



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:09 AM UTC

PDB ID : 7EZJ / pdb_00007ezj
Title : Crystal structure of p73 DNA binding domain complex bound with 1 bp and 2 bp spacer DNA response elements.
Authors : Koley, T.; Roy Chowdhury, S.; Kumar, M.; Kaur, P.; Singh, T.P.; Viadiu, H.; Ethayathulla, A.S.
Deposited on : 2021-06-01
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

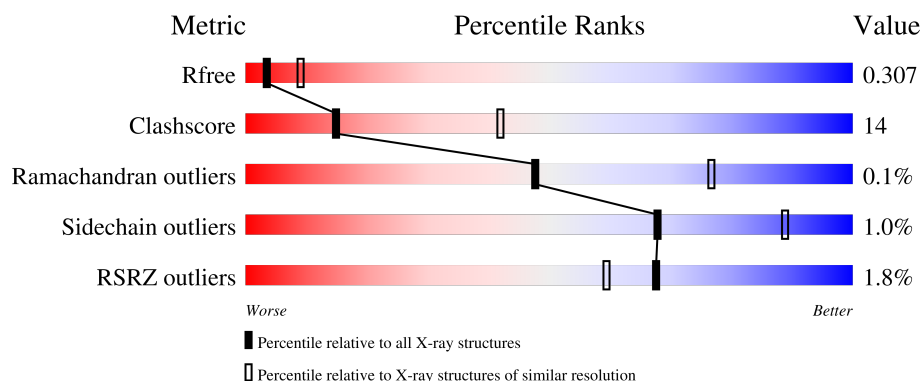
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	210	63% 32% • •
1	B	210	% 70% 24% • •
1	C	210	71% 24% •
1	D	210	74% 20% 5%
1	I	210	66% 28% 5%

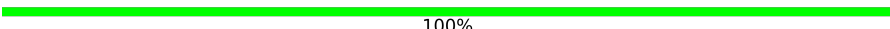
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Mol	Chain	Length	Quality of chain
1	J	210	
1	K	210	
1	L	210	
1	a	210	
1	b	210	
1	c	210	
1	d	210	
1	i	210	
1	j	210	
1	k	210	
1	l	210	
2	E	12	
2	F	12	
2	G	12	
2	H	12	
2	M	12	
2	N	12	
2	O	12	
2	P	12	
2	e	12	
2	f	12	
2	g	12	
2	h	12	
2	m	12	
2	n	12	

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Mol	Chain	Length	Quality of chain
2	o	12	 67% 33%
2	p	12	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29062 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
			1591	996	286	298	11			
1	B	201	Total	C	N	O	S	0	0	0
			1580	987	285	297	11			
1	C	201	Total	C	N	O	S	0	0	0
			1586	993	285	297	11			
1	D	199	Total	C	N	O	S	0	0	0
			1558	978	280	289	11			
1	I	199	Total	C	N	O	S	0	0	0
			1559	979	280	289	11			
1	J	197	Total	C	N	O	S	0	0	0
			1542	966	278	287	11			
1	K	201	Total	C	N	O	S	0	0	0
			1586	993	285	297	11			
1	L	200	Total	C	N	O	S	0	0	0
			1576	988	283	294	11			
1	a	199	Total	C	N	O	S	0	0	0
			1566	982	280	293	11			
1	b	199	Total	C	N	O	S	0	0	0
			1561	977	282	291	11			
1	c	200	Total	C	N	O	S	0	0	0
			1577	989	285	292	11			
1	d	198	Total	C	N	O	S	0	0	0
			1553	975	279	288	11			
1	i	201	Total	C	N	O	S	0	0	0
			1577	988	283	295	11			
1	j	196	Total	C	N	O	S	0	0	0
			1536	960	277	288	11			
1	k	206	Total	C	N	O	S	0	0	0
			1626	1018	297	300	11			
1	l	200	Total	C	N	O	S	0	0	0
			1576	988	283	294	11			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	MET	-	expression tag	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	-	expression tag	UNP O15350
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	-	expression tag	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	-	expression tag	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	-	expression tag	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
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	-	expression tag	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	-	expression tag	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

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Chain	Residue	Modelled	Actual	Comment	Reference
L	103	MET	-	expression tag	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
a	103	MET	-	expression tag	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	-	expression tag	UNP O15350
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	-	expression tag	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	-	expression tag	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	-	expression tag	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
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	-	expression tag	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

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Chain	Residue	Modelled	Actual	Comment	Reference
k	103	MET	-	expression tag	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	-	expression tag	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 12-mer DNA.

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	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
2	H	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
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	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
2	h	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
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 (CCD ID: 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		
3	a	1	Total	Zn	0	0
			1	1		
3	b	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	c	1	Total 1	Zn 1	0	0
3	d	1	Total 1	Zn 1	0	0
3	i	1	Total 1	Zn 1	0	0
3	j	1	Total 1	Zn 1	0	0
3	k	1	Total 1	Zn 1	0	0
3	l	1	Total 1	Zn 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total 4	O 4	0	0
4	B	5	Total 5	O 5	0	0
4	C	5	Total 5	O 5	0	0
4	D	2	Total 2	O 2	0	0
4	I	3	Total 3	O 3	0	0
4	J	2	Total 2	O 2	0	0
4	K	1	Total 1	O 1	0	0
4	L	14	Total 14	O 14	0	0
4	a	2	Total 2	O 2	0	0
4	b	4	Total 4	O 4	0	0
4	c	6	Total 6	O 6	0	0
4	d	5	Total 5	O 5	0	0
4	i	9	Total 9	O 9	0	0

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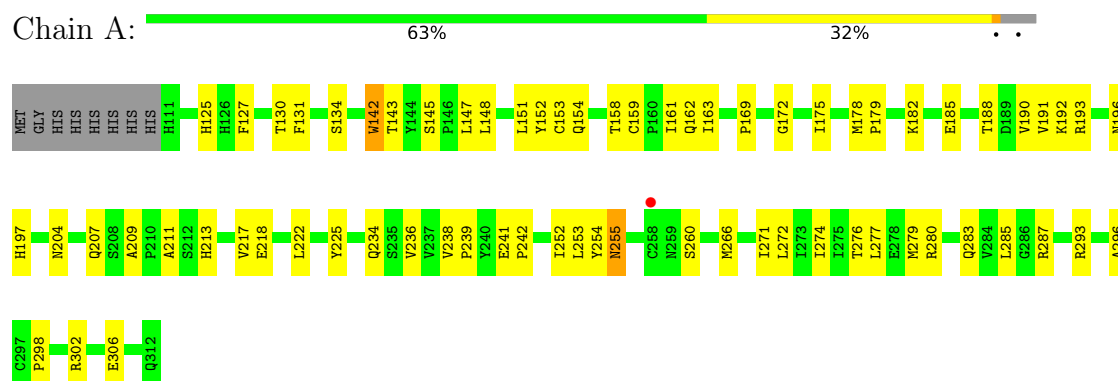
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	j	1	Total 1	O 1	0	0
4	k	11	Total 11	O 11	0	0
4	l	7	Total 7	O 7	0	0
4	H	1	Total 1	O 1	0	0
4	h	1	Total 1	O 1	0	0
4	o	1	Total 1	O 1	0	0

3 Residue-property plots

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

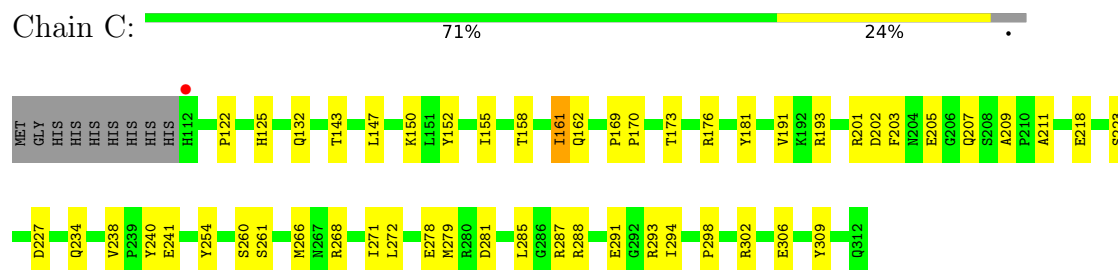
• Molecule 1: Tumor protein p73



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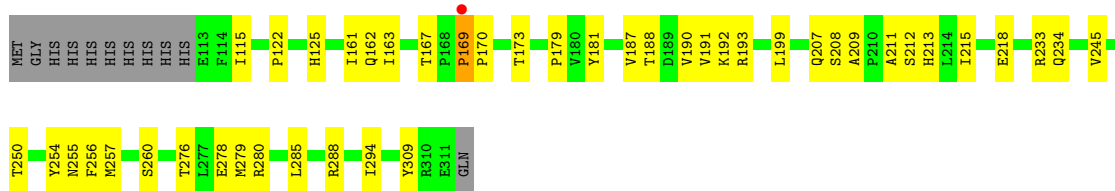


• Molecule 1: Tumor protein p73

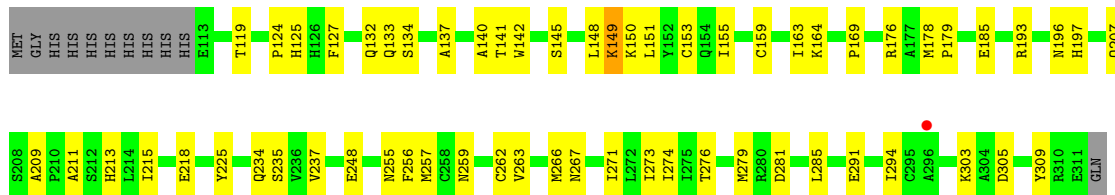


• Molecule 1: Tumor protein p73

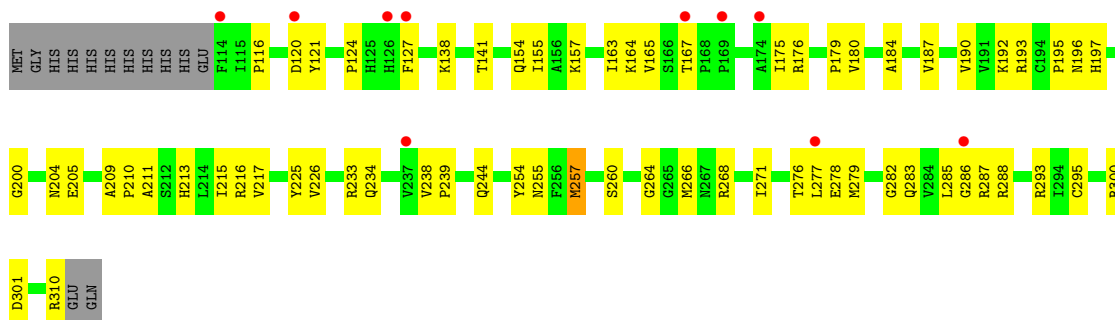




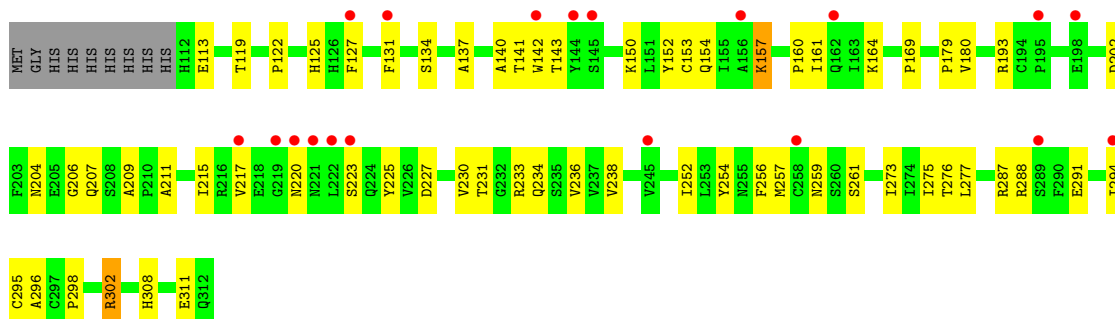
• Molecule 1: Tumor protein p73



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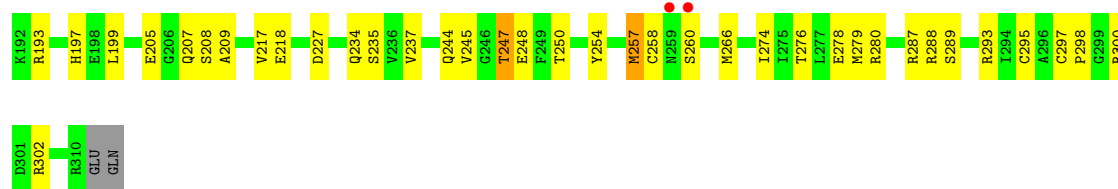
• Molecule 1: Tumor protein p73



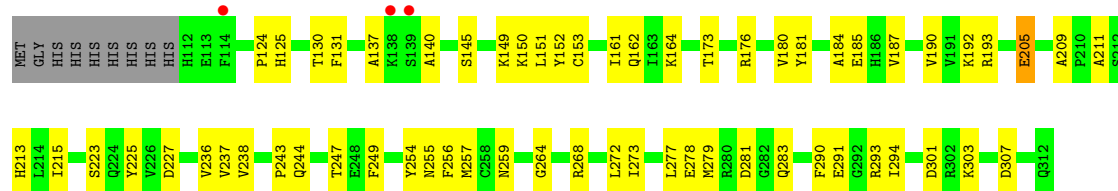
• Molecule 1: Tumor protein p73



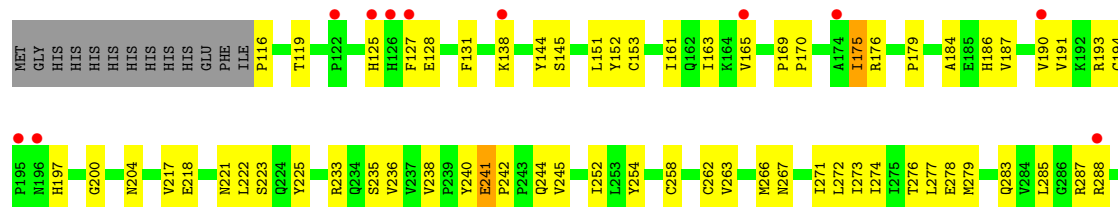




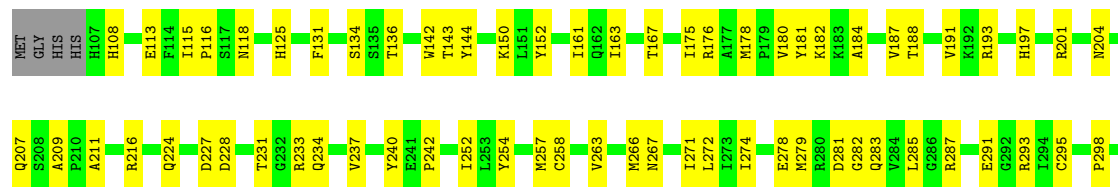
• Molecule 1: Tumor protein p73



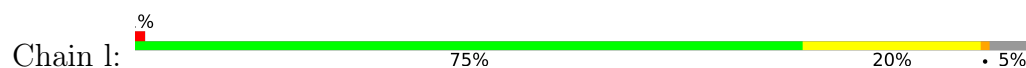
• Molecule 1: Tumor protein p73

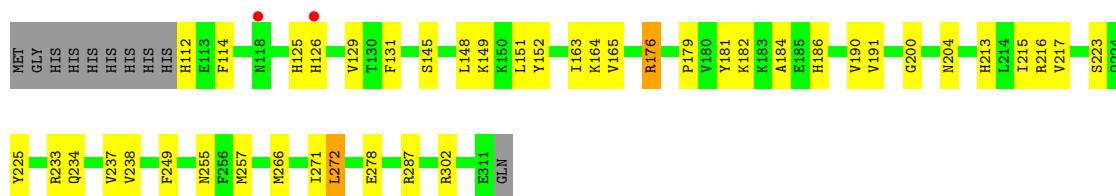


• Molecule 1: Tumor protein p73

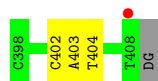


• Molecule 1: Tumor protein p73

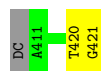




- Molecule 2: 12-mer DNA



- Molecule 2: 12-mer DNA



- Molecule 2: 12-mer DNA

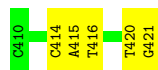


- Molecule 2: 12-mer DNA



There are no outlier residues recorded for this chain.

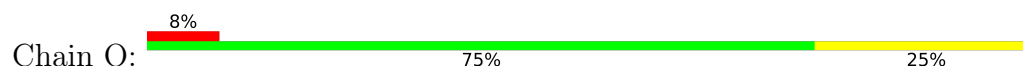
- Molecule 2: 12-mer DNA

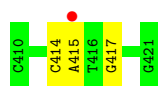


- Molecule 2: 12-mer DNA

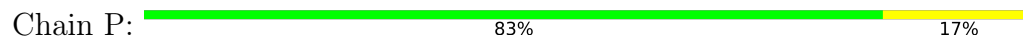


- Molecule 2: 12-mer DNA

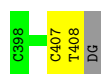




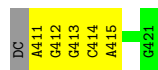
- Molecule 2: 12-mer DNA



- Molecule 2: 12-mer DNA



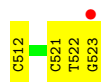
- Molecule 2: 12-mer DNA



- Molecule 2: 12-mer DNA



- Molecule 2: 12-mer DNA

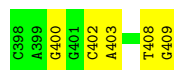


- Molecule 2: 12-mer DNA



There are no outlier residues recorded for this chain.

- Molecule 2: 12-mer DNA



- Molecule 2: 12-mer DNA

Chain o:  67% 33%



- Molecule 2: 12-mer DNA

Chain p:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	139.70Å 105.50Å 155.50Å 90.00° 112.36° 90.00°	Depositor
Resolution (Å)	40.93 – 2.90 40.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.0 (40.93-2.90) 95.4 (40.93-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.91Å)	Xtrriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.241 , 0.306 0.259 , 0.307	Depositor DCC
R_{free} test set	4387 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	78.8	Xtrriage
Anisotropy	0.139	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29062	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 86.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.5269e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.58	0/1632	0.85	2/2217 (0.1%)
1	B	0.63	0/1620	0.81	2/2201 (0.1%)
1	C	0.60	0/1627	0.81	2/2210 (0.1%)
1	D	0.74	1/1598 (0.1%)	1.05	5/2173 (0.2%)
1	I	0.56	0/1599	0.83	2/2174 (0.1%)
1	J	0.55	0/1581	0.92	1/2150 (0.0%)
1	K	0.53	0/1627	0.81	2/2210 (0.1%)
1	L	0.59	0/1617	0.82	1/2198 (0.0%)
1	a	0.63	0/1606	1.01	13/2183 (0.6%)
1	b	0.58	0/1601	0.84	3/2177 (0.1%)
1	c	0.59	1/1619 (0.1%)	0.80	2/2201 (0.1%)
1	d	0.51	0/1593	0.80	1/2166 (0.0%)
1	i	0.58	0/1617	0.84	2/2197 (0.1%)
1	j	0.61	1/1574 (0.1%)	0.92	4/2139 (0.2%)
1	k	0.56	0/1671	0.85	2/2272 (0.1%)
1	l	0.61	0/1617	0.83	0/2198
2	E	0.45	0/247	0.63	0/379
2	F	0.39	0/254	0.63	0/390
2	G	0.43	0/272	0.64	0/418
2	H	0.41	0/272	0.60	0/418
2	M	0.41	0/272	0.66	0/418
2	N	0.41	0/272	0.66	0/418
2	O	0.43	0/272	0.63	0/418
2	P	0.38	0/272	0.62	0/418
2	e	0.42	0/247	0.64	0/379
2	f	0.39	0/254	0.51	0/390
2	g	0.42	0/272	0.59	0/418
2	h	0.40	0/272	0.69	0/418
2	m	0.39	0/272	0.67	0/418
2	n	0.43	0/272	0.61	0/418
2	o	0.38	0/272	0.61	0/418
2	p	0.40	0/272	0.63	0/418

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.57	3/30065 (0.0%)	0.83	44/41620 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	169	PRO	C-N	19.35	1.50	1.33
1	c	242	PRO	CA-C	9.18	1.56	1.51
1	j	242	PRO	CA-C	-5.17	1.47	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	169	PRO	CA-C-N	21.72	135.52	119.66
1	D	169	PRO	C-N-CA	21.72	135.52	119.66
1	a	249	PHE	N-CA-C	8.48	123.44	109.95
1	a	242	PRO	CA-C-N	-8.41	112.19	120.52
1	a	242	PRO	C-N-CA	-8.41	112.19	120.52
1	k	242	PRO	CA-C-N	-8.13	112.47	120.52
1	k	242	PRO	C-N-CA	-8.13	112.47	120.52
1	J	257	MET	N-CA-C	8.11	122.95	112.89
1	a	208	SER	N-CA-C	-8.10	102.96	112.92
1	b	226	VAL	N-CA-C	8.01	119.38	108.17
1	D	257	MET	N-CA-C	7.70	122.49	113.18
1	C	241	GLU	CA-C-N	-6.62	114.89	119.66
1	C	241	GLU	C-N-CA	-6.62	114.89	119.66
1	j	116	PRO	N-CA-CB	6.42	110.06	103.00
1	a	244	GLN	N-CA-C	-6.37	101.68	110.35
1	b	149	LYS	N-CA-C	-6.20	102.91	111.28
1	j	153	CYS	N-CA-C	6.19	118.71	108.99
1	B	250	THR	N-CA-C	-6.15	98.49	108.52
1	c	271	ILE	CB-CA-C	-6.12	102.80	111.19
1	A	238	VAL	CA-C-N	-6.06	114.03	120.03
1	A	238	VAL	C-N-CA	-6.06	114.03	120.03
1	d	257	MET	N-CA-C	5.96	120.25	112.92
1	i	268	ARG	N-CA-C	-5.93	104.23	112.30
1	c	242	PRO	O-C-N	5.93	124.04	121.31
1	j	241	GLU	CA-C-N	-5.92	114.29	120.38
1	j	241	GLU	C-N-CA	-5.92	114.29	120.38
1	b	264	GLY	N-CA-C	-5.90	106.35	114.67
1	I	273	ILE	N-CA-C	-5.83	100.02	108.17
1	a	241	GLU	CA-C-N	-5.76	114.44	120.38
1	a	241	GLU	C-N-CA	-5.76	114.44	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	302	ARG	N-CA-C	-5.75	104.38	111.40
1	i	264	GLY	N-CA-C	-5.74	108.25	115.08
1	K	206	GLY	N-CA-C	5.71	122.72	114.10
1	D	309	TYR	N-CA-C	-5.60	106.30	113.02
1	a	198	GLU	N-CA-C	-5.53	105.36	111.71
1	I	149	LYS	N-CA-C	-5.52	103.80	111.52
1	a	167	THR	CA-C-N	-5.45	114.77	120.38
1	a	167	THR	C-N-CA	-5.45	114.77	120.38
1	L	262	CYS	CB-CA-C	5.43	116.48	109.80
1	B	231	THR	N-CA-C	5.24	119.16	112.87
1	D	162	GLN	CA-CB-CG	-5.20	103.70	114.10
1	a	238	VAL	CA-C-N	-5.18	115.39	120.52
1	a	238	VAL	C-N-CA	-5.18	115.39	120.52
1	a	241	GLU	N-CA-C	-5.17	102.05	109.24

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	1591	0	1553	64	0
1	B	1580	0	1545	69	0
1	C	1586	0	1551	35	0
1	D	1558	0	1528	32	0
1	I	1559	0	1530	43	0
1	J	1542	0	1517	59	0
1	K	1586	0	1551	47	0
1	L	1576	0	1543	40	0
1	a	1566	0	1536	56	0
1	b	1561	0	1530	45	0
1	c	1577	0	1544	43	0
1	d	1553	0	1526	63	0
1	i	1577	0	1542	42	0
1	j	1536	0	1505	51	0
1	k	1626	0	1575	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	l	1576	0	1543	26	0
2	E	221	0	125	2	0
2	F	227	0	124	1	0
2	G	243	0	136	5	0
2	H	243	0	136	0	0
2	M	243	0	136	6	0
2	N	243	0	136	2	0
2	O	243	0	136	2	0
2	P	243	0	136	1	0
2	e	221	0	125	1	0
2	f	227	0	124	4	0
2	g	243	0	136	3	0
2	h	243	0	136	5	0
2	m	243	0	136	0	0
2	n	243	0	136	4	0
2	o	243	0	136	2	0
2	p	243	0	136	0	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
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	4	0	0	1	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	2	0	0	0	0
4	H	1	0	0	0	0
4	I	3	0	0	0	0
4	J	2	0	0	1	0
4	K	1	0	0	1	0
4	L	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	a	2	0	0	0	0
4	b	4	0	0	0	0
4	c	6	0	0	0	0
4	d	5	0	0	1	0
4	h	1	0	0	0	0
4	i	9	0	0	0	0
4	j	1	0	0	0	0
4	k	11	0	0	0	0
4	l	7	0	0	1	0
4	o	1	0	0	0	0
All	All	29062	0	26749	771	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 14.

All (771) 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:a:284:VAL:CG2	1:d:245:VAL:HG11	1.54	1.37
1:a:284:VAL:HG21	1:d:245:VAL:CG1	1.64	1.25
1:B:127:PHE:CE2	1:B:277:LEU:HB2	1.82	1.15
1:I:197:HIS:HE1	1:I:262:CYS:SG	1.81	1.03
1:a:158:THR:HA	1:a:255:ASN:HD21	1.21	1.02
1:b:193:ARG:HH21	1:b:197:HIS:HB3	1.21	1.01
1:B:193:ARG:HD3	1:B:257:MET:HB3	1.42	1.01
1:j:176:ARG:HH12	1:j:278:GLU:CD	1.69	1.00
1:b:178:MET:HE2	1:b:233:ARG:HB3	1.43	1.00
1:l:176:ARG:HB2	1:l:237:VAL:HG22	1.43	0.98
1:A:204:ASN:HD21	1:A:211:ALA:CB	1.76	0.97
1:B:230:VAL:HG23	1:B:231:THR:H	1.25	0.96
1:c:293:ARG:NH1	1:c:295:CYS:SG	2.41	0.93
1:C:170:PRO:HG2	1:C:279:MET:HE2	1.51	0.92
1:D:173:THR:HG23	1:D:278:GLU:O	1.70	0.91
1:B:127:PHE:CE2	1:B:277:LEU:CB	2.54	0.89
1:K:142:TRP:NE1	1:K:160:PRO:HD2	1.87	0.89
1:B:193:ARG:HD3	1:B:257:MET:CB	2.03	0.89
1:L:255:ASN:HB3	1:L:257:MET:CE	2.03	0.88
1:A:204:ASN:ND2	1:A:211:ALA:HB2	1.89	0.87
1:i:205:GLU:OE2	1:i:205:GLU:N	2.08	0.86
1:d:163:ILE:HD11	1:d:250:THR:HB	1.55	0.85
1:A:204:ASN:ND2	1:A:211:ALA:CB	2.40	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:144:TYR:OH	1:c:149:LYS:HD2	1.79	0.83
1:B:312:GLN:HG3	1:B:312:GLN:O	1.77	0.82
1:b:145:SER:HA	1:b:302:ARG:HH21	1.45	0.82
1:j:176:ARG:NH1	1:j:278:GLU:CD	2.37	0.81
1:L:193:ARG:HD2	1:L:197:HIS:HB2	1.60	0.81
1:j:223:SER:HB3	1:j:238:VAL:HG12	1.62	0.81
1:d:115:ILE:HD12	1:d:187:VAL:HG22	1.64	0.79
1:D:163:ILE:HD11	1:D:250:THR:HB	1.65	0.79
1:a:158:THR:HA	1:a:255:ASN:ND2	1.97	0.79
1:j:179:PRO:HB2	1:j:191:VAL:HG11	1.63	0.79
1:b:178:MET:CE	1:b:233:ARG:HB3	2.12	0.79
1:A:204:ASN:HD21	1:A:211:ALA:HB1	1.47	0.79
1:k:266:MET:HE2	1:k:271:ILE:HG21	1.65	0.78
1:C:279:MET:HE3	1:C:285:LEU:HD11	1.63	0.78
1:I:125:HIS:CE1	1:I:169:PRO:HA	2.19	0.78
1:B:117:SER:OG	1:B:287:ARG:CZ	2.33	0.77
1:D:193:ARG:HD3	1:D:211:ALA:O	1.85	0.77
1:j:184:ALA:HA	1:j:187:VAL:HG23	1.66	0.76
1:j:218:GLU:HG2	1:k:188:THR:HG21	1.67	0.76
1:d:293:ARG:NH1	1:d:295:CYS:SG	2.59	0.76
1:j:221:ASN:O	1:j:221:ASN:ND2	2.18	0.76
1:J:176:ARG:HH12	1:J:226:VAL:HG21	1.51	0.76
1:a:138:LYS:HG3	1:a:300:ARG:HB2	1.68	0.75
1:d:163:ILE:O	1:d:163:ILE:HD12	1.87	0.75
1:a:161:ILE:HD13	1:a:254:TYR:HD2	1.51	0.75
1:j:274:ILE:HD11	1:j:287:ARG:HG3	1.67	0.75
1:d:276:THR:HG22	1:d:287:ARG:HG3	1.69	0.75
1:J:213:HIS:CE1	1:J:234:GLN:HB2	2.21	0.75
1:i:185:GLU:N	1:i:185:GLU:OE1	2.19	0.75
1:k:161:ILE:HG13	1:k:254:TYR:HD2	1.52	0.75
1:B:193:ARG:HG2	1:B:258:CYS:SG	2.27	0.74
1:L:193:ARG:HD2	1:L:197:HIS:CB	2.15	0.74
1:j:245:VAL:O	1:k:287:ARG:NH2	2.20	0.74
1:D:161:ILE:HD12	1:D:254:TYR:HD2	1.51	0.74
1:i:176:ARG:NH1	1:i:278:GLU:OE1	2.21	0.74
1:b:245:VAL:O	1:c:287:ARG:NH1	2.21	0.73
1:J:278:GLU:OE2	1:J:282:GLY:HA2	1.88	0.73
1:d:193:ARG:HD2	1:d:257:MET:HB2	1.71	0.73
1:B:285:LEU:HD12	1:B:285:LEU:N	2.02	0.73
1:j:194:CYS:HB3	1:j:262:CYS:HB3	1.70	0.73
1:K:142:TRP:NE1	1:K:160:PRO:CD	2.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:293:ARG:NH1	1:b:301:ASP:OD2	2.20	0.73
1:L:193:ARG:HH22	1:L:216:ARG:NH2	1.87	0.72
1:I:207:GLN:N	1:I:207:GLN:OE1	2.22	0.72
1:d:163:ILE:HD12	1:d:163:ILE:C	2.14	0.72
1:B:176:ARG:HB2	1:B:237:VAL:HG22	1.71	0.71
1:d:171:PRO:O	1:d:279:MET:HE1	1.91	0.71
1:j:184:ALA:HA	1:j:187:VAL:CG2	2.20	0.71
1:I:176:ARG:HB2	1:I:237:VAL:HG22	1.73	0.71
1:J:193:ARG:HH21	1:J:197:HIS:HB3	1.56	0.70
1:d:138:LYS:NZ	2:g:503:DG:O6	2.24	0.70
1:A:279:MET:HG3	1:A:285:LEU:HD21	1.72	0.70
1:I:185:GLU:N	1:I:185:GLU:OE2	2.25	0.70
1:k:178:MET:HE3	1:k:233:ARG:HB3	1.74	0.69
2:G:505:DA:H2"	2:G:506:DT:H5"	1.73	0.69
1:a:284:VAL:HG21	1:d:245:VAL:HG11	0.75	0.69
1:B:245:VAL:O	1:C:287:ARG:NH2	2.25	0.69
1:J:163:ILE:HD11	1:J:175:ILE:HD13	1.74	0.69
1:K:230:VAL:HG23	1:K:231:THR:HG23	1.75	0.69
1:a:124:PRO:HG2	1:a:125:HIS:CD2	2.28	0.68
1:b:138:LYS:HG3	1:b:300:ARG:HB2	1.72	0.68
1:B:230:VAL:HG23	1:B:231:THR:N	2.04	0.68
1:b:145:SER:HB2	1:b:302:ARG:HE	1.56	0.68
1:a:255:ASN:HB3	1:a:257:MET:HE1	1.75	0.68
1:j:279:MET:HE3	1:j:285:LEU:HD11	1.74	0.68
1:L:255:ASN:HB3	1:L:257:MET:HE1	1.74	0.68
1:a:222:LEU:HD22	1:a:239:PRO:HD3	1.76	0.67
1:B:127:PHE:HE2	1:B:277:LEU:N	1.92	0.67
1:L:141:THR:HG22	1:L:157:LYS:HD3	1.75	0.67
1:d:181:TYR:CE1	1:d:191:VAL:HB	2.29	0.67
1:J:155:ILE:HD11	1:J:257:MET:O	1.94	0.67
1:C:176:ARG:NH1	1:C:278:GLU:OE2	2.28	0.67
1:c:223:SER:HB3	1:c:238:VAL:HG12	1.77	0.67
1:K:217:VAL:HG11	1:K:238:VAL:HG11	1.77	0.66
1:D:279:MET:HE3	1:D:280:ARG:H	1.60	0.66
1:b:184:ALA:HA	1:b:187:VAL:HG12	1.77	0.66
1:L:193:ARG:HH11	1:L:197:HIS:HB3	1.58	0.66
1:j:176:ARG:NH1	1:j:278:GLU:OE1	2.28	0.66
1:A:193:ARG:HD3	1:A:211:ALA:O	1.96	0.66
1:C:281:ASP:OD1	1:C:281:ASP:N	2.26	0.66
1:K:119:THR:O	1:K:287:ARG:HD2	1.96	0.66
1:k:116:PRO:HG3	1:k:178:MET:HE2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:THR:HG22	1:B:131:PHE:H	1.61	0.66
1:B:278:GLU:HA	1:B:285:LEU:HD13	1.78	0.66
1:D:161:ILE:HD12	1:D:254:TYR:CD2	2.30	0.66
1:c:132:GLN:HB3	1:c:162:GLN:HE21	1.61	0.65
1:a:183:LYS:HG3	1:a:185:GLU:H	1.61	0.65
1:k:224:GLN:HB3	1:k:237:VAL:HG13	1.77	0.65
1:d:293:ARG:HD2	4:d:505:HOH:O	1.96	0.65
1:B:278:GLU:HA	1:B:285:LEU:CD1	2.27	0.64
1:d:193:ARG:HH21	1:d:197:HIS:HB3	1.62	0.64
1:k:152:TYR:HB3	1:k:298:PRO:HB3	1.80	0.64
1:D:122:PRO:HG3	1:D:288:ARG:NH2	2.11	0.64
1:d:260:SER:HA	1:d:266:MET:HE3	1.80	0.64
1:K:152:TYR:HB3	1:K:298:PRO:HB3	1.78	0.64
1:j:145:SER:HA	1:j:302:ARG:HH21	1.62	0.64
1:A:134:SER:HB3	1:A:142:TRP:CZ3	2.33	0.64
1:B:127:PHE:HE2	1:B:277:LEU:CB	2.09	0.64
2:h:521:DC:H2'	2:h:522:DT:H71	1.80	0.64
1:B:266:MET:HE3	1:B:271:ILE:CG2	2.28	0.64
1:K:179:PRO:HD3	1:K:215:ILE:HD12	1.78	0.64
1:b:280:ARG:HH12	1:i:303:LYS:HG3	1.60	0.63
1:b:178:MET:HE2	1:b:233:ARG:CB	2.24	0.63
1:c:176:ARG:HB2	1:c:237:VAL:HG22	1.80	0.63
1:J:268:ARG:NH1	2:M:415:DA:O3'	2.31	0.63
1:C:207:GLN:HG3	1:C:209:ALA:H	1.64	0.63
1:K:161:ILE:HD12	1:K:254:TYR:HD2	1.64	0.63
1:d:293:ARG:HH11	1:d:293:ARG:HG2	1.64	0.63
1:K:142:TRP:HE1	1:K:160:PRO:CD	2.11	0.63
1:K:227:ASP:OD1	1:K:234:GLN:HG2	1.97	0.62
1:k:163:ILE:HD11	1:k:240:TYR:HE1	1.63	0.62
1:A:260:SER:HA	1:A:266:MET:HE2	1.80	0.62
1:B:283:GLN:O	1:B:285:LEU:HD12	1.99	0.62
1:A:241:GLU:HG2	1:A:242:PRO:HD2	1.82	0.62
1:B:228:ASP:CG	1:B:231:THR:OG1	2.43	0.62
1:J:163:ILE:CD1	1:J:175:ILE:HD13	2.29	0.62
2:G:504:DC:H2''	2:G:505:DA:C8	2.35	0.62
1:B:117:SER:OG	1:B:287:ARG:NH2	2.33	0.62
1:k:161:ILE:HG13	1:k:254:TYR:CD2	2.35	0.62
1:D:179:PRO:HD3	1:D:215:ILE:HD12	1.81	0.62
1:A:125:HIS:CE1	1:A:169:PRO:HA	2.35	0.61
1:C:152:TYR:HB3	1:C:298:PRO:HB3	1.82	0.61
1:a:165:VAL:HG21	1:a:169:PRO:HD3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:132:GLN:HB3	1:c:162:GLN:NE2	2.16	0.61
1:k:263:VAL:HG12	1:k:267:ASN:OD1	2.01	0.61
1:a:163:ILE:HB	1:a:250:THR:HB	1.81	0.61
1:j:200:GLY:O	1:j:204:ASN:ND2	2.26	0.61
1:k:115:ILE:HD12	1:k:187:VAL:HG22	1.83	0.61
1:D:125:HIS:CE1	1:D:169:PRO:HA	2.36	0.60
1:c:125:HIS:CE1	1:c:169:PRO:HA	2.36	0.60
1:j:119:THR:O	1:j:287:ARG:HD2	2.01	0.60
1:C:293:ARG:NH2	2:G:506:DT:H5'	2.16	0.60
1:K:127:PHE:CD1	1:K:277:LEU:HD13	2.37	0.60
1:k:201:ARG:HA	1:k:204:ASN:HB2	1.84	0.60
1:D:173:THR:CG2	1:D:278:GLU:O	2.47	0.60
1:a:155:ILE:HD11	1:a:257:MET:O	2.02	0.60
1:j:175:ILE:HG12	1:j:277:LEU:HB3	1.84	0.60
1:J:268:ARG:NH1	2:M:416:DT:OP1	2.35	0.60
1:j:144:TYR:O	1:j:302:ARG:NH2	2.35	0.60
1:K:134:SER:HB3	1:K:143:THR:HA	1.84	0.59
1:b:193:ARG:HD2	1:b:257:MET:HB2	1.83	0.59
1:c:176:ARG:NH1	1:c:278:GLU:OE2	2.35	0.59
1:j:263:VAL:HA	1:j:267:ASN:OD1	2.02	0.59
1:b:193:ARG:NH2	1:b:197:HIS:HB3	2.05	0.59
1:C:132:GLN:HB3	1:C:162:GLN:NE2	2.17	0.59
1:k:193:ARG:HD3	1:k:211:ALA:O	2.03	0.59
1:B:283:GLN:O	1:B:285:LEU:CD1	2.51	0.59
1:k:207:GLN:HG3	1:k:209:ALA:H	1.68	0.59
1:b:138:LYS:HE3	1:b:300:ARG:HD3	1.85	0.59
1:I:178:MET:HB2	1:I:235:SER:HB3	1.85	0.58
1:a:284:VAL:HG23	1:a:284:VAL:O	2.01	0.58
1:i:176:ARG:HB2	1:i:237:VAL:HG22	1.84	0.58
1:A:287:ARG:NH1	1:D:245:VAL:O	2.35	0.58
1:I:132:GLN:HG3	1:I:133:GLN:H	1.68	0.58
1:d:179:PRO:HG2	1:d:191:VAL:HG13	1.84	0.58
1:A:127:PHE:CD1	1:A:277:LEU:HD22	2.38	0.58
1:J:209:ALA:HA	1:J:225:TYR:CE2	2.38	0.58
1:B:156:ALA:HB2	1:B:257:MET:HE1	1.86	0.58
1:J:268:ARG:HH12	2:M:416:DT:P	2.26	0.58
1:A:192:LYS:HG2	1:A:234:GLN:NE2	2.19	0.58
1:A:217:VAL:HG23	1:A:236:VAL:HG11	1.86	0.58
1:i:173:THR:CG2	1:i:277:LEU:HD11	2.34	0.58
1:C:272:LEU:HD23	1:C:291:GLU:HA	1.86	0.58
1:d:120:ASP:HB3	1:d:288:ARG:NH2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:207:GLN:OE1	1:d:208:SER:N	2.36	0.58
1:L:161:ILE:HD12	1:L:254:TYR:CD2	2.39	0.57
1:a:161:ILE:HD13	1:a:254:TYR:CD2	2.38	0.57
1:c:293:ARG:HG2	1:c:293:ARG:HH11	1.68	0.57
1:d:297:CYS:HB2	1:d:300:ARG:HH21	1.68	0.57
1:J:266:MET:HE3	1:J:271:ILE:HG23	1.87	0.57
1:L:193:ARG:NH2	1:L:216:ARG:NH2	2.50	0.57
1:c:138:LYS:HG3	1:c:300:ARG:HB2	1.86	0.57
1:i:213:HIS:NE2	1:i:227:ASP:OD1	2.35	0.57
1:C:193:ARG:HD3	1:C:211:ALA:O	2.04	0.57
1:b:193:ARG:HD2	1:b:257:MET:CB	2.34	0.57
1:l:223:SER:HB3	1:l:238:VAL:HG12	1.86	0.57
1:A:185:GLU:HG3	1:A:185:GLU:O	2.04	0.57
1:B:266:MET:HE3	1:B:271:ILE:HG23	1.85	0.57
1:L:138:LYS:HE3	1:L:300:ARG:HD3	1.87	0.57
1:j:152:TYR:OH	1:j:305:ASP:HB2	2.05	0.57
2:h:521:DC:H2"	2:h:522:DT:C6	2.40	0.57
1:I:148:LEU:O	1:I:149:LYS:HB2	2.04	0.57
1:K:180:VAL:HG23	1:K:233:ARG:HH12	1.70	0.57
1:L:153:CYS:O	1:L:294:ILE:HA	2.05	0.56
1:A:279:MET:HG3	1:A:285:LEU:CD2	2.35	0.56
1:K:180:VAL:HG23	1:K:233:ARG:NH1	2.20	0.56
1:A:161:ILE:HG13	1:A:254:TYR:HD2	1.71	0.56
1:J:268:ARG:NH1	2:M:416:DT:P	2.79	0.56
1:K:142:TRP:CE2	1:K:160:PRO:HD2	2.40	0.56
1:J:141:THR:HG22	1:J:157:LYS:HE3	1.87	0.56
1:d:207:GLN:HG3	1:d:209:ALA:H	1.70	0.56
1:K:122:PRO:HG3	1:K:288:ARG:HH21	1.69	0.56
1:b:274:ILE:HG22	1:b:276:THR:CG2	2.36	0.56
1:J:200:GLY:O	1:J:204:ASN:ND2	2.34	0.56
1:d:120:ASP:HB3	1:d:288:ARG:HH21	1.69	0.56
1:A:134:SER:HB3	1:A:142:TRP:CH2	2.40	0.56
1:A:213:HIS:CD2	1:A:234:GLN:HB3	2.41	0.56
1:b:176:ARG:NH1	1:b:278:GLU:OE2	2.38	0.56
1:A:154:GLN:NE2	1:A:296:ALA:O	2.39	0.55
1:A:188:THR:HG21	1:D:218:GLU:HG2	1.88	0.55
1:A:266:MET:HE3	1:A:271:ILE:HG23	1.87	0.55
1:B:127:PHE:HE2	1:B:277:LEU:H	1.53	0.55
1:k:227:ASP:OD1	1:k:234:GLN:HG2	2.07	0.55
1:K:202:ASP:O	1:K:204:ASN:ND2	2.36	0.55
1:b:125:HIS:HD1	1:b:167:THR:HB	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:420:DT:H2"	2:F:421:DG:C8	2.41	0.55
1:B:228:ASP:HB3	1:B:231:THR:OG1	2.06	0.55
1:K:252:ILE:HD12	4:K:501:HOH:O	2.06	0.55
1:a:277:LEU:O	1:a:285:LEU:N	2.33	0.55
1:k:163:ILE:HD13	1:k:175:ILE:HD11	1.88	0.55
1:l:213:HIS:CD2	1:l:225:TYR:HD2	2.24	0.55
1:j:161:ILE:HD12	1:j:254:TYR:CD2	2.42	0.55
1:k:116:PRO:HG2	1:k:180:VAL:CG1	2.37	0.55
1:l:179:PRO:HD3	1:l:215:ILE:HD12	1.88	0.55
1:d:176:ARG:NH1	1:d:278:GLU:OE2	2.39	0.55
1:I:193:ARG:HD3	1:I:211:ALA:O	2.07	0.55
1:j:190:VAL:HG12	1:j:233:ARG:HH11	1.72	0.55
1:K:153:CYS:SG	1:K:294:ILE:HD13	2.47	0.55
1:a:179:PRO:HG2	1:a:191:VAL:HB	1.88	0.55
1:c:213:HIS:CE1	1:c:234:GLN:HB3	2.41	0.55
1:i:293:ARG:NH1	1:i:301:ASP:HB3	2.21	0.55
1:C:143:THR:OG1	1:C:302:ARG:NH2	2.39	0.54
1:b:190:VAL:HG23	1:b:192:LYS:HG3	1.88	0.54
1:b:193:ARG:NH1	1:b:216:ARG:NH2	2.55	0.54
1:C:181:TYR:CE2	1:C:191:VAL:HG22	2.43	0.54
1:k:279:MET:HG3	1:k:285:LEU:HD13	1.89	0.54
1:C:261:SER:HA	1:C:268:ARG:H	1.72	0.54
1:a:254:TYR:C	1:a:255:ASN:HD22	2.14	0.54
1:j:194:CYS:CB	1:j:262:CYS:HB3	2.38	0.54
1:A:142:TRP:CE3	1:A:142:TRP:C	2.85	0.54
1:I:259:ASN:OD1	1:I:294:ILE:HG22	2.07	0.54
1:A:161:ILE:HG13	1:A:254:TYR:CD2	2.42	0.54
1:B:293:ARG:HH22	2:E:404:DT:P	2.31	0.54
1:a:209:ALA:CB	1:a:216:ARG:HD3	2.38	0.54
1:d:227:ASP:OD1	1:d:234:GLN:HG2	2.07	0.54
1:D:181:TYR:CE2	1:D:191:VAL:HG22	2.43	0.54
1:k:116:PRO:HG2	1:k:180:VAL:HG11	1.89	0.54
1:J:193:ARG:HD3	1:J:211:ALA:O	2.07	0.54
1:b:152:TYR:HB3	1:b:298:PRO:HB3	1.88	0.54
1:K:308:HIS:ND1	1:K:311:GLU:OE1	2.39	0.54
1:l:216:ARG:HB2	1:l:255:ASN:HB2	1.90	0.54
1:I:151:LEU:HD22	1:I:153:CYS:HB2	1.89	0.53
1:B:154:GLN:HB2	1:B:157:LYS:HG3	1.88	0.53
1:D:169:PRO:HB2	1:D:173:THR:HG21	1.90	0.53
1:L:138:LYS:HG3	1:L:300:ARG:HB2	1.90	0.53
1:a:193:ARG:HD3	1:a:211:ALA:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:129:VAL:HG12	1:d:163:ILE:HG22	1.90	0.53
1:A:131:PHE:CE2	1:A:151:LEU:HD13	2.43	0.53
1:A:130:THR:HG22	1:A:131:PHE:H	1.73	0.53
1:A:193:ARG:HH11	1:A:197:HIS:HB3	1.73	0.53
1:A:225:TYR:CD1	1:A:236:VAL:HG22	2.43	0.53
1:a:225:TYR:CD1	1:a:236:VAL:HG12	2.43	0.53
1:c:293:ARG:NH1	1:c:293:ARG:HG2	2.23	0.53
1:d:293:ARG:NH1	1:d:293:ARG:HG2	2.22	0.53
1:b:272:LEU:HD23	1:b:291:GLU:HA	1.90	0.53
1:i:223:SER:HB3	1:i:238:VAL:HG12	1.89	0.53
1:I:279:MET:HG2	1:I:285:LEU:HD11	1.90	0.53
1:d:125:HIS:CE1	1:d:169:PRO:HA	2.43	0.53
1:j:179:PRO:HB2	1:j:191:VAL:CG1	2.34	0.53
1:k:293:ARG:NH1	1:k:295:CYS:SG	2.81	0.53
1:D:192:LYS:HE2	1:D:234:GLN:NE2	2.24	0.53
1:J:209:ALA:HA	1:J:225:TYR:HE2	1.74	0.53
1:a:175:ILE:HD12	1:a:252:ILE:HD11	1.89	0.53
1:L:266:MET:HE3	1:L:271:ILE:CG2	2.39	0.53
1:c:138:LYS:HE3	1:c:300:ARG:HD3	1.91	0.53
1:A:218:GLU:HB3	1:A:253:LEU:HB3	1.91	0.53
1:J:121:TYR:O	1:J:286:GLY:HA2	2.09	0.52
1:J:244:GLN:NE2	1:K:113:GLU:HB3	2.25	0.52
1:L:266:MET:HE3	1:L:271:ILE:HG21	1.91	0.52
1:a:195:PRO:HB3	1:b:199:LEU:HD12	1.91	0.52
1:B:266:MET:CE	1:B:271:ILE:HG12	2.39	0.52
2:O:414:DC:H2''	2:O:415:DA:C8	2.45	0.52
1:I:193:ARG:HD2	1:I:213:HIS:O	2.09	0.52
1:K:131:PHE:CE2	1:K:161:ILE:HG12	2.45	0.52
1:k:125:HIS:ND1	1:k:167:THR:O	2.43	0.52
1:A:179:PRO:HG2	1:A:191:VAL:HB	1.92	0.52
1:J:163:ILE:CD1	1:J:175:ILE:CD1	2.87	0.52
1:J:210:PRO:HD3	1:J:225:TYR:HD2	1.74	0.52
1:a:158:THR:CA	1:a:255:ASN:HD21	2.07	0.52
1:b:179:PRO:HG2	1:b:191:VAL:HB	1.92	0.52
1:A:207:GLN:HG3	1:A:209:ALA:HB3	1.92	0.52
1:c:259:ASN:HA	1:c:294:ILE:HG22	1.90	0.52
1:A:266:MET:HE3	1:A:271:ILE:CG2	2.40	0.52
1:B:161:ILE:HG13	1:B:254:TYR:HD2	1.74	0.52
1:B:230:VAL:CG2	1:B:231:THR:H	2.07	0.52
1:a:155:ILE:CD1	1:a:257:MET:O	2.56	0.52
1:B:145:SER:HA	1:B:302:ARG:NH2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:295:CYS:SG	1:K:296:ALA:N	2.83	0.51
1:L:193:ARG:NH2	1:L:216:ARG:HH21	2.05	0.51
1:j:277:LEU:HD12	1:j:285:LEU:HB2	1.91	0.51
1:l:145:SER:O	1:l:149:LYS:N	2.43	0.51
2:g:511:DG:H1	2:h:512:DC:H42	1.58	0.51
1:I:137:ALA:HB3	1:I:140:ALA:HB2	1.91	0.51
1:J:190:VAL:HG13	1:J:233:ARG:HD3	1.92	0.51
1:J:260:SER:O	1:J:268:ARG:N	2.39	0.51
1:L:255:ASN:CB	1:L:257:MET:CE	2.83	0.51
1:a:215:ILE:O	1:a:236:VAL:HG11	2.11	0.51
1:c:184:ALA:HA	1:c:187:VAL:HG23	1.93	0.51
1:K:220:ASN:HB3	1:K:223:SER:HB3	1.92	0.51
1:d:178:MET:HB2	1:d:235:SER:HB3	1.92	0.51
1:i:150:LYS:HD3	1:i:152:TYR:CZ	2.45	0.51
1:B:193:ARG:CG	1:B:258:CYS:SG	2.97	0.51
1:K:142:TRP:CZ2	1:K:160:PRO:HG2	2.45	0.51
1:L:161:ILE:HD12	1:L:254:TYR:HD2	1.75	0.51
1:L:179:PRO:HG2	1:L:191:VAL:HB	1.91	0.51
1:b:274:ILE:HG22	1:b:276:THR:HG22	1.93	0.51
1:k:178:MET:CE	1:k:233:ARG:HD2	2.40	0.51
1:C:150:LYS:HD2	1:C:152:TYR:CZ	2.45	0.51
1:D:199:LEU:HD21	1:L:166:SER:HB2	1.93	0.51
1:B:193:ARG:HD3	1:B:257:MET:HB2	1.89	0.51
1:d:117:SER:OG	1:d:287:ARG:NH2	2.44	0.51
1:k:231:THR:HG22	1:k:233:ARG:H	1.75	0.51
1:l:126:HIS:O	1:l:165:VAL:HA	2.11	0.51
1:A:175:ILE:HD11	1:A:252:ILE:HG13	1.93	0.51
1:i:193:ARG:NE	1:i:257:MET:HB3	2.24	0.51
1:B:230:VAL:HG23	1:B:231:THR:HG23	1.92	0.51
1:J:184:ALA:HA	1:J:187:VAL:HG13	1.93	0.51
1:L:276:THR:HG22	1:L:278:GLU:HG2	1.93	0.51
1:b:125:HIS:ND1	1:b:167:THR:O	2.43	0.51
1:k:134:SER:HB3	1:k:142:TRP:CZ3	2.46	0.51
1:d:207:GLN:HG3	1:d:209:ALA:N	2.25	0.50
1:D:125:HIS:ND1	1:D:167:THR:O	2.39	0.50
1:J:192:LYS:HG2	1:J:193:ARG:O	2.12	0.50
1:b:308:HIS:O	1:b:308:HIS:ND1	2.41	0.50
1:k:193:ARG:NH1	1:k:197:HIS:HB3	2.25	0.50
1:C:240:TYR:CD1	1:C:240:TYR:C	2.88	0.50
1:D:115:ILE:HD12	1:D:187:VAL:HG23	1.92	0.50
1:c:153:CYS:SG	1:c:159:CYS:SG	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:163:ILE:O	1:k:163:ILE:HG13	2.11	0.50
2:f:414:DC:H2"	2:f:415:DA:C8	2.46	0.50
1:A:277:LEU:O	1:A:285:LEU:N	2.34	0.50
1:K:207:GLN:HG3	1:K:209:ALA:H	1.77	0.50
1:A:152:TYR:HB3	1:A:298:PRO:HB3	1.92	0.50
1:A:274:ILE:HG22	1:A:276:THR:HG23	1.94	0.50
1:A:296:ALA:C	1:A:298:PRO:HD3	2.36	0.50
1:a:209:ALA:HB1	1:a:216:ARG:HD3	1.93	0.50
1:b:164:LYS:HB2	1:b:249:PHE:HD2	1.77	0.50
1:K:261:SER:OG	2:O:417:DG:OP1	2.20	0.50
1:B:156:ALA:CB	1:B:257:MET:HE1	2.42	0.50
1:A:279:MET:CE	1:A:283:GLN:HB2	2.41	0.50
1:B:228:ASP:CB	1:B:231:THR:OG1	2.60	0.50
1:C:201:ARG:NH1	1:C:205:GLU:HB2	2.27	0.50
1:J:193:ARG:NH2	1:J:197:HIS:HB3	2.24	0.50
1:L:193:ARG:HD2	1:L:197:HIS:HB3	1.93	0.50
1:L:255:ASN:HB3	1:L:257:MET:HE2	1.89	0.50
1:i:193:ARG:HE	1:i:257:MET:HB3	1.76	0.50
2:N:398:DC:H2"	2:N:399:DA:C8	2.46	0.50
1:J:127:PHE:CD2	1:J:277:LEU:HD11	2.46	0.49
1:c:122:PRO:HG3	1:c:288:ARG:NH2	2.27	0.49
1:c:210:PRO:HB2	1:c:213:HIS:HD2	1.77	0.49
1:d:130:THR:N	1:d:162:GLN:O	2.35	0.49
1:C:223:SER:HB3	1:C:238:VAL:HG12	1.94	0.49
1:K:215:ILE:HG12	1:K:256:PHE:CE1	2.47	0.49
1:k:281:ASP:OD1	1:k:282:GLY:N	2.44	0.49
1:B:210:PRO:HG2	1:B:213:HIS:CE1	2.47	0.49
1:K:122:PRO:HG3	1:K:288:ARG:NH2	2.27	0.49
1:c:122:PRO:HG3	1:c:288:ARG:HH21	1.78	0.49
1:c:184:ALA:HA	1:c:187:VAL:CG2	2.42	0.49
1:j:240:TYR:CD2	1:j:241:GLU:N	2.80	0.49
1:C:147:LEU:HD23	1:C:306:GLU:HG2	1.94	0.49
1:L:176:ARG:HB2	1:L:237:VAL:HG22	1.94	0.49
1:c:120:ASP:HA	1:c:287:ARG:O	2.12	0.49
1:i:131:PHE:CE2	1:i:161:ILE:HD11	2.47	0.49
1:A:143:THR:OG1	1:A:302:ARG:NH2	2.44	0.49
2:o:420:DT:H2"	2:o:421:DG:C8	2.47	0.49
1:K:125:HIS:CE1	1:K:169:PRO:HA	2.47	0.49
1:c:226:VAL:O	1:c:234:GLN:HA	2.12	0.49
1:A:225:TYR:HD1	1:A:236:VAL:HG22	1.77	0.49
2:n:408:DT:H2"	2:n:409:DG:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:ILE:HG23	1:C:155:ILE:O	2.12	0.49
1:a:134:SER:HB2	1:a:143:THR:HA	1.95	0.49
1:K:209:ALA:HB2	1:K:225:TYR:CZ	2.48	0.49
1:a:124:PRO:HG2	1:a:125:HIS:HD2	1.77	0.49
1:d:193:ARG:NH2	1:d:197:HIS:O	2.46	0.49
1:l:131:PHE:CE1	1:l:151:LEU:HD13	2.47	0.49
1:B:163:ILE:HD12	1:B:252:ILE:HD12	1.94	0.49
1:K:193:ARG:HD3	1:K:211:ALA:O	2.12	0.49
1:c:129:VAL:HG23	1:c:288:ARG:HG3	1.94	0.49
1:K:142:TRP:CE3	1:K:142:TRP:C	2.91	0.48
1:c:150:LYS:HD2	1:c:152:TYR:CZ	2.48	0.48
1:j:238:VAL:HG21	1:j:252:ILE:HD13	1.94	0.48
1:k:178:MET:HE2	1:k:233:ARG:HD2	1.95	0.48
1:a:141:THR:HG23	1:a:157:LYS:HB3	1.94	0.48
1:d:184:ALA:O	1:d:187:VAL:HG12	2.13	0.48
1:I:145:SER:O	1:I:149:LYS:N	2.42	0.48
1:J:154:GLN:HA	1:J:295:CYS:O	2.13	0.48
1:K:127:PHE:CE1	1:K:277:LEU:HB2	2.48	0.48
1:c:259:ASN:HA	1:c:294:ILE:CG2	2.44	0.48
1:d:163:ILE:CD1	1:d:250:THR:HB	2.36	0.48
1:a:141:THR:CG2	1:a:157:LYS:HB3	2.43	0.48
1:d:125:HIS:HE1	1:d:168:PRO:O	1.95	0.48
1:i:259:ASN:HA	1:i:294:ILE:HB	1.95	0.48
1:k:216:ARG:NH1	1:k:257:MET:HE2	2.29	0.48
1:J:155:ILE:CD1	1:J:257:MET:O	2.60	0.48
1:L:259:ASN:HA	1:L:294:ILE:HG22	1.95	0.48
1:B:127:PHE:CD2	1:B:277:LEU:CB	2.97	0.48
1:i:279:MET:HE2	1:i:283:GLN:HG2	1.96	0.48
1:D:115:ILE:HD11	1:D:188:THR:HG22	1.95	0.48
1:I:209:ALA:HB2	1:I:225:TYR:CZ	2.49	0.48
2:h:522:DT:H2''	2:h:523:DG:C8	2.49	0.48
1:J:226:VAL:O	1:J:234:GLN:HA	2.13	0.48
1:L:150:LYS:HD3	1:L:152:TYR:OH	2.14	0.48
1:k:118:ASN:HA	1:k:274:ILE:HD12	1.96	0.48
1:D:207:GLN:OE1	1:D:208:SER:N	2.47	0.48
1:A:142:TRP:CE3	1:A:143:THR:CA	2.97	0.48
1:K:150:LYS:HD2	1:K:152:TYR:CZ	2.49	0.48
1:l:287:ARG:NH1	4:l:501:HOH:O	2.30	0.48
1:B:228:ASP:OD1	1:B:230:VAL:HG22	2.14	0.47
1:D:276:THR:HG22	1:D:278:GLU:HG2	1.95	0.47
1:K:276:THR:HG22	1:K:287:ARG:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:145:SER:HA	1:b:302:ARG:NH2	2.23	0.47
1:b:153:CYS:O	1:b:294:ILE:HA	2.14	0.47
1:B:266:MET:HE3	1:B:271:ILE:HG12	1.97	0.47
1:k:266:MET:CE	1:k:271:ILE:HD13	2.44	0.47
1:D:190:VAL:HG22	1:D:233:ARG:HD3	1.97	0.47
1:L:218:GLU:HB2	1:L:255:ASN:ND2	2.29	0.47
1:b:193:ARG:NH1	1:b:216:ARG:HH21	2.12	0.47
1:j:240:TYR:CG	1:j:241:GLU:N	2.82	0.47
1:j:271:ILE:HD12	1:j:273:ILE:HD11	1.97	0.47
1:k:228:ASP:CG	1:k:231:THR:HB	2.39	0.47
1:l:182:LYS:HG3	1:l:272:LEU:HD13	1.95	0.47
1:D:170:PRO:HB2	1:D:279:MET:SD	2.55	0.47
1:J:176:ARG:O	1:J:276:THR:N	2.36	0.47
1:a:181:TYR:CE2	1:a:191:VAL:HG22	2.49	0.47
1:b:153:CYS:SG	1:b:256:PHE:CD2	3.08	0.47
1:i:164:LYS:HB2	1:i:249:PHE:HD1	1.79	0.47
1:j:152:TYR:HB3	1:j:298:PRO:HB3	1.96	0.47
1:l:184:ALA:C	1:l:186:HIS:H	2.22	0.47
1:D:213:HIS:CD2	1:D:234:GLN:HB3	2.49	0.47
1:I:125:HIS:HE1	1:I:169:PRO:HA	1.71	0.47
1:I:134:SER:OG	1:I:142:TRP:O	2.24	0.47
2:g:504:DC:H2"	2:g:505:DA:C8	2.49	0.47
1:D:207:GLN:HG3	1:D:209:ALA:N	2.29	0.47
1:J:238:VAL:HG22	1:J:239:PRO:HD2	1.96	0.47
1:J:278:GLU:HG2	1:J:279:MET:O	2.15	0.47
1:K:150:LYS:HG3	1:K:291:GLU:HB3	1.96	0.47
1:d:119:THR:HB	1:d:287:ARG:HH22	1.80	0.47
1:d:217:VAL:HG22	1:d:254:TYR:CE1	2.50	0.47
1:d:244:GLN:O	1:d:247:THR:HG23	2.15	0.47
1:k:131:PHE:CE2	1:k:161:ILE:HD13	2.50	0.47
1:k:150:LYS:HG3	1:k:291:GLU:HB3	1.97	0.47
1:d:163:ILE:C	1:d:163:ILE:CD1	2.85	0.47
1:i:153:CYS:SG	1:i:256:PHE:CD2	3.08	0.47
1:k:108:HIS:ND1	1:k:283:GLN:HG3	2.30	0.47
1:I:148:LEU:HD11	1:I:305:ASP:HB3	1.96	0.47
1:I:263:VAL:O	1:J:196:ASN:ND2	2.48	0.47
1:A:130:THR:HG22	1:A:131:PHE:N	2.30	0.47
1:a:201:ARG:HA	1:a:204:ASN:HB2	1.96	0.47
1:d:125:HIS:CE1	1:d:167:THR:OG1	2.67	0.47
1:C:260:SER:HA	1:C:266:MET:HE2	1.97	0.46
1:I:124:PRO:HB2	1:I:125:HIS:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:188:THR:HG21	1:d:218:GLU:HG2	1.97	0.46
1:B:279:MET:HE2	1:B:279:MET:HB3	1.68	0.46
1:J:116:PRO:HG2	1:J:180:VAL:HG21	1.98	0.46
1:L:244:GLN:HB2	1:L:247:THR:OG1	2.16	0.46
1:d:144:TYR:OH	1:d:149:LYS:HA	2.14	0.46
2:N:402:DC:H2"	2:N:403:DA:C8	2.51	0.46
1:C:147:LEU:HD21	1:C:309:TYR:CD2	2.51	0.46
1:I:279:MET:HB2	1:I:281:ASP:OD1	2.15	0.46
1:d:193:ARG:HG2	1:d:258:CYS:SG	2.56	0.46
1:i:272:LEU:HD23	1:i:291:GLU:HA	1.96	0.46
1:i:279:MET:HB2	1:i:281:ASP:OD1	2.15	0.46
1:j:274:ILE:CD1	1:j:287:ARG:HG3	2.42	0.46
1:k:163:ILE:HD13	1:k:175:ILE:CD1	2.46	0.46
1:J:244:GLN:HE21	1:K:113:GLU:HB3	1.80	0.46
1:a:125:HIS:CE1	1:a:169:PRO:HA	2.51	0.46
1:i:190:VAL:HG13	1:i:192:LYS:HD2	1.96	0.46
1:j:125:HIS:HB3	1:j:165:VAL:HG13	1.98	0.46
1:k:176:ARG:HE	1:k:278:GLU:CD	2.23	0.46
1:l:213:HIS:HA	1:l:234:GLN:NE2	2.31	0.46
1:A:147:LEU:HG	1:A:148:LEU:HD12	1.98	0.46
1:A:207:GLN:HG3	1:A:209:ALA:H	1.80	0.46
1:J:138:LYS:HG3	1:J:300:ARG:HB2	1.97	0.46
1:i:244:GLN:O	1:i:247:THR:OG1	2.31	0.46
1:a:184:ALA:O	1:a:187:VAL:HG12	2.16	0.46
1:D:207:GLN:HG3	1:D:209:ALA:H	1.81	0.46
1:i:254:TYR:O	1:i:255:ASN:ND2	2.48	0.46
1:l:152:TYR:CZ	1:l:302:ARG:HA	2.51	0.46
2:f:411:DA:H2"	2:f:412:DG:C8	2.51	0.46
1:I:213:HIS:ND1	1:I:234:GLN:OE1	2.49	0.46
1:d:125:HIS:ND1	1:d:167:THR:O	2.40	0.46
1:C:158:THR:HG23	1:C:218:GLU:OE1	2.16	0.45
1:D:173:THR:HG21	1:D:285:LEU:HD12	1.98	0.45
1:l:190:VAL:HG13	1:l:233:ARG:HD3	1.97	0.45
2:P:402:DC:H2"	2:P:403:DA:C8	2.51	0.45
1:C:202:ASP:HB3	1:C:203:PHE:CD2	2.52	0.45
1:k:175:ILE:HD12	1:k:252:ILE:HD11	1.99	0.45
1:l:266:MET:SD	1:l:271:ILE:HD13	2.56	0.45
1:I:218:GLU:HB2	1:I:255:ASN:ND2	2.32	0.45
1:L:153:CYS:SG	1:L:159:CYS:HB2	2.56	0.45
1:j:272:LEU:HD12	1:j:291:GLU:HA	1.97	0.45
1:D:260:SER:OG	1:D:294:ILE:N	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:205:GLU:H	1:J:205:GLU:HG2	1.52	0.45
1:L:261:SER:O	1:L:262:CYS:C	2.59	0.45
1:a:254:TYR:O	1:a:255:ASN:ND2	2.36	0.45
1:a:273:ILE:CD1	1:a:292:GLY:HA3	2.47	0.45
1:c:132:GLN:O	1:c:142:TRP:HH2	1.99	0.45
1:j:152:TYR:CE2	1:j:302:ARG:HA	2.52	0.45
1:J:121:TYR:O	1:J:121:TYR:CG	2.69	0.45
1:K:215:ILE:HG12	1:K:256:PHE:HE1	1.81	0.45
1:j:131:PHE:CE2	1:j:151:LEU:HD13	2.52	0.45
1:A:182:LYS:HG3	1:A:272:LEU:HD21	1.99	0.45
1:B:150:LYS:NZ	1:B:305:ASP:OD2	2.39	0.45
1:B:278:GLU:CA	1:B:285:LEU:HD13	2.46	0.45
1:K:273:ILE:HG22	1:K:275:ILE:HD11	1.98	0.45
1:j:128:GLU:HA	1:j:288:ARG:HE	1.82	0.45
1:B:193:ARG:CD	1:B:257:MET:HB3	2.30	0.45
1:K:142:TRP:CE3	1:K:142:TRP:O	2.70	0.45
1:c:153:CYS:SG	1:c:154:GLN:N	2.89	0.45
1:c:207:GLN:HG3	1:c:209:ALA:H	1.81	0.45
1:i:273:ILE:HB	1:i:290:PHE:CE1	2.52	0.45
2:e:407:DC:C6	2:e:408:DT:H72	2.52	0.45
1:C:147:LEU:HD11	1:C:309:TYR:CE2	2.52	0.45
1:I:256:PHE:HB3	1:I:294:ILE:HG12	1.98	0.45
1:a:209:ALA:CB	1:a:225:TYR:HE2	2.30	0.45
1:a:284:VAL:CG2	1:d:245:VAL:CG1	2.51	0.45
1:b:184:ALA:HA	1:b:187:VAL:CG1	2.46	0.45
1:c:256:PHE:CE1	1:c:273:ILE:HD13	2.51	0.45
1:k:181:TYR:CE2	1:k:191:VAL:HG22	2.52	0.45
2:o:414:DC:H2"	2:o:415:DA:C8	2.52	0.45
1:A:178:MET:HE2	1:A:178:MET:HB3	1.82	0.45
1:B:118:ASN:OD1	1:B:118:ASN:N	2.49	0.45
1:c:112:HIS:CG	1:c:230:VAL:HG11	2.51	0.45
1:A:204:ASN:HD22	1:A:211:ALA:HB2	1.73	0.44
1:I:124:PRO:HB2	1:I:125:HIS:CD2	2.53	0.44
1:k:178:MET:HE3	1:k:233:ARG:CB	2.45	0.44
1:c:193:ARG:HD3	1:c:211:ALA:O	2.17	0.44
1:A:142:TRP:HE3	1:A:143:THR:N	2.15	0.44
1:A:279:MET:HE1	1:A:283:GLN:OE1	2.18	0.44
1:I:164:LYS:HE3	1:I:248:GLU:HG3	1.98	0.44
1:a:213:HIS:NE2	1:a:227:ASP:OD1	2.51	0.44
1:c:114:PHE:CE1	1:c:231:THR:HA	2.52	0.44
1:d:125:HIS:ND1	1:d:167:THR:OG1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:195:PRO:HD2	1:J:264:GLY:HA3	2.00	0.44
1:a:132:GLN:HB3	1:a:162:GLN:NE2	2.32	0.44
2:h:521:DC:C2'	2:h:522:DT:H71	2.47	0.44
1:A:130:THR:O	1:A:162:GLN:HB2	2.16	0.44
1:d:279:MET:HE3	1:d:280:ARG:H	1.82	0.44
1:j:194:CYS:N	1:j:258:CYS:SG	2.86	0.44
1:B:130:THR:HG22	1:B:131:PHE:N	2.30	0.44
1:B:161:ILE:HG13	1:B:254:TYR:CD2	2.50	0.44
1:k:143:THR:OG1	1:k:302:ARG:NH2	2.51	0.44
1:A:279:MET:HE2	1:A:283:GLN:HB2	1.99	0.44
1:J:279:MET:HE3	1:J:285:LEU:HD11	1.99	0.44
1:L:125:HIS:ND1	1:L:167:THR:HB	2.33	0.44
1:i:184:ALA:HA	1:i:187:VAL:HG23	1.99	0.44
2:E:402:DC:H2''	2:E:403:DA:C8	2.53	0.44
1:A:158:THR:HA	1:A:255:ASN:HD21	1.83	0.44
1:B:272:LEU:HD23	1:B:291:GLU:HA	2.00	0.44
1:J:179:PRO:HD3	1:J:215:ILE:HD12	1.99	0.44
1:a:213:HIS:HA	1:a:234:GLN:NE2	2.33	0.44
1:A:142:TRP:C	1:A:142:TRP:CD2	2.96	0.43
1:B:118:ASN:HB3	1:B:274:ILE:HD11	1.98	0.43
1:I:151:LEU:CD2	1:I:153:CYS:HB2	2.48	0.43
1:L:223:SER:HB3	1:L:238:VAL:HG12	1.99	0.43
1:a:158:THR:HG22	1:a:218:GLU:OE1	2.17	0.43
1:a:168:PRO:HA	1:a:169:PRO:HD3	1.83	0.43
1:a:222:LEU:HD13	1:a:239:PRO:HG3	1.98	0.43
2:M:420:DT:H2''	2:M:421:DG:N7	2.33	0.43
1:B:193:ARG:HG3	1:B:213:HIS:O	2.18	0.43
1:j:240:TYR:O	1:j:241:GLU:HG3	2.18	0.43
1:k:224:GLN:HB3	1:k:237:VAL:CG1	2.47	0.43
1:l:200:GLY:O	1:l:204:ASN:ND2	2.46	0.43
1:A:127:PHE:CZ	1:A:163:ILE:HD12	2.53	0.43
1:L:124:PRO:HG2	1:L:125:HIS:CD2	2.53	0.43
1:i:215:ILE:O	1:i:236:VAL:HG21	2.18	0.43
1:j:225:TYR:CD2	1:j:236:VAL:HG12	2.53	0.43
1:A:190:VAL:HG23	4:A:504:HOH:O	2.19	0.43
1:A:213:HIS:NE2	1:A:234:GLN:HB3	2.34	0.43
1:I:274:ILE:HG22	1:I:276:THR:HG23	2.00	0.43
1:a:155:ILE:HG13	1:a:257:MET:O	2.18	0.43
1:b:178:MET:CE	1:b:233:ARG:CB	2.89	0.43
1:C:125:HIS:CE1	1:C:169:PRO:HA	2.52	0.43
1:J:154:GLN:OE1	1:J:157:LYS:HE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:278:GLU:HG3	1:J:283:GLN:O	2.18	0.43
1:J:293:ARG:NH1	1:J:301:ASP:HB3	2.34	0.43
1:d:116:PRO:HG3	1:d:178:MET:SD	2.58	0.43
1:i:205:GLU:O	1:i:205:GLU:HG2	2.19	0.43
1:j:152:TYR:CZ	1:j:302:ARG:HA	2.54	0.43
1:j:304:ALA:O	1:j:308:HIS:ND1	2.52	0.43
1:k:184:ALA:O	1:k:187:VAL:HG12	2.19	0.43
2:M:414:DC:H2"	2:M:415:DA:C8	2.53	0.43
1:J:121:TYR:H	1:J:287:ARG:HB3	1.84	0.43
1:J:295:CYS:HB2	4:J:501:HOH:O	2.18	0.43
1:K:259:ASN:HA	1:K:294:ILE:HB	2.00	0.43
1:k:134:SER:HB3	1:k:142:TRP:CH2	2.54	0.43
1:k:182:LYS:HG3	1:k:272:LEU:HD21	2.00	0.43
1:c:209:ALA:HB2	1:c:225:TYR:CZ	2.54	0.43
1:i:193:ARG:HD3	1:i:211:ALA:O	2.19	0.43
1:j:278:GLU:HB2	1:j:283:GLN:O	2.18	0.43
1:I:179:PRO:HD3	1:I:215:ILE:CD1	2.49	0.43
1:I:196:ASN:N	1:J:196:ASN:OD1	2.51	0.43
1:L:262:CYS:O	1:L:267:ASN:N	2.48	0.43
1:b:154:GLN:HB2	1:b:157:LYS:HG3	2.01	0.43
1:c:138:LYS:HE3	1:c:300:ARG:HB2	2.01	0.43
1:c:168:PRO:HA	1:c:169:PRO:HD3	1.87	0.43
1:j:138:LYS:NZ	2:n:400:DG:N7	2.66	0.43
1:j:176:ARG:HG3	1:j:235:SER:OG	2.18	0.43
1:I:119:THR:HG21	1:L:245:VAL:H	1.84	0.43
1:J:277:LEU:HD12	1:J:277:LEU:H	1.84	0.43
1:l:181:TYR:CE2	1:l:191:VAL:HG22	2.53	0.43
1:a:209:ALA:HA	1:a:225:TYR:CE2	2.53	0.43
1:c:162:GLN:HB3	1:c:249:PHE:HB3	2.01	0.43
1:c:172:GLY:HA3	1:c:280:ARG:NE	2.34	0.43
1:d:152:TYR:HB3	1:d:298:PRO:HB3	2.01	0.43
1:l:164:LYS:HB2	1:l:249:PHE:CD1	2.53	0.43
1:A:222:LEU:HD13	1:A:239:PRO:HG3	1.99	0.42
1:D:193:ARG:HG3	1:D:212:SER:O	2.19	0.42
1:J:184:ALA:O	1:J:187:VAL:HG22	2.18	0.42
1:L:218:GLU:HB2	1:L:255:ASN:HD21	1.84	0.42
1:a:152:TYR:CZ	1:a:302:ARG:HA	2.54	0.42
1:a:164:LYS:HD3	1:a:249:PHE:CE1	2.53	0.42
1:i:131:PHE:CE2	1:i:151:LEU:HD13	2.53	0.42
1:K:152:TYR:CZ	1:K:302:ARG:HA	2.54	0.42
2:n:402:DC:H2"	2:n:403:DA:H8	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:ARG:HH22	2:G:506:DT:H5'	1.81	0.42
1:b:143:THR:HG22	1:b:152:TYR:HB2	2.00	0.42
1:c:129:VAL:HG22	1:c:163:ILE:CD1	2.48	0.42
1:B:178:MET:O	1:B:273:ILE:HD12	2.19	0.42
1:B:193:ARG:HD2	1:B:258:CYS:SG	2.60	0.42
1:B:231:THR:C	1:B:233:ARG:H	2.27	0.42
1:C:122:PRO:HG3	1:C:288:ARG:NH2	2.33	0.42
1:c:128:GLU:OE2	1:c:164:LYS:NZ	2.52	0.42
1:d:205:GLU:O	1:d:205:GLU:HG3	2.19	0.42
1:d:287:ARG:CB	1:d:287:ARG:HH11	2.32	0.42
1:i:124:PRO:HG2	1:i:125:HIS:CD2	2.55	0.42
1:i:130:THR:HG23	1:i:162:GLN:HB2	1.99	0.42
1:B:228:ASP:OD1	1:B:230:VAL:CG2	2.68	0.42
1:D:254:TYR:C	1:D:255:ASN:HD22	2.28	0.42
1:d:193:ARG:NH2	1:d:197:HIS:HB3	2.33	0.42
2:G:510:DT:H2''	2:G:511:DG:C8	2.54	0.42
1:A:142:TRP:HE3	1:A:143:THR:CA	2.33	0.42
1:B:124:PRO:HG2	1:B:125:HIS:CD2	2.54	0.42
1:B:285:LEU:N	1:B:285:LEU:CD1	2.73	0.42
1:C:227:ASP:OD1	1:C:234:GLN:HG2	2.18	0.42
1:J:120:ASP:HB2	1:J:288:ARG:HD3	2.01	0.42
1:K:217:VAL:HG23	1:K:236:VAL:HG21	2.01	0.42
1:c:294:ILE:HD12	1:c:294:ILE:HG23	1.84	0.42
1:i:161:ILE:HD13	1:i:161:ILE:HA	1.64	0.42
1:d:145:SER:HB2	1:d:302:ARG:HG3	2.02	0.42
1:d:175:ILE:O	1:d:237:VAL:HA	2.20	0.42
1:i:161:ILE:HG23	1:i:161:ILE:HD12	1.74	0.42
1:l:216:ARG:NH1	1:l:257:MET:HE2	2.34	0.42
1:B:163:ILE:HD12	1:B:252:ILE:CD1	2.50	0.42
1:d:122:PRO:HG3	1:d:288:ARG:NH1	2.34	0.42
1:i:173:THR:HG21	1:i:277:LEU:HD11	2.02	0.42
1:j:217:VAL:HG22	1:j:254:TYR:CE1	2.54	0.42
1:j:276:THR:HG22	1:j:287:ARG:HB2	2.02	0.42
1:k:144:TYR:O	1:k:302:ARG:NH2	2.53	0.42
1:I:196:ASN:OD1	1:J:264:GLY:HA3	2.19	0.42
1:K:137:ALA:HB3	1:K:140:ALA:HB2	2.01	0.42
1:L:128:GLU:HB2	1:L:164:LYS:HB3	2.00	0.42
1:L:149:LYS:HB3	1:L:149:LYS:HE2	1.82	0.42
1:d:179:PRO:HG2	1:d:191:VAL:CG1	2.50	0.42
2:n:402:DC:H2''	2:n:403:DA:C8	2.54	0.42
1:C:181:TYR:CZ	1:C:191:VAL:HG22	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:SER:HG	1:C:294:ILE:H	1.63	0.42
1:J:127:PHE:HE1	1:J:163:ILE:HG23	1.84	0.42
1:b:231:THR:CG2	1:b:233:ARG:HG2	2.50	0.42
1:d:150:LYS:HD3	1:d:152:TYR:OH	2.20	0.42
1:i:303:LYS:HE2	1:i:307:ASP:OD2	2.19	0.42
1:l:217:VAL:HG11	1:l:238:VAL:HG11	2.02	0.42
1:a:117:SER:OG	1:d:247:THR:HG22	2.20	0.41
1:c:223:SER:HB3	1:c:238:VAL:CG1	2.48	0.41
1:l:148:LEU:HD23	1:l:148:LEU:HA	1.80	0.41
1:B:145:SER:HA	1:B:302:ARG:HH21	1.86	0.41
1:B:280:ARG:HH12	1:I:303:LYS:HE2	1.84	0.41
1:D:215:ILE:HG12	1:D:256:PHE:CE1	2.56	0.41
1:b:231:THR:HG22	1:b:233:ARG:HG2	2.02	0.41
1:j:169:PRO:HB2	1:j:170:PRO:HD2	2.02	0.41
1:K:257:MET:HE3	1:K:257:MET:HB3	1.91	0.41
1:a:157:LYS:O	1:a:255:ASN:ND2	2.52	0.41
1:i:145:SER:O	1:i:149:LYS:N	2.53	0.41
1:B:127:PHE:CD2	1:B:277:LEU:HB3	2.55	0.41
1:b:115:ILE:HD12	1:b:187:VAL:HG13	2.02	0.41
1:b:197:HIS:HE1	1:b:262:CYS:SG	2.42	0.41
1:B:148:LEU:HD23	1:B:148:LEU:HA	1.79	0.41
1:I:127:PHE:CE1	1:I:163:ILE:HG23	2.55	0.41
1:a:150:LYS:HG3	1:a:291:GLU:HB3	2.02	0.41
1:b:161:ILE:HG13	1:b:254:TYR:HD2	1.84	0.41
1:k:304:ALA:O	1:k:308:HIS:HB2	2.20	0.41
1:B:145:SER:HB2	1:B:302:ARG:HE	1.85	0.41
1:C:173:THR:HA	1:C:279:MET:HA	2.02	0.41
1:I:150:LYS:HE3	1:I:291:GLU:OE1	2.20	0.41
1:I:256:PHE:CB	1:I:294:ILE:HG12	2.51	0.41
1:I:266:MET:HE3	1:I:271:ILE:HG12	2.03	0.41
1:J:216:ARG:HB2	1:J:255:ASN:HB2	2.01	0.41
1:j:222:LEU:HD23	1:j:222:LEU:HA	1.76	0.41
1:l:164:LYS:HB2	1:l:249:PHE:HD1	1.85	0.41
1:C:161:ILE:HG13	1:C:254:TYR:HD2	1.86	0.41
1:I:151:LEU:HD11	1:I:159:CYS:SG	2.60	0.41
1:i:209:ALA:HB2	1:i:225:TYR:CZ	2.56	0.41
1:A:145:SER:OG	1:A:306:GLU:OE2	2.34	0.41
1:A:153:CYS:HB2	1:A:159:CYS:SG	2.61	0.41
1:B:193:ARG:NH1	1:B:257:MET:HB3	2.35	0.41
1:B:215:ILE:CD1	1:B:273:ILE:HD13	2.51	0.41
1:b:193:ARG:HH12	1:b:216:ARG:NH2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:243:PRO:HB3	1:i:249:PHE:O	2.21	0.41
1:j:244:GLN:NE2	1:k:113:GLU:HB3	2.36	0.41
1:A:152:TYR:CE2	1:A:293:ARG:HD3	2.56	0.41
1:C:266:MET:HE3	1:C:271:ILE:CG2	2.51	0.41
1:D:276:THR:HG22	1:D:278:GLU:CG	2.50	0.41
1:I:140:ALA:O	1:I:141:THR:C	2.64	0.41
1:J:165:VAL:HG12	1:J:167:THR:H	1.86	0.41
1:L:131:PHE:CE1	1:L:151:LEU:HD13	2.56	0.41
1:a:178:MET:HG3	1:a:235:SER:HB3	2.03	0.41
1:i:137:ALA:HB3	1:i:140:ALA:HB2	2.02	0.41
1:i:193:ARG:HD2	1:i:213:HIS:O	2.21	0.41
2:f:413:DG:H2''	2:f:414:DC:C6	2.55	0.41
1:A:225:TYR:CE1	1:A:236:VAL:HG13	2.56	0.41
1:I:263:VAL:HG12	1:I:267:ASN:ND2	2.36	0.41
1:J:127:PHE:CE1	1:J:163:ILE:HG23	2.56	0.41
1:L:262:CYS:O	1:L:267:ASN:HA	2.21	0.41
1:I:155:ILE:HG13	1:I:257:MET:O	2.20	0.40
1:b:149:LYS:HB2	1:b:149:LYS:HE2	1.71	0.40
1:b:176:ARG:HH11	1:b:176:ARG:HD2	1.73	0.40
1:i:180:VAL:HG12	1:i:181:TYR:O	2.21	0.40
1:k:266:MET:HE1	1:k:271:ILE:HD13	2.03	0.40
1:l:112:HIS:CE1	1:l:114:PHE:HB2	2.56	0.40
1:l:125:HIS:O	1:l:126:HIS:C	2.62	0.40
2:f:411:DA:H2''	2:f:412:DG:H8	1.86	0.40
1:C:150:LYS:HG3	1:C:291:GLU:HG2	2.03	0.40
1:c:199:LEU:HD11	1:d:199:LEU:CD2	2.52	0.40
1:d:125:HIS:HE1	1:d:168:PRO:C	2.28	0.40
1:j:127:PHE:HE1	1:j:163:ILE:HD13	1.86	0.40
1:k:279:MET:HG3	1:k:285:LEU:CD1	2.50	0.40
1:l:176:ARG:NH1	1:l:278:GLU:OE2	2.55	0.40
1:J:217:VAL:HG22	1:J:254:TYR:CE1	2.57	0.40
1:K:154:GLN:HB2	1:K:157:LYS:HG3	2.02	0.40
1:L:127:PHE:CD1	1:L:277:LEU:HD22	2.57	0.40
1:i:184:ALA:HA	1:i:187:VAL:CG2	2.51	0.40
1:i:193:ARG:NE	1:i:257:MET:CB	2.85	0.40
1:k:136:THR:HG22	1:k:136:THR:O	2.20	0.40
1:k:279:MET:HE2	1:k:279:MET:HB3	2.01	0.40
1:A:172:GLY:HA3	1:A:280:ARG:HE	1.87	0.40
1:B:179:PRO:HG2	1:B:191:VAL:HB	2.03	0.40
1:b:193:ARG:NE	1:b:257:MET:HB3	2.36	0.40
1:d:131:PHE:CE1	1:d:144:TYR:CE2	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:129:VAL:HG22	1:l:163:ILE:CD1	2.51	0.40
1:A:142:TRP:CE3	1:A:143:THR:N	2.89	0.40
1:B:147:LEU:HD12	1:B:306:GLU:HG2	2.04	0.40
1:B:196:ASN:HD22	1:B:196:ASN:HA	1.75	0.40
1:I:309:TYR:CD1	1:I:309:TYR:C	3.00	0.40
1:J:163:ILE:CG2	1:J:164:LYS:N	2.84	0.40
1:J:225:TYR:HD1	1:J:225:TYR:HA	1.76	0.40
1:a:132:GLN:O	1:a:142:TRP:HH2	2.05	0.40
1:d:274:ILE:HG12	1:d:289:SER:HB3	2.04	0.40
1:j:193:ARG:NE	1:j:197:HIS:HB3	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	200/210 (95%)	189 (94%)	11 (6%)	0	100	100
1	B	199/210 (95%)	186 (94%)	12 (6%)	1 (0%)	24	54
1	C	199/210 (95%)	190 (96%)	9 (4%)	0	100	100
1	D	197/210 (94%)	188 (95%)	9 (5%)	0	100	100
1	I	197/210 (94%)	184 (93%)	13 (7%)	0	100	100
1	J	195/210 (93%)	188 (96%)	6 (3%)	1 (0%)	24	54
1	K	199/210 (95%)	195 (98%)	4 (2%)	0	100	100
1	L	198/210 (94%)	186 (94%)	12 (6%)	0	100	100
1	a	197/210 (94%)	193 (98%)	4 (2%)	0	100	100
1	b	197/210 (94%)	188 (95%)	8 (4%)	1 (0%)	24	54
1	c	198/210 (94%)	194 (98%)	4 (2%)	0	100	100
1	d	196/210 (93%)	188 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	i	199/210 (95%)	192 (96%)	7 (4%)	0	100	100
1	j	194/210 (92%)	182 (94%)	12 (6%)	0	100	100
1	k	204/210 (97%)	200 (98%)	4 (2%)	0	100	100
1	l	198/210 (94%)	185 (93%)	13 (7%)	0	100	100
All	All	3167/3360 (94%)	3028 (96%)	136 (4%)	3 (0%)	48	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	124	PRO
1	b	179	PRO
1	B	232	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	178/186 (96%)	175 (98%)	3 (2%)	53	82
1	B	177/186 (95%)	174 (98%)	3 (2%)	53	82
1	C	178/186 (96%)	177 (99%)	1 (1%)	78	93
1	D	174/186 (94%)	174 (100%)	0	100	100
1	I	174/186 (94%)	174 (100%)	0	100	100
1	J	173/186 (93%)	172 (99%)	1 (1%)	78	93
1	K	178/186 (96%)	175 (98%)	3 (2%)	53	82
1	L	177/186 (95%)	176 (99%)	1 (1%)	78	93
1	a	176/186 (95%)	174 (99%)	2 (1%)	65	88
1	b	175/186 (94%)	171 (98%)	4 (2%)	44	76
1	c	177/186 (95%)	177 (100%)	0	100	100
1	d	174/186 (94%)	172 (99%)	2 (1%)	65	88
1	i	176/186 (95%)	175 (99%)	1 (1%)	78	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	j	172/186 (92%)	169 (98%)	3 (2%)	53	82
1	k	181/186 (97%)	180 (99%)	1 (1%)	78	93
1	l	177/186 (95%)	175 (99%)	2 (1%)	65	88
All	All	2817/2976 (95%)	2790 (99%)	27 (1%)	68	89

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	TRP
1	A	196	ASN
1	A	255	ASN
1	B	196	ASN
1	B	257	MET
1	B	312	GLN
1	C	161	ILE
1	J	310	ARG
1	K	141	THR
1	K	157	LYS
1	K	164	LYS
1	L	193	ARG
1	a	241	GLU
1	a	279	MET
1	b	119	THR
1	b	226	VAL
1	b	250	THR
1	b	276	THR
1	d	247	THR
1	d	248	GLU
1	i	205	GLU
1	j	175	ILE
1	j	186	HIS
1	j	266	MET
1	k	258	CYS
1	l	176	ARG
1	l	272	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	HIS

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Mol	Chain	Res	Type
1	A	196	ASN
1	A	207	GLN
1	A	255	ASN
1	B	154	GLN
1	B	196	ASN
1	B	224	GLN
1	B	244	GLN
1	C	126	HIS
1	C	207	GLN
1	C	224	GLN
1	C	255	ASN
1	C	267	ASN
1	D	186	HIS
1	D	255	ASN
1	I	125	HIS
1	I	255	ASN
1	I	267	ASN
1	J	132	GLN
1	J	224	GLN
1	J	267	ASN
1	K	112	HIS
1	K	234	GLN
1	K	259	ASN
1	L	132	GLN
1	L	133	GLN
1	L	162	GLN
1	L	207	GLN
1	L	213	HIS
1	L	234	GLN
1	a	255	ASN
1	a	283	GLN
1	b	162	GLN
1	b	186	HIS
1	b	213	HIS
1	b	221	ASN
1	b	259	ASN
1	i	207	GLN
1	i	234	GLN
1	i	267	ASN
1	i	283	GLN
1	j	162	GLN
1	j	259	ASN

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Mol	Chain	Res	Type
1	k	111	HIS
1	k	162	GLN
1	k	224	GLN
1	l	112	HIS
1	l	162	GLN
1	l	213	HIS
1	l	224	GLN
1	l	234	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	202/210 (96%)	0.07	1 (0%) 87 83	54, 86, 126, 174	0
1	B	201/210 (95%)	0.04	2 (0%) 79 73	53, 84, 120, 150	0
1	C	201/210 (95%)	-0.16	1 (0%) 87 83	53, 76, 109, 155	0
1	D	199/210 (94%)	-0.06	1 (0%) 87 83	57, 80, 120, 201	0
1	I	199/210 (94%)	-0.07	1 (0%) 87 83	56, 76, 120, 144	0
1	J	197/210 (93%)	0.42	10 (5%) 33 26	63, 105, 167, 196	0
1	K	201/210 (95%)	0.72	19 (9%) 14 11	80, 110, 151, 210	0
1	L	200/210 (95%)	-0.19	0 100 100	45, 63, 94, 120	0
1	a	199/210 (94%)	0.27	3 (1%) 72 64	61, 95, 141, 163	0
1	b	199/210 (94%)	0.09	1 (0%) 87 83	59, 92, 131, 169	0
1	c	200/210 (95%)	0.03	1 (0%) 87 83	58, 81, 119, 144	0
1	d	198/210 (94%)	0.16	3 (1%) 72 64	68, 93, 133, 157	0
1	i	201/210 (95%)	0.04	3 (1%) 72 64	56, 78, 119, 150	0
1	j	196/210 (93%)	0.30	11 (5%) 30 23	62, 93, 143, 179	0
1	k	206/210 (98%)	-0.20	0 100 100	52, 72, 123, 170	0
1	l	200/210 (95%)	-0.00	2 (1%) 79 73	49, 71, 98, 128	0
2	E	11/12 (91%)	0.58	1 (9%) 15 12	81, 92, 103, 117	0
2	F	11/12 (91%)	0.12	0 100 100	72, 94, 115, 119	0
2	G	12/12 (100%)	0.27	0 100 100	78, 97, 120, 121	0
2	H	12/12 (100%)	0.09	0 100 100	72, 101, 113, 120	0
2	M	12/12 (100%)	0.17	0 100 100	70, 95, 109, 110	0
2	N	12/12 (100%)	0.25	0 100 100	77, 95, 112, 119	0
2	O	12/12 (100%)	0.65	1 (8%) 17 14	93, 113, 165, 165	0
2	P	12/12 (100%)	0.60	0 100 100	87, 101, 171, 178	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	e	11/12 (91%)	0.19	0 100 100	81, 96, 113, 148	0
2	f	11/12 (91%)	0.32	0 100 100	79, 103, 124, 129	0
2	g	12/12 (100%)	0.47	0 100 100	87, 107, 148, 152	0
2	h	12/12 (100%)	0.87	1 (8%) 17 14	44, 88, 143, 156	0
2	m	12/12 (100%)	0.38	0 100 100	67, 86, 109, 109	0
2	n	12/12 (100%)	0.36	0 100 100	74, 97, 114, 121	0
2	o	12/12 (100%)	0.54	0 100 100	74, 86, 108, 110	0
2	p	12/12 (100%)	0.28	0 100 100	69, 89, 114, 124	0
All	All	3387/3552 (95%)	0.11	62 (1%) 67 59	44, 85, 134, 210	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	i	139	SER	4.2
2	h	523	DG	3.9
1	K	222	LEU	3.9
1	j	174	ALA	3.6
1	K	223	SER	3.5
1	j	126	HIS	3.5
1	D	169	PRO	3.3
1	J	277	LEU	3.2
1	c	159	CYS	3.1
1	a	169	PRO	3.1
1	j	127	PHE	3.0
1	K	217	VAL	2.9
1	j	190	VAL	2.9
1	C	112	HIS	2.8
1	K	258	CYS	2.8
1	j	196	ASN	2.8
1	a	278	GLU	2.7
1	K	294	ILE	2.7
2	E	408	DT	2.7
1	K	127	PHE	2.6
1	B	258	CYS	2.6
1	K	144	TYR	2.6
1	J	126	HIS	2.6
1	K	145	SER	2.6
1	d	260	SER	2.6
1	j	165	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	286	GLY	2.5
1	J	120	ASP	2.5
1	J	127	PHE	2.5
1	i	114	PHE	2.5
1	a	177	ALA	2.5
1	j	288	ARG	2.5
1	K	221	ASN	2.5
1	d	139	SER	2.4
1	K	195	PRO	2.4
1	j	122	PRO	2.4
1	l	126	HIS	2.4
1	J	237	VAL	2.4
1	A	258	CYS	2.3
1	K	142	TRP	2.3
1	J	167	THR	2.3
1	i	138	LYS	2.3
1	j	195	PRO	2.3
1	j	138	LYS	2.3
1	K	289	SER	2.3
2	O	415	DA	2.2
1	j	125	HIS	2.2
1	K	219	GLY	2.2
1	K	162	GLN	2.2
1	J	169	PRO	2.1
1	K	156	ALA	2.1
1	K	198	GLU	2.1
1	l	118	ASN	2.1
1	K	245	VAL	2.1
1	J	174	ALA	2.1
1	K	220	ASN	2.1
1	K	131	PHE	2.1
1	b	127	PHE	2.1
1	d	259	ASN	2.0
1	B	127	PHE	2.0
1	I	296	ALA	2.0
1	J	114	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZN	B	401	1/1	0.96	0.07	59,59,59,59	0
3	ZN	K	401	1/1	0.96	0.06	101,101,101,101	0
3	ZN	i	401	1/1	0.96	0.07	86,86,86,86	0
3	ZN	a	401	1/1	0.97	0.04	85,85,85,85	0
3	ZN	L	401	1/1	0.97	0.06	63,63,63,63	0
3	ZN	A	401	1/1	0.98	0.03	84,84,84,84	0
3	ZN	k	401	1/1	0.98	0.05	69,69,69,69	0
3	ZN	l	401	1/1	0.98	0.05	68,68,68,68	0
3	ZN	I	401	1/1	0.99	0.02	76,76,76,76	0
3	ZN	b	401	1/1	0.99	0.03	59,59,59,59	0
3	ZN	c	401	1/1	0.99	0.08	65,65,65,65	0
3	ZN	d	401	1/1	0.99	0.04	76,76,76,76	0
3	ZN	J	401	1/1	0.99	0.05	81,81,81,81	0
3	ZN	j	401	1/1	0.99	0.02	79,79,79,79	0
3	ZN	C	401	1/1	0.99	0.08	63,63,63,63	0
3	ZN	D	401	1/1	0.99	0.02	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.