	UNP O15350
D	105	HIS	-	expression tag	UNP O15350
D	106	HIS	-	expression tag	UNP O15350
D	107	HIS	-	expression tag	UNP O15350
D	108	HIS	-	expression tag	UNP O15350
D	109	HIS	-	expression tag	UNP O15350
D	110	HIS	-	expression tag	UNP O15350
D	111	HIS	-	expression tag	UNP O15350
D	112	HIS	-	expression tag	UNP O15350
D	113	GLU	-	expression tag	UNP O15350
D	114	PHE	-	expression tag	UNP O15350
I	103	MET	-	initiating methionine	UNP O15350
I	104	GLY	-	expression tag	UNP O15350
I	105	HIS	-	expression tag	UNP O15350
I	106	HIS	-	expression tag	UNP O15350
I	107	HIS	-	expression tag	UNP O15350
I	108	HIS	-	expression tag	UNP O15350
I	109	HIS	-	expression tag	UNP O15350

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Chain	Residue	Modelled	Actual	Comment	Reference
I	110	HIS	-	expression tag	UNP O15350
I	111	HIS	-	expression tag	UNP O15350
I	112	HIS	-	expression tag	UNP O15350
I	113	GLU	-	expression tag	UNP O15350
I	114	PHE	-	expression tag	UNP O15350
J	103	MET	-	initiating methionine	UNP O15350
J	104	GLY	-	expression tag	UNP O15350
J	105	HIS	-	expression tag	UNP O15350
J	106	HIS	-	expression tag	UNP O15350
J	107	HIS	-	expression tag	UNP O15350
J	108	HIS	-	expression tag	UNP O15350
J	109	HIS	-	expression tag	UNP O15350
J	110	HIS	-	expression tag	UNP O15350
J	111	HIS	-	expression tag	UNP O15350
J	112	HIS	-	expression tag	UNP O15350
J	113	GLU	-	expression tag	UNP O15350
J	114	PHE	-	expression tag	UNP O15350
K	103	MET	-	initiating methionine	UNP O15350
K	104	GLY	-	expression tag	UNP O15350
K	105	HIS	-	expression tag	UNP O15350
K	106	HIS	-	expression tag	UNP O15350
K	107	HIS	-	expression tag	UNP O15350
K	108	HIS	-	expression tag	UNP O15350
K	109	HIS	-	expression tag	UNP O15350
K	110	HIS	-	expression tag	UNP O15350
K	111	HIS	-	expression tag	UNP O15350
K	112	HIS	-	expression tag	UNP O15350
K	113	GLU	-	expression tag	UNP O15350
K	114	PHE	-	expression tag	UNP O15350
L	103	MET	-	initiating methionine	UNP O15350
L	104	GLY	-	expression tag	UNP O15350
L	105	HIS	-	expression tag	UNP O15350
L	106	HIS	-	expression tag	UNP O15350
L	107	HIS	-	expression tag	UNP O15350
L	108	HIS	-	expression tag	UNP O15350
L	109	HIS	-	expression tag	UNP O15350
L	110	HIS	-	expression tag	UNP O15350
L	111	HIS	-	expression tag	UNP O15350
L	112	HIS	-	expression tag	UNP O15350
L	113	GLU	-	expression tag	UNP O15350
L	114	PHE	-	expression tag	UNP O15350

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*GP*GP*GP*CP*AP*AP*GP*CP*CP*

CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	12	Total	C	N	O	P	0	0	0
			244	115	50	68	11			
2	G	11	Total	C	N	O	P	0	0	0
			228	106	47	64	11			
2	M	12	Total	C	N	O	P	0	0	0
			244	115	50	68	11			
2	O	12	Total	C	N	O	P	0	0	0
			244	115	50	68	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	12	Total	C	N	O	P	0	0	0
			242	115	44	72	11			
3	H	12	Total	C	N	O	P	0	0	0
			242	115	44	72	11			
3	N	12	Total	C	N	O	P	0	0	0
			242	115	44	72	11			
3	P	12	Total	C	N	O	P	0	0	0
			242	115	44	72	11			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	I	1	Total	Zn	0	0
			1	1		
4	J	1	Total	Zn	0	0
			1	1		
4	K	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	16	Total O 16 16	0	0
5	B	15	Total O 15 15	0	0
5	C	21	Total O 21 21	0	0
5	D	18	Total O 18 18	0	0
5	I	14	Total O 14 14	0	0
5	J	10	Total O 10 10	0	0
5	K	18	Total O 18 18	0	0
5	L	20	Total O 20 20	0	0
5	E	1	Total O 1 1	0	0
5	H	1	Total O 1 1	0	0
5	N	1	Total O 1 1	0	0
5	P	1	Total O 1 1	0	0

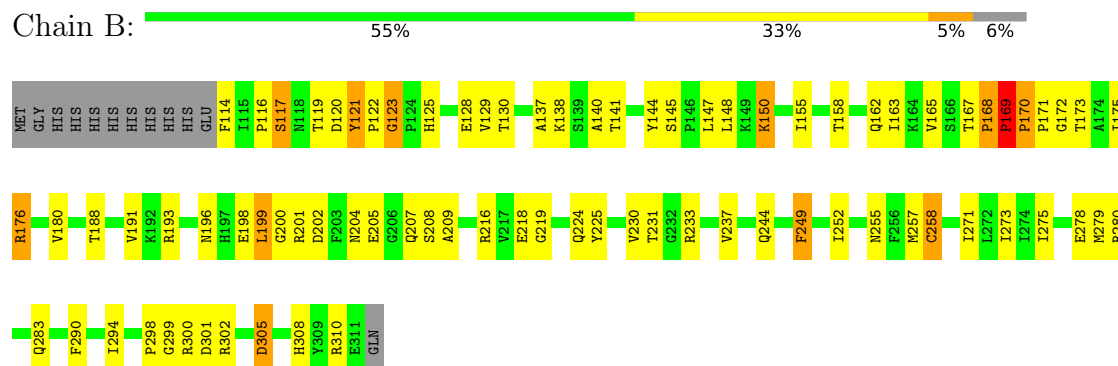
3 Residue-property plots

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

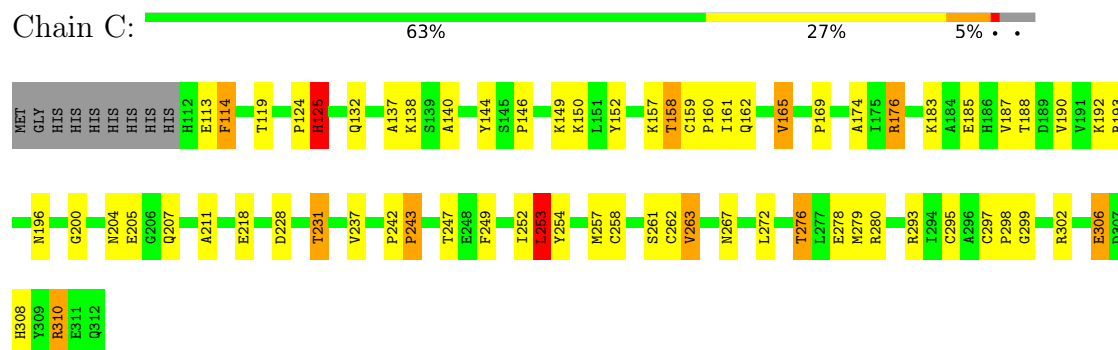
• Molecule 1: Tumor protein p73



• Molecule 1: Tumor protein p73

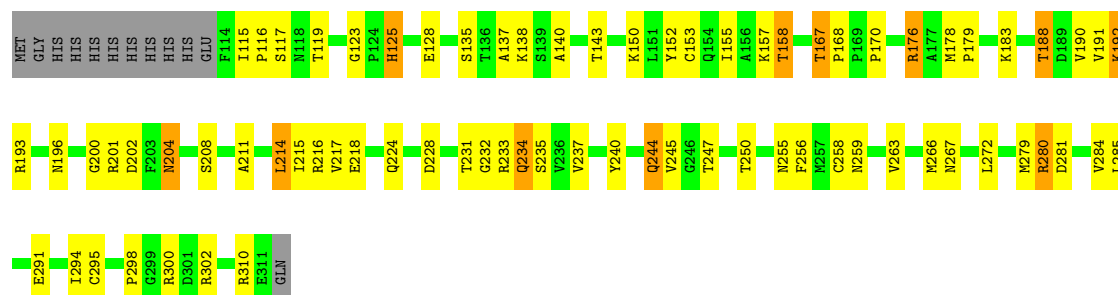


• Molecule 1: Tumor protein p73



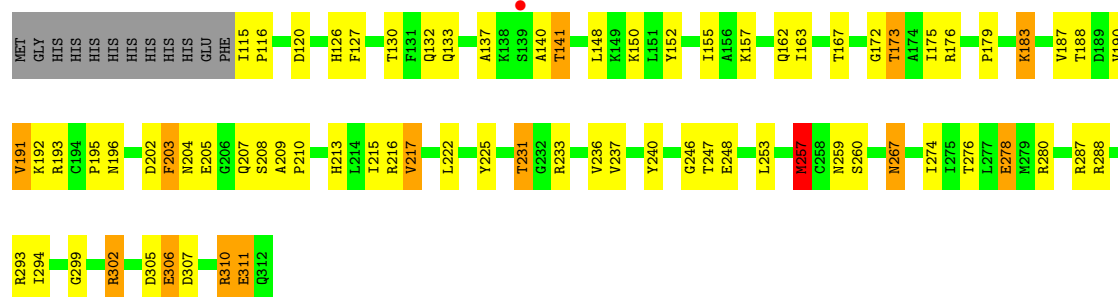
- Molecule 1: Tumor protein p73

Chain D: 



- Molecule 1: Tumor protein p73

Chain I: 



- Molecule 1: Tumor protein p73

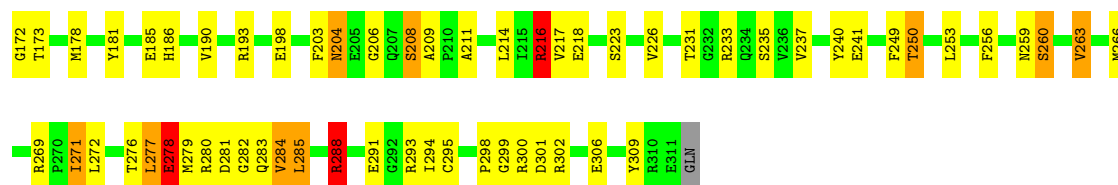
Chain J: 



- Molecule 1: Tumor protein p73

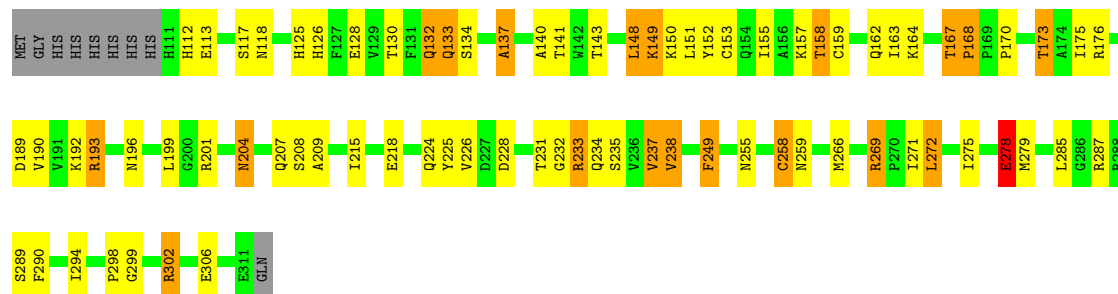
Chain K: 





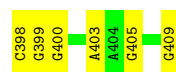
- Molecule 1: Tumor protein p73

Chain L: 59% 28% 9% .



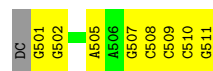
- Molecule 2: DNA (5'-D(*CP*GP*GP*GP*CP*AP*AP*GP*CP*CP*CP*G)-3')

Chain E: 50% 50%



- Molecule 2: DNA (5'-D(*CP*GP*GP*GP*CP*AP*AP*GP*CP*CP*CP*G)-3')

Chain G: 25% 67% 8%



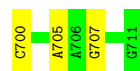
- Molecule 2: DNA (5'-D(*CP*GP*GP*GP*CP*AP*AP*GP*CP*CP*CP*G)-3')

Chain M: 83% 8% 8%

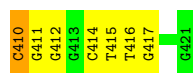


- Molecule 2: DNA (5'-D(*CP*GP*GP*GP*CP*AP*AP*GP*CP*CP*CP*G)-3')

Chain O: 75% 25%



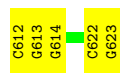
- Molecule 3: DNA (5'-D(*CP*GP*GP*GP*CP*TP*TP*GP*CP*CP*CP*G)-3')



- Molecule 3: DNA (5'-D(*CP*GP*GP*GP*CP*TP*TP*GP*CP*CP*CP*G)-3')



- Molecule 3: DNA (5'-D(*CP*GP*GP*GP*CP*TP*TP*GP*CP*CP*CP*G)-3')



- Molecule 3: DNA (5'-D(*CP*GP*GP*GP*CP*TP*TP*GP*CP*CP*CP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.25Å 104.33Å 123.32Å 90.00° 96.38° 90.00°	Depositor
Resolution (Å)	44.01 – 3.19 44.01 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.01-3.19) 99.1 (44.01-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.208 , 0.270 (Not available) , 0.252	Depositor DCC
R_{free} test set	1738 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	80.8	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14607	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.78	0/1610	1.06	4/2188 (0.2%)
1	B	0.78	0/1593	1.21	8/2166 (0.4%)
1	C	0.76	0/1627	1.04	2/2210 (0.1%)
1	D	0.76	0/1590	1.16	7/2162 (0.3%)
1	I	0.78	0/1595	1.13	5/2167 (0.2%)
1	J	0.81	1/1600 (0.1%)	1.18	6/2174 (0.3%)
1	K	0.83	2/1616 (0.1%)	1.17	7/2197 (0.3%)
1	L	0.80	0/1622	1.10	5/2205 (0.2%)
2	E	0.55	0/274	0.73	1/421 (0.2%)
2	G	0.34	0/256	0.65	0/393
2	M	0.62	1/274 (0.4%)	0.85	1/421 (0.2%)
2	O	0.45	0/274	0.78	1/421 (0.2%)
3	F	0.47	0/270	0.91	1/415 (0.2%)
3	H	0.41	0/270	0.96	1/415 (0.2%)
3	N	0.49	0/270	0.96	1/415 (0.2%)
3	P	0.50	0/270	0.98	1/415 (0.2%)
All	All	0.75	4/15011 (0.0%)	1.09	51/20785 (0.2%)

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	K	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	168	PRO	CA-C	5.77	1.55	1.51
2	M	600	DC	O3'-P	-5.49	1.52	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	168	PRO	C-O	-5.49	1.18	1.24
1	K	166	SER	CA-C	5.46	1.60	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	168	PRO	N-CA-C	10.05	120.12	110.47
1	D	208	SER	N-CA-C	9.96	122.21	111.36
1	J	282	GLY	N-CA-C	9.33	127.87	112.85
1	B	168	PRO	N-CA-C	8.66	121.26	110.70
1	B	168	PRO	CA-C-N	8.42	129.06	120.38
1	B	168	PRO	C-N-CA	8.42	129.06	120.38
1	J	136	THR	N-CA-C	8.09	120.36	110.41
2	O	700	DC	C5'-C4'-O4'	7.66	120.89	109.40
1	J	168	PRO	CA-C-N	7.35	127.95	120.38
1	J	168	PRO	C-N-CA	7.35	127.95	120.38
3	H	512	DC	C5'-C4'-O4'	7.33	120.39	109.40
2	M	600	DC	C5'-C4'-O4'	7.25	120.28	109.40
1	L	132	GLN	N-CA-C	7.23	119.06	111.03
1	B	169	PRO	N-CA-C	7.21	119.50	110.70
1	A	151	LEU	N-CA-CB	7.19	121.88	110.23
1	K	134	SER	N-CA-C	-7.02	99.50	109.96
1	D	125	HIS	N-CA-C	-6.96	97.86	109.07
1	C	125	HIS	N-CA-C	-6.54	100.15	109.96
1	D	123	GLY	CA-C-N	6.50	126.00	119.24
1	D	123	GLY	C-N-CA	6.50	126.00	119.24
1	B	150	LYS	N-CA-C	6.29	119.38	108.76
1	B	170	PRO	N-CA-C	6.26	118.34	110.70
1	K	284	VAL	N-CA-C	6.13	116.94	107.99
3	N	612	DC	C5'-C4'-O4'	6.07	118.51	109.40
1	I	202	ASP	N-CA-C	6.01	118.60	111.33
1	I	278	GLU	N-CA-C	6.00	118.19	109.07
3	F	410	DC	C5'-C4'-O4'	5.85	118.18	109.40
2	E	398	DC	C5'-C4'-O4'	5.79	118.08	109.40
1	L	249	PHE	N-CA-C	5.66	117.79	109.24
1	D	188	THR	CB-CA-C	-5.58	101.19	110.68
1	C	253	LEU	CB-CA-C	5.58	119.42	110.16
1	L	278	GLU	N-CA-C	5.55	117.50	109.07
1	K	216	ARG	NE-CZ-NH2	5.52	124.17	119.20
1	D	202	ASP	N-CA-C	5.50	117.98	111.33
1	L	168	PRO	CB-CA-C	-5.48	106.24	111.39
1	B	202	ASP	N-CA-C	5.48	118.01	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	257	MET	N-CA-C	5.45	119.99	113.23
1	K	278	GLU	N-CA-C	5.45	117.46	109.24
3	P	716	DC	C4'-C3'-O3'	5.44	118.16	110.00
1	K	136	THR	N-CA-C	5.36	117.45	110.43
1	A	249	PHE	N-CA-C	5.34	117.30	109.24
1	I	208	SER	N-CA-C	5.33	117.09	111.28
1	J	168	PRO	O-C-N	5.25	123.72	121.31
1	D	217	VAL	CB-CA-C	-5.22	102.90	110.63
1	K	208	SER	N-CA-C	-5.15	106.50	112.89
1	K	288	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	B	278	GLU	N-CA-C	5.09	117.12	109.23
1	A	303	LYS	N-CA-CB	5.09	117.39	110.01
1	L	137	ALA	N-CA-C	-5.07	101.37	109.23
1	A	206	GLY	N-CA-C	-5.04	106.11	114.48
1	I	267	ASN	N-CA-C	5.04	118.55	111.74

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	283	GLN	Peptide

5.2 Too-close contacts [i](#)

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	1571	0	1535	70	0
1	B	1553	0	1526	55	0
1	C	1586	0	1551	45	0
1	D	1551	0	1523	55	0
1	I	1556	0	1529	54	0
1	J	1561	0	1531	69	0
1	K	1576	0	1540	71	0
1	L	1581	0	1545	60	0
2	E	244	0	134	6	0
2	G	228	0	122	7	0
2	M	244	0	134	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	244	0	134	2	0
3	F	242	0	136	16	0
3	H	242	0	136	4	0
3	N	242	0	136	3	0
3	P	242	0	136	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	A	16	0	0	2	0
5	B	15	0	0	1	0
5	C	21	0	0	4	0
5	D	18	0	0	0	0
5	E	1	0	0	1	0
5	H	1	0	0	0	0
5	I	14	0	0	5	0
5	J	10	0	0	2	0
5	K	18	0	0	0	0
5	L	20	0	0	2	0
5	N	1	0	0	0	0
5	P	1	0	0	0	0
All	All	14607	0	13348	487	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 (487) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:233:ARG:O	1:L:233:ARG:HD3	1.47	1.14
1:L:279:MET:HG3	1:L:285:LEU:HD11	1.32	1.09
1:J:255:ASN:HB3	1:J:257:MET:CE	1.84	1.08
1:K:169:PRO:HB2	1:K:170:PRO:HD2	1.37	1.07
3:F:415:DT:H2''	3:F:416:DT:H5''	1.42	0.98
1:J:158:THR:HB	1:J:218:GLU:OE1	1.67	0.92
1:D:115:ILE:HG21	1:D:231:THR:HG21	1.51	0.91
3:N:613:DG:H2''	3:N:614:DG:OP2	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:PHE:HB3	1:B:231:THR:HG23	1.53	0.90
3:F:416:DT:H2''	3:F:417:DG:C8	2.08	0.89
1:L:233:ARG:HD3	1:L:233:ARG:C	1.98	0.89
1:D:176:ARG:HB2	1:D:237:VAL:HG12	1.53	0.89
1:J:255:ASN:HB3	1:J:257:MET:HE2	1.55	0.86
1:A:185:GLU:HA	1:D:158:THR:HG23	1.56	0.86
3:F:414:DC:H2''	3:F:415:DT:O5'	1.77	0.85
1:D:263:VAL:HA	1:D:267:ASN:HD22	1.39	0.85
1:A:127:PHE:O	1:A:288:ARG:NH1	2.10	0.84
1:J:155:ILE:HA	1:J:294:ILE:HD11	1.59	0.84
1:A:150:LYS:HB2	1:A:291:GLU:HB3	1.60	0.84
1:A:284:VAL:HB	1:D:245:VAL:HG11	1.60	0.83
3:F:415:DT:C2'	3:F:416:DT:H5''	2.09	0.83
1:I:141:THR:HG22	1:I:157:LYS:HD3	1.59	0.83
1:B:199:LEU:HD23	1:I:167:THR:HG22	1.59	0.82
1:J:255:ASN:HB3	1:J:257:MET:HE1	1.59	0.82
1:K:288:ARG:HG3	1:K:288:ARG:HH21	1.45	0.82
1:J:117:SER:O	1:J:274:ILE:HD12	1.79	0.82
1:I:216:ARG:HD3	5:I:503:HOH:O	1.80	0.81
1:I:225:TYR:HD1	1:I:236:VAL:HG22	1.44	0.81
1:I:204:ASN:HA	1:I:207:GLN:HG3	1.63	0.81
1:L:163:ILE:HD13	1:L:175:ILE:HD13	1.63	0.80
1:L:193:ARG:HG3	1:L:258:CYS:SG	2.21	0.80
1:L:167:THR:HG22	1:L:168:PRO:HD2	1.64	0.79
1:K:300:ARG:NH2	2:O:707:DG:N7	2.31	0.79
1:B:170:PRO:HB2	1:B:173:THR:OG1	1.83	0.78
1:J:150:LYS:HE2	1:J:152:TYR:OH	1.83	0.78
1:J:279:MET:H	1:J:282:GLY:HA3	1.47	0.78
1:A:247:THR:HG22	1:A:249:PHE:H	1.47	0.77
1:K:169:PRO:CB	1:K:170:PRO:HD2	2.15	0.77
1:D:200:GLY:O	1:D:204:ASN:ND2	2.19	0.76
1:I:231:THR:HB	1:I:233:ARG:HG3	1.66	0.76
1:L:279:MET:CG	1:L:285:LEU:HD11	2.13	0.75
1:B:116:PRO:HG2	1:B:180:VAL:HG21	1.68	0.75
1:C:196:ASN:HB2	1:D:196:ASN:OD1	1.85	0.75
1:K:279:MET:HG2	1:K:285:LEU:HD21	1.69	0.75
1:L:158:THR:HB	1:L:218:GLU:OE1	1.87	0.75
1:C:137:ALA:HB3	1:C:140:ALA:HB2	1.69	0.74
1:J:150:LYS:HE2	1:J:152:TYR:CZ	2.23	0.74
1:L:207:GLN:HG3	1:L:209:ALA:H	1.53	0.74
1:K:169:PRO:HB2	1:K:170:PRO:CD	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:279:MET:HG3	1:L:285:LEU:CD1	2.17	0.72
1:A:212:SER:HB2	1:A:234:GLN:HE22	1.53	0.72
1:J:255:ASN:CB	1:J:257:MET:CE	2.66	0.72
1:D:176:ARG:CB	1:D:237:VAL:HG12	2.20	0.72
1:D:125:HIS:HD2	1:D:167:THR:HB	1.54	0.72
1:J:178:MET:HB2	1:J:235:SER:OG	1.89	0.72
1:B:279:MET:HG3	1:B:283:GLN:HB2	1.72	0.71
1:I:195:PRO:HB3	1:J:199:LEU:HD12	1.72	0.71
1:K:169:PRO:HG2	1:K:173:THR:HB	1.72	0.71
1:B:176:ARG:HB2	1:B:237:VAL:HG22	1.72	0.71
1:A:204:ASN:O	1:A:207:GLN:HB3	1.91	0.71
1:I:210:PRO:HG2	1:I:213:HIS:ND1	2.06	0.71
1:K:150:LYS:HG3	1:K:291:GLU:HB3	1.72	0.70
1:L:266:MET:O	1:L:269:ARG:HG2	1.91	0.70
1:L:112:HIS:HB3	5:L:507:HOH:O	1.91	0.70
1:D:158:THR:HB	1:D:218:GLU:OE2	1.91	0.70
1:A:256:PHE:HB3	1:A:294:ILE:HD13	1.75	0.69
1:B:168:PRO:N	1:B:169:PRO:HD2	2.08	0.68
1:B:169:PRO:HB2	1:B:170:PRO:HD3	1.74	0.68
1:A:217:VAL:HG23	1:A:236:VAL:HG11	1.74	0.68
1:A:247:THR:HG22	1:A:249:PHE:N	2.08	0.68
1:K:276:THR:HG22	1:K:278:GLU:HG2	1.75	0.68
1:J:195:PRO:HA	1:J:198:GLU:HG2	1.75	0.67
1:A:185:GLU:HA	1:D:158:THR:CG2	2.23	0.67
1:K:168:PRO:HB2	1:K:169:PRO:HD2	1.77	0.67
1:B:168:PRO:N	1:B:169:PRO:CD	2.58	0.67
1:J:223:SER:HB3	1:J:238:VAL:HG12	1.76	0.67
1:J:155:ILE:HA	1:J:294:ILE:CD1	2.26	0.66
1:L:140:ALA:O	1:L:298:PRO:HG2	1.96	0.66
1:A:247:THR:HG21	1:A:249:PHE:O	1.96	0.66
1:L:231:THR:O	1:L:233:ARG:N	2.28	0.66
1:C:263:VAL:HA	1:C:267:ASN:HD22	1.61	0.65
1:D:150:LYS:HE3	1:D:152:TYR:OH	1.97	0.65
1:I:173:THR:HG22	1:I:240:TYR:HB3	1.79	0.65
1:I:163:ILE:HD13	1:I:175:ILE:HD13	1.77	0.65
1:A:184:ALA:HA	1:A:187:VAL:HG23	1.77	0.64
1:D:167:THR:HG22	1:D:168:PRO:HD2	1.80	0.64
1:L:266:MET:HE3	1:L:271:ILE:HG23	1.79	0.64
1:A:163:ILE:HD13	1:A:175:ILE:HD13	1.79	0.64
1:L:150:LYS:HE2	1:L:152:TYR:OH	1.97	0.63
3:F:411:DG:H2"	3:F:412:DG:C8	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:ILE:CG2	1:D:231:THR:HG21	2.27	0.63
3:P:722:DC:H2"	3:P:723:DG:C8	2.33	0.63
1:B:145:SER:O	1:B:148:LEU:O	2.15	0.63
1:C:242:PRO:O	1:C:243:PRO:O	2.14	0.63
1:J:127:PHE:CE1	1:J:129:VAL:CG2	2.81	0.63
1:K:158:THR:HB	1:K:218:GLU:OE2	1.98	0.63
1:A:287:ARG:NH2	1:D:245:VAL:O	2.29	0.63
1:C:242:PRO:O	1:C:243:PRO:C	2.41	0.63
1:C:280:ARG:HD2	5:C:503:HOH:O	1.98	0.63
1:I:137:ALA:HB3	1:I:140:ALA:HB2	1.80	0.63
1:K:170:PRO:O	1:K:172:GLY:N	2.33	0.62
1:B:137:ALA:HB3	1:B:140:ALA:HB2	1.82	0.62
1:B:163:ILE:HD13	1:B:175:ILE:HD13	1.81	0.62
1:J:141:THR:HG22	1:J:142:TRP:HD1	1.64	0.62
1:I:215:ILE:O	1:I:236:VAL:HG21	1.99	0.62
1:A:183:LYS:HG3	1:A:186:HIS:HD2	1.64	0.62
1:J:127:PHE:CE1	1:J:129:VAL:HG23	2.35	0.62
1:A:185:GLU:OE1	1:D:157:LYS:HD3	1.98	0.62
1:D:115:ILE:O	1:D:115:ILE:HG13	1.99	0.62
1:C:150:LYS:HD2	1:C:152:TYR:CZ	2.34	0.62
1:J:155:ILE:CA	1:J:294:ILE:HD11	2.29	0.62
1:L:233:ARG:O	1:L:233:ARG:CD	2.35	0.61
1:A:215:ILE:O	1:A:236:VAL:HG21	2.00	0.61
1:A:287:ARG:O	1:A:288:ARG:HD2	2.00	0.61
1:B:158:THR:HG23	1:B:218:GLU:OE2	2.00	0.61
1:A:253:LEU:N	1:A:253:LEU:HD22	2.16	0.61
1:I:225:TYR:CD1	1:I:236:VAL:HG22	2.32	0.61
3:F:416:DT:H2"	3:F:417:DG:N7	2.16	0.61
1:L:266:MET:HE3	1:L:271:ILE:CG2	2.31	0.61
1:I:302:ARG:HH21	1:I:306:GLU:HB2	1.66	0.61
1:B:167:THR:C	1:B:169:PRO:HD2	2.25	0.61
1:B:150:LYS:NZ	1:B:305:ASP:OD2	2.31	0.60
1:D:140:ALA:O	1:D:298:PRO:HG2	2.01	0.60
1:D:214:LEU:CD1	1:D:266:MET:HE2	2.31	0.60
1:K:168:PRO:HG3	1:K:240:TYR:CE2	2.36	0.60
1:D:224:GLN:HB3	1:D:237:VAL:HG22	1.82	0.60
1:D:228:ASP:HB3	1:D:231:THR:O	2.02	0.60
1:I:196:ASN:N	1:J:196:ASN:OD1	2.35	0.60
1:I:302:ARG:NH2	1:I:306:GLU:HB2	2.16	0.59
1:C:293:ARG:HG2	1:C:295:CYS:SG	2.42	0.59
1:A:185:GLU:OE1	1:D:157:LYS:CD	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:HIS:HB3	1:B:165:VAL:CG1	2.32	0.59
1:J:244:GLN:OE1	1:K:117:SER:HB2	2.01	0.59
1:J:279:MET:N	1:J:282:GLY:HA3	2.17	0.59
1:A:150:LYS:CB	1:A:291:GLU:HB3	2.33	0.59
1:D:216:ARG:HB3	1:D:255:ASN:HB2	1.85	0.59
1:A:306:GLU:O	1:A:310:ARG:HG3	2.03	0.59
1:C:247:THR:HG22	1:C:249:PHE:H	1.67	0.59
1:L:228:ASP:HB2	1:L:233:ARG:HD2	1.85	0.59
1:I:191:VAL:HG23	5:I:506:HOH:O	2.03	0.58
1:I:193:ARG:NE	1:I:257:MET:HB3	2.17	0.58
1:K:279:MET:CG	1:K:285:LEU:HD21	2.31	0.58
1:B:114:PHE:HB3	1:B:231:THR:CG2	2.29	0.58
1:L:231:THR:O	1:L:231:THR:HG23	2.03	0.58
1:A:201:ARG:HB2	1:A:201:ARG:HH11	1.67	0.58
1:C:176:ARG:HG2	1:C:276:THR:OG1	2.04	0.58
1:L:266:MET:O	1:L:269:ARG:CG	2.51	0.58
1:C:253:LEU:H	1:C:253:LEU:HD23	1.69	0.58
3:P:716:DC:H2''	3:P:717:DT:C6	2.39	0.57
1:I:173:THR:CG2	1:I:240:TYR:HB3	2.34	0.57
1:J:279:MET:HG2	1:J:282:GLY:CA	2.35	0.57
2:M:600:DC:H1'	2:M:601:DG:C8	2.40	0.57
1:B:170:PRO:HB2	1:B:173:THR:HG1	1.69	0.57
1:A:244:GLN:OE1	1:A:245:VAL:N	2.37	0.57
1:C:193:ARG:HD3	1:C:211:ALA:O	2.05	0.57
1:K:114:PHE:HA	1:K:231:THR:HG23	1.86	0.56
1:K:288:ARG:HG3	1:K:288:ARG:NH2	2.13	0.56
1:L:153:CYS:SG	1:L:159:CYS:HB2	2.45	0.56
1:B:140:ALA:O	1:B:298:PRO:HG2	2.05	0.56
1:A:263:VAL:HA	1:A:267:ASN:HB3	1.88	0.56
1:D:115:ILE:HG21	1:D:231:THR:CG2	2.32	0.56
1:B:138:LYS:N	3:F:411:DG:OP2	2.33	0.56
1:B:193:ARG:HD3	1:B:257:MET:HB2	1.87	0.56
1:B:200:GLY:O	1:B:204:ASN:ND2	2.39	0.56
1:L:152:TYR:HB3	1:L:298:PRO:HB3	1.87	0.56
1:I:137:ALA:O	1:I:299:GLY:HA3	2.06	0.55
1:I:193:ARG:CZ	1:I:257:MET:HB3	2.35	0.55
1:D:150:LYS:HD3	1:D:291:GLU:CD	2.31	0.55
1:A:193:ARG:HD3	1:A:211:ALA:O	2.05	0.55
1:A:150:LYS:HE3	1:A:152:TYR:OH	2.07	0.55
1:A:201:ARG:HH11	1:A:201:ARG:CB	2.19	0.55
1:K:154:GLN:HB2	1:K:157:LYS:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:147:LEU:HD12	1:J:306:GLU:HG2	1.88	0.55
1:J:176:ARG:HB2	1:J:237:VAL:HG12	1.89	0.55
1:J:244:GLN:OE1	1:K:117:SER:N	2.40	0.55
1:D:231:THR:O	1:D:233:ARG:N	2.33	0.55
1:K:204:ASN:OD1	1:K:204:ASN:N	2.39	0.55
1:A:130:THR:HG23	5:A:511:HOH:O	2.06	0.55
1:K:166:SER:OG	1:K:167:THR:N	2.39	0.55
1:K:141:THR:HG22	1:K:142:TRP:HD1	1.71	0.54
1:K:169:PRO:CB	1:K:170:PRO:CD	2.82	0.54
1:K:226:VAL:CG2	1:K:235:SER:OG	2.55	0.54
1:I:310:ARG:HB2	5:I:509:HOH:O	2.07	0.54
1:J:135:SER:HB2	1:J:142:TRP:O	2.08	0.54
1:J:213:HIS:CE1	1:J:234:GLN:HB2	2.43	0.54
1:K:217:VAL:HG11	1:K:223:SER:HB3	1.89	0.54
1:K:263:VAL:O	1:L:196:ASN:ND2	2.41	0.54
3:F:411:DG:C2'	3:F:412:DG:C8	2.91	0.54
1:B:137:ALA:O	1:B:299:GLY:HA3	2.08	0.54
1:A:256:PHE:HB3	1:A:294:ILE:CD1	2.38	0.54
1:J:186:HIS:CD2	1:J:269:ARG:HD3	2.43	0.54
1:K:193:ARG:HD3	1:K:211:ALA:O	2.07	0.54
1:L:137:ALA:O	1:L:299:GLY:HA3	2.07	0.54
1:A:161:ILE:HG13	1:A:254:TYR:HD2	1.74	0.53
1:D:135:SER:O	1:D:143:THR:CG2	2.56	0.53
1:J:125:HIS:HD2	1:J:167:THR:O	1.91	0.53
1:L:170:PRO:HD2	1:L:173:THR:HG21	1.89	0.53
2:G:510:DC:H2''	2:G:511:DG:C8	2.43	0.53
1:J:279:MET:HG2	1:J:282:GLY:HA2	1.90	0.53
1:K:277:LEU:HD13	1:K:285:LEU:HD12	1.91	0.53
3:N:622:DC:H2''	3:N:623:DG:C8	2.44	0.53
1:D:193:ARG:HD3	1:D:211:ALA:O	2.09	0.53
1:L:233:ARG:C	1:L:233:ARG:CD	2.67	0.53
1:J:125:HIS:CD2	1:J:167:THR:O	2.62	0.53
1:A:247:THR:CG2	1:A:249:PHE:O	2.57	0.53
1:J:127:PHE:HE1	1:J:129:VAL:CG2	2.21	0.53
1:L:272:LEU:HD13	1:L:289:SER:HB2	1.91	0.53
1:J:127:PHE:HE1	1:J:129:VAL:HG22	1.74	0.52
1:L:190:VAL:HG12	1:L:192:LYS:HG3	1.91	0.52
1:A:151:LEU:HD12	1:A:151:LEU:O	2.09	0.52
1:L:285:LEU:HD12	1:L:285:LEU:N	2.25	0.52
1:C:125:HIS:H	1:C:125:HIS:CD2	2.25	0.52
1:C:263:VAL:O	1:D:196:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:613:DG:C2'	3:N:614:DG:OP2	2.53	0.52
1:L:275:ILE:HD12	1:L:290:PHE:HE1	1.75	0.52
1:B:244:GLN:HE22	1:C:113:GLU:HB3	1.75	0.52
1:C:262:CYS:HA	5:C:514:HOH:O	2.09	0.52
1:C:247:THR:HG21	5:C:502:HOH:O	2.09	0.51
1:I:203:PHE:HD1	1:I:204:ASN:H	1.57	0.51
1:L:137:ALA:HB3	1:L:140:ALA:HB2	1.92	0.51
1:B:169:PRO:O	1:B:170:PRO:C	2.53	0.51
1:K:153:CYS:SG	1:K:256:PHE:HD2	2.33	0.51
1:K:156:ALA:CB	1:K:203:PHE:CZ	2.93	0.51
1:A:161:ILE:HG13	1:A:254:TYR:CD2	2.46	0.51
1:C:125:HIS:CE1	1:C:169:PRO:HA	2.46	0.51
1:L:228:ASP:HB3	1:L:231:THR:O	2.10	0.51
1:K:131:PHE:CE2	1:K:161:ILE:HD12	2.45	0.51
1:A:242:PRO:O	1:A:243:PRO:C	2.54	0.51
1:K:132:GLN:OE1	1:K:133:GLN:HB2	2.11	0.51
1:B:117:SER:OG	1:B:119:THR:HG22	2.10	0.51
1:D:138:LYS:CG	1:D:300:ARG:HB2	2.40	0.51
1:J:250:THR:O	1:J:250:THR:OG1	2.24	0.51
1:L:170:PRO:HG2	1:L:279:MET:HE3	1.93	0.51
1:K:129:VAL:HG13	1:K:288:ARG:HD3	1.93	0.51
1:K:138:LYS:HA	1:K:299:GLY:HA3	1.93	0.51
2:E:405:DG:H1	3:F:414:DC:H42	1.57	0.51
1:I:141:THR:CG2	1:I:157:LYS:HD3	2.37	0.51
1:J:127:PHE:CE1	1:J:129:VAL:HG22	2.46	0.51
1:J:150:LYS:HB2	1:J:291:GLU:HB3	1.92	0.51
1:D:135:SER:O	1:D:143:THR:HG22	2.11	0.50
1:B:258:CYS:O	1:B:294:ILE:HD13	2.11	0.50
1:K:231:THR:HG22	1:K:233:ARG:HG2	1.92	0.50
1:K:241:GLU:O	1:K:250:THR:HG21	2.10	0.50
1:L:117:SER:HB3	1:L:287:ARG:HH12	1.76	0.50
1:B:138:LYS:HG3	1:B:300:ARG:HB2	1.93	0.50
1:B:193:ARG:HD3	1:B:257:MET:CB	2.42	0.50
1:J:127:PHE:HD1	1:J:128:GLU:N	2.10	0.50
1:K:138:LYS:HG2	1:K:139:SER:N	2.26	0.50
1:C:176:ARG:NE	1:C:278:GLU:OE2	2.39	0.50
1:B:207:GLN:HG3	1:B:208:SER:N	2.27	0.50
1:K:129:VAL:HG13	1:K:288:ARG:CD	2.42	0.50
1:K:253:LEU:N	1:K:253:LEU:HD22	2.27	0.50
1:B:158:THR:OG1	1:C:185:GLU:HA	2.12	0.49
1:I:141:THR:HG22	1:I:157:LYS:CD	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:247:THR:HG22	1:I:248:GLU:N	2.27	0.49
1:C:162:GLN:HE21	1:C:162:GLN:HA	1.77	0.49
1:K:209:ALA:HB3	1:K:216:ARG:HD2	1.93	0.49
1:A:150:LYS:HE3	1:A:152:TYR:CZ	2.47	0.49
1:J:200:GLY:O	1:J:204:ASN:ND2	2.44	0.49
1:L:128:GLU:HG3	1:L:164:LYS:HB3	1.94	0.49
1:C:137:ALA:O	1:C:299:GLY:HA3	2.13	0.49
1:I:183:LYS:O	1:I:187:VAL:HG23	2.12	0.49
1:J:126:HIS:HB2	1:J:166:SER:HB2	1.93	0.49
1:L:132:GLN:HB3	1:L:162:GLN:OE1	2.13	0.49
2:E:403:DA:N6	3:F:415:DT:O4	2.45	0.49
1:J:127:PHE:CD1	1:J:127:PHE:C	2.91	0.49
1:L:143:THR:CG2	1:L:298:PRO:O	2.61	0.49
1:L:152:TYR:CZ	1:L:302:ARG:HA	2.48	0.49
1:B:125:HIS:CB	1:B:165:VAL:CG1	2.90	0.49
1:D:244:GLN:O	1:D:247:THR:HB	2.12	0.49
1:K:226:VAL:HG23	1:K:235:SER:OG	2.13	0.49
1:C:261:SER:HB3	2:G:507:DG:OP1	2.13	0.48
1:D:214:LEU:HD11	1:D:266:MET:CE	2.43	0.48
1:I:116:PRO:HD3	1:I:233:ARG:HE	1.77	0.48
1:K:127:PHE:CE1	1:K:277:LEU:HB2	2.48	0.48
1:I:217:VAL:HG23	1:I:253:LEU:O	2.13	0.48
1:J:255:ASN:CB	1:J:257:MET:HE2	2.32	0.48
1:B:163:ILE:O	1:B:249:PHE:HB3	2.13	0.48
1:B:168:PRO:HD2	1:B:169:PRO:HD3	1.95	0.48
1:D:190:VAL:HG22	1:D:233:ARG:HD3	1.94	0.48
1:B:273:ILE:HD12	1:B:290:PHE:HE1	1.78	0.48
1:J:127:PHE:HD1	1:J:127:PHE:C	2.21	0.48
1:K:156:ALA:HB1	1:K:203:PHE:CZ	2.47	0.48
1:L:176:ARG:NH1	1:L:278:GLU:OE2	2.43	0.48
1:A:132:GLN:HE21	1:A:162:GLN:HE22	1.61	0.48
1:A:190:VAL:HG12	1:A:192:LYS:HG3	1.94	0.48
1:I:120:ASP:OD2	1:I:288:ARG:NE	2.43	0.48
1:I:209:ALA:HB2	1:I:225:TYR:CZ	2.48	0.48
1:K:279:MET:HB2	1:K:282:GLY:O	2.13	0.48
1:I:307:ASP:O	1:I:311:GLU:HB2	2.12	0.48
1:J:216:ARG:HD2	1:J:257:MET:HE3	1.96	0.48
1:A:158:THR:HG22	1:A:253:LEU:HD12	1.95	0.48
1:A:304:ALA:O	1:A:308:HIS:HB2	2.14	0.48
1:J:266:MET:O	1:J:269:ARG:HG3	2.14	0.48
1:L:209:ALA:HB2	1:L:225:TYR:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:LYS:HG2	1:D:300:ARG:HB2	1.96	0.47
1:A:151:LEU:HD12	1:A:151:LEU:C	2.39	0.47
1:I:196:ASN:HB2	1:J:196:ASN:OD1	2.15	0.47
3:F:410:DC:O4'	3:H:523:DG:OP1	2.32	0.47
1:C:138:LYS:NZ	3:H:514:DG:N7	2.53	0.47
2:G:509:DC:H2''	2:G:510:DC:C6	2.50	0.47
1:K:150:LYS:HD2	1:K:152:TYR:CZ	2.49	0.47
1:L:118:ASN:OD1	1:L:118:ASN:C	2.57	0.47
1:A:185:GLU:OE2	1:D:158:THR:CG2	2.63	0.47
1:B:121:TYR:CE2	1:B:123:GLY:CA	2.98	0.47
1:J:149:LYS:HG3	1:J:149:LYS:O	2.15	0.47
1:J:149:LYS:O	1:J:149:LYS:CG	2.63	0.47
1:K:114:PHE:HA	1:K:231:THR:CG2	2.44	0.47
1:L:272:LEU:CD1	1:L:289:SER:HB2	2.44	0.47
2:G:501:DG:H2''	2:G:502:DG:C8	2.49	0.47
1:A:179:PRO:HD3	1:A:215:ILE:HD12	1.97	0.47
1:D:259:ASN:HD22	1:D:295:CYS:HA	1.80	0.47
1:K:259:ASN:HA	1:K:294:ILE:HB	1.97	0.47
1:K:300:ARG:HG3	1:K:301:ASP:OD1	2.15	0.47
1:C:193:ARG:NE	1:C:257:MET:HB3	2.31	0.47
1:K:141:THR:HG22	1:K:142:TRP:CD1	2.48	0.47
2:E:409:DG:O6	3:H:522:DC:N4	2.47	0.47
3:F:414:DC:C2'	3:F:415:DT:O5'	2.58	0.47
1:I:172:GLY:HA3	1:I:280:ARG:NH1	2.30	0.46
1:J:130:THR:HG22	1:J:131:PHE:H	1.80	0.46
1:D:240:TYR:CD1	1:D:240:TYR:C	2.92	0.46
1:L:204:ASN:N	1:L:204:ASN:OD1	2.48	0.46
1:L:234:GLN:HE21	1:L:234:GLN:HA	1.79	0.46
1:A:225:TYR:HD1	1:A:236:VAL:HG22	1.80	0.46
1:B:121:TYR:CE2	1:B:123:GLY:HA2	2.50	0.46
1:D:137:ALA:HB3	1:D:140:ALA:HB2	1.98	0.46
1:B:216:ARG:HA	1:B:225:TYR:HE2	1.79	0.46
1:C:144:TYR:HE1	1:C:146:PRO:HA	1.81	0.46
1:J:223:SER:HB3	1:J:238:VAL:CG1	2.45	0.46
1:J:277:LEU:H	1:J:284:VAL:HG13	1.81	0.46
3:F:416:DT:C2'	3:F:417:DG:C8	2.91	0.46
1:D:158:THR:HB	1:D:218:GLU:CD	2.40	0.46
1:D:214:LEU:HD11	1:D:266:MET:HE2	1.97	0.46
1:I:148:LEU:CD1	1:I:305:ASP:HB3	2.46	0.46
1:J:152:TYR:CZ	1:J:302:ARG:HA	2.51	0.46
1:K:198:GLU:O	1:K:204:ASN:ND2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PHE:HB2	1:A:277:LEU:HD12	1.97	0.46
1:A:307:ASP:HA	1:A:310:ARG:HD2	1.97	0.46
2:O:705:DA:C8	2:O:705:DA:H5'	2.51	0.46
1:B:207:GLN:HG3	1:B:209:ALA:N	2.31	0.46
1:I:132:GLN:O	1:I:133:GLN:C	2.58	0.46
1:K:138:LYS:HB3	3:P:713:DG:OP2	2.16	0.46
1:K:302:ARG:O	1:K:306:GLU:HG2	2.16	0.46
1:C:144:TYR:CE1	1:C:146:PRO:HA	2.51	0.45
1:C:253:LEU:HD23	1:C:253:LEU:N	2.31	0.45
1:I:150:LYS:HE2	1:I:293:ARG:HB2	1.99	0.45
1:J:279:MET:HG2	1:J:282:GLY:HA3	1.97	0.45
1:L:125:HIS:O	1:L:126:HIS:C	2.58	0.45
1:B:169:PRO:HB2	1:B:170:PRO:CD	2.42	0.45
1:J:141:THR:HG22	1:J:142:TRP:CD1	2.47	0.45
1:J:158:THR:HG23	5:J:503:HOH:O	2.14	0.45
1:K:127:PHE:CZ	1:K:277:LEU:HB2	2.51	0.45
1:K:140:ALA:O	1:K:298:PRO:HG2	2.17	0.45
1:L:148:LEU:HD12	1:L:149:LYS:N	2.30	0.45
1:A:130:THR:CG2	1:A:131:PHE:N	2.79	0.45
1:C:152:TYR:CZ	1:C:302:ARG:HA	2.51	0.45
1:D:259:ASN:HA	1:D:294:ILE:HB	1.99	0.45
1:J:259:ASN:HA	1:J:294:ILE:HG12	1.98	0.45
1:K:168:PRO:CB	1:K:169:PRO:HD2	2.43	0.45
1:A:140:ALA:O	1:A:298:PRO:HG2	2.17	0.45
1:A:303:LYS:HG3	1:A:304:ALA:N	2.31	0.45
1:C:125:HIS:HB3	1:C:165:VAL:CG1	2.47	0.45
1:C:174:ALA:HB1	1:C:237:VAL:HG12	1.99	0.45
1:C:306:GLU:O	1:C:310:ARG:HD2	2.17	0.45
1:A:184:ALA:HA	1:A:187:VAL:CG2	2.43	0.45
1:B:144:TYR:O	1:B:302:ARG:NH2	2.49	0.45
1:I:127:PHE:O	1:I:288:ARG:NH1	2.50	0.45
1:J:178:MET:HE2	1:J:233:ARG:HB3	1.97	0.45
1:D:263:VAL:HA	1:D:267:ASN:ND2	2.19	0.45
1:L:148:LEU:O	1:L:150:LYS:N	2.50	0.45
1:L:302:ARG:HD3	1:L:306:GLU:OE2	2.17	0.45
1:D:192:LYS:HE2	1:D:234:GLN:OE1	2.17	0.45
1:C:140:ALA:O	1:C:298:PRO:HG2	2.16	0.44
1:I:148:LEU:HD11	1:I:305:ASP:HB3	1.99	0.44
1:I:190:VAL:HG12	1:I:192:LYS:HG3	1.98	0.44
1:K:181:TYR:CD1	1:K:271:ILE:HG22	2.52	0.44
1:B:301:ASP:O	1:B:305:ASP:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:117:SER:CB	1:L:287:ARG:HH12	2.29	0.44
1:I:193:ARG:NH2	1:I:257:MET:HB3	2.32	0.44
1:J:128:GLU:HB3	1:J:164:LYS:HB3	1.99	0.44
1:A:179:PRO:HG2	1:A:191:VAL:HB	1.99	0.44
1:I:306:GLU:HG3	1:I:307:ASP:N	2.32	0.44
1:A:132:GLN:NE2	1:A:162:GLN:HE22	2.16	0.44
1:B:175:ILE:HD12	1:B:252:ILE:HD11	1.99	0.44
1:C:150:LYS:HD2	1:C:152:TYR:CE1	2.51	0.44
1:K:170:PRO:C	1:K:172:GLY:N	2.76	0.44
2:E:409:DG:H2'	2:G:501:DG:O4'	2.16	0.44
1:A:212:SER:HB2	1:A:234:GLN:NE2	2.27	0.44
1:I:216:ARG:NH2	5:I:505:HOH:O	2.48	0.44
1:D:125:HIS:CD2	1:D:167:THR:HB	2.43	0.44
1:I:190:VAL:HA	1:I:233:ARG:HH12	1.83	0.44
1:K:125:HIS:ND1	1:K:167:THR:O	2.51	0.44
1:A:210:PRO:HG2	1:A:213:HIS:CD2	2.53	0.44
1:K:170:PRO:C	1:K:172:GLY:H	2.26	0.44
2:E:399:DG:H2''	2:E:400:DG:OP2	2.18	0.44
1:A:223:SER:HA	1:A:238:VAL:HG12	2.00	0.43
1:A:268:ARG:HD3	5:E:501:HOH:O	2.18	0.43
1:C:200:GLY:O	1:C:204:ASN:ND2	2.50	0.43
1:D:150:LYS:HE3	1:D:152:TYR:CZ	2.53	0.43
1:I:179:PRO:HG2	1:I:191:VAL:HB	2.00	0.43
1:B:231:THR:HG22	1:B:233:ARG:HG2	1.99	0.43
1:C:157:LYS:N	5:C:510:HOH:O	2.45	0.43
1:C:190:VAL:HG12	1:C:192:LYS:HG3	2.00	0.43
1:A:130:THR:HG22	1:A:131:PHE:N	2.32	0.43
1:A:244:GLN:O	1:A:247:THR:HB	2.18	0.43
1:I:196:ASN:HB2	1:J:196:ASN:CG	2.43	0.43
1:L:133:GLN:HG2	1:L:134:SER:N	2.33	0.43
1:A:284:VAL:HB	1:D:245:VAL:CG1	2.40	0.43
1:B:219:GLY:N	5:B:506:HOH:O	2.18	0.43
1:D:150:LYS:HG2	1:D:152:TYR:CE1	2.53	0.43
1:K:281:ASP:C	1:K:282:GLY:O	2.60	0.43
2:G:508:DC:H1'	2:G:509:DC:C6	2.53	0.43
1:D:179:PRO:HD3	1:D:215:ILE:HD12	2.00	0.43
1:D:279:MET:HG3	1:D:280:ARG:HD3	2.01	0.43
1:C:114:PHE:CD1	1:C:231:THR:HG23	2.54	0.43
1:A:263:VAL:C	1:A:265:GLY:H	2.27	0.43
1:K:172:GLY:CA	1:K:280:ARG:HB2	2.49	0.43
1:K:218:GLU:HB3	1:K:253:LEU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:HIS:CB	1:C:165:VAL:CG1	2.97	0.43
1:J:132:GLN:O	1:J:133:GLN:C	2.60	0.43
1:A:150:LYS:HG3	1:A:152:TYR:CE1	2.54	0.42
1:A:152:TYR:CZ	1:A:302:ARG:HA	2.54	0.42
2:G:505:DA:N6	3:H:517:DT:O4	2.52	0.42
1:I:259:ASN:HA	1:I:294:ILE:HB	2.00	0.42
1:J:127:PHE:CD1	1:J:128:GLU:N	2.87	0.42
1:K:164:LYS:O	1:K:165:VAL:HG13	2.18	0.42
1:L:170:PRO:O	1:L:173:THR:HG23	2.18	0.42
1:J:229:PRO:HD3	5:J:505:HOH:O	2.19	0.42
1:B:172:GLY:HA3	1:B:280:ARG:HD3	2.01	0.42
1:J:124:PRO:HG2	1:J:125:HIS:CE1	2.54	0.42
1:L:164:LYS:HB2	5:L:514:HOH:O	2.19	0.42
1:A:196:ASN:HB2	1:B:196:ASN:CG	2.44	0.42
1:A:185:GLU:OE2	1:D:158:THR:HG23	2.20	0.42
1:C:158:THR:HB	1:C:218:GLU:OE1	2.19	0.42
1:L:259:ASN:HA	1:L:294:ILE:HG22	2.00	0.42
1:C:161:ILE:HD11	1:C:254:TYR:HE2	1.85	0.42
1:C:193:ARG:HG3	1:C:258:CYS:SG	2.60	0.42
1:I:247:THR:CG2	1:I:248:GLU:H	2.33	0.42
1:K:171:PRO:C	1:K:173:THR:N	2.76	0.42
1:B:125:HIS:CB	1:B:165:VAL:HG13	2.49	0.42
1:L:237:VAL:CG2	1:L:238:VAL:N	2.83	0.42
3:P:716:DC:H2'	3:P:717:DT:H71	2.02	0.42
1:B:162:GLN:HE21	1:B:162:GLN:HB3	1.70	0.41
1:A:200:GLY:HA3	5:A:516:HOH:O	2.20	0.41
1:I:140:ALA:O	1:I:141:THR:C	2.60	0.41
1:L:224:GLN:HB3	1:L:237:VAL:HG13	2.02	0.41
1:C:152:TYR:CE2	1:C:302:ARG:HA	2.55	0.41
1:J:138:LYS:HA	1:J:299:GLY:HA3	2.01	0.41
1:K:153:CYS:O	1:K:294:ILE:HA	2.20	0.41
1:D:152:TYR:CZ	1:D:302:ARG:HA	2.55	0.41
1:A:151:LEU:C	1:A:151:LEU:CD1	2.94	0.41
1:C:159:CYS:HA	1:C:160:PRO:HD3	1.78	0.41
1:K:147:LEU:HD21	1:K:309:TYR:CD2	2.56	0.41
1:B:121:TYR:HA	1:B:122:PRO:HD3	1.79	0.41
1:B:172:GLY:HA3	1:B:280:ARG:HH11	1.85	0.41
1:J:152:TYR:CE2	1:J:302:ARG:HA	2.56	0.41
1:K:116:PRO:HB3	1:K:178:MET:HE3	2.01	0.41
1:L:233:ARG:HE	1:L:235:SER:HB2	1.84	0.41
1:L:218:GLU:HB2	1:L:255:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:226:VAL:HB	1:L:235:SER:HB3	2.03	0.41
1:B:198:GLU:O	1:I:126:HIS:HE1	2.04	0.41
1:I:287:ARG:O	1:I:288:ARG:HG2	2.21	0.41
1:K:260:SER:O	1:K:266:MET:O	2.39	0.41
1:K:293:ARG:HD2	1:K:295:CYS:SG	2.61	0.41
3:F:415:DT:C3'	3:F:416:DT:H5''	2.51	0.41
1:C:252:ILE:HD13	1:C:252:ILE:HA	1.92	0.41
1:I:216:ARG:CD	5:I:503:HOH:O	2.54	0.41
1:A:154:GLN:NE2	1:A:296:ALA:O	2.53	0.40
1:B:170:PRO:HA	1:B:171:PRO:HD3	1.93	0.40
1:D:256:PHE:CB	1:D:294:ILE:HD12	2.51	0.40
1:J:163:ILE:O	1:J:249:PHE:HA	2.21	0.40
1:L:231:THR:O	1:L:231:THR:CG2	2.69	0.40
1:A:123:GLY:C	1:A:125:HIS:N	2.77	0.40
1:J:153:CYS:O	1:J:294:ILE:HA	2.22	0.40
3:F:415:DT:H2'	3:F:416:DT:C6	2.55	0.40
1:B:275:ILE:HD11	1:B:290:PHE:CE2	2.56	0.40
1:K:130:THR:OG1	1:K:162:GLN:HB2	2.21	0.40
1:B:125:HIS:ND1	1:B:167:THR:O	2.55	0.40
1:I:152:TYR:CE2	1:I:302:ARG:HG2	2.56	0.40
1:I:176:ARG:HH21	1:I:278:GLU:CD	2.29	0.40
1:J:125:HIS:HE1	1:J:285:LEU:HD22	1.87	0.40
2:E:405:DG:H1	3:F:414:DC:N4	2.20	0.40
1:A:217:VAL:HG23	1:A:236:VAL:CG1	2.47	0.40
1:D:178:MET:HE3	1:D:235:SER:HB3	2.03	0.40
1:D:224:GLN:HB3	1:D:237:VAL:CG2	2.50	0.40
1:J:178:MET:CE	1:J:233:ARG:HB3	2.52	0.40
1:K:186:HIS:CD2	1:K:269:ARG:HE	2.39	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	199/210 (95%)	189 (95%)	10 (5%)	0	100	100
1	B	196/210 (93%)	179 (91%)	15 (8%)	2 (1%)	12	45
1	C	199/210 (95%)	188 (94%)	9 (4%)	2 (1%)	12	45
1	D	196/210 (93%)	187 (95%)	6 (3%)	3 (2%)	8	37
1	I	196/210 (93%)	188 (96%)	7 (4%)	1 (0%)	24	59
1	J	197/210 (94%)	188 (95%)	8 (4%)	1 (0%)	24	59
1	K	199/210 (95%)	184 (92%)	10 (5%)	5 (2%)	4	27
1	L	199/210 (95%)	187 (94%)	11 (6%)	1 (0%)	24	59
All	All	1581/1680 (94%)	1490 (94%)	76 (5%)	15 (1%)	14	47

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	123	GLY
1	B	169	PRO
1	C	243	PRO
1	D	116	PRO
1	J	122	PRO
1	D	232	GLY
1	I	246	GLY
1	K	169	PRO
1	L	232	GLY
1	K	171	PRO
1	K	168	PRO
1	C	124	PRO
1	K	206	GLY
1	D	170	PRO
1	K	165	VAL

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	175/186 (94%)	156 (89%)	19 (11%)	6	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	174/186 (94%)	150 (86%)	24 (14%)	3	18
1	C	178/186 (96%)	154 (86%)	24 (14%)	4	19
1	D	174/186 (94%)	149 (86%)	25 (14%)	3	16
1	I	175/186 (94%)	151 (86%)	24 (14%)	3	18
1	J	175/186 (94%)	144 (82%)	31 (18%)	2	10
1	K	176/186 (95%)	143 (81%)	33 (19%)	1	9
1	L	177/186 (95%)	149 (84%)	28 (16%)	2	13
All	All	1404/1488 (94%)	1196 (85%)	208 (15%)	3	15

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	119	THR
1	A	134	SER
1	A	151	LEU
1	A	155	ILE
1	A	183	LYS
1	A	201	ARG
1	A	203	PHE
1	A	212	SER
1	A	227	ASP
1	A	231	THR
1	A	249	PHE
1	A	258	CYS
1	A	263	VAL
1	A	272	LEU
1	A	276	THR
1	A	277	LEU
1	A	281	ASP
1	A	303	LYS
1	B	117	SER
1	B	120	ASP
1	B	121	TYR
1	B	128	GLU
1	B	129	VAL
1	B	130	THR
1	B	141	THR
1	B	147	LEU
1	B	155	ILE

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Mol	Chain	Res	Type
1	B	176	ARG
1	B	188	THR
1	B	191	VAL
1	B	199	LEU
1	B	201	ARG
1	B	205	GLU
1	B	224	GLN
1	B	230	VAL
1	B	249	PHE
1	B	255	ASN
1	B	258	CYS
1	B	271	ILE
1	B	305	ASP
1	B	308	HIS
1	B	310	ARG
1	C	114	PHE
1	C	119	THR
1	C	125	HIS
1	C	132	GLN
1	C	149	LYS
1	C	158	THR
1	C	165	VAL
1	C	176	ARG
1	C	183	LYS
1	C	187	VAL
1	C	188	THR
1	C	205	GLU
1	C	207	GLN
1	C	228	ASP
1	C	231	THR
1	C	253	LEU
1	C	263	VAL
1	C	272	LEU
1	C	276	THR
1	C	279	MET
1	C	297	CYS
1	C	306	GLU
1	C	308	HIS
1	C	310	ARG
1	D	117	SER
1	D	119	THR
1	D	128	GLU

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Mol	Chain	Res	Type
1	D	153	CYS
1	D	155	ILE
1	D	158	THR
1	D	167	THR
1	D	176	ARG
1	D	183	LYS
1	D	188	THR
1	D	191	VAL
1	D	192	LYS
1	D	201	ARG
1	D	204	ASN
1	D	214	LEU
1	D	234	GLN
1	D	244	GLN
1	D	250	THR
1	D	258	CYS
1	D	272	LEU
1	D	280	ARG
1	D	281	ASP
1	D	284	VAL
1	D	285	LEU
1	D	310	ARG
1	I	115	ILE
1	I	130	THR
1	I	141	THR
1	I	155	ILE
1	I	162	GLN
1	I	173	THR
1	I	183	LYS
1	I	188	THR
1	I	191	VAL
1	I	203	PHE
1	I	205	GLU
1	I	217	VAL
1	I	222	LEU
1	I	231	THR
1	I	237	VAL
1	I	257	MET
1	I	260	SER
1	I	267	ASN
1	I	274	ILE
1	I	276	THR

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Mol	Chain	Res	Type
1	I	302	ARG
1	I	306	GLU
1	I	310	ARG
1	I	311	GLU
1	J	115	ILE
1	J	117	SER
1	J	119	THR
1	J	130	THR
1	J	133	GLN
1	J	136	THR
1	J	141	THR
1	J	147	LEU
1	J	149	LYS
1	J	158	THR
1	J	161	ILE
1	J	173	THR
1	J	187	VAL
1	J	188	THR
1	J	189	ASP
1	J	191	VAL
1	J	197	HIS
1	J	244	GLN
1	J	250	THR
1	J	251	THR
1	J	258	CYS
1	J	263	VAL
1	J	269	ARG
1	J	271	ILE
1	J	272	LEU
1	J	274	ILE
1	J	279	MET
1	J	284	VAL
1	J	294	ILE
1	J	306	GLU
1	J	311	GLU
1	K	113	GLU
1	K	119	THR
1	K	129	VAL
1	K	132	GLN
1	K	133	GLN
1	K	136	THR
1	K	139	SER

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Mol	Chain	Res	Type
1	K	141	THR
1	K	153	CYS
1	K	155	ILE
1	K	157	LYS
1	K	158	THR
1	K	162	GLN
1	K	164	LYS
1	K	165	VAL
1	K	185	GLU
1	K	190	VAL
1	K	204	ASN
1	K	208	SER
1	K	214	LEU
1	K	216	ARG
1	K	237	VAL
1	K	249	PHE
1	K	250	THR
1	K	260	SER
1	K	263	VAL
1	K	271	ILE
1	K	272	LEU
1	K	277	LEU
1	K	278	GLU
1	K	284	VAL
1	K	285	LEU
1	K	288	ARG
1	L	113	GLU
1	L	130	THR
1	L	133	GLN
1	L	141	THR
1	L	148	LEU
1	L	149	LYS
1	L	151	LEU
1	L	155	ILE
1	L	157	LYS
1	L	158	THR
1	L	167	THR
1	L	173	THR
1	L	189	ASP
1	L	193	ARG
1	L	199	LEU
1	L	201	ARG

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Mol	Chain	Res	Type
1	L	204	ASN
1	L	208	SER
1	L	215	ILE
1	L	233	ARG
1	L	237	VAL
1	L	238	VAL
1	L	249	PHE
1	L	258	CYS
1	L	269	ARG
1	L	272	LEU
1	L	278	GLU
1	L	302	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	132	GLN
1	A	186	HIS
1	A	234	GLN
1	A	255	ASN
1	B	133	GLN
1	B	162	GLN
1	B	186	HIS
1	B	224	GLN
1	C	112	HIS
1	C	125	HIS
1	C	133	GLN
1	C	154	GLN
1	C	162	GLN
1	C	267	ASN
1	D	125	HIS
1	D	126	HIS
1	D	162	GLN
1	D	213	HIS
1	D	234	GLN
1	D	255	ASN
1	D	259	ASN
1	D	267	ASN
1	I	126	HIS
1	I	133	GLN
1	I	154	GLN

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Mol	Chain	Res	Type
1	I	162	GLN
1	I	234	GLN
1	I	267	ASN
1	J	125	HIS
1	J	132	GLN
1	J	133	GLN
1	J	186	HIS
1	J	207	GLN
1	J	267	ASN
1	K	133	GLN
1	K	154	GLN
1	K	186	HIS
1	K	283	GLN
1	K	308	HIS
1	L	112	HIS
1	L	154	GLN
1	L	213	HIS
1	L	221	ASN
1	L	234	GLN
1	L	255	ASN
1	L	259	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	201/210 (95%)	-0.34	0	100 100	50, 98, 147, 172	1 (0%)
1	B	198/210 (94%)	-0.40	0	100 100	58, 92, 126, 145	2 (1%)
1	C	201/210 (95%)	-0.43	0	100 100	55, 83, 126, 141	0
1	D	198/210 (94%)	-0.42	0	100 100	63, 89, 132, 160	0
1	I	198/210 (94%)	-0.44	1 (0%)	87 76	64, 87, 129, 156	0
1	J	199/210 (94%)	-0.16	2 (1%)	79 63	75, 111, 158, 195	0
1	K	201/210 (95%)	-0.28	3 (1%)	72 52	63, 87, 144, 164	0
1	L	201/210 (95%)	-0.54	0	100 100	48, 73, 108, 138	0
2	E	12/12 (100%)	-0.17	0	100 100	73, 100, 152, 178	0
2	G	11/12 (91%)	-0.36	0	100 100	85, 106, 135, 142	0
2	M	12/12 (100%)	-0.56	0	100 100	72, 90, 103, 106	0
2	O	12/12 (100%)	-0.40	0	100 100	92, 106, 140, 146	0
3	F	12/12 (100%)	-0.31	0	100 100	69, 102, 138, 158	0
3	H	12/12 (100%)	-0.22	0	100 100	79, 115, 157, 170	0
3	N	12/12 (100%)	-0.45	0	100 100	72, 84, 105, 117	0
3	P	12/12 (100%)	-0.33	0	100 100	80, 99, 150, 160	0
All	All	1692/1776 (95%)	-0.38	6 (0%)	88 79	48, 89, 141, 195	3 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	174	ALA	2.4
1	K	171	PRO	2.4
1	I	139	SER	2.3
1	K	131	PHE	2.1
1	J	285	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	K	161	ILE	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ZN	A	401	1/1	0.99	0.02	87,87,87,87	0
4	ZN	B	401	1/1	0.99	0.03	63,63,63,63	0
4	ZN	C	401	1/1	0.99	0.05	59,59,59,59	0
4	ZN	I	401	1/1	0.99	0.04	98,98,98,98	0
4	ZN	J	401	1/1	0.99	0.03	84,84,84,84	0
4	ZN	D	401	1/1	1.00	0.02	71,71,71,71	0
4	ZN	K	401	1/1	1.00	0.02	89,89,89,89	0
4	ZN	L	401	1/1	1.00	0.01	76,76,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.