



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:28 PM GMT

PDB ID : 3Q2K
Title : Crystal structure of the WlbA dehydrogenase from Bordetella pertussis in complex with NADH and UDP-GlcNAcA
Authors : Holden, H.M.; Thoden, J.B.
Deposited on : 2010-12-20
Resolution : 2.13 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

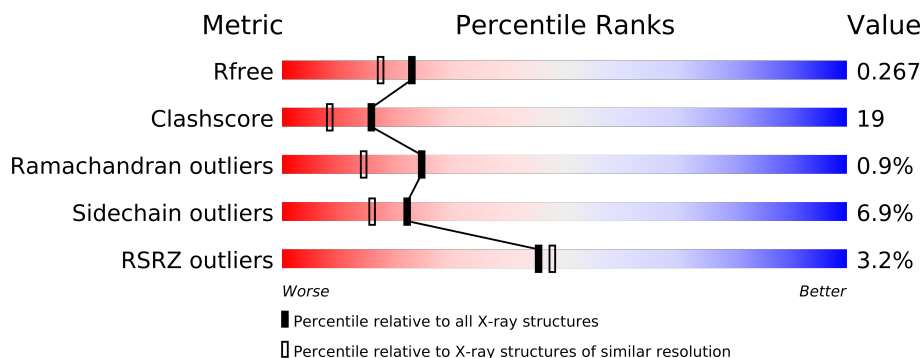
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.13 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}	66092	1116 (2.16-2.12)
Clashscore	79885	1302 (2.16-2.12)
Ramachandran outliers	78287	1281 (2.16-2.12)
Sidechain outliers	78261	1281 (2.16-2.12)
RSRZ outliers	66119	1116 (2.16-2.12)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	370	
1	B	370	
1	C	370	
1	D	370	
1	E	370	
1	F	370	
1	G	370	
1	H	370	
1	I	370	
1	J	370	
1	K	370	
1	L	370	
1	M	370	
1	N	370	

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Mol	Chain	Length	Quality of chain
1	O	370	
1	P	370	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 43985 atoms, of which 0 are hydrogen and 0 are deuterium.

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 oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2707	1699	492	504	12			
1	B	329	Total	C	N	O	S	0	2	0
			2587	1625	476	474	12			
1	C	347	Total	C	N	O	S	0	0	0
			2712	1702	493	505	12			
1	D	343	Total	C	N	O	S	0	1	0
			2693	1689	492	500	12			
1	E	321	Total	C	N	O	S	0	0	0
			2501	1572	457	460	12			
1	F	327	Total	C	N	O	S	0	0	0
			2552	1600	468	472	12			
1	G	342	Total	C	N	O	S	0	0	0
			2677	1680	488	497	12			
1	H	342	Total	C	N	O	S	0	1	0
			2681	1684	488	497	12			
1	I	342	Total	C	N	O	S	0	0	0
			2677	1680	488	497	12			
1	J	346	Total	C	N	O	S	0	0	0
			2707	1699	492	504	12			
1	K	322	Total	C	N	O	S	0	0	0
			2511	1577	461	461	12			
1	L	321	Total	C	N	O	S	0	1	0
			2514	1579	463	460	12			
1	M	346	Total	C	N	O	S	0	0	0
			2707	1699	492	504	12			
1	N	342	Total	C	N	O	S	0	0	0
			2677	1680	488	497	12			
1	O	334	Total	C	N	O	S	0	0	0
			2610	1637	479	482	12			
1	P	322	Total	C	N	O	S	0	0	0
			2511	1577	461	461	12			

There are 320 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q79H45
A	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
A	-17	SER	-	EXPRESSION TAG	UNP Q79H45
A	-16	SER	-	EXPRESSION TAG	UNP Q79H45
A	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
A	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
A	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
A	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
A	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
A	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
A	-9	SER	-	EXPRESSION TAG	UNP Q79H45
A	-8	SER	-	EXPRESSION TAG	UNP Q79H45
A	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
A	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
A	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
A	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
A	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
A	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
A	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
A	0	HIS	-	EXPRESSION TAG	UNP Q79H45
B	-19	MET	-	EXPRESSION TAG	UNP Q79H45
B	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
B	-17	SER	-	EXPRESSION TAG	UNP Q79H45
B	-16	SER	-	EXPRESSION TAG	UNP Q79H45
B	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
B	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
B	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
B	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
B	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
B	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
B	-9	SER	-	EXPRESSION TAG	UNP Q79H45
B	-8	SER	-	EXPRESSION TAG	UNP Q79H45
B	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
B	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
B	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
B	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
B	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
B	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
B	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
B	0	HIS	-	EXPRESSION TAG	UNP Q79H45
C	-19	MET	-	EXPRESSION TAG	UNP Q79H45
C	-18	GLY	-	EXPRESSION TAG	UNP Q79H45

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	SER	-	EXPRESSION TAG	UNP Q79H45
C	-16	SER	-	EXPRESSION TAG	UNP Q79H45
C	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
C	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
C	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
C	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
C	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
C	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
C	-9	SER	-	EXPRESSION TAG	UNP Q79H45
C	-8	SER	-	EXPRESSION TAG	UNP Q79H45
C	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
C	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
C	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
C	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
C	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
C	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
C	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
C	0	HIS	-	EXPRESSION TAG	UNP Q79H45
D	-19	MET	-	EXPRESSION TAG	UNP Q79H45
D	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
D	-17	SER	-	EXPRESSION TAG	UNP Q79H45
D	-16	SER	-	EXPRESSION TAG	UNP Q79H45
D	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
D	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
D	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
D	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
D	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
D	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
D	-9	SER	-	EXPRESSION TAG	UNP Q79H45
D	-8	SER	-	EXPRESSION TAG	UNP Q79H45
D	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
D	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
D	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
D	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
D	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
D	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
D	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
D	0	HIS	-	EXPRESSION TAG	UNP Q79H45
E	-19	MET	-	EXPRESSION TAG	UNP Q79H45
E	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
E	-17	SER	-	EXPRESSION TAG	UNP Q79H45
E	-16	SER	-	EXPRESSION TAG	UNP Q79H45

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
E	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
E	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
E	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
E	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
E	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
E	-9	SER	-	EXPRESSION TAG	UNP Q79H45
E	-8	SER	-	EXPRESSION TAG	UNP Q79H45
E	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
E	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
E	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
E	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
E	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
E	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
E	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
E	0	HIS	-	EXPRESSION TAG	UNP Q79H45
F	-19	MET	-	EXPRESSION TAG	UNP Q79H45
F	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
F	-17	SER	-	EXPRESSION TAG	UNP Q79H45
F	-16	SER	-	EXPRESSION TAG	UNP Q79H45
F	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
F	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
F	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
F	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
F	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
F	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
F	-9	SER	-	EXPRESSION TAG	UNP Q79H45
F	-8	SER	-	EXPRESSION TAG	UNP Q79H45
F	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
F	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
F	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
F	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
F	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
F	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
F	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
F	0	HIS	-	EXPRESSION TAG	UNP Q79H45
G	-19	MET	-	EXPRESSION TAG	UNP Q79H45
G	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
G	-17	SER	-	EXPRESSION TAG	UNP Q79H45
G	-16	SER	-	EXPRESSION TAG	UNP Q79H45
G	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
G	-14	HIS	-	EXPRESSION TAG	UNP Q79H45

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
G	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
G	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
G	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
G	-9	SER	-	EXPRESSION TAG	UNP Q79H45
G	-8	SER	-	EXPRESSION TAG	UNP Q79H45
G	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
G	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
G	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
G	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
G	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
G	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
G	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
G	0	HIS	-	EXPRESSION TAG	UNP Q79H45
H	-19	MET	-	EXPRESSION TAG	UNP Q79H45
H	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
H	-17	SER	-	EXPRESSION TAG	UNP Q79H45
H	-16	SER	-	EXPRESSION TAG	UNP Q79H45
H	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
H	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
H	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
H	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
H	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
H	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
H	-9	SER	-	EXPRESSION TAG	UNP Q79H45
H	-8	SER	-	EXPRESSION TAG	UNP Q79H45
H	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
H	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
H	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
H	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
H	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
H	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
H	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
H	0	HIS	-	EXPRESSION TAG	UNP Q79H45
I	-19	MET	-	EXPRESSION TAG	UNP Q79H45
I	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
I	-17	SER	-	EXPRESSION TAG	UNP Q79H45
I	-16	SER	-	EXPRESSION TAG	UNP Q79H45
I	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
I	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
I	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
I	-12	HIS	-	EXPRESSION TAG	UNP Q79H45

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
I	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
I	-9	SER	-	EXPRESSION TAG	UNP Q79H45
I	-8	SER	-	EXPRESSION TAG	UNP Q79H45
I	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
I	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
I	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
I	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
I	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
I	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
I	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
I	0	HIS	-	EXPRESSION TAG	UNP Q79H45
J	-19	MET	-	EXPRESSION TAG	UNP Q79H45
J	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
J	-17	SER	-	EXPRESSION TAG	UNP Q79H45
J	-16	SER	-	EXPRESSION TAG	UNP Q79H45
J	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
J	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
J	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
J	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
J	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
J	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
J	-9	SER	-	EXPRESSION TAG	UNP Q79H45
J	-8	SER	-	EXPRESSION TAG	UNP Q79H45
J	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
J	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
J	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
J	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
J	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
J	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
J	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
J	0	HIS	-	EXPRESSION TAG	UNP Q79H45
K	-19	MET	-	EXPRESSION TAG	UNP Q79H45
K	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
K	-17	SER	-	EXPRESSION TAG	UNP Q79H45
K	-16	SER	-	EXPRESSION TAG	UNP Q79H45
K	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
K	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
K	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
K	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
K	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
K	-10	HIS	-	EXPRESSION TAG	UNP Q79H45

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-9	SER	-	EXPRESSION TAG	UNP Q79H45
K	-8	SER	-	EXPRESSION TAG	UNP Q79H45
K	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
K	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
K	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
K	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
K	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
K	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
K	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
K	0	HIS	-	EXPRESSION TAG	UNP Q79H45
L	-19	MET	-	EXPRESSION TAG	UNP Q79H45
L	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
L	-17	SER	-	EXPRESSION TAG	UNP Q79H45
L	-16	SER	-	EXPRESSION TAG	UNP Q79H45
L	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
L	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
L	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
L	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
L	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
L	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
L	-9	SER	-	EXPRESSION TAG	UNP Q79H45
L	-8	SER	-	EXPRESSION TAG	UNP Q79H45
L	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
L	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
L	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
L	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
L	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
L	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
L	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
L	0	HIS	-	EXPRESSION TAG	UNP Q79H45
M	-19	MET	-	EXPRESSION TAG	UNP Q79H45
M	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
M	-17	SER	-	EXPRESSION TAG	UNP Q79H45
M	-16	SER	-	EXPRESSION TAG	UNP Q79H45
M	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
M	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
M	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
M	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
M	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
M	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
M	-9	SER	-	EXPRESSION TAG	UNP Q79H45
M	-8	SER	-	EXPRESSION TAG	UNP Q79H45

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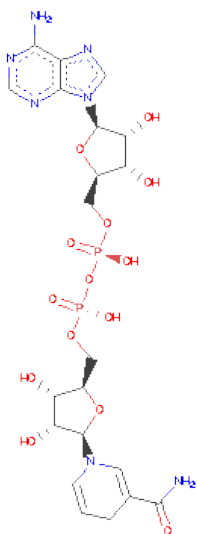
Chain	Residue	Modelled	Actual	Comment	Reference
M	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
M	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
M	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
M	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
M	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
M	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
M	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
M	0	HIS	-	EXPRESSION TAG	UNP Q79H45
N	-19	MET	-	EXPRESSION TAG	UNP Q79H45
N	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
N	-17	SER	-	EXPRESSION TAG	UNP Q79H45
N	-16	SER	-	EXPRESSION TAG	UNP Q79H45
N	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
N	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
N	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
N	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
N	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
N	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
N	-9	SER	-	EXPRESSION TAG	UNP Q79H45
N	-8	SER	-	EXPRESSION TAG	UNP Q79H45
N	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
N	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
N	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
N	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
N	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
N	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
N	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
N	0	HIS	-	EXPRESSION TAG	UNP Q79H45
O	-19	MET	-	EXPRESSION TAG	UNP Q79H45
O	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
O	-17	SER	-	EXPRESSION TAG	UNP Q79H45
O	-16	SER	-	EXPRESSION TAG	UNP Q79H45
O	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
O	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
O	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
O	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
O	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
O	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
O	-9	SER	-	EXPRESSION TAG	UNP Q79H45
O	-8	SER	-	EXPRESSION TAG	UNP Q79H45
O	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
O	-6	ASN	-	EXPRESSION TAG	UNP Q79H45

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
O	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
O	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
O	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
O	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
O	0	HIS	-	EXPRESSION TAG	UNP Q79H45
P	-19	MET	-	EXPRESSION TAG	UNP Q79H45
P	-18	GLY	-	EXPRESSION TAG	UNP Q79H45
P	-17	SER	-	EXPRESSION TAG	UNP Q79H45
P	-16	SER	-	EXPRESSION TAG	UNP Q79H45
P	-15	HIS	-	EXPRESSION TAG	UNP Q79H45
P	-14	HIS	-	EXPRESSION TAG	UNP Q79H45
P	-13	HIS	-	EXPRESSION TAG	UNP Q79H45
P	-12	HIS	-	EXPRESSION TAG	UNP Q79H45
P	-11	HIS	-	EXPRESSION TAG	UNP Q79H45
P	-10	HIS	-	EXPRESSION TAG	UNP Q79H45
P	-9	SER	-	EXPRESSION TAG	UNP Q79H45
P	-8	SER	-	EXPRESSION TAG	UNP Q79H45
P	-7	GLU	-	EXPRESSION TAG	UNP Q79H45
P	-6	ASN	-	EXPRESSION TAG	UNP Q79H45
P	-5	LEU	-	EXPRESSION TAG	UNP Q79H45
P	-4	TYR	-	EXPRESSION TAG	UNP Q79H45
P	-3	PHE	-	EXPRESSION TAG	UNP Q79H45
P	-2	GLN	-	EXPRESSION TAG	UNP Q79H45
P	-1	GLY	-	EXPRESSION TAG	UNP Q79H45
P	0	HIS	-	EXPRESSION TAG	UNP Q79H45

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDEADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



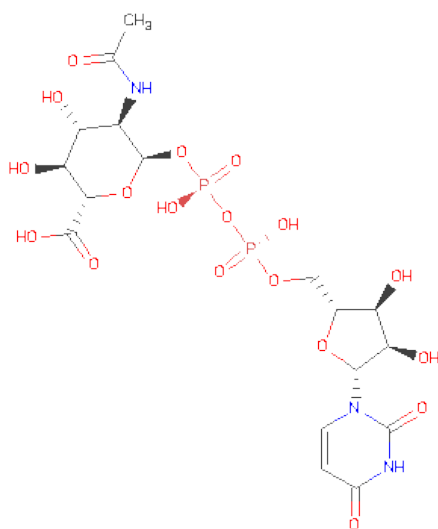
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	I	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	J	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	K	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	L	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	M	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	N	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	P	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is (2S,3S,4R,5R,6R)-5-ACETAMIDO-6-[[[(2R,3S,4R,5R)-5-(2,4-DIOXOPYRIMIDIN-1-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHOXY-HYDROXY-PHOSPHORYL]OXY-HYDROXY-PHOSPHORYL]OXY-3,4-DIHYDROXY-OXANE-2-CARBOXYLIC ACID (three-letter code: HP7) (formula: C₁₇H₂₅N₃O₁₈P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	B	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	C	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	D	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	E	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	F	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	G	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	H	1	Total	C	N	O	P	0	0
			40	17	3	18	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	I	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	J	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	K	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	L	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	M	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	N	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	O	1	Total	C	N	O	P	0	0
			40	17	3	18	2		
3	P	1	Total	C	N	O	P	0	0
			40	17	3	18	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	85	Total	O	0	0
			85	85		
4	B	54	Total	O	0	0
			54	54		
4	C	58	Total	O	0	0
			58	58		
4	D	51	Total	O	0	0
			51	51		
4	E	21	Total	O	0	0
			21	21		
4	F	24	Total	O	0	0
			24	24		
4	G	49	Total	O	0	0
			49	49		
4	H	35	Total	O	0	0
			35	35		
4	I	36	Total	O	0	0
			36	36		
4	J	30	Total	O	0	0
			30	30		
4	K	26	Total	O	0	0
			26	26		

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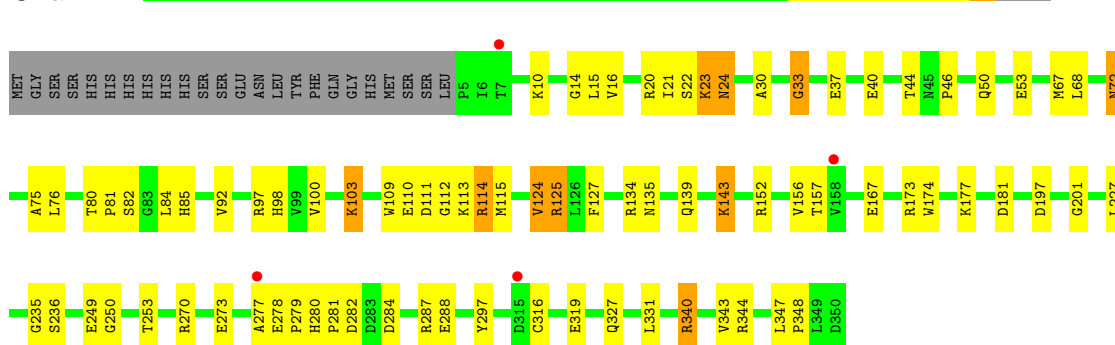
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	37	Total 37	O 37	0	0
4	M	36	Total 36	O 36	0	0
4	N	34	Total 34	O 34	0	0
4	O	17	Total 17	O 17	0	0
4	P	24	Total 24	O 24	0	0

3 Residue-property plots

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.

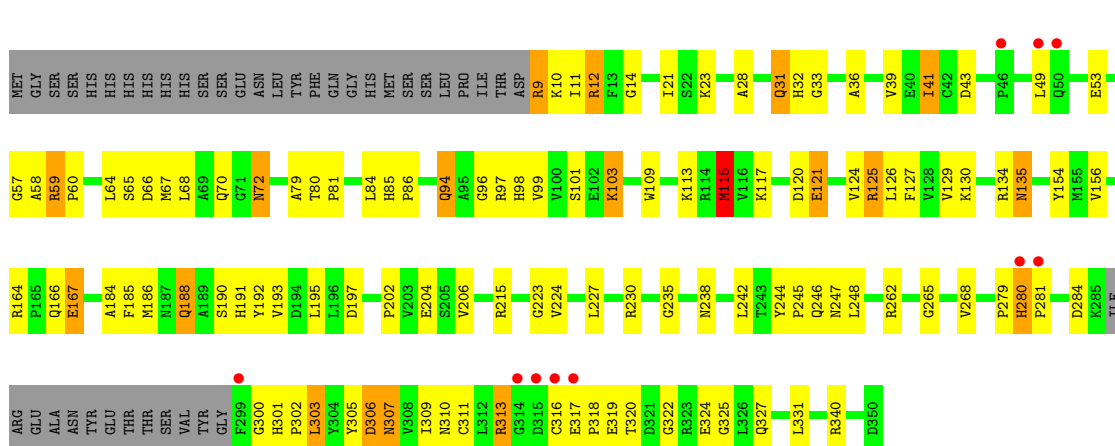
- Molecule 1: oxidoreductase

Chain A:



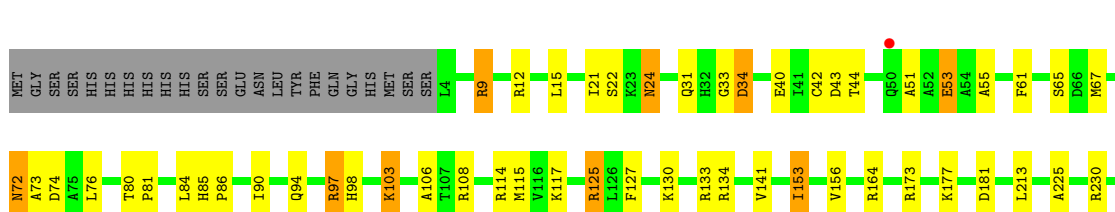
- Molecule 1: oxidoreductase

Chain B:



- Molecule 1: oxidoreductase

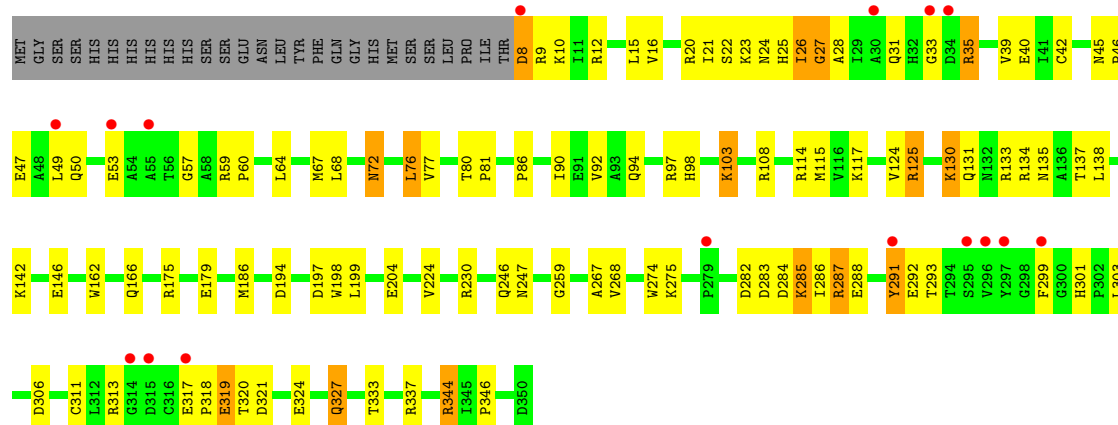
Chain C:





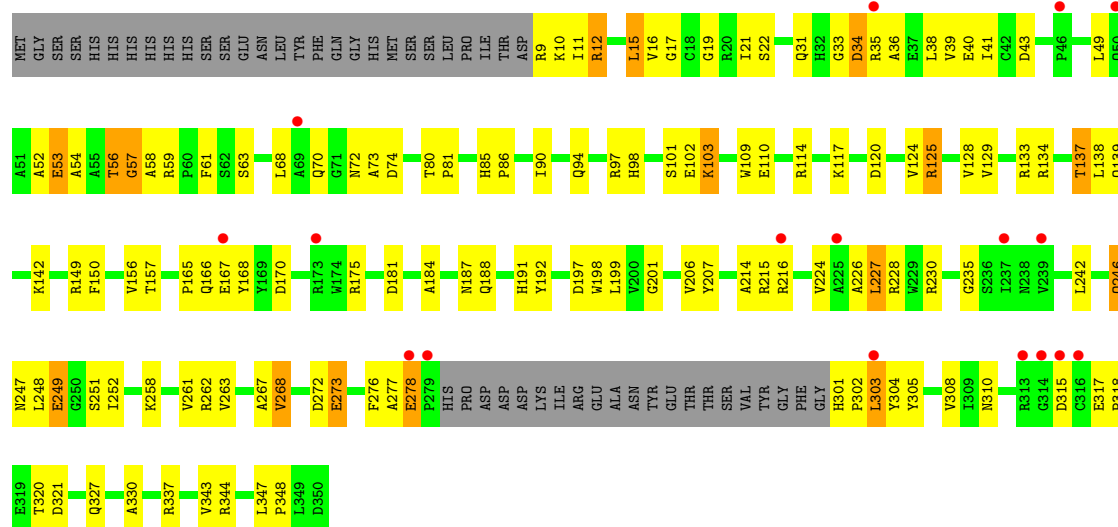
• Molecule 1: oxidoreductase

Chain D:



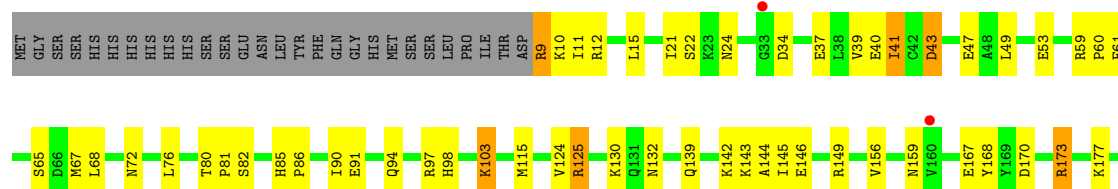
• Molecule 1: oxidoreductase

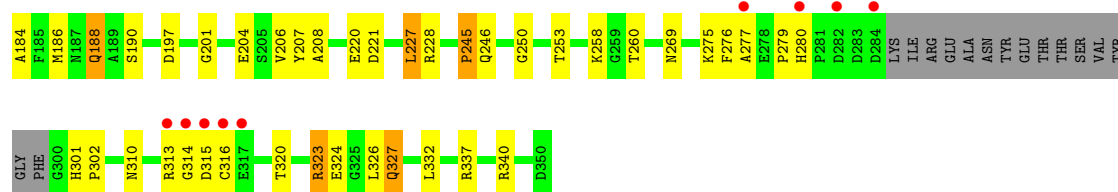
Chain E:



• Molecule 1: oxidoreductase

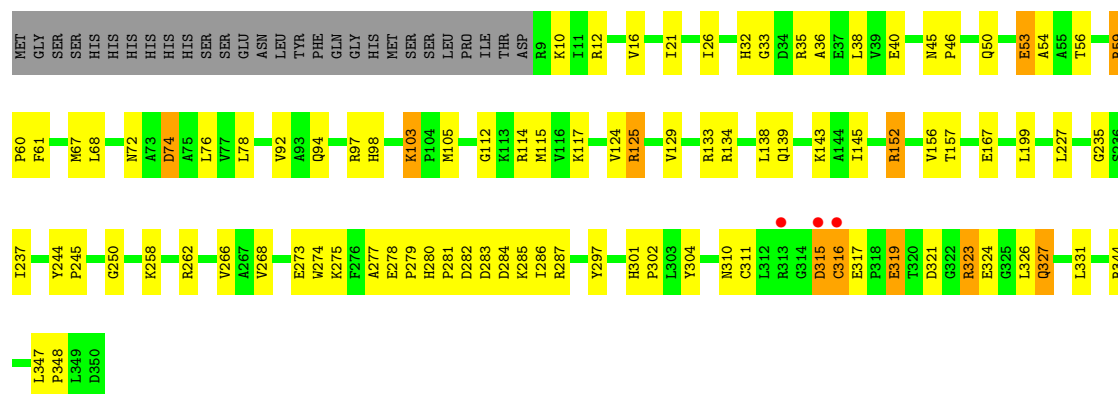
Chain F:





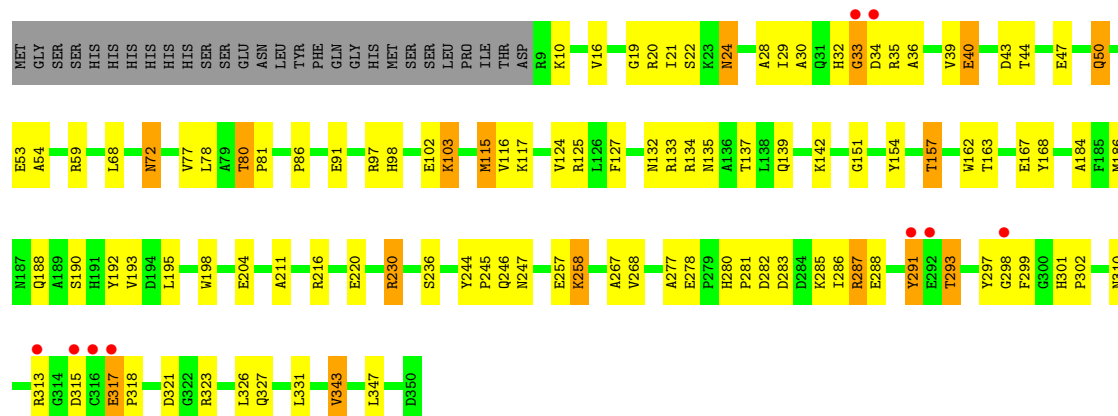
• Molecule 1: oxidoreductase

Chain G:



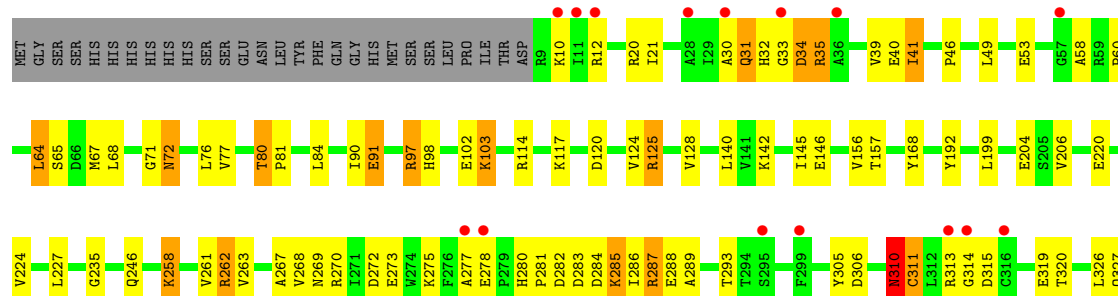
• Molecule 1: oxidoreductase

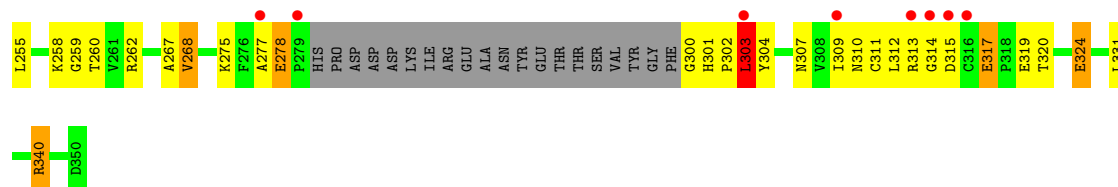
Chain H:



• Molecule 1: oxidoreductase

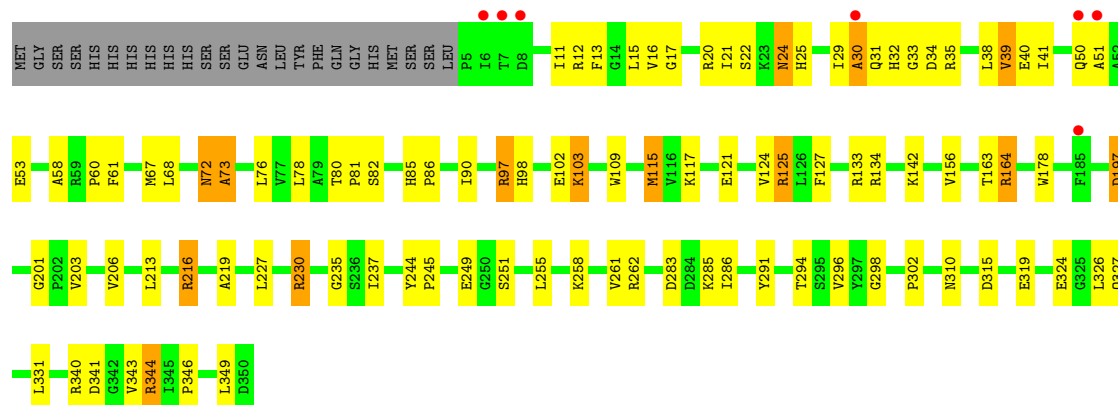
Chain I:





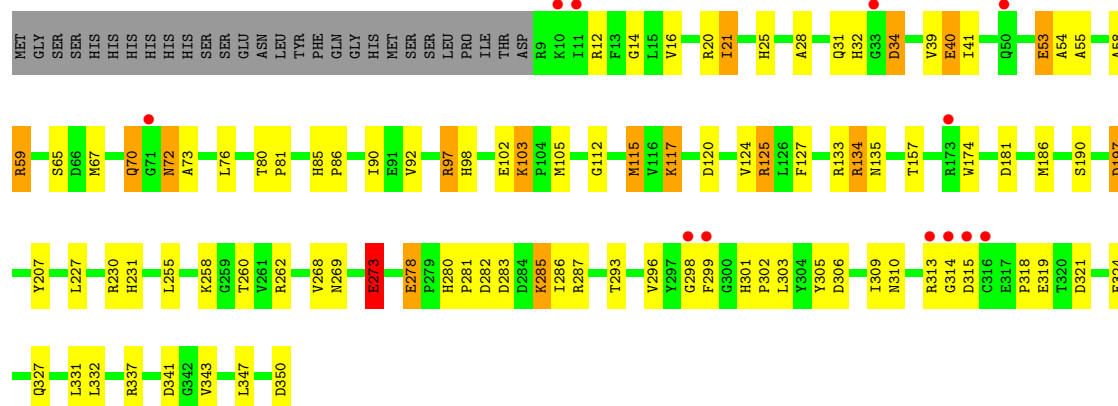
- Molecule 1: oxidoreductase

Chain M:



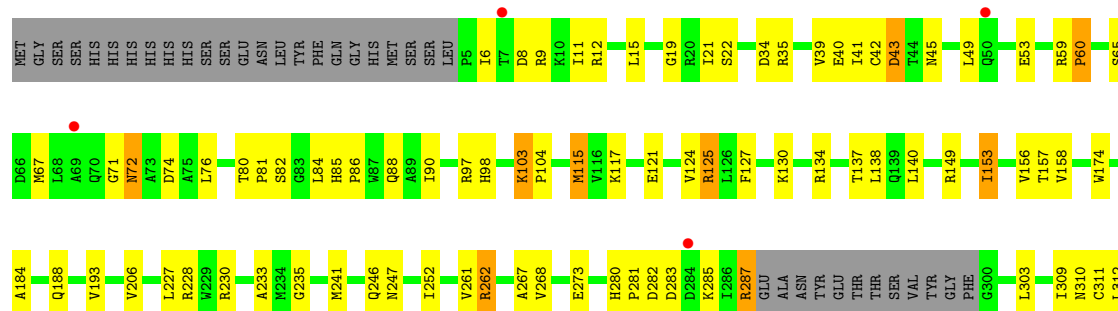
- Molecule 1: oxidoreductase

Chain N:



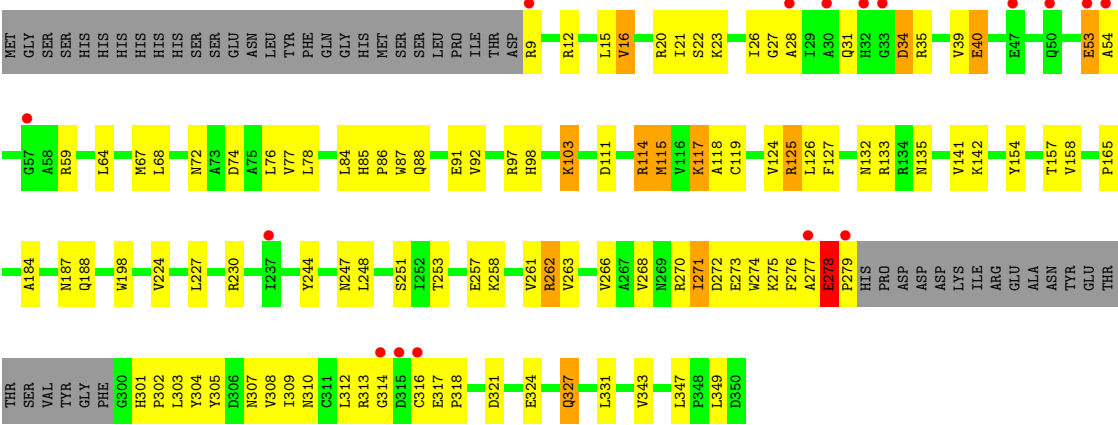
- Molecule 1: oxidoreductase

Chain 0:





● Molecule 1: oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.26Å 319.98Å 103.80Å 90.00° 119.07° 90.00°	Depositor
Resolution (Å)	30.00 – 2.13 34.28 – 2.13	Depositor EDS
% Data completeness (in resolution range)	92.6 (30.00-2.13) 92.6 (34.28-2.13)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.54 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.183 , 0.269 0.184 , 0.267	Depositor DCC
R_{free} test set	15038 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 34.1	EDS
Estimated twinning fraction	0.007 for -h-l,k,h 0.007 for l,k,-h-l 0.026 for h,-k,-h-l 0.024 for -h-l,-k,l 0.024 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 297987 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	43985	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAI, HP7

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	0.32	0/2767	1.16	14/3755 (0.4%)
1	B	0.28	0/2650	1.07	7/3593 (0.2%)
1	C	0.28	0/2772	1.08	5/3763 (0.1%)
1	D	0.27	0/2755	1.06	2/3737 (0.1%)
1	E	0.27	0/2554	1.06	6/3464 (0.2%)
1	F	0.28	0/2607	1.09	10/3536 (0.3%)
1	G	0.29	0/2736	1.11	8/3712 (0.2%)
1	H	0.28	0/2743	1.08	6/3722 (0.2%)
1	I	0.27	0/2736	1.05	1/3712 (0.0%)
1	J	0.27	0/2767	1.06	7/3755 (0.2%)
1	K	0.27	0/2564	1.06	7/3476 (0.2%)
1	L	0.26	0/2569	1.02	8/3480 (0.2%)
1	M	0.29	0/2767	1.16	14/3755 (0.4%)
1	N	0.30	0/2736	1.10	8/3712 (0.2%)
1	O	0.27	0/2666	1.19	7/3615 (0.2%)
1	P	0.26	0/2564	1.05	3/3476 (0.1%)
All	All	0.28	0/42953	1.09	113/58263 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	1

There are no bond length outliers.

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	230	ARG	NE-CZ-NH2	-20.32	110.14	120.30
1	O	230	ARG	NE-CZ-NH1	19.79	130.20	120.30
1	M	230	ARG	NE-CZ-NH2	-11.89	114.35	120.30
1	K	340	ARG	NE-CZ-NH1	-10.26	115.17	120.30
1	F	221	ASP	CB-CG-OD1	9.39	126.75	118.30
1	A	270	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	A	181	ASP	CB-CG-OD1	8.96	126.37	118.30
1	J	340	ARG	NE-CZ-NH1	-8.85	115.87	120.30
1	M	230	ARG	CG-CD-NE	-8.85	93.22	111.80
1	B	9	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	C	164	ARG	NE-CZ-NH2	-8.61	115.99	120.30
1	M	340	ARG	NE-CZ-NH1	-8.17	116.22	120.30
1	M	344	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	K	340	ARG	NE-CZ-NH2	7.70	124.15	120.30
1	C	181	ASP	CB-CG-OD1	7.65	125.18	118.30
1	N	341	ASP	CB-CG-OD2	-7.44	111.60	118.30
1	F	170	ASP	CB-CG-OD1	7.44	124.99	118.30
1	G	152	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	E	230	ARG	CG-CD-NE	-7.35	96.36	111.80
1	F	9	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	N	181	ASP	CB-CG-OD1	7.25	124.82	118.30
1	K	323	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	B	340	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	A	270	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	D	344	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	J	230	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	A	10	LYS	CD-CE-NZ	-6.87	95.90	111.70
1	L	340	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	O	228	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	K	323	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	A	177	LYS	CD-CE-NZ	-6.65	96.41	111.70
1	C	337	ARG	NE-CZ-NH1	-6.59	117.01	120.30
1	P	133	ARG	NE-CZ-NH1	-6.57	117.02	120.30
1	N	337	ARG	NE-CZ-NH1	-6.55	117.03	120.30
1	B	9	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	G	74	ASP	CB-CG-OD1	-6.43	112.51	118.30
1	J	181	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	P	115	MET	CG-SD-CE	6.33	110.32	100.20
1	N	341	ASP	CB-CG-OD1	6.31	123.98	118.30
1	N	115	MET	CG-SD-CE	-6.28	90.16	100.20
1	O	344	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	C	76	LEU	CA-CB-CG	-6.21	101.02	115.30
1	A	227	LEU	CB-CG-CD2	-6.16	100.53	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	76	LEU	CA-CB-CG	-6.16	101.14	115.30
1	M	255	LEU	CB-CG-CD2	-6.15	100.55	111.00
1	J	9	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	O	262	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	J	213	LEU	CB-CG-CD1	6.12	121.40	111.00
1	F	337	ARG	NE-CZ-NH1	-6.11	117.25	120.30
1	P	349	LEU	CB-CG-CD1	-6.11	100.62	111.00
1	H	323	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	B	306	ASP	CB-CG-OD1	5.98	123.68	118.30
1	G	114	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	K	177	LYS	CD-CE-NZ	-5.95	98.02	111.70
1	M	78	LEU	CB-CG-CD1	-5.88	101.00	111.00
1	F	177	LYS	CD-CE-NZ	-5.86	98.21	111.70
1	O	115	MET	CB-CA-C	-5.86	98.68	110.40
1	M	230	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	I	262	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	M	164	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	J	160	VAL	N-CA-C	-5.72	95.56	111.00
1	L	181	ASP	CB-CG-OD1	5.68	123.41	118.30
1	L	303	LEU	CB-CG-CD1	5.68	120.65	111.00
1	H	151	GLY	N-CA-C	-5.67	98.93	113.10
1	A	340	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	H	59	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	N	197	ASP	CB-CG-OD2	5.64	123.38	118.30
1	K	331	LEU	CB-CG-CD1	-5.63	101.43	111.00
1	D	76	LEU	CA-CB-CG	-5.62	102.37	115.30
1	N	181	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	M	341	ASP	CB-CG-OD2	5.58	123.32	118.30
1	F	332	LEU	CB-CG-CD2	-5.56	101.55	111.00
1	E	224	VAL	CB-CA-C	-5.51	100.93	111.40
1	E	344	ARG	NE-CZ-NH1	-5.51	117.54	120.30
1	M	97	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	F	323	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	344	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	A	250	GLY	N-CA-C	-5.40	99.60	113.10
1	H	230	ARG	CG-CD-NE	-5.39	100.47	111.80
1	C	108	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	340	ARG	NE-CZ-NH2	5.35	122.98	120.30
1	H	115	MET	CA-CB-CG	5.35	122.40	113.30
1	L	250	GLY	N-CA-C	-5.35	99.73	113.10
1	L	49	LEU	CB-CG-CD2	-5.31	101.98	111.00
1	G	250	GLY	N-CA-C	-5.24	100.00	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	43	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	G	331	LEU	CB-CG-CD2	-5.23	102.11	111.00
1	A	84	LEU	CA-CB-CG	5.23	127.33	115.30
1	B	284	ASP	CB-CG-OD2	5.22	123.00	118.30
1	M	142	LYS	CD-CE-NZ	-5.20	99.74	111.70
1	A	331	LEU	CB-CG-CD2	-5.19	102.17	111.00
1	L	199	LEU	CB-CG-CD1	-5.18	102.19	111.00
1	G	78	LEU	CB-CG-CD2	-5.16	102.22	111.00
1	E	278	GLU	C-N-CD	-5.16	109.25	120.60
1	B	115	MET	CA-CB-CG	5.15	122.05	113.30
1	F	340	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	A	111	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	F	323	ARG	CG-CD-NE	-5.14	101.01	111.80
1	G	344	ARG	NE-CZ-NH2	5.13	122.86	120.30
1	M	349	LEU	CB-CG-CD1	-5.12	102.29	111.00
1	M	115	MET	CB-CA-C	-5.11	100.18	110.40
1	G	152	ARG	CG-CD-NE	5.09	122.48	111.80
1	N	273	GLU	N-CA-C	-5.07	97.30	111.00
1	B	164	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	E	337	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	H	343	VAL	CG1-CB-CG2	5.07	119.01	110.90
1	M	115	MET	CB-CG-SD	-5.07	97.19	112.40
1	A	152	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	L	115	MET	CB-CA-C	-5.03	100.35	110.40
1	E	207	TYR	N-CA-C	-5.02	97.44	111.00
1	J	258	LYS	CB-CA-C	-5.02	100.36	110.40
1	K	228	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	L	228	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	315	ASP	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2707	0	2654	65	0
1	B	2587	0	2547	122	0
1	C	2712	0	2655	72	0
1	D	2693	0	2641	133	0
1	E	2501	0	2465	136	0
1	F	2552	0	2505	82	0
1	G	2677	0	2624	71	0
1	H	2681	0	2633	110	2
1	I	2677	0	2624	108	1
1	J	2707	0	2654	80	1
1	K	2511	0	2479	104	0
1	L	2514	0	2486	130	0
1	M	2707	0	2654	85	0
1	N	2677	0	2624	98	0
1	O	2610	0	2572	87	0
1	P	2511	0	2479	98	0
2	A	44	0	27	1	0
2	B	44	0	27	6	0
2	C	44	0	27	6	0
2	D	44	0	27	7	0
2	E	44	0	27	7	0
2	F	44	0	27	4	0
2	G	44	0	27	4	0
2	H	44	0	27	8	0
2	I	44	0	27	12	0
2	J	44	0	27	7	0
2	K	44	0	27	4	0
2	L	44	0	27	6	0
2	M	44	0	27	4	0
2	N	44	0	27	4	0
2	O	44	0	27	3	0
2	P	44	0	27	5	0
3	A	40	0	22	2	0
3	B	40	0	22	1	0
3	C	40	0	22	1	0
3	D	40	0	22	1	0
3	E	40	0	22	5	0
3	F	40	0	22	2	0
3	G	40	0	22	2	0
3	H	40	0	22	3	0
3	I	40	0	22	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	40	0	22	3	0
3	K	40	0	22	6	0
3	L	40	0	22	0	0
3	M	40	0	22	4	0
3	N	40	0	22	1	0
3	O	40	0	22	2	0
3	P	40	0	22	1	0
4	A	85	0	0	8	0
4	B	54	0	0	6	0
4	C	58	0	0	3	0
4	D	51	0	0	3	0
4	E	21	0	0	2	0
4	F	24	0	0	0	0
4	G	49	0	0	4	0
4	H	35	0	0	2	0
4	I	36	0	0	2	0
4	J	30	0	0	1	0
4	K	26	0	0	2	0
4	L	37	0	0	3	0
4	M	36	0	0	1	0
4	N	34	0	0	4	0
4	O	17	0	0	1	0
4	P	24	0	0	0	0
All	All	43985	0	42080	1583	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (1583) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:39:VAL:HG12	1:K:40:GLU:CG	1.49	1.43
1:I:64:LEU:HD23	1:I:67:MET:CE	1.59	1.31
1:B:12:ARG:HG2	1:B:39:VAL:CG2	1.61	1.28
1:B:12:ARG:CG	1:B:39:VAL:HG21	1.64	1.27
1:N:12:ARG:NH1	1:N:72:ASN:OD1	1.70	1.25
1:E:317:GLU:OE1	1:E:318:PRO:CD	1.84	1.23
1:E:98:HIS:HA	1:E:124:VAL:CG1	1.71	1.20
1:B:98:HIS:HA	1:B:124:VAL:CG1	1.73	1.19
1:O:98:HIS:HA	1:O:124:VAL:CG1	1.74	1.16
2:J:500:NAI:H51N	2:J:500:NAI:H6N	1.20	1.12
1:K:39:VAL:HG12	1:K:40:GLU:HG2	1.28	1.12
1:O:39:VAL:HG12	1:O:40:GLU:HG3	1.20	1.11

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:39:VAL:CG1	1:D:40:GLU:HG3	1.78	1.11
1:P:39:VAL:HG12	1:P:40:GLU:CG	1.79	1.11
2:J:500:NAI:C6N	2:J:500:NAI:H51N	1.81	1.11
1:B:166:GLN:HB2	4:B:366:HOH:O	1.47	1.11
1:O:125:ARG:NH1	1:O:311:CYS:SG	2.25	1.10
1:K:39:VAL:HG12	1:K:40:GLU:HG3	1.21	1.10
1:M:216:ARG:CG	1:M:216:ARG:HH11	1.65	1.09
1:E:103:LYS:O	1:E:103:LYS:HD3	1.50	1.09
1:N:98:HIS:HA	1:N:124:VAL:CG1	1.82	1.08
1:K:278:GLU:O	1:K:278:GLU:HG2	1.46	1.08
1:E:317:GLU:OE1	1:E:318:PRO:HD2	1.51	1.07
1:M:216:ARG:NH1	1:M:216:ARG:HG3	1.51	1.07
1:E:97:ARG:O	1:E:124:VAL:HG11	1.52	1.06
1:K:9:ARG:HG2	1:K:9:ARG:HH11	0.93	1.06
1:P:277:ALA:C	1:P:278:GLU:HG2	1.76	1.06
1:L:324:GLU:HA	1:L:324:GLU:OE2	1.56	1.06
1:E:98:HIS:HA	1:E:124:VAL:HG13	1.34	1.05
1:E:317:GLU:OE1	1:E:318:PRO:HD3	1.48	1.05
1:D:98:HIS:HA	1:D:124:VAL:CG1	1.86	1.05
1:B:127:PHE:HE1	1:B:318:PRO:HB3	1.17	1.04
1:P:97:ARG:O	1:P:124:VAL:HG11	1.57	1.04
1:I:39:VAL:HG12	1:I:40:GLU:HG3	1.36	1.04
1:D:39:VAL:HG12	1:D:40:GLU:CG	1.86	1.04
1:E:12:ARG:HG2	1:E:74:ASP:OD2	1.58	1.03
1:E:137:THR:HG22	1:E:138:LEU:N	1.71	1.03
1:B:307:ASN:HD21	1:B:318:PRO:HA	1.20	1.03
1:H:327:GLN:HA	1:H:327:GLN:NE2	1.74	1.03
1:E:305:TYR:HA	1:E:308:VAL:CG2	1.88	1.03
1:K:103:LYS:HD3	1:K:103:LYS:O	1.59	1.03
1:B:124:VAL:HG12	1:B:125:ARG:H	1.18	1.02
1:E:12:ARG:NH2	1:E:72:ASN:OD1	1.91	1.02
1:P:270:ARG:HG2	1:P:272:ASP:OD1	1.59	1.02
1:K:278:GLU:O	1:K:278:GLU:CG	2.05	1.01
1:O:97:ARG:O	1:O:124:VAL:HG11	1.59	1.01
1:O:53:GLU:HG3	1:O:60:PRO:HG3	1.40	1.01
1:B:98:HIS:HA	1:B:124:VAL:HG11	1.36	1.00
1:B:166:GLN:CB	4:B:366:HOH:O	1.99	1.00
1:B:313:ARG:HG2	1:B:313:ARG:HH11	1.25	1.00
1:D:287:ARG:NH1	1:M:24:ASN:OD1	1.94	0.99
1:B:124:VAL:HG12	1:B:125:ARG:N	1.74	0.99
1:C:327:GLN:HA	1:C:327:GLN:HE21	1.23	0.99
1:D:39:VAL:HG12	1:D:40:GLU:HG3	0.99	0.99

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:313:ARG:CG	1:B:313:ARG:HH11	1.76	0.99
1:P:39:VAL:CG1	1:P:40:GLU:HG3	1.92	0.99
1:B:12:ARG:HG2	1:B:39:VAL:HG21	0.99	0.98
1:F:67:MET:HE2	1:F:76:LEU:HD21	1.46	0.97
1:N:97:ARG:O	1:N:124:VAL:HG11	1.65	0.97
2:D:500:NAI:H42N	3:D:550:HP7:H3'	1.46	0.97
1:I:98:HIS:HA	1:I:124:VAL:CG1	1.93	0.97
1:D:103:LYS:HD3	1:D:103:LYS:O	1.64	0.97
2:D:500:NAI:H6N	2:D:500:NAI:H51N	1.47	0.97
1:K:39:VAL:CG1	1:K:40:GLU:CG	2.41	0.96
1:P:103:LYS:HD3	1:P:103:LYS:C	1.85	0.96
1:O:340:ARG:HD3	1:O:341:ASP:OD1	1.66	0.96
1:I:64:LEU:HD23	1:I:67:MET:HE1	1.42	0.96
1:P:39:VAL:HG12	1:P:40:GLU:HG3	0.97	0.96
1:H:43:ASP:OD2	2:H:500:NAI:O3B	1.84	0.96
4:A:390:HOH:O	1:D:230:ARG:HD3	1.65	0.95
1:M:98:HIS:HA	1:M:124:VAL:CG1	1.95	0.95
1:L:262:ARG:HH11	1:L:262:ARG:HG2	1.28	0.95
1:M:97:ARG:O	1:M:124:VAL:HG11	1.66	0.95
1:I:39:VAL:HG12	1:I:40:GLU:CG	1.97	0.95
1:J:75:ALA:C	1:J:76:LEU:HD23	1.87	0.95
1:G:53:GLU:OE1	1:G:60:PRO:HG3	1.66	0.95
1:P:98:HIS:HA	1:P:124:VAL:CG1	1.95	0.95
1:L:32:HIS:CE1	1:L:35:ARG:HH11	1.85	0.94
1:K:39:VAL:CG1	1:K:40:GLU:HG2	1.95	0.94
1:J:76:LEU:HD23	1:J:76:LEU:N	1.83	0.94
1:J:173:ARG:O	1:J:177:LYS:HE2	1.66	0.94
1:G:98:HIS:HA	1:G:124:VAL:HG13	1.49	0.94
1:E:305:TYR:HA	1:E:308:VAL:HG23	1.49	0.94
2:B:500:NAI:H6N	2:B:500:NAI:H51N	1.45	0.94
1:K:9:ARG:HG2	1:K:9:ARG:NH1	1.74	0.94
1:K:9:ARG:CG	1:K:9:ARG:HH11	1.81	0.94
1:J:58:ALA:O	1:J:60:PRO:HD3	1.68	0.94
1:A:114:ARG:HH11	1:A:114:ARG:HB2	1.32	0.93
1:K:206:VAL:HG12	1:K:227:LEU:HD23	1.49	0.93
1:P:277:ALA:O	1:P:278:GLU:HG2	1.66	0.92
1:H:327:GLN:HA	1:H:327:GLN:HE21	1.29	0.92
1:L:11:ILE:H	1:L:11:ILE:HD13	1.31	0.92
1:O:281:PRO:O	1:O:282:ASP:HB2	1.66	0.92
1:H:97:ARG:O	1:H:124:VAL:HG11	1.69	0.92
1:D:103:LYS:HD3	1:D:103:LYS:C	1.87	0.92
1:K:103:LYS:C	1:K:103:LYS:HD3	1.89	0.91

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:127:PHE:CE1	1:B:318:PRO:HB3	2.05	0.91
1:D:133:ARG:HH12	1:D:324:GLU:HG2	1.35	0.91
1:F:206:VAL:HG12	1:F:227:LEU:HD23	1.51	0.91
1:K:103:LYS:NZ	3:K:550:HP7:O3'	2.02	0.90
1:B:310:ASN:HB3	1:B:316:CYS:SG	2.11	0.90
1:I:10:LYS:HG2	1:I:34:ASP:O	1.70	0.90
1:L:29:ILE:O	1:L:32:HIS:N	2.04	0.90
1:I:10:LYS:CG	1:I:34:ASP:O	2.20	0.90
1:L:9:ARG:HG3	1:L:10:LYS:N	1.84	0.90
1:H:39:VAL:HG12	1:H:40:GLU:HG3	1.52	0.89
1:O:340:ARG:CD	1:O:341:ASP:OD1	2.21	0.89
1:C:86:PRO:HA	1:C:115:MET:HG2	1.52	0.89
1:I:103:LYS:O	1:I:103:LYS:HD3	1.73	0.89
1:O:98:HIS:HA	1:O:124:VAL:HG13	1.53	0.89
1:L:108:ARG:HG2	1:L:108:ARG:HH11	1.36	0.88
1:F:142:LYS:HE3	1:F:146:GLU:OE2	1.72	0.88
1:L:184:ALA:HA	1:L:188:GLN:NE2	1.90	0.87
2:K:500:NAI:H42N	3:K:550:HP7:H3'	1.57	0.87
1:H:288:GLU:HA	1:H:291:TYR:HB2	1.56	0.87
1:P:98:HIS:HA	1:P:124:VAL:HG12	1.55	0.86
1:I:97:ARG:O	1:I:124:VAL:HG11	1.76	0.85
1:D:344:ARG:NH1	4:D:571:HOH:O	2.09	0.85
1:B:124:VAL:CG1	1:B:125:ARG:H	1.89	0.85
1:E:103:LYS:C	1:E:103:LYS:HD3	1.96	0.85
2:M:500:NAI:H42N	3:M:550:HP7:H3'	1.57	0.85
1:I:284:ASP:C	1:I:285:LYS:HD3	1.97	0.85
1:I:64:LEU:HD23	1:I:67:MET:HE2	1.58	0.85
1:B:313:ARG:NH1	1:B:313:ARG:HG2	1.90	0.85
1:D:15:LEU:HD21	1:D:22:SER:HB2	1.59	0.85
1:L:108:ARG:HH11	1:L:108:ARG:CG	1.87	0.84
1:O:42:CYS:HB2	1:O:67:MET:HE1	1.59	0.84
1:C:114:ARG:HG2	1:C:117:LYS:HE2	1.59	0.84
2:N:500:NAI:H42N	3:N:550:HP7:H3'	1.58	0.84
1:I:64:LEU:CD2	1:I:67:MET:CE	2.51	0.84
1:B:280[B]:HIS:CD2	1:B:281:PRO:HD2	2.12	0.84
2:N:500:NAI:H6N	2:N:500:NAI:H51N	1.58	0.84
1:H:103:LYS:O	1:H:103:LYS:HD3	1.78	0.84
1:B:80:THR:HB	1:B:81:PRO:HD2	1.58	0.83
1:P:86:PRO:HA	1:P:115:MET:HG2	1.59	0.83
1:F:98:HIS:HA	1:F:124:VAL:CG1	2.08	0.83
1:B:317:GLU:HG3	1:C:173:ARG:HH12	1.43	0.83
1:K:216:ARG:HG3	1:K:216:ARG:O	1.78	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:39:VAL:CG1	1:M:40:GLU:HG3	2.08	0.83
1:K:97:ARG:O	1:K:124:VAL:HG21	1.79	0.83
1:E:305:TYR:HA	1:E:308:VAL:HG21	1.59	0.82
1:O:98:HIS:HA	1:O:124:VAL:HG12	1.61	0.82
1:L:32:HIS:CE1	1:L:35:ARG:NH1	2.46	0.82
1:H:35:ARG:HG2	1:H:313:ARG:NH1	1.94	0.82
1:N:282:ASP:OD1	1:N:285:LYS:HE2	1.77	0.82
1:C:34:ASP:N	1:C:34:ASP:OD2	2.06	0.82
2:D:500:NAI:C6N	2:D:500:NAI:H51N	2.09	0.82
1:H:98:HIS:HA	1:H:124:VAL:CG1	2.08	0.82
2:N:500:NAI:C6N	2:N:500:NAI:H51N	2.10	0.82
1:N:76:LEU:HD12	1:N:92:VAL:HG13	1.61	0.82
1:N:280:HIS:CG	1:N:281:PRO:HD2	2.13	0.82
1:I:310:ASN:HD22	1:I:310:ASN:N	1.75	0.82
2:H:500:NAI:H42N	3:H:550:HP7:H3'	1.61	0.82
1:E:59:ARG:NH2	1:E:70:GLN:HB3	1.95	0.82
1:G:16:VAL:HG22	1:G:67:MET:HE1	1.60	0.82
1:N:310:ASN:O	1:N:315:ASP:HB2	1.80	0.82
1:L:174:TRP:O	1:L:177:LYS:HB2	1.79	0.82
1:L:324:GLU:CA	1:L:324:GLU:OE2	2.28	0.82
1:B:311:CYS:SG	1:B:318:PRO:HD3	2.20	0.82
1:C:21:ILE:HD13	2:C:500:NAI:H4N	1.62	0.82
1:D:86:PRO:HA	1:D:115:MET:HG2	1.60	0.82
1:N:39:VAL:O	1:N:58:ALA:HB1	1.79	0.82
1:F:98:HIS:HA	1:F:124:VAL:HG13	1.60	0.81
1:E:59:ARG:HH22	1:E:70:GLN:HB3	1.45	0.81
1:C:103:LYS:C	1:C:103:LYS:HD3	2.00	0.81
1:A:67:MET:HE1	1:A:76:LEU:HD22	1.62	0.81
1:D:9:ARG:NH2	1:D:12:ARG:HH21	1.78	0.81
1:I:21:ILE:HD13	2:I:500:NAI:H4N	1.60	0.81
1:G:310:ASN:O	1:G:315:ASP:HB2	1.80	0.81
1:O:206:VAL:HG12	1:O:227:LEU:HD23	1.61	0.80
2:B:500:NAI:C6N	2:B:500:NAI:H51N	2.10	0.80
1:L:11:ILE:N	1:L:11:ILE:HD13	1.91	0.80
1:J:53:GLU:OE2	1:J:60:PRO:HG3	1.82	0.80
1:E:165:PRO:HB2	1:E:167:GLU:HG2	1.64	0.80
1:H:33:GLY:HA2	1:H:36:ALA:O	1.80	0.80
1:F:15:LEU:HD21	1:F:22:SER:HB2	1.62	0.79
1:D:16:VAL:HG22	1:D:67:MET:HE1	1.64	0.79
1:H:280:HIS:ND1	1:H:281:PRO:HD2	1.98	0.79
1:M:15:LEU:HD21	1:M:17:GLY:O	1.81	0.79
1:D:197:ASP:OD1	1:D:327:GLN:HG2	1.82	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:305:TYR:CA	1:E:308:VAL:HG23	2.13	0.79
1:E:310:ASN:O	1:E:315:ASP:HB2	1.83	0.79
1:B:135:ASN:HD22	1:B:135:ASN:N	1.78	0.79
1:P:9:ARG:HH22	1:P:12:ARG:NH2	1.79	0.79
1:M:216:ARG:HH11	1:M:216:ARG:HG3	0.72	0.79
1:F:90:ILE:O	1:F:94:GLN:HG3	1.83	0.79
1:C:9:ARG:HG3	1:C:9:ARG:HH11	1.48	0.79
1:C:103:LYS:O	1:C:103:LYS:HD3	1.83	0.79
1:C:327:GLN:CA	1:C:327:GLN:HE21	1.95	0.79
1:F:41:ILE:HD12	1:F:49:LEU:HD11	1.64	0.79
1:D:26:ILE:HG22	1:D:27:GLY:N	1.97	0.78
1:K:86:PRO:HA	1:K:115:MET:HG2	1.64	0.78
1:E:327:GLN:HA	1:E:327:GLN:OE1	1.83	0.78
1:N:98:HIS:HA	1:N:124:VAL:HG12	1.63	0.78
1:E:12:ARG:HD3	1:E:72:ASN:OD1	1.83	0.78
1:I:34:ASP:N	1:I:34:ASP:OD2	2.13	0.78
1:K:10:LYS:HD3	1:K:34:ASP:O	1.83	0.78
1:I:157:THR:HG21	4:I:362:HOH:O	1.84	0.78
1:L:76:LEU:N	1:L:76:LEU:HD23	1.98	0.78
1:B:124:VAL:CG1	1:B:125:ARG:N	2.47	0.78
1:L:277:ALA:C	1:L:278:GLU:HG2	2.04	0.78
1:J:29:ILE:O	1:J:31:GLN:N	2.16	0.78
1:O:42:CYS:HB2	1:O:67:MET:CE	2.14	0.77
1:N:14:GLY:HA3	1:N:76:LEU:HD23	1.63	0.77
1:B:12:ARG:CG	1:B:39:VAL:CG2	2.42	0.77
1:L:21:ILE:HD13	2:L:500:NAI:H4N	1.64	0.77
1:M:72:ASN:H	1:M:72:ASN:HD22	1.32	0.77
1:C:24:ASN:H	1:C:24:ASN:HD22	1.32	0.77
1:B:184:ALA:HA	1:B:188:GLN:NE2	2.00	0.77
1:O:310:ASN:HB2	1:O:316:CYS:SG	2.26	0.76
1:P:21:ILE:HG22	2:P:500:NAI:H52N	1.66	0.76
1:J:109:TRP:NE1	1:J:113:LYS:HE2	2.01	0.76
1:A:20:ARG:O	1:A:23:LYS:HE3	1.86	0.76
1:D:86:PRO:HA	1:D:115:MET:CG	2.15	0.76
1:A:114:ARG:HH11	1:A:114:ARG:CB	1.99	0.76
1:D:133:ARG:HH12	1:D:324:GLU:CG	1.98	0.76
1:N:53:GLU:HG2	1:N:54:ALA:N	2.01	0.76
1:M:39:VAL:HG13	1:M:40:GLU:HG3	1.68	0.76
1:E:39:VAL:O	1:E:58:ALA:HB1	1.85	0.75
1:I:269:ASN:HA	1:I:293:THR:HG21	1.68	0.75
1:I:21:ILE:HG22	2:I:500:NAI:O2N	1.87	0.75
1:O:98:HIS:CA	1:O:124:VAL:CG1	2.63	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:154:TYR:OH	4:B:353:HOH:O	2.04	0.75
2:J:500:NAI:H42N	3:J:550:HP7:H3'	1.67	0.75
1:B:307:ASN:ND2	1:B:318:PRO:HA	2.01	0.75
2:G:500:NAI:H42N	3:G:550:HP7:H3'	1.68	0.75
1:I:285:LYS:HD3	1:I:285:LYS:N	2.02	0.75
1:N:76:LEU:HD12	1:N:92:VAL:CG1	2.16	0.75
1:D:98:HIS:HA	1:D:124:VAL:HG11	1.67	0.74
1:F:41:ILE:HD12	1:F:49:LEU:CD1	2.17	0.74
1:G:21:ILE:HD13	2:G:500:NAI:H4N	1.68	0.74
1:L:108:ARG:NH1	1:L:108:ARG:CG	2.49	0.74
1:E:98:HIS:CA	1:E:124:VAL:HG13	2.16	0.74
1:D:125:ARG:HH11	1:D:125:ARG:HG2	1.52	0.74
1:A:114:ARG:NH1	1:A:114:ARG:HB2	2.00	0.74
1:D:35:ARG:HD2	1:D:313:ARG:HH12	1.52	0.74
1:K:25:HIS:ND1	1:K:305:TYR:OH	2.20	0.74
1:E:137:THR:HG21	1:E:263:VAL:HG11	1.70	0.74
1:D:291:TYR:OH	1:M:302:PRO:HD3	1.88	0.74
1:H:257:GLU:OE2	1:H:258:LYS:HE2	1.87	0.74
1:J:80:THR:HB	1:J:81:PRO:HD2	1.68	0.74
1:D:9:ARG:CZ	1:D:12:ARG:NH2	2.50	0.73
1:L:25:HIS:O	1:L:29:ILE:HG13	1.88	0.73
1:L:98:HIS:HA	1:L:124:VAL:CG1	2.17	0.73
2:C:500:NAI:H42N	3:C:550:HP7:H3'	1.68	0.73
1:O:6:ILE:HG21	1:O:11:ILE:HD13	1.69	0.73
1:O:39:VAL:CG1	1:O:40:GLU:HG3	2.11	0.73
1:D:142:LYS:NZ	1:D:146:GLU:OE2	2.20	0.73
1:N:98:HIS:CA	1:N:124:VAL:CG1	2.64	0.73
1:F:173:ARG:NH2	1:G:317:GLU:OE1	2.20	0.73
2:I:500:NAI:H42N	3:I:550:HP7:H3'	1.68	0.73
1:L:98:HIS:HA	1:L:124:VAL:HG13	1.70	0.73
1:P:9:ARG:HH12	1:P:12:ARG:CZ	2.02	0.72
1:D:53:GLU:OE1	1:D:60:PRO:HG3	1.89	0.72
1:I:103:LYS:C	1:I:103:LYS:HD3	2.09	0.72
1:I:128:VAL:O	1:I:320:THR:HG22	1.89	0.72
1:H:19:GLY:O	1:H:22:SER:OG	2.08	0.72
1:P:103:LYS:HD3	1:P:103:LYS:O	1.88	0.72
1:G:76:LEU:HD12	1:G:92:VAL:HG22	1.69	0.72
1:M:30:ALA:O	1:M:32:HIS:N	2.22	0.72
1:L:307:ASN:CG	1:L:319:GLU:HG3	2.10	0.72
1:N:103:LYS:O	1:N:103:LYS:HD3	1.90	0.72
1:D:133:ARG:NH1	1:D:324:GLU:HG2	2.04	0.71
1:D:59:ARG:HG2	1:D:60:PRO:HD2	1.72	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:274:TRP:CD1	1:D:286:ILE:HD11	2.24	0.71
1:K:253:THR:OG1	1:K:262:ARG:HG3	1.90	0.71
2:I:500:NAI:H6N	2:I:500:NAI:H51N	1.71	0.71
1:I:310:ASN:HD22	1:I:310:ASN:H	1.37	0.71
1:L:23:LYS:HA	1:L:26:ILE:HD12	1.72	0.71
1:F:86:PRO:HA	1:F:115:MET:HG2	1.73	0.71
1:H:16:VAL:HG11	1:H:78:LEU:HD23	1.72	0.71
1:L:262:ARG:HH11	1:L:262:ARG:CG	2.02	0.71
1:H:43:ASP:CG	2:H:500:NAI:O3B	2.29	0.71
1:A:67:MET:CE	1:A:76:LEU:HD22	2.20	0.71
1:J:12:ARG:HG2	1:J:39:VAL:HG21	1.73	0.71
1:L:80:THR:HB	1:L:81:PRO:HD2	1.74	0.70
1:P:39:VAL:CG1	1:P:40:GLU:CG	2.62	0.70
1:H:21:ILE:HD13	2:H:500:NAI:H4N	1.73	0.70
1:G:98:HIS:HA	1:G:124:VAL:CG1	2.19	0.70
1:D:97:ARG:O	1:D:124:VAL:HG11	1.91	0.70
1:M:86:PRO:O	1:M:90:ILE:HG13	1.91	0.70
1:B:23:LYS:HD2	1:B:23:LYS:H	1.57	0.70
1:C:327:GLN:HA	1:C:327:GLN:NE2	2.00	0.70
1:D:90:ILE:HD11	1:D:114:ARG:HG2	1.72	0.70
1:D:9:ARG:CZ	1:D:12:ARG:HH21	2.03	0.70
1:G:68:LEU:HD21	1:G:76:LEU:HD11	1.73	0.70
1:B:64:LEU:HD11	1:B:68:LEU:HD11	1.71	0.70
1:E:61:PHE:HE1	1:E:70:GLN:OE1	1.74	0.70
1:H:280:HIS:CE1	1:H:281:PRO:HD2	2.26	0.70
1:J:29:ILE:C	1:J:31:GLN:H	1.92	0.70
1:C:80:THR:HB	1:C:81:PRO:HD2	1.74	0.70
1:N:12:ARG:NH1	1:N:72:ASN:CG	2.45	0.70
1:E:168:TYR:OH	3:E:550:HP7:O'Q	2.09	0.70
1:C:86:PRO:HA	1:C:115:MET:CG	2.22	0.70
4:D:368:HOH:O	1:H:230:ARG:HD3	1.92	0.70
1:B:98:HIS:CA	1:B:124:VAL:CG1	2.62	0.70
1:H:103:LYS:C	1:H:103:LYS:HE2	2.12	0.69
1:M:310:ASN:O	1:M:315:ASP:HB2	1.92	0.69
1:K:98:HIS:ND1	1:K:125:ARG:HB2	2.07	0.69
1:F:67:MET:CE	1:F:76:LEU:HD21	2.22	0.69
1:N:98:HIS:ND1	1:N:124:VAL:HG13	2.08	0.69
1:B:80:THR:HB	1:B:81:PRO:CD	2.22	0.69
1:C:51:ALA:O	1:C:55:ALA:HB2	1.93	0.69
2:A:500:NAI:H42N	3:A:550:HP7:H3'	1.74	0.69
1:K:246:GLN:O	1:K:247:ASN:C	2.30	0.69
1:I:64:LEU:HD13	1:I:91:GLU:OE2	1.92	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:64:LEU:HD23	1:I:67:MET:HE3	1.69	0.69
1:P:9:ARG:NH2	1:P:12:ARG:NH2	2.39	0.69
1:I:310:ASN:O	1:I:313:ARG:N	2.21	0.69
1:N:31:GLN:O	1:N:31:GLN:HG2	1.93	0.69
1:D:318:PRO:HB2	1:D:321:ASP:HB3	1.74	0.69
1:L:262:ARG:HG2	1:L:262:ARG:NH1	2.07	0.69
1:D:35:ARG:HD2	1:D:313:ARG:NH1	2.06	0.69
1:B:130:LYS:CG	1:B:320:THR:HG21	2.23	0.69
1:I:90:ILE:HD11	1:I:114:ARG:HG2	1.75	0.68
1:B:12:ARG:HG2	1:B:39:VAL:HG23	1.71	0.68
1:B:127:PHE:HE1	1:B:318:PRO:CB	2.01	0.68
1:I:41:ILE:HD13	1:I:58:ALA:HB3	1.75	0.68
1:K:45:ASN:OD1	1:K:48:ALA:N	2.23	0.68
3:O:550:HP7:O2A	3:O:550:HP7:O2B	2.10	0.68
1:O:49:LEU:HD12	1:O:49:LEU:O	1.93	0.68
2:I:500:NAI:C6N	2:I:500:NAI:H51N	2.24	0.68
1:D:76:LEU:HD12	1:D:92:VAL:HG13	1.73	0.68
1:P:270:ARG:CG	1:P:272:ASP:OD1	2.40	0.68
1:J:76:LEU:CD2	1:J:76:LEU:N	2.57	0.68
1:B:130:LYS:HG3	1:B:320:THR:HG21	1.76	0.68
1:A:68:LEU:HD21	1:A:76:LEU:HD11	1.75	0.68
1:G:310:ASN:HB3	1:G:316:CYS:SG	2.33	0.68
1:D:274:TRP:CG	1:D:286:ILE:HD11	2.29	0.68
1:I:98:HIS:HA	1:I:124:VAL:HG13	1.76	0.68
1:E:103:LYS:NZ	3:E:550:HP7:O3'	2.26	0.67
1:F:206:VAL:CG1	1:F:227:LEU:HD23	2.25	0.67
1:F:97:ARG:O	1:F:124:VAL:HG11	1.94	0.67
1:N:40:GLU:C	1:N:41:ILE:HG23	2.14	0.67
1:P:277:ALA:C	1:P:278:GLU:CG	2.60	0.67
1:E:12:ARG:HH21	1:E:72:ASN:CG	1.94	0.67
1:L:32:HIS:ND1	1:L:35:ARG:NH1	2.37	0.67
1:M:39:VAL:HG12	1:M:40:GLU:HG3	1.76	0.67
1:A:80:THR:HB	1:A:81:PRO:HD2	1.75	0.67
1:I:64:LEU:CD2	1:I:67:MET:HE1	2.18	0.67
1:F:67:MET:HE2	1:F:76:LEU:CD2	2.23	0.67
1:H:127:PHE:CE1	1:H:318:PRO:HB3	2.29	0.67
1:H:86:PRO:HA	1:H:115:MET:HG2	1.75	0.67
1:H:327:GLN:CA	1:H:327:GLN:HE21	1.99	0.67
1:C:125:ARG:NH2	1:C:317:GLU:OE1	2.27	0.67
1:F:184:ALA:HA	1:F:188:GLN:NE2	2.10	0.67
1:N:280:HIS:CE1	1:N:281:PRO:HG2	2.28	0.67
1:P:21:ILE:HD13	2:P:500:NAI:H4N	1.75	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:10:LYS:HE2	1:F:34:ASP:O	1.94	0.67
1:M:15:LEU:C	1:M:15:LEU:HD23	2.14	0.67
1:H:16:VAL:CG1	1:H:78:LEU:HD23	2.25	0.67
1:H:32:HIS:O	1:H:34:ASP:N	2.27	0.66
1:G:16:VAL:HG22	1:G:67:MET:CE	2.25	0.66
1:E:35:ARG:O	1:E:36:ALA:HB2	1.96	0.66
1:L:14:GLY:HA3	1:L:67:MET:CE	2.25	0.66
1:A:110:GLU:HB2	4:A:362:HOH:O	1.94	0.66
1:O:15:LEU:HD21	1:O:22:SER:HB2	1.77	0.66
1:E:11:ILE:O	1:E:36:ALA:HB1	1.95	0.66
1:B:86:PRO:HA	1:B:115:MET:HG2	1.78	0.66
1:K:59:ARG:HG2	1:K:60:PRO:CD	2.26	0.66
2:F:500:NAI:H42N	3:F:550:HP7:H3'	1.78	0.66
1:A:46:PRO:O	1:A:50:GLN:HG3	1.94	0.66
1:M:117:LYS:HD3	1:M:121:GLU:OE2	1.96	0.66
1:I:128:VAL:O	1:I:320:THR:CG2	2.44	0.66
1:A:197:ASP:OD1	1:A:327:GLN:HG2	1.95	0.66
1:O:98:HIS:CA	1:O:124:VAL:HG13	2.26	0.66
1:H:154:TYR:OH	1:H:257:GLU:HB2	1.96	0.66
1:K:59:ARG:HG2	1:K:60:PRO:HD2	1.78	0.66
1:E:39:VAL:C	1:E:58:ALA:HB1	2.16	0.65
1:B:41:ILE:HG13	1:B:49:LEU:CD1	2.25	0.65
2:H:500:NAI:H51N	2:H:500:NAI:H6N	1.77	0.65
1:L:310:ASN:O	1:L:315:ASP:HB2	1.96	0.65
1:P:86:PRO:CA	1:P:115:MET:HG2	2.26	0.65
1:H:16:VAL:HG11	1:H:78:LEU:CD2	2.26	0.65
1:L:103:LYS:O	1:L:103:LYS:HD3	1.97	0.65
1:P:261:VAL:HA	1:P:273:GLU:O	1.96	0.65
1:O:103:LYS:HD2	1:O:103:LYS:C	2.16	0.65
1:H:16:VAL:CG1	1:H:78:LEU:HA	2.27	0.65
1:E:98:HIS:HA	1:E:124:VAL:HG11	1.76	0.65
1:O:310:ASN:CB	1:O:316:CYS:SG	2.85	0.65
1:P:21:ILE:CG2	2:P:500:NAI:H52N	2.27	0.65
1:P:117:LYS:CD	1:P:117:LYS:C	2.66	0.65
1:F:139:GLN:O	1:F:143:LYS:HG2	1.97	0.65
1:P:142:LYS:HE2	1:P:198:TRP:NE1	2.12	0.65
1:E:15:LEU:HD11	1:E:17:GLY:O	1.97	0.65
1:E:166:GLN:NE2	1:E:216:ARG:H	1.94	0.65
1:H:317:GLU:HA	1:H:317:GLU:OE2	1.97	0.65
1:J:206:VAL:HG12	1:J:227:LEU:HD23	1.79	0.64
1:E:301:HIS:N	1:E:302:PRO:HD2	2.11	0.64
1:B:166:GLN:N	4:B:366:HOH:O	1.77	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:259:GLY:HA2	1:L:275:LYS:O	1.98	0.64
1:K:16:VAL:HG22	1:K:67:MET:HE1	1.80	0.64
1:P:97:ARG:O	1:P:124:VAL:CG1	2.42	0.64
1:B:12:ARG:CD	1:B:39:VAL:HG21	2.28	0.64
1:O:97:ARG:O	1:O:124:VAL:CG1	2.42	0.64
1:K:86:PRO:HA	1:K:115:MET:CG	2.26	0.64
1:E:327:GLN:CA	1:E:327:GLN:OE1	2.45	0.64
1:F:43:ASP:OD2	2:F:500:NAI:O3B	2.14	0.64
1:O:86:PRO:HA	1:O:115:MET:HG2	1.79	0.64
1:M:13:PHE:O	1:M:38:LEU:HD12	1.98	0.64
1:G:32:HIS:ND1	1:G:35:ARG:NH1	2.46	0.64
1:A:110:GLU:HG3	4:A:363:HOH:O	1.98	0.64
1:O:267:ALA:O	1:O:268:VAL:C	2.37	0.64
1:E:38:LEU:HD21	1:E:41:ILE:CG2	2.28	0.64
1:A:80:THR:HB	1:A:81:PRO:CD	2.28	0.64
1:L:176:GLY:O	1:L:218:GLU:HB2	1.97	0.64
1:L:20:ARG:HG2	1:L:20:ARG:HH11	1.61	0.64
1:B:127:PHE:CE1	1:B:318:PRO:CB	2.80	0.63
1:E:304:TYR:O	1:E:308:VAL:HG23	1.98	0.63
1:O:340:ARG:HD2	1:O:341:ASP:OD1	1.96	0.63
1:K:25:HIS:O	1:K:29:ILE:HG13	1.97	0.63
1:L:20:ARG:NH1	1:L:20:ARG:HG2	2.13	0.63
1:A:16:VAL:HG22	1:A:67:MET:CE	2.28	0.63
1:D:35:ARG:NH1	1:D:306:ASP:OD1	2.32	0.63
1:L:92:VAL:CG1	1:L:92:VAL:O	2.46	0.63
1:H:28:ALA:O	1:H:32:HIS:HD2	1.81	0.63
1:N:86:PRO:O	1:N:90:ILE:HG13	1.98	0.63
1:I:224:VAL:HG21	1:J:235:GLY:HA2	1.80	0.63
1:P:253:THR:OG1	1:P:262:ARG:HG3	1.98	0.63
1:L:11:ILE:N	1:L:11:ILE:CD1	2.62	0.63
1:F:67:MET:CE	1:F:76:LEU:CD2	2.77	0.63
2:C:500:NAI:H51N	2:C:500:NAI:H6N	1.80	0.63
1:J:80:THR:HB	1:J:81:PRO:CD	2.28	0.63
1:L:92:VAL:HG12	1:L:92:VAL:O	1.98	0.63
1:O:184:ALA:HA	1:O:188:GLN:HE21	1.64	0.63
1:B:97:ARG:O	1:B:124:VAL:HG11	1.99	0.63
1:D:86:PRO:O	1:D:90:ILE:HG13	1.99	0.63
1:I:142:LYS:HE3	1:I:146:GLU:OE2	1.99	0.63
1:O:39:VAL:HG11	1:O:72:ASN:HD21	1.64	0.63
1:E:103:LYS:C	1:E:103:LYS:CD	2.67	0.63
1:H:98:HIS:HA	1:H:124:VAL:HG13	1.80	0.63
1:E:90:ILE:O	1:E:94:GLN:HG3	1.99	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:246:GLN:O	1:L:247:ASN:C	2.36	0.63
1:C:24:ASN:N	1:C:24:ASN:HD22	1.97	0.62
1:B:301:HIS:N	1:B:302:PRO:HD2	2.14	0.62
1:F:40:GLU:OE2	1:F:72:ASN:N	2.32	0.62
1:E:38:LEU:HD11	1:E:40:GLU:O	1.99	0.62
1:F:21:ILE:HD13	2:F:500:NAI:H4N	1.80	0.62
1:J:134:ARG:NH2	1:J:319:GLU:OE2	2.28	0.62
1:M:98:HIS:ND1	1:M:124:VAL:HG13	2.14	0.62
1:L:29:ILE:O	1:L:31:GLN:N	2.33	0.62
1:B:184:ALA:HA	1:B:188:GLN:HE21	1.63	0.62
1:H:133:ARG:O	1:H:139:GLN:OE1	2.16	0.62
1:M:291:TYR:CD1	1:M:291:TYR:C	2.72	0.62
1:E:12:ARG:NH2	1:E:72:ASN:CG	2.53	0.62
1:K:18:CYS:HA	1:K:22:SER:OG	2.00	0.62
1:O:80:THR:HB	1:O:81:PRO:HD2	1.82	0.62
1:E:43:ASP:OD2	2:E:500:NAI:O3B	2.16	0.62
1:L:317:GLU:HA	1:L:317:GLU:OE2	1.95	0.62
1:B:135:ASN:H	1:B:135:ASN:HD22	1.47	0.62
1:M:30:ALA:O	1:M:33:GLY:N	2.33	0.62
1:B:101:SER:O	1:B:129:VAL:HG23	1.99	0.62
1:E:181:ASP:OD1	1:E:187:ASN:ND2	2.28	0.61
1:I:41:ILE:HD11	1:I:53:GLU:HA	1.81	0.61
1:J:310:ASN:O	1:J:315:ASP:HB2	2.00	0.61
1:I:30:ALA:O	1:I:33:GLY:N	2.32	0.61
1:M:86:PRO:HA	1:M:115:MET:CG	2.30	0.61
1:K:82:SER:HB3	1:K:104:PRO:HD2	1.81	0.61
1:L:97:ARG:O	1:L:124:VAL:HG11	2.00	0.61
1:L:37:GLU:O	1:L:37:GLU:HG3	2.00	0.61
1:J:262:ARG:HG2	1:J:262:ARG:HH11	1.66	0.61
1:M:216:ARG:CG	1:M:216:ARG:NH1	2.36	0.61
1:G:76:LEU:CD1	1:G:92:VAL:HG22	2.31	0.61
1:L:14:GLY:HA3	1:L:67:MET:HE1	1.81	0.61
1:C:301:HIS:N	1:C:302:PRO:HD2	2.16	0.61
1:P:184:ALA:HA	1:P:188:GLN:OE1	1.99	0.61
1:D:333:THR:O	1:D:337:ARG:HG3	2.00	0.61
1:G:280:HIS:CG	1:G:281:PRO:HD2	2.36	0.61
1:H:72:ASN:H	1:H:72:ASN:HD22	1.48	0.61
1:N:59:ARG:NH1	1:N:59:ARG:HG3	2.15	0.61
1:H:103:LYS:HD3	1:H:103:LYS:C	2.21	0.61
1:C:81:PRO:HD2	1:C:84:LEU:HD12	1.83	0.61
1:M:80:THR:HB	1:M:81:PRO:HD2	1.82	0.61
1:L:40:GLU:OE1	1:L:71:GLY:HA3	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:90:ILE:HD13	1:E:114:ARG:HD3	1.83	0.61
1:D:287:ARG:NH2	3:M:550:HP7:O1B	2.34	0.60
1:I:77:VAL:HG21	1:I:305:TYR:OH	2.01	0.60
1:E:98:HIS:CA	1:E:124:VAL:CG1	2.64	0.60
1:C:156:VAL:O	1:C:235:GLY:HA3	2.02	0.60
1:L:137:THR:O	1:L:141:VAL:HG23	2.01	0.60
1:A:98:HIS:HA	1:A:124:VAL:HG13	1.82	0.60
1:E:117:LYS:O	1:E:120:ASP:HB2	2.01	0.60
1:K:39:VAL:C	1:K:40:GLU:CG	2.69	0.60
1:D:287:ARG:NH1	1:M:24:ASN:CG	2.54	0.60
1:N:230:ARG:NE	4:N:452:HOH:O	2.30	0.60
1:L:110:GLU:HG3	4:L:437:HOH:O	2.02	0.60
1:E:175:ARG:HH21	1:E:175:ARG:HG2	1.67	0.60
1:B:98:HIS:CA	1:B:124:VAL:HG11	2.22	0.60
1:K:34:ASP:OD1	1:K:35:ARG:HG3	2.01	0.60
1:D:287:ARG:NE	1:M:298:GLY:O	2.34	0.60
1:I:21:ILE:CD1	2:I:500:NAI:H4N	2.31	0.60
1:D:53:GLU:O	1:D:57:GLY:N	2.34	0.60
1:D:39:VAL:CG1	1:D:40:GLU:CG	2.59	0.60
1:A:249:GLU:OE2	1:B:262:ARG:NH2	2.30	0.60
1:E:267:ALA:O	1:E:268:VAL:C	2.39	0.60
1:P:98:HIS:CA	1:P:124:VAL:CG1	2.74	0.60
1:G:103:LYS:HD3	1:G:103:LYS:O	2.02	0.60
1:L:184:ALA:HA	1:L:188:GLN:HE21	1.62	0.60
1:M:53:GLU:HG3	1:M:60:PRO:HG3	1.83	0.60
1:F:86:PRO:HA	1:F:115:MET:CG	2.32	0.59
1:O:184:ALA:HA	1:O:188:GLN:NE2	2.17	0.59
1:I:80:THR:HB	1:I:81:PRO:HD2	1.84	0.59
1:B:265:GLY:N	4:B:380:HOH:O	2.06	0.59
1:L:86:PRO:HA	1:L:115:MET:CG	2.32	0.59
1:I:64:LEU:HA	1:I:67:MET:HE2	1.83	0.59
1:N:12:ARG:HB3	1:N:39:VAL:HG21	1.83	0.59
1:I:306:ASP:O	1:I:310:ASN:ND2	2.34	0.59
1:L:80:THR:HB	1:L:81:PRO:CD	2.32	0.59
1:I:39:VAL:HG12	1:I:40:GLU:HG2	1.84	0.59
1:K:206:VAL:CG1	1:K:227:LEU:HD23	2.27	0.59
1:H:29:ILE:O	1:H:32:HIS:N	2.26	0.59
1:P:87:TRP:HH2	1:P:114:ARG:HH21	1.50	0.59
1:E:98:HIS:ND1	1:E:125:ARG:HB2	2.17	0.59
1:P:97:ARG:C	1:P:124:VAL:HG11	2.21	0.59
1:M:58:ALA:O	1:M:60:PRO:HD3	2.02	0.59
1:I:35:ARG:HB3	1:I:313:ARG:NH1	2.17	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:9:ARG:NH2	1:D:12:ARG:NH2	2.51	0.59
2:E:500:NAI:H42N	3:E:550:HP7:H3'	1.85	0.59
2:H:500:NAI:C6N	2:H:500:NAI:H51N	2.33	0.59
1:J:58:ALA:O	1:J:60:PRO:CD	2.47	0.59
1:A:76:LEU:HD12	1:A:92:VAL:HG22	1.85	0.59
1:E:248:LEU:HD22	1:F:260:THR:HG21	1.84	0.59
1:M:25:HIS:O	1:M:29:ILE:HD12	2.03	0.59
1:G:10:LYS:HB3	1:G:36:ALA:HA	1.85	0.59
1:D:125:ARG:HH11	1:D:125:ARG:CG	2.15	0.59
3:K:550:HP7:O5C	3:K:550:HP7:H6	2.03	0.59
1:D:68:LEU:HD21	1:D:76:LEU:CD1	2.33	0.59
1:K:39:VAL:O	1:K:40:GLU:HG2	2.03	0.59
1:B:23:LYS:HD2	1:B:23:LYS:N	2.17	0.59
1:A:81:PRO:HB3	1:A:174:TRP:CD2	2.38	0.59
1:O:42:CYS:CB	1:O:67:MET:HE1	2.31	0.58
1:H:28:ALA:HB2	1:H:302:PRO:HD3	1.85	0.58
1:E:15:LEU:HD12	1:E:16:VAL:O	2.02	0.58
1:E:246:GLN:O	1:E:247:ASN:C	2.41	0.58
1:I:64:LEU:HD22	1:I:64:LEU:O	2.03	0.58
1:D:47:GLU:HG3	1:D:50:GLN:NE2	2.18	0.58
1:F:11:ILE:N	1:F:11:ILE:HD13	2.17	0.58
1:N:12:ARG:HH12	1:N:72:ASN:CG	2.06	0.58
1:J:173:ARG:O	1:J:177:LYS:CE	2.48	0.58
1:B:43:ASP:OD1	2:B:500:NAI:O2B	2.16	0.58
1:G:124:VAL:CG1	1:G:125:ARG:N	2.66	0.58
1:C:328:SER:HB3	4:C:373:HOH:O	2.02	0.58
1:I:310:ASN:ND2	1:I:310:ASN:N	2.48	0.58
1:L:98:HIS:ND1	1:L:125:ARG:HB2	2.19	0.58
1:P:248:LEU:HD12	1:P:248:LEU:O	2.04	0.58
1:E:137:THR:CG2	1:E:263:VAL:HG11	2.32	0.58
1:F:61:PHE:CD2	1:F:67:MET:HG3	2.38	0.58
1:L:29:ILE:O	1:L:30:ALA:C	2.42	0.58
1:L:310:ASN:HB3	1:L:315:ASP:HB3	1.86	0.58
1:D:24:ASN:O	1:D:28:ALA:HB2	2.04	0.58
1:K:278:GLU:HG3	1:K:278:GLU:O	2.01	0.58
1:H:43:ASP:OD1	2:H:500:NAI:O3B	2.22	0.58
1:O:130:LYS:HB2	1:O:320:THR:HG21	1.85	0.58
1:H:193:VAL:HG13	1:H:331:LEU:HD13	1.86	0.58
1:P:9:ARG:HH22	1:P:12:ARG:HH21	1.48	0.58
1:E:166:GLN:HE22	1:E:216:ARG:H	1.51	0.58
1:D:98:HIS:HA	1:D:124:VAL:HG12	1.83	0.57
1:I:140:LEU:HD11	1:I:289:ALA:HB2	1.84	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:301:HIS:N	1:K:302:PRO:HD2	2.19	0.57
1:N:278:GLU:HG2	4:N:503:HOH:O	2.02	0.57
1:N:97:ARG:C	1:N:124:VAL:HG11	2.24	0.57
1:H:103:LYS:O	1:H:103:LYS:CD	2.51	0.57
1:C:21:ILE:CD1	2:C:500:NAI:H4N	2.33	0.57
1:O:188:GLN:HG2	1:O:241:MET:SD	2.44	0.57
1:O:261:VAL:HA	1:O:273:GLU:O	2.04	0.57
1:C:24:ASN:ND2	1:C:24:ASN:N	2.53	0.57
1:H:245:PRO:HD2	1:H:246:GLN:HG2	1.85	0.57
1:K:10:LYS:CD	1:K:34:ASP:O	2.51	0.57
1:O:21:ILE:HD13	2:O:500:NAI:H4N	1.86	0.57
1:D:68:LEU:HD21	1:D:76:LEU:HD13	1.86	0.57
1:H:283:ASP:O	1:H:286:ILE:HD12	2.05	0.57
1:L:157:THR:HG22	1:L:236:SER:OG	2.03	0.57
1:N:72:ASN:H	1:N:72:ASN:HD22	1.52	0.57
1:B:98:HIS:HA	1:B:124:VAL:HG12	1.81	0.57
1:D:288:GLU:O	1:D:291:TYR:HB2	2.05	0.57
1:B:72:ASN:HD22	1:B:72:ASN:H	1.52	0.57
1:C:127:PHE:CE1	1:C:318:PRO:HB3	2.40	0.57
1:J:298:GLY:C	1:J:299:PHE:CD2	2.77	0.57
1:D:39:VAL:C	1:D:40:GLU:HG3	2.23	0.57
1:K:20:ARG:NH2	3:K:550:HP7:H5C	2.20	0.57
1:H:72:ASN:N	1:H:72:ASN:HD22	2.03	0.57
1:H:80:THR:HB	1:H:81:PRO:HD2	1.86	0.57
1:D:175:ARG:HH21	1:D:175:ARG:HG2	1.70	0.57
1:M:206:VAL:HG12	1:M:227:LEU:HD23	1.87	0.57
1:I:10:LYS:CD	1:I:34:ASP:O	2.53	0.57
1:L:267:ALA:O	1:L:268:VAL:HG23	2.04	0.57
1:D:108:ARG:NH2	1:D:179:GLU:HG3	2.20	0.57
1:E:305:TYR:C	1:E:308:VAL:HG23	2.26	0.56
1:H:103:LYS:CD	1:H:103:LYS:C	2.73	0.56
1:N:282:ASP:HA	1:N:285:LYS:HE2	1.87	0.56
1:H:157:THR:HG22	1:H:236:SER:OG	2.05	0.56
1:E:80:THR:HB	1:E:81:PRO:HD2	1.87	0.56
1:M:61:PHE:CD1	1:M:67:MET:HA	2.40	0.56
1:P:68:LEU:HD21	1:P:76:LEU:CD1	2.34	0.56
1:K:51:ALA:O	1:K:55:ALA:HB2	2.04	0.56
1:B:9:ARG:HH11	1:B:9:ARG:HG3	1.70	0.56
1:N:98:HIS:HA	1:N:124:VAL:HG11	1.80	0.56
2:K:500:NAI:H51N	2:K:500:NAI:H6N	1.86	0.56
1:M:98:HIS:HA	1:M:124:VAL:HG11	1.85	0.56
1:L:14:GLY:CA	1:L:67:MET:CE	2.83	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:26:ILE:HD13	1:G:56:THR:CG2	2.35	0.56
1:N:133:ARG:HH12	1:N:324:GLU:HG2	1.70	0.56
1:N:157:THR:HG21	4:N:473:HOH:O	2.04	0.56
1:G:12:ARG:HB2	1:G:74:ASP:OD2	2.05	0.56
1:J:194:ASP:OD2	4:J:386:HOH:O	2.18	0.56
1:E:53:GLU:HG3	1:E:54:ALA:N	2.18	0.56
1:B:72:ASN:HD22	1:B:72:ASN:N	2.04	0.56
1:A:297:TYR:HA	4:A:401:HOH:O	2.05	0.56
1:G:139:GLN:O	1:G:143:LYS:HG3	2.05	0.56
1:K:184:ALA:HA	1:K:188:GLN:NE2	2.21	0.56
1:G:134:ARG:HH21	1:G:319:GLU:HG2	1.69	0.56
1:B:307:ASN:ND2	1:B:307:ASN:C	2.59	0.56
1:I:310:ASN:O	1:I:311:CYS:C	2.42	0.56
1:L:15:LEU:HD23	1:L:16:VAL:H	1.69	0.56
1:P:273:GLU:OE2	1:P:275:LYS:HE3	2.06	0.56
1:E:15:LEU:HD12	1:E:16:VAL:N	2.21	0.56
1:L:301:HIS:HB2	1:L:302:PRO:HD3	1.87	0.56
1:J:197:ASP:OD1	1:J:327:GLN:HG2	2.06	0.56
1:G:21:ILE:CD1	2:G:500:NAI:H4N	2.36	0.56
1:N:309:ILE:O	1:N:313:ARG:HG3	2.06	0.56
1:D:134:ARG:O	1:D:135:ASN:C	2.42	0.56
1:E:303:LEU:H	1:E:303:LEU:HD12	1.71	0.56
1:H:297:TYR:C	1:H:297:TYR:CD2	2.79	0.56
1:K:39:VAL:CG1	1:K:39:VAL:O	2.54	0.55
1:P:76:LEU:HD12	1:P:92:VAL:HG13	1.89	0.55
1:B:244:TYR:CE1	1:B:245:PRO:HB3	2.41	0.55
1:A:109:TRP:NE1	1:A:113:LYS:HE2	2.21	0.55
1:O:40:GLU:OE2	1:O:71:GLY:CA	2.55	0.55
1:H:288:GLU:CA	1:H:291:TYR:HB2	2.33	0.55
1:C:80:THR:HB	1:C:81:PRO:CD	2.36	0.55
1:G:266:VAL:HG22	4:G:389:HOH:O	2.05	0.55
1:N:34:ASP:OD2	1:N:34:ASP:N	2.32	0.55
1:A:68:LEU:HD21	1:A:76:LEU:CD1	2.37	0.55
1:P:154:TYR:OH	1:P:257:GLU:HB2	2.06	0.55
1:B:10:LYS:HE2	1:B:33:GLY:O	2.06	0.55
1:D:166:GLN:HG3	1:D:166:GLN:O	2.06	0.55
1:O:53:GLU:CG	1:O:60:PRO:HG3	2.27	0.55
1:H:24:ASN:N	1:H:24:ASN:HD22	2.04	0.55
1:N:39:VAL:O	1:N:58:ALA:CB	2.52	0.55
1:C:328:SER:CB	4:C:373:HOH:O	2.53	0.55
1:I:31:GLN:O	1:I:31:GLN:CG	2.55	0.55
1:J:40:GLU:OE2	1:J:72:ASN:N	2.35	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:317:GLU:HB3	1:P:318:PRO:HD2	1.89	0.55
1:P:277:ALA:O	1:P:278:GLU:CG	2.49	0.55
1:F:68:LEU:CD1	1:F:91:GLU:HG2	2.36	0.55
1:B:313:ARG:CG	1:B:313:ARG:NH1	2.46	0.55
1:O:42:CYS:O	1:O:43:ASP:HB2	2.07	0.55
1:N:282:ASP:HA	1:N:285:LYS:CE	2.35	0.55
2:C:500:NAI:H51N	2:C:500:NAI:C6N	2.37	0.55
1:M:15:LEU:HD11	1:M:22:SER:HB2	1.88	0.55
1:B:28:ALA:HB2	1:B:302:PRO:HD3	1.88	0.55
1:H:135:ASN:O	1:H:139:GLN:HG2	2.06	0.55
1:P:88:GLN:O	1:P:92:VAL:HG23	2.06	0.55
1:F:245:PRO:HD2	1:F:246:GLN:H	1.72	0.55
1:N:124:VAL:HG12	1:N:125:ARG:N	2.21	0.55
1:E:12:ARG:HG2	1:E:74:ASP:CG	2.24	0.55
1:E:12:ARG:HG3	1:E:73:ALA:HA	1.89	0.55
1:N:53:GLU:C	1:N:55:ALA:H	2.10	0.55
1:L:222:THR:HG23	1:L:240:THR:HB	1.88	0.55
1:M:98:HIS:HA	1:M:124:VAL:HG13	1.84	0.55
1:L:246:GLN:O	1:L:247:ASN:O	2.25	0.55
1:L:86:PRO:HA	1:L:115:MET:HG2	1.87	0.55
1:B:206:VAL:HG12	1:B:227:LEU:HD23	1.89	0.55
1:J:285:LYS:NZ	1:J:288:GLU:OE1	2.30	0.55
1:H:280:HIS:ND1	1:H:281:PRO:CD	2.69	0.54
1:K:301:HIS:N	1:K:302:PRO:CD	2.70	0.54
1:A:157:THR:HG22	1:A:253:THR:HB	1.89	0.54
1:H:39:VAL:C	1:H:40:GLU:HG3	2.27	0.54
1:J:156:VAL:O	1:J:235:GLY:HA3	2.07	0.54
1:E:80:THR:HB	1:E:81:PRO:CD	2.36	0.54
1:E:101:SER:O	1:E:129:VAL:HG23	2.07	0.54
1:C:15:LEU:HD21	1:C:22:SER:HB2	1.89	0.54
1:E:133:ARG:O	1:E:139:GLN:NE2	2.37	0.54
1:I:310:ASN:ND2	1:I:310:ASN:H	2.02	0.54
1:E:10:LYS:HE2	1:E:33:GLY:O	2.06	0.54
1:P:35:ARG:NH2	1:P:310:ASN:OD1	2.40	0.54
1:A:16:VAL:HG22	1:A:67:MET:HE1	1.89	0.54
1:B:135:ASN:ND2	1:B:135:ASN:N	2.52	0.54
1:E:38:LEU:HD21	1:E:41:ILE:HG23	1.89	0.54
1:L:76:LEU:CD2	1:L:76:LEU:N	2.69	0.54
1:M:82:SER:HA	1:M:85:HIS:CE1	2.43	0.54
1:L:310:ASN:C	1:L:315:ASP:HB2	2.27	0.54
1:N:59:ARG:CG	1:N:59:ARG:HH11	2.19	0.54
1:J:296:VAL:O	1:J:297:TYR:C	2.44	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:46:PRO:O	1:L:49:LEU:HB3	2.07	0.54
1:N:331:LEU:HD23	1:N:347:LEU:HD11	1.90	0.54
1:F:149:ARG:O	1:F:258:LYS:HG3	2.07	0.54
1:G:124:VAL:HG12	1:G:125:ARG:N	2.23	0.54
4:I:362:HOH:O	1:J:157:THR:HG21	2.06	0.54
1:C:318:PRO:HG2	1:C:321:ASP:HB3	1.89	0.54
1:P:271:ILE:HD13	1:P:274:TRP:CE3	2.43	0.54
1:P:271:ILE:O	1:P:271:ILE:HG22	2.08	0.54
1:E:214:ALA:HB3	1:E:242:LEU:HD22	1.89	0.54
1:D:90:ILE:CD1	1:D:114:ARG:HG2	2.38	0.54
1:D:46:PRO:O	1:D:50:GLN:HG3	2.08	0.54
1:M:203:VAL:HG21	1:M:331:LEU:HD11	1.89	0.54
1:F:310:ASN:HB3	1:F:316:CYS:SG	2.48	0.54
1:I:224:VAL:HG21	1:J:235:GLY:CA	2.37	0.54
1:L:300:GLY:O	1:L:303:LEU:HB2	2.07	0.54
1:K:24:ASN:H	1:K:24:ASN:HD22	1.56	0.54
1:I:346:PRO:HB2	1:O:340:ARG:HG2	1.90	0.53
1:L:262:ARG:CG	1:L:262:ARG:NH1	2.66	0.53
1:F:98:HIS:ND1	1:F:125:ARG:HB2	2.23	0.53
1:G:68:LEU:HD21	1:G:76:LEU:CD1	2.36	0.53
1:G:68:LEU:CD2	1:G:76:LEU:HD11	2.39	0.53
1:C:173:ARG:O	1:C:177:LYS:HE3	2.08	0.53
1:E:12:ARG:NH2	1:E:72:ASN:HD21	2.06	0.53
1:L:9:ARG:HG3	1:L:10:LYS:H	1.67	0.53
1:J:167:GLU:H	1:J:167:GLU:CD	2.12	0.53
1:E:12:ARG:NH2	1:E:72:ASN:ND2	2.56	0.53
1:H:16:VAL:HG12	1:H:77:VAL:O	2.07	0.53
1:D:35:ARG:HB3	1:D:313:ARG:NH1	2.24	0.53
1:P:53:GLU:HG3	1:P:54:ALA:N	2.23	0.53
1:C:141:VAL:HG22	1:C:261:VAL:HG11	1.91	0.53
1:N:301:HIS:N	1:N:302:PRO:CD	2.72	0.53
1:E:12:ARG:HH22	1:E:72:ASN:HD21	1.55	0.53
1:E:175:ARG:NH2	1:E:175:ARG:HG2	2.23	0.53
1:L:43:ASP:OD2	2:L:500:NAI:O3B	2.27	0.53
1:J:103:LYS:HD3	1:J:103:LYS:C	2.29	0.53
1:M:102:GLU:HG3	2:M:500:NAI:O4D	2.09	0.53
1:E:272:ASP:O	1:E:273:GLU:HB2	2.09	0.53
1:K:307:ASN:ND2	1:K:307:ASN:O	2.42	0.53
1:A:16:VAL:HG22	1:A:67:MET:HE2	1.89	0.53
1:P:317:GLU:HB3	1:P:318:PRO:CD	2.39	0.53
1:B:11:ILE:HB	1:B:36:ALA:HB2	1.91	0.53
1:M:125:ARG:HG2	1:M:127:PHE:CE2	2.44	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:344:ARG:HD3	1:L:207:TYR:OH	2.08	0.53
1:E:228:ARG:HD3	4:E:358:HOH:O	2.08	0.53
1:B:66:ASP:O	1:B:70:GLN:HG3	2.09	0.53
1:O:39:VAL:HG12	1:O:40:GLU:CG	2.14	0.53
1:N:40:GLU:C	1:N:41:ILE:CG2	2.77	0.53
1:G:157:THR:HG21	4:H:375:HOH:O	2.07	0.53
4:L:454:HOH:O	1:N:231:HIS:HB3	2.08	0.53
1:L:340:ARG:HH22	1:N:350:ASP:CG	2.12	0.53
1:J:20:ARG:NH2	3:J:550:HP7:O2A	2.40	0.52
1:N:98:HIS:CA	1:N:124:VAL:HG13	2.39	0.52
1:B:313:ARG:HH11	1:B:313:ARG:HG3	1.69	0.52
1:N:98:HIS:HA	1:N:124:VAL:HG13	1.82	0.52
1:G:97:ARG:O	1:G:124:VAL:HG11	2.09	0.52
1:B:309:ILE:O	1:B:310:ASN:C	2.48	0.52
1:H:32:HIS:C	1:H:34:ASP:H	2.10	0.52
1:O:81:PRO:HD2	1:O:84:LEU:HD12	1.90	0.52
1:O:156:VAL:O	1:O:235:GLY:HA3	2.07	0.52
1:I:21:ILE:CG2	2:I:500:NAI:H52N	2.39	0.52
1:B:130:LYS:HG2	1:B:320:THR:HG21	1.90	0.52
1:L:40:GLU:HB2	1:L:67:MET:CE	2.39	0.52
1:F:39:VAL:HG12	1:F:40:GLU:HG3	1.90	0.52
1:H:133:ARG:HD3	1:H:198:TRP:CE2	2.43	0.52
1:A:235:GLY:HA2	1:B:224:VAL:HG21	1.91	0.52
1:I:204:GLU:HG2	1:I:204:GLU:O	2.07	0.52
1:D:197:ASP:OD1	1:D:327:GLN:CG	2.56	0.52
1:O:80:THR:HB	1:O:81:PRO:CD	2.38	0.52
1:G:129:VAL:HG22	1:G:304:TYR:CE1	2.45	0.52
1:D:98:HIS:ND1	1:D:124:VAL:HG13	2.24	0.52
1:L:108:ARG:NH1	1:L:108:ARG:HG3	2.24	0.52
1:H:68:LEU:CD1	1:H:91:GLU:HG2	2.40	0.52
1:O:98:HIS:CD2	1:O:312:LEU:HD22	2.45	0.52
1:D:130:LYS:HB2	1:D:320:THR:HG21	1.91	0.52
1:L:10:LYS:O	1:L:12:ARG:HG3	2.10	0.52
1:P:103:LYS:CD	1:P:103:LYS:C	2.70	0.52
1:L:20:ARG:CG	1:L:20:ARG:HH11	2.21	0.52
1:N:301:HIS:N	1:N:302:PRO:HD2	2.25	0.52
1:B:134:ARG:HB3	1:B:303:LEU:HD13	1.92	0.52
1:A:15:LEU:HD21	1:A:22:SER:HB2	1.91	0.52
1:M:34:ASP:OD1	1:M:35:ARG:HG3	2.09	0.52
1:E:187:ASN:OD1	3:E:550:HP7:O4'	2.22	0.52
1:K:103:LYS:O	1:K:103:LYS:CD	2.46	0.52
1:G:53:GLU:HG3	1:G:60:PRO:HB3	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:35:ARG:HG2	1:H:313:ARG:HH12	1.71	0.52
1:H:127:PHE:HE1	1:H:318:PRO:HB3	1.72	0.52
1:G:277:ALA:HA	1:H:244:TYR:OH	2.10	0.52
1:K:9:ARG:CG	1:K:9:ARG:NH1	2.51	0.52
1:E:40:GLU:OE1	1:E:73:ALA:HB2	2.09	0.52
1:J:73:ALA:HB3	1:J:76:LEU:HD21	1.91	0.52
1:G:59:ARG:HG2	1:G:60:PRO:HD2	1.91	0.52
1:A:110:GLU:CG	4:A:363:HOH:O	2.55	0.52
1:J:127:PHE:CE1	1:J:318:PRO:HB3	2.45	0.52
1:J:21:ILE:HD13	2:J:500:NAI:H4N	1.92	0.52
1:O:6:ILE:HG21	1:O:11:ILE:CD1	2.37	0.52
1:A:72:ASN:H	1:A:72:ASN:HD22	1.57	0.52
1:I:220:GLU:O	1:I:220:GLU:HG2	2.09	0.52
1:K:20:ARG:HH22	3:K:550:HP7:H5C	1.73	0.51
1:B:53:GLU:O	1:B:57:GLY:N	2.31	0.51
1:B:39:VAL:O	1:B:58:ALA:HB1	2.10	0.51
1:G:50:GLN:O	1:G:53:GLU:HB2	2.10	0.51
1:A:76:LEU:CD1	1:A:92:VAL:HG22	2.40	0.51
1:H:280:HIS:CG	1:H:281:PRO:HD2	2.45	0.51
1:H:16:VAL:HG12	1:H:78:LEU:HA	1.92	0.51
1:N:59:ARG:CG	1:N:59:ARG:NH1	2.72	0.51
1:G:16:VAL:CG2	1:G:67:MET:HE1	2.37	0.51
1:K:67:MET:HE1	1:K:76:LEU:HD22	1.92	0.51
1:E:184:ALA:HA	1:E:188:GLN:OE1	2.10	0.51
1:N:72:ASN:N	1:N:72:ASN:HD22	2.08	0.51
1:D:318:PRO:O	1:D:320:THR:N	2.44	0.51
1:I:10:LYS:HD3	1:I:34:ASP:O	2.11	0.51
1:N:282:ASP:OD1	1:N:285:LYS:CE	2.53	0.51
2:G:500:NAI:C4N	3:G:550:HP7:H3'	2.40	0.51
1:M:85:HIS:N	1:M:86:PRO:CD	2.74	0.51
1:H:86:PRO:HA	1:H:115:MET:CG	2.41	0.51
1:P:117:LYS:HD2	1:P:118:ALA:N	2.26	0.51
1:J:127:PHE:CD1	1:J:318:PRO:HB3	2.45	0.51
1:J:145:ILE:HG22	1:J:146:GLU:N	2.24	0.51
1:B:109:TRP:NE1	1:B:113:LYS:HE2	2.26	0.51
1:K:39:VAL:C	1:K:40:GLU:HG3	2.31	0.51
1:H:20:ARG:NH2	3:H:550:HP7:O2A	2.43	0.51
1:D:59:ARG:HG2	1:D:60:PRO:CD	2.41	0.51
1:F:86:PRO:HB3	1:F:115:MET:HG3	1.92	0.51
1:F:10:LYS:CE	1:F:34:ASP:O	2.59	0.51
1:O:137:THR:OG1	1:O:138:LEU:N	2.44	0.51
1:F:80:THR:HB	1:F:81:PRO:HD2	1.91	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:97:ARG:C	1:E:124:VAL:HG11	2.27	0.51
1:B:307:ASN:ND2	1:B:307:ASN:O	2.43	0.51
1:O:282:ASP:OD1	1:O:285:LYS:NZ	2.40	0.51
1:O:117:LYS:HG2	1:O:121:GLU:OE2	2.11	0.51
1:M:261:VAL:HG12	1:M:262:ARG:N	2.26	0.51
1:J:154:TYR:OH	1:J:257:GLU:HB2	2.11	0.51
1:A:112:GLY:O	1:A:115:MET:HG2	2.11	0.51
1:F:103:LYS:C	1:F:103:LYS:HD3	2.31	0.51
1:E:9:ARG:HH12	1:E:12:ARG:HD2	1.75	0.51
1:D:103:LYS:HD2	2:D:500:NAI:H2N	1.92	0.51
1:O:6:ILE:HB	1:O:11:ILE:HD11	1.91	0.51
1:C:127:PHE:CD1	1:C:318:PRO:HB3	2.46	0.51
1:A:197:ASP:HB3	4:A:385:HOH:O	2.10	0.51
1:C:42:CYS:HA	1:C:61:PHE:O	2.11	0.51
1:N:255:LEU:CD2	1:N:260:THR:HG23	2.41	0.51
1:D:98:HIS:CA	1:D:124:VAL:CG1	2.76	0.51
1:N:102:GLU:OE2	2:N:500:NAI:H2N	2.10	0.51
1:M:72:ASN:N	1:M:72:ASN:HD22	1.99	0.51
1:L:124:VAL:CG1	1:L:125:ARG:N	2.73	0.51
1:L:15:LEU:CD2	1:L:16:VAL:N	2.74	0.51
1:F:245:PRO:CD	1:F:246:GLN:H	2.24	0.51
1:N:80:THR:HB	1:N:81:PRO:HD2	1.93	0.51
1:K:13:PHE:O	1:K:38:LEU:HD12	2.11	0.51
1:M:41:ILE:HD11	1:M:53:GLU:HB2	1.92	0.51
1:N:305:TYR:O	1:N:309:ILE:HG13	2.11	0.51
1:P:64:LEU:HD23	1:P:91:GLU:OE2	2.11	0.51
1:H:116:VAL:HG21	1:H:326:LEU:HD11	1.93	0.51
1:P:324:GLU:OE2	1:P:324:GLU:HA	2.10	0.51
1:K:9:ARG:CG	1:K:10:LYS:N	2.73	0.50
1:P:21:ILE:CG2	2:P:500:NAI:C5D	2.89	0.50
1:E:197:ASP:HA	1:E:201:GLY:O	2.11	0.50
1:N:186:MET:O	1:N:190:SER:HB3	2.11	0.50
1:I:64:LEU:HD22	1:I:68:LEU:HG	1.93	0.50
1:I:12:ARG:HH21	1:I:39:VAL:HG21	1.76	0.50
1:I:98:HIS:CA	1:I:124:VAL:CG1	2.79	0.50
1:B:84:LEU:O	1:B:85:HIS:C	2.49	0.50
1:E:15:LEU:HD12	1:E:16:VAL:C	2.31	0.50
1:J:85:HIS:N	1:J:86:PRO:CD	2.75	0.50
1:C:86:PRO:O	1:C:90:ILE:HG13	2.11	0.50
1:H:103:LYS:C	1:H:103:LYS:CE	2.80	0.50
1:K:184:ALA:HA	1:K:188:GLN:HE21	1.75	0.50
1:L:15:LEU:HD23	1:L:16:VAL:N	2.27	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:20:ARG:HG2	1:N:20:ARG:HH11	1.76	0.50
1:O:281:PRO:O	1:O:282:ASP:CB	2.46	0.50
1:L:277:ALA:O	1:L:278:GLU:HG2	2.11	0.50
1:L:313:ARG:O	1:L:315:ASP:N	2.45	0.50
1:M:11:ILE:N	1:M:35:ARG:O	2.34	0.50
1:A:24:ASN:N	1:A:24:ASN:HD22	2.09	0.50
1:K:103:LYS:HE2	1:K:190:SER:OG	2.11	0.50
1:M:310:ASN:HB3	1:M:315:ASP:HB2	1.94	0.50
1:L:92:VAL:HG11	1:L:99:VAL:HG22	1.94	0.50
1:I:71:GLY:C	1:I:72:ASN:HD22	2.15	0.50
1:F:323:ARG:O	1:F:326:LEU:HB2	2.12	0.50
1:M:294:THR:HG22	1:M:294:THR:O	2.10	0.50
1:N:73:ALA:O	1:N:97:ARG:NE	2.37	0.50
1:D:318:PRO:O	1:D:319:GLU:C	2.50	0.50
1:K:98:HIS:HA	1:K:124:VAL:HG22	1.94	0.50
1:N:103:LYS:C	1:N:103:LYS:HD3	2.31	0.50
1:N:40:GLU:O	1:N:41:ILE:CG2	2.60	0.50
1:F:9:ARG:NH1	1:F:12:ARG:HE	2.09	0.50
1:A:98:HIS:ND1	1:A:125:ARG:HB2	2.26	0.50
1:B:99:VAL:O	1:B:126:LEU:HA	2.12	0.50
1:B:197:ASP:OD1	1:B:327:GLN:HG2	2.12	0.50
1:N:262:ARG:HB3	1:N:273:GLU:HB2	1.93	0.50
1:H:53:GLU:HG3	1:H:54:ALA:H	1.76	0.50
1:O:40:GLU:OE2	1:O:72:ASN:N	2.44	0.50
1:I:103:LYS:HD2	2:I:500:NAI:H2N	1.94	0.50
1:N:14:GLY:HA3	1:N:76:LEU:CD2	2.40	0.50
1:B:41:ILE:HG13	1:B:49:LEU:HD12	1.92	0.50
1:L:267:ALA:O	1:L:268:VAL:C	2.50	0.50
1:H:310:ASN:O	1:H:315:ASP:HB2	2.12	0.50
1:J:52:ALA:O	1:J:56:THR:OG1	2.23	0.50
1:N:12:ARG:HB3	1:N:39:VAL:CG2	2.42	0.50
1:E:318:PRO:HG2	1:E:321:ASP:HB3	1.94	0.50
1:D:103:LYS:HB2	1:D:130:LYS:HZ1	1.76	0.50
1:G:61:PHE:CE2	1:G:67:MET:HG3	2.46	0.50
1:F:245:PRO:CD	1:F:246:GLN:N	2.73	0.50
1:D:125:ARG:NH1	1:D:311:CYS:SG	2.84	0.50
1:B:85:HIS:CE1	2:B:500:NAI:O3D	2.64	0.49
1:G:273:GLU:HG3	1:G:275:LYS:HE3	1.94	0.49
1:M:197:ASP:HA	1:M:201:GLY:O	2.12	0.49
1:B:167:GLU:OE2	1:B:167:GLU:N	2.33	0.49
1:H:135:ASN:CB	1:H:293:THR:HG23	2.42	0.49
1:B:94:GLN:C	1:B:96:GLY:H	2.15	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:64:LEU:O	1:B:64:LEU:HD12	2.13	0.49
1:M:156:VAL:O	1:M:235:GLY:HA2	2.12	0.49
1:M:16:VAL:HG22	1:M:67:MET:CE	2.42	0.49
1:D:26:ILE:HG22	1:D:27:GLY:H	1.75	0.49
1:A:72:ASN:N	1:A:72:ASN:HD22	2.10	0.49
1:J:263:VAL:HG12	1:J:268:VAL:HA	1.93	0.49
1:J:43:ASP:OD2	2:J:500:NAI:O3B	2.20	0.49
1:P:97:ARG:C	1:P:124:VAL:CG1	2.79	0.49
1:H:163:THR:OG1	1:H:246:GLN:HA	2.12	0.49
1:B:32:HIS:HE1	1:B:306:ASP:HB2	1.77	0.49
1:G:323:ARG:CG	1:G:323:ARG:HH11	2.25	0.49
1:H:10:LYS:HE2	1:H:34:ASP:HA	1.93	0.49
1:F:49:LEU:HD21	1:F:60:PRO:HB2	1.94	0.49
1:N:331:LEU:CD2	1:N:347:LEU:HD11	2.42	0.49
1:F:130:LYS:HG2	1:F:320:THR:HG21	1.94	0.49
1:P:12:ARG:N	1:P:74:ASP:OD2	2.39	0.49
1:P:74:ASP:O	1:P:97:ARG:HB3	2.12	0.49
1:C:85:HIS:N	1:C:86:PRO:CD	2.75	0.49
1:N:280:HIS:CD2	1:N:281:PRO:HD2	2.48	0.49
1:L:53:GLU:OE2	1:L:60:PRO:HG3	2.13	0.49
1:B:262:ARG:HD3	4:B:379:HOH:O	2.13	0.49
1:I:98:HIS:HA	1:I:124:VAL:HG12	1.88	0.49
1:K:97:ARG:C	1:K:124:VAL:HG21	2.32	0.49
1:B:10:LYS:HB3	1:B:36:ALA:HA	1.95	0.49
1:B:215:ARG:HG2	1:B:242:LEU:HD21	1.95	0.49
1:P:125:ARG:HG2	1:P:127:PHE:CZ	2.48	0.49
1:I:102:GLU:OE2	2:I:500:NAI:H2N	2.13	0.49
1:J:7:THR:HG22	1:J:313:ARG:O	2.12	0.49
1:H:184:ALA:HA	1:H:188:GLN:NE2	2.28	0.49
1:P:98:HIS:ND1	1:P:125:ARG:HB2	2.28	0.48
1:B:322:GLY:O	1:B:325:GLY:N	2.46	0.48
1:E:137:THR:CG2	1:E:138:LEU:N	2.42	0.48
1:E:252:ILE:HG22	1:E:263:VAL:HB	1.95	0.48
1:P:310:ASN:HB3	1:P:316:CYS:SG	2.52	0.48
1:H:287:ARG:HH11	1:H:287:ARG:HB3	1.78	0.48
1:D:9:ARG:NE	1:D:12:ARG:NH2	2.61	0.48
1:M:344:ARG:HD3	1:N:207:TYR:OH	2.12	0.48
1:O:309:ILE:O	1:O:313:ARG:HG3	2.12	0.48
1:P:165:PRO:HD3	3:P:550:HP7:O2	2.13	0.48
1:D:10:LYS:HE2	1:D:33:GLY:O	2.13	0.48
1:E:19:GLY:O	1:E:22:SER:OG	2.31	0.48
1:P:327:GLN:HA	1:P:327:GLN:HE21	1.78	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:103:LYS:O	1:H:103:LYS:HE2	2.13	0.48
1:I:313:ARG:C	1:I:315:ASP:H	2.16	0.48
1:E:35:ARG:O	1:E:36:ALA:CB	2.62	0.48
1:L:14:GLY:CA	1:L:67:MET:HE1	2.42	0.48
1:K:76:LEU:HD12	1:K:92:VAL:HG13	1.96	0.48
1:O:86:PRO:HA	1:O:115:MET:CG	2.43	0.48
1:J:222:THR:HG23	1:J:240:THR:HB	1.95	0.48
1:H:186:MET:O	1:H:190:SER:HB3	2.13	0.48
2:J:500:NAI:C5D	2:J:500:NAI:H6N	2.14	0.48
1:E:103:LYS:O	1:E:103:LYS:CD	2.41	0.48
1:C:153:ILE:O	1:C:233:ALA:HB2	2.14	0.48
1:O:347:LEU:HB3	1:O:348:PRO:HA	1.95	0.48
1:E:85:HIS:N	1:E:86:PRO:HD2	2.28	0.48
1:P:34:ASP:N	1:P:34:ASP:OD2	2.46	0.48
1:I:98:HIS:CA	1:I:124:VAL:HG13	2.44	0.48
1:B:64:LEU:CD1	1:B:68:LEU:HD11	2.43	0.48
1:P:117:LYS:HD2	1:P:117:LYS:C	2.33	0.48
1:H:135:ASN:HB3	1:H:293:THR:CG2	2.44	0.48
1:N:16:VAL:HG22	1:N:67:MET:CE	2.43	0.48
1:C:43:ASP:OD1	1:C:44:THR:N	2.47	0.48
1:H:192:TYR:HA	1:H:195:LEU:HG	1.95	0.48
1:K:331:LEU:HD23	1:K:347:LEU:HD11	1.96	0.48
1:N:117:LYS:O	1:N:120:ASP:HB2	2.13	0.48
2:E:500:NAI:H6N	2:E:500:NAI:H51N	1.95	0.48
1:H:21:ILE:CD1	2:H:500:NAI:H4N	2.44	0.48
1:C:86:PRO:HG3	1:C:106:ALA:HB2	1.94	0.48
1:G:138:LEU:HD11	1:G:268:VAL:HG21	1.96	0.48
1:M:103:LYS:C	1:M:103:LYS:HE2	2.34	0.48
1:B:125:ARG:NH2	1:B:317:GLU:OE1	2.46	0.48
1:P:98:HIS:HA	1:P:124:VAL:HG11	1.90	0.48
1:I:140:LEU:HD11	1:I:289:ALA:CB	2.44	0.48
1:E:150:PHE:CZ	1:E:261:VAL:HG23	2.49	0.48
1:C:40:GLU:HB3	1:C:67:MET:HE3	1.95	0.48
1:E:277:ALA:O	1:E:278:GLU:CG	2.61	0.48
1:M:249:GLU:OE1	1:M:251:SER:OG	2.20	0.48
1:M:178:TRP:CZ2	1:M:219:ALA:HA	2.49	0.48
1:I:263:VAL:HG12	1:I:268:VAL:HA	1.96	0.48
1:L:184:ALA:HA	1:L:188:GLN:HE22	1.73	0.48
1:K:29:ILE:C	1:K:31:GLN:H	2.17	0.48
1:H:86:PRO:HB3	1:H:115:MET:HG3	1.96	0.48
1:F:12:ARG:NH1	1:F:72:ASN:OD1	2.41	0.48
1:C:134:ARG:NH2	1:C:319:GLU:OE2	2.47	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:312:LEU:C	1:P:314:GLY:H	2.17	0.48
1:J:139:GLN:O	1:J:143:LYS:HG3	2.13	0.48
1:C:333:THR:HG23	4:C:363:HOH:O	2.13	0.48
1:N:21:ILE:HD12	1:N:21:ILE:HA	1.67	0.48
1:J:338:SER:HB2	1:J:345:ILE:HG12	1.96	0.48
1:P:278:GLU:HA	1:P:279:PRO:HD2	1.55	0.48
1:E:41:ILE:HD11	1:E:53:GLU:HA	1.95	0.48
1:E:53:GLU:O	1:E:57:GLY:HA2	2.13	0.48
1:F:184:ALA:HA	1:F:188:GLN:HE22	1.79	0.48
1:P:318:PRO:HG2	1:P:321:ASP:HB3	1.96	0.48
1:C:320:THR:HG23	1:C:324:GLU:HB3	1.96	0.48
1:E:347:LEU:HB3	1:E:348:PRO:HA	1.96	0.48
1:K:9:ARG:HG3	1:K:10:LYS:H	1.78	0.47
1:D:287:ARG:CZ	1:M:24:ASN:OD1	2.60	0.47
1:B:135:ASN:H	1:B:135:ASN:ND2	2.11	0.47
1:I:30:ALA:O	1:I:32:HIS:N	2.47	0.47
1:E:149:ARG:HB3	1:E:276:PHE:CD1	2.49	0.47
1:I:117:LYS:O	1:I:120:ASP:HB2	2.13	0.47
1:O:82:SER:HA	1:O:85:HIS:CE1	2.49	0.47
1:L:134:ARG:O	1:L:135:ASN:C	2.51	0.47
1:O:45:ASN:C	1:O:45:ASN:OD1	2.52	0.47
1:E:21:ILE:CG2	2:E:500:NAI:H52N	2.44	0.47
1:H:327:GLN:CA	1:H:327:GLN:NE2	2.53	0.47
1:F:124:VAL:CG1	1:F:125:ARG:N	2.77	0.47
1:P:68:LEU:HD21	1:P:76:LEU:HD11	1.96	0.47
1:J:136:ALA:HB3	1:J:293:THR:OG1	2.13	0.47
1:J:213:LEU:HD23	1:J:213:LEU:HA	1.66	0.47
1:O:72:ASN:C	1:O:72:ASN:HD22	2.16	0.47
1:P:77:VAL:HG21	1:P:305:TYR:OH	2.14	0.47
1:B:14:GLY:HA3	1:B:67:MET:CE	2.45	0.47
1:J:94:GLN:C	1:J:96:GLY:H	2.17	0.47
1:O:12:ARG:O	1:O:74:ASP:N	2.42	0.47
1:H:282:ASP:HA	1:H:285:LYS:HD3	1.96	0.47
1:A:75:ALA:HB2	1:A:98:HIS:HB2	1.97	0.47
1:L:86:PRO:HG3	1:L:106:ALA:CB	2.44	0.47
1:N:269:ASN:HA	1:N:293:THR:HG21	1.96	0.47
1:F:156:VAL:HA	1:F:253:THR:O	2.15	0.47
1:J:29:ILE:C	1:J:31:GLN:N	2.59	0.47
1:I:269:ASN:HA	1:I:293:THR:CG2	2.42	0.47
1:O:6:ILE:O	1:O:6:ILE:HG22	2.14	0.47
1:O:86:PRO:O	1:O:90:ILE:HD12	2.15	0.47
1:E:214:ALA:HB3	1:E:242:LEU:CD2	2.45	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:59:ARG:HH12	1:L:70:GLN:CG	2.28	0.47
1:K:39:VAL:O	1:K:39:VAL:HG13	2.13	0.47
1:J:59:ARG:HA	1:J:60:PRO:HD2	1.64	0.47
1:H:103:LYS:O	1:H:103:LYS:CE	2.62	0.47
1:J:109:TRP:CE2	1:J:113:LYS:HE2	2.48	0.47
2:O:500:NAI:H42N	3:O:550:HP7:H3'	1.96	0.47
1:F:34:ASP:N	1:F:34:ASP:OD2	2.48	0.47
1:N:70:GLN:HB3	1:N:70:GLN:HE21	1.43	0.47
1:E:12:ARG:HB2	1:E:39:VAL:HG21	1.96	0.47
1:E:304:TYR:O	1:E:308:VAL:CG2	2.63	0.47
1:E:167:GLU:HA	1:E:170:ASP:HB2	1.96	0.47
1:A:20:ARG:NH2	3:A:550:HP7:O2A	2.43	0.47
1:A:347:LEU:HB3	1:A:348:PRO:HA	1.96	0.47
1:E:109:TRP:CZ3	1:E:330:ALA:HB2	2.50	0.47
1:G:244:TYR:CE1	1:G:245:PRO:HB3	2.50	0.47
1:B:310:ASN:CB	1:B:316:CYS:SG	2.96	0.47
1:L:72:ASN:HA	1:L:97:ARG:NH1	2.29	0.47
1:B:246:GLN:O	1:B:247:ASN:C	2.51	0.47
1:M:237:ILE:O	1:M:237:ILE:HG23	2.13	0.47
1:H:347:LEU:HD23	1:H:347:LEU:HA	1.68	0.47
1:D:125:ARG:NH1	1:D:125:ARG:CG	2.75	0.47
1:D:21:ILE:HG22	2:D:500:NAI:H52N	1.97	0.47
1:I:346:PRO:HG2	1:O:340:ARG:HD3	1.95	0.47
1:L:267:ALA:C	1:L:268:VAL:CG2	2.83	0.47
1:A:139:GLN:O	1:A:143:LYS:HG3	2.15	0.47
1:M:109:TRP:CZ3	1:M:326:LEU:HD22	2.50	0.47
1:B:280[B]:HIS:CD2	1:B:281:PRO:CD	2.93	0.47
1:D:327:GLN:HE21	1:D:327:GLN:HA	1.80	0.47
1:L:41:ILE:HD11	1:L:53:GLU:HA	1.97	0.47
1:N:28:ALA:O	1:N:32:HIS:HD2	1.98	0.47
1:K:46:PRO:O	1:K:47:GLU:C	2.49	0.47
1:G:145:ILE:HD13	1:G:199:LEU:O	2.14	0.47
1:I:273:GLU:OE2	1:I:275:LYS:HE3	2.14	0.47
1:D:117:LYS:HB3	1:D:117:LYS:HE2	1.35	0.47
1:A:134:ARG:O	1:A:135:ASN:C	2.53	0.47
1:D:12:ARG:HG2	1:D:39:VAL:HG21	1.97	0.46
1:N:124:VAL:CG1	1:N:125:ARG:N	2.77	0.46
1:K:278:GLU:HA	1:K:279:PRO:HD3	1.63	0.46
1:J:130:LYS:HG2	1:J:320:THR:HG21	1.96	0.46
1:C:72:ASN:HD22	1:C:72:ASN:H	1.63	0.46
1:N:296:VAL:O	1:N:296:VAL:HG23	2.14	0.46
1:E:103:LYS:HD2	2:E:500:NAI:C2N	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:16:VAL:CG2	1:D:67:MET:HE1	2.41	0.46
1:H:133:ARG:NH1	1:H:198:TRP:CD1	2.83	0.46
1:F:149:ARG:HB3	1:F:276:PHE:CD1	2.50	0.46
1:O:137:THR:O	1:O:140:LEU:HB2	2.14	0.46
1:A:273:GLU:HG2	1:B:248:LEU:HD11	1.97	0.46
1:G:274:TRP:CG	1:G:286:ILE:HD11	2.50	0.46
1:A:280:HIS:CG	1:A:281:PRO:HD2	2.50	0.46
1:B:12:ARG:HB2	1:B:12:ARG:HE	1.47	0.46
1:E:15:LEU:CD1	1:E:17:GLY:O	2.63	0.46
1:G:280:HIS:ND1	1:G:281:PRO:HD2	2.30	0.46
1:I:206:VAL:HG12	1:I:227:LEU:HD23	1.97	0.46
1:N:283:ASP:O	1:N:286:ILE:HD12	2.16	0.46
1:H:29:ILE:HG22	1:H:30:ALA:N	2.30	0.46
1:C:125:ARG:HG2	1:C:127:PHE:CZ	2.51	0.46
1:G:40:GLU:OE2	1:G:72:ASN:N	2.47	0.46
1:N:28:ALA:HB1	1:N:302:PRO:HA	1.97	0.46
1:B:134:ARG:CB	1:B:303:LEU:HD13	2.45	0.46
1:D:137:THR:CG2	1:D:293:THR:HG21	2.46	0.46
1:G:347:LEU:HB3	1:G:348:PRO:HA	1.98	0.46
1:C:230:ARG:HD3	4:G:357:HOH:O	2.14	0.46
1:M:283:ASP:O	1:M:286:ILE:HD12	2.16	0.46
1:L:309:ILE:O	1:L:312:LEU:N	2.48	0.46
1:H:220:GLU:OE1	1:H:220:GLU:N	2.42	0.46
1:I:21:ILE:HG21	2:I:500:NAI:H52N	1.97	0.46
1:H:80:THR:HB	1:H:81:PRO:CD	2.45	0.46
1:F:258:LYS:HB2	1:F:277:ALA:HB2	1.98	0.46
1:F:103:LYS:C	1:F:103:LYS:CD	2.84	0.46
1:C:133:ARG:HH12	1:C:324:GLU:HG3	1.80	0.46
1:L:74:ASP:OD2	1:L:74:ASP:N	2.48	0.46
1:L:39:VAL:HG12	1:L:40:GLU:HG3	1.97	0.46
1:H:142:LYS:HE2	1:H:198:TRP:CE2	2.50	0.46
1:N:197:ASP:OD1	1:N:327:GLN:HG2	2.16	0.46
1:F:76:LEU:N	1:F:76:LEU:HD12	2.31	0.46
1:J:61:PHE:CD1	1:J:67:MET:HA	2.51	0.46
1:I:145:ILE:HD13	1:I:199:LEU:O	2.16	0.46
1:D:287:ARG:HE	1:M:298:GLY:HA2	1.81	0.46
1:I:97:ARG:C	1:I:124:VAL:HG11	2.35	0.46
1:K:86:PRO:O	1:K:90:ILE:HG13	2.16	0.46
1:B:9:ARG:NH1	1:B:9:ARG:HG3	2.31	0.46
1:J:38:LEU:HD23	1:J:56:THR:HG21	1.98	0.46
1:F:144:ALA:O	1:F:145:ILE:C	2.53	0.46
1:E:192:TYR:N	1:E:192:TYR:CD2	2.84	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:271:ILE:H	1:C:290:ASN:ND2	2.14	0.46
1:O:206:VAL:CG1	1:O:227:LEU:HD23	2.39	0.46
1:A:20:ARG:O	1:A:23:LYS:CE	2.61	0.46
1:H:297:TYR:CD2	1:H:297:TYR:O	2.69	0.46
1:E:262:ARG:HB3	1:E:273:GLU:HB3	1.98	0.46
1:D:285:LYS:NZ	1:D:285:LYS:HB3	2.30	0.46
1:E:90:ILE:CD1	1:E:114:ARG:HD3	2.46	0.46
1:H:132:ASN:HB2	4:H:380:HOH:O	2.15	0.46
1:K:52:ALA:O	1:K:56:THR:HG23	2.16	0.46
1:K:165:PRO:HD3	3:K:550:HP7:O2	2.16	0.45
1:F:188:GLN:HB2	1:F:188:GLN:HE21	1.38	0.45
1:F:103:LYS:HD3	1:F:103:LYS:O	2.16	0.45
1:K:130:LYS:HG2	1:K:194:ASP:OD2	2.16	0.45
1:F:279:PRO:O	1:F:280:HIS:HD2	1.99	0.45
1:M:76:LEU:HD23	1:M:76:LEU:HA	1.60	0.45
1:E:15:LEU:CD1	1:E:16:VAL:O	2.65	0.45
1:F:245:PRO:HD2	1:F:246:GLN:N	2.31	0.45
1:O:82:SER:OG	1:O:104:PRO:HD2	2.16	0.45
1:G:133:ARG:HH22	1:G:324:GLU:HG3	1.81	0.45
1:B:185:PHE:HE2	1:B:223:GLY:HA3	1.82	0.45
1:F:82:SER:HA	1:F:85:HIS:CE1	2.51	0.45
1:D:138:LEU:HA	1:D:138:LEU:HD23	1.67	0.45
1:B:305:TYR:O	1:B:309:ILE:HG13	2.16	0.45
1:L:92:VAL:CG1	1:L:99:VAL:HG22	2.46	0.45
1:E:102:GLU:HA	1:E:129:VAL:CG2	2.46	0.45
1:E:133:ARG:HD3	1:E:198:TRP:CE2	2.51	0.45
1:P:301:HIS:O	1:P:304:TYR:N	2.50	0.45
1:K:105:MET:HG2	4:K:406:HOH:O	2.16	0.45
1:P:158:VAL:HA	1:P:251:SER:O	2.16	0.45
1:E:142:LYS:HD2	1:E:199:LEU:HD23	1.99	0.45
1:I:280:HIS:O	1:I:281:PRO:C	2.55	0.45
1:D:72:ASN:H	1:D:72:ASN:ND2	2.14	0.45
1:K:306:ASP:OD1	1:K:306:ASP:C	2.55	0.45
1:D:287:ARG:HH11	1:M:24:ASN:HD21	1.63	0.45
1:C:98:HIS:ND1	1:C:125:ARG:HB2	2.31	0.45
1:K:263:VAL:HG22	1:K:271:ILE:HG12	1.98	0.45
1:I:46:PRO:O	1:I:49:LEU:HB3	2.16	0.45
1:G:45:ASN:HA	1:G:46:PRO:HD2	1.67	0.45
1:E:68:LEU:O	1:E:97:ARG:NH2	2.48	0.45
1:L:320:THR:HG23	1:L:324:GLU:HG3	1.97	0.45
1:C:327:GLN:CA	1:C:327:GLN:NE2	2.67	0.45
1:F:67:MET:HE1	1:F:76:LEU:CD2	2.46	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:103:LYS:CD	1:D:103:LYS:C	2.74	0.45
1:G:97:ARG:O	1:G:124:VAL:HG21	2.17	0.45
1:H:142:LYS:HE2	1:H:198:TRP:NE1	2.32	0.45
1:O:117:LYS:HE2	1:O:117:LYS:HB3	1.64	0.45
1:N:16:VAL:HG22	1:N:67:MET:HE2	1.99	0.45
1:L:59:ARG:HH12	1:L:70:GLN:HG3	1.81	0.45
1:D:25:HIS:ND1	1:D:77:VAL:HG11	2.32	0.45
1:P:119:CYS:SG	1:P:126:LEU:HB2	2.57	0.45
1:D:291:TYR:OH	1:M:302:PRO:CD	2.63	0.45
1:E:277:ALA:O	1:E:278:GLU:HG2	2.17	0.45
1:I:273:GLU:OE2	1:I:275:LYS:CE	2.65	0.45
1:D:72:ASN:C	1:D:72:ASN:HD22	2.20	0.45
2:E:500:NAI:H51N	2:E:500:NAI:C6N	2.46	0.45
1:C:9:ARG:HH11	1:C:9:ARG:CG	2.24	0.45
1:O:103:LYS:HD2	1:O:103:LYS:O	2.17	0.45
1:H:162:TRP:HA	1:H:247:ASN:HA	1.99	0.45
1:E:261:VAL:HG12	1:E:262:ARG:N	2.31	0.45
1:N:20:ARG:NH1	1:N:20:ARG:HG2	2.32	0.45
1:I:347:LEU:HB3	1:I:348:PRO:HA	1.98	0.45
1:N:321:ASP:OD2	1:N:321:ASP:C	2.54	0.45
1:I:124:VAL:HG12	1:I:125:ARG:N	2.31	0.45
3:H:550:HP7:H6	3:H:550:HP7:O5C	2.17	0.45
1:G:310:ASN:CB	1:G:316:CYS:SG	3.03	0.45
1:H:10:LYS:HB3	1:H:36:ALA:HA	1.99	0.45
1:L:103:LYS:HD2	2:L:500:NAI:H2N	1.99	0.45
1:F:10:LYS:HG2	1:F:34:ASP:O	2.17	0.45
1:N:21:ILE:O	1:N:25:HIS:HD2	1.99	0.45
1:F:204:GLU:OE2	1:F:228:ARG:NE	2.47	0.45
1:K:269:ASN:N	1:K:269:ASN:OD1	2.33	0.45
1:I:68:LEU:HD21	1:I:76:LEU:CD1	2.47	0.45
1:O:125:ARG:HB3	1:O:127:PHE:CE2	2.52	0.45
1:P:85:HIS:N	1:P:86:PRO:HD2	2.32	0.45
1:I:80:THR:HB	1:I:81:PRO:CD	2.46	0.45
1:L:301:HIS:O	1:L:304:TYR:N	2.50	0.45
1:P:307:ASN:O	1:P:308:VAL:C	2.54	0.45
1:G:282:ASP:C	1:G:284:ASP:N	2.69	0.45
1:L:66:ASP:C	1:L:68:LEU:N	2.70	0.45
1:B:58:ALA:O	1:B:60:PRO:HD3	2.17	0.45
1:I:58:ALA:O	1:I:60:PRO:HD3	2.17	0.45
1:E:301:HIS:N	1:E:302:PRO:CD	2.78	0.45
1:P:327:GLN:HA	1:P:327:GLN:NE2	2.31	0.45
1:G:282:ASP:OD1	1:G:285:LYS:HE2	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:98:HIS:HA	1:D:124:VAL:HG13	1.87	0.44
4:A:391:HOH:O	1:D:230:ARG:HD2	2.17	0.44
1:I:20:ARG:NH1	3:I:550:HP7:O2B	2.42	0.44
1:A:20:ARG:HD3	4:A:353:HOH:O	2.17	0.44
1:E:262:ARG:HB3	1:E:273:GLU:CB	2.47	0.44
1:F:186:MET:O	1:F:190:SER:HB3	2.17	0.44
1:J:53:GLU:O	1:J:57:GLY:N	2.47	0.44
1:L:40:GLU:HB2	1:L:67:MET:HE2	1.98	0.44
1:L:40:GLU:CD	1:L:71:GLY:HA3	2.38	0.44
1:L:310:ASN:HB3	1:L:315:ASP:CB	2.47	0.44
1:O:81:PRO:HB3	1:O:174:TRP:CE3	2.52	0.44
1:C:73:ALA:O	1:C:97:ARG:HD2	2.17	0.44
1:K:235:GLY:CA	1:L:224:VAL:HG21	2.47	0.44
1:B:117:LYS:HD2	1:B:121:GLU:OE2	2.17	0.44
1:K:9:ARG:CG	1:K:10:LYS:H	2.31	0.44
1:L:81:PRO:HD2	1:L:84:LEU:HD12	2.00	0.44
1:D:42:CYS:HB2	1:D:67:MET:SD	2.57	0.44
1:L:313:ARG:C	1:L:315:ASP:N	2.70	0.44
1:N:133:ARG:HH22	1:N:324:GLU:HG3	1.82	0.44
1:N:32:HIS:HE1	1:N:306:ASP:HB2	1.83	0.44
1:H:195:LEU:N	1:H:195:LEU:HD23	2.32	0.44
1:C:320:THR:HA	1:C:324:GLU:HG2	2.00	0.44
1:D:287:ARG:HE	1:M:298:GLY:CA	2.29	0.44
1:I:282:ASP:HA	1:I:285:LYS:HG2	1.98	0.44
1:J:39:VAL:C	1:J:40:GLU:HG3	2.38	0.44
1:K:307:ASN:OD1	1:K:319:GLU:HG3	2.18	0.44
1:P:230:ARG:NH1	1:P:347:LEU:O	2.48	0.44
2:J:500:NAI:C4N	3:J:550:HP7:H3'	2.44	0.44
1:M:21:ILE:HD13	2:M:500:NAI:H4N	1.99	0.44
1:D:64:LEU:HD12	1:D:67:MET:HE3	1.99	0.44
1:L:74:ASP:O	1:L:97:ARG:HB3	2.17	0.44
1:J:103:LYS:HD3	1:J:103:LYS:O	2.16	0.44
1:K:222:THR:HG23	1:K:240:THR:HB	1.99	0.44
1:G:105:MET:HG2	4:G:377:HOH:O	2.16	0.44
1:E:156:VAL:O	1:E:235:GLY:HA3	2.18	0.44
1:D:64:LEU:CD1	1:D:67:MET:CE	2.96	0.44
1:O:310:ASN:HB3	1:O:316:CYS:SG	2.58	0.44
1:K:16:VAL:HG22	1:K:67:MET:CE	2.46	0.44
1:M:53:GLU:HG3	1:M:60:PRO:HD3	2.00	0.44
1:H:116:VAL:HG21	1:H:326:LEU:CD1	2.46	0.44
1:D:137:THR:HG23	1:D:293:THR:CB	2.47	0.44
1:A:278:GLU:HA	1:A:279:PRO:HD3	1.71	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:206:VAL:HG12	1:E:227:LEU:HD23	1.99	0.44
1:E:138:LEU:HG	1:E:138:LEU:H	1.62	0.44
1:K:73:ALA:O	1:K:97:ARG:HD2	2.16	0.44
1:L:103:LYS:C	1:L:103:LYS:HD3	2.37	0.44
1:B:86:PRO:CA	1:B:115:MET:HG2	2.46	0.44
1:N:85:HIS:N	1:N:86:PRO:CD	2.80	0.44
1:J:102:GLU:OE1	1:J:129:VAL:HG11	2.18	0.44
2:M:500:NAI:C4N	3:M:550:HP7:H3'	2.37	0.44
1:L:26:ILE:O	1:L:27:GLY:C	2.56	0.44
1:H:16:VAL:HG13	1:H:16:VAL:O	2.18	0.44
1:L:255:LEU:CD2	1:L:260:THR:HG23	2.47	0.44
1:C:309:ILE:HG22	1:C:313:ARG:HD3	2.00	0.44
1:K:310:ASN:O	1:K:315:ASP:HB2	2.18	0.44
1:J:155:MET:HA	1:J:234:MET:O	2.18	0.44
1:G:167:GLU:H	1:G:167:GLU:CD	2.21	0.44
1:A:82:SER:HA	1:A:85:HIS:CE1	2.53	0.44
1:E:38:LEU:O	1:E:58:ALA:HB2	2.18	0.44
1:K:80:THR:O	2:K:500:NAI:H4D	2.18	0.44
1:N:14:GLY:O	1:N:76:LEU:HA	2.18	0.44
1:D:76:LEU:HD23	1:D:76:LEU:HA	1.59	0.44
1:F:21:ILE:CD1	2:F:500:NAI:H4N	2.47	0.44
1:P:117:LYS:HD3	1:P:117:LYS:C	2.39	0.44
1:C:235:GLY:HA2	1:D:224:VAL:HG21	1.98	0.44
1:A:109:TRP:CE2	1:A:113:LYS:HE2	2.52	0.44
1:J:267:ALA:O	1:J:268:VAL:HG23	2.18	0.44
1:J:278:GLU:O	1:J:278:GLU:HG2	2.18	0.44
1:H:318:PRO:HG2	1:H:321:ASP:HB3	1.99	0.43
1:I:326:LEU:HD23	1:I:326:LEU:HA	1.68	0.43
1:M:133:ARG:HH12	1:M:324:GLU:CG	2.31	0.43
1:K:103:LYS:HA	1:K:104:PRO:C	2.39	0.43
1:K:131:GLN:HE22	2:K:500:NAI:C7N	2.30	0.43
1:C:103:LYS:HD2	2:C:500:NAI:H2N	1.99	0.43
1:A:68:LEU:CD2	1:A:76:LEU:HD11	2.44	0.43
1:L:101:SER:O	1:L:129:VAL:HG23	2.18	0.43
1:F:24:ASN:ND2	1:F:24:ASN:H	2.16	0.43
4:E:360:HOH:O	1:H:211:ALA:HB1	2.17	0.43
1:A:97:ARG:O	1:A:124:VAL:HG11	2.18	0.43
1:I:267:ALA:O	1:I:268:VAL:C	2.56	0.43
1:G:156:VAL:O	1:G:235:GLY:CA	2.67	0.43
1:N:127:PHE:CE1	1:N:318:PRO:HB3	2.54	0.43
1:L:142:LYS:HB2	1:L:199:LEU:CD2	2.48	0.43
1:A:173:ARG:HH22	1:D:317:GLU:HG3	1.82	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:297:TYR:HA	4:G:391:HOH:O	2.19	0.43
1:L:24:ASN:O	1:L:28:ALA:HB2	2.18	0.43
1:E:85:HIS:N	1:E:86:PRO:CD	2.81	0.43
1:J:45:ASN:HA	1:J:46:PRO:HD2	1.72	0.43
1:C:225:ALA:HB3	1:C:237:ILE:CG2	2.48	0.43
1:K:15:LEU:HD12	1:K:77:VAL:HB	2.01	0.43
1:E:128:VAL:O	1:E:320:THR:HG21	2.19	0.43
1:G:321:ASP:OD2	1:G:321:ASP:C	2.55	0.43
1:A:21:ILE:HG13	1:A:21:ILE:O	2.18	0.43
1:I:64:LEU:CD2	1:I:64:LEU:O	2.67	0.43
1:H:288:GLU:O	1:H:291:TYR:CB	2.66	0.43
1:J:82:SER:HB3	1:J:104:PRO:HD2	2.01	0.43
1:P:305:TYR:HA	1:P:308:VAL:HG23	2.01	0.43
1:A:134:ARG:NE	1:A:319:GLU:OE2	2.51	0.43
1:A:236:SER:OG	1:B:238:ASN:ND2	2.49	0.43
1:E:52:ALA:O	1:E:56:THR:OG1	2.36	0.43
1:A:30:ALA:O	1:A:33:GLY:N	2.45	0.43
1:A:282:ASP:C	1:A:284:ASP:H	2.21	0.43
1:B:192:TYR:N	1:B:192:TYR:CD2	2.86	0.43
1:D:130:LYS:HG2	1:D:194:ASP:OD2	2.19	0.43
1:M:15:LEU:HD23	1:M:16:VAL:N	2.34	0.43
1:F:168:TYR:OH	3:F:550:HP7:O'Q	2.31	0.43
1:N:133:ARG:NH1	1:N:324:GLU:HG2	2.32	0.43
1:F:275:LYS:C	1:F:276:PHE:CD2	2.91	0.43
1:D:137:THR:HG23	1:D:293:THR:HG21	2.00	0.43
1:G:117:LYS:HE2	1:G:117:LYS:HB3	1.30	0.43
1:L:320:THR:HG23	1:L:324:GLU:HB3	1.99	0.43
1:K:82:SER:CB	1:K:104:PRO:HD2	2.48	0.43
1:D:103:LYS:HD2	2:D:500:NAI:C2N	2.49	0.43
1:B:103:LYS:NZ	3:B:550:HP7:O3'	2.51	0.43
1:K:97:ARG:O	1:K:124:VAL:CG2	2.60	0.43
1:D:46:PRO:O	1:D:49:LEU:HB3	2.19	0.43
1:A:277:ALA:HA	1:B:244:TYR:OH	2.18	0.43
1:E:33:GLY:O	1:E:34:ASP:C	2.56	0.43
1:J:38:LEU:CD2	1:J:56:THR:HG21	2.49	0.43
1:B:156:VAL:O	1:B:235:GLY:HA3	2.18	0.43
1:F:324:GLU:O	1:F:327:GLN:HB2	2.18	0.43
1:P:263:VAL:HG12	1:P:268:VAL:HA	2.00	0.43
1:M:134:ARG:NE	1:M:319:GLU:OE1	2.51	0.43
1:I:331:LEU:HD23	1:I:331:LEU:HA	1.81	0.43
1:K:39:VAL:O	1:K:40:GLU:CG	2.65	0.43
1:B:301:HIS:N	1:B:302:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:37:GLU:HG3	1:F:39:VAL:HG23	2.00	0.43
1:J:262:ARG:CG	1:J:262:ARG:HH11	2.31	0.43
1:C:235:GLY:CA	1:D:224:VAL:HG21	2.49	0.43
1:H:246:GLN:O	1:H:247:ASN:C	2.56	0.43
1:C:40:GLU:HB3	1:C:67:MET:CE	2.48	0.43
1:D:162:TRP:HA	1:D:247:ASN:HA	2.00	0.43
1:H:53:GLU:HG3	1:H:54:ALA:N	2.34	0.43
1:I:270:ARG:NE	1:I:272:ASP:OD1	2.36	0.43
1:B:59:ARG:HA	1:B:60:PRO:HD2	1.87	0.43
1:C:85:HIS:HB2	1:C:86:PRO:HD3	2.01	0.43
1:N:53:GLU:C	1:N:55:ALA:N	2.72	0.43
1:L:310:ASN:O	1:L:311:CYS:C	2.56	0.43
1:D:72:ASN:H	1:D:72:ASN:HD22	1.67	0.43
1:M:50:GLN:O	1:M:51:ALA:C	2.58	0.43
1:J:259:GLY:HA2	1:J:275:LYS:O	2.19	0.43
1:B:202:PRO:HB2	1:B:230[A]:ARG:HD3	2.00	0.43
1:O:6:ILE:CG2	1:O:11:ILE:HD13	2.44	0.42
1:P:64:LEU:HD12	1:P:67:MET:HE3	1.99	0.42
1:N:21:ILE:O	1:N:21:ILE:HG23	2.18	0.42
1:O:153:ILE:O	1:O:233:ALA:HB2	2.18	0.42
1:I:192:TYR:N	1:I:192:TYR:CD2	2.87	0.42
1:J:187:ASN:C	1:J:187:ASN:OD1	2.56	0.42
1:D:259:GLY:HA2	1:D:275:LYS:O	2.19	0.42
1:I:65:SER:HB3	1:I:91:GLU:OE1	2.20	0.42
1:D:133:ARG:NH1	1:D:324:GLU:CG	2.74	0.42
1:C:86:PRO:HG3	1:C:106:ALA:CB	2.49	0.42
1:O:19:GLY:HA3	2:O:500:NAI:O2A	2.19	0.42
1:L:86:PRO:CB	1:L:111:ASP:HB3	2.50	0.42
1:M:163:THR:O	1:M:164:ARG:HD3	2.19	0.42
1:D:142:LYS:HG3	1:D:146:GLU:OE2	2.19	0.42
1:P:141:VAL:O	1:P:142:LYS:C	2.56	0.42
1:L:245:PRO:HG2	1:L:246:GLN:N	2.34	0.42
1:E:102:GLU:HA	1:E:129:VAL:HG23	2.01	0.42
1:K:307:ASN:ND2	1:K:307:ASN:C	2.72	0.42
1:A:14:GLY:HA2	1:A:40:GLU:O	2.19	0.42
1:P:16:VAL:CG1	1:P:78:LEU:HD23	2.48	0.42
1:G:301:HIS:N	1:G:302:PRO:CD	2.82	0.42
1:M:98:HIS:HA	1:M:124:VAL:HG12	1.91	0.42
1:F:142:LYS:CE	1:F:146:GLU:OE2	2.56	0.42
1:P:111:ASP:O	1:P:115:MET:HG3	2.19	0.42
1:E:117:LYS:HE2	1:E:117:LYS:HB3	1.86	0.42
1:C:133:ARG:NH1	1:C:324:GLU:HG3	2.35	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:283:ASP:O	1:M:286:ILE:CD1	2.67	0.42
1:M:213:LEU:HD23	1:M:213:LEU:HA	1.82	0.42
1:K:86:PRO:HG3	1:K:106:ALA:HB2	2.01	0.42
1:G:103:LYS:C	1:G:103:LYS:HD3	2.40	0.42
1:J:82:SER:CB	1:J:104:PRO:HD2	2.48	0.42
1:A:156:VAL:O	1:A:235:GLY:HA3	2.20	0.42
1:G:237:ILE:O	1:G:237:ILE:HG23	2.19	0.42
1:P:12:ARG:HG2	1:P:39:VAL:HG21	2.01	0.42
1:L:98:HIS:HA	1:L:124:VAL:HG11	1.99	0.42
1:A:81:PRO:HB3	1:A:174:TRP:CE3	2.55	0.42
1:O:267:ALA:C	1:O:268:VAL:CG2	2.87	0.42
1:J:197:ASP:OD2	1:J:202:PRO:HA	2.19	0.42
1:F:24:ASN:H	1:F:24:ASN:HD22	1.68	0.42
1:E:128:VAL:O	1:E:320:THR:CG2	2.67	0.42
1:H:267:ALA:O	1:H:268:VAL:C	2.58	0.42
1:K:133:ARG:O	1:K:139:GLN:NE2	2.51	0.42
1:D:8:ASP:N	1:D:8:ASP:OD1	2.53	0.42
1:D:124:VAL:HG12	1:D:125:ARG:O	2.19	0.42
1:B:103:LYS:HE2	2:B:500:NAI:C2N	2.49	0.42
1:K:162:TRP:HA	1:K:247:ASN:HA	2.02	0.42
1:D:246:GLN:O	1:D:247:ASN:C	2.58	0.42
1:J:301:HIS:N	1:J:302:PRO:CD	2.82	0.42
1:P:31:GLN:HE21	1:P:31:GLN:HB2	1.58	0.42
1:I:39:VAL:O	1:I:58:ALA:HB1	2.19	0.42
1:K:98:HIS:ND1	1:K:125:ARG:CB	2.80	0.42
1:L:131:GLN:HE22	2:L:500:NAI:C7N	2.27	0.42
1:O:80:THR:OG1	1:O:88:GLN:NE2	2.51	0.42
1:M:331:LEU:HA	1:M:331:LEU:HD23	1.54	0.42
1:E:226:ALA:C	1:E:227:LEU:HG	2.39	0.42
1:C:282:ASP:OD1	1:C:285:LYS:HE2	2.20	0.42
1:I:261:VAL:HG12	1:I:262:ARG:N	2.34	0.42
1:D:31:GLN:HB2	1:D:31:GLN:HE21	1.53	0.42
1:M:20:ARG:NH1	3:M:550:HP7:H5C	2.35	0.42
1:L:9:ARG:CG	1:L:10:LYS:H	2.30	0.42
1:I:313:ARG:O	1:I:315:ASP:N	2.52	0.42
1:J:12:ARG:CG	1:J:39:VAL:HG21	2.46	0.42
1:N:133:ARG:HH12	1:N:324:GLU:CG	2.32	0.42
1:F:258:LYS:HB2	1:F:277:ALA:CB	2.50	0.42
1:A:280:HIS:ND1	1:A:281:PRO:HD2	2.35	0.42
1:K:39:VAL:HG12	1:K:40:GLU:CD	2.31	0.42
1:E:21:ILE:HG22	2:E:500:NAI:H52N	2.01	0.42
1:O:6:ILE:CG2	1:O:11:ILE:CD1	2.97	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:59:ARG:HA	1:K:60:PRO:HD3	1.75	0.42
1:O:86:PRO:HB3	1:O:115:MET:HG3	2.02	0.42
1:F:68:LEU:HD12	1:F:91:GLU:HG2	2.02	0.42
1:I:156:VAL:O	1:I:235:GLY:HA3	2.20	0.42
1:K:255:LEU:HD11	1:L:161:PHE:CG	2.55	0.42
1:I:258:LYS:HB2	1:I:277:ALA:HB2	2.01	0.42
1:P:28:ALA:HB1	1:P:302:PRO:HA	2.01	0.42
1:L:156:VAL:O	1:L:235:GLY:HA3	2.20	0.42
1:D:39:VAL:C	1:D:40:GLU:CG	2.88	0.41
1:E:191:HIS:CD2	3:E:550:HP7:C7'	3.02	0.41
1:D:125:ARG:HD2	1:D:125:ARG:HA	1.72	0.41
1:P:103:LYS:CD	1:P:103:LYS:O	2.65	0.41
1:M:85:HIS:N	1:M:86:PRO:HD2	2.34	0.41
1:I:140:LEU:CD1	1:I:289:ALA:CB	2.97	0.41
1:I:72:ASN:ND2	1:I:72:ASN:N	2.68	0.41
1:J:136:ALA:H	1:J:293:THR:HG1	1.67	0.41
1:O:193:VAL:HG21	1:O:332:LEU:HD21	2.00	0.41
1:E:249:GLU:OE1	1:E:251:SER:OG	2.30	0.41
1:O:40:GLU:OE2	1:O:71:GLY:HA3	2.20	0.41
1:B:307:ASN:CG	1:B:319:GLU:H	2.24	0.41
1:E:49:LEU:HD21	1:E:61:PHE:C	2.41	0.41
1:F:188:GLN:NE2	1:F:188:GLN:H	2.18	0.41
1:F:9:ARG:HH12	1:F:12:ARG:HE	1.68	0.41
1:M:80:THR:HB	1:M:81:PRO:CD	2.45	0.41
1:J:298:GLY:O	1:J:299:PHE:CD2	2.73	0.41
1:J:103:LYS:HB2	1:J:104:PRO:HA	2.02	0.41
1:H:50:GLN:O	1:H:53:GLU:HG3	2.19	0.41
1:M:244:TYR:HA	1:M:245:PRO:HA	1.89	0.41
1:K:224:VAL:HG23	1:L:234:MET:HB3	2.01	0.41
1:J:305:TYR:O	1:J:306:ASP:C	2.56	0.41
1:P:15:LEU:HD21	1:P:22:SER:HB2	2.02	0.41
1:C:312:LEU:HD23	1:C:312:LEU:HA	1.80	0.41
1:P:84:LEU:HA	1:P:84:LEU:HD23	1.82	0.41
1:K:80:THR:OG1	1:K:88:GLN:NE2	2.53	0.41
1:C:90:ILE:O	1:C:94:GLN:HG3	2.20	0.41
1:I:320:THR:O	1:I:320:THR:HG22	2.20	0.41
1:G:76:LEU:HD12	1:G:92:VAL:CG2	2.46	0.41
1:B:320:THR:HG23	1:B:324:GLU:HG2	2.03	0.41
1:J:262:ARG:HG2	1:J:262:ARG:NH1	2.34	0.41
1:P:274:TRP:CE2	1:P:276:PHE:HE2	2.38	0.41
1:B:192:TYR:O	1:B:193:VAL:C	2.56	0.41
1:F:159:ASN:O	1:F:250:GLY:HA2	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:100:VAL:HG22	1:A:127:PHE:HB2	2.02	0.41
1:O:158:VAL:HG22	1:O:252:ILE:HG13	2.01	0.41
1:O:283:ASP:O	1:O:287:ARG:HB2	2.20	0.41
1:E:215:ARG:HD3	1:E:215:ARG:HA	1.96	0.41
1:F:125:ARG:HA	1:F:125:ARG:HD2	1.89	0.41
1:D:142:LYS:HE2	1:D:198:TRP:O	2.20	0.41
1:A:197:ASP:HA	1:A:201:GLY:O	2.20	0.41
1:K:42:CYS:HB2	1:K:67:MET:SD	2.60	0.41
1:D:72:ASN:ND2	1:D:72:ASN:N	2.68	0.41
1:B:117:LYS:O	1:B:120:ASP:HB2	2.21	0.41
1:L:202:PRO:HD2	4:L:458:HOH:O	2.20	0.41
1:N:112:GLY:O	1:N:115:MET:HB3	2.20	0.41
1:B:21:ILE:CG2	1:B:79:ALA:HB1	2.50	0.41
1:E:137:THR:O	1:E:138:LEU:C	2.58	0.41
1:O:59:ARG:HA	1:O:60:PRO:HD3	1.84	0.41
1:M:16:VAL:HG22	1:M:67:MET:HE1	2.02	0.41
1:L:21:ILE:CD1	2:L:500:NAI:H4N	2.42	0.41
1:H:154:TYR:HE2	1:H:257:GLU:HA	1.85	0.41
1:C:301:HIS:N	1:C:302:PRO:CD	2.82	0.41
1:K:53:GLU:C	1:K:55:ALA:H	2.23	0.41
1:C:42:CYS:HB2	1:C:67:MET:SD	2.60	0.41
1:J:136:ALA:N	1:J:293:THR:OG1	2.54	0.41
1:D:282:ASP:HA	1:D:285:LYS:CD	2.51	0.41
1:F:207:TYR:CD2	1:F:208:ALA:N	2.89	0.41
1:P:247:ASN:HB3	1:P:266:VAL:CG1	2.50	0.41
1:K:117:LYS:HB3	1:K:117:LYS:HE2	1.51	0.41
1:I:246:GLN:HB3	1:I:246:GLN:HE21	1.74	0.41
1:E:125:ARG:HD2	1:E:125:ARG:HA	1.87	0.41
1:B:191:HIS:HE1	2:B:500:NAI:O7N	2.04	0.41
1:P:86:PRO:HB3	1:P:115:MET:CG	2.50	0.41
1:M:72:ASN:O	1:M:73:ALA:C	2.59	0.41
1:J:309:ILE:O	1:J:310:ASN:C	2.55	0.41
1:I:81:PRO:HD2	1:I:84:LEU:HD12	2.02	0.41
1:E:248:LEU:HD22	1:F:260:THR:CG2	2.49	0.41
1:D:282:ASP:C	1:D:284:ASP:N	2.74	0.41
1:H:298:GLY:C	1:H:299:PHE:CD2	2.93	0.41
1:N:332:LEU:HA	1:N:332:LEU:HD23	1.95	0.41
1:D:21:ILE:CG2	2:D:500:NAI:H52N	2.50	0.41
1:I:124:VAL:CG1	1:I:125:ARG:N	2.84	0.41
1:F:98:HIS:HA	1:F:124:VAL:HG11	1.99	0.41
1:M:15:LEU:CD2	1:M:15:LEU:C	2.86	0.41
1:H:244:TYR:HA	1:H:245:PRO:HA	1.89	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:331:LEU:HD23	1:N:331:LEU:HA	1.87	0.41
1:L:68:LEU:HD22	1:L:95:ALA:HB3	2.02	0.41
1:N:134:ARG:O	1:N:135:ASN:C	2.58	0.41
1:B:186:MET:O	1:B:190:SER:HB3	2.20	0.41
1:K:244:TYR:HA	1:K:245:PRO:HA	1.71	0.41
1:D:186:MET:O	1:D:186:MET:HG2	2.21	0.41
1:J:6:ILE:O	1:J:6:ILE:HG22	2.21	0.41
1:H:168:TYR:C	1:H:168:TYR:CD2	2.93	0.41
1:B:195:LEU:HD23	1:B:195:LEU:HA	1.88	0.41
1:N:12:ARG:HH11	1:N:12:ARG:HD2	1.70	0.41
1:H:301:HIS:O	1:H:302:PRO:C	2.57	0.41
1:H:32:HIS:C	1:H:34:ASP:N	2.72	0.41
1:P:35:ARG:HG2	1:P:313:ARG:NH1	2.36	0.41
1:J:267:ALA:O	1:J:268:VAL:C	2.58	0.41
1:P:20:ARG:HA	1:P:23:LYS:NZ	2.34	0.41
1:G:53:GLU:OE1	1:G:60:PRO:CG	2.54	0.41
1:A:16:VAL:CG2	1:A:67:MET:HE1	2.50	0.41
1:D:142:LYS:HD3	1:D:199:LEU:HD23	2.02	0.41
1:I:90:ILE:CD1	1:I:114:ARG:HG2	2.48	0.41
1:L:310:ASN:CA	1:L:315:ASP:HB2	2.51	0.41
1:H:135:ASN:HB3	1:H:293:THR:HG23	2.01	0.41
1:D:47:GLU:HA	1:D:50:GLN:HG3	2.02	0.41
1:G:26:ILE:HD13	1:G:26:ILE:HG21	1.78	0.41
1:N:81:PRO:HB3	1:N:174:TRP:CD2	2.56	0.41
1:B:197:ASP:CG	1:B:327:GLN:HG2	2.41	0.41
1:N:273:GLU:HA	4:N:620:HOH:O	2.19	0.41
1:G:324:GLU:O	1:G:327:GLN:HB2	2.21	0.41
1:I:261:VAL:CG1	1:I:262:ARG:N	2.84	0.41
1:K:78:LEU:HB2	1:K:101:SER:HA	2.02	0.41
1:C:246:GLN:O	1:C:247:ASN:C	2.59	0.41
1:P:187:ASN:C	1:P:187:ASN:OD1	2.59	0.41
1:F:220:GLU:O	1:F:220:GLU:HG2	2.17	0.41
1:G:278:GLU:HA	1:G:279:PRO:HD3	1.89	0.41
1:K:127:PHE:HB3	1:K:304:TYR:OH	2.21	0.41
1:N:298:GLY:C	1:N:299:PHE:CD2	2.94	0.41
1:K:80:THR:HB	1:K:81:PRO:HD2	2.03	0.41
1:D:287:ARG:NH1	1:M:24:ASN:ND2	2.68	0.41
1:I:285:LYS:O	1:I:286:ILE:C	2.59	0.41
1:P:86:PRO:HA	1:P:115:MET:CG	2.39	0.41
1:K:98:HIS:ND1	1:K:125:ARG:N	2.51	0.41
1:L:21:ILE:HD13	2:L:500:NAI:C4N	2.43	0.41
2:P:500:NAI:C6N	2:P:500:NAI:H51N	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:53:GLU:C	1:C:55:ALA:N	2.74	0.41
1:N:85:HIS:HB2	1:N:105:MET:O	2.21	0.41
1:D:267:ALA:C	1:D:268:VAL:HG22	2.41	0.41
1:A:340:ARG:HG3	1:D:346:PRO:HB2	2.02	0.41
1:O:246:GLN:O	1:O:247:ASN:C	2.59	0.41
1:C:213:LEU:HA	1:C:213:LEU:HD23	1.75	0.41
1:B:31:GLN:HB3	1:B:31:GLN:HE21	1.75	0.41
1:D:124:VAL:HG12	1:D:125:ARG:N	2.36	0.40
1:M:310:ASN:HB3	1:M:315:ASP:CB	2.51	0.40
1:H:135:ASN:ND2	1:H:293:THR:CG2	2.84	0.40
1:D:45:ASN:HA	1:D:46:PRO:HD2	1.92	0.40
1:O:235:GLY:HA2	1:P:224:VAL:HG21	2.04	0.40
1:C:134:ARG:CD	1:C:319:GLU:OE1	2.68	0.40
1:C:320:THR:HA	1:C:324:GLU:CG	2.52	0.40
1:G:244:TYR:OH	1:H:277:ALA:HA	2.20	0.40
1:D:282:ASP:C	1:D:284:ASP:H	2.24	0.40
1:K:197:ASP:OD2	4:K:420:HOH:O	2.22	0.40
1:F:301:HIS:N	1:F:302:PRO:CD	2.83	0.40
1:G:112:GLY:O	1:G:115:MET:HG2	2.21	0.40
1:O:40:GLU:O	1:O:41:ILE:HG23	2.20	0.40
1:B:279:PRO:C	1:B:280[A]:HIS:HD1	2.24	0.40
1:L:81:PRO:HB3	1:L:174:TRP:CD2	2.56	0.40
1:L:40:GLU:O	1:L:41:ILE:CG2	2.69	0.40
1:L:42:CYS:HB2	1:L:67:MET:SD	2.61	0.40
1:G:12:ARG:NH1	1:G:72:ASN:O	2.54	0.40
1:C:12:ARG:O	1:C:74:ASP:N	2.45	0.40
1:O:8:ASP:O	1:O:9:ARG:HB3	2.21	0.40
1:G:53:GLU:O	1:G:54:ALA:C	2.59	0.40
1:I:21:ILE:HG22	2:I:500:NAI:H52N	2.02	0.40
1:I:21:ILE:HG21	2:I:500:NAI:C5D	2.52	0.40
1:I:168:TYR:OH	3:I:550:HP7:O'Q	2.32	0.40
1:N:76:LEU:HD12	1:N:92:VAL:HG11	1.99	0.40
1:D:64:LEU:HD12	1:D:67:MET:CE	2.52	0.40
1:M:30:ALA:C	1:M:32:HIS:N	2.75	0.40
1:L:28:ALA:HA	1:L:302:PRO:HG3	2.03	0.40
1:P:154:TYR:CZ	1:P:257:GLU:HB2	2.56	0.40
1:E:134:ARG:HA	1:E:139:GLN:HE21	1.86	0.40
1:P:309:ILE:O	1:P:310:ASN:C	2.59	0.40
1:M:197:ASP:HB2	4:M:478:HOH:O	2.20	0.40
1:G:323:ARG:O	1:G:326:LEU:HB2	2.21	0.40
1:G:156:VAL:O	1:G:235:GLY:HA3	2.20	0.40
1:D:204:GLU:OE1	4:D:559:HOH:O	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:197:ASP:HA	1:F:201:GLY:O	2.22	0.40
1:D:80:THR:HB	1:D:81:PRO:HD2	2.02	0.40
1:F:269:ASN:OD1	1:F:269:ASN:N	2.39	0.40
1:H:137:THR:HG23	1:H:293:THR:OG1	2.21	0.40
1:L:301:HIS:CB	1:L:302:PRO:HD3	2.52	0.40
1:B:11:ILE:HD12	1:B:11:ILE:HG23	1.80	0.40
1:C:40:GLU:HG2	1:C:61:PHE:HE2	1.86	0.40
1:A:103:LYS:HE2	1:A:103:LYS:C	2.42	0.40
1:A:76:LEU:HD12	1:A:92:VAL:CG2	2.50	0.40
1:O:35:ARG:NH2	1:O:310:ASN:OD1	2.54	0.40
1:P:310:ASN:CB	1:P:316:CYS:SG	3.10	0.40
1:E:149:ARG:NH1	1:E:278:GLU:O	2.35	0.40
1:G:282:ASP:C	1:G:284:ASP:H	2.25	0.40
1:D:131:GLN:NE2	1:D:301:HIS:CE1	2.89	0.40
1:O:149:ARG:HD2	4:O:519:HOH:O	2.20	0.40
1:P:244:TYR:CD1	1:P:244:TYR:C	2.95	0.40
1:M:68:LEU:HA	1:M:68:LEU:HD23	1.95	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:297:TYR:CE2	1:I:287:ARG:CD[2_746]	1.84	0.36
1:H:287:ARG:NH2	1:J:273:GLU:OE2[2_746]	2.12	0.08

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	344/370 (93%)	323 (94%)	20 (6%)	1 (0%)	50	46
1	B	327/370 (88%)	306 (94%)	20 (6%)	1 (0%)	50	46
1	C	345/370 (93%)	322 (93%)	21 (6%)	2 (1%)	33	25
1	D	342/370 (92%)	309 (90%)	29 (8%)	4 (1%)	19	9
1	E	317/370 (86%)	278 (88%)	34 (11%)	5 (2%)	14	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	323/370 (87%)	297 (92%)	25 (8%)	1 (0%)	50	46
1	G	340/370 (92%)	317 (93%)	20 (6%)	3 (1%)	25	14
1	H	341/370 (92%)	317 (93%)	23 (7%)	1 (0%)	50	46
1	I	340/370 (92%)	306 (90%)	28 (8%)	6 (2%)	13	4
1	J	344/370 (93%)	309 (90%)	31 (9%)	4 (1%)	19	9
1	K	318/370 (86%)	287 (90%)	26 (8%)	5 (2%)	14	5
1	L	316/370 (85%)	281 (89%)	27 (8%)	8 (2%)	9	2
1	M	344/370 (93%)	321 (93%)	20 (6%)	3 (1%)	25	14
1	N	340/370 (92%)	313 (92%)	26 (8%)	1 (0%)	50	46
1	O	330/370 (89%)	299 (91%)	29 (9%)	2 (1%)	33	25
1	P	318/370 (86%)	291 (92%)	24 (8%)	3 (1%)	25	14
All	All	5329/5920 (90%)	4876 (92%)	403 (8%)	50 (1%)	25	14

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	30	ALA
1	L	26	ILE
1	L	30	ALA
1	M	30	ALA
1	M	31	GLN
1	G	33	GLY
1	H	33	GLY
1	I	31	GLN
1	I	72	ASN
1	I	310	ASN
1	J	95	ALA
1	K	30	ALA
1	K	39	VAL
1	K	314	GLY
1	L	57	GLY
1	L	72	ASN
1	L	314	GLY
1	M	73	ALA
1	P	27	GLY
1	E	137	THR
1	G	283	ASP
1	G	315	ASP

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Mol	Chain	Res	Type
1	I	283	ASP
1	I	311	CYS
1	I	314	GLY
1	D	283	ASP
1	E	273	GLU
1	P	278	GLU
1	C	9	ARG
1	E	31	GLN
1	F	314	GLY
1	L	71	GLY
1	O	43	ASP
1	O	60	PRO
1	P	26	ILE
1	D	26	ILE
1	D	319	GLU
1	J	281	PRO
1	L	11	ILE
1	E	57	GLY
1	E	268	VAL
1	K	278	GLU
1	N	314	GLY
1	J	129	VAL
1	C	33	GLY
1	D	27	GLY
1	L	29	ILE
1	A	33	GLY
1	K	268	VAL
1	B	300	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	277/299 (93%)	261 (94%)	16 (6%)	28	23
1	B	264/299 (88%)	242 (92%)	22 (8%)	16	10
1	C	277/299 (93%)	262 (95%)	15 (5%)	31	25
1	D	275/299 (92%)	259 (94%)	16 (6%)	28	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	254/299 (85%)	238 (94%)	16 (6%)	25	19
1	F	260/299 (87%)	244 (94%)	16 (6%)	26	20
1	G	273/299 (91%)	257 (94%)	16 (6%)	28	22
1	H	274/299 (92%)	251 (92%)	23 (8%)	16	9
1	I	273/299 (91%)	256 (94%)	17 (6%)	26	20
1	J	277/299 (93%)	259 (94%)	18 (6%)	24	18
1	K	255/299 (85%)	233 (91%)	22 (9%)	15	8
1	L	256/299 (86%)	231 (90%)	25 (10%)	12	6
1	M	277/299 (93%)	262 (95%)	15 (5%)	31	25
1	N	273/299 (91%)	250 (92%)	23 (8%)	16	9
1	O	267/299 (89%)	251 (94%)	16 (6%)	27	21
1	P	255/299 (85%)	233 (91%)	22 (9%)	15	8
All	All	4287/4784 (90%)	3989 (93%)	298 (7%)	22	15

All (298) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	24	ASN
1	A	37	GLU
1	A	44	THR
1	A	53	GLU
1	A	72	ASN
1	A	103	LYS
1	A	114	ARG
1	A	124	VAL
1	A	125	ARG
1	A	143	LYS
1	A	167	GLU
1	A	287	ARG
1	A	288	GLU
1	A	316	CYS
1	A	343	VAL
1	B	12	ARG
1	B	31	GLN
1	B	41	ILE
1	B	59	ARG
1	B	65	SER

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Mol	Chain	Res	Type
1	B	72	ASN
1	B	94	GLN
1	B	103	LYS
1	B	115	MET
1	B	121	GLU
1	B	125	ARG
1	B	135	ASN
1	B	167	GLU
1	B	188	GLN
1	B	204	GLU
1	B	268	VAL
1	B	280[A]	HIS
1	B	280[B]	HIS
1	B	303	LEU
1	B	307	ASN
1	B	313	ARG
1	B	331	LEU
1	C	24	ASN
1	C	31	GLN
1	C	34	ASP
1	C	53	GLU
1	C	65	SER
1	C	72	ASN
1	C	97	ARG
1	C	103	LYS
1	C	125	ARG
1	C	130	LYS
1	C	153	ILE
1	C	258	LYS
1	C	295	SER
1	C	324	GLU
1	C	327	GLN
1	D	8	ASP
1	D	20	ARG
1	D	23	LYS
1	D	35	ARG
1	D	72	ASN
1	D	94	GLN
1	D	103	LYS
1	D	125	ARG
1	D	130	LYS
1	D	285	LYS

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Mol	Chain	Res	Type
1	D	287	ARG
1	D	291	TYR
1	D	292	GLU
1	D	299	PHE
1	D	303	LEU
1	D	327	GLN
1	E	12	ARG
1	E	15	LEU
1	E	34	ASP
1	E	53	GLU
1	E	56	THR
1	E	63	SER
1	E	103	LYS
1	E	110	GLU
1	E	125	ARG
1	E	157	THR
1	E	227	LEU
1	E	246	GLN
1	E	249	GLU
1	E	258	LYS
1	E	303	LEU
1	E	343	VAL
1	F	41	ILE
1	F	47	GLU
1	F	53	GLU
1	F	59	ARG
1	F	65	SER
1	F	103	LYS
1	F	125	ARG
1	F	132	ASN
1	F	167	GLU
1	F	173	ARG
1	F	188	GLN
1	F	227	LEU
1	F	245	PRO
1	F	313	ARG
1	F	315	ASP
1	F	327	GLN
1	G	38	LEU
1	G	53	GLU
1	G	59	ARG
1	G	94	GLN

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Mol	Chain	Res	Type
1	G	103	LYS
1	G	125	ARG
1	G	152	ARG
1	G	227	LEU
1	G	258	LYS
1	G	262	ARG
1	G	287	ARG
1	G	311	CYS
1	G	316	CYS
1	G	319	GLU
1	G	323	ARG
1	G	327	GLN
1	H	24	ASN
1	H	40	GLU
1	H	44	THR
1	H	47	GLU
1	H	50	GLN
1	H	72	ASN
1	H	80	THR
1	H	102	GLU
1	H	103	LYS
1	H	117	LYS
1	H	125	ARG
1	H	134	ARG
1	H	157	THR
1	H	167	GLU
1	H	204	GLU
1	H	216	ARG
1	H	258	LYS
1	H	278	GLU
1	H	287	ARG
1	H	291	TYR
1	H	293	THR
1	H	317	GLU
1	H	343	VAL
1	I	34	ASP
1	I	35	ARG
1	I	41	ILE
1	I	64	LEU
1	I	80	THR
1	I	91	GLU
1	I	97	ARG

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Mol	Chain	Res	Type
1	I	103	LYS
1	I	125	ARG
1	I	258	LYS
1	I	278	GLU
1	I	285	LYS
1	I	287	ARG
1	I	288	GLU
1	I	310	ASN
1	I	319	GLU
1	I	327	GLN
1	J	16	VAL
1	J	24	ASN
1	J	65	SER
1	J	72	ASN
1	J	76	LEU
1	J	103	LYS
1	J	117	LYS
1	J	125	ARG
1	J	153	ILE
1	J	167	GLU
1	J	177	LYS
1	J	230	ARG
1	J	268	VAL
1	J	278	GLU
1	J	287	ARG
1	J	288	GLU
1	J	319	GLU
1	J	327	GLN
1	K	9	ARG
1	K	40	GLU
1	K	44	THR
1	K	53	GLU
1	K	59	ARG
1	K	66	ASP
1	K	70	GLN
1	K	72	ASN
1	K	82	SER
1	K	103	LYS
1	K	117	LYS
1	K	130	LYS
1	K	153	ILE
1	K	204	GLU

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Mol	Chain	Res	Type
1	K	268	VAL
1	K	302	PRO
1	K	307	ASN
1	K	315	ASP
1	K	316	CYS
1	K	317	GLU
1	K	327	GLN
1	K	343	VAL
1	L	11	ILE
1	L	15	LEU
1	L	16	VAL
1	L	20	ARG
1	L	31	GLN
1	L	44	THR
1	L	47	GLU
1	L	74	ASP
1	L	76	LEU
1	L	97	ARG
1	L	103	LYS
1	L	108	ARG
1	L	125	ARG
1	L	130	LYS
1	L	177	LYS
1	L	216	ARG
1	L	230	ARG
1	L	245	PRO
1	L	258	LYS
1	L	268	VAL
1	L	278	GLU
1	L	303	LEU
1	L	317	GLU
1	L	324	GLU
1	L	331	LEU
1	M	12	ARG
1	M	24	ASN
1	M	39	VAL
1	M	72	ASN
1	M	103	LYS
1	M	125	ARG
1	M	197	ASP
1	M	216	ARG
1	M	230	ARG

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Mol	Chain	Res	Type
1	M	258	LYS
1	M	285	LYS
1	M	296	VAL
1	M	327	GLN
1	M	343	VAL
1	M	346	PRO
1	N	21	ILE
1	N	34	ASP
1	N	40	GLU
1	N	53	GLU
1	N	59	ARG
1	N	65	SER
1	N	70	GLN
1	N	72	ASN
1	N	97	ARG
1	N	103	LYS
1	N	117	LYS
1	N	125	ARG
1	N	134	ARG
1	N	227	LEU
1	N	258	LYS
1	N	268	VAL
1	N	273	GLU
1	N	278	GLU
1	N	285	LYS
1	N	287	ARG
1	N	303	LEU
1	N	319	GLU
1	N	343	VAL
1	O	34	ASP
1	O	65	SER
1	O	72	ASN
1	O	103	LYS
1	O	125	ARG
1	O	134	ARG
1	O	153	ILE
1	O	157	THR
1	O	262	ARG
1	O	280	HIS
1	O	287	ARG
1	O	303	LEU
1	O	316	CYS

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Mol	Chain	Res	Type
1	O	328	SER
1	O	331	LEU
1	O	343	VAL
1	P	16	VAL
1	P	34	ASP
1	P	40	GLU
1	P	53	GLU
1	P	59	ARG
1	P	72	ASN
1	P	103	LYS
1	P	114	ARG
1	P	117	LYS
1	P	125	ARG
1	P	132	ASN
1	P	135	ASN
1	P	157	THR
1	P	227	LEU
1	P	258	LYS
1	P	262	ARG
1	P	271	ILE
1	P	278	GLU
1	P	303	LEU
1	P	327	GLN
1	P	331	LEU
1	P	343	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	88	GLN
1	A	246	GLN
1	B	24	ASN
1	B	50	GLN
1	B	72	ASN
1	B	88	GLN
1	B	135	ASN
1	B	188	GLN
1	B	191	HIS
1	B	238	ASN
1	C	24	ASN
1	C	31	GLN

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Mol	Chain	Res	Type
1	C	72	ASN
1	C	88	GLN
1	C	246	GLN
1	C	290	ASN
1	C	327	GLN
1	D	24	ASN
1	D	31	GLN
1	D	50	GLN
1	D	72	ASN
1	D	88	GLN
1	D	147	GLN
1	D	246	GLN
1	D	327	GLN
1	E	88	GLN
1	E	166	GLN
1	E	191	HIS
1	E	246	GLN
1	F	24	ASN
1	F	31	GLN
1	F	88	GLN
1	F	139	GLN
1	F	188	GLN
1	F	246	GLN
1	F	280	HIS
1	G	88	GLN
1	H	24	ASN
1	H	72	ASN
1	H	88	GLN
1	H	188	GLN
1	H	327	GLN
1	I	31	GLN
1	I	72	ASN
1	I	88	GLN
1	I	246	GLN
1	I	310	ASN
1	J	31	GLN
1	J	88	GLN
1	K	24	ASN
1	K	31	GLN
1	K	88	GLN
1	K	139	GLN
1	K	188	GLN

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Mol	Chain	Res	Type
1	K	246	GLN
1	K	327	GLN
1	L	88	GLN
1	L	188	GLN
1	M	31	GLN
1	M	72	ASN
1	M	88	GLN
1	N	31	GLN
1	N	70	GLN
1	N	88	GLN
1	N	246	GLN
1	O	72	ASN
1	O	88	GLN
1	O	188	GLN
1	P	31	GLN
1	P	88	GLN
1	P	135	ASN
1	P	246	GLN
1	P	269	ASN
1	P	327	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

32 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAI	A	500	-	48,48,48	1.39	4 (8%)	73,73,73	2.26	21 (28%)
3	HP7	A	550	-	42,42,42	1.01	2 (4%)	60,64,64	2.25	17 (28%)
2	NAI	B	500	-	48,48,48	1.44	5 (10%)	73,73,73	2.29	26 (35%)
3	HP7	B	550	-	42,42,42	0.91	2 (4%)	60,64,64	1.76	14 (23%)
2	NAI	C	500	-	48,48,48	1.42	4 (8%)	73,73,73	2.32	26 (35%)
3	HP7	C	550	-	42,42,42	0.92	2 (4%)	60,64,64	1.78	21 (35%)
2	NAI	D	500	-	48,48,48	1.41	5 (10%)	73,73,73	2.36	21 (28%)
3	HP7	D	550	-	42,42,42	0.96	2 (4%)	60,64,64	1.61	7 (11%)
2	NAI	E	500	-	48,48,48	1.42	5 (10%)	73,73,73	2.32	19 (26%)
3	HP7	E	550	-	42,42,42	0.94	2 (4%)	60,64,64	1.57	9 (15%)
2	NAI	F	500	-	48,48,48	1.42	6 (12%)	73,73,73	2.36	27 (36%)
3	HP7	F	550	-	42,42,42	0.92	2 (4%)	60,64,64	1.40	9 (15%)
2	NAI	G	500	-	48,48,48	1.40	6 (12%)	73,73,73	2.39	26 (35%)
3	HP7	G	550	-	42,42,42	0.95	1 (2%)	60,64,64	1.81	10 (16%)
2	NAI	H	500	-	48,48,48	1.40	5 (10%)	73,73,73	2.74	28 (38%)
3	HP7	H	550	-	42,42,42	0.93	1 (2%)	60,64,64	1.94	12 (20%)
2	NAI	I	500	-	48,48,48	1.38	5 (10%)	73,73,73	2.33	22 (30%)
3	HP7	I	550	-	42,42,42	1.01	1 (2%)	60,64,64	1.67	15 (25%)
2	NAI	J	500	-	48,48,48	1.41	5 (10%)	73,73,73	2.47	26 (35%)
3	HP7	J	550	-	42,42,42	0.93	2 (4%)	60,64,64	1.83	15 (25%)
2	NAI	K	500	-	48,48,48	1.39	5 (10%)	73,73,73	2.65	29 (39%)
3	HP7	K	550	-	42,42,42	0.98	2 (4%)	60,64,64	1.95	12 (20%)
2	NAI	L	500	-	48,48,48	1.41	5 (10%)	73,73,73	2.59	28 (38%)
3	HP7	L	550	-	42,42,42	0.94	2 (4%)	60,64,64	1.80	11 (18%)
2	NAI	M	500	-	48,48,48	1.42	5 (10%)	73,73,73	2.30	24 (32%)
3	HP7	M	550	-	42,42,42	0.92	2 (4%)	60,64,64	2.11	15 (25%)
2	NAI	N	500	-	48,48,48	1.41	6 (12%)	73,73,73	2.43	23 (31%)
3	HP7	N	550	-	42,42,42	0.91	1 (2%)	60,64,64	2.10	13 (21%)
2	NAI	O	500	-	48,48,48	1.41	5 (10%)	73,73,73	2.48	23 (31%)
3	HP7	O	550	-	42,42,42	0.97	2 (4%)	60,64,64	1.76	9 (15%)
2	NAI	P	500	-	48,48,48	1.40	5 (10%)	73,73,73	2.10	23 (31%)
3	HP7	P	550	-	42,42,42	0.95	2 (4%)	60,64,64	1.51	9 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAI	A	500	-	-	0/30/72/72	0/3/5/5
3	HP7	A	550	-	-	0/27/65/65	0/3/3/3
2	NAI	B	500	-	-	0/30/72/72	0/3/5/5
3	HP7	B	550	-	-	0/27/65/65	0/3/3/3
2	NAI	C	500	-	-	0/30/72/72	0/3/5/5
3	HP7	C	550	-	-	0/27/65/65	0/3/3/3
2	NAI	D	500	-	-	0/30/72/72	0/3/5/5
3	HP7	D	550	-	-	0/27/65/65	0/3/3/3
2	NAI	E	500	-	-	0/30/72/72	0/3/5/5
3	HP7	E	550	-	-	0/27/65/65	0/3/3/3
2	NAI	F	500	-	-	0/30/72/72	0/3/5/5
3	HP7	F	550	-	-	0/27/65/65	0/3/3/3
2	NAI	G	500	-	-	0/30/72/72	0/3/5/5
3	HP7	G	550	-	-	0/27/65/65	0/3/3/3
2	NAI	H	500	-	-	0/30/72/72	0/3/5/5
3	HP7	H	550	-	-	0/27/65/65	0/3/3/3
2	NAI	I	500	-	-	0/30/72/72	0/3/5/5
3	HP7	I	550	-	-	0/27/65/65	0/3/3/3
2	NAI	J	500	-	-	0/30/72/72	0/3/5/5
3	HP7	J	550	-	-	0/27/65/65	0/3/3/3
2	NAI	K	500	-	-	0/30/72/72	0/3/5/5
3	HP7	K	550	-	-	0/27/65/65	0/3/3/3
2	NAI	L	500	-	-	0/30/72/72	0/3/5/5
3	HP7	L	550	-	-	0/27/65/65	0/3/3/3
2	NAI	M	500	-	-	0/30/72/72	0/3/5/5
3	HP7	M	550	-	-	0/27/65/65	0/3/3/3
2	NAI	N	500	-	-	0/30/72/72	0/3/5/5
3	HP7	N	550	-	-	0/27/65/65	0/3/3/3
2	NAI	O	500	-	-	0/30/72/72	0/3/5/5
3	HP7	O	550	-	-	0/27/65/65	0/3/3/3
2	NAI	P	500	-	-	0/30/72/72	0/3/5/5
3	HP7	P	550	-	-	0/27/65/65	0/3/3/3

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	NAI	C4N-C3N	-5.35	1.39	1.50
2	F	500	NAI	C4N-C3N	-5.12	1.40	1.50
2	B	500	NAI	C4N-C3N	-5.02	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	500	NAI	C4N-C3N	-5.02	1.40	1.50
2	O	500	NAI	C4N-C3N	-4.95	1.40	1.50
2	L	500	NAI	C4N-C3N	-4.95	1.40	1.50
2	P	500	NAI	C4N-C3N	-4.94	1.40	1.50
2	D	500	NAI	C4N-C3N	-4.92	1.40	1.50
2	N	500	NAI	C4N-C3N	-4.91	1.40	1.50
2	H	500	NAI	C4N-C3N	-4.86	1.40	1.50
2	I	500	NAI	C4N-C3N	-4.86	1.40	1.50
2	M	500	NAI	C4N-C3N	-4.83	1.40	1.50
2	J	500	NAI	C4N-C3N	-4.80	1.40	1.50
2	G	500	NAI	C4N-C3N	-4.80	1.40	1.50
2	G	500	NAI	C4N-C5N	-4.80	1.38	1.49
2	A	500	NAI	C4N-C3N	-4.80	1.40	1.50
2	K	500	NAI	C4N-C3N	-4.78	1.40	1.50
2	C	500	NAI	C4N-C5N	-4.77	1.38	1.49
2	L	500	NAI	C4N-C5N	-4.76	1.38	1.49
2	F	500	NAI	C4N-C5N	-4.75	1.38	1.49
2	E	500	NAI	C4N-C5N	-4.70	1.38	1.49
2	O	500	NAI	C4N-C5N	-4.69	1.38	1.49
2	H	500	NAI	C4N-C5N	-4.69	1.38	1.49
2	I	500	NAI	C4N-C5N	-4.68	1.38	1.49
2	D	500	NAI	C4N-C5N	-4.65	1.38	1.49
2	M	500	NAI	C4N-C5N	-4.65	1.38	1.49
2	K	500	NAI	C4N-C5N	-4.64	1.38	1.49
2	J	500	NAI	C4N-C5N	-4.64	1.38	1.49
2	A	500	NAI	C4N-C5N	-4.58	1.39	1.49
2	N	500	NAI	C4N-C5N	-4.50	1.39	1.49
2	B	500	NAI	C4N-C5N	-4.48	1.39	1.49
2	P	500	NAI	C4N-C5N	-4.46	1.39	1.49
3	I	550	HP7	C2-N1	-4.45	1.33	1.38
3	A	550	HP7	C2-N1	-4.30	1.33	1.38
3	D	550	HP7	C2-N1	-4.16	1.33	1.38
3	G	550	HP7	C2-N1	-4.13	1.33	1.38
3	O	550	HP7	C2-N1	-4.10	1.33	1.38
3	P	550	HP7	C2-N1	-4.07	1.34	1.38
3	K	550	HP7	C2-N1	-4.06	1.34	1.38
3	H	550	HP7	C2-N1	-3.95	1.34	1.38
3	E	550	HP7	C2-N1	-3.90	1.34	1.38
3	B	550	HP7	C2-N1	-3.81	1.34	1.38
3	J	550	HP7	C2-N1	-3.62	1.34	1.38
3	L	550	HP7	C2-N1	-3.59	1.34	1.38
3	C	550	HP7	C2-N1	-3.55	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	550	HP7	C2-N1	-3.48	1.34	1.38
3	N	550	HP7	C2-N1	-3.45	1.34	1.38
3	M	550	HP7	C2-N1	-3.42	1.34	1.38
2	B	500	NAI	C2N-C3N	2.96	1.40	1.34
2	A	500	NAI	C6N-C5N	2.90	1.39	1.33
2	K	500	NAI	C2N-C3N	2.85	1.40	1.34
2	M	500	NAI	C6N-C5N	2.85	1.39	1.33
2	M	500	NAI	C2N-C3N	2.81	1.40	1.34
2	J	500	NAI	C2N-C3N	2.81	1.40	1.34
2	D	500	NAI	C2N-C3N	2.77	1.40	1.34
2	P	500	NAI	C6N-C5N	2.77	1.39	1.33
2	N	500	NAI	C6N-C5N	2.76	1.39	1.33
2	O	500	NAI	C2N-C3N	2.75	1.40	1.34
2	D	500	NAI	C6N-C5N	2.74	1.39	1.33
2	J	500	NAI	C6N-C5N	2.73	1.39	1.33
2	E	500	NAI	C6N-C5N	2.71	1.39	1.33
2	L	500	NAI	C2N-C3N	2.71	1.40	1.34
2	B	500	NAI	O4B-C1B	2.69	1.45	1.41
2	I	500	NAI	C6N-C5N	2.69	1.39	1.33
2	E	500	NAI	C2N-C3N	2.68	1.40	1.34
2	G	500	NAI	C6N-C5N	2.68	1.38	1.33
2	I	500	NAI	C2N-C3N	2.68	1.40	1.34
2	P	500	NAI	C2N-C3N	2.68	1.40	1.34
2	B	500	NAI	C6N-C5N	2.68	1.38	1.33
2	N	500	NAI	C2N-C3N	2.67	1.39	1.34
2	H	500	NAI	C2N-C3N	2.66	1.39	1.34
2	A	500	NAI	C2N-C3N	2.66	1.39	1.34
2	L	500	NAI	C6N-C5N	2.66	1.38	1.33
2	G	500	NAI	C2N-C3N	2.63	1.39	1.34
2	F	500	NAI	C6N-C5N	2.62	1.38	1.33
2	H	500	NAI	O4B-C1B	2.60	1.45	1.41
2	K	500	NAI	C6N-C5N	2.59	1.38	1.33
2	N	500	NAI	O4B-C1B	2.54	1.45	1.41
2	O	500	NAI	C6N-C5N	2.53	1.38	1.33
2	C	500	NAI	C6N-C5N	2.52	1.38	1.33
2	F	500	NAI	C2N-C3N	2.48	1.39	1.34
3	A	550	HP7	C6-C5	2.47	1.40	1.36
2	H	500	NAI	C6N-C5N	2.46	1.38	1.33
3	M	550	HP7	C6-C5	2.43	1.40	1.36
3	L	550	HP7	C6-C5	2.40	1.39	1.36
3	C	550	HP7	C6-C5	2.40	1.39	1.36
2	J	500	NAI	O4B-C1B	2.39	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	500	NAI	O4B-C1B	2.37	1.45	1.41
2	C	500	NAI	C2N-C3N	2.37	1.39	1.34
3	J	550	HP7	C6-C5	2.36	1.39	1.36
2	L	500	NAI	O4B-C1B	2.35	1.44	1.41
2	D	500	NAI	O4B-C1B	2.30	1.44	1.41
2	E	500	NAI	O4B-C1B	2.27	1.44	1.41
2	I	500	NAI	O4B-C1B	2.22	1.44	1.41
3	F	550	HP7	C6-C5	2.20	1.39	1.36
3	E	550	HP7	C6-C5	2.20	1.39	1.36
2	F	500	NAI	C2N-N1N	-2.19	1.31	1.36
2	P	500	NAI	O4B-C1B	2.18	1.44	1.41
3	O	550	HP7	C6-C5	2.12	1.39	1.36
2	K	500	NAI	O4B-C1B	2.12	1.44	1.41
2	G	500	NAI	O4B-C1B	2.12	1.44	1.41
3	D	550	HP7	C6-C5	2.09	1.39	1.36
2	O	500	NAI	O4B-C1B	2.09	1.44	1.41
2	F	500	NAI	O4B-C1B	2.07	1.44	1.41
3	K	550	HP7	C6-C5	2.06	1.39	1.36
2	N	500	NAI	C2N-N1N	-2.05	1.31	1.36
2	G	500	NAI	C2N-N1N	-2.01	1.32	1.36
3	P	550	HP7	C6-C5	2.00	1.39	1.36
3	B	550	HP7	C6-C5	2.00	1.39	1.36

All (590) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	500	NAI	O4B-C1B-N9A	12.29	119.87	108.44
2	G	500	NAI	N3A-C2A-N1A	-11.44	119.15	128.71
2	N	500	NAI	N3A-C2A-N1A	-11.03	119.48	128.71
3	A	550	HP7	C2-N1-C1C	-10.72	111.49	118.21
2	K	500	NAI	N3A-C2A-N1A	-10.56	119.88	128.71
2	L	500	NAI	N3A-C2A-N1A	-10.37	120.04	128.71
2	O	500	NAI	N3A-C2A-N1A	-10.07	120.29	128.71
2	A	500	NAI	N3A-C2A-N1A	-10.03	120.32	128.71
2	E	500	NAI	N3A-C2A-N1A	-9.13	121.08	128.71
2	J	500	NAI	N3A-C2A-N1A	-8.74	121.40	128.71
2	D	500	NAI	N3A-C2A-N1A	-8.67	121.46	128.71
2	B	500	NAI	N3A-C2A-N1A	-8.14	121.90	128.71
2	I	500	NAI	N3A-C2A-N1A	-8.08	121.96	128.71
2	C	500	NAI	N3A-C2A-N1A	-7.74	122.24	128.71
2	H	500	NAI	N3A-C2A-N1A	-7.56	122.39	128.71
2	P	500	NAI	N3A-C2A-N1A	-7.54	122.40	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	550	HP7	N3-C2-N1	7.51	122.24	115.97
3	M	550	HP7	N3-C2-N1	7.41	122.16	115.97
3	J	550	HP7	N3-C2-N1	7.37	122.13	115.97
3	O	550	HP7	N3-C2-N1	7.30	122.07	115.97
3	K	550	HP7	N3-C2-N1	7.29	122.06	115.97
3	N	550	HP7	C2-N1-C1C	-7.11	113.75	118.21
2	L	500	NAI	C4B-O4B-C1B	-6.68	102.49	109.75
3	K	550	HP7	O5'-C1'-O3B	-6.58	102.77	111.36
2	D	500	NAI	C4B-O4B-C1B	-6.56	102.62	109.75
2	I	500	NAI	C4B-O4B-C1B	-6.51	102.67	109.75
2	J	500	NAI	C5B-C4B-C3B	-6.42	89.48	115.21
2	C	500	NAI	C4B-O4B-C1B	-6.35	102.85	109.75
2	L	500	NAI	PN-O3-PA	-6.35	113.07	131.68
2	D	500	NAI	C5B-C4B-C3B	-6.34	89.82	115.21
2	M	500	NAI	N3A-C2A-N1A	-6.33	123.41	128.71
3	B	550	HP7	N3-C2-N1	6.24	121.18	115.97
3	L	550	HP7	O5'-C1'-O3B	-6.23	103.22	111.36
2	J	500	NAI	O4B-C1B-N9A	6.19	114.20	108.44
2	O	500	NAI	PN-O3-PA	-6.12	113.75	131.68
2	K	500	NAI	PN-O3-PA	-6.06	113.91	131.68
3	D	550	HP7	O5'-C1'-O3B	-6.04	103.47	111.36
3	E	550	HP7	N3-C2-N1	6.04	121.01	115.97
2	H	500	NAI	O4D-C4D-C5D	-6.01	87.92	109.36
2	J	500	NAI	PN-O3-PA	-6.00	114.10	131.68
3	M	550	HP7	O5'-C1'-O3B	-5.95	103.59	111.36
3	H	550	HP7	N3-C2-N1	5.91	120.91	115.97
2	M	500	NAI	C4A-C5A-N7A	-5.90	104.47	109.52
2	M	500	NAI	C5B-C4B-C3B	-5.90	91.58	115.21
2	E	500	NAI	PN-O3-PA	-5.82	114.61	131.68
2	E	500	NAI	O4B-C1B-N9A	5.80	113.83	108.44
2	K	500	NAI	O4D-C4D-C5D	-5.78	88.72	109.36
2	L	500	NAI	O4B-C1B-N9A	5.74	113.78	108.44
2	I	500	NAI	O4D-C4D-C5D	-5.73	88.90	109.36
2	B	500	NAI	C4B-O4B-C1B	-5.68	103.58	109.75
2	F	500	NAI	PN-O3-PA	-5.63	115.17	131.68
2	O	500	NAI	N3A-C4A-N9A	5.62	135.58	125.43
2	H	500	NAI	C3B-C2B-C1B	-5.61	92.13	100.91
2	P	500	NAI	PN-O3-PA	-5.61	115.25	131.68
2	F	500	NAI	C4B-O4B-C1B	-5.51	103.76	109.75
2	E	500	NAI	O4B-C1B-C2B	-5.47	98.39	106.77
3	H	550	HP7	O5'-C1'-O3B	-5.45	104.23	111.36
2	H	500	NAI	PN-O3-PA	-5.43	115.76	131.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	500	NAI	C5B-C4B-C3B	-5.39	93.63	115.21
3	H	550	HP7	C2-N1-C1C	5.38	121.58	118.21
2	K	500	NAI	O4B-C1B-N9A	5.34	113.40	108.44
2	O	500	NAI	O5B-C5B-C4B	5.29	128.36	108.94
2	I	500	NAI	N3A-C4A-N9A	5.29	134.98	125.43
2	A	500	NAI	C4A-C5A-N7A	-5.27	105.01	109.52
2	C	500	NAI	C4A-C5A-N7A	-5.24	105.03	109.52
3	N	550	HP7	N3-C2-N1	5.19	120.31	115.97
2	C	500	NAI	PN-O3-PA	-5.12	116.68	131.68
2	F	500	NAI	C5B-C4B-C3B	-5.11	94.73	115.21
2	P	500	NAI	C5B-C4B-C3B	-5.09	94.84	115.21
2	N	500	NAI	PN-O3-PA	-5.08	116.77	131.68
2	N	500	NAI	C5B-C4B-C3B	-5.08	94.86	115.21
3	N	550	HP7	C8'-C7'-N2'	5.03	125.95	116.11
2	H	500	NAI	C6N-N1N-C2N	4.98	125.95	119.44
2	L	500	NAI	N3A-C4A-N9A	4.97	134.40	125.43
2	D	500	NAI	N3A-C4A-N9A	4.89	134.27	125.43
2	N	500	NAI	C1B-N9A-C4A	-4.88	118.20	126.64
2	M	500	NAI	PN-O3-PA	-4.88	117.38	131.68
2	G	500	NAI	C1B-N9A-C4A	-4.86	118.23	126.64
2	B	500	NAI	O4D-C1D-N1N	4.83	118.28	108.05
2	K	500	NAI	C1B-N9A-C4A	-4.82	118.31	126.64
3	D	550	HP7	N3-C2-N1	4.80	119.98	115.97
2	F	500	NAI	N3A-C4A-N9A	4.79	134.07	125.43
2	A	500	NAI	PN-O3-PA	-4.76	117.72	131.68
2	B	500	NAI	C5B-C4B-C3B	-4.73	96.26	115.21
3	L	550	HP7	C1'-C2'-N2'	-4.72	102.09	111.02
3	M	550	HP7	C8'-C7'-N2'	4.72	125.33	116.11
3	N	550	HP7	O7'-C7'-N2'	-4.71	112.08	121.90
2	B	500	NAI	PN-O3-PA	-4.69	117.92	131.68
2	L	500	NAI	C3B-C2B-C1B	-4.68	93.58	100.91
2	K	500	NAI	N3A-C4A-N9A	4.65	133.83	125.43
2	O	500	NAI	O4D-C1D-N1N	4.63	117.84	108.05
3	A	550	HP7	C8'-C7'-N2'	4.59	125.07	116.11
2	D	500	NAI	O4D-C1D-N1N	4.56	117.70	108.05
2	E	500	NAI	C5B-C4B-C3B	-4.56	96.96	115.21
2	M	500	NAI	O3-PA-O5B	4.54	123.71	103.41
2	J	500	NAI	N3A-C4A-N9A	4.54	133.63	125.43
2	D	500	NAI	PN-O3-PA	-4.54	118.38	131.68
2	A	500	NAI	N3A-C4A-N9A	4.53	133.61	125.43
2	M	500	NAI	C3N-C7N-N7N	4.52	126.18	117.48
2	N	500	NAI	C1D-N1N-C2N	-4.51	113.33	121.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	500	NAI	N3A-C2A-N1A	-4.51	124.94	128.71
3	I	550	HP7	O5'-C5'-C4'	-4.47	102.40	110.02
2	K	500	NAI	O3-PA-O5B	4.42	123.16	103.41
2	L	500	NAI	C5B-C4B-C3B	-4.42	97.52	115.21
2	K	500	NAI	C4B-O4B-C1B	-4.41	104.95	109.75
2	P	500	NAI	N3A-C4A-N9A	4.40	133.38	125.43
2	C	500	NAI	N3A-C4A-N9A	4.39	133.37	125.43
3	G	550	HP7	C8'-C7'-N2'	4.39	124.69	116.11
2	E	500	NAI	C4A-C5A-N7A	-4.39	105.76	109.52
3	O	550	HP7	PB-O3A-PA	-4.37	118.87	131.68
2	C	500	NAI	O3-PA-O5B	4.36	122.88	103.41
3	J	550	HP7	PB-O3A-PA	-4.35	118.91	131.68
2	A	500	NAI	O3-PA-O5B	4.35	122.85	103.41
3	H	550	HP7	C3'-C2'-N2'	-4.34	101.34	110.56
3	G	550	HP7	C2-N1-C1C	4.34	120.93	118.21
3	A	550	HP7	N3-C2-N1	4.33	119.59	115.97
2	L	500	NAI	C4N-C3N-C2N	-4.33	116.41	121.68
2	E	500	NAI	O3-PA-O5B	4.31	122.69	103.41
2	I	500	NAI	O4B-C1B-N9A	4.26	112.40	108.44
2	N	500	NAI	C8A-N9A-C1B	4.26	134.77	126.38
2	K	500	NAI	C4A-C5A-N7A	-4.24	105.89	109.52
2	C	500	NAI	C6N-N1N-C2N	4.24	124.98	119.44
2	B	500	NAI	C4A-C5A-N7A	-4.22	105.90	109.52
2	M	500	NAI	C4N-C3N-C2N	-4.22	116.54	121.68
2	J	500	NAI	C1D-N1N-C2N	-4.21	113.84	121.02
3	P	550	HP7	C2-N1-C1C	4.20	120.84	118.21
2	F	500	NAI	O4B-C1B-N9A	4.19	112.34	108.44
2	O	500	NAI	O4D-C4D-C5D	-4.17	94.46	109.36
2	D	500	NAI	C4N-C3N-C2N	-4.13	116.65	121.68
2	B	500	NAI	O3-PA-O5B	4.13	121.89	103.41
3	C	550	HP7	N3-C2-N1	4.12	119.41	115.97
2	O	500	NAI	C4A-C5A-N7A	-4.11	106.01	109.52
2	F	500	NAI	O3-PA-O5B	4.09	121.70	103.41
2	E	500	NAI	O4D-C1D-N1N	4.08	116.70	108.05
2	C	500	NAI	C5B-C4B-C3B	-4.07	98.89	115.21
2	F	500	NAI	C4A-C5A-N7A	-4.05	106.06	109.52
2	N	500	NAI	N3A-C4A-N9A	4.03	132.72	125.43
2	H	500	NAI	C3N-C2N-N1N	-4.02	117.34	123.05
3	M	550	HP7	O'Q-C6'-O'P	-4.02	114.99	124.07
2	I	500	NAI	C4N-C3N-C2N	-3.98	116.83	121.68
2	G	500	NAI	N3A-C4A-N9A	3.97	132.61	125.43
2	N	500	NAI	C6N-N1N-C2N	3.95	124.61	119.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	500	NAI	C6N-N1N-C2N	3.94	124.59	119.44
2	B	500	NAI	O4D-C4D-C5D	-3.92	95.35	109.36
2	G	500	NAI	PN-O3-PA	-3.91	120.22	131.68
2	O	500	NAI	C5A-C4A-N3A	-3.90	117.20	125.70
2	O	500	NAI	C4B-O4B-C1B	-3.89	105.52	109.75
2	F	500	NAI	C6N-N1N-C2N	3.89	124.53	119.44
2	J	500	NAI	C6N-N1N-C2N	3.89	124.52	119.44
3	L	550	HP7	C1'-O5'-C5'	-3.88	106.65	112.20
3	D	550	HP7	C3C-C2C-C1C	3.88	106.97	100.91
3	P	550	HP7	C4C-O4C-C1C	-3.86	105.56	109.75
2	J	500	NAI	O4D-C4D-C5D	-3.84	95.67	109.36
2	P	500	NAI	C4N-C3N-C2N	-3.83	117.01	121.68
3	A	550	HP7	O7'-C7'-C8'	-3.83	114.56	122.04
3	N	550	HP7	O2C-C2C-C1C	-3.83	99.64	111.23
2	A	500	NAI	C3N-C7N-N7N	3.83	124.84	117.48
2	H	500	NAI	C5B-C4B-C3B	-3.82	99.90	115.21
3	J	550	HP7	C4'-C3'-C2'	-3.81	105.04	110.44
2	D	500	NAI	O4D-C4D-C5D	-3.78	95.85	109.36
2	J	500	NAI	C4D-O4D-C1D	-3.78	100.90	109.51
3	K	550	HP7	C8'-C7'-N2'	3.76	123.47	116.11
2	O	500	NAI	O3-PA-O5B	3.74	120.15	103.41
2	L	500	NAI	C1B-N9A-C4A	-3.74	120.18	126.64
3	B	550	HP7	C2C-C1C-N1	-3.73	103.64	113.26
2	K	500	NAI	C3N-C2N-N1N	-3.73	117.75	123.05
2	G	500	NAI	O5B-C5B-C4B	3.72	122.59	108.94
3	O	550	HP7	C2-N1-C1C	3.71	120.53	118.21
2	K	500	NAI	O2A-PA-O5B	-3.71	89.80	108.51
2	G	500	NAI	C5B-C4B-C3B	-3.69	100.44	115.21
3	K	550	HP7	C5-C6-N1	-3.69	117.04	121.21
3	N	550	HP7	C4'-C5'-C6'	-3.69	104.36	110.84
2	F	500	NAI	C5A-C4A-N3A	-3.69	117.68	125.70
2	F	500	NAI	C3N-C2N-N1N	-3.68	117.82	123.05
2	H	500	NAI	N3A-C4A-N9A	3.68	132.08	125.43
3	F	550	HP7	N3-C2-N1	3.66	119.03	115.97
2	O	500	NAI	C2A-N3A-C4A	3.66	124.44	114.01
2	B	500	NAI	C4N-C3N-C2N	-3.65	117.23	121.68
3	O	550	HP7	O2C-C2C-C1C	-3.65	100.19	111.23
3	P	550	HP7	PB-O3A-PA	-3.64	121.00	131.68
2	F	500	NAI	O1N-PN-O5D	-3.63	90.22	108.51
2	A	500	NAI	O7N-C7N-C3N	-3.61	113.72	120.51
3	F	550	HP7	O3'-C3'-C2'	-3.61	102.19	109.61
2	E	500	NAI	N3A-C4A-N9A	3.61	131.95	125.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	550	HP7	O5'-C5'-C4'	-3.58	103.90	110.02
3	G	550	HP7	O5C-C5C-C4C	-3.58	95.78	108.94
3	L	550	HP7	N3-C2-N1	3.58	118.96	115.97
2	I	500	NAI	O3-PA-O5B	3.56	119.34	103.41
2	D	500	NAI	O2D-C2D-C1D	-3.55	97.94	110.04
2	P	500	NAI	O4B-C1B-C2B	-3.53	101.36	106.77
3	B	550	HP7	C1'-C2'-N2'	-3.52	104.36	111.02
2	H	500	NAI	O1N-PN-O2N	-3.51	92.60	112.21
2	G	500	NAI	C8A-N9A-C1B	3.50	133.28	126.38
3	I	550	HP7	PB-O3A-PA	-3.49	121.45	131.68
2	M	500	NAI	O2A-PA-O5B	-3.43	91.23	108.51
3	I	550	HP7	O3A-PB-O3B	-3.42	94.83	103.48
3	C	550	HP7	O5'-C1'-O3B	-3.41	106.91	111.36
2	G	500	NAI	C2A-N1A-C6A	3.41	124.92	118.77
2	A	500	NAI	C5A-C4A-N3A	-3.41	118.28	125.70
2	N	500	NAI	O3-PA-O5B	3.41	118.64	103.41
2	O	500	NAI	O4B-C1B-C2B	-3.39	101.57	106.77
3	E	550	HP7	O5'-C1'-C2'	3.39	118.08	110.78
2	K	500	NAI	C5B-C4B-C3B	-3.39	101.65	115.21
2	C	500	NAI	O4D-C4D-C5D	-3.39	97.27	109.36
2	K	500	NAI	C8A-N9A-C4A	3.38	109.48	106.90
2	C	500	NAI	C3N-C2N-N1N	-3.38	118.25	123.05
2	M	500	NAI	C8A-N9A-C1B	3.37	133.03	126.38
2	K	500	NAI	C4N-C5N-C6N	-3.37	116.43	122.61
3	P	550	HP7	O5'-C1'-O3B	-3.37	106.97	111.36
3	L	550	HP7	O5'-C5'-C6'	-3.36	99.79	107.23
2	J	500	NAI	C3D-C2D-C1D	-3.35	94.70	101.35
3	C	550	HP7	O'Q-C6'-O'P	-3.34	116.51	124.07
2	J	500	NAI	O3-PA-O5B	3.33	118.31	103.41
2	F	500	NAI	C1D-N1N-C2N	-3.33	115.35	121.02
2	M	500	NAI	O7N-C7N-N7N	-3.32	114.53	122.93
3	M	550	HP7	O2C-C2C-C1C	-3.32	101.19	111.23
2	I	500	NAI	C1D-N1N-C2N	-3.32	115.36	121.02
2	L	500	NAI	O5B-C5B-C4B	3.32	121.11	108.94
3	H	550	HP7	PB-O3A-PA	-3.31	121.98	131.68
3	M	550	HP7	O3C-C3C-C4C	-3.26	101.48	111.08
2	L	500	NAI	O3-PA-O5B	3.25	117.94	103.41
2	F	500	NAI	O4D-C4D-C3D	3.24	111.75	105.17
2	B	500	NAI	C2D-C3D-C4D	-3.23	96.22	102.65
2	J	500	NAI	C3N-C2N-N1N	-3.23	118.47	123.05
2	L	500	NAI	C8A-N9A-C4A	3.22	109.36	106.90
2	B	500	NAI	O5B-C5B-C4B	3.22	120.75	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	550	HP7	N3-C2-N1	3.21	118.65	115.97
3	M	550	HP7	O4C-C1C-N1	3.21	114.83	108.06
2	I	500	NAI	O4D-C1D-N1N	3.21	114.84	108.05
3	L	550	HP7	C2-N1-C1C	-3.20	116.20	118.21
3	L	550	HP7	C4C-O4C-C1C	-3.19	106.28	109.75
3	E	550	HP7	C4'-C3'-C2'	-3.19	105.92	110.44
2	M	500	NAI	C1B-N9A-C4A	-3.18	121.14	126.64
2	O	500	NAI	C4N-C3N-C2N	-3.17	117.82	121.68
3	A	550	HP7	O2C-C2C-C1C	-3.17	101.65	111.23
3	C	550	HP7	O4C-C4C-C3C	-3.16	98.76	105.17
2	F	500	NAI	O2B-C2B-C3B	-3.16	101.56	111.83
3	O	550	HP7	O5'-C1'-O3B	-3.16	107.24	111.36
2	G	500	NAI	O4D-C4D-C5D	-3.15	98.10	109.36
2	K	500	NAI	O3D-C3D-C4D	-3.15	101.80	111.08
3	M	550	HP7	O7'-C7'-C8'	-3.14	115.91	122.04
2	G	500	NAI	O3-PN-O5D	3.14	117.44	103.41
2	H	500	NAI	O2D-C2D-C1D	-3.13	99.37	110.04
2	L	500	NAI	O4D-C1D-N1N	3.12	114.66	108.05
3	N	550	HP7	C5-C6-N1	-3.11	117.69	121.21
3	E	550	HP7	O2C-C2C-C1C	-3.11	101.82	111.23
2	H	500	NAI	O3-PA-O5B	3.11	117.31	103.41
3	B	550	HP7	C3C-C2C-C1C	3.11	105.77	100.91
2	A	500	NAI	C2A-N3A-C4A	3.10	122.84	114.01
3	G	550	HP7	C3C-C2C-C1C	3.09	105.75	100.91
3	G	550	HP7	C1'-O5'-C5'	3.09	116.61	112.20
2	J	500	NAI	C4B-O4B-C1B	-3.09	106.39	109.75
3	A	550	HP7	O3A-PB-O3B	-3.09	95.67	103.48
2	K	500	NAI	O5D-C5D-C4D	3.08	120.25	108.94
3	N	550	HP7	C5-C4-N3	3.08	122.51	116.70
3	N	550	HP7	O5C-C5C-C4C	-3.08	97.65	108.94
3	N	550	HP7	C6-N1-C2	3.05	123.77	119.51
3	D	550	HP7	PB-O3A-PA	-3.05	122.74	131.68
2	G	500	NAI	O3D-C3D-C4D	-3.03	102.14	111.08
3	C	550	HP7	C6-N1-C2	3.03	123.74	119.51
2	K	500	NAI	C6N-N1N-C2N	3.03	123.40	119.44
3	K	550	HP7	C3'-C2'-N2'	-3.03	104.14	110.56
3	A	550	HP7	C5-C4-N3	3.02	122.40	116.70
3	J	550	HP7	C4'-C5'-C6'	-3.01	105.56	110.84
3	I	550	HP7	O2C-C2C-C1C	-3.00	102.14	111.23
2	N	500	NAI	C2A-N3A-C4A	3.00	122.55	114.01
3	K	550	HP7	O2C-C2C-C1C	-3.00	102.16	111.23
2	P	500	NAI	C5N-C4N-C3N	2.99	120.70	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	500	NAI	C4N-C3N-C2N	-2.99	118.04	121.68
2	M	500	NAI	N3A-C4A-N9A	2.97	130.80	125.43
2	J	500	NAI	O4D-C1D-C2D	2.97	113.43	106.60
2	K	500	NAI	C2A-N3A-C4A	2.96	122.45	114.01
3	L	550	HP7	O3A-PB-O3B	2.96	110.96	103.48
3	A	550	HP7	C6-N1-C2	2.96	123.63	119.51
3	C	550	HP7	O2C-C2C-C3C	-2.95	102.23	111.83
2	I	500	NAI	PN-O3-PA	-2.93	123.08	131.68
3	B	550	HP7	O4C-C1C-N1	2.93	114.24	108.06
2	K	500	NAI	C8A-N9A-C1B	2.93	132.15	126.38
3	K	550	HP7	C4C-O4C-C1C	-2.92	106.58	109.75
3	F	550	HP7	C4'-C3'-C2'	2.91	114.58	110.44
2	N	500	NAI	O4D-C4D-C5D	-2.90	98.99	109.36
2	H	500	NAI	C1D-N1N-C2N	-2.90	116.07	121.02
3	P	550	HP7	O5'-C5'-C4'	-2.90	105.07	110.02
3	K	550	HP7	PB-O3A-PA	-2.89	123.22	131.68
3	H	550	HP7	O2C-C2C-C1C	-2.89	102.49	111.23
2	F	500	NAI	O4B-C1B-C2B	-2.89	102.35	106.77
2	H	500	NAI	C5N-C4N-C3N	2.88	120.42	112.60
3	M	550	HP7	C3C-C2C-C1C	2.88	105.42	100.91
2	G	500	NAI	O3-PA-O5B	2.88	116.28	103.41
3	J	550	HP7	C5-C6-N1	-2.88	117.96	121.21
2	D	500	NAI	C3B-C2B-C1B	-2.88	96.41	100.91
2	G	500	NAI	C4N-C3N-C2N	-2.87	118.18	121.68
2	E	500	NAI	C1D-N1N-C2N	-2.86	116.15	121.02
3	M	550	HP7	C5-C6-N1	-2.86	117.98	121.21
2	F	500	NAI	O4B-C4B-C3B	2.85	110.95	105.17
2	O	500	NAI	O3B-C3B-C4B	-2.84	102.70	111.08
3	H	550	HP7	O5'-C1'-C2'	2.84	116.89	110.78
2	I	500	NAI	C5N-C4N-C3N	2.84	120.29	112.60
2	M	500	NAI	O4B-C1B-C2B	-2.81	102.46	106.77
2	P	500	NAI	C1D-N1N-C2N	-2.81	116.23	121.02
3	I	550	HP7	C4C-O4C-C1C	-2.81	106.70	109.75
2	F	500	NAI	O3-PN-O5D	2.81	115.95	103.41
3	A	550	HP7	O2C-C2C-C3C	-2.80	102.72	111.83
3	I	550	HP7	O5C-C5C-C4C	-2.80	98.67	108.94
2	M	500	NAI	C1D-N1N-C2N	-2.79	116.26	121.02
3	H	550	HP7	O2A-PA-O1A	2.79	127.80	112.21
2	I	500	NAI	C6N-N1N-C2N	2.79	123.08	119.44
2	N	500	NAI	O5B-PA-O1A	2.77	120.24	109.37
3	G	550	HP7	O3B-PB-O1B	-2.76	98.53	109.65
2	H	500	NAI	O4B-C1B-C2B	-2.76	102.54	106.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	550	HP7	C4'-C3'-C2'	2.76	114.36	110.44
2	C	500	NAI	C8A-N7A-C5A	2.75	112.12	103.58
2	E	500	NAI	C5A-C4A-N3A	-2.75	119.71	125.70
2	H	500	NAI	C4A-C5A-N7A	-2.74	107.17	109.52
2	P	500	NAI	O3-PA-O5B	2.73	115.61	103.41
2	J	500	NAI	C4A-C5A-N7A	-2.73	107.19	109.52
2	L	500	NAI	O4D-C4D-C5D	-2.72	99.65	109.36
2	E	500	NAI	C3N-C2N-N1N	-2.72	119.19	123.05
2	I	500	NAI	C8A-N9A-C4A	2.72	108.97	106.90
2	B	500	NAI	C2B-C1B-N9A	-2.72	106.29	113.27
2	K	500	NAI	C5N-C4N-C3N	2.72	119.96	112.60
2	K	500	NAI	C8A-N7A-C5A	2.71	111.99	103.58
3	C	550	HP7	C5-C4-N3	2.71	121.81	116.70
2	A	500	NAI	O4B-C1B-C2B	-2.71	102.61	106.77
3	C	550	HP7	C5-C6-N1	-2.70	118.16	121.21
2	J	500	NAI	C1B-N9A-C4A	-2.69	121.99	126.64
2	G	500	NAI	O1N-PN-O5D	-2.68	95.00	108.51
3	C	550	HP7	C3'-C2'-N2'	-2.68	104.88	110.56
2	D	500	NAI	C5N-C4N-C3N	2.68	119.86	112.60
2	O	500	NAI	O2A-PA-O5B	-2.67	95.04	108.51
2	C	500	NAI	C5A-C4A-N3A	-2.67	119.88	125.70
2	B	500	NAI	C1D-N1N-C2N	-2.66	116.48	121.02
2	D	500	NAI	O3-PA-O5B	2.66	115.30	103.41
3	N	550	HP7	O'Q-C6'-O'P	-2.65	118.08	124.07
2	G	500	NAI	C4D-O4D-C1D	2.65	115.55	109.51
2	K	500	NAI	N7A-C8A-N9A	-2.65	106.87	114.36
2	H	500	NAI	C4N-C5N-C6N	-2.65	117.75	122.61
2	G	500	NAI	C4B-O4B-C1B	-2.65	106.88	109.75
2	P	500	NAI	O3D-C3D-C2D	-2.64	103.23	111.83
3	F	550	HP7	C3C-C2C-C1C	2.64	105.04	100.91
2	D	500	NAI	C6N-N1N-C2N	2.63	122.89	119.44
2	J	500	NAI	C5A-C4A-N3A	-2.63	119.98	125.70
3	O	550	HP7	O3A-PB-O3B	2.62	110.11	103.48
2	K	500	NAI	O4B-C4B-C3B	2.62	110.48	105.17
3	K	550	HP7	O3A-PB-O3B	2.62	110.09	103.48
2	A	500	NAI	O3-PN-O5D	2.61	115.08	103.41
2	L	500	NAI	C3N-C7N-N7N	2.61	122.50	117.48
2	P	500	NAI	O2A-PA-O5B	-2.61	95.35	108.51
2	N	500	NAI	O4B-C4B-C5B	2.61	118.67	109.36
3	F	550	HP7	C8'-C7'-N2'	2.61	121.21	116.11
3	I	550	HP7	O2B-PB-O3B	2.61	116.67	105.71
2	O	500	NAI	C5N-C4N-C3N	2.61	119.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	550	HP7	C2-N1-C1C	2.60	119.84	118.21
2	M	500	NAI	C5N-C4N-C3N	2.60	119.65	112.60
3	E	550	HP7	O5'-C1'-O3B	-2.59	107.98	111.36
2	F	500	NAI	C8A-N9A-C4A	-2.58	104.93	106.90
2	G	500	NAI	O4B-C1B-C2B	-2.58	102.82	106.77
2	H	500	NAI	C2A-N1A-C6A	2.57	123.42	118.77
3	C	550	HP7	C8'-C7'-N2'	2.56	121.12	116.11
3	C	550	HP7	O5'-C5'-C4'	-2.56	105.65	110.02
2	A	500	NAI	O4D-C1D-N1N	2.56	113.47	108.05
3	F	550	HP7	O'Q-C6'-C5'	2.56	122.81	113.49
2	E	500	NAI	C2A-N3A-C4A	2.55	121.26	114.01
2	M	500	NAI	C5A-C4A-N3A	-2.54	120.17	125.70
2	C	500	NAI	O2A-PA-O5B	-2.54	95.71	108.51
3	E	550	HP7	C2C-C3C-C4C	-2.54	97.60	102.65
2	H	500	NAI	O4B-C4B-C5B	2.54	118.41	109.36
3	K	550	HP7	O7'-C7'-N2'	-2.53	116.62	121.90
3	C	550	HP7	O3'-C3'-C2'	2.53	114.80	109.61
2	B	500	NAI	C4D-O4D-C1D	-2.53	103.75	109.51
3	N	550	HP7	O4C-C1C-N1	2.52	113.38	108.06
2	N	500	NAI	C5N-C4N-C3N	2.52	119.43	112.60
2	C	500	NAI	O4B-C4B-C3B	2.51	110.25	105.17
2	F	500	NAI	O2D-C2D-C3D	-2.50	103.72	111.83
3	J	550	HP7	O3'-C3'-C4'	2.50	115.95	110.35
2	J	500	NAI	C2A-N3A-C4A	2.49	121.11	114.01
3	P	550	HP7	O5C-C5C-C4C	-2.49	99.80	108.94
2	D	500	NAI	C2A-N1A-C6A	2.49	123.26	118.77
2	L	500	NAI	O1N-PN-O2N	-2.49	98.32	112.21
3	I	550	HP7	O3B-C1'-C2'	2.49	111.87	107.91
2	H	500	NAI	O1N-PN-O3	2.49	116.93	105.14
2	B	500	NAI	C2A-N1A-C6A	2.49	123.26	118.77
3	P	550	HP7	C2C-C3C-C4C	-2.48	97.70	102.65
2	C	500	NAI	O4B-C1B-C2B	-2.47	102.98	106.77
2	L	500	NAI	O7N-C7N-N7N	-2.47	116.70	122.93
3	B	550	HP7	C5C-C4C-C3C	-2.46	105.34	115.21
3	J	550	HP7	O5'-C1'-O3B	-2.46	108.15	111.36
2	L	500	NAI	C2A-N3A-C4A	2.46	121.01	114.01
2	P	500	NAI	C5A-C4A-N3A	-2.46	120.34	125.70
3	K	550	HP7	C2C-C1C-N1	-2.45	106.96	113.26
2	M	500	NAI	C5A-C6A-N6A	2.45	126.25	120.72
3	J	550	HP7	O2A-PA-O1A	2.44	125.87	112.21
3	G	550	HP7	O7'-C7'-C8'	-2.44	117.27	122.04
2	A	500	NAI	C2D-C1D-N1N	2.44	119.44	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	500	NAI	C3B-C2B-C1B	-2.44	97.08	100.91
2	H	500	NAI	O7N-C7N-C3N	-2.44	115.93	120.51
3	O	550	HP7	O4C-C4C-C3C	-2.43	100.24	105.17
2	K	500	NAI	C5A-C4A-N3A	-2.43	120.41	125.70
2	O	500	NAI	C5B-C4B-C3B	-2.43	105.48	115.21
2	G	500	NAI	O5B-PA-O1A	2.43	118.87	109.37
3	I	550	HP7	O4C-C4C-C3C	-2.42	100.27	105.17
2	I	500	NAI	C5A-C4A-N3A	-2.41	120.44	125.70
2	M	500	NAI	O2B-C2B-C1B	-2.41	103.94	111.23
2	N	500	NAI	C3N-C2N-N1N	-2.40	119.64	123.05
3	A	550	HP7	C3'-C2'-N2'	-2.40	105.47	110.56
3	I	550	HP7	C5-C4-N3	2.39	121.21	116.70
2	M	500	NAI	C8A-N7A-C5A	2.38	110.97	103.58
2	I	500	NAI	C3B-C2B-C1B	-2.38	97.18	100.91
3	B	550	HP7	O2C-C2C-C1C	-2.38	104.02	111.23
2	E	500	NAI	C6N-N1N-C2N	2.38	122.55	119.44
3	C	550	HP7	C1'-C2'-N2'	2.37	115.51	111.02
2	A	500	NAI	C8A-N7A-C5A	2.37	110.94	103.58
2	D	500	NAI	C1B-N9A-C4A	-2.37	122.54	126.64
2	B	500	NAI	C6N-N1N-C2N	2.37	122.54	119.44
2	C	500	NAI	N7A-C8A-N9A	-2.37	107.65	114.36
3	J	550	HP7	O2A-PA-O5C	-2.35	96.65	108.51
3	M	550	HP7	O5C-PA-O1A	-2.35	100.17	109.37
2	M	500	NAI	O3D-C3D-C4D	-2.35	104.16	111.08
3	H	550	HP7	C5-C6-N1	-2.34	118.56	121.21
2	B	500	NAI	O2B-C2B-C1B	-2.34	104.14	111.23
2	H	500	NAI	C4N-C3N-C2N	-2.34	118.83	121.68
2	B	500	NAI	C3N-C7N-N7N	2.34	121.97	117.48
2	C	500	NAI	C1D-N1N-C2N	-2.34	117.04	121.02
2	D	500	NAI	C2D-C1D-N1N	-2.33	107.27	113.21
3	J	550	HP7	O4'-C4'-C3'	-2.32	105.14	110.35
2	J	500	NAI	C8A-N9A-C1B	2.32	130.96	126.38
2	J	500	NAI	O2B-C2B-C1B	-2.32	104.22	111.23
3	E	550	HP7	O7'-C7'-C8'	-2.32	117.52	122.04
2	F	500	NAI	C4D-O4D-C1D	-2.31	104.23	109.51
3	A	550	HP7	O4'-C4'-C5'	-2.31	104.17	109.81
3	C	550	HP7	O'Q-C6'-C5'	2.31	121.91	113.49
3	A	550	HP7	C5-C6-N1	-2.31	118.60	121.21
2	O	500	NAI	C4N-C5N-C6N	-2.30	118.39	122.61
2	I	500	NAI	C1B-N9A-C4A	-2.29	122.67	126.64
2	F	500	NAI	C5D-C4D-C3D	-2.28	106.06	115.21
3	C	550	HP7	O5'-C1'-C2'	2.28	115.68	110.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	550	HP7	C5C-C4C-C3C	-2.28	106.10	115.21
2	J	500	NAI	C2D-C3D-C4D	-2.27	98.12	102.65
3	C	550	HP7	C4'-C3'-C2'	-2.27	107.22	110.44
2	B	500	NAI	O4B-C4B-C3B	2.27	109.77	105.17
2	L	500	NAI	C5N-C6N-N1N	-2.26	118.42	123.03
2	P	500	NAI	O7N-C7N-N7N	-2.26	117.22	122.93
3	C	550	HP7	C5C-C4C-C3C	-2.25	106.18	115.21
3	B	550	HP7	O2A-PA-O3A	2.25	115.82	105.14
3	B	550	HP7	O5'-C1'-O3B	-2.25	108.42	111.36
3	C	550	HP7	O7'-C7'-N2'	-2.24	117.22	121.90
3	M	550	HP7	O5C-C5C-C4C	-2.24	100.70	108.94
3	L	550	HP7	O4C-C1C-C2C	2.24	110.21	106.77
3	O	550	HP7	C4'-C5'-C6'	-2.24	106.91	110.84
3	B	550	HP7	C2'-N2'-C7'	2.24	128.99	123.02
3	B	550	HP7	O'Q-C6'-C5'	2.24	121.65	113.49
2	P	500	NAI	C4A-C5A-N7A	-2.23	107.61	109.52
2	A	500	NAI	C5B-C4B-C3B	-2.23	106.26	115.21
3	A	550	HP7	C6-N1-C1C	2.23	124.87	119.33
2	B	500	NAI	C5N-C6N-N1N	-2.23	118.48	123.03
2	B	500	NAI	O4B-C4B-C5B	2.22	117.30	109.36
3	J	550	HP7	O5'-C5'-C6'	2.22	112.15	107.23
2	L	500	NAI	O1N-PN-O3	2.22	115.65	105.14
3	J	550	HP7	C3'-C2'-N2'	-2.21	105.86	110.56
3	B	550	HP7	O'Q-C6'-O'P	-2.21	119.07	124.07
2	H	500	NAI	C1B-N9A-C4A	-2.20	122.83	126.64
2	F	500	NAI	O2A-PA-O1A	-2.20	99.92	112.21
3	A	550	HP7	O'Q-C6'-O'P	-2.20	119.10	124.07
3	E	550	HP7	O4'-C4'-C3'	2.20	115.28	110.35
2	C	500	NAI	O4B-C1B-N9A	2.20	110.48	108.44
2	P	500	NAI	C4N-C3N-C7N	2.20	124.37	118.38
2	I	500	NAI	C2A-N3A-C4A	2.19	120.26	114.01
3	M	550	HP7	C2-N1-C1C	-2.19	116.83	118.21
2	O	500	NAI	O5B-PA-O1A	2.19	117.94	109.37
3	L	550	HP7	O5C-C5C-C4C	-2.18	100.92	108.94
3	M	550	HP7	O5'-C5'-C6'	2.18	112.07	107.23
3	P	550	HP7	C8'-C7'-N2'	2.18	120.37	116.11
2	G	500	NAI	C2A-N3A-C4A	2.18	120.21	114.01
3	C	550	HP7	PB-O3A-PA	-2.18	125.30	131.68
2	E	500	NAI	C8A-N9A-C1B	2.17	130.66	126.38
3	M	550	HP7	O4'-C4'-C3'	-2.17	105.49	110.35
2	K	500	NAI	O4D-C1D-N1N	2.16	112.64	108.05
2	N	500	NAI	C5A-C4A-N3A	-2.16	120.99	125.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	NAI	O7N-C7N-N7N	-2.16	117.46	122.93
2	H	500	NAI	PN-O5D-C5D	-2.16	106.48	122.03
2	B	500	NAI	O4B-C1B-N9A	2.16	110.45	108.44
3	I	550	HP7	C6-N1-C2	2.16	122.52	119.51
2	B	500	NAI	PA-O5B-C5B	-2.16	106.49	122.03
2	K	500	NAI	C6A-C5A-N7A	2.15	139.56	131.34
2	I	500	NAI	PN-O5D-C5D	-2.15	106.56	122.03
2	L	500	NAI	PA-O5B-C5B	-2.15	106.58	122.03
2	A	500	NAI	O2A-PA-O5B	-2.15	97.68	108.51
3	G	550	HP7	C4'-C3'-C2'	2.15	113.49	110.44
2	P	500	NAI	C3N-C2N-N1N	-2.15	120.00	123.05
2	A	500	NAI	C3D-C2D-C1D	2.15	105.61	101.35
2	N	500	NAI	C4A-C5A-N7A	-2.14	107.69	109.52
2	L	500	NAI	O4B-C4B-C5B	2.14	117.00	109.36
2	I	500	NAI	PA-O5B-C5B	-2.14	106.61	122.03
2	H	500	NAI	C5A-C6A-N6A	2.14	125.56	120.72
2	P	500	NAI	O4B-C4B-C5B	2.14	116.99	109.36
2	K	500	NAI	PN-O5D-C5D	-2.14	106.67	122.03
3	E	550	HP7	C3C-C2C-C1C	2.14	104.25	100.91
2	O	500	NAI	C6N-N1N-C2N	2.13	122.23	119.44
2	B	500	NAI	PN-O5D-C5D	-2.13	106.67	122.03
2	A	500	NAI	C1D-N1N-C2N	-2.13	117.39	121.02
2	C	500	NAI	O3D-C3D-C2D	-2.13	104.92	111.83
2	E	500	NAI	PA-O5B-C5B	-2.13	106.74	122.03
2	G	500	NAI	O4B-C4B-C3B	2.12	109.47	105.17
2	P	500	NAI	C4N-C5N-C6N	-2.12	118.72	122.61
2	O	500	NAI	PN-O5D-C5D	-2.12	106.78	122.03
2	L	500	NAI	C2A-N1A-C6A	2.12	122.60	118.77
2	E	500	NAI	PN-O5D-C5D	-2.12	106.80	122.03
2	D	500	NAI	C5A-C4A-N3A	-2.12	121.09	125.70
2	C	500	NAI	C5N-C4N-C3N	2.12	118.33	112.60
2	G	500	NAI	C5N-C4N-C3N	2.11	118.32	112.60
3	F	550	HP7	O2A-PA-O1A	2.11	124.00	112.21
3	O	550	HP7	O4C-C1C-N1	2.11	112.51	108.06
3	A	550	HP7	C3'-C4'-C5'	-2.11	105.65	109.48
2	M	500	NAI	O5B-PA-O1A	2.11	117.62	109.37
2	M	500	NAI	C4N-C3N-C7N	2.11	124.12	118.38
2	L	500	NAI	C5N-C4N-C3N	2.10	118.30	112.60
2	I	500	NAI	C2D-C3D-C4D	-2.10	98.46	102.65
2	M	500	NAI	PN-O5D-C5D	-2.10	106.91	122.03
2	C	500	NAI	C2B-C1B-N9A	-2.10	107.87	113.27
2	C	500	NAI	C2A-N3A-C4A	2.10	119.99	114.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	500	NAI	PN-O5D-C5D	-2.10	106.94	122.03
3	I	550	HP7	O5'-C1'-O3B	-2.10	108.62	111.36
2	G	500	NAI	O1N-PN-O3	-2.10	95.19	105.14
3	B	550	HP7	O5C-C5C-C4C	-2.10	101.24	108.94
2	J	500	NAI	PA-O5B-C5B	-2.09	106.96	122.03
2	O	500	NAI	C8A-N7A-C5A	2.09	110.07	103.58
2	D	500	NAI	PN-O5D-C5D	-2.09	106.97	122.03
3	B	550	HP7	O4'-C4'-C3'	2.09	115.04	110.35
2	J	500	NAI	PN-O5D-C5D	-2.09	106.99	122.03
3	J	550	HP7	O5'-C1'-C2'	2.09	115.27	110.78
3	D	550	HP7	O'Q-C6'-C5'	2.09	121.10	113.49
3	A	550	HP7	O3'-C3'-C2'	-2.09	105.33	109.61
2	H	500	NAI	PA-O5B-C5B	-2.08	107.04	122.03
2	D	500	NAI	PA-O5B-C5B	-2.08	107.05	122.03
2	P	500	NAI	C2A-N1A-C6A	2.08	122.53	118.77
2	G	500	NAI	C8A-N9A-C4A	2.08	108.49	106.90
2	L	500	NAI	C5A-C4A-N9A	-2.08	104.16	107.16
2	C	500	NAI	PA-O5B-C5B	-2.08	107.09	122.03
2	E	500	NAI	C8A-N9A-C4A	-2.07	105.32	106.90
3	G	550	HP7	O2B-PB-O3B	2.07	114.41	105.71
2	C	500	NAI	C5N-C6N-N1N	-2.07	118.80	123.03
2	L	500	NAI	C8A-N9A-C1B	2.07	130.46	126.38
2	F	500	NAI	PA-O5B-C5B	-2.07	107.14	122.03
2	G	500	NAI	PN-O5D-C5D	-2.07	107.16	122.03
2	N	500	NAI	C4B-O4B-C1B	-2.07	107.50	109.75
3	N	550	HP7	O2B-PB-O1B	2.07	123.76	112.21
2	P	500	NAI	O4D-C4D-C5D	-2.07	101.98	109.36
2	F	500	NAI	C2B-C3B-C4B	-2.07	98.54	102.65
3	I	550	HP7	O3C-C3C-C2C	2.06	118.54	111.83
3	H	550	HP7	C1'-C2'-N2'	2.06	114.92	111.02
2	J	500	NAI	C5N-C4N-C3N	2.06	118.18	112.60
2	G	500	NAI	O4D-C1D-C2D	-2.06	101.87	106.60
3	I	550	HP7	C8'-C7'-N2'	2.05	120.12	116.11
2	H	500	NAI	C8A-N9A-C1B	2.05	130.42	126.38
2	B	500	NAI	N3A-C4A-N9A	2.05	129.13	125.43
3	L	550	HP7	C6-N1-C2	2.04	122.36	119.51
2	N	500	NAI	C5N-C6N-N1N	-2.04	118.86	123.03
2	N	500	NAI	PN-O5D-C5D	-2.04	107.36	122.03
2	C	500	NAI	PN-O5D-C5D	-2.04	107.36	122.03
2	M	500	NAI	PA-O5B-C5B	-2.04	107.38	122.03
3	H	550	HP7	O3'-C3'-C4'	2.04	114.92	110.35
2	H	500	NAI	C3N-C7N-N7N	2.04	121.40	117.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	500	NAI	C2D-C1D-N1N	-2.03	108.03	113.21
2	D	500	NAI	O5D-PN-O2N	2.03	117.34	109.37
2	P	500	NAI	PN-O5D-C5D	-2.03	107.42	122.03
2	A	500	NAI	C8A-N9A-C1B	2.03	130.38	126.38
2	N	500	NAI	PA-O5B-C5B	-2.03	107.44	122.03
2	F	500	NAI	C2B-C1B-N9A	2.03	118.47	113.27
2	F	500	NAI	PN-O5D-C5D	-2.03	107.44	122.03
2	I	500	NAI	C3N-C7N-N7N	2.03	121.38	117.48
3	H	550	HP7	O5C-C5C-C4C	-2.03	101.50	108.94
3	C	550	HP7	O2B-PB-O1B	2.02	123.52	112.21
2	P	500	NAI	PA-O5B-C5B	-2.02	107.47	122.03
3	F	550	HP7	O2C-C2C-C3C	-2.02	105.25	111.83
3	K	550	HP7	C3'-C4'-C5'	2.02	113.15	109.48
2	G	500	NAI	C1D-N1N-C2N	-2.02	117.58	121.02
3	C	550	HP7	O4'-C4'-C3'	-2.02	105.83	110.35
2	K	500	NAI	PA-O5B-C5B	-2.02	107.52	122.03
2	C	500	NAI	C8A-N9A-C4A	2.01	108.44	106.90
3	I	550	HP7	C5-C6-N1	2.01	123.49	121.21
2	O	500	NAI	PA-O5B-C5B	-2.01	107.55	122.03
3	J	550	HP7	C5-C4-N3	2.01	120.49	116.70
3	D	550	HP7	O'Q-C6'-O'P	-2.01	119.53	124.07
2	B	500	NAI	C8A-N7A-C5A	2.01	109.81	103.58
2	A	500	NAI	PN-O5D-C5D	-2.01	107.59	122.03
2	L	500	NAI	N6A-C6A-N1A	2.00	123.30	119.36
2	E	500	NAI	C3N-C7N-N7N	2.00	121.33	117.48
2	A	500	NAI	C5N-C4N-C3N	2.00	118.03	112.60
2	J	500	NAI	O5D-C5D-C4D	-2.00	101.58	108.94
2	N	500	NAI	C6A-C5A-C4A	-2.00	113.57	117.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	346/370 (93%)	-0.18	4 (1%) 75 79	16, 29, 45, 62	0
1	B	329/370 (88%)	0.02	10 (3%) 48 51	15, 37, 68, 94	0
1	C	347/370 (93%)	-0.18	3 (0%) 81 84	13, 34, 62, 82	0
1	D	343/370 (92%)	-0.01	16 (4%) 30 33	17, 39, 75, 90	0
1	E	321/370 (86%)	0.17	17 (5%) 25 28	16, 46, 74, 89	0
1	F	327/370 (88%)	-0.04	11 (3%) 43 45	16, 38, 69, 87	0
1	G	342/370 (92%)	-0.20	3 (0%) 81 84	13, 31, 59, 75	0
1	H	342/370 (92%)	-0.14	9 (2%) 53 56	16, 36, 72, 88	0
1	I	342/370 (92%)	0.04	15 (4%) 33 36	17, 39, 72, 91	0
1	J	346/370 (93%)	0.09	15 (4%) 34 36	20, 40, 73, 86	0
1	K	322/370 (87%)	0.11	10 (3%) 47 49	15, 42, 75, 97	0
1	L	321/370 (86%)	0.25	21 (6%) 18 20	18, 47, 83, 93	0
1	M	346/370 (93%)	-0.24	7 (2%) 62 65	12, 31, 61, 84	0
1	N	342/370 (92%)	-0.05	12 (3%) 42 44	13, 34, 69, 80	0
1	O	334/370 (90%)	-0.12	4 (1%) 75 79	16, 39, 64, 86	0
1	P	322/370 (87%)	0.10	16 (4%) 28 30	16, 40, 74, 93	0
All	All	5372/5920 (90%)	-0.03	173 (3%) 45 48	12, 37, 72, 97	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	30	ALA	8.0
1	P	30	ALA	6.8
1	L	33	GLY	5.3
1	P	279	PRO	4.6
1	P	316	CYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	O	50	GLN	4.5
1	D	295	SER	4.4
1	E	316	CYS	4.4
1	L	316	CYS	4.3
1	K	316	CYS	4.3
1	D	299	PHE	4.1
1	D	297	TYR	4.1
1	H	291	TYR	4.1
1	F	315	ASP	4.0
1	G	315	ASP	3.9
1	J	316	CYS	3.8
1	M	7	THR	3.7
1	P	314	GLY	3.7
1	L	309	ILE	3.6
1	L	10	LYS	3.6
1	J	54	ALA	3.6
1	N	314	GLY	3.5
1	L	11	ILE	3.5
1	L	315	ASP	3.4
1	I	278	GLU	3.4
1	L	34	ASP	3.4
1	M	6	ILE	3.4
1	P	53	GLU	3.3
1	L	279	PRO	3.3
1	P	33	GLY	3.3
1	K	315	ASP	3.3
1	E	69	ALA	3.3
1	I	316	CYS	3.3
1	K	69	ALA	3.3
1	J	7	THR	3.2
1	H	316	CYS	3.2
1	D	33	GLY	3.2
1	B	299	PHE	3.2
1	F	316	CYS	3.1
1	P	50	GLN	3.1
1	D	30	ALA	3.1
1	L	277	ALA	3.0
1	J	69	ALA	3.0
1	L	303	LEU	3.0
1	L	158	VAL	3.0
1	J	62	SER	3.0
1	E	314	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	313	ARG	2.9
1	O	69	ALA	2.9
1	A	7	THR	2.8
1	F	33	GLY	2.8
1	B	316	CYS	2.7
1	G	316	CYS	2.7
1	H	33	GLY	2.7
1	K	33	GLY	2.7
1	I	10	LYS	2.7
1	I	295	SER	2.7
1	H	34	ASP	2.7
1	F	317	GLU	2.7
1	B	281	PRO	2.6
1	E	303	LEU	2.6
1	M	51	ALA	2.6
1	J	285	LYS	2.6
1	A	315	ASP	2.5
1	C	278	GLU	2.5
1	P	28	ALA	2.5
1	E	315	ASP	2.5
1	K	317	GLU	2.5
1	D	55	ALA	2.5
1	B	280[A]	HIS	2.5
1	N	11	ILE	2.5
1	P	315	ASP	2.5
1	D	317	GLU	2.5
1	M	50	GLN	2.5
1	I	314	GLY	2.4
1	N	33	GLY	2.4
1	J	282	ASP	2.4
1	I	277	ALA	2.4
1	I	299	PHE	2.4
1	D	53	GLU	2.4
1	H	317	GLU	2.4
1	M	30	ALA	2.4
1	N	299	PHE	2.4
1	K	35	ARG	2.4
1	D	314	GLY	2.4
1	N	10	LYS	2.4
1	A	277	ALA	2.4
1	L	9	ARG	2.4
1	J	315	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	36	ALA	2.4
1	P	32	HIS	2.4
1	D	49	LEU	2.3
1	P	54	ALA	2.3
1	M	185	PHE	2.3
1	B	49	LEU	2.3
1	J	8	ASP	2.3
1	K	279	PRO	2.3
1	D	8	ASP	2.3
1	D	34	ASP	2.3
1	J	33	GLY	2.3
1	L	314	GLY	2.3
1	M	8	ASP	2.3
1	I	33	GLY	2.2
1	J	50	GLN	2.2
1	K	278	GLU	2.2
1	F	277	ALA	2.2
1	E	50	GLN	2.2
1	J	287	ARG	2.2
1	N	315	ASP	2.2
1	C	50	GLN	2.2
1	B	315	ASP	2.2
1	P	57	GLY	2.2
1	N	173	ARG	2.2
1	C	279	PRO	2.2
1	F	280	HIS	2.2
1	F	282	ASP	2.2
1	H	315	ASP	2.2
1	E	237	ILE	2.2
1	L	156	VAL	2.2
1	O	7	THR	2.2
1	E	216	ARG	2.2
1	F	313	ARG	2.2
1	I	30	ALA	2.2
1	F	160	VAL	2.2
1	D	279	PRO	2.2
1	E	173	ARG	2.1
1	E	225	ALA	2.1
1	L	32	HIS	2.1
1	A	158	VAL	2.1
1	I	57	GLY	2.1
1	H	313	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	72	ASN	2.1
1	N	50	GLN	2.1
1	E	279	PRO	2.1
1	B	317	GLU	2.1
1	P	47	GLU	2.1
1	E	239	VAL	2.1
1	P	277	ALA	2.1
1	B	314	GLY	2.1
1	N	298	GLY	2.1
1	G	313	ARG	2.1
1	K	313	ARG	2.1
1	E	46	PRO	2.1
1	F	284	ASP	2.1
1	P	9	ARG	2.1
1	L	193	VAL	2.1
1	D	291	TYR	2.1
1	D	315	ASP	2.1
1	E	313	ARG	2.1
1	I	12	ARG	2.1
1	I	313	ARG	2.1
1	J	52	ALA	2.1
1	P	237	ILE	2.1
1	B	46	PRO	2.1
1	F	314	GLY	2.1
1	N	71	GLY	2.1
1	O	284	ASP	2.1
1	B	50	GLN	2.0
1	E	278	GLU	2.0
1	L	69	ALA	2.0
1	I	11	ILE	2.0
1	E	35	ARG	2.0
1	D	296	VAL	2.0
1	H	292	GLU	2.0
1	J	57	GLY	2.0
1	L	237	ILE	2.0
1	N	313	ARG	2.0
1	N	316	CYS	2.0
1	E	167	GLU	2.0
1	I	28	ALA	2.0
1	J	189	ALA	2.0
1	L	157	THR	2.0
1	H	298	GLY	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAI	M	500	44/44	0.11	0.06	15,32,49,84	0
2	NAI	C	500	44/44	0.10	0.03	14,28,44,71	0
2	NAI	H	500	44/44	0.10	-0.03	21,34,60,100	0
2	NAI	F	500	44/44	0.10	-0.03	15,28,43,64	0
2	NAI	G	500	44/44	0.10	-0.17	17,28,38,57	0
3	HP7	O	550	40/40	0.11	-0.20	22,56,100,100	0
3	HP7	A	550	40/40	0.11	-0.22	11,25,50,100	0
2	NAI	A	500	44/44	0.10	-0.26	19,25,31,45	0
2	NAI	O	500	44/44	0.10	-0.32	19,35,52,63	0
3	HP7	P	550	40/40	0.12	-0.33	28,48,100,100	0
2	NAI	I	500	44/44	0.09	-0.33	20,35,46,59	0
3	HP7	J	550	40/40	0.10	-0.34	14,36,75,100	0
2	NAI	E	500	44/44	0.10	-0.41	23,43,87,98	0
2	NAI	K	500	44/44	0.09	-0.47	18,33,53,100	0
3	HP7	G	550	40/40	0.09	-0.48	14,32,77,100	0
3	HP7	B	550	40/40	0.10	-0.50	25,45,100,100	0
3	HP7	K	550	40/40	0.11	-0.51	17,53,100,100	0
3	HP7	E	550	40/40	0.12	-0.51	32,64,100,100	0
2	NAI	L	500	44/44	0.10	-0.51	23,40,63,100	0
2	NAI	N	500	44/44	0.09	-0.53	17,32,48,63	0
3	HP7	N	550	40/40	0.08	-0.54	15,27,50,56	0
3	HP7	L	550	40/40	0.11	-0.55	20,56,100,100	0
2	NAI	P	500	44/44	0.09	-0.56	24,37,54,73	0
2	NAI	J	500	44/44	0.10	-0.61	18,37,60,78	0
3	HP7	F	550	40/40	0.10	-0.62	24,43,100,100	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	HP7	D	550	40/40	0.09	-0.68	23,47,99,100	0
3	HP7	C	550	40/40	0.09	-0.68	17,30,76,100	0
2	NAI	B	500	44/44	0.09	-0.68	21,36,58,79	0
3	HP7	H	550	40/40	0.10	-0.69	21,34,59,90	0
3	HP7	M	550	40/40	0.09	-0.77	17,31,42,59	0
2	NAI	D	500	44/44	0.08	-0.84	20,36,52,70	0
3	HP7	I	550	40/40	0.08	-1.01	19,40,82,100	0

6.5 Other polymers

There are no such residues in this entry.