Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:02 PM GMT

PDB ID	:	4GUO
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

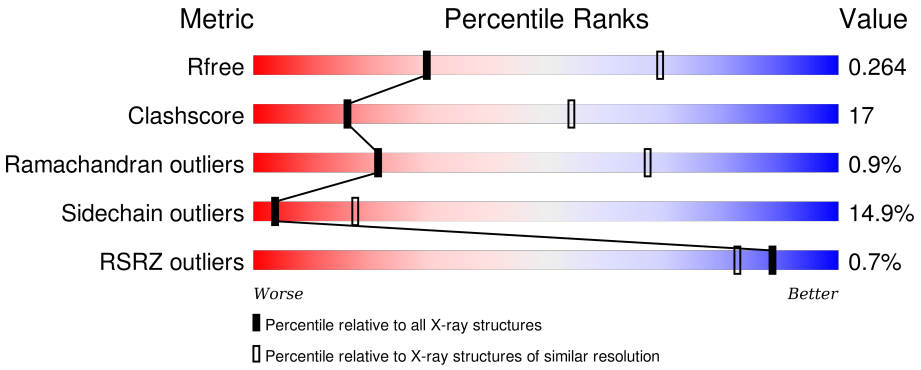
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.19 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	60% 31% • • •
1	B	210	55% 36% • 6%
1	C	210	63% 28% 5% •
1	D	210	60% 29% 5% 6%
1	I	210	59% 30% 5% 6%

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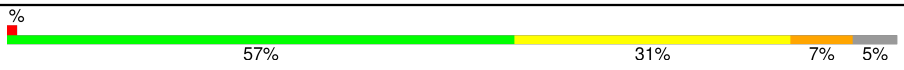
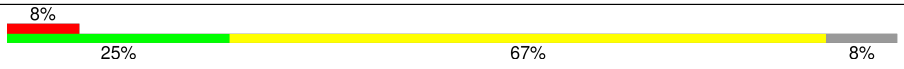
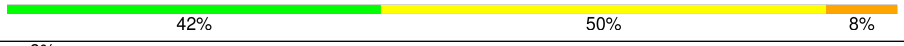
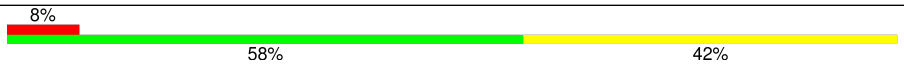
Mol	Chain	Length	Quality of chain
1	J	210	
1	K	210	
1	L	210	
2	E	12	
2	G	12	
2	M	12	
2	O	12	
3	F	12	
3	H	12	
3	N	12	
3	P	12	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ZN	C	401	-	-	-	X

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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is water.

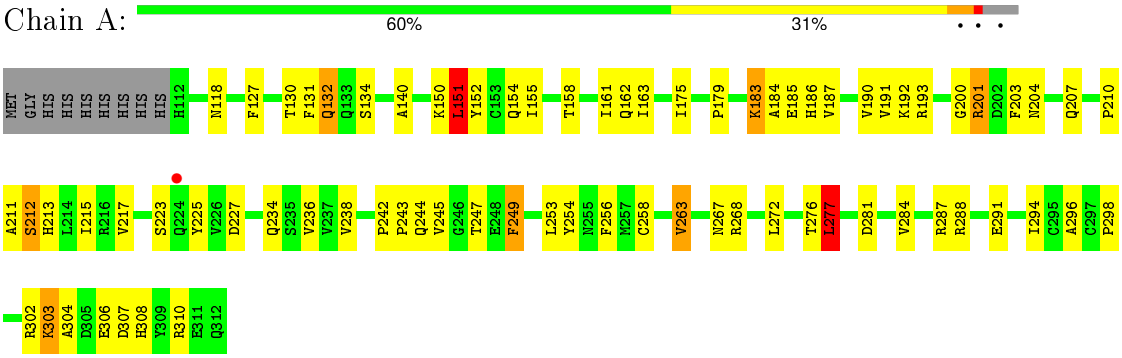
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	16	Total O 16 16	0	0
5	B	15	Total O 15 15	0	0
5	C	21	Total O 21 21	0	0
5	D	18	Total O 18 18	0	0
5	I	14	Total O 14 14	0	0
5	J	10	Total O 10 10	0	0
5	K	18	Total O 18 18	0	0
5	L	20	Total O 20 20	0	0
5	E	1	Total O 1 1	0	0
5	H	1	Total O 1 1	0	0
5	N	1	Total O 1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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

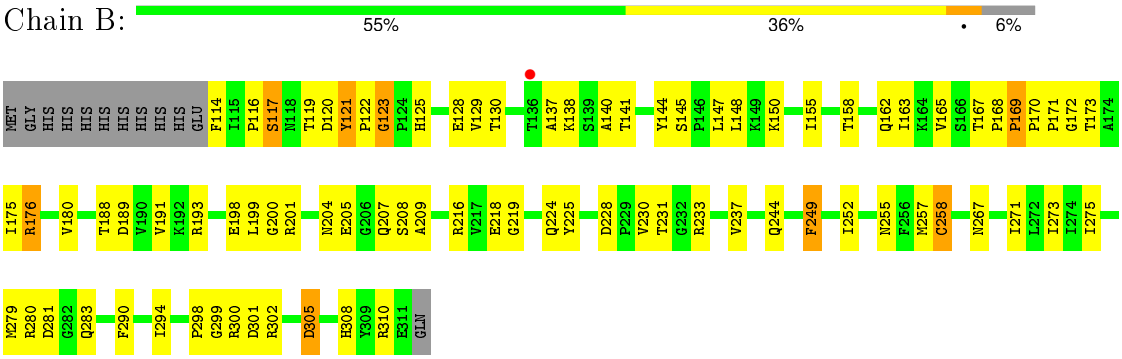
- Molecule 1: Tumor protein p73

Chain A:



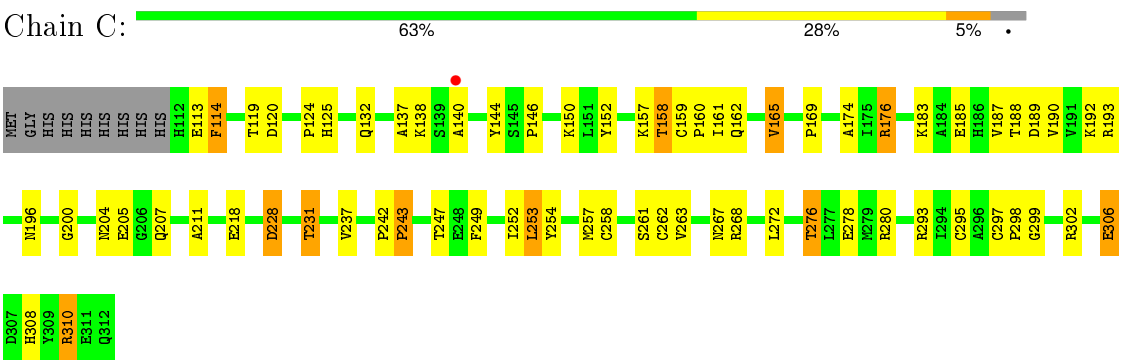
- Molecule 1: Tumor protein p73

Chain B:



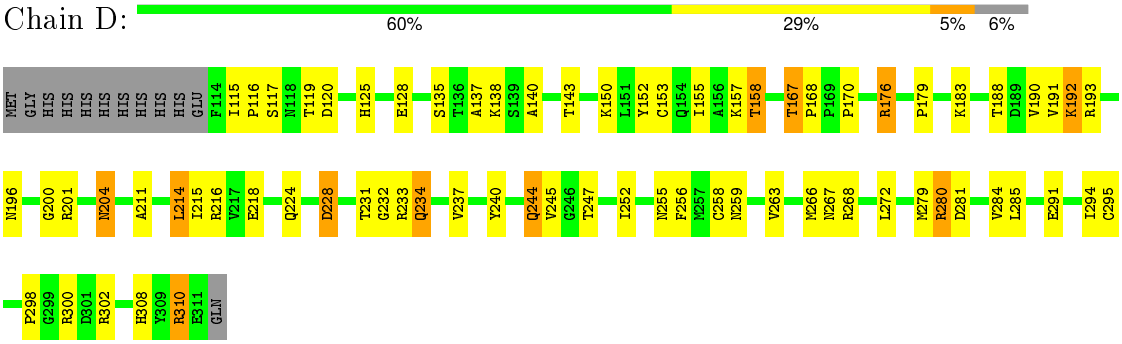
- Molecule 1: Tumor protein p73

Chain C:



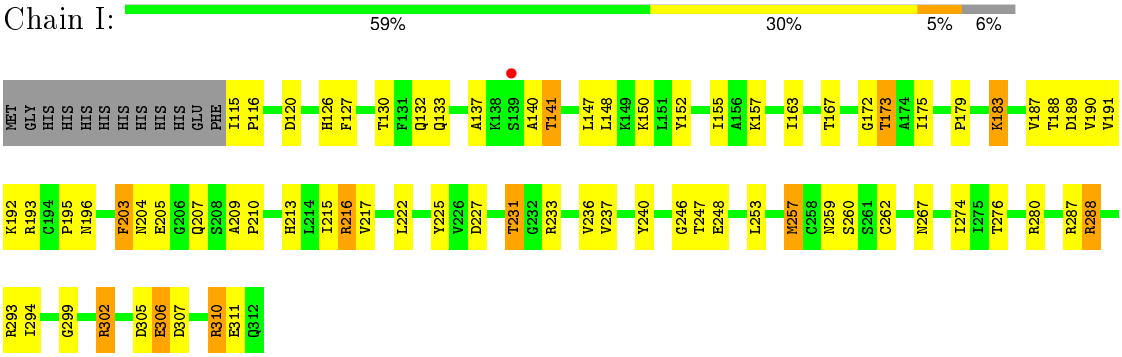
• Molecule 1: Tumor protein p73

Chain D:



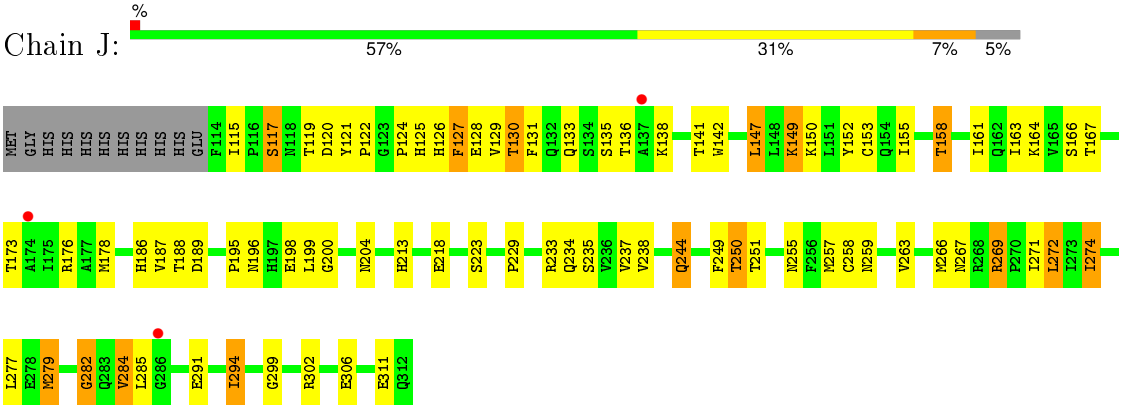
• Molecule 1: Tumor protein p73

Chain I:



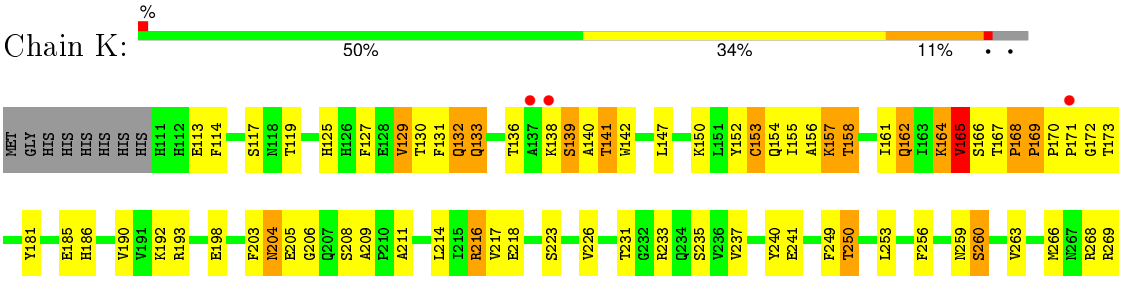
• Molecule 1: Tumor protein p73

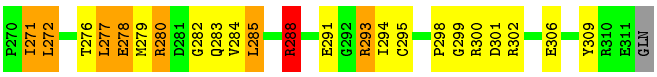
Chain J:



• Molecule 1: Tumor protein p73

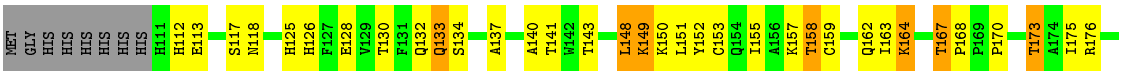
Chain K:

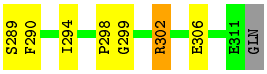




• Molecule 1: Tumor protein p73

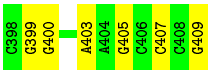
Chain L:





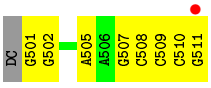
• Molecule 2: DNA (5'-D(*CP*GP*GP*GP*CP*AP*AP*GP*CP*CP*CP*G)-3')

Chain E:



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

Chain G:



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

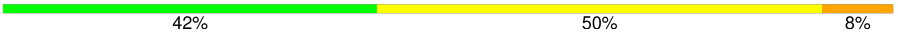
Chain M:

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

Chain O:

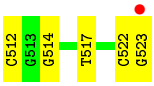
• Molecule 3: DNA (5'-D(*CP*GP*GP*GP*CP*TP*TP*GP*CP*CP*CP*G)-3')

Chain F:



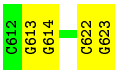
• Molecule 3: DNA (5'-D(*CP*GP*GP*GP*CP*TP*TP*GP*CP*CP*CP*G)-3')

Chain H:



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

Chain N:



• Molecule 3: DNA (5'-D(*CP*GP*GP*GP*CP*TP*TP*GP*CP*CP*CP*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	82.25Å 104.33Å 123.32Å 90.00° 96.38° 90.00°	Depositor
Resolution (Å)	44.01 – 3.19 43.97 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.01-3.19) 99.1 (43.97-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.208 , 0.270 0.202 , 0.264	Depositor DCC
R_{free} test set	1738 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	80.8	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 42.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 34474 reflections (0.003%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.55	0/1610	0.85	2/2188 (0.1%)
1	B	0.57	0/1593	0.93	4/2166 (0.2%)
1	C	0.59	0/1627	0.86	1/2210 (0.0%)
1	D	0.57	0/1590	0.91	5/2162 (0.2%)
1	I	0.57	0/1595	0.90	2/2167 (0.1%)
1	J	0.57	0/1600	0.89	2/2174 (0.1%)
1	K	0.59	0/1616	0.95	5/2197 (0.2%)
1	L	0.59	0/1622	0.89	0/2205
2	E	0.67	1/274 (0.4%)	0.77	0/421
2	G	0.33	0/256	0.66	0/393
2	M	0.76	1/274 (0.4%)	0.87	1/421 (0.2%)
2	O	0.51	0/274	0.82	1/421 (0.2%)
3	F	0.58	0/270	0.88	1/415 (0.2%)
3	H	0.47	0/270	1.00	1/415 (0.2%)
3	N	0.58	0/270	0.92	0/415
3	P	0.61	0/270	1.01	1/415 (0.2%)
All	All	0.57	2/15011 (0.0%)	0.89	26/20785 (0.1%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	600	DC	O3'-P	-6.87	1.52	1.61
2	E	407	DC	O3'-P	-5.18	1.54	1.61

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	216	ARG	NE-CZ-NH2	7.74	124.17	120.30
1	K	288	ARG	NE-CZ-NH2	7.01	123.81	120.30
1	A	277	LEU	CA-CB-CG	6.93	131.25	115.30
1	D	228	ASP	CB-CG-OD2	6.81	124.43	118.30
3	P	716	DC	O5'-P-OP2	-6.29	100.04	105.70
1	B	281	ASP	CB-CG-OD2	-6.15	112.77	118.30
2	O	700	DC	C5'-C4'-O4'	6.10	120.89	109.30
1	B	189	ASP	CB-CG-OD1	5.92	123.63	118.30
1	J	282	GLY	N-CA-C	5.91	127.87	113.10
1	K	288	ARG	NE-CZ-NH1	-5.87	117.37	120.30
3	H	512	DC	C5'-C4'-O4'	5.84	120.39	109.30
2	M	600	DC	C5'-C4'-O4'	5.78	120.28	109.30
1	A	151	LEU	N-CA-CB	5.74	121.88	110.40
1	I	216	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	C	228	ASP	CB-CG-OD2	5.67	123.40	118.30
1	B	281	ASP	CB-CG-OD1	5.61	123.35	118.30
1	D	252	ILE	CG1-CB-CG2	-5.57	99.14	111.40
3	F	414	DC	P-O3'-C3'	5.52	126.33	119.70
1	B	228	ASP	CB-CG-OD1	5.51	123.25	118.30
1	D	228	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	J	272	LEU	CA-CB-CG	5.39	127.69	115.30
1	K	216	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	D	268	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	I	189	ASP	CB-CG-OD1	5.22	123.00	118.30
1	K	272	LEU	CA-CB-CG	5.12	127.07	115.30
1	D	310	ARG	NE-CZ-NH1	5.11	122.85	120.30

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	66	0
1	B	1553	0	1526	54	0
1	C	1586	0	1551	45	0
1	D	1551	0	1523	54	0
1	I	1556	0	1529	51	0
1	J	1561	0	1531	65	0
1	K	1576	0	1540	68	0
1	L	1581	0	1545	58	0
2	E	244	0	134	6	0
2	G	228	0	122	7	0
2	M	244	0	134	1	0
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	471	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 17.

All (471) 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:J:255:ASN:HB3	1:J:257:MET:HE1	1.30	1.11
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
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:D:176:ARG:HB2	1:D:237:VAL:HG12	1.53	0.89
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:L:233:ARG:C	1:L:233:ARG:HD3	1.98	0.84
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:K:288:ARG:HH21	1:K:288:ARG:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:153:CYS:HG	1:K:256:PHE:HD2	1.34	0.74
1:K:169:PRO:HB2	1:K:170:PRO:CD	2.17	0.73
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:K:168:PRO:HB2	1:K:169:PRO:HD2	1.77	0.67
1:A:185:GLU:HA	1:D:158:THR:CG2	2.23	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:L:231:THR:O	1:L:233:ARG:N	2.28	0.66
1:A:247:THR:HG21	1:A:249:PHE:O	1.96	0.66
1:C:263:VAL:HA	1:C:267:ASN:HD22	1.61	0.65
1:I:173:THR:HG22	1:I:240:TYR:HB3	1.79	0.65
1:D:150:LYS:HE3	1:D:152:TYR:OH	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:B:145:SER:O	1:B:148:LEU:O	2.15	0.63
1:D:115:ILE:HG13	1:D:115:ILE:O	1.99	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: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:163:ILE:HD13	1:B:175:ILE:HD13	1.81	0.62
1:B:137:ALA:HB3	1:B:140:ALA:HB2	1.82	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:J:127:PHE:CE1	1:J:129:VAL:HG23	2.35	0.62
1:A:183:LYS:HG3	1:A:186:HIS:HD2	1.64	0.62
1:A:185:GLU:OE1	1:D:157:LYS:HD3	1.98	0.62
1:J:155:ILE:CA	1:J:294:ILE:HD11	2.29	0.62
1:C:150:LYS:HD2	1:C:152:TYR:CZ	2.34	0.62
1:L:233:ARG:CD	1:L:233:ARG:O	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
3:F:416:DT:H2"	3:F:417:DG:N7	2.16	0.61
1:I:225:TYR:CD1	1:I:236:VAL:HG22	2.32	0.61
1:A:253:LEU:HD22	1:A:253:LEU:N	2.16	0.61
1:I:302:ARG:HH21	1:I:306:GLU:HB2	1.66	0.61
1:D:140:ALA:O	1:D:298:PRO:HG2	2.01	0.60
1:B:150:LYS:NZ	1:B:305:ASP:OD2	2.31	0.60
1:K:168:PRO:HG3	1:K:240:TYR:CE2	2.36	0.60
1:D:228:ASP:HB3	1:D:231:THR:O	2.02	0.60
1:D:224:GLN:HB3	1:D:237:VAL:HG22	1.82	0.60
1:B:170:PRO:HB2	1:B:173:THR:HG1	1.67	0.60
1:I:196:ASN:N	1:J:196:ASN:OD1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:125:HIS:HB3	1:B:165:VAL:CG1	2.32	0.59
1:J:279:MET:N	1:J:282:GLY:HA3	2.17	0.59
1:J:244:GLN:OE1	1:K:117:SER:HB2	2.01	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:L:228:ASP:HB2	1:L:233:ARG:HD2	1.85	0.59
1:C:247:THR:HG22	1:C:249:PHE:H	1.67	0.59
1:I:191:VAL:HG23	5:I:506:HOH:O	2.03	0.58
1:K:279:MET:CG	1:K:285:LEU:HD21	2.31	0.58
1:I:193:ARG:NE	1:I:257:MET:HB3	2.17	0.58
1:B:114:PHE:HB3	1:B:231:THR:CG2	2.29	0.58
1:L:231:THR:HG23	1:L:231:THR:O	2.03	0.58
1:C:242:PRO:O	1:C:243:PRO:C	2.41	0.58
1:L:266:MET:O	1:L:269:ARG:CG	2.51	0.58
1:C:176:ARG:HG2	1:C:276:THR:OG1	2.04	0.58
1:A:201:ARG:HB2	1:A:201:ARG:HH11	1.67	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:J:279:MET:HG2	1:J:282:GLY:CA	2.35	0.57
1:I:173:THR:CG2	1:I:240:TYR:HB3	2.34	0.57
2:M:600:DC:H1'	2:M:601:DG:C8	2.40	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:288:ARG:NH2	1:K:288:ARG:HG3	2.13	0.56
1:K:114:PHE:HA	1:K:231:THR:HG23	1.86	0.56
1:B:167:THR:C	1:B:169:PRO:HD2	2.25	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:L:152:TYR:HB3	1:L:298:PRO:HB3	1.87	0.56
1:B:200:GLY:O	1:B:204:ASN:ND2	2.39	0.56
1:L:233:ARG:CD	1:L:233:ARG:C	2.67	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:J:176:ARG:HB2	1:J:237:VAL:HG12	1.89	0.55
1:J:147:LEU:HD12	1:J:306:GLU:HG2	1.88	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:K:166:SER:OG	1:K:167:THR:N	2.39	0.55
1:A:130:THR:HG23	5:A:511:HOH:O	2.06	0.55
1:K:169:PRO:CB	1:K:170:PRO:CD	2.82	0.54
1:K:141:THR:HG22	1:K:142:TRP:HD1	1.71	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
3:F:411:DG:C2'	3:F:412:DG:C8	2.91	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:263:VAL:O	1:L:196:ASN:ND2	2.41	0.54
1:K:217:VAL:HG11	1:K:223:SER:HB3	1.89	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:L:137:ALA:O	1:L:299:GLY:HA3	2.07	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: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
1:A:161:ILE:HG13	1:A:254:TYR:HD2	1.74	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: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:L:285:LEU:HD12	1:L:285:LEU:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:HD12	1:A:151:LEU:O	2.09	0.52
3:N:613:DG:C2'	3:N:614:DG:OP2	2.53	0.52
1:C:263:VAL:O	1:D:196:ASN:ND2	2.42	0.52
1:C:125:HIS:H	1:C:125:HIS:CD2	2.25	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: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:C:247:THR:HG21	5:C:502:HOH:O	2.09	0.51
1:K:156:ALA:CB	1:K:203:PHE:CZ	2.93	0.51
1:L:228:ASP:HB3	1:L:231:THR:O	2.10	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:K:131:PHE:CE2	1:K:161:ILE:HD12	2.45	0.51
1:K:132:GLN:OE1	1:K:133:GLN:HB2	2.11	0.51
1:D:138:LYS:CG	1:D:300:ARG:HB2	2.40	0.51
1:J:250:THR:OG1	1:J:250:THR:O	2.24	0.51
1:B:117:SER:OG	1:B:119:THR:HG22	2.10	0.51
2:E:405:DG:H1	3:F:414:DC:H42	1.57	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
1:I:141:THR:CG2	1:I:157:LYS:HD3	2.37	0.51
1:J:150:LYS:HB2	1:J:291:GLU:HB3	1.92	0.51
1:J:127:PHE:CE1	1:J:129:VAL:HG22	2.46	0.51
1:D:150:LYS:HD3	1:D:291:GLU:CD	2.31	0.50
1:D:135:SER:O	1:D:143:THR:HG22	2.11	0.50
1:K:231:THR:HG22	1:K:233:ARG:HG2	1.92	0.50
1:B:258:CYS:O	1:B:294:ILE:HD13	2.11	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:D:214:LEU:CD1	1:D:266:MET:HE2	2.41	0.50
1:C:176:ARG:NE	1:C:278:GLU:OE2	2.39	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:207:GLN:HG3	1:B:208:SER:N	2.27	0.50
1:B:158:THR:OG1	1:C:185:GLU:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:141:THR:HG22	1:I:157:LYS:CD	2.37	0.49
1:I:247:THR:HG22	1:I:248:GLU:N	2.27	0.49
1:J:150:LYS:HE2	1:J:152:TYR:HH	1.77	0.49
1:K:209:ALA:HB3	1:K:216:ARG:HD2	1.93	0.49
1:C:162:GLN:HE21	1:C:162:GLN:HA	1.77	0.49
1:A:150:LYS:HE3	1:A:152:TYR:CZ	2.47	0.49
1:L:128:GLU:HG3	1:L:164:LYS:HB3	1.94	0.49
1:J:200:GLY:O	1:J:204:ASN:ND2	2.44	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
2:E:403:DA:N6	3:F:415:DT:O4	2.45	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
1:K:153:CYS:SG	1:K:256:PHE:HD2	2.33	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:K:226:VAL:HG23	1:K:235:SER:OG	2.13	0.49
1:D:244:GLN:O	1:D:247:THR:HB	2.12	0.49
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:D:214:LEU:HD11	1:D:266:MET:CE	2.43	0.48
1:C:261:SER:HB3	2:G:507:DG:OP1	2.13	0.48
1:I:217:VAL:HG23	1:I:253:LEU:O	2.13	0.48
1:D:190:VAL:HG22	1:D:233:ARG:HD3	1.94	0.48
1:B:168:PRO:HD2	1:B:169:PRO:HD3	1.95	0.48
1:B:163:ILE:O	1:B:249:PHE:HB3	2.13	0.48
1:K:156:ALA:HB1	1:K:203:PHE:CZ	2.47	0.48
1:B:273:ILE:HD12	1:B:290:PHE:HE1	1.78	0.48
1:L:176:ARG:NH1	1:L:278:GLU:OE2	2.43	0.48
1:I:209:ALA:HB2	1:I:225:TYR:CZ	2.48	0.48
1:A:190:VAL:HG12	1:A:192:LYS:HG3	1.94	0.48
1:A:132:GLN:HE21	1:A:162:GLN:HE22	1.61	0.48
1:I:120:ASP:OD2	1:I:288:ARG:NE	2.43	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:A:158:THR:HG22	1:A:253:LEU:HD12	1.95	0.48
1:B:169:PRO:O	1:B:170:PRO:C	2.53	0.48
1:L:209:ALA:HB2	1:L:225:TYR:CZ	2.49	0.48
1:J:266:MET:O	1:J:269:ARG:HG3	2.14	0.48
1:A:304:ALA:O	1:A:308:HIS:HB2	2.14	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: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
2:G:509:DC:H2"	2:G:510:DC:C6	2.50	0.47
1:C:138:LYS:NZ	3:H:514:DG:N7	2.53	0.47
1:K:150:LYS:HD2	1:K:152:TYR:CZ	2.49	0.47
1:A:185:GLU:OE2	1:D:158:THR:CG2	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
1:J:149:LYS:O	1:J:149:LYS:HG3	2.15	0.47
1:J:149:LYS:O	1:J:149:LYS:CG	2.63	0.47
2:G:501:DG:H2"	2:G:502:DG:C8	2.49	0.47
1:B:121:TYR:CE2	1:B:123:GLY:CA	2.98	0.47
1:K:300:ARG:HG3	1:K:301:ASP:OD1	2.15	0.47
1:K:259:ASN:HA	1:K:294:ILE:HB	1.97	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
3:F:414:DC:C2'	3:F:415:DT:O5'	2.58	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
1:J:130:THR:HG22	1:J:131:PHE:H	1.80	0.46
1:I:172:GLY:HA3	1:I:280:ARG:NH1	2.30	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:242:PRO:O	1:A:243:PRO:C	2.54	0.46
1:A:225:TYR:HD1	1:A:236:VAL:HG22	1.80	0.46
1:D:137:ALA:HB3	1:D:140:ALA:HB2	1.98	0.46
1:B:121:TYR:CE2	1:B:123:GLY:HA2	2.50	0.46
1:C:144:TYR:HE1	1:C:146:PRO:HA	1.81	0.46
1:B:216:ARG:HA	1:B:225:TYR:HE2	1.79	0.46
3:F:416:DT:C2'	3:F:417:DG:C8	2.91	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
1:J:152:TYR:CZ	1:J:302:ARG:HA	2.51	0.46
1:I:148:LEU:CD1	1:I:305:ASP:HB3	2.46	0.46
1:K:198:GLU:O	1:K:204:ASN:ND2	2.49	0.46
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:K:138:LYS:HB3	3:P:713:DG:OP2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:GLN:HG3	1:B:209:ALA:N	2.31	0.46
1:K:302:ARG:O	1:K:306:GLU:HG2	2.16	0.46
1:J:279:MET:HG2	1:J:282:GLY:HA3	1.97	0.45
1:C:253:LEU:HD23	1:C:253:LEU:N	2.31	0.45
1:C:144:TYR:CE1	1:C:146:PRO:HA	2.51	0.45
1:I:150:LYS:HE2	1:I:293:ARG:HB2	1.99	0.45
1:J:158:THR:HG23	5:J:503:HOH:O	2.14	0.45
1:B:169:PRO:HB2	1:B:170:PRO:CD	2.42	0.45
1:K:127:PHE:CZ	1:K:277:LEU:HB2	2.51	0.45
1:J:141:THR:HG22	1:J:142:TRP:CD1	2.47	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:C:152:TYR:CZ	1:C:302:ARG:HA	2.51	0.45
1:A:130:THR:CG2	1:A:131:PHE:N	2.79	0.45
1:K:168:PRO:CB	1:K:169:PRO:HD2	2.43	0.45
1:J:259:ASN:HA	1:J:294:ILE:HG12	1.98	0.45
1:D:259:ASN:HA	1:D:294:ILE:HB	1.99	0.45
1:C:125:HIS:HB3	1:C:165:VAL:CG1	2.47	0.45
1:A:303:LYS:HG3	1:A:304:ALA:N	2.31	0.45
1:C:174:ALA:HB1	1:C:237:VAL:HG12	1.99	0.45
1:A:140:ALA:O	1:A:298:PRO:HG2	2.17	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:I:127:PHE:O	1:I:288:ARG:NH1	2.50	0.45
1:B:144:TYR:O	1:B:302:ARG:NH2	2.49	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:I:190:VAL:HG12	1:I:192:LYS:HG3	1.98	0.44
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: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
1:L:117:SER:CB	1:L:287:ARG:HH12	2.29	0.44
1:J:128:GLU:HB3	1:J:164:LYS:HB3	1.99	0.44
1:I:193:ARG:NH2	1:I:257:MET:HB3	2.32	0.44
1:J:178:MET:HE1	1:J:233:ARG:HB3	2.00	0.44
1:A:179:PRO:HG2	1:A:191:VAL:HB	1.99	0.44
1:J:127:PHE:CD1	1:J:127:PHE:C	2.91	0.44
1:I:306:GLU:HG3	1:I:307:ASP:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:266:MET:HE3	1:L:271:ILE:HG23	1.99	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:A:132:GLN:NE2	1:A:162:GLN:HE22	2.16	0.44
2:E:409:DG:H2'	2:G:501:DG:O4'	2.16	0.44
1:I:216:ARG:NH2	5:I:505:HOH:O	2.48	0.44
1:A:212:SER:HB2	1:A:234:GLN:NE2	2.27	0.44
1:I:190:VAL:HA	1:I:233:ARG:HH12	1.83	0.44
1:D:125:HIS:CD2	1:D:167:THR:HB	2.43	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
2:E:399:DG:H2"	2:E:400:DG:OP2	2.18	0.44
1:D:150:LYS:HE3	1:D:152:TYR:CZ	2.53	0.43
1:J:127:PHE:HD1	1:J:127:PHE:C	2.21	0.43
1:I:179:PRO:HG2	1:I:191:VAL:HB	2.00	0.43
1:A:268:ARG:HD3	5:E:501:HOH:O	2.18	0.43
1:A:223:SER:HA	1:A:238:VAL:HG12	2.00	0.43
1:C:200:GLY:O	1:C:204:ASN:ND2	2.50	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:244:GLN:O	1:A:247:THR:HB	2.18	0.43
1:A:130:THR:HG22	1:A:131:PHE:N	2.32	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:D:150:LYS:HG2	1:D:152:TYR:CE1	2.53	0.43
2:G:508:DC:H1'	2:G:509:DC:C6	2.53	0.43
1:B:219:GLY:N	5:B:506:HOH:O	2.18	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: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
1:A:151:LEU:C	1:A:151:LEU:HD12	2.39	0.43
1:C:125:HIS:CB	1:C:165:VAL:CG1	2.97	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:J:127:PHE:CD1	1:J:128:GLU:N	2.87	0.42
1:I:259:ASN:HA	1:I:294:ILE:HB	2.00	0.42
1:L:170:PRO:O	1:L:173:THR:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:118:ASN:C	1:L:118:ASN:OD1	2.57	0.42
1:K:164:LYS:O	1:K:165:VAL:HG13	2.18	0.42
1:J:229:PRO:HD3	5:J:505:HOH:O	2.19	0.42
1:J:124:PRO:HG2	1:J:125:HIS:CE1	2.54	0.42
1:B:172:GLY:HA3	1:B:280:ARG:HD3	2.01	0.42
1:D:259:ASN:O	1:D:266:MET:HE3	2.19	0.42
1:L:164:LYS:HB2	5:L:514:HOH:O	2.19	0.42
1:A:185:GLU:OE2	1:D:158:THR:HG23	2.20	0.42
1:L:259:ASN:HA	1:L:294:ILE:HG22	2.00	0.42
1:C:158:THR:HB	1:C:218:GLU:OE1	2.19	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:C:161:ILE:HD11	1:C:254:TYR:HE2	1.85	0.42
1:B:125:HIS:CB	1:B:165:VAL:HG13	2.49	0.42
3:P:716:DC:H2'	3:P:717:DT:H71	2.02	0.42
1:D:240:TYR:C	1:D:240:TYR:CD1	2.92	0.42
1:L:237:VAL:CG2	1:L:238:VAL:N	2.83	0.42
1:K:266:MET:HE3	1:K:271:ILE:HD12	2.02	0.41
1:B:162:GLN:HE21	1:B:162:GLN:HB3	1.70	0.41
1:L:224:GLN:HB3	1:L:237:VAL:HG13	2.02	0.41
1:A:200:GLY:HA3	5:A:516:HOH:O	2.20	0.41
1:K:153:CYS:O	1:K:294:ILE:HA	2.20	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:D:152:TYR:CZ	1:D:302:ARG:HA	2.55	0.41
1:K:147:LEU:HD21	1:K:309:TYR:CD2	2.56	0.41
1:C:159:CYS:HA	1:C:160:PRO:HD3	1.78	0.41
1:L:233:ARG:HE	1:L:235:SER:HB2	1.84	0.41
1:J:152:TYR:CE2	1:J:302:ARG:HA	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:L:226:VAL:HB	1:L:235:SER:HB3	2.03	0.41
1:L:218:GLU:HB2	1:L:255:ASN:ND2	2.36	0.41
1:I:132:GLN:O	1:I:133:GLN:C	2.58	0.41
3:F:415:DT:C3'	3:F:416:DT:H5"	2.51	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:L:125:HIS:O	1:L:126:HIS:C	2.58	0.41
1:B:198:GLU:O	1:I:126:HIS:HE1	2.04	0.41
1:K:293:ARG:HD2	1:K:295:CYS:SG	2.61	0.41
1:I:216:ARG:CD	5:I:503:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ILE:HA	1:C:252:ILE:HD13	1.92	0.41
1:L:231:THR:CG2	1:L:231:THR:O	2.69	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:A:154:GLN:NE2	1:A:296:ALA:O	2.53	0.40
1:J:163:ILE:O	1:J:249:PHE:HA	2.21	0.40
3:F:415:DT:H2'	3:F:416:DT:C6	2.55	0.40
1:J:153:CYS:O	1:J:294:ILE:HA	2.22	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
2:E:405:DG:H1	3:F:414:DC:N4	2.20	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:J:125:HIS:HE1	1:J:285:LEU:HD22	1.87	0.40
1:D:224:GLN:HB3	1:D:237:VAL:CG2	2.50	0.40
1:D:158:THR:HB	1:D:218:GLU:CD	2.40	0.40
1:J:178:MET:CE	1:J:233:ARG:HB3	2.52	0.40
1:A:217:VAL:HG23	1:A:236:VAL:CG1	2.47	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%)	19	65
1	C	199/210 (95%)	188 (94%)	9 (4%)	2 (1%)	19	65
1	D	196/210 (93%)	187 (95%)	6 (3%)	3 (2%)	13	55
1	I	196/210 (93%)	188 (96%)	7 (4%)	1 (0%)	34	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	J	197/210 (94%)	188 (95%)	8 (4%)	1 (0%)	34 78
1	K	199/210 (95%)	184 (92%)	10 (5%)	5 (2%)	7 41
1	L	199/210 (95%)	187 (94%)	11 (6%)	1 (0%)	34 78
All	All	1581/1680 (94%)	1490 (94%)	76 (5%)	15 (1%)	21 67

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 (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	175/186 (94%)	157 (90%)	18 (10%)	9 36
1	B	174/186 (94%)	150 (86%)	24 (14%)	4 21
1	C	178/186 (96%)	155 (87%)	23 (13%)	5 24
1	D	174/186 (94%)	148 (85%)	26 (15%)	4 17
1	I	175/186 (94%)	151 (86%)	24 (14%)	4 21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	175/186 (94%)	144 (82%)	31 (18%)	2 11
1	K	176/186 (95%)	140 (80%)	36 (20%)	1 7
1	L	177/186 (95%)	150 (85%)	27 (15%)	3 17
All	All	1404/1488 (94%)	1195 (85%)	209 (15%)	4 17

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	132	GLN
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	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
1	B	176	ARG
1	B	188	THR
1	B	191	VAL
1	B	201	ARG
1	B	205	GLU
1	B	224	GLN

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Mol	Chain	Res	Type
1	B	230	VAL
1	B	249	PHE
1	B	255	ASN
1	B	258	CYS
1	B	267	ASN
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	120	ASP
1	C	132	GLN
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	189	ASP
1	C	205	GLU
1	C	207	GLN
1	C	228	ASP
1	C	231	THR
1	C	253	LEU
1	C	268	ARG
1	C	272	LEU
1	C	276	THR
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	120	ASP
1	D	128	GLU
1	D	153	CYS
1	D	155	ILE
1	D	158	THR
1	D	167	THR
1	D	176	ARG
1	D	183	LYS

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Mol	Chain	Res	Type
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	258	CYS
1	D	272	LEU
1	D	280	ARG
1	D	281	ASP
1	D	284	VAL
1	D	285	LEU
1	D	308	HIS
1	D	310	ARG
1	I	115	ILE
1	I	130	THR
1	I	141	THR
1	I	147	LEU
1	I	155	ILE
1	I	173	THR
1	I	183	LYS
1	I	188	THR
1	I	203	PHE
1	I	205	GLU
1	I	222	LEU
1	I	227	ASP
1	I	231	THR
1	I	237	VAL
1	I	257	MET
1	I	260	SER
1	I	262	CYS
1	I	267	ASN
1	I	274	ILE
1	I	276	THR
1	I	288	ARG
1	I	302	ARG
1	I	306	GLU
1	I	310	ARG
1	J	115	ILE
1	J	117	SER

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Mol	Chain	Res	Type
1	J	119	THR
1	J	120	ASP
1	J	121	TYR
1	J	127	PHE
1	J	130	THR
1	J	133	GLN
1	J	136	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	244	GLN
1	J	250	THR
1	J	251	THR
1	J	258	CYS
1	J	263	VAL
1	J	267	ASN
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	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
1	K	141	THR
1	K	153	CYS
1	K	155	ILE
1	K	157	LYS
1	K	158	THR
1	K	162	GLN

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Mol	Chain	Res	Type
1	K	164	LYS
1	K	165	VAL
1	K	185	GLU
1	K	190	VAL
1	K	192	LYS
1	K	204	ASN
1	K	205	GLU
1	K	208	SER
1	K	214	LEU
1	K	237	VAL
1	K	249	PHE
1	K	250	THR
1	K	260	SER
1	K	268	ARG
1	K	271	ILE
1	K	272	LEU
1	K	277	LEU
1	K	278	GLU
1	K	280	ARG
1	K	284	VAL
1	K	285	LEU
1	K	288	ARG
1	K	293	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	164	LYS
1	L	167	THR
1	L	173	THR
1	L	189	ASP
1	L	193	ARG
1	L	199	LEU
1	L	201	ARG
1	L	204	ASN
1	L	208	SER

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Mol	Chain	Res	Type
1	L	215	ILE
1	L	233	ARG
1	L	238	VAL
1	L	249	PHE
1	L	269	ARG
1	L	272	LEU
1	L	278	GLU
1	L	302	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) 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	B	162	GLN
1	B	207	GLN
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	154	GLN
1	D	213	HIS
1	D	255	ASN
1	D	259	ASN
1	D	267	ASN
1	I	126	HIS
1	I	133	GLN
1	I	154	GLN
1	I	267	ASN
1	J	125	HIS
1	J	133	GLN
1	J	186	HIS
1	J	213	HIS
1	J	234	GLN
1	J	267	ASN
1	K	186	HIS

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Mol	Chain	Res	Type
1	K	283	GLN
1	L	112	HIS
1	L	154	GLN
1	L	213	HIS
1	L	234	GLN
1	L	259	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates 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	201/210 (95%)	-0.21	1 (0%) 91 87	59, 98, 147, 172	1 (0%)
1	B	198/210 (94%)	-0.36	1 (0%) 91 87	60, 92, 126, 145	2 (1%)
1	C	201/210 (95%)	-0.40	1 (0%) 91 87	55, 84, 126, 141	0
1	D	198/210 (94%)	-0.37	0 100 100	63, 89, 132, 160	1 (0%)
1	I	198/210 (94%)	-0.31	1 (0%) 91 87	64, 87, 129, 156	0
1	J	199/210 (94%)	-0.00	3 (1%) 76 63	75, 111, 158, 195	0
1	K	201/210 (95%)	-0.24	3 (1%) 76 63	63, 87, 144, 164	0
1	L	201/210 (95%)	-0.48	0 100 100	48, 73, 108, 138	0
2	E	12/12 (100%)	-0.15	0 100 100	73, 100, 152, 178	0
2	G	11/12 (91%)	-0.01	1 (9%) 11 6	85, 106, 135, 142	0
2	M	12/12 (100%)	-0.57	0 100 100	72, 90, 103, 106	0
2	O	12/12 (100%)	-0.60	0 100 100	92, 106, 140, 146	0
3	F	12/12 (100%)	-0.28	0 100 100	69, 102, 138, 158	0
3	H	12/12 (100%)	0.29	1 (8%) 14 7	79, 115, 157, 170	0
3	N	12/12 (100%)	-0.65	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%)	-0.30	12 (0%) 89 83	48, 90, 141, 195	4 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	286	GLY	5.4
3	H	523	DG	4.6
1	K	137	ALA	4.6
1	J	137	ALA	4.4
1	I	139	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	K	171	PRO	3.7
1	J	174	ALA	3.5
1	K	138	LYS	3.0
1	C	140	ALA	2.6
1	B	136	THR	2.3
1	A	224	GLN	2.1
2	G	511	DG	2.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
4	ZN	C	401	1/1	0.99	0.18	3.70	59,59,59,59	0
4	ZN	B	401	1/1	0.99	0.16	0.18	63,63,63,63	0
4	ZN	L	401	1/1	0.99	0.11	-1.31	76,76,76,76	0
4	ZN	J	401	1/1	0.99	0.12	-1.63	84,84,84,84	0
4	ZN	A	401	1/1	0.98	0.11	-2.36	87,87,87,87	0
4	ZN	K	401	1/1	0.99	0.07	-2.65	89,89,89,89	0
4	ZN	D	401	1/1	0.99	0.14	-	71,71,71,71	0
4	ZN	I	401	1/1	0.96	0.13	-	98,98,98,98	0

6.5 Other polymers (i)

There are no such residues in this entry.