Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2023 – 08:14 PM EDT

PDB ID	:	3VD0
Title	:	structure of p73 DNA binding domain tetramer modulates p73 transactivation
Authors	:	Ethayathulla, A.S.; Tse, P.W.; Nguyen, S.; Viadiu, H.
Deposited on	:	2012-01-04
Resolution	:	2.95 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:

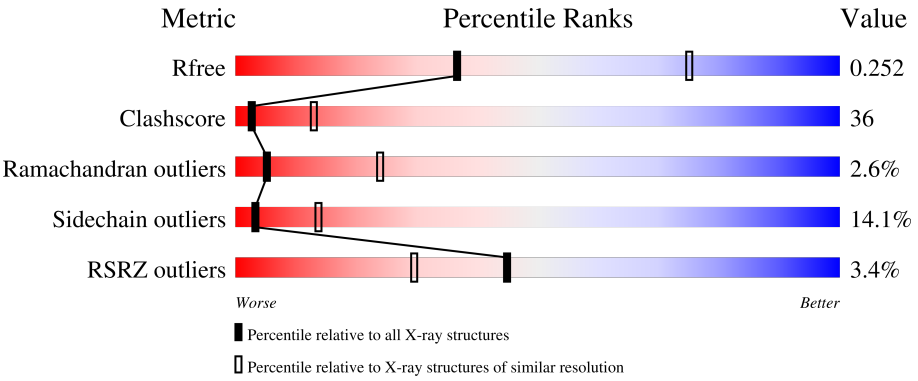
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 <=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	5% 34% 48% 14% ·
1	B	210	3% 35% 49% 11% ·
1	C	210	4% 42% 49% 5% ·
1	D	210	2% 40% 47% 9% 5%
1	I	210	2% 45% 43% 7% 5%

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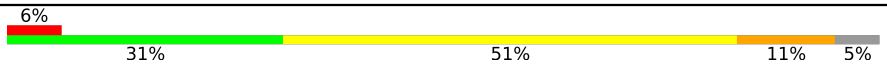
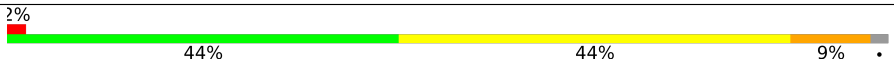
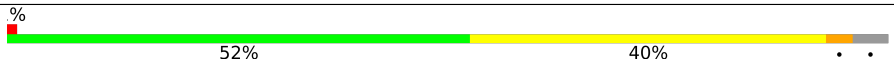
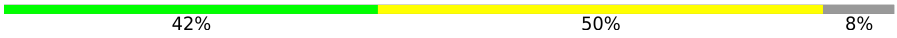
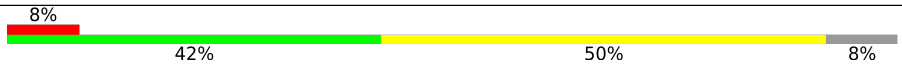
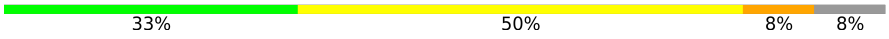
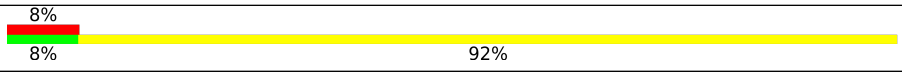
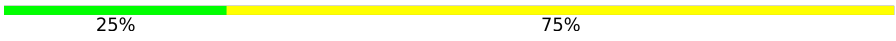
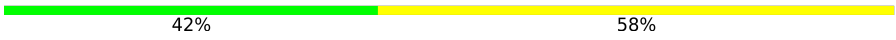
Mol	Chain	Length	Quality of chain
1	J	210	
1	K	210	
1	L	210	
2	E	12	
2	F	12	
2	G	12	
2	H	12	
2	M	12	
2	N	12	
2	O	12	
2	P	12	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14734 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	202	Total	C	N	O	S	0	0	0
			1596	999	288	298	11			
1	B	201	Total	C	N	O	S	0	0	0
			1580	987	285	297	11			
1	C	202	Total	C	N	O	S	0	0	0
			1596	999	288	298	11			
1	D	200	Total	C	N	O	S	2	0	0
			1572	985	282	294	11			
1	I	199	Total	C	N	O	S	0	0	0
			1567	982	281	293	11			
1	J	199	Total	C	N	O	S	1	0	0
			1561	976	281	293	11			
1	K	206	Total	C	N	O	S	0	0	0
			1631	1020	298	302	11			
1	L	201	Total	C	N	O	S	1	0	0
			1586	993	285	297	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*AP*GP*GP*CP*AP*TP*GP*CP*CP*

TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	11	Total	C	N	O	P	0	0	0
			221	106	41	64	10			
2	F	11	Total	C	N	O	P	0	0	0
			227	107	43	66	11			
2	G	11	Total	C	N	O	P	0	0	0
			227	107	43	66	11			
2	H	11	Total	C	N	O	P	0	0	0
			221	106	41	64	10			
2	M	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
2	N	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
2	O	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
2	P	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		

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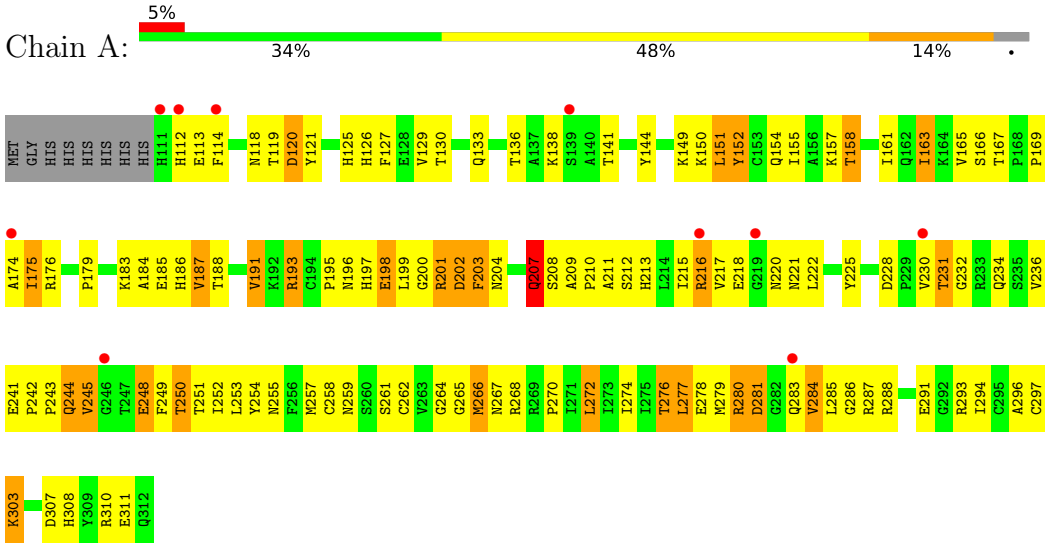
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	19	Total O 19 19	0	0
4	C	19	Total O 19 19	0	0
4	D	13	Total O 13 13	0	0
4	I	19	Total O 19 19	0	0
4	J	14	Total O 14 14	0	0
4	K	34	Total O 34 34	0	0
4	L	30	Total O 30 30	0	0
4	E	1	Total O 1 1	0	0
4	N	1	Total O 1 1	0	0
4	O	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

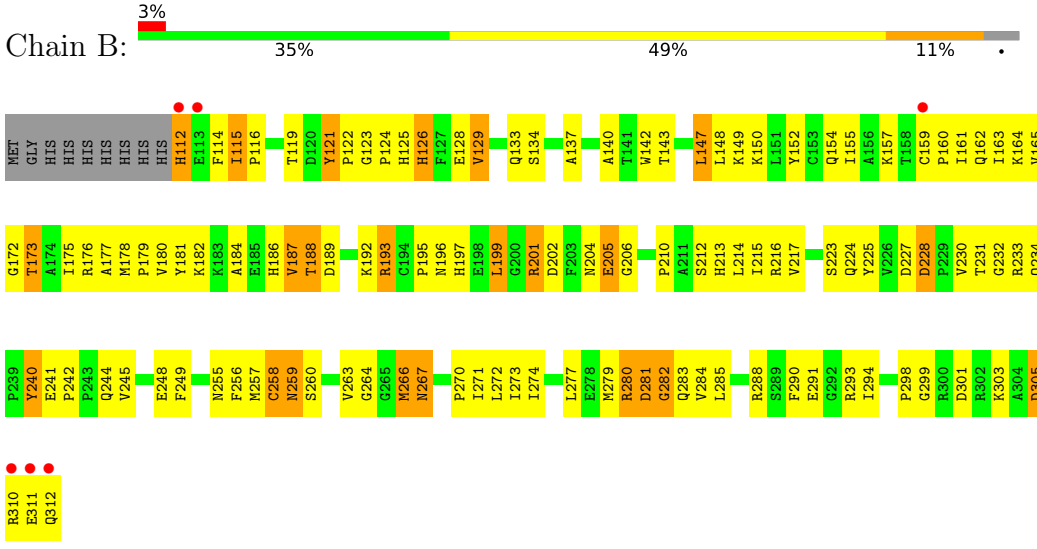
• Molecule 1: Tumor protein p73

Chain A:



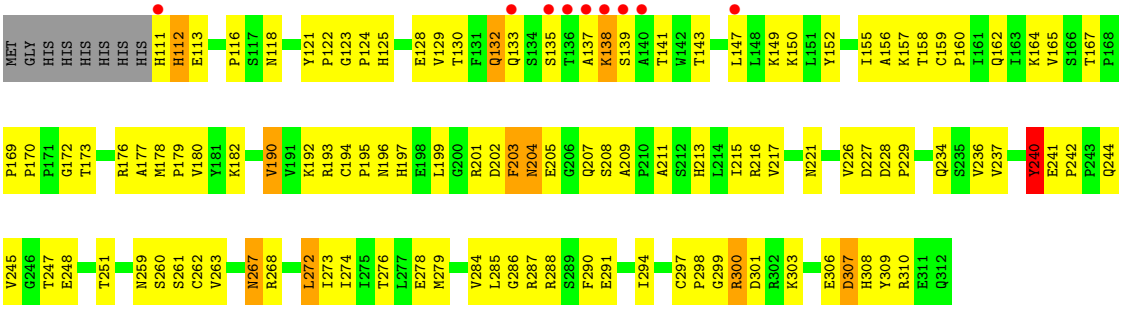
• Molecule 1: Tumor protein p73

Chain B:



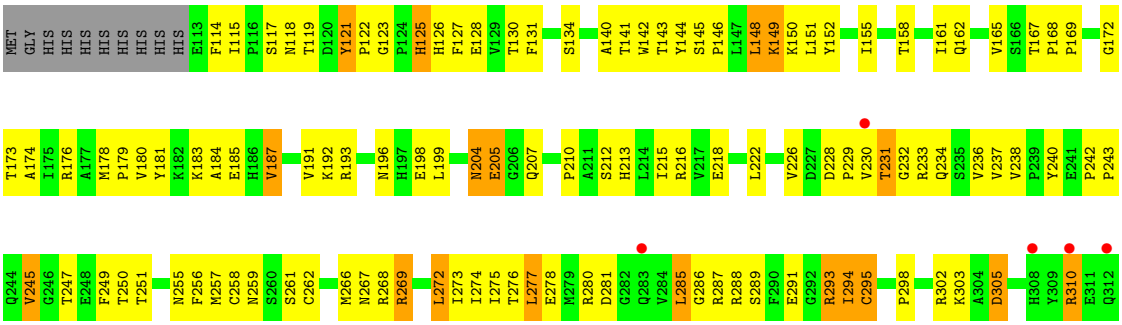
• Molecule 1: Tumor protein p73

Chain C:



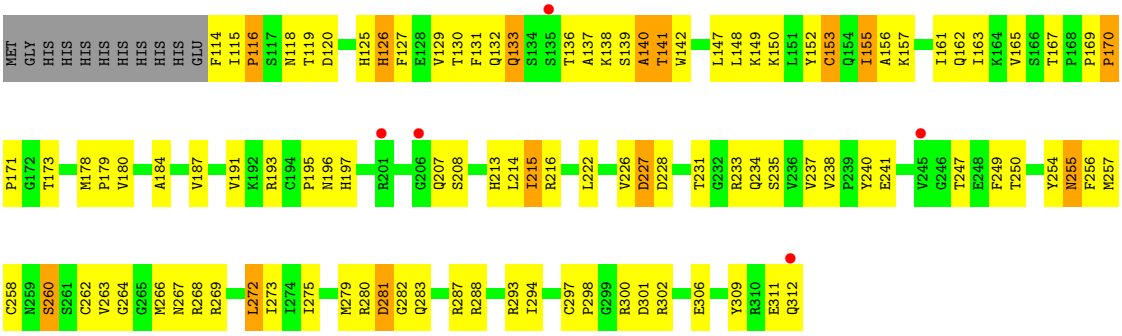
• Molecule 1: Tumor protein p73

Chain D:



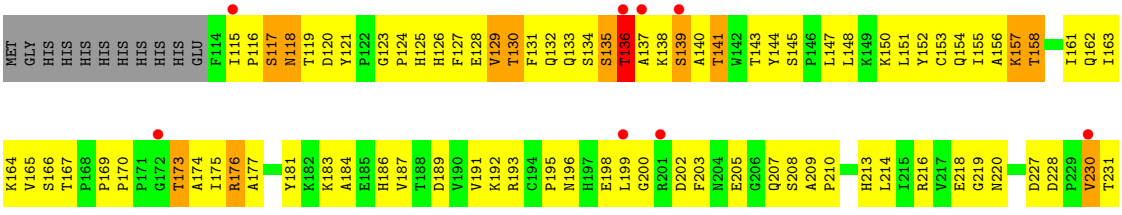
• Molecule 1: Tumor protein p73

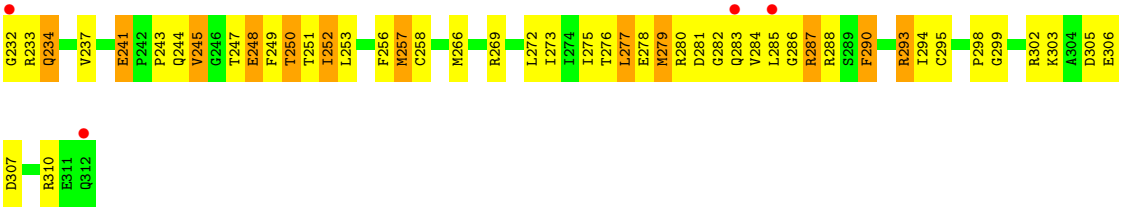
Chain I:



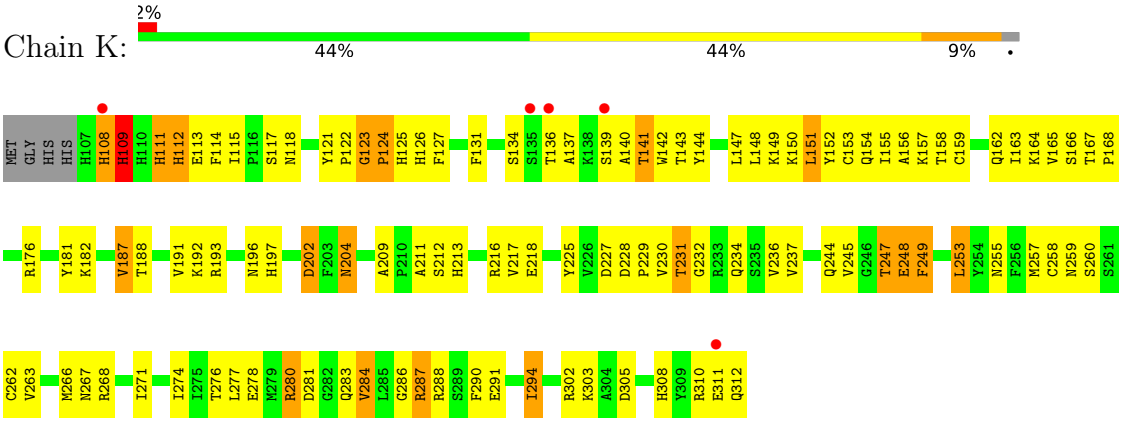
• Molecule 1: Tumor protein p73

Chain J:

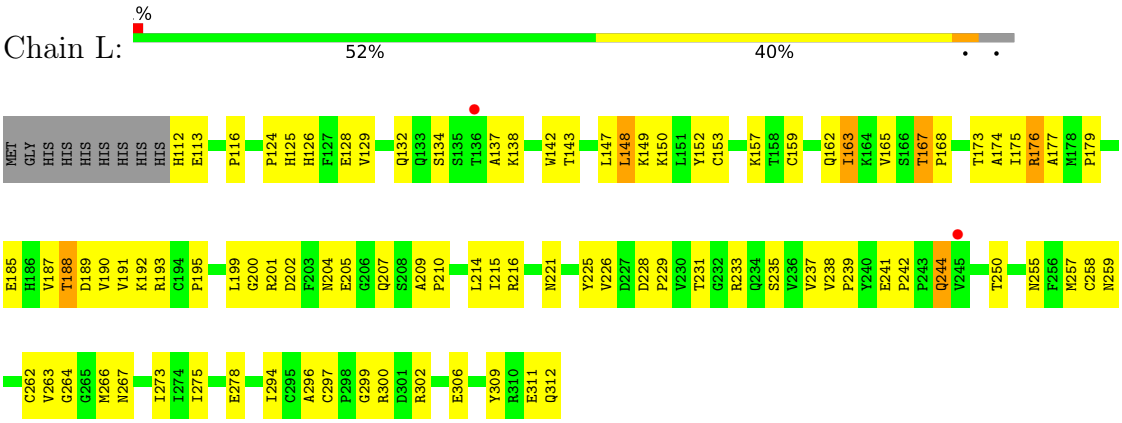




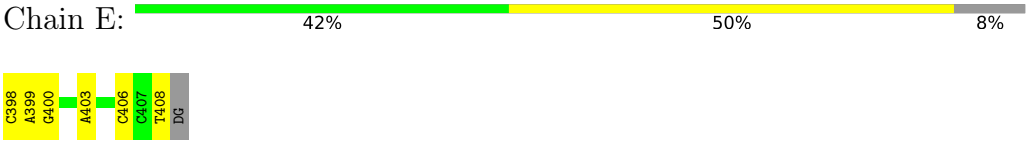
• Molecule 1: Tumor protein p73



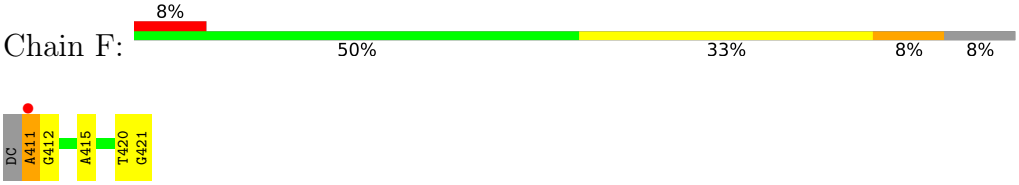
• Molecule 1: Tumor protein p73



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



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

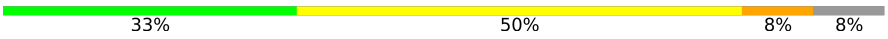


• Molecule 2: DNA (5'-D(*CP*AP*GP*GP*CP*AP*TP*GP*CP*CP*TP*G)-3')

Chain G:

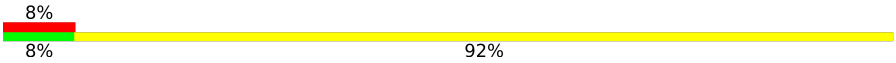
• Molecule 2: DNA (5'-D(*CP*AP*GP*GP*CP*AP*TP*GP*CP*CP*TP*G)-3')

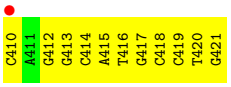
Chain H:



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

Chain M:



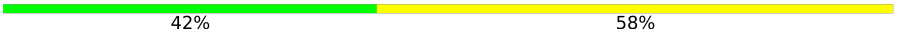


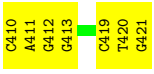
• Molecule 2: DNA (5'-D(*CP*AP*GP*GP*CP*AP*TP*GP*CP*CP*TP*G)-3')

Chain N:

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

Chain O:





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

Chain P:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.09Å 104.52Å 122.99Å 90.00° 96.18° 90.00°	Depositor
Resolution (Å)	19.92 – 2.95 19.92 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.92-2.95) 99.7 (19.92-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.00 (at 2.93Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.235 , 0.254 0.234 , 0.252	Depositor DCC
R_{free} test set	877 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å^2)	69.5	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 53.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14734	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.44	0/1638	0.77	1/2225 (0.0%)
1	B	0.44	0/1620	0.77	0/2201
1	C	0.55	2/1638 (0.1%)	0.75	0/2225
1	D	0.41	0/1612	0.71	1/2190 (0.0%)
1	I	0.48	0/1607	0.77	1/2183 (0.0%)
1	J	0.41	0/1600	0.73	0/2174
1	K	0.44	0/1676	0.74	1/2277 (0.0%)
1	L	0.49	0/1627	0.79	1/2210 (0.0%)
2	E	0.43	0/247	0.81	0/379
2	F	0.68	0/254	0.97	1/390 (0.3%)
2	G	0.75	0/254	0.81	0/390
2	H	0.84	0/247	0.91	1/379 (0.3%)
2	M	0.65	0/272	0.89	0/418
2	N	0.60	0/272	1.08	0/418
2	O	0.50	0/272	0.86	0/418
2	P	0.52	0/272	0.81	0/418
All	All	0.49	2/15108 (0.0%)	0.78	7/20895 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	240	TYR	CB-CG	-5.84	1.42	1.51
1	C	240	TYR	CE2-CZ	-5.46	1.31	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	109	HIS	N-CA-C	-5.47	96.23	111.00
1	D	125	HIS	N-CA-C	-5.26	96.80	111.00
1	L	250	THR	N-CA-C	-5.24	96.85	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	411	DA	OP1-P-OP2	-5.24	111.74	119.60
1	A	207	GLN	N-CA-C	5.12	124.83	111.00
2	H	515	DG	O5'-P-OP1	-5.09	101.11	105.70
1	I	140	ALA	N-CA-C	-5.05	97.35	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1596	0	1558	155	0
1	B	1580	0	1544	148	0
1	C	1596	0	1558	113	0
1	D	1572	0	1540	132	0
1	I	1567	0	1538	107	0
1	J	1561	0	1531	145	0
1	K	1631	0	1581	123	0
1	L	1586	0	1551	65	0
2	E	221	0	125	8	0
2	F	227	0	124	8	0
2	G	227	0	124	5	0
2	H	221	0	125	6	0
2	M	243	0	136	11	0
2	N	243	0	136	14	0
2	O	243	0	136	10	0
2	P	243	0	136	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	18	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	19	0	0	1	0
4	C	19	0	0	1	0
4	D	13	0	0	0	0
4	E	1	0	0	0	0
4	I	19	0	0	3	0
4	J	14	0	0	2	0
4	K	34	0	0	0	0
4	L	30	0	0	3	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
All	All	14734	0	13443	1008	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 36.

All (1008) 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:K:280:ARG:HG2	1:K:280:ARG:HH11	1.02	1.13
1:I:231:THR:CG2	1:I:233:ARG:HG2	1.83	1.08
2:N:401:DG:H2"	2:N:402:DC:H5"	1.33	1.08
1:C:240:TYR:C	1:C:240:TYR:CD2	2.30	1.01
1:B:169:PRO:HG2	1:B:170:PRO:HD3	1.43	1.00
1:D:121:TYR:HE2	1:D:123:GLY:HA2	1.27	0.99
1:C:240:TYR:CD2	1:C:241:GLU:N	2.30	0.99
1:C:204:ASN:HB3	1:C:216:ARG:HH22	1.28	0.98
1:B:170:PRO:HB2	1:B:173:THR:HG23	1.46	0.97
1:D:122:PRO:HG3	1:D:288:ARG:HH21	1.29	0.97
1:I:231:THR:HG21	1:I:233:ARG:HG2	1.46	0.97
1:A:204:ASN:HA	1:A:207:GLN:HB3	1.45	0.96
2:F:420:DT:H2'	2:F:421:DG:C8	2.00	0.96
1:D:277:LEU:H	1:D:277:LEU:HD23	1.29	0.94
1:A:280:ARG:HG3	1:A:280:ARG:HH11	1.32	0.93
1:A:203:PHE:O	1:A:204:ASN:OD1	1.87	0.92
1:C:132:GLN:HG3	1:C:160:PRO:HG2	1.51	0.92
1:J:127:PHE:HE1	1:J:163:ILE:HG23	1.34	0.92
1:J:164:LYS:HE2	1:J:248:GLU:HB2	1.51	0.91
1:J:193:ARG:NE	1:J:257:MET:HB3	1.86	0.91
1:K:122:PRO:HG3	1:K:288:ARG:NH1	1.86	0.91
1:L:176:ARG:HB2	1:L:237:VAL:HG22	1.53	0.89
1:A:296:ALA:O	1:A:298:PRO:HD3	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:157:LYS:O	1:I:255:ASN:HB3	1.73	0.88
1:B:280:ARG:HH21	1:I:136:THR:HG21	1.37	0.88
1:K:280:ARG:HG2	1:K:280:ARG:NH1	1.81	0.87
1:D:243:PRO:HG3	1:D:250:THR:HG23	1.55	0.87
1:D:293:ARG:HH11	1:D:293:ARG:CG	1.87	0.87
1:D:176:ARG:HB2	1:D:237:VAL:HG22	1.56	0.87
1:J:118:ASN:C	1:J:118:ASN:HD22	1.75	0.87
1:K:259:ASN:HA	1:K:294:ILE:HB	1.57	0.87
1:B:193:ARG:NH1	1:B:197:HIS:HB3	1.90	0.86
2:M:418:DC:H2"	2:M:419:DC:H5'	1.57	0.86
1:A:209:ALA:HB3	1:A:216:ARG:HH21	1.41	0.85
1:B:115:ILE:HG13	1:B:115:ILE:O	1.74	0.85
1:C:193:ARG:HH11	1:C:197:HIS:HB3	1.39	0.85
1:D:172:GLY:HA3	1:D:280:ARG:HB3	1.56	0.85
1:K:109:HIS:HB3	1:K:111:HIS:CE1	2.12	0.85
1:J:141:THR:HG22	1:J:157:LYS:HB3	1.59	0.85
1:D:207:GLN:HG2	1:D:216:ARG:NH1	1.92	0.84
1:I:228:ASP:HB3	1:I:231:THR:HB	1.59	0.84
1:C:132:GLN:OE1	1:C:162:GLN:HG3	1.76	0.84
2:N:401:DG:C2'	2:N:402:DC:H5"	2.07	0.84
1:D:231:THR:HG22	1:D:233:ARG:HG2	1.62	0.82
1:B:179:PRO:HB2	1:B:271:ILE:HD11	1.60	0.82
1:A:202:ASP:O	1:A:203:PHE:HB2	1.77	0.82
1:B:169:PRO:CG	1:B:170:PRO:HD3	2.09	0.81
1:J:181:TYR:CE1	1:J:191:VAL:HG22	2.15	0.81
1:K:312:GLN:HA	1:K:312:GLN:HE21	1.45	0.81
2:O:410:DC:H5"	2:O:410:DC:H6	1.45	0.81
1:D:293:ARG:HH11	1:D:293:ARG:HG3	1.46	0.81
1:J:125:HIS:HB3	1:J:165:VAL:HG13	1.61	0.81
1:B:192:LYS:HE3	1:B:234:GLN:HE22	1.43	0.81
1:D:121:TYR:CE2	1:D:123:GLY:HA2	2.15	0.80
1:L:188:THR:HG23	4:L:517:HOH:O	1.80	0.80
2:E:408:DT:H2"	2:G:501:DA:N7	1.96	0.80
1:L:167:THR:HG22	1:L:168:PRO:HD2	1.63	0.79
1:D:274:ILE:HG22	1:D:289:SER:HB3	1.63	0.79
1:I:231:THR:HG22	1:I:233:ARG:HG2	1.61	0.79
1:D:259:ASN:HA	1:D:294:ILE:HB	1.64	0.78
1:C:207:GLN:HG3	1:C:209:ALA:H	1.47	0.78
1:I:148:LEU:O	1:I:149:LYS:HB2	1.83	0.78
1:B:231:THR:HG22	1:B:233:ARG:HG2	1.66	0.78
1:I:263:VAL:HA	1:I:267:ASN:HB3	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:399:DA:H2"	2:E:400:DG:OP2	1.82	0.78
2:P:399:DA:H2"	2:P:400:DG:C8	2.18	0.78
1:J:276:THR:HG22	1:J:287:ARG:HB3	1.66	0.78
1:B:240:TYR:HD2	1:B:241:GLU:N	1.80	0.77
1:B:263:VAL:HA	1:B:267:ASN:HB3	1.66	0.77
1:C:128:GLU:OE2	1:C:164:LYS:HG2	1.85	0.77
1:A:126:HIS:HB2	1:A:166:SER:OG	1.84	0.77
1:C:276:THR:HG22	1:C:278:GLU:HG3	1.63	0.77
1:D:114:PHE:HA	1:D:231:THR:HG23	1.65	0.77
1:D:207:GLN:HG2	1:D:216:ARG:HH12	1.48	0.77
1:D:276:THR:HG22	1:D:287:ARG:HG3	1.66	0.77
1:K:137:ALA:HB3	1:K:140:ALA:HB2	1.67	0.77
1:C:138:LYS:HE3	1:C:297:CYS:SG	2.25	0.76
1:C:138:LYS:HA	1:C:300:ARG:H	1.50	0.76
1:A:266:MET:O	1:A:266:MET:HG3	1.86	0.76
1:C:240:TYR:C	1:C:240:TYR:HD2	1.89	0.75
1:A:209:ALA:HB3	1:A:216:ARG:NH2	2.00	0.75
1:J:266:MET:O	1:J:269:ARG:HG3	1.87	0.75
1:B:301:ASP:O	1:B:305:ASP:HB2	1.86	0.75
1:K:230:VAL:HG12	1:K:231:THR:N	2.02	0.75
1:J:184:ALA:O	1:J:187:VAL:HB	1.86	0.75
1:A:259:ASN:HA	1:A:294:ILE:HB	1.69	0.75
2:G:504:DC:H2"	2:G:505:DA:C8	2.22	0.74
1:C:138:LYS:HD3	1:C:139:SER:HB2	1.69	0.74
1:B:240:TYR:HD2	1:B:240:TYR:C	1.89	0.74
1:K:244:GLN:O	1:K:247:THR:HB	1.87	0.74
1:B:137:ALA:O	1:B:299:GLY:HA3	1.88	0.74
1:C:310:ARG:HG2	1:C:310:ARG:HH11	1.52	0.74
1:A:293:ARG:HG3	1:A:293:ARG:HH11	1.52	0.74
1:J:287:ARG:O	1:J:288:ARG:HD3	1.88	0.74
1:A:280:ARG:HH11	1:A:280:ARG:CG	2.02	0.73
1:B:217:VAL:HG23	1:B:236:VAL:HG21	1.70	0.73
1:A:255:ASN:HB3	1:A:257:MET:CE	2.19	0.73
1:J:127:PHE:CE1	1:J:163:ILE:HG23	2.23	0.73
1:B:280:ARG:HH21	1:I:136:THR:CG2	2.02	0.72
1:A:170:PRO:HB2	1:A:173:THR:CG2	2.19	0.72
1:C:125:HIS:HD1	1:C:167:THR:HB	1.54	0.72
1:B:244:GLN:NE2	1:C:113:GLU:HB3	2.05	0.72
1:J:164:LYS:HE2	1:J:248:GLU:CB	2.19	0.72
1:J:293:ARG:HD3	1:J:295:CYS:SG	2.29	0.72
1:L:179:PRO:HD3	1:L:215:ILE:HD12	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LYS:HB2	1:A:291:GLU:HB3	1.71	0.71
1:A:213:HIS:HA	1:A:234:GLN:NE2	2.04	0.71
1:K:280:ARG:HH11	1:K:280:ARG:CG	1.91	0.71
1:A:276:THR:HG23	1:A:287:ARG:HG3	1.73	0.71
2:P:398:DC:H2"	2:P:399:DA:C8	2.25	0.71
1:C:193:ARG:HD3	1:C:211:ALA:O	1.90	0.71
1:C:193:ARG:NH1	1:C:197:HIS:HB3	2.04	0.71
1:K:193:ARG:HD3	1:K:211:ALA:O	1.90	0.71
1:K:158:THR:CG2	1:K:253:LEU:HD12	2.21	0.71
2:N:401:DG:H2"	2:N:402:DC:C5'	2.14	0.71
1:I:213:HIS:CE1	1:I:234:GLN:HB3	2.25	0.71
1:A:141:THR:HA	1:A:154:GLN:HE21	1.54	0.70
1:C:204:ASN:HB3	1:C:216:ARG:NH2	2.06	0.70
1:L:147:LEU:HD23	1:L:148:LEU:HD21	1.71	0.70
1:B:147:LEU:HB3	1:B:148:LEU:HD12	1.73	0.70
1:L:112:HIS:CD2	1:L:113:GLU:H	2.08	0.70
1:A:255:ASN:HB3	1:A:257:MET:HE1	1.73	0.69
1:C:310:ARG:HG2	1:C:310:ARG:NH1	2.05	0.69
1:B:150:LYS:HB3	1:B:152:TYR:CE1	2.26	0.69
1:A:203:PHE:C	1:A:204:ASN:OD1	2.31	0.69
1:I:281:ASP:O	1:I:283:GLN:N	2.26	0.69
1:J:193:ARG:HE	1:J:257:MET:HB3	1.57	0.69
1:J:277:LEU:HG	1:J:286:GLY:HA3	1.74	0.69
1:L:195:PRO:HD3	1:L:264:GLY:O	1.93	0.69
1:A:170:PRO:HB3	1:A:171:PRO:HD2	1.73	0.69
1:C:111:HIS:HA	1:I:312:GLN:O	1.93	0.69
1:I:263:VAL:HA	1:I:267:ASN:CB	2.23	0.69
1:C:204:ASN:CB	1:C:216:ARG:HH22	2.02	0.69
1:A:277:LEU:O	1:A:285:LEU:N	2.22	0.68
1:C:182:LYS:HD2	1:C:291:GLU:OE1	1.92	0.68
1:A:196:ASN:HB2	1:B:196:ASN:OD1	1.93	0.68
1:B:281:ASP:O	1:B:283:GLN:HG2	1.93	0.68
1:A:207:GLN:HG2	1:A:208:SER:N	2.07	0.68
1:D:293:ARG:HD3	1:D:295:CYS:SG	2.33	0.68
1:D:176:ARG:HB2	1:D:237:VAL:CG2	2.23	0.68
1:A:125:HIS:NE2	1:A:169:PRO:HA	2.09	0.68
1:A:119:THR:HB	1:A:287:ARG:HH21	1.58	0.67
1:C:118:ASN:HB3	1:C:274:ILE:HD11	1.76	0.67
1:I:247:THR:HG22	1:I:249:PHE:H	1.58	0.67
1:A:112:HIS:NE2	1:A:230:VAL:HG11	2.10	0.67
1:A:125:HIS:HE2	1:A:169:PRO:HA	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ILE:O	1:B:115:ILE:CG1	2.42	0.67
1:C:306:GLU:O	1:C:310:ARG:HG3	1.94	0.67
1:D:151:LEU:HD12	1:D:152:TYR:N	2.10	0.67
1:C:201:ARG:O	1:C:203:PHE:N	2.27	0.67
1:D:184:ALA:O	1:D:187:VAL:HG13	1.95	0.67
1:D:277:LEU:HD23	1:D:277:LEU:N	2.07	0.67
1:A:170:PRO:HB2	1:A:173:THR:HG23	1.77	0.67
1:J:210:PRO:HG2	1:J:213:HIS:ND1	2.10	0.67
1:B:195:PRO:HD3	1:B:264:GLY:O	1.94	0.66
1:I:130:THR:HG22	1:I:131:PHE:H	1.61	0.66
1:I:294:ILE:HD12	1:I:294:ILE:H	1.60	0.66
1:A:268:ARG:NH1	2:E:406:DC:H4'	2.11	0.66
1:D:231:THR:CG2	1:D:233:ARG:HG2	2.25	0.66
1:D:310:ARG:HG3	1:D:310:ARG:O	1.95	0.66
1:I:179:PRO:HG3	1:I:214:LEU:HD23	1.75	0.66
1:J:135:SER:O	1:J:136:THR:O	2.14	0.66
1:J:173:THR:OG1	1:J:174:ALA:N	2.28	0.66
1:A:129:VAL:HG23	1:A:288:ARG:HG3	1.77	0.66
1:L:132:GLN:HG2	1:L:162:GLN:NE2	2.11	0.66
1:A:174:ALA:HB1	1:A:238:VAL:O	1.96	0.65
1:J:121:TYR:CE1	1:J:123:GLY:HA2	2.30	0.65
1:K:216:ARG:HB2	1:K:255:ASN:HB2	1.77	0.65
1:A:152:TYR:CD1	1:A:293:ARG:HD3	2.31	0.65
1:A:120:ASP:OD2	1:A:288:ARG:HD2	1.96	0.65
1:B:192:LYS:HE3	1:B:234:GLN:NE2	2.12	0.65
1:C:164:LYS:NZ	1:C:248:GLU:HG3	2.12	0.65
1:A:293:ARG:HG3	1:A:293:ARG:NH1	2.11	0.65
1:I:268:ARG:HH21	1:I:268:ARG:HG3	1.62	0.65
1:B:240:TYR:C	1:B:240:TYR:CD2	2.63	0.64
1:B:240:TYR:HE2	1:B:242:PRO:HA	1.63	0.64
1:I:179:PRO:HD3	1:I:215:ILE:CD1	2.27	0.64
1:D:127:PHE:CD2	1:D:277:LEU:HD22	2.32	0.64
1:D:176:ARG:HH21	1:D:237:VAL:HG21	1.61	0.64
1:B:163:ILE:CD1	1:B:175:ILE:HD13	2.28	0.64
1:C:267:ASN:O	1:C:267:ASN:ND2	2.31	0.64
1:B:170:PRO:CB	1:B:173:THR:HG23	2.25	0.64
1:J:155:ILE:HA	1:J:294:ILE:HD11	1.80	0.64
1:A:193:ARG:HG2	1:A:258:CYS:SG	2.38	0.64
1:A:151:LEU:HD13	1:A:151:LEU:O	1.98	0.64
1:D:228:ASP:HB3	1:D:231:THR:HB	1.80	0.64
1:I:231:THR:HG21	1:I:233:ARG:CG	2.24	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:312:GLN:HA	1:K:312:GLN:NE2	2.11	0.63
1:A:158:THR:HB	1:A:218:GLU:OE1	1.97	0.63
1:B:169:PRO:CD	1:B:170:PRO:HD3	2.28	0.63
1:J:130:THR:OG1	1:J:131:PHE:N	2.30	0.63
1:J:183:LYS:HB3	1:J:186:HIS:HD2	1.63	0.63
1:K:112:HIS:CD2	1:K:230:VAL:HG11	2.33	0.63
2:O:419:DC:H1'	2:O:420:DT:H5'	1.81	0.63
1:A:179:PRO:C	1:A:191:VAL:HG21	2.18	0.63
1:D:277:LEU:HD21	1:D:286:GLY:HA3	1.79	0.63
1:D:302:ARG:HG3	1:D:303:LYS:N	2.13	0.63
1:I:228:ASP:CB	1:I:231:THR:HB	2.29	0.63
2:P:409:DG:OP2	2:P:409:DG:H2'	1.97	0.63
1:D:144:TYR:OH	1:D:149:LYS:HA	1.98	0.63
1:I:179:PRO:HD3	1:I:215:ILE:HD11	1.81	0.63
1:A:240:TYR:OH	1:A:243:PRO:HD3	1.99	0.63
1:B:303:LYS:O	1:B:307:ASP:HB2	1.99	0.63
1:D:272:LEU:HD12	1:D:291:GLU:HA	1.81	0.63
1:I:127:PHE:HE2	1:I:163:ILE:HG23	1.64	0.63
1:A:222:LEU:HD21	1:A:239:PRO:HG2	1.81	0.62
1:C:125:HIS:ND1	1:C:167:THR:HB	2.14	0.62
1:A:141:THR:HG23	1:A:157:LYS:HB3	1.81	0.62
1:L:148:LEU:O	1:L:150:LYS:N	2.33	0.62
1:B:223:SER:HB3	1:B:238:VAL:HG12	1.81	0.62
1:K:143:THR:HG22	1:K:152:TYR:HB2	1.80	0.62
1:C:259:ASN:HA	1:C:294:ILE:HB	1.81	0.62
1:J:138:LYS:HA	1:J:299:GLY:HA3	1.80	0.62
1:A:151:LEU:HD12	1:A:151:LEU:H	1.65	0.62
1:A:161:ILE:HG13	1:A:254:TYR:HD2	1.63	0.62
1:B:195:PRO:O	1:B:199:LEU:HG	1.99	0.62
1:J:118:ASN:HD22	1:J:119:THR:N	1.97	0.62
1:B:274:ILE:HG13	1:B:274:ILE:O	2.00	0.62
1:J:118:ASN:C	1:J:118:ASN:ND2	2.48	0.62
1:C:138:LYS:HA	1:C:300:ARG:N	2.14	0.61
1:J:127:PHE:CE2	1:J:277:LEU:HD21	2.35	0.61
1:J:124:PRO:HG2	1:J:125:HIS:CD2	2.34	0.61
1:K:108:HIS:ND1	1:K:108:HIS:C	2.53	0.61
1:C:138:LYS:HD2	2:H:513:DA:N7	2.14	0.61
1:J:205:GLU:O	1:J:205:GLU:HG3	2.00	0.61
1:D:240:TYR:OH	1:D:242:PRO:HA	2.00	0.61
1:K:158:THR:HG22	1:K:253:LEU:HD12	1.82	0.61
1:L:239:PRO:HD2	4:L:525:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:165:VAL:HG12	1:J:167:THR:H	1.64	0.61
1:K:181:TYR:CE1	1:K:191:VAL:HG22	2.36	0.61
1:L:148:LEU:HD23	1:L:148:LEU:N	2.16	0.61
1:C:125:HIS:CE1	1:C:169:PRO:HA	2.35	0.61
1:J:158:THR:HB	1:J:218:GLU:OE1	2.00	0.61
1:D:114:PHE:HA	1:D:231:THR:CG2	2.30	0.61
1:D:204:ASN:OD1	1:D:204:ASN:N	2.32	0.61
1:I:267:ASN:O	1:I:268:ARG:HB2	2.00	0.61
1:I:197:HIS:HD2	4:I:509:HOH:O	1.83	0.60
1:K:164:LYS:O	1:K:165:VAL:HG22	2.01	0.60
1:C:137:ALA:O	1:C:299:GLY:HA3	2.01	0.60
1:I:155:ILE:HG12	1:I:156:ALA:N	2.16	0.60
1:J:127:PHE:CZ	1:J:277:LEU:HD21	2.37	0.60
1:J:290:PHE:N	1:J:290:PHE:CD2	2.69	0.60
1:K:114:PHE:HA	1:K:231:THR:CG2	2.30	0.60
1:C:111:HIS:CD2	1:C:112:HIS:H	2.20	0.60
1:L:176:ARG:NH1	1:L:278:GLU:OE2	2.35	0.60
1:D:114:PHE:CD2	1:D:231:THR:HA	2.36	0.60
1:L:193:ARG:NH2	1:L:204:ASN:OD1	2.34	0.60
1:C:150:LYS:HB3	1:C:291:GLU:HB3	1.84	0.60
1:L:167:THR:HG22	1:L:168:PRO:CD	2.31	0.60
1:A:204:ASN:CA	1:A:207:GLN:HB3	2.27	0.60
1:D:114:PHE:HD2	1:D:231:THR:HA	1.66	0.60
1:J:258:CYS:O	1:J:294:ILE:HD13	2.02	0.60
1:J:277:LEU:HG	1:J:286:GLY:CA	2.31	0.60
1:L:237:VAL:HG12	1:L:238:VAL:N	2.17	0.60
1:B:260:SER:O	1:B:266:MET:O	2.20	0.59
2:O:420:DT:H2"	2:O:421:DG:C8	2.36	0.59
1:D:134:SER:HB3	1:D:142:TRP:CZ3	2.37	0.59
1:I:114:PHE:HE1	1:I:231:THR:HG23	1.67	0.59
1:J:273:ILE:HB	1:J:290:PHE:CE2	2.37	0.59
1:K:122:PRO:HG3	1:K:288:ARG:HH12	1.64	0.59
1:K:310:ARG:O	1:K:310:ARG:HD3	2.01	0.59
1:A:198:GLU:HG2	1:A:198:GLU:O	2.00	0.59
1:A:284:VAL:HG22	1:D:245:VAL:HG11	1.84	0.59
1:B:244:GLN:HE21	1:C:113:GLU:HB3	1.67	0.59
1:L:138:LYS:O	1:L:297:CYS:HB3	2.01	0.59
1:J:125:HIS:NE2	1:J:285:LEU:HD23	2.17	0.59
1:A:244:GLN:HE21	1:A:244:GLN:CA	2.16	0.59
1:B:140:ALA:O	1:B:298:PRO:HG2	2.03	0.59
1:I:125:HIS:HB3	1:I:167:THR:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:204:ASN:ND2	1:K:211:ALA:HB1	2.17	0.59
1:B:173:THR:HG21	1:B:285:LEU:HD11	1.84	0.59
1:D:267:ASN:H	1:D:269:ARG:HG3	1.68	0.59
1:I:142:TRP:HB2	1:I:153:CYS:HB2	1.84	0.59
1:J:228:ASP:O	1:J:232:GLY:N	2.34	0.59
1:K:122:PRO:O	1:K:123:GLY:O	2.20	0.59
1:I:191:VAL:HG12	1:I:214:LEU:HD22	1.84	0.58
1:J:130:THR:HG23	1:J:162:GLN:HB2	1.85	0.58
2:G:510:DT:H2"	2:G:511:DG:OP2	2.03	0.58
1:A:193:ARG:HD3	1:A:211:ALA:O	2.04	0.58
1:C:204:ASN:HD22	1:C:204:ASN:C	2.07	0.58
1:J:277:LEU:HD23	1:J:277:LEU:N	2.19	0.58
1:B:181:TYR:HE2	1:B:266:MET:HB3	1.68	0.58
1:J:138:LYS:O	1:J:299:GLY:N	2.35	0.58
1:A:161:ILE:HG13	1:A:254:TYR:CD2	2.39	0.58
1:A:204:ASN:HB3	1:A:207:GLN:NE2	2.18	0.58
1:B:258:CYS:O	1:B:294:ILE:HG21	2.04	0.58
2:M:420:DT:H2"	2:M:421:DG:C8	2.38	0.58
1:C:199:LEU:HD11	1:D:199:LEU:HD11	1.85	0.58
1:J:140:ALA:O	1:J:141:THR:C	2.42	0.58
1:I:152:TYR:CE1	1:I:302:ARG:HG3	2.38	0.58
1:J:138:LYS:CG	1:J:139:SER:N	2.67	0.58
1:J:220:ASN:HA	1:K:114:PHE:CD1	2.39	0.58
1:I:147:LEU:HD21	1:I:309:TYR:CD2	2.39	0.58
1:K:204:ASN:HD22	1:K:211:ALA:CB	2.17	0.58
1:L:214:LEU:O	1:L:257:MET:HG2	2.04	0.58
1:A:173:THR:HG22	1:A:279:MET:HA	1.86	0.57
1:B:279:MET:O	1:B:281:ASP:N	2.37	0.57
1:J:220:ASN:HA	1:K:114:PHE:CE1	2.38	0.57
1:B:217:VAL:HG23	1:B:236:VAL:CG2	2.33	0.57
1:C:138:LYS:HD2	2:H:513:DA:C8	2.38	0.57
1:J:138:LYS:O	1:J:299:GLY:HA3	2.04	0.57
1:J:213:HIS:CE1	1:J:234:GLN:HE21	2.22	0.57
1:B:186:HIS:O	1:B:189:ASP:N	2.33	0.57
1:D:131:PHE:CE1	1:D:161:ILE:HG12	2.39	0.57
1:D:247:THR:HG22	1:D:249:PHE:H	1.69	0.57
1:A:185:GLU:OE2	1:D:141:THR:HG21	2.04	0.57
1:J:119:THR:O	1:J:287:ARG:HD3	2.04	0.57
1:J:306:GLU:O	1:J:310:ARG:HG3	2.03	0.57
1:B:164:LYS:HB2	1:B:249:PHE:CE1	2.39	0.57
1:B:170:PRO:HB2	1:B:173:THR:CG2	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:ASP:HB3	1:B:231:THR:HB	1.87	0.57
1:K:144:TYR:OH	1:K:149:LYS:HA	2.04	0.57
1:B:277:LEU:HD22	1:B:285:LEU:HD12	1.87	0.57
1:C:303:LYS:O	1:C:307:ASP:HB2	2.05	0.57
1:D:193:ARG:HD3	1:D:257:MET:HB2	1.87	0.57
1:D:256:PHE:HB3	1:D:294:ILE:HD12	1.84	0.57
1:B:150:LYS:HD3	1:B:152:TYR:CZ	2.40	0.57
1:D:176:ARG:HE	1:D:237:VAL:CG2	2.18	0.57
1:D:293:ARG:HH11	1:D:293:ARG:HG2	1.68	0.57
2:F:411:DA:H2"	2:F:412:DG:C8	2.39	0.57
1:D:262:CYS:O	1:D:266:MET:O	2.23	0.57
1:D:273:ILE:HD12	1:D:273:ILE:N	2.19	0.57
1:L:150:LYS:HD3	1:L:152:TYR:CZ	2.40	0.57
1:J:243:PRO:HB2	1:J:247:THR:O	2.05	0.57
1:K:280:ARG:NH1	1:K:280:ARG:CG	2.58	0.57
1:B:121:TYR:CE1	1:B:123:GLY:HA2	2.40	0.56
1:C:300:ARG:HD3	1:C:301:ASP:OD1	2.05	0.56
1:L:302:ARG:O	1:L:306:GLU:HG3	2.05	0.56
1:D:181:TYR:CE2	1:D:269:ARG:NH1	2.73	0.56
1:K:197:HIS:HE1	1:K:262:CYS:SG	2.27	0.56
1:B:193:ARG:HH11	1:B:197:HIS:HB3	1.69	0.56
1:D:122:PRO:HG3	1:D:288:ARG:NH2	2.10	0.56
1:I:197:HIS:CD2	4:I:509:HOH:O	2.58	0.56
1:I:140:ALA:C	1:I:142:TRP:N	2.52	0.56
1:A:183:LYS:HE2	1:A:270:PRO:HD2	1.86	0.56
1:D:119:THR:O	1:D:287:ARG:HD2	2.06	0.56
1:A:198:GLU:C	1:A:199:LEU:HG	2.26	0.56
1:A:228:ASP:O	1:A:232:GLY:N	2.37	0.56
1:D:125:HIS:CE1	1:D:169:PRO:HA	2.41	0.56
2:M:417:DG:H2"	2:M:418:DC:O5'	2.05	0.56
1:B:228:ASP:CB	1:B:231:THR:HB	2.35	0.56
1:D:293:ARG:HG3	1:D:293:ARG:NH1	2.18	0.56
1:D:243:PRO:CG	1:D:250:THR:HG23	2.33	0.56
1:I:169:PRO:HD2	1:I:240:TYR:HE2	1.71	0.56
1:I:193:ARG:HD3	1:I:257:MET:CB	2.36	0.56
1:L:138:LYS:HE3	1:L:300:ARG:HD3	1.88	0.56
1:D:216:ARG:HB2	1:D:255:ASN:HB2	1.87	0.56
1:I:120:ASP:OD1	1:I:288:ARG:HA	2.05	0.55
1:I:191:VAL:CG1	1:I:214:LEU:HD22	2.35	0.55
1:A:136:THR:HG22	1:A:136:THR:O	2.05	0.55
1:B:140:ALA:H	1:B:298:PRO:HD2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:183:LYS:HB3	1:J:186:HIS:CD2	2.40	0.55
1:J:277:LEU:N	1:J:286:GLY:O	2.36	0.55
1:K:151:LEU:HD23	1:K:152:TYR:H	1.70	0.55
1:J:293:ARG:HH11	1:J:295:CYS:HB3	1.71	0.55
1:D:114:PHE:CA	1:D:231:THR:HG23	2.34	0.55
1:A:138:LYS:HG3	1:A:300:ARG:HB2	1.88	0.55
1:J:158:THR:HG23	4:J:505:HOH:O	2.06	0.55
1:J:278:GLU:HG2	1:J:284:VAL:HG12	1.88	0.55
1:C:190:VAL:HG23	1:C:192:LYS:HG3	1.89	0.55
1:D:277:LEU:H	1:D:277:LEU:CD2	2.13	0.55
1:B:112:HIS:CB	1:B:230:VAL:O	2.55	0.55
1:J:157:LYS:HE3	4:J:508:HOH:O	2.05	0.55
1:B:149:LYS:O	1:B:291:GLU:N	2.39	0.55
1:B:284:VAL:HG23	1:B:284:VAL:O	2.06	0.55
1:I:137:ALA:C	1:I:139:SER:N	2.60	0.55
1:L:126:HIS:O	1:L:165:VAL:HA	2.06	0.55
1:C:122:PRO:HD3	1:C:288:ARG:HH11	1.72	0.55
1:C:176:ARG:HG2	1:C:177:ALA:N	2.21	0.55
1:I:132:GLN:O	1:I:133:GLN:HB2	2.05	0.55
1:I:231:THR:HG22	1:I:233:ARG:H	1.72	0.55
1:J:136:THR:HG22	1:J:137:ALA:H	1.72	0.55
1:J:181:TYR:CD1	1:J:191:VAL:HG22	2.42	0.55
1:K:125:HIS:HB3	1:K:165:VAL:CG1	2.36	0.55
1:L:116:PRO:HG3	1:L:233:ARG:CD	2.36	0.55
1:A:152:TYR:CE1	1:A:293:ARG:HD3	2.41	0.55
1:A:179:PRO:HD3	1:A:215:ILE:HD12	1.88	0.55
1:K:143:THR:CG2	1:K:302:ARG:HD2	2.37	0.55
1:L:311:GLU:HG2	1:L:312:GLN:H	1.72	0.54
1:B:271:ILE:HG12	1:B:272:LEU:N	2.22	0.54
1:J:143:THR:HG22	1:J:302:ARG:HH11	1.72	0.54
1:K:113:GLU:N	1:K:113:GLU:OE1	2.41	0.54
1:A:112:HIS:CE1	1:A:230:VAL:HG11	2.42	0.54
1:B:134:SER:OG	1:B:143:THR:HA	2.07	0.54
1:A:244:GLN:HE21	1:A:244:GLN:HA	1.71	0.54
1:I:125:HIS:CD2	1:I:169:PRO:HB3	2.42	0.54
1:A:179:PRO:HD3	1:A:215:ILE:CD1	2.37	0.54
1:D:276:THR:CG2	1:D:287:ARG:HG3	2.37	0.54
1:J:245:VAL:HG21	1:K:284:VAL:HB	1.88	0.54
1:K:204:ASN:HD22	1:K:211:ALA:HB1	1.71	0.54
1:A:127:PHE:HZ	1:A:163:ILE:HD11	1.73	0.54
1:B:240:TYR:CD2	1:B:241:GLU:N	2.69	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:216:ARG:HD2	1:I:257:MET:CE	2.38	0.54
1:I:273:ILE:HG22	1:I:275:ILE:CD1	2.38	0.54
1:J:207:GLN:O	1:J:209:ALA:N	2.33	0.54
1:L:193:ARG:HD3	1:L:257:MET:O	2.08	0.54
1:A:307:ASP:O	1:A:310:ARG:HB2	2.08	0.54
2:N:402:DC:H2"	2:N:403:DA:C5'	2.37	0.54
1:K:276:THR:HG22	1:K:287:ARG:HG3	1.90	0.53
1:L:311:GLU:O	1:L:312:GLN:C	2.47	0.53
1:J:256:PHE:HB2	1:J:294:ILE:HD12	1.90	0.53
1:L:311:GLU:CG	1:L:312:GLN:H	2.20	0.53
1:A:287:ARG:NH2	1:D:245:VAL:O	2.39	0.53
1:D:280:ARG:HG3	1:D:281:ASP:OD1	2.08	0.53
1:J:281:ASP:O	1:J:283:GLN:N	2.41	0.53
1:B:293:ARG:NH2	1:B:301:ASP:OD2	2.34	0.53
1:D:148:LEU:O	1:D:150:LYS:N	2.41	0.53
1:A:175:ILE:HD12	1:A:252:ILE:HD11	1.91	0.53
1:A:213:HIS:HA	1:A:234:GLN:HE22	1.72	0.53
1:D:183:LYS:HD3	1:D:185:GLU:OE2	2.08	0.53
1:D:192:LYS:HG2	1:D:234:GLN:OE1	2.09	0.53
1:D:277:LEU:HD21	1:D:286:GLY:CA	2.39	0.53
1:K:131:PHE:CE1	1:K:151:LEU:HG	2.44	0.53
2:E:403:DA:N6	2:F:415:DA:N6	2.57	0.53
1:C:129:VAL:HG23	1:C:288:ARG:HG3	1.91	0.53
1:I:266:MET:O	1:I:266:MET:HG3	2.09	0.53
1:J:129:VAL:CG1	1:J:288:ARG:HG3	2.39	0.53
1:A:152:TYR:CD2	1:A:152:TYR:N	2.74	0.53
1:A:204:ASN:O	1:A:207:GLN:OE1	2.26	0.53
1:J:115:ILE:HG23	1:J:116:PRO:HD2	1.89	0.53
1:K:117:SER:O	1:K:274:ILE:HD13	2.09	0.53
1:K:260:SER:O	1:K:266:MET:O	2.26	0.53
1:A:284:VAL:CG1	1:D:245:VAL:HG21	2.38	0.53
2:M:421:DG:H1	2:N:398:DC:H42	1.56	0.53
1:B:193:ARG:NH2	1:B:204:ASN:OD1	2.42	0.53
1:C:147:LEU:HD21	1:C:309:TYR:CE2	2.42	0.53
1:J:207:GLN:OE1	1:J:216:ARG:NH1	2.42	0.53
1:L:311:GLU:CG	1:L:312:GLN:N	2.72	0.53
1:A:170:PRO:HB2	1:A:173:THR:HG21	1.91	0.52
1:B:224:GLN:HG3	1:B:224:GLN:O	2.09	0.52
1:D:228:ASP:HB3	1:D:232:GLY:H	1.74	0.52
1:J:145:SER:HB2	1:J:302:ARG:HG3	1.91	0.52
1:K:126:HIS:O	1:K:165:VAL:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:THR:HG23	1:C:157:LYS:HB3	1.90	0.52
1:A:126:HIS:HB2	1:A:166:SER:CB	2.39	0.52
1:A:262:CYS:O	1:A:267:ASN:HB3	2.09	0.52
1:B:271:ILE:O	1:B:272:LEU:HD12	2.09	0.52
1:C:147:LEU:HD21	1:C:309:TYR:HE2	1.75	0.52
1:D:183:LYS:O	1:D:187:VAL:HG12	2.08	0.52
1:J:163:ILE:O	1:J:163:ILE:HG22	2.07	0.52
1:J:176:ARG:HD3	1:J:237:VAL:HG12	1.90	0.52
1:J:183:LYS:CB	1:J:186:HIS:HD2	2.21	0.52
1:J:210:PRO:CG	1:J:213:HIS:ND1	2.72	0.52
1:K:143:THR:HG21	1:K:302:ARG:HD2	1.92	0.52
1:K:123:GLY:O	1:K:124:PRO:C	2.48	0.52
1:L:153:CYS:O	1:L:294:ILE:HA	2.09	0.52
1:B:179:PRO:CB	1:B:271:ILE:HD11	2.35	0.52
1:J:121:TYR:HD1	1:J:286:GLY:HA2	1.73	0.52
1:B:149:LYS:HG2	1:B:290:PHE:HA	1.91	0.52
1:C:150:LYS:CB	1:C:291:GLU:HB3	2.40	0.52
1:A:199:LEU:O	1:A:200:GLY:C	2.48	0.52
1:B:244:GLN:NE2	1:C:113:GLU:CB	2.72	0.52
1:I:179:PRO:CD	1:I:215:ILE:HD11	2.38	0.52
1:K:193:ARG:HA	1:K:258:CYS:SG	2.50	0.52
1:A:197:HIS:C	1:A:199:LEU:H	2.12	0.52
1:K:112:HIS:ND1	1:K:112:HIS:N	2.57	0.52
1:A:193:ARG:NE	1:A:257:MET:HB3	2.25	0.52
1:A:244:GLN:HE21	1:A:245:VAL:N	2.08	0.52
1:A:308:HIS:HB3	4:A:510:HOH:O	2.09	0.52
1:K:228:ASP:O	1:K:232:GLY:HA2	2.10	0.52
1:B:142:TRP:CE2	1:B:160:PRO:HD2	2.45	0.52
1:B:169:PRO:HD2	1:B:170:PRO:HD3	1.91	0.52
1:B:187:VAL:O	1:B:233:ARG:NH2	2.38	0.52
2:N:401:DG:C2'	2:N:402:DC:OP1	2.56	0.52
1:B:217:VAL:HG21	1:B:238:VAL:HG13	1.92	0.51
1:A:179:PRO:O	1:A:191:VAL:HG21	2.10	0.51
1:A:204:ASN:O	1:A:207:GLN:CD	2.49	0.51
1:A:284:VAL:CG2	1:D:245:VAL:HG21	2.40	0.51
1:B:124:PRO:HG2	1:B:125:HIS:H	1.75	0.51
1:D:173:THR:HA	1:D:278:GLU:O	2.11	0.51
1:B:193:ARG:CZ	1:B:257:MET:HB3	2.39	0.51
1:J:193:ARG:HG2	1:J:193:ARG:HH11	1.76	0.51
2:M:415:DA:H5'	2:M:415:DA:C8	2.45	0.51
1:D:205:GLU:O	1:D:205:GLU:HG2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:140:ALA:O	1:I:141:THR:C	2.45	0.51
1:I:268:ARG:HG3	1:I:268:ARG:NH2	2.25	0.51
2:O:412:DG:H2"	2:O:413:DG:OP2	2.09	0.51
1:A:176:ARG:HD2	1:A:278:GLU:OE2	2.11	0.51
1:B:114:PHE:CB	1:B:231:THR:HG23	2.40	0.51
1:C:170:PRO:HB2	1:C:279:MET:CE	2.41	0.51
1:J:170:PRO:O	1:J:173:THR:HG22	2.11	0.51
1:K:204:ASN:OD1	1:K:204:ASN:N	2.43	0.51
1:B:217:VAL:HG21	1:B:238:VAL:CG1	2.40	0.51
1:B:299:GLY:O	1:B:303:LYS:HG3	2.11	0.51
1:C:279:MET:SD	1:C:285:LEU:HD11	2.51	0.51
1:I:148:LEU:O	1:I:149:LYS:CB	2.48	0.51
1:I:216:ARG:HD2	1:I:257:MET:HE3	1.92	0.51
1:J:162:GLN:HB3	1:J:249:PHE:CG	2.45	0.51
2:F:415:DA:H5'	2:F:415:DA:H8	1.76	0.51
1:A:253:LEU:N	1:A:253:LEU:HD22	2.26	0.51
1:A:255:ASN:HB3	1:A:257:MET:HE3	1.92	0.51
1:I:179:PRO:CG	1:I:214:LEU:HD23	2.41	0.51
1:J:120:ASP:OD1	1:J:121:TYR:N	2.44	0.51
1:D:274:ILE:HA	1:D:289:SER:HB3	1.93	0.51
1:J:288:ARG:HG3	1:J:288:ARG:NH1	2.25	0.51
2:F:415:DA:H5'	2:F:415:DA:C8	2.46	0.51
2:N:407:DC:H2"	2:N:408:DT:C6	2.46	0.51
1:A:266:MET:O	1:A:266:MET:CG	2.56	0.50
1:B:122:PRO:HG3	1:B:288:ARG:NH2	2.26	0.50
1:C:272:LEU:HD12	1:C:291:GLU:HA	1.93	0.50
1:I:114:PHE:O	1:I:114:PHE:CD1	2.64	0.50
1:B:172:GLY:HA3	1:B:280:ARG:HB2	1.93	0.50
2:F:420:DT:H2"	2:F:421:DG:O4'	2.11	0.50
1:C:240:TYR:CG	1:C:241:GLU:N	2.75	0.50
1:D:273:ILE:HG22	1:D:275:ILE:CD1	2.40	0.50
1:K:151:LEU:HD12	1:K:290:PHE:CE2	2.46	0.50
1:L:138:LYS:HG3	1:L:300:ARG:HB2	1.92	0.50
1:B:165:VAL:HG11	1:B:240:TYR:OH	2.11	0.50
1:C:122:PRO:HD3	1:C:288:ARG:NH1	2.26	0.50
1:I:147:LEU:HD21	1:I:309:TYR:CE2	2.47	0.50
1:C:173:THR:HG23	1:C:240:TYR:HB3	1.93	0.50
1:C:196:ASN:HB2	1:D:196:ASN:OD1	2.10	0.50
1:A:225:TYR:CE1	1:A:236:VAL:HG13	2.46	0.50
1:A:280:ARG:CG	1:A:280:ARG:NH1	2.68	0.50
1:K:141:THR:HG22	1:K:142:TRP:HD1	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:413:DG:H2"	2:M:414:DC:OP2	2.11	0.50
1:B:184:ALA:O	1:B:187:VAL:HG12	2.11	0.50
1:D:151:LEU:HD12	1:D:152:TYR:H	1.76	0.50
1:J:126:HIS:HB2	1:J:166:SER:OG	2.12	0.50
1:I:279:MET:HG3	1:I:283:GLN:HB3	1.93	0.49
1:L:163:ILE:HD12	1:L:175:ILE:HD13	1.94	0.49
1:A:179:PRO:HG2	1:A:191:VAL:CG2	2.42	0.49
1:J:117:SER:HB3	1:J:287:ARG:HH21	1.77	0.49
1:J:186:HIS:CE1	1:J:269:ARG:HD2	2.47	0.49
1:K:125:HIS:ND1	1:K:167:THR:HB	2.27	0.49
1:K:181:TYR:HA	1:K:271:ILE:HG22	1.94	0.49
2:O:421:DG:H2'	2:O:421:DG:OP2	2.13	0.49
1:B:199:LEU:N	1:B:199:LEU:HD23	2.26	0.49
1:B:272:LEU:HD12	1:B:291:GLU:HA	1.95	0.49
1:B:310:ARG:NH1	1:B:310:ARG:HG3	2.27	0.49
1:J:138:LYS:O	1:J:299:GLY:CA	2.60	0.49
2:O:410:DC:H42	2:P:409:DG:H1	1.59	0.49
1:C:213:HIS:CE1	1:C:234:GLN:HB3	2.47	0.49
1:D:274:ILE:HG22	1:D:289:SER:CB	2.40	0.49
1:I:193:ARG:HD3	1:I:257:MET:HB3	1.94	0.49
1:I:237:VAL:HG12	1:I:238:VAL:N	2.27	0.49
1:K:121:TYR:CE1	1:K:123:GLY:HA2	2.47	0.49
1:K:182:LYS:HE3	1:K:291:GLU:OE1	2.12	0.49
1:A:175:ILE:CD1	1:A:252:ILE:HD11	2.42	0.49
1:C:179:PRO:HD3	1:C:215:ILE:HD12	1.95	0.49
1:J:276:THR:HA	1:J:287:ARG:HA	1.93	0.49
2:N:402:DC:H2"	2:N:403:DA:H5'	1.93	0.49
1:A:112:HIS:CD2	1:A:230:VAL:HG11	2.47	0.49
1:A:173:THR:HB	1:A:278:GLU:O	2.13	0.49
1:C:259:ASN:C	1:C:261:SER:H	2.16	0.49
1:K:111:HIS:CD2	1:K:111:HIS:H	2.24	0.49
1:K:165:VAL:HG12	1:K:166:SER:H	1.77	0.49
1:K:228:ASP:HB3	1:K:232:GLY:H	1.76	0.49
1:K:263:VAL:HA	1:K:267:ASN:HB3	1.94	0.49
1:L:312:GLN:O	1:L:312:GLN:HG2	2.11	0.49
1:B:205:GLU:OE2	1:B:206:GLY:N	2.44	0.49
1:D:126:HIS:O	1:D:165:VAL:HA	2.13	0.49
1:I:169:PRO:HB2	1:I:173:THR:HG21	1.95	0.49
1:A:209:ALA:HB2	1:A:225:TYR:CE2	2.48	0.49
1:B:164:LYS:HB2	1:B:249:PHE:HE1	1.77	0.49
1:J:152:TYR:HB3	1:J:298:PRO:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:296:ALA:HB2	2:P:405:DG:H2'	1.93	0.49
1:A:198:GLU:O	1:A:199:LEU:HG	2.13	0.49
1:I:281:ASP:C	1:I:283:GLN:H	2.15	0.49
2:N:403:DA:H5'	2:N:403:DA:C8	2.48	0.49
1:A:244:GLN:HA	1:A:244:GLN:NE2	2.27	0.49
1:C:286:GLY:O	1:C:287:ARG:HB2	2.12	0.49
1:D:212:SER:HB2	1:D:234:GLN:HE22	1.77	0.49
1:I:137:ALA:O	1:I:139:SER:N	2.46	0.49
1:J:141:THR:CG2	1:J:157:LYS:HB3	2.39	0.49
1:L:177:ALA:O	1:L:235:SER:HB2	2.13	0.49
1:B:181:TYR:CE2	1:B:266:MET:HB3	2.48	0.48
1:C:244:GLN:O	1:C:247:THR:HB	2.12	0.48
1:J:117:SER:HB3	1:J:287:ARG:NH2	2.28	0.48
1:J:202:ASP:O	1:J:203:PHE:HB2	2.13	0.48
1:B:310:ARG:O	1:B:311:GLU:HB2	2.13	0.48
1:I:213:HIS:ND1	1:I:234:GLN:HB3	2.28	0.48
1:I:300:ARG:NH2	2:N:405:DG:N7	2.53	0.48
1:K:139:SER:O	1:K:154:GLN:NE2	2.46	0.48
1:B:112:HIS:HB2	1:B:230:VAL:O	2.12	0.48
1:B:205:GLU:OE2	1:B:205:GLU:HA	2.13	0.48
1:B:273:ILE:HD13	1:B:290:PHE:CE1	2.48	0.48
1:C:111:HIS:CG	1:C:112:HIS:H	2.31	0.48
1:C:121:TYR:CG	1:C:121:TYR:O	2.64	0.48
1:C:217:VAL:HG23	1:C:236:VAL:HG21	1.95	0.48
1:J:134:SER:O	1:J:135:SER:O	2.31	0.48
1:C:310:ARG:HH11	1:C:310:ARG:CG	2.23	0.48
1:J:213:HIS:CD2	1:J:234:GLN:HG3	2.48	0.48
2:F:421:DG:OP2	2:F:421:DG:H2'	2.13	0.48
1:B:201:ARG:O	1:B:201:ARG:HG3	2.10	0.48
1:B:273:ILE:HD13	1:B:290:PHE:HE1	1.78	0.48
1:C:240:TYR:CD2	1:C:241:GLU:CA	2.97	0.48
1:D:121:TYR:CE2	1:D:123:GLY:CA	2.94	0.48
1:I:150:LYS:HD3	1:I:152:TYR:CZ	2.49	0.48
1:K:158:THR:HG23	1:K:218:GLU:OE1	2.13	0.48
1:L:259:ASN:O	1:L:266:MET:HE3	2.12	0.48
1:J:127:PHE:CG	1:J:277:LEU:HD11	2.48	0.48
1:J:231:THR:HG22	1:J:233:ARG:HG3	1.95	0.48
1:B:121:TYR:O	1:B:121:TYR:HD1	1.96	0.48
1:C:240:TYR:HD2	1:C:240:TYR:O	1.94	0.48
1:J:153:CYS:O	1:J:294:ILE:HA	2.14	0.48
1:K:151:LEU:HD23	1:K:152:TYR:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:164:LYS:HG3	1:K:249:PHE:HD2	1.78	0.48
1:A:296:ALA:C	1:A:298:PRO:HD3	2.33	0.48
1:B:240:TYR:HE2	1:B:242:PRO:CA	2.27	0.48
1:B:267:ASN:ND2	1:B:267:ASN:H	2.12	0.48
1:C:204:ASN:CB	1:C:216:ARG:NH2	2.73	0.48
1:C:263:VAL:O	1:D:196:ASN:ND2	2.46	0.48
1:D:121:TYR:C	1:D:121:TYR:CD2	2.87	0.48
1:D:210:PRO:HB2	1:D:213:HIS:ND1	2.29	0.48
1:I:222:LEU:N	1:I:222:LEU:HD23	2.28	0.48
1:A:217:VAL:HG12	1:A:218:GLU:N	2.29	0.48
1:B:241:GLU:OE1	1:C:111:HIS:HB3	2.14	0.48
1:B:248:GLU:HG3	1:B:249:PHE:CD2	2.49	0.48
1:J:228:ASP:HB3	1:J:231:THR:HB	1.95	0.48
1:L:209:ALA:HB2	1:L:225:TYR:CZ	2.48	0.48
1:D:144:TYR:HE2	1:D:146:PRO:HA	1.79	0.47
1:I:178:MET:HB2	1:I:235:SER:HB3	1.95	0.47
1:C:150:LYS:HA	1:C:291:GLU:O	2.14	0.47
1:D:117:SER:O	1:D:287:ARG:HD3	2.15	0.47
1:I:302:ARG:O	1:I:306:GLU:HG3	2.14	0.47
1:J:151:LEU:HD22	1:J:290:PHE:HE1	1.77	0.47
1:L:179:PRO:HB2	1:L:191:VAL:HG11	1.96	0.47
1:A:176:ARG:HA	1:A:236:VAL:O	2.14	0.47
1:A:258:CYS:O	1:A:294:ILE:HG13	2.14	0.47
1:D:240:TYR:CD2	1:D:240:TYR:C	2.88	0.47
1:J:152:TYR:HB3	1:J:298:PRO:CB	2.44	0.47
1:J:210:PRO:HG3	1:J:213:HIS:CE1	2.49	0.47
1:J:230:VAL:HG12	1:J:231:THR:N	2.28	0.47
1:K:136:THR:HG22	1:K:302:ARG:NH2	2.30	0.47
1:K:151:LEU:CD2	1:K:152:TYR:N	2.77	0.47
2:O:410:DC:H2'	2:O:411:DA:C8	2.49	0.47
1:B:169:PRO:CD	1:B:170:PRO:CD	2.91	0.47
1:C:260:SER:O	1:C:268:ARG:N	2.47	0.47
1:J:193:ARG:HG2	1:J:193:ARG:NH1	2.29	0.47
1:J:250:THR:O	1:J:250:THR:OG1	2.30	0.47
1:L:262:CYS:O	1:L:266:MET:O	2.32	0.47
2:N:401:DG:H2"	2:N:402:DC:OP1	2.15	0.47
1:J:207:GLN:C	1:J:209:ALA:H	2.17	0.47
1:K:150:LYS:HD3	1:K:152:TYR:OH	2.13	0.47
1:A:207:GLN:HB2	1:A:216:ARG:HH22	1.79	0.47
1:C:116:PRO:HG2	1:C:178:MET:SD	2.55	0.47
1:I:267:ASN:C	1:I:269:ARG:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:131:PHE:CE2	1:J:151:LEU:HD13	2.50	0.47
1:B:173:THR:CG2	1:B:285:LEU:HD11	2.44	0.47
1:C:172:GLY:HA3	4:C:510:HOH:O	2.15	0.47
1:C:195:PRO:HB2	1:D:196:ASN:HA	1.96	0.47
1:C:276:THR:HG22	1:C:278:GLU:CG	2.41	0.47
1:I:263:VAL:O	1:J:196:ASN:ND2	2.47	0.47
1:K:151:LEU:HD12	1:K:290:PHE:HE2	1.79	0.47
1:B:231:THR:CG2	1:B:233:ARG:HG2	2.42	0.47
1:B:279:MET:O	1:B:280:ARG:C	2.53	0.47
1:C:259:ASN:C	1:C:261:SER:N	2.68	0.47
1:J:290:PHE:N	1:J:290:PHE:HD2	2.12	0.47
1:K:162:GLN:O	1:K:163:ILE:HD13	2.15	0.47
1:A:279:MET:HB2	1:A:281:ASP:O	2.14	0.47
1:B:182:LYS:HE2	1:B:291:GLU:OE2	2.15	0.47
1:D:277:LEU:HG	1:D:285:LEU:HB3	1.96	0.47
1:I:260:SER:HA	1:I:266:MET:HE2	1.97	0.47
2:M:420:DT:H2"	2:M:421:DG:N7	2.30	0.47
1:A:244:GLN:CA	1:A:244:GLN:NE2	2.78	0.46
1:C:143:THR:CG2	1:C:152:TYR:HB2	2.45	0.46
1:J:157:LYS:N	1:J:157:LYS:HD2	2.30	0.46
1:K:218:GLU:HB3	1:K:253:LEU:HB3	1.95	0.46
1:K:286:GLY:O	1:K:287:ARG:HB2	2.15	0.46
1:C:207:GLN:HG3	1:C:208:SER:N	2.30	0.46
1:J:125:HIS:HB3	1:J:165:VAL:CG1	2.41	0.46
1:L:193:ARG:HD3	1:L:257:MET:HB2	1.96	0.46
1:A:114:PHE:HE2	1:A:188:THR:HG22	1.80	0.46
1:B:176:ARG:HG2	1:B:177:ALA:N	2.30	0.46
1:I:196:ASN:OD1	1:J:195:PRO:HG2	2.15	0.46
1:J:170:PRO:O	1:J:173:THR:CG2	2.64	0.46
1:K:112:HIS:HD2	1:K:230:VAL:HG11	1.79	0.46
1:B:170:PRO:HG2	1:B:279:MET:HG3	1.96	0.46
1:I:163:ILE:HB	1:I:250:THR:HB	1.96	0.46
1:A:184:ALA:HA	1:A:187:VAL:HB	1.98	0.46
1:A:277:LEU:HB3	1:A:286:GLY:N	2.30	0.46
1:D:193:ARG:HD3	1:D:257:MET:CB	2.46	0.46
1:D:274:ILE:CG2	1:D:289:SER:HB3	2.37	0.46
1:I:118:ASN:OD1	1:L:244:GLN:HG2	2.16	0.46
1:J:129:VAL:HG12	1:J:288:ARG:HG3	1.98	0.46
1:A:210:PRO:C	1:A:212:SER:H	2.18	0.46
1:C:123:GLY:O	1:C:125:HIS:O	2.33	0.46
1:C:150:LYS:HD3	1:C:152:TYR:OH	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:141:THR:HG22	1:J:157:LYS:CB	2.37	0.46
1:K:147:LEU:HG	1:K:148:LEU:CD2	2.46	0.46
1:A:243:PRO:O	1:A:244:GLN:C	2.53	0.46
1:B:186:HIS:O	1:B:189:ASP:HB2	2.16	0.46
1:D:121:TYR:C	1:D:121:TYR:HD2	2.18	0.46
1:J:293:ARG:NH1	1:J:295:CYS:HB3	2.30	0.46
1:L:174:ALA:HB1	1:L:238:VAL:O	2.15	0.46
1:B:259:ASN:HD22	1:B:259:ASN:HA	1.57	0.45
1:C:129:VAL:HG21	1:C:288:ARG:HB2	1.97	0.45
1:D:179:PRO:HB2	1:D:191:VAL:HG11	1.97	0.45
1:J:279:MET:O	1:J:280:ARG:C	2.55	0.45
2:N:400:DG:H2"	2:N:401:DG:OP2	2.16	0.45
1:C:190:VAL:CG2	1:C:192:LYS:HG3	2.45	0.45
1:D:115:ILE:HG12	1:D:115:ILE:O	2.16	0.45
1:D:178:MET:O	1:D:274:ILE:HG12	2.16	0.45
1:D:302:ARG:HA	1:D:305:ASP:HB2	1.97	0.45
1:K:131:PHE:HE1	1:K:151:LEU:HG	1.80	0.45
1:B:121:TYR:HE1	1:B:123:GLY:HA2	1.81	0.45
1:B:310:ARG:HG3	1:B:310:ARG:HH11	1.81	0.45
1:C:194:CYS:SG	1:C:196:ASN:HB3	2.56	0.45
1:I:170:PRO:HA	1:I:171:PRO:HD3	1.76	0.45
1:I:301:ASP:OD1	1:I:301:ASP:N	2.47	0.45
1:K:164:LYS:HG3	1:K:249:PHE:CD2	2.51	0.45
1:B:154:GLN:HB2	1:B:157:LYS:HG3	1.98	0.45
1:D:261:SER:HA	1:D:268:ARG:HG2	1.98	0.45
1:I:226:VAL:CG1	1:I:227:ASP:N	2.80	0.45
1:L:233:ARG:HG2	1:L:233:ARG:HH11	1.82	0.45
1:C:143:THR:HG22	1:C:152:TYR:HB2	1.99	0.45
1:D:158:THR:OG1	1:D:218:GLU:OE1	2.31	0.45
1:J:214:LEU:CD1	1:J:258:CYS:H	2.29	0.45
1:B:256:PHE:HB3	1:B:294:ILE:HD13	1.99	0.45
1:I:129:VAL:O	1:I:129:VAL:HG23	2.17	0.45
1:J:176:ARG:O	1:J:275:ILE:HA	2.15	0.45
1:J:276:THR:C	1:J:277:LEU:HD23	2.37	0.45
1:D:174:ALA:HA	1:D:240:TYR:H	1.82	0.45
1:I:119:THR:CG2	1:I:287:ARG:HH21	2.29	0.45
1:L:179:PRO:HG2	1:L:191:VAL:HB	1.99	0.45
1:L:199:LEU:C	1:L:200:GLY:O	2.53	0.45
1:C:138:LYS:HG2	1:C:297:CYS:HB3	1.99	0.45
1:J:132:GLN:O	1:J:133:GLN:C	2.55	0.45
1:K:114:PHE:HA	1:K:231:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:267:ASN:O	1:K:268:ARG:HB2	2.16	0.45
1:B:128:GLU:OE1	1:B:164:LYS:HD2	2.17	0.45
1:B:169:PRO:HD2	1:B:170:PRO:CD	2.46	0.45
1:B:216:ARG:HB2	1:B:255:ASN:HB2	1.99	0.45
1:C:176:ARG:HG3	1:C:237:VAL:HG22	1.99	0.45
1:K:155:ILE:O	1:K:156:ALA:HB3	2.17	0.45
1:B:274:ILE:O	1:B:274:ILE:CG1	2.65	0.45
1:C:199:LEU:CD1	1:D:199:LEU:HD11	2.47	0.45
1:D:145:SER:HB3	1:D:148:LEU:CD1	2.47	0.45
2:M:415:DA:H2"	2:M:416:DT:O5'	2.17	0.45
1:A:126:HIS:O	1:A:165:VAL:HA	2.17	0.44
1:B:126:HIS:O	1:B:165:VAL:HA	2.17	0.44
1:D:130:THR:OG1	1:D:162:GLN:HB2	2.16	0.44
1:I:148:LEU:HD13	1:I:150:LYS:HD2	1.99	0.44
1:J:125:HIS:ND1	1:J:167:THR:O	2.46	0.44
1:J:129:VAL:HA	1:J:162:GLN:O	2.17	0.44
1:B:180:VAL:O	1:B:271:ILE:HG13	2.16	0.44
1:B:210:PRO:HB2	1:B:213:HIS:CD2	2.52	0.44
1:C:111:HIS:CD2	1:C:112:HIS:N	2.84	0.44
1:C:199:LEU:HD11	1:D:199:LEU:CD1	2.47	0.44
1:D:181:TYR:CE1	1:D:191:VAL:HG22	2.52	0.44
1:D:216:ARG:NE	1:D:257:MET:HG3	2.33	0.44
1:I:114:PHE:HE1	1:I:231:THR:CG2	2.30	0.44
1:J:145:SER:HB2	1:J:302:ARG:CD	2.47	0.44
1:J:176:ARG:HG3	1:J:177:ALA:N	2.32	0.44
1:K:164:LYS:C	1:K:165:VAL:CG2	2.85	0.44
1:L:137:ALA:O	1:L:299:GLY:HA3	2.18	0.44
2:O:410:DC:N4	2:P:409:DG:H1	2.14	0.44
1:B:205:GLU:OE2	1:B:205:GLU:CA	2.65	0.44
1:C:207:GLN:HG3	1:C:208:SER:H	1.82	0.44
1:J:148:LEU:N	1:J:148:LEU:HD23	2.32	0.44
1:J:155:ILE:O	1:J:156:ALA:HB3	2.17	0.44
1:K:181:TYR:OH	1:K:266:MET:HB3	2.17	0.44
1:K:271:ILE:HD12	1:K:271:ILE:C	2.37	0.44
2:M:410:DC:H42	2:N:409:DG:H1	1.65	0.44
1:B:150:LYS:HE3	1:B:291:GLU:OE1	2.17	0.44
1:J:241:GLU:HG2	1:K:111:HIS:HB2	1.99	0.44
1:K:312:GLN:HE21	1:K:312:GLN:CA	2.15	0.44
1:A:241:GLU:O	1:A:250:THR:HG21	2.18	0.44
1:D:134:SER:HB2	1:D:143:THR:HA	1.99	0.44
1:I:137:ALA:HB3	1:I:139:SER:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:226:VAL:O	1:I:234:GLN:HA	2.17	0.44
1:J:288:ARG:HG3	1:J:288:ARG:HH11	1.83	0.44
1:L:241:GLU:HA	1:L:242:PRO:HD3	1.79	0.44
2:M:412:DG:H2"	2:M:413:DG:O5'	2.18	0.44
1:A:138:LYS:HG3	1:A:297:CYS:HB3	2.00	0.44
1:B:129:VAL:O	1:B:129:VAL:CG2	2.65	0.44
1:I:125:HIS:O	1:I:126:HIS:C	2.55	0.44
1:I:156:ALA:HA	1:I:255:ASN:HB2	2.00	0.44
1:K:157:LYS:HD3	1:K:157:LYS:HA	1.79	0.44
1:L:157:LYS:O	1:L:255:ASN:HB3	2.17	0.44
2:H:515:DG:H2"	2:H:516:DC:OP2	2.18	0.44
2:P:408:DT:H2"	2:P:409:DG:C8	2.53	0.44
1:A:198:GLU:O	1:A:198:GLU:CG	2.65	0.44
1:B:169:PRO:O	1:B:170:PRO:C	2.56	0.44
1:C:170:PRO:HB2	1:C:279:MET:HE3	1.99	0.44
1:C:204:ASN:C	1:C:204:ASN:ND2	2.71	0.44
1:D:172:GLY:HA3	1:D:280:ARG:HE	1.83	0.44
1:B:122:PRO:HG3	1:B:288:ARG:HH21	1.82	0.44
1:C:241:GLU:HA	1:C:242:PRO:HD3	1.82	0.44
1:D:134:SER:CB	1:D:143:THR:HA	2.47	0.44
1:B:216:ARG:HA	1:B:225:TYR:HE2	1.83	0.44
1:B:228:ASP:HB3	1:B:232:GLY:H	1.82	0.44
1:I:119:THR:HG23	1:I:287:ARG:HH21	1.83	0.44
1:I:137:ALA:O	1:I:138:LYS:C	2.55	0.44
1:J:115:ILE:CG2	1:J:116:PRO:HD2	2.47	0.44
1:J:303:LYS:O	1:J:307:ASP:OD1	2.35	0.44
1:K:155:ILE:HG12	1:K:156:ALA:N	2.33	0.44
1:A:197:HIS:C	1:A:199:LEU:N	2.71	0.43
1:A:265:GLY:O	1:A:267:ASN:N	2.50	0.43
1:B:125:HIS:CE1	1:B:169:PRO:HD3	2.53	0.43
1:B:282:GLY:O	1:B:283:GLN:HG2	2.18	0.43
1:I:115:ILE:O	1:I:116:PRO:C	2.55	0.43
1:I:161:ILE:HD11	1:I:254:TYR:HE2	1.83	0.43
1:L:112:HIS:ND1	1:L:231:THR:HA	2.32	0.43
2:M:421:DG:H2"	2:O:410:DC:C2	2.52	0.43
1:C:156:ALA:HB1	1:C:203:PHE:CZ	2.54	0.43
1:J:245:VAL:HG23	1:J:245:VAL:O	2.18	0.43
1:K:162:GLN:C	1:K:163:ILE:HD13	2.39	0.43
1:K:253:LEU:N	1:K:253:LEU:CD2	2.81	0.43
1:L:132:GLN:HG2	1:L:162:GLN:HE21	1.81	0.43
1:L:193:ARG:HD3	1:L:257:MET:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:PRO:HG2	1:B:170:PRO:CD	2.31	0.43
1:D:267:ASN:N	1:D:269:ARG:HG3	2.31	0.43
1:K:244:GLN:OE1	1:K:244:GLN:HA	2.16	0.43
1:L:134:SER:OG	1:L:143:THR:HA	2.19	0.43
1:A:174:ALA:HB1	1:A:238:VAL:C	2.39	0.43
1:A:259:ASN:HA	1:A:294:ILE:CB	2.46	0.43
1:A:272:LEU:HD12	1:A:291:GLU:HA	2.01	0.43
1:D:140:ALA:O	1:D:298:PRO:HD2	2.18	0.43
1:L:142:TRP:HA	1:L:152:TYR:O	2.19	0.43
1:L:148:LEU:N	1:L:148:LEU:CD2	2.80	0.43
1:L:153:CYS:SG	1:L:159:CYS:HB2	2.59	0.43
1:A:284:VAL:CG2	1:D:245:VAL:HG11	2.47	0.43
1:I:131:PHE:CE1	1:I:161:ILE:HG22	2.54	0.43
1:I:140:ALA:O	1:I:142:TRP:N	2.51	0.43
1:J:144:TYR:O	1:J:302:ARG:NH1	2.51	0.43
1:K:118:ASN:H	1:K:118:ASN:ND2	2.17	0.43
1:K:181:TYR:CZ	1:K:191:VAL:HG22	2.54	0.43
2:H:519:DG:H1'	2:H:520:DC:H5'	2.00	0.43
1:B:121:TYR:O	1:B:121:TYR:CD1	2.72	0.43
1:B:182:LYS:HD3	1:B:272:LEU:HD11	2.01	0.43
1:D:181:TYR:CZ	1:D:191:VAL:HG22	2.54	0.43
1:K:125:HIS:HB3	1:K:165:VAL:HG11	1.99	0.43
1:A:183:LYS:CE	1:A:270:PRO:HD2	2.49	0.43
1:I:240:TYR:CD1	1:I:241:GLU:N	2.87	0.43
1:K:176:ARG:HB2	1:K:237:VAL:HG22	2.00	0.43
1:A:118:ASN:HA	1:A:274:ILE:HD11	2.00	0.43
1:D:114:PHE:O	1:D:115:ILE:HG22	2.19	0.43
1:D:277:LEU:N	1:D:277:LEU:CD2	2.78	0.43
1:A:261:SER:HA	1:A:268:ARG:HG3	2.01	0.43
1:A:279:MET:HG2	1:A:285:LEU:CD1	2.48	0.43
1:J:141:THR:O	1:J:154:GLN:HG3	2.19	0.43
1:K:266:MET:O	1:K:266:MET:HG3	2.19	0.43
2:E:403:DA:N6	2:F:415:DA:C6	2.87	0.43
1:A:196:ASN:HB2	1:B:196:ASN:CG	2.38	0.42
1:C:226:VAL:O	1:C:234:GLN:HA	2.20	0.42
1:I:130:THR:HG22	1:I:131:PHE:N	2.29	0.42
1:K:217:VAL:HG23	1:K:236:VAL:HG21	2.00	0.42
1:K:308:HIS:C	1:K:308:HIS:ND1	2.72	0.42
1:L:190:VAL:HG12	1:L:192:LYS:HG3	2.01	0.42
1:L:228:ASP:HA	1:L:229:PRO:HD3	1.83	0.42
1:B:245:VAL:HG11	1:C:284:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:ARG:O	1:D:305:ASP:N	2.51	0.42
1:I:263:VAL:HG12	1:I:264:GLY:N	2.34	0.42
1:J:145:SER:HB2	1:J:302:ARG:CG	2.49	0.42
1:L:216:ARG:HB2	1:L:255:ASN:OD1	2.19	0.42
2:P:398:DC:H2"	2:P:399:DA:N7	2.34	0.42
1:I:147:LEU:O	1:I:147:LEU:HD23	2.20	0.42
2:E:398:DC:H2"	2:E:399:DA:C8	2.54	0.42
1:A:150:LYS:HE2	1:A:152:TYR:CZ	2.54	0.42
1:A:217:VAL:HG22	1:A:254:TYR:CE1	2.55	0.42
1:D:179:PRO:HD3	1:D:215:ILE:HD12	2.01	0.42
1:D:228:ASP:HA	1:D:229:PRO:HD3	1.88	0.42
1:I:260:SER:HA	1:I:266:MET:CE	2.50	0.42
1:K:165:VAL:HG12	1:K:166:SER:N	2.33	0.42
1:L:273:ILE:HG22	1:L:275:ILE:CD1	2.49	0.42
2:E:408:DT:H2"	2:G:501:DA:C5	2.55	0.42
1:A:150:LYS:HG2	1:A:152:TYR:CE2	2.54	0.42
1:A:272:LEU:HD12	1:A:272:LEU:HA	1.74	0.42
1:C:111:HIS:CG	1:C:112:HIS:N	2.87	0.42
1:K:140:ALA:O	1:K:141:THR:C	2.56	0.42
1:K:153:CYS:SG	1:K:159:CYS:SG	3.17	0.42
1:A:201:ARG:NH2	4:A:502:HOH:O	2.52	0.42
1:A:238:VAL:HA	1:A:239:PRO:HD3	1.83	0.42
1:B:280:ARG:NH2	1:I:136:THR:HG21	2.18	0.42
1:C:159:CYS:O	1:C:159:CYS:SG	2.78	0.42
1:C:180:VAL:O	1:C:272:LEU:N	2.47	0.42
1:C:201:ARG:C	1:C:203:PHE:N	2.73	0.42
1:D:144:TYR:CE2	1:D:146:PRO:HA	2.55	0.42
1:J:244:GLN:NE2	1:K:113:GLU:HB2	2.35	0.42
1:L:147:LEU:HD21	1:L:309:TYR:CD2	2.55	0.42
1:C:228:ASP:HA	1:C:229:PRO:HD3	1.90	0.42
1:D:226:VAL:O	1:D:234:GLN:HA	2.20	0.42
1:K:136:THR:HG22	1:K:302:ARG:HH22	1.85	0.42
1:K:209:ALA:HB2	1:K:225:TYR:CZ	2.55	0.42
1:A:144:TYR:HD1	1:A:151:LEU:HB3	1.84	0.42
1:A:186:HIS:O	1:A:188:THR:N	2.52	0.42
1:A:248:GLU:H	1:A:248:GLU:HG2	1.51	0.42
1:A:303:LYS:HE3	1:A:303:LYS:HB2	1.83	0.42
1:B:284:VAL:O	1:B:284:VAL:CG2	2.68	0.42
1:I:114:PHE:CE1	1:I:231:THR:CG2	3.03	0.42
1:J:288:ARG:HH11	1:J:288:ARG:CG	2.33	0.42
1:L:263:VAL:HG23	4:L:527:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:PRO:CG	1:B:170:PRO:CD	2.91	0.42
1:D:155:ILE:HA	1:D:256:PHE:O	2.20	0.42
1:D:273:ILE:HG22	1:D:275:ILE:HD11	2.01	0.42
1:D:273:ILE:HG22	1:D:275:ILE:HD12	2.01	0.42
1:J:307:ASP:OD1	1:J:307:ASP:N	2.52	0.42
1:K:122:PRO:CG	1:K:288:ARG:HH12	2.31	0.42
1:K:228:ASP:HA	1:K:229:PRO:HD3	1.92	0.42
1:K:276:THR:HG22	1:K:287:ARG:CG	2.49	0.42
1:A:138:LYS:NZ	2:E:400:DG:N7	2.65	0.42
1:A:220:ASN:OD1	1:A:222:LEU:HB3	2.19	0.42
1:B:114:PHE:C	1:B:115:ILE:HG23	2.41	0.42
1:B:176:ARG:HD3	1:B:235:SER:OG	2.20	0.42
1:C:132:GLN:HA	1:C:162:GLN:NE2	2.35	0.42
1:D:179:PRO:HG2	1:D:191:VAL:HB	2.01	0.42
1:J:219:GLY:O	1:K:114:PHE:CB	2.67	0.42
1:L:173:THR:HG22	1:L:174:ALA:N	2.35	0.42
1:A:170:PRO:CB	1:A:171:PRO:HD2	2.42	0.41
1:A:279:MET:HG2	1:A:285:LEU:HD11	2.02	0.41
1:B:121:TYR:O	1:B:122:PRO:C	2.59	0.41
1:B:201:ARG:NH1	1:B:205:GLU:HG3	2.35	0.41
1:C:164:LYS:HG3	1:C:165:VAL:N	2.34	0.41
1:D:114:PHE:O	1:D:115:ILE:CG2	2.68	0.41
1:I:184:ALA:O	1:I:187:VAL:HG12	2.19	0.41
1:K:141:THR:HG22	1:K:142:TRP:CD1	2.55	0.41
1:L:124:PRO:HG2	1:L:125:HIS:H	1.85	0.41
1:B:179:PRO:HD3	1:B:215:ILE:HD12	2.01	0.41
1:B:267:ASN:ND2	1:B:267:ASN:N	2.68	0.41
1:D:275:ILE:HD12	1:D:275:ILE:N	2.35	0.41
1:J:123:GLY:C	1:J:125:HIS:H	2.24	0.41
1:J:128:GLU:O	1:J:130:THR:HG22	2.20	0.41
1:J:138:LYS:C	1:J:140:ALA:H	2.23	0.41
1:K:258:CYS:O	1:K:294:ILE:HG13	2.20	0.41
1:K:303:LYS:HE3	1:K:303:LYS:HB2	1.89	0.41
1:L:147:LEU:HD23	1:L:148:LEU:CD2	2.46	0.41
2:O:410:DC:H5"	2:O:410:DC:C6	2.37	0.41
1:A:209:ALA:CB	1:A:225:TYR:CE2	3.03	0.41
1:A:259:ASN:CA	1:A:294:ILE:HB	2.46	0.41
1:D:180:VAL:HG12	1:D:181:TYR:O	2.21	0.41
1:D:198:GLU:O	1:D:204:ASN:ND2	2.53	0.41
1:I:207:GLN:NE2	1:I:207:GLN:HA	2.35	0.41
1:K:127:PHE:CD1	1:K:277:LEU:HD22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:HIS:CE1	1:B:169:PRO:CD	3.03	0.41
1:B:129:VAL:O	1:B:129:VAL:HG22	2.21	0.41
1:B:186:HIS:O	1:B:188:THR:N	2.53	0.41
1:C:262:CYS:O	1:C:267:ASN:HB3	2.20	0.41
1:D:167:THR:HB	1:D:168:PRO:HD2	2.02	0.41
1:J:195:PRO:HA	1:J:198:GLU:HB3	2.02	0.41
1:J:219:GLY:O	1:K:114:PHE:HB3	2.20	0.41
1:K:281:ASP:OD1	1:K:281:ASP:C	2.59	0.41
2:G:501:DA:H2"	2:G:502:DG:OP2	2.21	0.41
1:A:114:PHE:HA	1:A:231:THR:CG2	2.50	0.41
1:C:132:GLN:H	1:C:132:GLN:HG2	1.55	0.41
1:C:240:TYR:CE2	1:C:241:GLU:C	2.93	0.41
1:D:242:PRO:O	1:D:243:PRO:C	2.58	0.41
1:I:260:SER:O	1:I:266:MET:O	2.39	0.41
1:J:176:ARG:HE	1:J:176:ARG:HB2	1.68	0.41
1:K:213:HIS:CD2	1:K:213:HIS:N	2.88	0.41
1:L:147:LEU:HG	1:L:148:LEU:HD23	2.02	0.41
1:B:116:PRO:CB	1:B:178:MET:HE1	2.51	0.41
1:B:308:HIS:ND1	1:B:308:HIS:C	2.73	0.41
1:I:140:ALA:C	1:I:142:TRP:H	2.24	0.41
1:J:244:GLN:OE1	1:K:117:SER:HB2	2.20	0.41
1:A:136:THR:O	1:A:136:THR:CG2	2.69	0.41
1:A:141:THR:HG23	1:A:157:LYS:CB	2.50	0.41
1:C:150:LYS:HG3	1:C:152:TYR:CE2	2.56	0.41
1:I:142:TRP:CB	1:I:153:CYS:HB2	2.48	0.41
1:K:192:LYS:HG2	1:K:234:GLN:OE1	2.20	0.41
1:A:121:TYR:O	1:A:286:GLY:HA2	2.21	0.41
1:A:195:PRO:CG	1:A:264:GLY:HA3	2.51	0.41
1:A:195:PRO:HD2	1:A:264:GLY:HA3	2.02	0.41
1:B:133:GLN:O	1:B:133:GLN:HG3	2.18	0.41
1:C:164:LYS:HZ1	1:C:248:GLU:HG3	1.81	0.41
1:D:176:ARG:HA	1:D:236:VAL:O	2.21	0.41
1:D:302:ARG:HG3	1:D:303:LYS:H	1.84	0.41
1:I:155:ILE:HG12	1:I:256:PHE:O	2.20	0.41
1:J:138:LYS:HG3	1:J:139:SER:N	2.32	0.41
1:A:174:ALA:HB2	1:A:239:PRO:HA	2.02	0.41
1:A:215:ILE:O	1:A:236:VAL:HG21	2.21	0.41
1:A:277:LEU:HD12	1:A:285:LEU:HB3	2.02	0.41
1:B:176:ARG:HD3	1:B:235:SER:CB	2.50	0.41
1:D:118:ASN:HA	1:D:274:ILE:HG21	2.01	0.41
1:D:152:TYR:CE2	1:D:302:ARG:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:294:ILE:HD12	1:I:294:ILE:N	2.33	0.41
1:J:241:GLU:CG	1:K:111:HIS:HB2	2.51	0.41
1:J:252:ILE:HG13	1:J:253:LEU:N	2.36	0.41
1:K:148:LEU:O	1:K:149:LYS:C	2.59	0.41
1:K:152:TYR:CE1	1:K:302:ARG:HA	2.56	0.41
1:K:165:VAL:HG12	1:K:167:THR:H	1.86	0.41
1:K:193:ARG:HH11	1:K:197:HIS:HB3	1.86	0.41
1:K:216:ARG:HG3	1:K:257:MET:SD	2.61	0.41
2:N:402:DC:H2"	2:N:403:DA:H5"	2.02	0.41
1:A:195:PRO:CD	1:A:264:GLY:HA3	2.51	0.41
1:A:209:ALA:HB2	1:A:225:TYR:HE2	1.86	0.41
1:A:210:PRO:C	1:A:212:SER:N	2.74	0.41
1:C:118:ASN:CG	1:C:118:ASN:O	2.60	0.41
1:D:174:ALA:O	1:D:277:LEU:HA	2.21	0.41
1:D:268:ARG:HD3	2:H:518:DT:OP1	2.21	0.41
1:L:209:ALA:HA	1:L:210:PRO:HD3	1.99	0.41
1:A:151:LEU:HD13	1:A:151:LEU:C	2.42	0.40
1:A:176:ARG:HD2	1:A:278:GLU:CD	2.42	0.40
1:B:129:VAL:HA	1:B:162:GLN:O	2.21	0.40
1:K:121:TYR:CD1	1:K:121:TYR:C	2.94	0.40
1:K:248:GLU:H	1:K:248:GLU:HG2	1.24	0.40
1:K:288:ARG:HA	1:K:288:ARG:HD2	1.95	0.40
1:L:173:THR:HG23	1:L:278:GLU:O	2.21	0.40
2:P:401:DG:H2"	2:P:402:DC:OP2	2.20	0.40
1:B:176:ARG:HD2	4:B:505:HOH:O	2.20	0.40
1:B:277:LEU:HD23	1:B:277:LEU:C	2.41	0.40
1:I:180:VAL:O	1:I:272:LEU:N	2.53	0.40
1:I:215:ILE:HG23	1:I:256:PHE:CE2	2.56	0.40
1:K:134:SER:HB3	1:K:142:TRP:CZ3	2.56	0.40
1:A:179:PRO:O	1:A:191:VAL:CG2	2.69	0.40
1:A:308:HIS:HA	1:A:311:GLU:HG3	2.03	0.40
1:J:162:GLN:HB3	1:J:249:PHE:HB3	2.02	0.40
1:B:260:SER:HA	1:B:266:MET:HE3	2.03	0.40
1:I:165:VAL:HG22	4:I:512:HOH:O	2.19	0.40
1:I:297:CYS:O	1:I:298:PRO:C	2.59	0.40
1:J:155:ILE:O	1:J:155:ILE:CG1	2.70	0.40
1:K:167:THR:HA	1:K:168:PRO:HD3	1.96	0.40
2:H:512:DC:C4	2:H:513:DA:N6	2.89	0.40
1:A:197:HIS:O	1:A:199:LEU:N	2.55	0.40
1:C:273:ILE:HD12	1:C:290:PHE:CE1	2.57	0.40
1:I:279:MET:O	1:I:280:ARG:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:150:LYS:HD3	1:J:152:TYR:OH	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	200/210 (95%)	168 (84%)	23 (12%)	9 (4%)	2	12
1	B	199/210 (95%)	173 (87%)	20 (10%)	6 (3%)	4	20
1	C	200/210 (95%)	180 (90%)	18 (9%)	2 (1%)	15	48
1	D	198/210 (94%)	177 (89%)	20 (10%)	1 (0%)	29	64
1	I	197/210 (94%)	172 (87%)	18 (9%)	7 (4%)	3	16
1	J	197/210 (94%)	164 (83%)	26 (13%)	7 (4%)	3	16
1	K	204/210 (97%)	180 (88%)	16 (8%)	8 (4%)	3	14
1	L	199/210 (95%)	174 (87%)	24 (12%)	1 (0%)	29	64
All	All	1594/1680 (95%)	1388 (87%)	165 (10%)	41 (3%)	5	24

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	PRO
1	A	207	GLN
1	B	169	PRO
1	C	202	ASP
1	I	282	GLY
1	J	135	SER
1	J	136	THR
1	J	282	GLY
1	L	149	LYS

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Mol	Chain	Res	Type
1	A	171	PRO
1	A	187	VAL
1	B	280	ARG
1	B	282	GLY
1	B	307	ASP
1	D	149	LYS
1	I	126	HIS
1	J	200	GLY
1	J	208	SER
1	K	123	GLY
1	K	187	VAL
1	K	202	ASP
1	A	198	GLU
1	A	266	MET
1	B	202	ASP
1	K	287	ARG
1	A	203	PHE
1	I	116	PRO
1	I	262	CYS
1	K	141	THR
1	A	242	PRO
1	B	187	VAL
1	I	133	GLN
1	J	245	VAL
1	K	245	VAL
1	K	196	ASN
1	I	170	PRO
1	I	195	PRO
1	K	124	PRO
1	C	298	PRO
1	A	245	VAL
1	J	169	PRO

5.3.2 Protein sidechains (i)

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	179/186 (96%)	146 (82%)	33 (18%)	1 7
1	B	177/186 (95%)	146 (82%)	31 (18%)	2 8
1	C	179/186 (96%)	155 (87%)	24 (13%)	4 15
1	D	176/186 (95%)	154 (88%)	22 (12%)	4 17
1	I	176/186 (95%)	162 (92%)	14 (8%)	12 37
1	J	175/186 (94%)	142 (81%)	33 (19%)	1 7
1	K	182/186 (98%)	158 (87%)	24 (13%)	4 16
1	L	178/186 (96%)	159 (89%)	19 (11%)	6 23
All	All	1422/1488 (96%)	1222 (86%)	200 (14%)	3 14

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	GLU
1	A	120	ASP
1	A	130	THR
1	A	133	GLN
1	A	149	LYS
1	A	151	LEU
1	A	152	TYR
1	A	155	ILE
1	A	158	THR
1	A	163	ILE
1	A	167	THR
1	A	175	ILE
1	A	191	VAL
1	A	193	ARG
1	A	201	ARG
1	A	202	ASP
1	A	207	GLN
1	A	216	ARG
1	A	221	ASN
1	A	231	THR
1	A	244	GLN
1	A	248	GLU
1	A	249	PHE
1	A	250	THR
1	A	251	THR
1	A	272	LEU
1	A	276	THR

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Mol	Chain	Res	Type
1	A	277	LEU
1	A	280	ARG
1	A	281	ASP
1	A	283	GLN
1	A	284	VAL
1	A	303	LYS
1	B	112	HIS
1	B	115	ILE
1	B	119	THR
1	B	121	TYR
1	B	126	HIS
1	B	129	VAL
1	B	147	LEU
1	B	155	ILE
1	B	159	CYS
1	B	161	ILE
1	B	173	THR
1	B	188	THR
1	B	193	ARG
1	B	199	LEU
1	B	201	ARG
1	B	205	GLU
1	B	212	SER
1	B	214	LEU
1	B	227	ASP
1	B	228	ASP
1	B	237	VAL
1	B	240	TYR
1	B	258	CYS
1	B	259	ASN
1	B	266	MET
1	B	267	ASN
1	B	270	PRO
1	B	281	ASP
1	B	305	ASP
1	B	307	ASP
1	B	312	GLN
1	C	112	HIS
1	C	124	PRO
1	C	130	THR
1	C	132	GLN
1	C	133	GLN

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Mol	Chain	Res	Type
1	C	135	SER
1	C	138	LYS
1	C	149	LYS
1	C	155	ILE
1	C	158	THR
1	C	190	VAL
1	C	203	PHE
1	C	204	ASN
1	C	205	GLU
1	C	221	ASN
1	C	227	ASP
1	C	240	TYR
1	C	245	VAL
1	C	251	THR
1	C	267	ASN
1	C	272	LEU
1	C	300	ARG
1	C	307	ASP
1	C	308	HIS
1	D	121	TYR
1	D	128	GLU
1	D	148	LEU
1	D	187	VAL
1	D	204	ASN
1	D	205	GLU
1	D	222	LEU
1	D	230	VAL
1	D	231	THR
1	D	238	VAL
1	D	245	VAL
1	D	251	THR
1	D	258	CYS
1	D	269	ARG
1	D	272	LEU
1	D	277	LEU
1	D	285	LEU
1	D	293	ARG
1	D	294	ILE
1	D	295	CYS
1	D	305	ASP
1	D	310	ARG
1	I	141	THR

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Mol	Chain	Res	Type
1	I	153	CYS
1	I	155	ILE
1	I	162	GLN
1	I	208	SER
1	I	215	ILE
1	I	227	ASP
1	I	255	ASN
1	I	258	CYS
1	I	260	SER
1	I	272	LEU
1	I	281	ASP
1	I	293	ARG
1	I	311	GLU
1	J	117	SER
1	J	118	ASN
1	J	129	VAL
1	J	130	THR
1	J	136	THR
1	J	139	SER
1	J	141	THR
1	J	147	LEU
1	J	157	LYS
1	J	158	THR
1	J	161	ILE
1	J	173	THR
1	J	175	ILE
1	J	176	ARG
1	J	189	ASP
1	J	192	LYS
1	J	199	LEU
1	J	227	ASP
1	J	230	VAL
1	J	234	GLN
1	J	241	GLU
1	J	248	GLU
1	J	250	THR
1	J	251	THR
1	J	252	ILE
1	J	257	MET
1	J	272	LEU
1	J	277	LEU
1	J	279	MET

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Mol	Chain	Res	Type
1	J	287	ARG
1	J	290	PHE
1	J	293	ARG
1	J	305	ASP
1	K	108	HIS
1	K	109	HIS
1	K	111	HIS
1	K	112	HIS
1	K	115	ILE
1	K	151	LEU
1	K	187	VAL
1	K	188	THR
1	K	202	ASP
1	K	204	ASN
1	K	212	SER
1	K	227	ASP
1	K	231	THR
1	K	247	THR
1	K	248	GLU
1	K	249	PHE
1	K	253	LEU
1	K	278	GLU
1	K	280	ARG
1	K	283	GLN
1	K	284	VAL
1	K	294	ILE
1	K	305	ASP
1	K	311	GLU
1	L	128	GLU
1	L	129	VAL
1	L	148	LEU
1	L	163	ILE
1	L	167	THR
1	L	176	ARG
1	L	185	GLU
1	L	187	VAL
1	L	188	THR
1	L	189	ASP
1	L	201	ARG
1	L	202	ASP
1	L	205	GLU
1	L	207	GLN

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Mol	Chain	Res	Type
1	L	221	ASN
1	L	226	VAL
1	L	244	GLN
1	L	258	CYS
1	L	267	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	154	GLN
1	A	162	GLN
1	A	186	HIS
1	A	213	HIS
1	A	234	GLN
1	A	244	GLN
1	A	255	ASN
1	B	162	GLN
1	B	234	GLN
1	B	244	GLN
1	B	259	ASN
1	B	267	ASN
1	C	111	HIS
1	C	133	GLN
1	C	204	ASN
1	C	224	GLN
1	C	267	ASN
1	D	255	ASN
1	I	132	GLN
1	I	196	ASN
1	I	207	GLN
1	I	255	ASN
1	J	118	ASN
1	J	186	HIS
1	J	234	GLN
1	J	255	ASN
1	J	267	ASN
1	J	283	GLN
1	K	111	HIS
1	K	118	ASN
1	K	154	GLN
1	K	312	GLN

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Mol	Chain	Res	Type
1	L	112	HIS
1	L	132	GLN
1	L	133	GLN
1	L	162	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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, 95^{th} 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	202/210 (96%)	0.30	10 (4%) 28 18	43, 89, 123, 127	3 (1%)
1	B	201/210 (95%)	0.06	7 (3%) 44 29	40, 75, 108, 136	1 (0%)
1	C	202/210 (96%)	-0.01	9 (4%) 33 21	41, 71, 108, 135	1 (0%)
1	D	200/210 (95%)	0.16	5 (2%) 57 40	49, 82, 112, 144	2 (1%)
1	I	199/210 (94%)	-0.03	5 (2%) 57 40	47, 70, 105, 114	1 (0%)
1	J	199/210 (94%)	0.40	12 (6%) 21 13	53, 88, 121, 129	1 (0%)
1	K	206/210 (98%)	-0.04	5 (2%) 59 42	32, 60, 108, 128	0
1	L	201/210 (95%)	-0.36	2 (0%) 82 68	26, 49, 80, 95	1 (0%)
2	E	11/12 (91%)	-0.02	0 100 100	59, 76, 97, 100	0
2	F	11/12 (91%)	0.06	1 (9%) 9 5	50, 80, 122, 133	0
2	G	11/12 (91%)	1.01	1 (9%) 9 5	91, 117, 128, 148	0
2	H	11/12 (91%)	0.29	0 100 100	76, 98, 129, 130	0
2	M	12/12 (100%)	0.10	1 (8%) 11 6	43, 75, 126, 136	0
2	N	12/12 (100%)	-0.11	0 100 100	50, 80, 93, 94	0
2	O	12/12 (100%)	-0.18	0 100 100	53, 66, 132, 133	0
2	P	12/12 (100%)	-0.19	0 100 100	49, 65, 121, 124	0
All	All	1702/1776 (95%)	0.06	58 (3%) 45 29	26, 73, 117, 148	10 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	159	CYS	7.3
1	C	137	ALA	6.0
1	C	139	SER	5.8
1	B	312	GLN	5.5
1	J	172	GLY	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	140	ALA	4.8
1	A	216	ARG	4.6
1	C	136	THR	4.5
1	D	308	HIS	4.3
1	A	139	SER	4.3
1	J	312	GLN	4.1
1	D	312	GLN	3.7
1	A	112	HIS	3.6
1	L	245	VAL	3.6
1	C	138	LYS	3.5
2	G	511	DG	3.5
1	B	309	TYR	3.4
1	K	311	GLU	3.3
1	B	311	GLU	3.2
1	J	285	LEU	3.1
1	A	114	PHE	3.1
1	K	136	THR	3.1
1	A	111	HIS	3.0
1	J	283	GLN	3.0
1	C	147	LEU	3.0
1	J	232	GLY	2.7
1	J	136	THR	2.7
1	J	115	ILE	2.7
1	I	245	VAL	2.7
1	K	139	SER	2.6
1	D	230	VAL	2.6
1	I	135	SER	2.6
1	K	135	SER	2.6
1	I	312	GLN	2.6
1	J	201	ARG	2.6
1	C	111	HIS	2.6
1	J	137	ALA	2.6
1	B	310	ARG	2.5
1	L	136	THR	2.5
1	D	310	ARG	2.4
1	I	201	ARG	2.3
1	B	113	GLU	2.3
1	A	283	GLN	2.3
1	B	112	HIS	2.2
1	J	199	LEU	2.2
1	A	246	GLY	2.2
1	D	283	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	M	410	DC	2.1
1	A	230	VAL	2.1
1	K	108	HIS	2.1
1	A	174	ALA	2.1
1	A	219	GLY	2.1
1	C	133	GLN	2.1
1	J	139	SER	2.1
2	F	411	DA	2.1
1	J	230	VAL	2.0
1	I	206	GLY	2.0
1	C	135	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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, 95^{th} 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
3	ZN	I	401	1/1	0.97	0.10	74,74,74,74	0
3	ZN	D	401	1/1	0.98	0.11	62,62,62,62	0
3	ZN	A	401	1/1	0.98	0.10	72,72,72,72	0
3	ZN	B	401	1/1	0.99	0.09	49,49,49,49	0
3	ZN	C	401	1/1	0.99	0.13	50,50,50,50	0
3	ZN	J	401	1/1	0.99	0.10	70,70,70,70	0
3	ZN	L	401	1/1	0.99	0.15	50,50,50,50	0
3	ZN	K	401	1/1	1.00	0.08	48,48,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.