



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 08:26 pm BST

PDB ID : 5UK4
Title : VESICULAR STOMATITIS VIRUS N PROTEIN IN COMPLEX WITH INHIBITORY NANOBODY 1307
Authors : Hanke, L.; Knockenhauer, K.E.; Ploegh, H.L.; Schwartz, T.U.
Deposited on : 2017-01-19
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

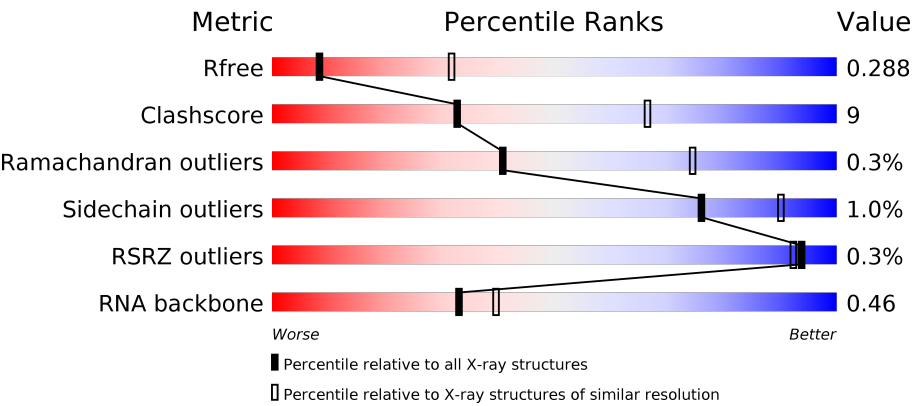
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 Å.

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





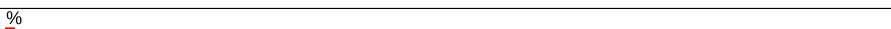



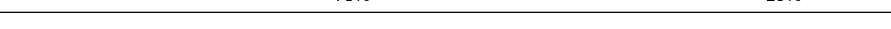



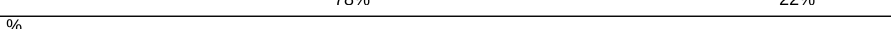














Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	422	<div><div></div><div>77%21%..</div></div>
1	B	422	<div><div></div><div>77%20%.</div></div>
1	C	422	<div><div>%</div><div>76%22%.</div></div>
1	D	422	<div><div></div><div>79%19%..</div></div>

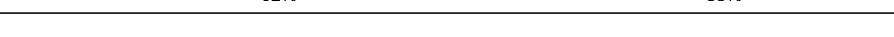
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Mol	Chain	Length	Quality of chain
1	E	422	 79% 18% .
1	F	422	 % 76% 23% .
1	G	422	 % 77% 22% .
1	H	422	 % 78% 20% .
1	I	422	 78% 19% ..
1	J	422	 76% 22% .
1	K	422	 78% 21%
1	L	422	 78% 22%
1	M	422	 % 77% 21% .
1	N	422	 76% 23% .
1	O	422	 77% 23%
1	P	422	 78% 19% ..
1	Q	422	 80% 19% .
1	R	422	 % 78% 21% .
1	S	422	 77% 22% .
1	T	422	 78% 22%
2	a	139	 90% 10%
2	b	139	 88% . 10%
2	c	139	 90% 10%
2	d	139	 89% . 10%
2	e	139	 89% . 10%
2	f	139	 90% 10%
2	g	139	 89% . 10%
2	h	139	 89% . 10%
2	i	139	 89% . 10%

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Mol	Chain	Length	Quality of chain
2	j	139	 89% 10%
2	k	139	 90% 10%
2	l	139	 90% 10%
2	m	139	 90% 10%
2	n	139	 90% 10%
2	o	139	 90% 10%
2	p	139	 88% 10%
2	q	139	 90% 10%
2	r	139	 90% 10%
2	s	139	 88% 10%
2	t	139	 90% 10%
3	u	45	 64% 36%
3	v	45	 64% 36%
3	w	45	 62% 38%
3	x	45	 64% 36%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 89086 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	414	Total	C	N	O	S	0	0	0
			3281	2090	551	622	18			
1	B	412	Total	C	N	O	S	0	0	0
			3270	2083	548	621	18			
1	Q	419	Total	C	N	O	S	0	0	0
			3316	2111	556	631	18			
1	C	417	Total	C	N	O	S	0	0	0
			3299	2102	554	625	18			
1	R	419	Total	C	N	O	S	0	0	0
			3315	2112	556	629	18			
1	D	418	Total	C	N	O	S	0	0	0
			3305	2106	552	629	18			
1	S	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			
1	E	413	Total	C	N	O	S	0	0	0
			3273	2084	550	621	18			
1	T	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			
1	K	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			
1	L	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			
1	N	418	Total	C	N	O	S	0	0	0
			3305	2106	552	629	18			
1	M	416	Total	C	N	O	S	0	0	0
			3291	2099	550	624	18			
1	F	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			
1	G	416	Total	C	N	O	S	0	0	0
			3295	2099	553	625	18			
1	H	420	Total	C	N	O	S	0	0	0
			3316	2112	554	632	18			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	415	Total	C	N	O	S	0	0	0
			3289	2094	552	625	18			
1	O	420	Total	C	N	O	S	0	0	0
			3323	2116	557	632	18			
1	J	420	Total	C	N	O	S	0	0	0
			3323	2116	557	632	18			
1	A	416	Total	C	N	O	S	0	0	0
			3290	2097	550	625	18			

- Molecule 2 is a protein called Anti-vesicular stomatitis virus N VHH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	p	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	b	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	q	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	c	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	r	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	d	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	s	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	e	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	t	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	k	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	l	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	n	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	m	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	f	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	g	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	h	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	i	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	o	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	j	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	a	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			

There are 280 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
p	126	GLY	-	expression tag	UNP A0A192B6J6
p	127	GLY	-	expression tag	UNP A0A192B6J6
p	128	LEU	-	expression tag	UNP A0A192B6J6
p	129	PRO	-	expression tag	UNP A0A192B6J6
p	130	GLU	-	expression tag	UNP A0A192B6J6
p	131	THR	-	expression tag	UNP A0A192B6J6
p	132	GLY	-	expression tag	UNP A0A192B6J6
p	133	GLY	-	expression tag	UNP A0A192B6J6
p	134	HIS	-	expression tag	UNP A0A192B6J6
p	135	HIS	-	expression tag	UNP A0A192B6J6
p	136	HIS	-	expression tag	UNP A0A192B6J6
p	137	HIS	-	expression tag	UNP A0A192B6J6
p	138	HIS	-	expression tag	UNP A0A192B6J6
p	139	HIS	-	expression tag	UNP A0A192B6J6
b	126	GLY	-	expression tag	UNP A0A192B6J6
b	127	GLY	-	expression tag	UNP A0A192B6J6
b	128	LEU	-	expression tag	UNP A0A192B6J6
b	129	PRO	-	expression tag	UNP A0A192B6J6
b	130	GLU	-	expression tag	UNP A0A192B6J6
b	131	THR	-	expression tag	UNP A0A192B6J6
b	132	GLY	-	expression tag	UNP A0A192B6J6
b	133	GLY	-	expression tag	UNP A0A192B6J6
b	134	HIS	-	expression tag	UNP A0A192B6J6
b	135	HIS	-	expression tag	UNP A0A192B6J6
b	136	HIS	-	expression tag	UNP A0A192B6J6
b	137	HIS	-	expression tag	UNP A0A192B6J6
b	138	HIS	-	expression tag	UNP A0A192B6J6
b	139	HIS	-	expression tag	UNP A0A192B6J6
q	126	GLY	-	expression tag	UNP A0A192B6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
q	127	GLY	-	expression tag	UNP A0A192B6J6
q	128	LEU	-	expression tag	UNP A0A192B6J6
q	129	PRO	-	expression tag	UNP A0A192B6J6
q	130	GLU	-	expression tag	UNP A0A192B6J6
q	131	THR	-	expression tag	UNP A0A192B6J6
q	132	GLY	-	expression tag	UNP A0A192B6J6
q	133	GLY	-	expression tag	UNP A0A192B6J6
q	134	HIS	-	expression tag	UNP A0A192B6J6
q	135	HIS	-	expression tag	UNP A0A192B6J6
q	136	HIS	-	expression tag	UNP A0A192B6J6
q	137	HIS	-	expression tag	UNP A0A192B6J6
q	138	HIS	-	expression tag	UNP A0A192B6J6
q	139	HIS	-	expression tag	UNP A0A192B6J6
c	126	GLY	-	expression tag	UNP A0A192B6J6
c	127	GLY	-	expression tag	UNP A0A192B6J6
c	128	LEU	-	expression tag	UNP A0A192B6J6
c	129	PRO	-	expression tag	UNP A0A192B6J6
c	130	GLU	-	expression tag	UNP A0A192B6J6
c	131	THR	-	expression tag	UNP A0A192B6J6
c	132	GLY	-	expression tag	UNP A0A192B6J6
c	133	GLY	-	expression tag	UNP A0A192B6J6
c	134	HIS	-	expression tag	UNP A0A192B6J6
c	135	HIS	-	expression tag	UNP A0A192B6J6
c	136	HIS	-	expression tag	UNP A0A192B6J6
c	137	HIS	-	expression tag	UNP A0A192B6J6
c	138	HIS	-	expression tag	UNP A0A192B6J6
c	139	HIS	-	expression tag	UNP A0A192B6J6
r	126	GLY	-	expression tag	UNP A0A192B6J6
r	127	GLY	-	expression tag	UNP A0A192B6J6
r	128	LEU	-	expression tag	UNP A0A192B6J6
r	129	PRO	-	expression tag	UNP A0A192B6J6
r	130	GLU	-	expression tag	UNP A0A192B6J6
r	131	THR	-	expression tag	UNP A0A192B6J6
r	132	GLY	-	expression tag	UNP A0A192B6J6
r	133	GLY	-	expression tag	UNP A0A192B6J6
r	134	HIS	-	expression tag	UNP A0A192B6J6
r	135	HIS	-	expression tag	UNP A0A192B6J6
r	136	HIS	-	expression tag	UNP A0A192B6J6
r	137	HIS	-	expression tag	UNP A0A192B6J6
r	138	HIS	-	expression tag	UNP A0A192B6J6
r	139	HIS	-	expression tag	UNP A0A192B6J6
d	126	GLY	-	expression tag	UNP A0A192B6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
d	127	GLY	-	expression tag	UNP A0A192B6J6
d	128	LEU	-	expression tag	UNP A0A192B6J6
d	129	PRO	-	expression tag	UNP A0A192B6J6
d	130	GLU	-	expression tag	UNP A0A192B6J6
d	131	THR	-	expression tag	UNP A0A192B6J6
d	132	GLY	-	expression tag	UNP A0A192B6J6
d	133	GLY	-	expression tag	UNP A0A192B6J6
d	134	HIS	-	expression tag	UNP A0A192B6J6
d	135	HIS	-	expression tag	UNP A0A192B6J6
d	136	HIS	-	expression tag	UNP A0A192B6J6
d	137	HIS	-	expression tag	UNP A0A192B6J6
d	138	HIS	-	expression tag	UNP A0A192B6J6
d	139	HIS	-	expression tag	UNP A0A192B6J6
s	126	GLY	-	expression tag	UNP A0A192B6J6
s	127	GLY	-	expression tag	UNP A0A192B6J6
s	128	LEU	-	expression tag	UNP A0A192B6J6
s	129	PRO	-	expression tag	UNP A0A192B6J6
s	130	GLU	-	expression tag	UNP A0A192B6J6
s	131	THR	-	expression tag	UNP A0A192B6J6
s	132	GLY	-	expression tag	UNP A0A192B6J6
s	133	GLY	-	expression tag	UNP A0A192B6J6
s	134	HIS	-	expression tag	UNP A0A192B6J6
s	135	HIS	-	expression tag	UNP A0A192B6J6
s	136	HIS	-	expression tag	UNP A0A192B6J6
s	137	HIS	-	expression tag	UNP A0A192B6J6
s	138	HIS	-	expression tag	UNP A0A192B6J6
s	139	HIS	-	expression tag	UNP A0A192B6J6
e	126	GLY	-	expression tag	UNP A0A192B6J6
e	127	GLY	-	expression tag	UNP A0A192B6J6
e	128	LEU	-	expression tag	UNP A0A192B6J6
e	129	PRO	-	expression tag	UNP A0A192B6J6
e	130	GLU	-	expression tag	UNP A0A192B6J6
e	131	THR	-	expression tag	UNP A0A192B6J6
e	132	GLY	-	expression tag	UNP A0A192B6J6
e	133	GLY	-	expression tag	UNP A0A192B6J6
e	134	HIS	-	expression tag	UNP A0A192B6J6
e	135	HIS	-	expression tag	UNP A0A192B6J6
e	136	HIS	-	expression tag	UNP A0A192B6J6
e	137	HIS	-	expression tag	UNP A0A192B6J6
e	138	HIS	-	expression tag	UNP A0A192B6J6
e	139	HIS	-	expression tag	UNP A0A192B6J6
t	126	GLY	-	expression tag	UNP A0A192B6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
t	127	GLY	-	expression tag	UNP A0A192B6J6
t	128	LEU	-	expression tag	UNP A0A192B6J6
t	129	PRO	-	expression tag	UNP A0A192B6J6
t	130	GLU	-	expression tag	UNP A0A192B6J6
t	131	THR	-	expression tag	UNP A0A192B6J6
t	132	GLY	-	expression tag	UNP A0A192B6J6
t	133	GLY	-	expression tag	UNP A0A192B6J6
t	134	HIS	-	expression tag	UNP A0A192B6J6
t	135	HIS	-	expression tag	UNP A0A192B6J6
t	136	HIS	-	expression tag	UNP A0A192B6J6
t	137	HIS	-	expression tag	UNP A0A192B6J6
t	138	HIS	-	expression tag	UNP A0A192B6J6
t	139	HIS	-	expression tag	UNP A0A192B6J6
k	126	GLY	-	expression tag	UNP A0A192B6J6
k	127	GLY	-	expression tag	UNP A0A192B6J6
k	128	LEU	-	expression tag	UNP A0A192B6J6
k	129	PRO	-	expression tag	UNP A0A192B6J6
k	130	GLU	-	expression tag	UNP A0A192B6J6
k	131	THR	-	expression tag	UNP A0A192B6J6
k	132	GLY	-	expression tag	UNP A0A192B6J6
k	133	GLY	-	expression tag	UNP A0A192B6J6
k	134	HIS	-	expression tag	UNP A0A192B6J6
k	135	HIS	-	expression tag	UNP A0A192B6J6
k	136	HIS	-	expression tag	UNP A0A192B6J6
k	137	HIS	-	expression tag	UNP A0A192B6J6
k	138	HIS	-	expression tag	UNP A0A192B6J6
k	139	HIS	-	expression tag	UNP A0A192B6J6
l	126	GLY	-	expression tag	UNP A0A192B6J6
l	127	GLY	-	expression tag	UNP A0A192B6J6
l	128	LEU	-	expression tag	UNP A0A192B6J6
l	129	PRO	-	expression tag	UNP A0A192B6J6
l	130	GLU	-	expression tag	UNP A0A192B6J6
l	131	THR	-	expression tag	UNP A0A192B6J6
l	132	GLY	-	expression tag	UNP A0A192B6J6
l	133	GLY	-	expression tag	UNP A0A192B6J6
l	134	HIS	-	expression tag	UNP A0A192B6J6
l	135	HIS	-	expression tag	UNP A0A192B6J6
l	136	HIS	-	expression tag	UNP A0A192B6J6
l	137	HIS	-	expression tag	UNP A0A192B6J6
l	138	HIS	-	expression tag	UNP A0A192B6J6
l	139	HIS	-	expression tag	UNP A0A192B6J6
n	126	GLY	-	expression tag	UNP A0A192B6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
n	127	GLY	-	expression tag	UNP A0A192B6J6
n	128	LEU	-	expression tag	UNP A0A192B6J6
n	129	PRO	-	expression tag	UNP A0A192B6J6
n	130	GLU	-	expression tag	UNP A0A192B6J6
n	131	THR	-	expression tag	UNP A0A192B6J6
n	132	GLY	-	expression tag	UNP A0A192B6J6
n	133	GLY	-	expression tag	UNP A0A192B6J6
n	134	HIS	-	expression tag	UNP A0A192B6J6
n	135	HIS	-	expression tag	UNP A0A192B6J6
n	136	HIS	-	expression tag	UNP A0A192B6J6
n	137	HIS	-	expression tag	UNP A0A192B6J6
n	138	HIS	-	expression tag	UNP A0A192B6J6
n	139	HIS	-	expression tag	UNP A0A192B6J6
m	126	GLY	-	expression tag	UNP A0A192B6J6
m	127	GLY	-	expression tag	UNP A0A192B6J6
m	128	LEU	-	expression tag	UNP A0A192B6J6
m	129	PRO	-	expression tag	UNP A0A192B6J6
m	130	GLU	-	expression tag	UNP A0A192B6J6
m	131	THR	-	expression tag	UNP A0A192B6J6
m	132	GLY	-	expression tag	UNP A0A192B6J6
m	133	GLY	-	expression tag	UNP A0A192B6J6
m	134	HIS	-	expression tag	UNP A0A192B6J6
m	135	HIS	-	expression tag	UNP A0A192B6J6
m	136	HIS	-	expression tag	UNP A0A192B6J6
m	137	HIS	-	expression tag	UNP A0A192B6J6
m	138	HIS	-	expression tag	UNP A0A192B6J6
m	139	HIS	-	expression tag	UNP A0A192B6J6
f	126	GLY	-	expression tag	UNP A0A192B6J6
f	127	GLY	-	expression tag	UNP A0A192B6J6
f	128	LEU	-	expression tag	UNP A0A192B6J6
f	129	PRO	-	expression tag	UNP A0A192B6J6
f	130	GLU	-	expression tag	UNP A0A192B6J6
f	131	THR	-	expression tag	UNP A0A192B6J6
f	132	GLY	-	expression tag	UNP A0A192B6J6
f	133	GLY	-	expression tag	UNP A0A192B6J6
f	134	HIS	-	expression tag	UNP A0A192B6J6
f	135	HIS	-	expression tag	UNP A0A192B6J6
f	136	HIS	-	expression tag	UNP A0A192B6J6
f	137	HIS	-	expression tag	UNP A0A192B6J6
f	138	HIS	-	expression tag	UNP A0A192B6J6
f	139	HIS	-	expression tag	UNP A0A192B6J6
g	126	GLY	-	expression tag	UNP A0A192B6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
g	127	GLY	-	expression tag	UNP A0A192B6J6
g	128	LEU	-	expression tag	UNP A0A192B6J6
g	129	PRO	-	expression tag	UNP A0A192B6J6
g	130	GLU	-	expression tag	UNP A0A192B6J6
g	131	THR	-	expression tag	UNP A0A192B6J6
g	132	GLY	-	expression tag	UNP A0A192B6J6
g	133	GLY	-	expression tag	UNP A0A192B6J6
g	134	HIS	-	expression tag	UNP A0A192B6J6
g	135	HIS	-	expression tag	UNP A0A192B6J6
g	136	HIS	-	expression tag	UNP A0A192B6J6
g	137	HIS	-	expression tag	UNP A0A192B6J6
g	138	HIS	-	expression tag	UNP A0A192B6J6
g	139	HIS	-	expression tag	UNP A0A192B6J6
h	126	GLY	-	expression tag	UNP A0A192B6J6
h	127	GLY	-	expression tag	UNP A0A192B6J6
h	128	LEU	-	expression tag	UNP A0A192B6J6
h	129	PRO	-	expression tag	UNP A0A192B6J6
h	130	GLU	-	expression tag	UNP A0A192B6J6
h	131	THR	-	expression tag	UNP A0A192B6J6
h	132	GLY	-	expression tag	UNP A0A192B6J6
h	133	GLY	-	expression tag	UNP A0A192B6J6
h	134	HIS	-	expression tag	UNP A0A192B6J6
h	135	HIS	-	expression tag	UNP A0A192B6J6
h	136	HIS	-	expression tag	UNP A0A192B6J6
h	137	HIS	-	expression tag	UNP A0A192B6J6
h	138	HIS	-	expression tag	UNP A0A192B6J6
h	139	HIS	-	expression tag	UNP A0A192B6J6
i	126	GLY	-	expression tag	UNP A0A192B6J6
i	127	GLY	-	expression tag	UNP A0A192B6J6
i	128	LEU	-	expression tag	UNP A0A192B6J6
i	129	PRO	-	expression tag	UNP A0A192B6J6
i	130	GLU	-	expression tag	UNP A0A192B6J6
i	131	THR	-	expression tag	UNP A0A192B6J6
i	132	GLY	-	expression tag	UNP A0A192B6J6
i	133	GLY	-	expression tag	UNP A0A192B6J6
i	134	HIS	-	expression tag	UNP A0A192B6J6
i	135	HIS	-	expression tag	UNP A0A192B6J6
i	136	HIS	-	expression tag	UNP A0A192B6J6
i	137	HIS	-	expression tag	UNP A0A192B6J6
i	138	HIS	-	expression tag	UNP A0A192B6J6
i	139	HIS	-	expression tag	UNP A0A192B6J6
o	126	GLY	-	expression tag	UNP A0A192B6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
o	127	GLY	-	expression tag	UNP A0A192B6J6
o	128	LEU	-	expression tag	UNP A0A192B6J6
o	129	PRO	-	expression tag	UNP A0A192B6J6
o	130	GLU	-	expression tag	UNP A0A192B6J6
o	131	THR	-	expression tag	UNP A0A192B6J6
o	132	GLY	-	expression tag	UNP A0A192B6J6
o	133	GLY	-	expression tag	UNP A0A192B6J6
o	134	HIS	-	expression tag	UNP A0A192B6J6
o	135	HIS	-	expression tag	UNP A0A192B6J6
o	136	HIS	-	expression tag	UNP A0A192B6J6
o	137	HIS	-	expression tag	UNP A0A192B6J6
o	138	HIS	-	expression tag	UNP A0A192B6J6
o	139	HIS	-	expression tag	UNP A0A192B6J6
j	126	GLY	-	expression tag	UNP A0A192B6J6
j	127	GLY	-	expression tag	UNP A0A192B6J6
j	128	LEU	-	expression tag	UNP A0A192B6J6
j	129	PRO	-	expression tag	UNP A0A192B6J6
j	130	GLU	-	expression tag	UNP A0A192B6J6
j	131	THR	-	expression tag	UNP A0A192B6J6
j	132	GLY	-	expression tag	UNP A0A192B6J6
j	133	GLY	-	expression tag	UNP A0A192B6J6
j	134	HIS	-	expression tag	UNP A0A192B6J6
j	135	HIS	-	expression tag	UNP A0A192B6J6
j	136	HIS	-	expression tag	UNP A0A192B6J6
j	137	HIS	-	expression tag	UNP A0A192B6J6
j	138	HIS	-	expression tag	UNP A0A192B6J6
j	139	HIS	-	expression tag	UNP A0A192B6J6
a	126	GLY	-	expression tag	UNP A0A192B6J6
a	127	GLY	-	expression tag	UNP A0A192B6J6
a	128	LEU	-	expression tag	UNP A0A192B6J6
a	129	PRO	-	expression tag	UNP A0A192B6J6
a	130	GLU	-	expression tag	UNP A0A192B6J6
a	131	THR	-	expression tag	UNP A0A192B6J6
a	132	GLY	-	expression tag	UNP A0A192B6J6
a	133	GLY	-	expression tag	UNP A0A192B6J6
a	134	HIS	-	expression tag	UNP A0A192B6J6
a	135	HIS	-	expression tag	UNP A0A192B6J6
a	136	HIS	-	expression tag	UNP A0A192B6J6
a	137	HIS	-	expression tag	UNP A0A192B6J6
a	138	HIS	-	expression tag	UNP A0A192B6J6
a	139	HIS	-	expression tag	UNP A0A192B6J6

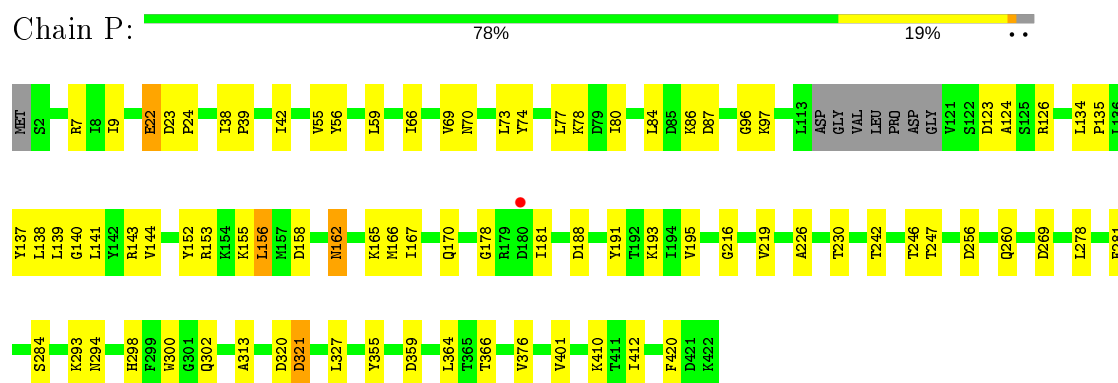
- Molecule 3 is a RNA chain called RNA (45-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	u	45	Total	C	N	O	P	0	0	0
			900	405	90	360	45			
3	v	45	Total	C	N	O	P	0	0	0
			900	405	90	360	45			
3	w	45	Total	C	N	O	P	0	0	0
			900	405	90	360	45			
3	x	45	Total	C	N	O	P	0	0	0
			900	405	90	360	45			

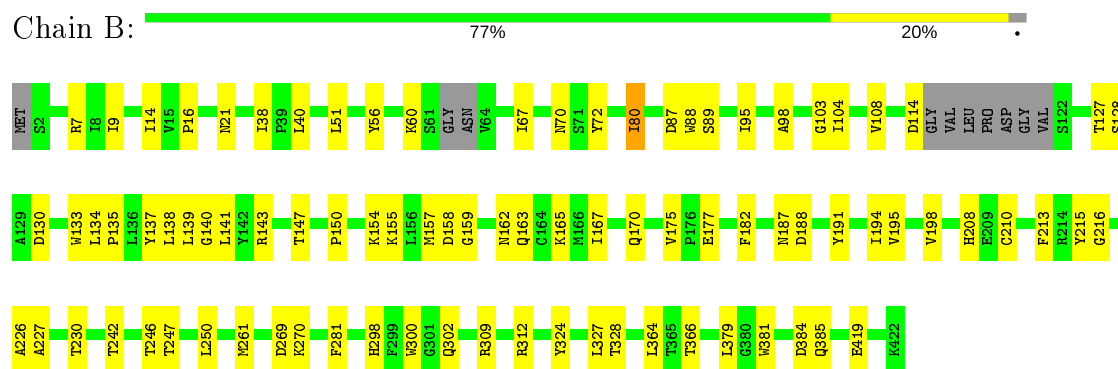
3 Residue-property plots

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

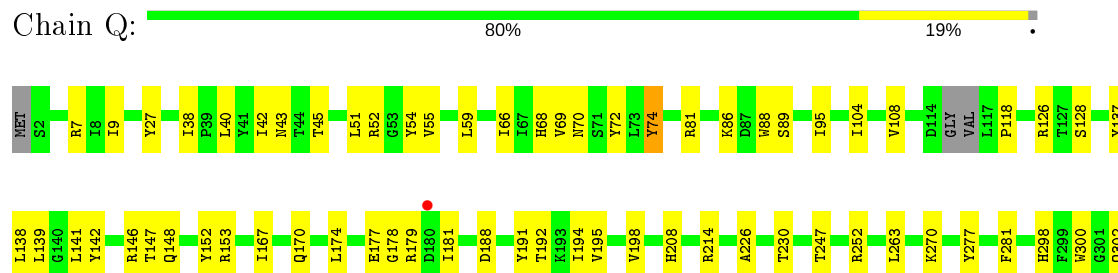
• Molecule 1: Nucleoprotein



• Molecule 1: Nucleoprotein

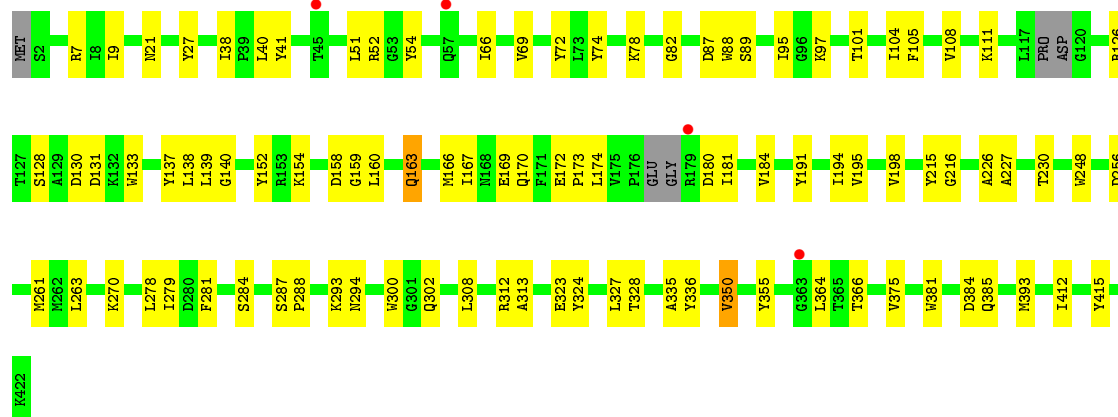
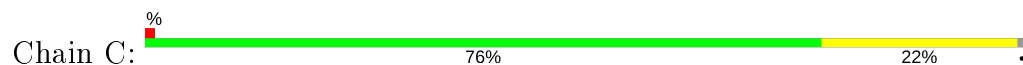


• Molecule 1: Nucleoprotein

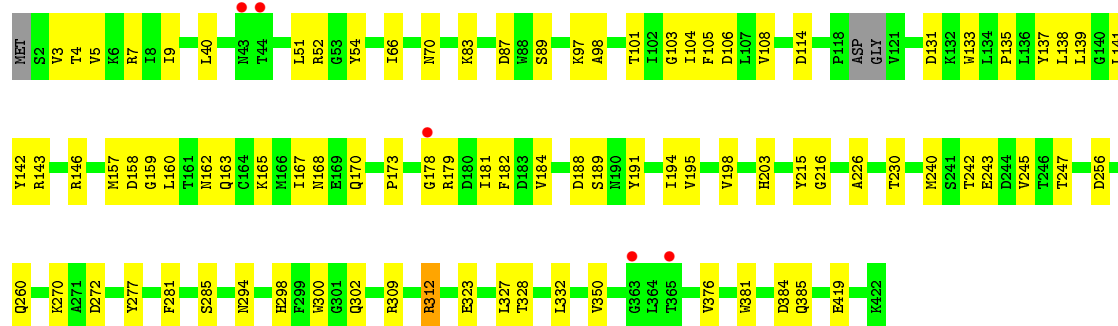
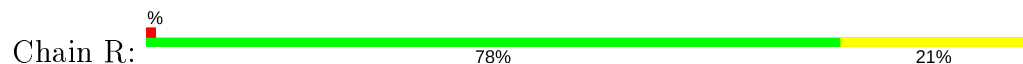




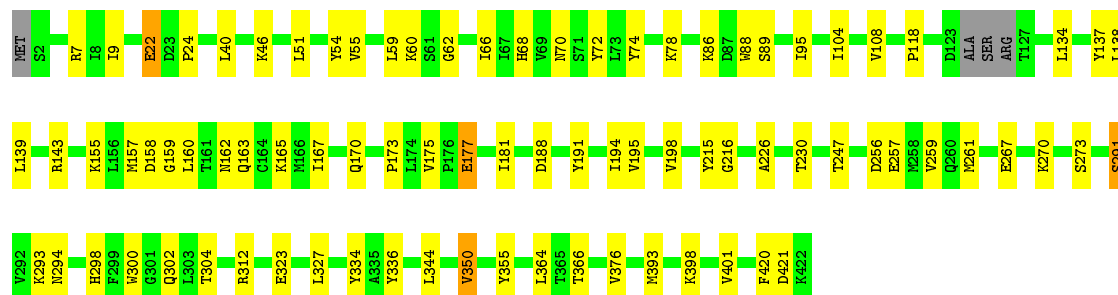
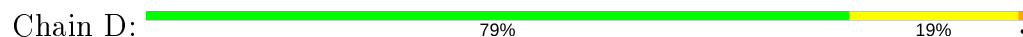
• Molecule 1: Nucleoprotein




• Molecule 1: Nucleoprotein

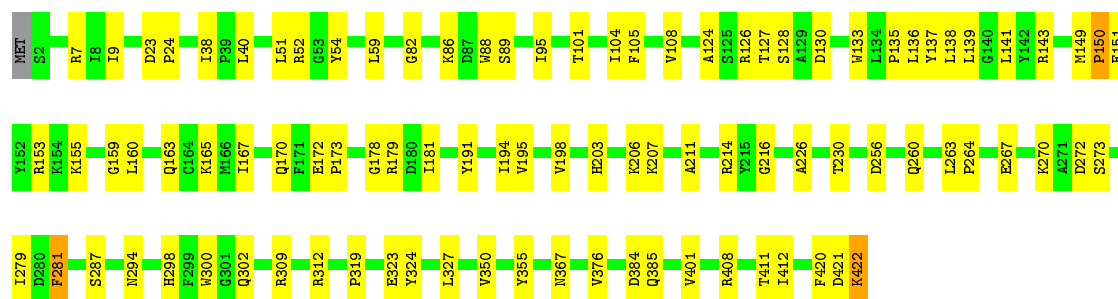


• Molecule 1: Nucleoprotein




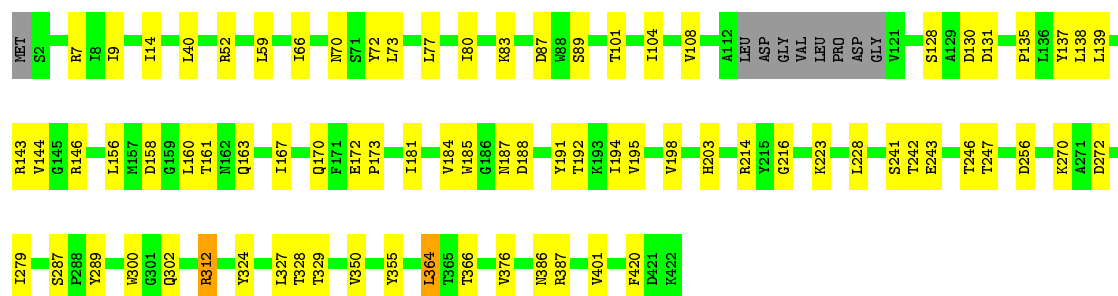
• Molecule 1: Nucleoprotein

Chain S:  77% 22%




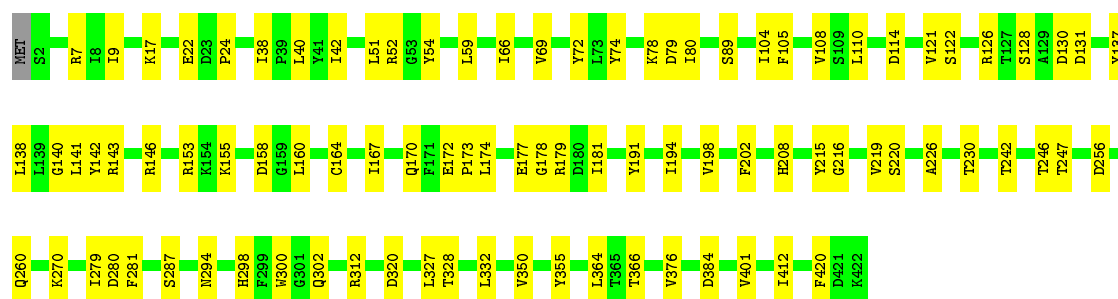
• Molecule 1: Nucleoprotein

Chain E:  79% 18%




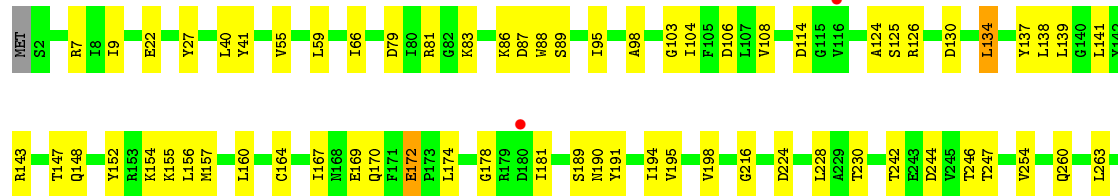
• Molecule 1: Nucleoprotein

Chain T:  78% 22%



• Molecule 1: Nucleoprotein

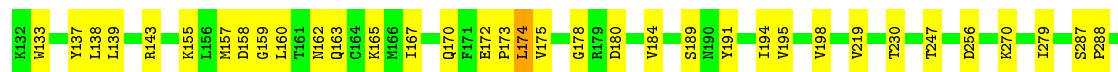
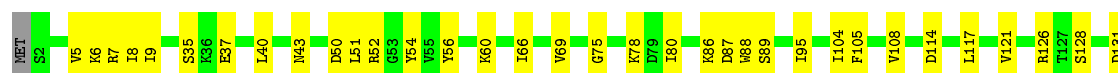
Chain K:  78% 21%





• Molecule 1: Nucleoprotein

Chain L: 78% 22%



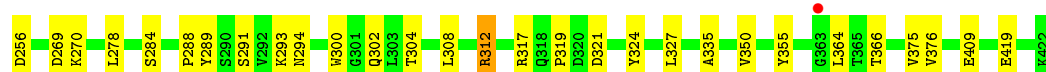
• Molecule 1: Nucleoprotein

Chain N: 76% 23%



• Molecule 1: Nucleoprotein

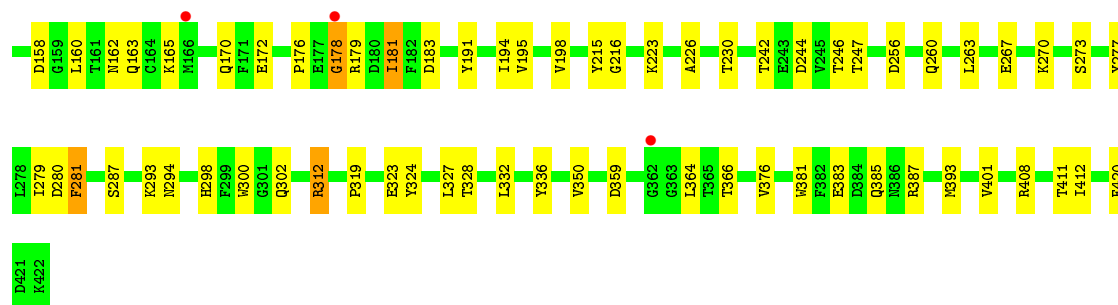
Chain M: 77% 21%



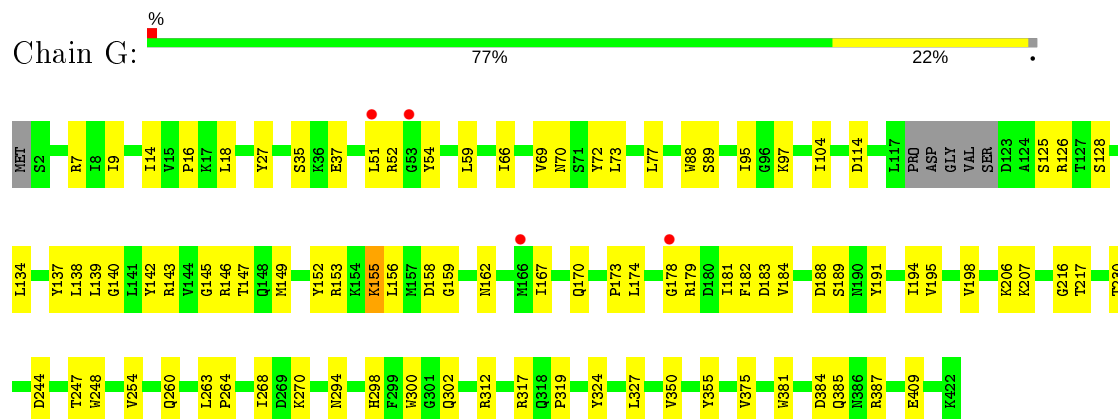
• Molecule 1: Nucleoprotein

Chain F: 76% 23%

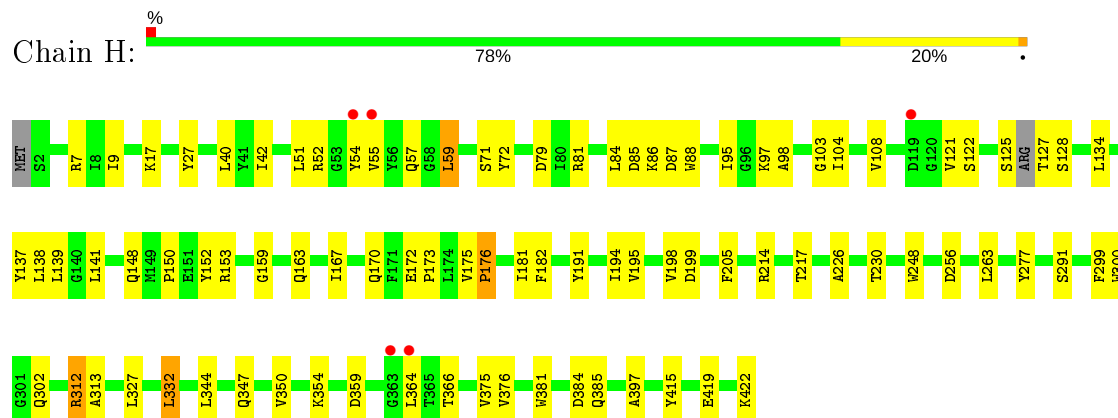




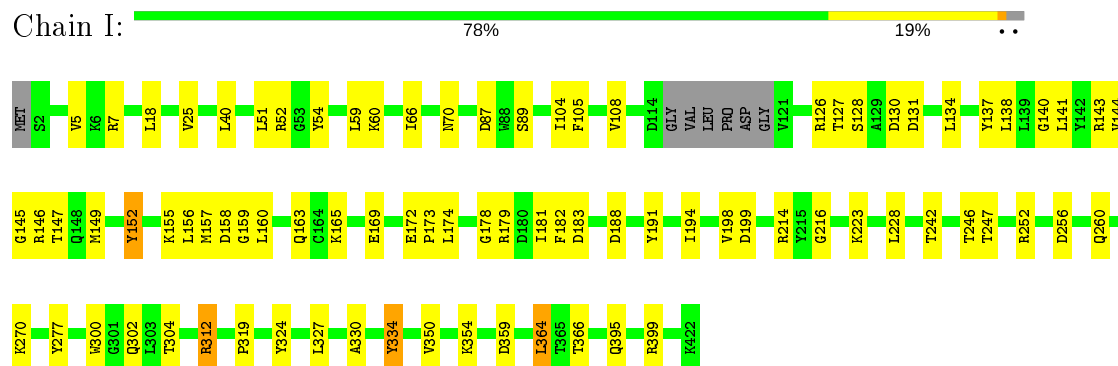
• Molecule 1: Nucleoprotein



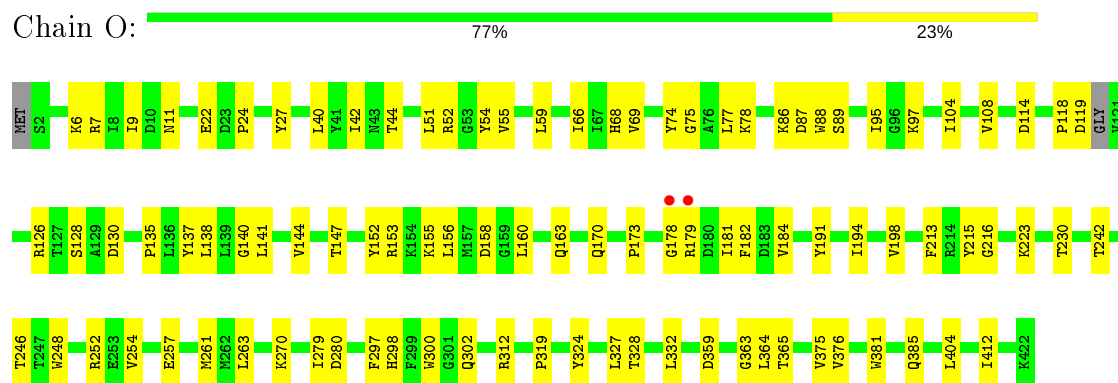
• Molecule 1: Nucleoprotein



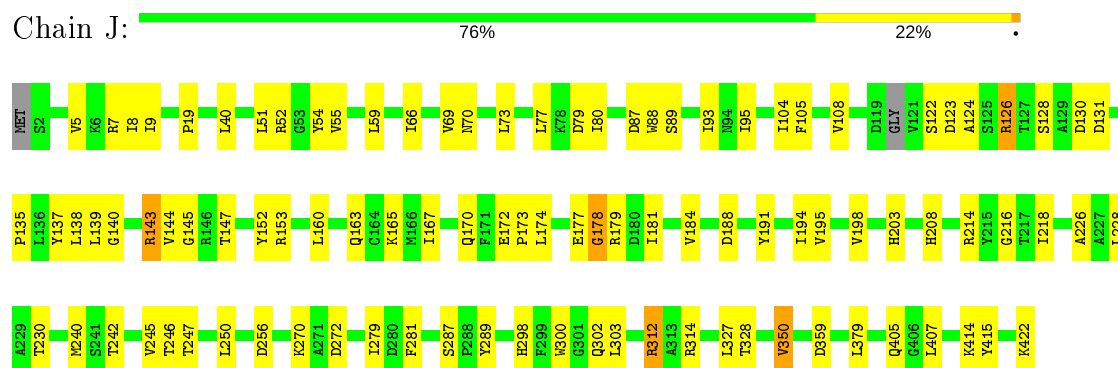
• Molecule 1: Nucleoprotein



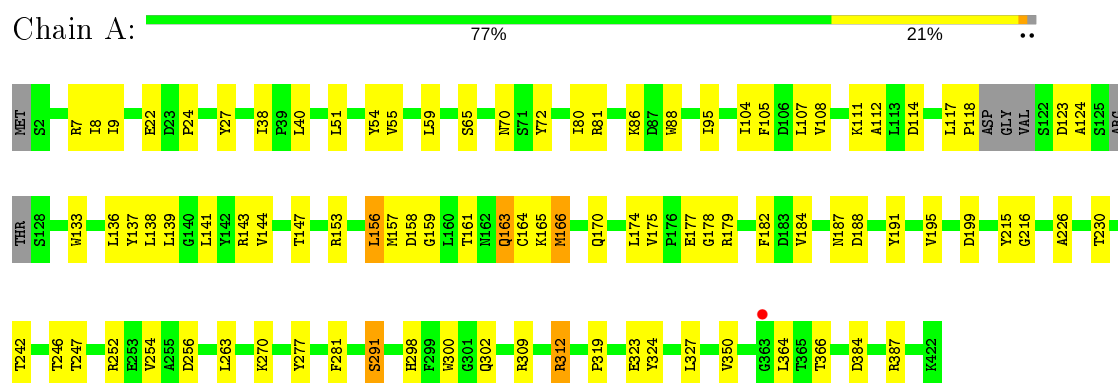
- Molecule 1: Nucleoprotein



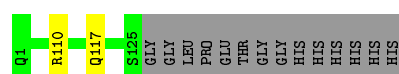
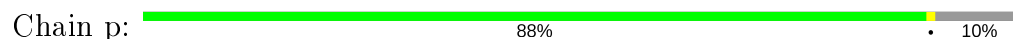
- Molecule 1: Nucleoprotein




- Molecule 1: Nucleoprotein

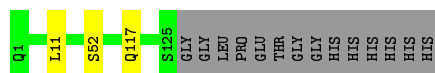


- Molecule 2: Anti-vesicular stomatitis virus N VHH




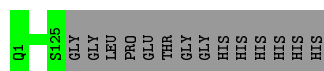
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain b:  88% 10%




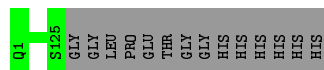
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain q:  90% 10%




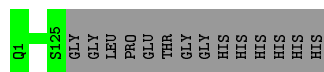
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain c:  90% 10%




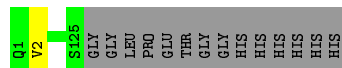
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain r:  90% 10%




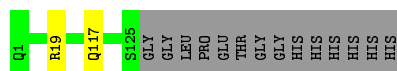
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain d:  89% 10%




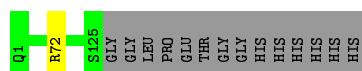
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain s:  88% 10%



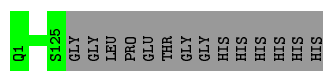
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain e:  89% 10%



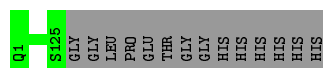
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain t:  90% 10%



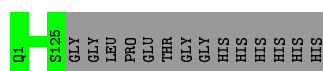
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain k: 90% 10%



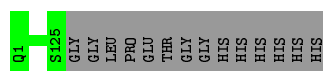
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain l: 90% 10%



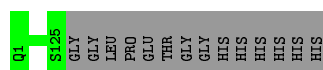
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain n: 90% 10%



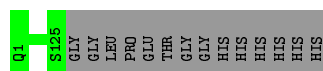
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain m: 90% 10%



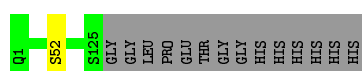
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain f: 90% 10%



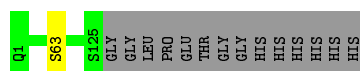
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain g: 89% 10%



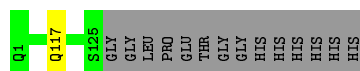
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain h: 89% 10%



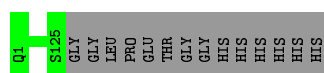
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain i: 89% 10%



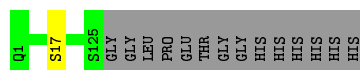
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain o: 90% 10%



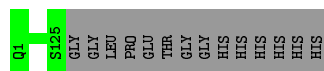
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain j: 89% 10%



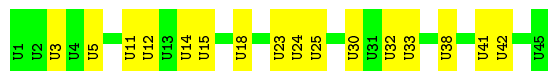
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain a: 90% 10%



- Molecule 3: RNA (45-MER)

Chain u: 64% 36%



- Molecule 3: RNA (45-MER)

Chain v: 64% 36%



- Molecule 3: RNA (45-MER)

Chain w: 62% 38%



● Molecule 3: RNA (45-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	147.56Å 156.01Å 217.45Å 79.24° 75.66° 62.27°	Depositor
Resolution (Å)	128.35 – 3.20 128.36 – 3.20	Depositor EDS
% Data completeness (in resolution range)	92.0 (128.35-3.20) 91.9 (128.36-3.20)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.236 , 0.288 0.237 , 0.288	Depositor DCC
R_{free} test set	1990 reflections (0.79%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.724	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 9.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	89086	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.25	0/3364	0.42	0/4551
1	B	0.24	0/3343	0.41	0/4521
1	C	0.24	0/3372	0.41	0/4561
1	D	0.25	0/3380	0.41	0/4575
1	E	0.24	0/3347	0.42	0/4528
1	F	0.24	0/3403	0.41	0/4607
1	G	0.24	0/3369	0.42	0/4558
1	H	0.25	0/3391	0.43	1/4590 (0.0%)
1	I	0.24	0/3363	0.42	1/4550 (0.0%)
1	J	0.24	0/3398	0.42	0/4599
1	K	0.24	0/3403	0.42	0/4607
1	L	0.25	0/3403	0.42	0/4607
1	M	0.24	0/3366	0.40	0/4556
1	N	0.24	0/3380	0.42	0/4575
1	O	0.24	0/3398	0.42	0/4599
1	P	0.24	0/3355	0.41	0/4539
1	Q	0.24	0/3391	0.42	0/4589
1	R	0.25	0/3390	0.43	0/4588
1	S	0.25	0/3403	0.44	1/4607 (0.0%)
1	T	0.24	0/3403	0.42	0/4607
2	a	0.25	0/988	0.44	0/1334
2	b	0.25	0/988	0.45	0/1334
2	c	0.26	0/988	0.45	0/1334
2	d	0.25	0/988	0.45	0/1334
2	e	0.26	0/988	0.45	0/1334
2	f	0.25	0/988	0.45	0/1334
2	g	0.26	0/988	0.44	0/1334
2	h	0.25	0/988	0.45	0/1334
2	i	0.26	0/988	0.45	0/1334
2	j	0.25	0/988	0.45	0/1334
2	k	0.25	0/988	0.46	0/1334
2	l	0.25	0/988	0.44	0/1334
2	m	0.25	0/988	0.45	0/1334
2	n	0.25	0/988	0.44	0/1334

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	o	0.25	0/988	0.45	0/1334
2	p	0.25	0/988	0.45	0/1334
2	q	0.25	0/988	0.45	0/1334
2	r	0.25	0/988	0.45	0/1334
2	s	0.25	0/988	0.45	0/1334
2	t	0.25	0/988	0.46	0/1334
3	u	0.20	0/989	0.94	1/1526 (0.1%)
3	v	0.20	0/989	0.93	2/1526 (0.1%)
3	w	0.19	0/989	0.92	2/1526 (0.1%)
3	x	0.21	0/989	0.99	3/1526 (0.2%)
All	All	0.24	0/91338	0.46	11/124298 (0.0%)

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	H	0	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	59	LEU	CB-CG-CD1	5.92	121.07	111.00
1	I	364	LEU	CA-CB-CG	5.81	128.66	115.30
1	H	59	LEU	CB-CG-CD1	5.78	120.82	111.00
3	x	9	U	C2-N1-C1'	5.48	124.28	117.70
3	v	18	U	C2-N1-C1'	5.45	124.24	117.70
3	u	18	U	C2-N1-C1'	5.42	124.21	117.70
3	x	18	U	C2-N1-C1'	5.28	124.04	117.70
3	x	27	U	C2-N1-C1'	5.26	124.02	117.70
3	w	9	U	C2-N1-C1'	5.23	123.98	117.70
3	w	18	U	C2-N1-C1'	5.18	123.92	117.70
3	v	9	U	C2-N1-C1'	5.13	123.85	117.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	152	TYR	Peptide

5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3290	0	3249	62	0
1	B	3270	0	3230	53	0
1	C	3299	0	3265	56	0
1	D	3305	0	3263	55	0
1	E	3273	0	3234	49	0
1	F	3327	0	3287	65	0
1	G	3295	0	3258	61	0
1	H	3316	0	3273	53	0
1	I	3289	0	3249	62	0
1	J	3323	0	3283	71	0
1	K	3327	0	3287	57	0
1	L	3327	0	3287	64	1
1	M	3291	0	3254	63	0
1	N	3305	0	3263	63	0
1	O	3323	0	3283	65	0
1	P	3281	0	3245	52	0
1	Q	3316	0	3274	51	1
1	R	3315	0	3279	59	0
1	S	3327	0	3287	63	0
1	T	3327	0	3287	65	0
2	a	968	0	932	0	0
2	b	968	0	932	0	0
2	c	968	0	932	0	0
2	d	968	0	932	0	0
2	e	968	0	932	0	0
2	f	968	0	932	0	0
2	g	968	0	932	0	0
2	h	968	0	932	0	0
2	i	968	0	932	0	0
2	j	968	0	932	0	0
2	k	968	0	932	0	0
2	l	968	0	932	0	0
2	m	968	0	932	0	0
2	n	968	0	932	0	0
2	o	968	0	932	0	0
2	p	968	0	932	0	0
2	q	968	0	932	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	r	968	0	932	0	0
2	s	968	0	932	0	0
2	t	968	0	932	0	0
3	u	900	0	451	0	0
3	v	900	0	451	0	0
3	w	900	0	451	0	0
3	x	900	0	451	0	0
All	All	89086	0	85781	1109	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (1109) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:ASP:O	1:D:162:ASN:HB2	1.45	1.14
1:M:55:VAL:O	1:M:59:LEU:HD13	1.63	0.97
1:G:158:ASP:O	1:G:162:ASN:HB2	1.66	0.93
1:L:300:TRP:HB2	1:L:327:LEU:HD12	1.51	0.93
1:K:300:TRP:HB2	1:K:327:LEU:HD12	1.51	0.92
1:N:157:MET:O	1:N:160:LEU:HB2	1.72	0.89
1:G:300:TRP:HB2	1:G:327:LEU:HD12	1.56	0.86
1:I:300:TRP:HB2	1:I:327:LEU:HD12	1.56	0.86
1:T:74:TYR:O	1:T:78:LYS:HB2	1.76	0.85
1:F:149:MET:HG3	1:F:150:PRO:HD2	1.57	0.85
1:M:300:TRP:HB2	1:M:327:LEU:HD12	1.58	0.84
1:N:55:VAL:O	1:N:59:LEU:HB2	1.77	0.83
1:D:300:TRP:HB2	1:D:327:LEU:HD12	1.60	0.83
1:Q:300:TRP:HB2	1:Q:327:LEU:HD12	1.59	0.83
1:N:300:TRP:HB2	1:N:327:LEU:HD12	1.61	0.82
1:C:300:TRP:HB2	1:C:327:LEU:HD12	1.62	0.81
1:F:27:TYR:CZ	1:F:263:LEU:HD22	2.16	0.80
1:B:300:TRP:HB2	1:B:327:LEU:HD12	1.63	0.80
1:H:300:TRP:HB2	1:H:327:LEU:HD12	1.62	0.79
1:F:300:TRP:HB2	1:F:327:LEU:HD12	1.63	0.79
1:H:175:VAL:HG22	1:H:176:PRO:HD2	1.65	0.78
1:H:167:ILE:HG23	1:H:170:GLN:HB2	1.67	0.77
1:S:300:TRP:HB2	1:S:327:LEU:HD12	1.64	0.77
1:R:300:TRP:HB2	1:R:327:LEU:HD12	1.64	0.77
1:P:300:TRP:HB2	1:P:327:LEU:HD12	1.67	0.76
1:I:147:THR:O	1:I:179:ARG:NH1	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:ILE:HD11	1:D:198:VAL:HG22	1.69	0.75
1:P:144:VAL:HG11	1:P:156:LEU:HG	1.69	0.75
1:T:143:ARG:HE	1:T:155:LYS:HE3	1.48	0.75
1:G:179:ARG:NH1	1:G:183:ASP:OD2	2.19	0.75
1:T:300:TRP:HB2	1:T:327:LEU:HD12	1.68	0.75
1:J:70:ASN:ND2	1:J:188:ASP:OD2	2.19	0.74
1:J:300:TRP:HB2	1:J:327:LEU:HD12	1.69	0.74
1:O:40:LEU:HD12	1:O:108:VAL:HG21	1.69	0.73
1:K:376:VAL:HG13	1:L:355:TYR:HA	1.70	0.73
1:R:133:TRP:HB2	1:R:163:GLN:HG3	1.70	0.73
1:J:40:LEU:HD12	1:J:108:VAL:HG21	1.71	0.72
1:B:104:ILE:HD11	1:B:198:VAL:HG22	1.72	0.72
1:H:159:GLY:O	1:H:163:GLN:NE2	2.23	0.72
1:D:165:LYS:NZ	1:E:184:VAL:O	2.23	0.71
1:N:104:ILE:HD11	1:N:198:VAL:HG22	1.71	0.71
1:C:230:THR:HG22	1:C:312:ARG:HH22	1.55	0.71
1:I:144:VAL:HG11	1:I:156:LEU:HG	1.72	0.71
1:E:163:GLN:OE1	1:E:163:GLN:N	2.23	0.71
1:E:300:TRP:HB2	1:E:327:LEU:HD12	1.71	0.71
1:O:68:HIS:NE2	1:O:118:PRO:O	2.24	0.70
1:O:279:ILE:HD12	1:O:280:ASP:H	1.54	0.70
1:S:260:GLN:OE1	1:S:294:ASN:ND2	2.23	0.70
1:F:256:ASP:OD1	1:G:7:ARG:NH2	2.25	0.70
1:K:104:ILE:HD11	1:K:198:VAL:HG22	1.74	0.70
1:A:40:LEU:HD12	1:A:108:VAL:HG21	1.73	0.69
1:O:300:TRP:HB2	1:O:327:LEU:HD12	1.74	0.69
1:Q:302:GLN:OE1	1:Q:312:ARG:NH1	2.25	0.69
1:J:167:ILE:HG23	1:J:170:GLN:HB2	1.73	0.69
1:G:147:THR:O	1:G:153:ARG:NH2	2.25	0.69
1:M:40:LEU:HD12	1:M:108:VAL:HG21	1.75	0.69
1:E:52:ARG:NH1	1:E:131:ASP:OD2	2.27	0.68
1:M:308:LEU:HD11	1:M:335:ALA:HA	1.75	0.68
1:O:89:SER:O	1:O:270:LYS:NZ	2.27	0.68
1:E:40:LEU:HD12	1:E:108:VAL:HG21	1.74	0.68
1:P:86:LYS:HD3	1:P:87:ASP:H	1.57	0.68
1:P:167:ILE:HG23	1:P:170:GLN:HB2	1.75	0.68
1:M:317:ARG:NH1	1:M:409:GLU:O	2.26	0.67
1:H:104:ILE:HD11	1:H:198:VAL:HG22	1.76	0.67
1:S:104:ILE:HD11	1:S:198:VAL:HG22	1.76	0.67
1:B:230:THR:HG22	1:B:312:ARG:HH22	1.59	0.67
1:F:137:TYR:HB2	1:F:163:GLN:HE22	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:GLN:OE1	1:C:312:ARG:NH2	2.27	0.67
1:Q:230:THR:HG22	1:Q:312:ARG:HH12	1.59	0.67
1:S:7:ARG:NH2	1:T:256:ASP:OD1	2.28	0.67
1:I:40:LEU:HD12	1:I:108:VAL:HG21	1.77	0.67
1:A:300:TRP:HB2	1:A:327:LEU:HD12	1.77	0.67
1:B:7:ARG:NH2	1:A:256:ASP:OD1	2.27	0.67
1:T:52:ARG:NH1	1:T:131:ASP:OD2	2.28	0.67
1:R:104:ILE:HD11	1:R:198:VAL:HG22	1.77	0.67
1:S:178:GLY:HA2	1:S:181:ILE:HG12	1.76	0.67
1:E:104:ILE:HD11	1:E:198:VAL:HG22	1.77	0.66
1:F:137:TYR:O	1:F:141:LEU:HD22	1.93	0.66
1:L:56:TYR:OH	1:L:126:ARG:NH2	2.28	0.66
1:G:138:LEU:O	1:G:191:TYR:OH	2.12	0.66
1:B:40:LEU:HD12	1:B:108:VAL:HG21	1.76	0.66
1:E:256:ASP:OD1	1:F:7:ARG:NH2	2.27	0.66
1:G:14:ILE:HG23	1:G:16:PRO:HD3	1.77	0.66
1:N:145:GLY:HA2	1:N:153:ARG:HH12	1.60	0.66
1:E:167:ILE:HG23	1:E:170:GLN:HB2	1.77	0.66
1:A:158:ASP:OD1	1:A:161:THR:OG1	2.14	0.66
1:J:144:VAL:O	1:J:153:ARG:NH2	2.29	0.65
1:L:89:SER:O	1:L:270:LYS:NZ	2.30	0.65
1:B:167:ILE:HG23	1:B:170:GLN:HB2	1.76	0.65
1:E:242:THR:O	1:E:246:THR:OG1	2.13	0.65
1:I:59:LEU:HD22	1:I:174:LEU:HD11	1.79	0.65
1:J:104:ILE:HD11	1:J:198:VAL:HG22	1.76	0.65
1:N:51:LEU:HB3	1:N:72:TYR:HB2	1.79	0.65
1:A:319:PRO:O	1:A:324:TYR:OH	2.10	0.65
1:Q:137:TYR:O	1:Q:141:LEU:HD22	1.97	0.65
1:Q:313:ALA:HB1	1:Q:412:ILE:HD11	1.78	0.65
1:K:137:TYR:O	1:K:141:LEU:HD22	1.96	0.65
1:I:178:GLY:HA2	1:I:181:ILE:HG12	1.78	0.65
1:Q:104:ILE:HD11	1:Q:198:VAL:HG22	1.79	0.64
1:D:355:TYR:HA	1:E:376:VAL:HG13	1.78	0.64
1:N:143:ARG:HG2	1:N:155:LYS:HZ1	1.62	0.64
1:Q:178:GLY:HA2	1:Q:181:ILE:HG12	1.79	0.64
1:C:174:LEU:HD11	1:C:181:ILE:HG13	1.78	0.64
1:J:178:GLY:HA2	1:J:181:ILE:HD13	1.79	0.64
1:K:89:SER:O	1:K:270:LYS:NZ	2.31	0.64
1:N:177:GLU:O	1:N:179:ARG:N	2.31	0.64
1:S:40:LEU:HD12	1:S:108:VAL:HG21	1.80	0.64
1:D:167:ILE:HG23	1:D:170:GLN:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:TYR:CE2	1:F:263:LEU:HD22	2.33	0.64
1:H:332:LEU:HD21	1:H:397:ALA:HB2	1.80	0.64
1:I:127:THR:HG22	1:I:128:SER:H	1.62	0.64
1:N:152:TYR:O	1:N:155:LYS:HB3	1.97	0.64
1:P:56:TYR:OH	1:P:126:ARG:NH2	2.30	0.63
1:J:52:ARG:NH1	1:J:131:ASP:OD2	2.31	0.63
1:Q:42:ILE:CD1	1:Q:74:TYR:HB2	2.27	0.63
1:R:139:LEU:HD22	1:R:195:VAL:HG12	1.79	0.63
1:G:104:ILE:HD11	1:G:198:VAL:HG22	1.81	0.63
1:N:77:LEU:HD13	1:N:104:ILE:HD13	1.81	0.63
1:E:138:LEU:O	1:E:191:TYR:OH	2.17	0.63
1:P:256:ASP:OD1	1:O:7:ARG:NH2	2.30	0.63
1:D:68:HIS:NE2	1:D:118:PRO:O	2.31	0.63
1:N:143:ARG:HB2	1:N:216:GLY:HA2	1.80	0.63
1:P:376:VAL:HG13	1:Q:355:TYR:HA	1.80	0.63
1:I:138:LEU:O	1:I:191:TYR:OH	2.17	0.63
1:F:138:LEU:O	1:F:191:TYR:OH	2.17	0.63
1:L:7:ARG:NH2	1:M:256:ASP:OD1	2.30	0.63
1:S:139:LEU:HD22	1:S:195:VAL:HG12	1.79	0.63
1:T:160:LEU:HD21	1:T:172:GLU:HB3	1.81	0.62
1:J:165:LYS:HZ1	1:A:187:ASN:HB2	1.63	0.62
1:B:70:ASN:ND2	1:B:188:ASP:OD2	2.28	0.62
1:I:179:ARG:NH2	1:I:183:ASP:OD1	2.32	0.62
1:J:153:ARG:NH1	1:J:179:ARG:O	2.31	0.62
1:R:137:TYR:O	1:R:141:LEU:HD22	1.98	0.62
1:O:137:TYR:O	1:O:141:LEU:HD22	1.99	0.62
1:R:157:MET:HA	1:R:160:LEU:HB2	1.81	0.62
1:L:40:LEU:HD12	1:L:108:VAL:HG21	1.82	0.62
1:P:178:GLY:HA2	1:P:181:ILE:HG12	1.81	0.62
1:T:167:ILE:HG23	1:T:170:GLN:HB2	1.82	0.62
1:T:137:TYR:O	1:T:141:LEU:HD22	2.01	0.61
1:N:137:TYR:O	1:N:141:LEU:HD22	1.99	0.61
1:P:138:LEU:O	1:P:191:TYR:OH	2.18	0.61
1:G:178:GLY:HA2	1:G:181:ILE:HG12	1.82	0.61
1:T:302:GLN:OE1	1:T:312:ARG:NH1	2.32	0.61
1:C:313:ALA:HB1	1:C:412:ILE:HD11	1.81	0.61
1:D:157:MET:HA	1:D:160:LEU:HB2	1.81	0.61
1:G:260:GLN:OE1	1:G:294:ASN:ND2	2.28	0.61
1:J:302:GLN:OE1	1:J:312:ARG:NH2	2.34	0.61
1:L:104:ILE:HD11	1:L:198:VAL:HG22	1.81	0.61
1:D:159:GLY:HA3	1:D:163:GLN:HG2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:GLY:O	1:B:163:GLN:HG2	2.01	0.61
1:E:203:HIS:ND1	1:E:272:ASP:OD1	2.31	0.61
1:H:40:LEU:HD12	1:H:108:VAL:HG21	1.83	0.61
1:P:139:LEU:HD22	1:P:195:VAL:HG12	1.81	0.61
1:K:138:LEU:O	1:K:191:TYR:OH	2.18	0.60
1:N:69:VAL:O	1:N:73:LEU:HB2	2.00	0.60
1:P:22:GLU:HB3	1:P:24:PRO:HD3	1.82	0.60
1:M:89:SER:O	1:M:270:LYS:NZ	2.34	0.60
1:F:143:ARG:HB2	1:F:216:GLY:HA2	1.84	0.60
1:Q:138:LEU:O	1:Q:191:TYR:OH	2.19	0.60
1:Q:51:LEU:HB3	1:Q:72:TYR:HB2	1.82	0.60
1:T:143:ARG:HB2	1:T:216:GLY:HA2	1.83	0.60
1:J:279:ILE:HD11	1:J:287:SER:HB2	1.84	0.60
1:E:279:ILE:HD11	1:E:287:SER:HB2	1.83	0.60
1:T:7:ARG:HG2	1:T:9:ILE:HG22	1.84	0.60
1:E:70:ASN:ND2	1:E:188:ASP:OD2	2.34	0.60
1:I:256:ASP:OD1	1:J:7:ARG:NH2	2.35	0.60
1:O:163:GLN:NE2	1:O:170:GLN:OE1	2.34	0.60
1:Q:40:LEU:HD12	1:Q:108:VAL:HG21	1.84	0.60
1:S:203:HIS:ND1	1:S:272:ASP:OD1	2.31	0.60
1:A:143:ARG:HB2	1:A:216:GLY:HA2	1.84	0.60
1:B:127:THR:OG1	1:B:128:SER:N	2.34	0.60
1:N:138:LEU:O	1:N:191:TYR:OH	2.19	0.60
1:I:147:THR:HG1	1:I:152:TYR:HD2	1.49	0.59
1:L:52:ARG:NH1	1:L:131:ASP:OD2	2.35	0.59
1:M:144:VAL:HG11	1:M:156:LEU:HB2	1.83	0.59
1:P:38:ILE:HD12	1:P:39:PRO:HD2	1.84	0.59
1:M:72:TYR:O	1:M:75:GLY:N	2.35	0.59
1:M:167:ILE:HG23	1:M:170:GLN:HB2	1.84	0.59
1:A:51:LEU:HB3	1:A:72:TYR:HB2	1.85	0.59
1:C:51:LEU:HA	1:C:54:TYR:HB2	1.85	0.59
1:J:123:ASP:OD1	1:J:124:ALA:N	2.35	0.59
1:I:228:LEU:HD21	1:J:19:PRO:HG2	1.84	0.59
1:K:143:ARG:HB2	1:K:216:GLY:HA2	1.85	0.59
1:L:160:LEU:HD11	1:L:172:GLU:HG3	1.83	0.59
1:A:242:THR:O	1:A:246:THR:OG1	2.21	0.59
1:C:104:ILE:HD11	1:C:198:VAL:HG22	1.84	0.59
1:J:230:THR:HG22	1:J:312:ARG:HH22	1.67	0.59
1:M:138:LEU:O	1:M:191:TYR:OH	2.20	0.59
1:E:302:GLN:OE1	1:E:312:ARG:NH1	2.36	0.59
1:H:139:LEU:HD22	1:H:195:VAL:HG12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:42:ILE:HD11	1:Q:74:TYR:HB2	1.85	0.59
1:R:184:VAL:O	1:S:165:LYS:NZ	2.36	0.59
1:E:139:LEU:HD22	1:E:195:VAL:HG12	1.85	0.58
1:J:145:GLY:HA2	1:J:153:ARG:HH22	1.67	0.58
1:M:86:LYS:HD3	1:M:87:ASP:H	1.68	0.58
1:L:298:HIS:O	1:L:302:GLN:HB2	2.03	0.58
1:C:40:LEU:HD12	1:C:108:VAL:HG21	1.84	0.58
1:A:88:TRP:CD2	1:A:95:ILE:HD11	2.38	0.58
1:C:279:ILE:HD11	1:C:287:SER:HB2	1.85	0.58
1:H:55:VAL:O	1:H:59:LEU:HB2	2.04	0.58
1:I:104:ILE:HD11	1:I:198:VAL:HG22	1.85	0.58
1:J:7:ARG:HG2	1:J:9:ILE:HG22	1.85	0.58
1:G:319:PRO:O	1:G:324:TYR:OH	2.17	0.58
1:T:242:THR:O	1:T:246:THR:OG1	2.18	0.58
1:Q:153:ARG:NH2	1:Q:179:ARG:O	2.36	0.58
1:R:260:GLN:OE1	1:R:294:ASN:ND2	2.33	0.58
1:S:367:ASN:OD1	1:S:385:GLN:NE2	2.28	0.58
1:H:302:GLN:OE1	1:H:312:ARG:NH1	2.37	0.58
1:R:52:ARG:NH1	1:R:131:ASP:OD2	2.37	0.58
1:J:165:LYS:NZ	1:A:187:ASN:HB2	2.18	0.58
1:N:230:THR:HG21	1:N:298:HIS:ND1	2.19	0.57
1:C:159:GLY:O	1:C:163:GLN:NE2	2.38	0.57
1:D:256:ASP:OD1	1:E:7:ARG:NH2	2.38	0.57
1:T:138:LEU:O	1:T:191:TYR:OH	2.22	0.57
1:N:165:LYS:HG2	1:M:184:VAL:HG22	1.87	0.57
1:T:364:LEU:HG	1:T:366:THR:HG23	1.87	0.57
1:O:178:GLY:HA2	1:O:181:ILE:HG12	1.87	0.57
1:J:165:LYS:HZ2	1:A:184:VAL:HA	1.69	0.57
1:B:143:ARG:HB3	1:B:216:GLY:HA2	1.86	0.57
1:D:159:GLY:CA	1:D:163:GLN:HG2	2.34	0.57
1:G:317:ARG:NH1	1:G:409:GLU:O	2.37	0.57
1:M:25:VAL:HG11	1:M:288:PRO:HB3	1.87	0.57
1:B:7:ARG:HG2	1:B:9:ILE:HG22	1.85	0.57
1:B:140:GLY:HA2	1:B:216:GLY:HA3	1.87	0.57
1:C:7:ARG:HG2	1:C:9:ILE:HG22	1.86	0.57
1:H:7:ARG:HG2	1:H:9:ILE:HG22	1.86	0.57
1:I:137:TYR:HD1	1:I:163:GLN:HE22	1.50	0.57
1:K:7:ARG:NH2	1:L:256:ASP:OD1	2.25	0.57
1:H:87:ASP:OD1	1:H:98:ALA:N	2.37	0.57
1:O:77:LEU:HD11	1:O:135:PRO:HB3	1.86	0.57
1:D:7:ARG:HG2	1:D:9:ILE:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:302:GLN:OE1	1:F:312:ARG:NH1	2.38	0.56
1:J:160:LEU:HD21	1:J:172:GLU:HB3	1.87	0.56
1:O:7:ARG:HG2	1:O:9:ILE:HG22	1.85	0.56
1:T:72:TYR:OH	1:T:131:ASP:OD1	2.17	0.56
1:F:154:LYS:HG2	1:F:179:ARG:HH22	1.71	0.56
1:I:149:MET:HB3	1:I:152:TYR:HB2	1.87	0.56
1:T:260:GLN:OE1	1:T:294:ASN:ND2	2.33	0.56
1:F:7:ARG:HG2	1:F:9:ILE:HG22	1.87	0.56
1:R:51:LEU:HA	1:R:54:TYR:HB2	1.86	0.56
1:S:153:ARG:HB2	1:S:179:ARG:HH21	1.69	0.56
1:J:256:ASP:OD1	1:A:7:ARG:NH2	2.38	0.56
1:E:144:VAL:HG11	1:E:156:LEU:HD12	1.86	0.56
1:J:230:THR:HG21	1:J:298:HIS:ND1	2.20	0.56
1:H:350:VAL:HG22	1:J:5:VAL:HG22	1.87	0.56
1:L:302:GLN:OE1	1:L:312:ARG:NH1	2.39	0.56
1:A:22:GLU:HB3	1:A:24:PRO:HD3	1.88	0.56
1:K:359:ASP:N	1:K:359:ASP:OD1	2.38	0.56
1:L:5:VAL:HG22	1:N:350:VAL:HG22	1.87	0.56
1:A:55:VAL:O	1:A:59:LEU:HB2	2.05	0.56
1:J:51:LEU:HA	1:J:54:TYR:HB2	1.86	0.56
1:K:279:ILE:HD11	1:K:287:SER:HB2	1.87	0.56
1:M:67:ILE:O	1:M:71:SER:OG	2.18	0.56
1:Q:139:LEU:HD22	1:Q:195:VAL:HG12	1.87	0.56
1:D:165:LYS:HZ2	1:E:184:VAL:HG13	1.71	0.56
1:K:419:GLU:OE2	1:L:309:ARG:NE	2.38	0.56
1:N:364:LEU:HG	1:N:366:THR:HG23	1.87	0.56
1:O:75:GLY:HA2	1:O:78:LYS:HE2	1.88	0.56
1:C:163:GLN:HB3	1:C:170:GLN:HG3	1.88	0.56
1:F:104:ILE:HD11	1:F:198:VAL:HA	1.86	0.56
1:M:319:PRO:O	1:M:324:TYR:OH	2.22	0.56
1:O:153:ARG:HD2	1:O:179:ARG:HD2	1.86	0.56
1:B:230:THR:HG22	1:B:312:ARG:NH2	2.21	0.56
1:C:138:LEU:O	1:C:191:TYR:OH	2.23	0.56
1:R:89:SER:O	1:R:270:LYS:NZ	2.39	0.56
1:A:7:ARG:HG2	1:A:9:ILE:HG22	1.86	0.56
1:D:70:ASN:ND2	1:D:188:ASP:OD2	2.38	0.56
1:K:139:LEU:HD22	1:K:195:VAL:HG12	1.88	0.56
1:L:162:ASN:HA	1:L:165:LYS:HD3	1.88	0.56
1:G:69:VAL:O	1:G:73:LEU:HB2	2.05	0.56
1:O:104:ILE:HD11	1:O:198:VAL:HG22	1.88	0.56
1:O:279:ILE:HD12	1:O:280:ASP:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:89:SER:O	1:Q:270:LYS:NZ	2.39	0.55
1:B:139:LEU:HD22	1:B:195:VAL:HG12	1.86	0.55
1:B:302:GLN:OE1	1:B:312:ARG:NH2	2.38	0.55
1:D:139:LEU:HD22	1:D:195:VAL:HG12	1.88	0.55
1:G:167:ILE:HG23	1:G:170:GLN:HB2	1.89	0.55
1:I:140:GLY:HA2	1:I:216:GLY:HA3	1.87	0.55
1:I:302:GLN:OE1	1:I:312:ARG:NH1	2.39	0.55
1:K:364:LEU:HG	1:K:366:THR:HG23	1.87	0.55
1:Q:324:TYR:O	1:Q:328:THR:OG1	2.19	0.55
1:Q:7:ARG:HG2	1:Q:9:ILE:HG22	1.88	0.55
1:S:88:TRP:CD2	1:S:95:ILE:HD11	2.41	0.55
1:J:139:LEU:HD22	1:J:195:VAL:HG12	1.88	0.55
1:M:66:ILE:O	1:M:70:ASN:ND2	2.40	0.55
1:O:55:VAL:O	1:O:59:LEU:HB2	2.05	0.55
1:A:144:VAL:HG22	1:A:156:LEU:HB3	1.88	0.55
1:G:153:ARG:HH11	1:G:182:PHE:HE1	1.55	0.55
1:M:133:TRP:HB2	1:M:163:GLN:HG2	1.88	0.55
1:R:184:VAL:HA	1:S:165:LYS:HZ2	1.72	0.55
1:B:230:THR:HG21	1:B:298:HIS:ND1	2.22	0.55
1:C:256:ASP:OD1	1:D:7:ARG:NH2	2.35	0.55
1:K:55:VAL:O	1:K:59:LEU:HB2	2.07	0.55
1:S:138:LEU:O	1:S:191:TYR:OH	2.24	0.55
1:H:51:LEU:HB3	1:H:72:TYR:HB2	1.89	0.55
1:K:126:ARG:HD2	1:K:130:ASP:OD2	2.07	0.55
1:N:137:TYR:CZ	1:N:173:PRO:HD2	2.42	0.55
1:T:160:LEU:O	1:T:164:CYS:HB2	2.07	0.55
1:P:247:THR:HG21	1:Q:350:VAL:HG23	1.89	0.54
1:J:138:LEU:O	1:J:191:TYR:OH	2.24	0.54
1:N:309:ARG:NE	1:M:419:GLU:OE2	2.41	0.54
1:B:143:ARG:HE	1:B:155:LYS:HD2	1.72	0.54
1:H:364:LEU:HG	1:H:366:THR:HG23	1.89	0.54
1:D:46:LYS:HD3	1:D:54:TYR:HE2	1.70	0.54
1:K:160:LEU:HD11	1:K:172:GLU:HG3	1.90	0.54
1:L:7:ARG:HG2	1:L:9:ILE:HG22	1.90	0.54
1:O:302:GLN:HB3	1:O:412:ILE:HD13	1.90	0.54
1:P:158:ASP:O	1:P:162:ASN:N	2.41	0.54
1:R:178:GLY:HA2	1:R:181:ILE:HG12	1.90	0.54
1:N:167:ILE:HG23	1:N:170:GLN:HB2	1.87	0.54
1:O:27:TYR:CZ	1:O:263:LEU:HD22	2.42	0.54
1:R:83:LYS:HA	1:R:101:THR:HA	1.88	0.54
1:T:376:VAL:HG13	1:K:355:TYR:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:103:GLY:N	1:R:106:ASP:OD2	2.30	0.54
1:R:167:ILE:HG23	1:R:170:GLN:HB2	1.90	0.54
1:B:208:HIS:HD1	1:B:210:CYS:H	1.55	0.54
1:K:88:TRP:CD2	1:K:95:ILE:HD11	2.43	0.54
1:E:160:LEU:HD21	1:E:172:GLU:HB3	1.88	0.53
1:R:70:ASN:ND2	1:R:188:ASP:OD2	2.37	0.53
1:I:172:GLU:OE2	1:I:172:GLU:N	2.32	0.53
1:R:230:THR:HG21	1:R:298:HIS:ND1	2.23	0.53
1:S:149:MET:HB2	1:S:150:PRO:HD2	1.91	0.53
1:S:137:TYR:CZ	1:S:173:PRO:HD2	2.43	0.53
1:T:22:GLU:HB3	1:T:24:PRO:HD3	1.89	0.53
1:H:354:LYS:HD3	1:J:8:ILE:HB	1.90	0.53
1:L:137:TYR:CZ	1:L:173:PRO:HD2	2.43	0.53
1:M:77:LEU:HD11	1:M:80:ILE:HG12	1.90	0.53
1:D:138:LEU:O	1:D:191:TYR:OH	2.25	0.53
1:J:59:LEU:HD22	1:J:174:LEU:HD11	1.91	0.53
1:G:59:LEU:HD23	1:G:173:PRO:HG2	1.90	0.53
1:M:104:ILE:HD11	1:M:198:VAL:HG22	1.91	0.53
1:R:137:TYR:CZ	1:R:173:PRO:HD2	2.43	0.53
1:T:51:LEU:HA	1:T:54:TYR:HB2	1.90	0.53
1:B:242:THR:O	1:B:246:THR:OG1	2.16	0.53
1:E:364:LEU:HG	1:E:366:THR:HG23	1.89	0.53
1:N:240:MET:HB2	1:N:245:VAL:HG23	1.90	0.53
1:R:302:GLN:OE1	1:R:312:ARG:NH1	2.42	0.53
1:F:89:SER:O	1:F:270:LYS:NZ	2.42	0.53
1:G:51:LEU:HA	1:G:54:TYR:HB2	1.90	0.53
1:H:148:GLN:HA	1:H:153:ARG:HH11	1.73	0.53
1:Q:174:LEU:HG	1:Q:178:GLY:HA3	1.89	0.53
1:A:138:LEU:O	1:A:191:TYR:OH	2.19	0.53
1:F:279:ILE:HD11	1:F:287:SER:HB2	1.90	0.53
1:N:139:LEU:HD22	1:N:195:VAL:HG12	1.91	0.53
1:S:7:ARG:HG2	1:S:9:ILE:HG22	1.90	0.53
1:L:158:ASP:OD1	1:L:159:GLY:N	2.42	0.53
1:N:293:LYS:O	1:N:294:ASN:ND2	2.41	0.53
1:P:364:LEU:HG	1:P:366:THR:HG23	1.90	0.53
1:S:38:ILE:HD12	1:S:281:PHE:O	2.08	0.53
1:C:51:LEU:HB3	1:C:72:TYR:HB2	1.90	0.52
1:J:140:GLY:HA2	1:J:216:GLY:HA3	1.90	0.52
1:M:67:ILE:O	1:M:71:SER:CB	2.56	0.52
1:Q:55:VAL:O	1:Q:59:LEU:HB2	2.08	0.52
1:J:73:LEU:O	1:J:77:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:167:ILE:HG23	1:L:170:GLN:HB2	1.90	0.52
1:M:304:THR:O	1:M:308:LEU:HD13	2.09	0.52
1:Q:27:TYR:CZ	1:Q:263:LEU:HD22	2.43	0.52
1:F:140:GLY:HA2	1:F:216:GLY:HA3	1.90	0.52
1:G:302:GLN:OE1	1:G:312:ARG:NH1	2.42	0.52
1:J:80:ILE:HG23	1:J:208:HIS:HE1	1.75	0.52
1:L:138:LEU:O	1:L:191:TYR:OH	2.26	0.52
1:N:144:VAL:O	1:N:153:ARG:NH1	2.42	0.52
1:N:147:THR:HG1	1:N:152:TYR:HD2	1.56	0.52
1:A:302:GLN:OE1	1:A:312:ARG:NH1	2.43	0.52
1:L:180:ASP:N	1:L:180:ASP:OD1	2.38	0.52
1:E:89:SER:O	1:E:270:LYS:NZ	2.42	0.52
1:I:137:TYR:CZ	1:I:173:PRO:HD2	2.44	0.52
1:J:137:TYR:CZ	1:J:173:PRO:HD2	2.44	0.52
1:L:50:ASP:HB3	1:L:54:TYR:HE2	1.73	0.52
1:Q:51:LEU:HA	1:Q:54:TYR:HB2	1.91	0.52
1:D:51:LEU:HD23	1:D:54:TYR:HD2	1.75	0.52
1:G:137:TYR:CZ	1:G:173:PRO:HD2	2.45	0.52
1:R:328:THR:O	1:R:332:LEU:HB2	2.09	0.52
1:N:7:ARG:HG2	1:N:9:ILE:HG22	1.91	0.52
1:S:143:ARG:HE	1:S:155:LYS:HD3	1.74	0.52
1:B:138:LEU:O	1:B:191:TYR:OH	2.27	0.52
1:E:73:LEU:O	1:E:77:LEU:HB2	2.10	0.52
1:F:260:GLN:OE1	1:F:294:ASN:ND2	2.35	0.52
1:I:350:VAL:HG23	1:J:247:THR:HG21	1.92	0.52
1:O:104:ILE:HD11	1:O:198:VAL:HA	1.92	0.52
1:O:135:PRO:HB2	1:O:213:PHE:HE2	1.75	0.52
1:G:142:TYR:CZ	1:G:146:ARG:HD2	2.44	0.52
1:G:69:VAL:HB	1:G:138:LEU:HD13	1.92	0.52
1:M:293:LYS:O	1:M:294:ASN:ND2	2.42	0.52
1:O:223:LYS:HD3	1:O:279:ILE:HD13	1.91	0.52
1:O:66:ILE:HA	1:O:69:VAL:HG22	1.92	0.52
1:Q:43:ASN:OD1	1:Q:45:THR:OG1	2.22	0.52
1:C:89:SER:O	1:C:270:LYS:NZ	2.43	0.51
1:E:66:ILE:HD12	1:E:66:ILE:H	1.75	0.51
1:F:163:GLN:OE1	1:F:170:GLN:NE2	2.43	0.51
1:I:152:TYR:CZ	1:I:155:LYS:HE3	2.45	0.51
1:I:89:SER:O	1:I:270:LYS:NZ	2.42	0.51
1:M:242:THR:OG1	1:M:243:GLU:OE1	2.27	0.51
1:N:152:TYR:O	1:N:155:LYS:CB	2.58	0.51
1:B:364:LEU:HG	1:B:366:THR:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:THR:HG21	1:F:298:HIS:ND1	2.26	0.51
1:I:157:MET:O	1:I:160:LEU:HB2	2.09	0.51
1:I:159:GLY:O	1:I:163:GLN:NE2	2.30	0.51
1:G:153:ARG:C	1:G:155:LYS:H	2.13	0.51
1:E:7:ARG:HG2	1:E:9:ILE:HG22	1.93	0.51
1:F:319:PRO:O	1:F:324:TYR:OH	2.19	0.51
1:F:350:VAL:HG23	1:G:247:THR:HG21	1.91	0.51
1:H:419:GLU:O	1:H:422:LYS:NZ	2.40	0.51
1:J:93:ILE:HG22	1:J:95:ILE:HG23	1.92	0.51
1:M:68:HIS:HE2	1:M:119:ASP:HA	1.74	0.51
1:R:138:LEU:O	1:R:191:TYR:OH	2.25	0.51
1:T:38:ILE:HD12	1:T:281:PHE:O	2.11	0.51
1:G:156:LEU:O	1:G:159:GLY:N	2.43	0.51
1:J:147:THR:HG21	1:J:152:TYR:HE2	1.75	0.51
1:J:89:SER:O	1:J:270:LYS:NZ	2.43	0.51
1:K:87:ASP:OD1	1:K:98:ALA:N	2.44	0.51
1:N:260:GLN:OE1	1:N:294:ASN:ND2	2.43	0.51
1:Q:177:GLU:OE1	1:R:168:ASN:ND2	2.32	0.51
1:I:242:THR:O	1:I:246:THR:OG1	2.16	0.51
1:J:203:HIS:ND1	1:J:272:ASP:OD1	2.44	0.51
1:D:40:LEU:HD12	1:D:108:VAL:HG21	1.93	0.51
1:K:167:ILE:HG23	1:K:170:GLN:HB2	1.92	0.51
1:K:194:ILE:O	1:K:198:VAL:HG23	2.10	0.51
1:A:136:LEU:HD22	1:A:163:GLN:HE21	1.75	0.51
1:G:145:GLY:HA2	1:G:153:ARG:NH1	2.26	0.51
1:H:137:TYR:CZ	1:H:173:PRO:HD2	2.46	0.51
1:J:314:ARG:NH2	1:J:405:GLN:O	2.26	0.51
1:L:279:ILE:HD11	1:L:287:SER:HB2	1.91	0.51
1:O:156:LEU:O	1:O:160:LEU:HG	2.11	0.51
1:R:242:THR:OG1	1:R:243:GLU:OE1	2.29	0.51
1:R:3:VAL:HG22	1:R:4:THR:H	1.76	0.51
1:R:7:ARG:HG2	1:R:9:ILE:HG22	1.93	0.51
1:P:152:TYR:CZ	1:P:155:LYS:HE3	2.46	0.51
1:S:401:VAL:HG21	1:S:420:PHE:HB2	1.93	0.51
1:T:172:GLU:OE2	1:T:172:GLU:N	2.41	0.51
1:F:114:ASP:N	1:F:114:ASP:OD1	2.44	0.51
1:L:194:ILE:O	1:L:198:VAL:HG23	2.11	0.51
1:S:159:GLY:O	1:S:163:GLN:HG2	2.11	0.51
1:C:139:LEU:HD22	1:C:195:VAL:HG12	1.92	0.50
1:L:366:THR:O	1:L:368:ALA:N	2.44	0.50
1:M:144:VAL:O	1:M:153:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:314:ARG:HE	1:Q:404:LEU:HD22	1.76	0.50
1:S:167:ILE:HG23	1:S:170:GLN:HB2	1.92	0.50
1:S:89:SER:O	1:S:270:LYS:NZ	2.43	0.50
1:T:178:GLY:HA2	1:T:181:ILE:HG12	1.93	0.50
1:F:165:LYS:HG2	1:G:184:VAL:HG22	1.93	0.50
1:K:40:LEU:HD12	1:K:108:VAL:HG21	1.92	0.50
1:R:5:VAL:HG22	1:T:350:VAL:HG22	1.92	0.50
1:A:139:LEU:HD22	1:A:195:VAL:HG12	1.92	0.50
1:D:89:SER:O	1:D:270:LYS:NZ	2.44	0.50
1:L:133:TRP:HB2	1:L:163:GLN:HG2	1.93	0.50
1:N:54:TYR:CE1	1:N:122:SER:HB2	2.46	0.50
1:N:70:ASN:ND2	1:N:188:ASP:OD2	2.43	0.50
1:D:259:VAL:HG22	1:E:14:ILE:HD12	1.93	0.50
1:K:156:LEU:O	1:K:160:LEU:HD23	2.10	0.50
1:S:52:ARG:NH1	1:S:128:SER:HA	2.26	0.50
1:A:254:VAL:HG21	1:A:327:LEU:HD11	1.94	0.50
1:D:22:GLU:HB3	1:D:24:PRO:HD3	1.94	0.50
1:F:51:LEU:HA	1:F:54:TYR:HB2	1.92	0.50
1:J:359:ASP:N	1:J:359:ASP:OD1	2.42	0.50
1:L:184:VAL:HG22	1:M:165:LYS:HG2	1.94	0.50
1:O:328:THR:O	1:O:332:LEU:HB2	2.12	0.50
1:D:401:VAL:HG21	1:D:420:PHE:HB2	1.93	0.50
1:F:66:ILE:HD12	1:F:66:ILE:H	1.76	0.50
1:G:59:LEU:HG	1:G:174:LEU:HD11	1.94	0.50
1:J:137:TYR:HD1	1:J:163:GLN:HE22	1.60	0.50
1:L:139:LEU:HD22	1:L:195:VAL:HG12	1.94	0.50
1:T:38:ILE:HG23	1:T:108:VAL:HG12	1.93	0.50
1:D:74:TYR:O	1:D:78:LYS:N	2.44	0.50
1:I:52:ARG:NH1	1:I:131:ASP:OD2	2.44	0.50
1:F:74:TYR:O	1:F:78:LYS:N	2.44	0.49
1:I:152:TYR:CE2	1:I:155:LYS:HE3	2.47	0.49
1:J:143:ARG:HB2	1:J:216:GLY:HA2	1.94	0.49
1:P:123:ASP:OD1	1:P:124:ALA:N	2.43	0.49
1:B:114:ASP:OD1	1:B:114:ASP:N	2.43	0.49
1:A:230:THR:HG21	1:A:298:HIS:ND1	2.27	0.49
1:L:35:SER:OG	1:L:37:GLU:O	2.27	0.49
1:A:159:GLY:HA3	1:A:215:TYR:OH	2.12	0.49
1:D:175:VAL:O	1:D:177:GLU:N	2.39	0.49
1:M:302:GLN:OE1	1:M:312:ARG:NH1	2.45	0.49
1:P:242:THR:O	1:P:246:THR:OG1	2.23	0.49
1:T:126:ARG:HD2	1:T:130:ASP:OD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:89:SER:O	1:T:270:LYS:NZ	2.46	0.49
1:L:114:ASP:N	1:L:114:ASP:OD1	2.40	0.49
1:L:247:THR:HG21	1:M:350:VAL:HG23	1.95	0.49
1:M:364:LEU:HG	1:M:366:THR:HG23	1.94	0.49
1:T:42:ILE:HD13	1:T:74:TYR:HB2	1.95	0.49
1:H:51:LEU:HA	1:H:54:TYR:HB2	1.94	0.49
1:T:17:LYS:HG3	1:K:268:ILE:HD11	1.95	0.49
1:M:137:TYR:CZ	1:M:173:PRO:HD2	2.47	0.49
1:O:248:TRP:CD1	1:O:375:VAL:HG22	2.47	0.49
1:S:149:MET:O	1:S:151:GLU:N	2.45	0.49
1:B:130:ASP:HA	1:B:133:TRP:NE1	2.28	0.49
1:I:395:GLN:O	1:I:399:ARG:HG2	2.13	0.49
1:K:242:THR:O	1:K:246:THR:OG1	2.17	0.49
1:O:138:LEU:O	1:O:191:TYR:OH	2.30	0.49
1:T:143:ARG:NE	1:T:155:LYS:HE3	2.24	0.49
1:J:350:VAL:HG23	1:A:247:THR:HG21	1.95	0.49
1:G:89:SER:O	1:G:270:LYS:NZ	2.46	0.49
1:Q:88:TRP:CD2	1:Q:95:ILE:HD11	2.48	0.49
1:N:256:ASP:OD1	1:M:7:ARG:NH2	2.42	0.49
1:Q:364:LEU:HG	1:Q:366:THR:HG23	1.94	0.49
1:A:364:LEU:HG	1:A:366:THR:HG23	1.94	0.48
1:C:323:GLU:HB2	1:C:327:LEU:HD23	1.95	0.48
1:C:355:TYR:HA	1:D:376:VAL:HG13	1.94	0.48
1:D:293:LYS:O	1:D:294:ASN:ND2	2.46	0.48
1:O:302:GLN:OE1	1:O:312:ARG:NH1	2.42	0.48
1:R:285:SER:O	1:S:207:LYS:NZ	2.46	0.48
1:B:158:ASP:O	1:B:162:ASN:HB2	2.13	0.48
1:K:103:GLY:N	1:K:106:ASP:OD2	2.39	0.48
1:N:226:ALA:HB3	1:N:291:SER:HB3	1.94	0.48
1:R:376:VAL:HG13	1:S:355:TYR:HA	1.95	0.48
1:T:153:ARG:NH2	1:T:179:ARG:HB3	2.28	0.48
1:B:247:THR:HG21	1:A:350:VAL:HG23	1.95	0.48
1:D:230:THR:HG21	1:D:298:HIS:ND1	2.28	0.48
1:G:149:MET:HB3	1:G:152:TYR:HB3	1.95	0.48
1:I:194:ILE:O	1:I:198:VAL:HG23	2.14	0.48
1:R:66:ILE:HD12	1:R:66:ILE:H	1.77	0.48
1:A:51:LEU:HA	1:A:54:TYR:HB2	1.96	0.48
1:D:364:LEU:HG	1:D:366:THR:HG23	1.93	0.48
1:G:52:ARG:NH1	1:G:128:SER:HA	2.28	0.48
1:I:359:ASP:OD1	1:I:359:ASP:N	2.37	0.48
1:L:51:LEU:HA	1:L:54:TYR:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:230:THR:HG21	1:S:298:HIS:ND1	2.28	0.48
1:C:364:LEU:HG	1:C:366:THR:HG23	1.96	0.48
1:E:137:TYR:CZ	1:E:173:PRO:HD2	2.48	0.48
1:O:137:TYR:CZ	1:O:173:PRO:HD2	2.49	0.48
1:A:70:ASN:ND2	1:A:188:ASP:OD2	2.43	0.48
1:D:194:ILE:O	1:D:198:VAL:HG23	2.13	0.48
1:F:178:GLY:HA2	1:F:181:ILE:HG12	1.96	0.48
1:I:319:PRO:O	1:I:324:TYR:OH	2.24	0.48
1:K:147:THR:OG1	1:K:155:LYS:NZ	2.46	0.48
1:Q:70:ASN:ND2	1:Q:188:ASP:OD2	2.41	0.48
1:S:421:ASP:O	1:S:422:LYS:HD3	2.13	0.48
1:D:344:LEU:HD11	1:E:329:THR:HG22	1.96	0.48
1:L:158:ASP:O	1:L:162:ASN:HB2	2.14	0.48
1:L:362:GLY:O	1:L:364:LEU:N	2.47	0.48
1:D:60:LYS:HA	1:D:173:PRO:O	2.14	0.48
1:F:158:ASP:HB3	1:F:215:TYR:OH	2.13	0.48
1:H:347:GLN:OE1	1:I:252:ARG:NH2	2.47	0.48
1:E:52:ARG:NH1	1:E:128:SER:HA	2.29	0.48
1:G:230:THR:HG21	1:G:298:HIS:ND1	2.29	0.48
1:I:399:ARG:HE	1:J:422:LYS:HZ2	1.62	0.48
1:T:114:ASP:OD1	1:T:114:ASP:N	2.45	0.48
1:L:159:GLY:HA2	1:L:163:GLN:H	1.79	0.47
1:R:158:ASP:OD1	1:R:159:GLY:N	2.44	0.47
1:A:137:TYR:HD1	1:A:163:GLN:OE1	1.98	0.47
1:A:199:ASP:OD1	1:A:277:TYR:OH	2.20	0.47
1:B:14:ILE:HG23	1:B:16:PRO:HD3	1.97	0.47
1:G:139:LEU:HD22	1:G:195:VAL:HG12	1.97	0.47
1:H:141:LEU:HD12	1:H:182:PHE:CZ	2.49	0.47
1:K:152:TYR:C	1:K:154:LYS:H	2.18	0.47
1:K:278:LEU:HA	1:K:283:LEU:HD12	1.97	0.47
1:N:80:ILE:HD11	1:N:208:HIS:HE2	1.79	0.47
1:N:86:LYS:HG3	1:N:87:ASP:H	1.78	0.47
1:O:144:VAL:HG22	1:O:155:LYS:HB3	1.95	0.47
1:P:143:ARG:HB3	1:P:216:GLY:HA2	1.96	0.47
1:R:381:TRP:O	1:R:385:GLN:HG2	2.14	0.47
1:R:419:GLU:OE2	1:S:309:ARG:NE	2.39	0.47
1:E:192:THR:HA	1:E:195:VAL:HG22	1.96	0.47
1:G:51:LEU:HB3	1:G:72:TYR:HB2	1.96	0.47
1:G:7:ARG:HG2	1:G:9:ILE:HG22	1.96	0.47
1:K:7:ARG:HG2	1:K:9:ILE:HG22	1.97	0.47
1:O:74:TYR:O	1:O:78:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:7:ARG:HG2	1:P:9:ILE:HG22	1.97	0.47
1:A:114:ASP:OD1	1:A:114:ASP:N	2.46	0.47
1:B:137:TYR:O	1:B:141:LEU:HG	2.14	0.47
1:C:248:TRP:CD1	1:C:375:VAL:HG22	2.49	0.47
1:J:126:ARG:NE	1:J:130:ASP:OD2	2.41	0.47
1:L:86:LYS:HA	1:L:86:LYS:HD3	1.63	0.47
1:O:42:ILE:HD13	1:O:74:TYR:HB2	1.96	0.47
1:P:278:LEU:HD12	1:P:284:SER:HB3	1.95	0.47
1:Q:42:ILE:HD13	1:Q:74:TYR:HB2	1.96	0.47
1:D:267:GLU:OE1	1:D:273:SER:OG	2.29	0.47
1:E:355:TYR:HA	1:F:376:VAL:HG13	1.97	0.47
1:F:66:ILE:HA	1:F:69:VAL:HG22	1.97	0.47
1:M:288:PRO:HG2	1:M:289:TYR:CE2	2.50	0.47
1:P:74:TYR:O	1:P:78:LYS:HG3	2.15	0.47
1:S:127:THR:HG22	1:S:128:SER:H	1.78	0.47
1:C:160:LEU:HD11	1:C:172:GLU:HB3	1.95	0.47
1:D:66:ILE:H	1:D:66:ILE:HD12	1.80	0.47
1:E:194:ILE:O	1:E:198:VAL:HG23	2.14	0.47
1:F:223:LYS:NZ	1:F:280:ASP:OD1	2.45	0.47
1:G:350:VAL:HG22	1:I:5:VAL:HG22	1.97	0.47
1:J:88:TRP:CD1	1:J:95:ILE:HG13	2.50	0.47
1:L:104:ILE:HG23	1:L:105:PHE:CD2	2.50	0.47
1:Q:66:ILE:HD12	1:Q:66:ILE:H	1.79	0.47
1:R:114:ASP:N	1:R:114:ASP:OD1	2.45	0.47
1:T:66:ILE:HA	1:T:69:VAL:HG22	1.96	0.47
1:G:77:LEU:HD13	1:G:104:ILE:HD13	1.97	0.47
1:H:194:ILE:O	1:H:198:VAL:HG23	2.15	0.47
1:T:247:THR:HG21	1:K:350:VAL:HG23	1.97	0.47
1:M:156:LEU:O	1:M:160:LEU:HG	2.14	0.47
1:S:135:PRO:O	1:S:139:LEU:HG	2.15	0.47
1:G:70:ASN:ND2	1:G:188:ASP:OD2	2.48	0.47
1:L:88:TRP:CD2	1:L:95:ILE:HD11	2.50	0.47
1:O:52:ARG:NH1	1:O:128:SER:HA	2.30	0.47
1:P:87:ASP:OD2	1:P:97:LYS:HG3	2.15	0.47
1:R:159:GLY:HA2	1:R:163:GLN:H	1.79	0.47
1:S:136:LEU:HB3	1:S:163:GLN:HE22	1.79	0.47
1:F:158:ASP:OD1	1:F:162:ASN:ND2	2.48	0.47
1:I:126:ARG:NE	1:I:130:ASP:OD2	2.46	0.47
1:O:298:HIS:O	1:O:302:GLN:HB2	2.15	0.47
1:O:319:PRO:O	1:O:324:TYR:OH	2.21	0.47
1:O:86:LYS:HD3	1:O:86:LYS:HA	1.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:319:PRO:O	1:S:324:TYR:OH	2.20	0.47
1:A:38:ILE:HD12	1:A:281:PHE:O	2.15	0.46
1:I:199:ASP:OD1	1:I:214:ARG:NE	2.40	0.46
1:M:269:ASP:OD1	1:M:269:ASP:N	2.48	0.46
1:M:7:ARG:HG2	1:M:9:ILE:HG22	1.96	0.46
1:P:66:ILE:HA	1:P:69:VAL:HG22	1.97	0.46
1:R:277:TYR:O	1:R:281:PHE:HB2	2.15	0.46
1:T:202:PHE:HE1	1:T:208:HIS:HD1	1.63	0.46
1:H:350:VAL:HG23	1:I:247:THR:HG21	1.97	0.46
1:K:228:LEU:HB2	1:K:289:TYR:HB3	1.97	0.46
1:N:319:PRO:O	1:N:324:TYR:OH	2.23	0.46
1:O:242:THR:O	1:O:246:THR:OG1	2.24	0.46
1:S:130:ASP:HA	1:S:133:TRP:NE1	2.30	0.46
1:T:40:LEU:HD12	1:T:108:VAL:HG21	1.97	0.46
1:T:105:PHE:HB3	1:T:110:LEU:HD21	1.97	0.46
1:J:165:LYS:NZ	1:A:184:VAL:O	2.47	0.46
1:D:350:VAL:HG23	1:E:247:THR:HG21	1.97	0.46
1:Q:167:ILE:HG23	1:Q:170:GLN:HB2	1.96	0.46
1:A:226:ALA:HB3	1:A:291:SER:HB3	1.98	0.46
1:B:226:ALA:O	1:B:230:THR:HG23	2.15	0.46
1:G:35:SER:OG	1:G:37:GLU:O	2.29	0.46
1:L:50:ASP:HB3	1:L:54:TYR:CE2	2.51	0.46
1:M:194:ILE:O	1:M:198:VAL:HG23	2.16	0.46
1:P:140:GLY:HA2	1:P:216:GLY:HA3	1.97	0.46
1:R:7:ARG:NH2	1:S:256:ASP:OD1	2.44	0.46
1:T:54:TYR:CE1	1:T:122:SER:HB2	2.51	0.46
1:D:226:ALA:HB3	1:D:291:SER:HB3	1.98	0.46
1:F:364:LEU:HG	1:F:366:THR:HG23	1.98	0.46
1:H:85:ASP:OD1	1:H:85:ASP:N	2.41	0.46
1:N:153:ARG:O	1:N:156:LEU:HB3	2.16	0.46
1:O:119:ASP:OD1	1:O:119:ASP:N	2.49	0.46
1:O:158:ASP:HB3	1:O:215:TYR:OH	2.14	0.46
1:Q:247:THR:HG21	1:R:350:VAL:HG23	1.98	0.46
1:T:298:HIS:O	1:T:302:GLN:HB2	2.15	0.46
1:C:82:GLY:O	1:C:101:THR:HA	2.16	0.46
1:B:165:LYS:HD2	1:C:184:VAL:HG13	1.96	0.46
1:G:254:VAL:HG21	1:G:327:LEU:HD11	1.97	0.46
1:G:66:ILE:H	1:G:66:ILE:HD12	1.79	0.46
1:I:143:ARG:HE	1:I:155:LYS:HE2	1.81	0.46
1:J:194:ILE:O	1:J:198:VAL:HG23	2.16	0.46
1:N:143:ARG:CB	1:N:216:GLY:HA2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:51:LEU:HA	1:O:54:TYR:HB2	1.98	0.46
1:Q:192:THR:HA	1:Q:195:VAL:HG22	1.96	0.46
1:B:80:ILE:HA	1:B:103:GLY:HA2	1.97	0.46
1:C:66:ILE:HA	1:C:69:VAL:HG22	1.98	0.46
1:I:52:ARG:NH1	1:I:128:SER:HA	2.31	0.46
1:L:404:LEU:HB3	1:L:407:LEU:HD21	1.97	0.46
1:H:226:ALA:O	1:H:230:THR:HG23	2.16	0.46
1:K:178:GLY:HA2	1:K:181:ILE:HG12	1.97	0.46
1:K:27:TYR:CZ	1:K:263:LEU:HD22	2.51	0.46
1:Q:38:ILE:HG23	1:Q:108:VAL:HG12	1.97	0.46
1:S:408:ARG:O	1:S:411:THR:OG1	2.24	0.46
1:E:181:ILE:O	1:E:185:TRP:NE1	2.48	0.46
1:G:114:ASP:OD1	1:G:114:ASP:N	2.49	0.46
1:G:355:TYR:HA	1:H:376:VAL:HG13	1.98	0.46
1:J:143:ARG:CB	1:J:216:GLY:HA2	2.46	0.46
1:M:67:ILE:HD12	1:M:67:ILE:H	1.80	0.46
1:Q:147:THR:HG21	1:Q:152:TYR:CE2	2.51	0.46
1:S:194:ILE:O	1:S:198:VAL:HG23	2.16	0.46
1:A:136:LEU:HD22	1:A:163:GLN:NE2	2.30	0.46
1:F:328:THR:O	1:F:332:LEU:HB2	2.16	0.46
1:J:66:ILE:HA	1:J:69:VAL:HG22	1.97	0.46
1:P:230:THR:HG21	1:P:298:HIS:ND1	2.31	0.46
1:F:293:LYS:O	1:F:294:ASN:ND2	2.49	0.45
1:G:88:TRP:CD2	1:G:95:ILE:HD11	2.52	0.45
1:H:125:SER:O	1:H:127:THR:OG1	2.34	0.45
1:H:27:TYR:CZ	1:H:263:LEU:HD22	2.51	0.45
1:O:141:LEU:HB3	1:O:182:PHE:CG	2.51	0.45
1:S:267:GLU:OE1	1:S:273:SER:OG	2.26	0.45
1:T:194:ILE:O	1:T:198:VAL:HG23	2.16	0.45
1:T:59:LEU:HD23	1:T:173:PRO:HG2	1.99	0.45
1:C:293:LYS:O	1:C:294:ASN:ND2	2.48	0.45
1:N:66:ILE:HD12	1:N:66:ILE:H	1.81	0.45
1:T:78:LYS:NZ	1:T:79:ASP:OD1	2.40	0.45
1:A:157:MET:CG	1:A:179:ARG:HH12	2.29	0.45
1:E:386:ASN:O	1:E:387:ARG:HG2	2.16	0.45
1:J:407:LEU:HD13	1:J:414:LYS:HA	1.97	0.45
1:L:88:TRP:O	1:L:95:ILE:HG12	2.17	0.45
1:N:194:ILE:O	1:N:198:VAL:HG23	2.15	0.45
1:P:401:VAL:HG21	1:P:420:PHE:HB2	1.99	0.45
1:P:70:ASN:ND2	1:P:188:ASP:OD2	2.49	0.45
1:S:422:LYS:HD2	1:S:422:LYS:HA	1.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:LEU:HB3	1:A:163:GLN:HE21	1.81	0.45
1:C:52:ARG:NH1	1:C:128:SER:HA	2.31	0.45
1:D:55:VAL:O	1:D:59:LEU:HB2	2.16	0.45
1:J:242:THR:O	1:J:246:THR:OG1	2.28	0.45
1:J:328:THR:HG21	1:J:415:TYR:HE2	1.81	0.45
1:K:124:ALA:O	1:K:125:SER:OG	2.28	0.45
1:L:8:ILE:HB	1:N:354:LYS:HD3	1.98	0.45
1:M:147:THR:HG21	1:M:152:TYR:CD2	2.51	0.45
1:P:143:ARG:HD2	1:P:219:VAL:HG13	1.98	0.45
1:P:55:VAL:O	1:P:59:LEU:HG	2.16	0.45
1:R:247:THR:HG21	1:S:350:VAL:HG23	1.98	0.45
1:H:86:LYS:HA	1:H:86:LYS:HD3	1.80	0.45
1:N:27:TYR:CZ	1:N:263:LEU:HD22	2.52	0.45
1:Q:126:ARG:HD3	1:Q:126:ARG:HA	1.68	0.45
1:R:40:LEU:HD12	1:R:108:VAL:HG21	1.97	0.45
1:S:143:ARG:HB2	1:S:216:GLY:HA2	1.99	0.45
1:G:194:ILE:O	1:G:198:VAL:HG23	2.16	0.45
1:N:149:MET:O	1:N:153:ARG:HG2	2.17	0.45
1:N:51:LEU:HA	1:N:54:TYR:HB2	1.99	0.45
1:T:104:ILE:HD11	1:T:198:VAL:HG22	1.99	0.45
1:D:165:LYS:HD2	1:E:184:VAL:HG13	1.98	0.45
1:E:83:LYS:HA	1:E:101:THR:HA	1.98	0.45
1:F:53:GLY:HA3	1:F:123:ASP:HB3	1.97	0.45
1:F:151:GLU:HG3	1:F:154:LYS:HB2	1.98	0.45
1:I:146:ARG:HH22	1:I:223:LYS:HE3	1.80	0.45
1:I:60:LYS:HA	1:I:60:LYS:HD2	1.69	0.45
1:P:320:ASP:OD1	1:P:410:LYS:NZ	2.48	0.45
1:R:270:LYS:HE2	1:R:270:LYS:HB3	1.81	0.45
1:S:279:ILE:HD11	1:S:287:SER:HB2	1.99	0.45
1:C:226:ALA:O	1:C:230:THR:HG23	2.17	0.45
1:F:267:GLU:OE1	1:F:273:SER:OG	2.28	0.45
1:F:302:GLN:HB3	1:F:412:ILE:HD13	1.98	0.45
1:H:256:ASP:OD1	1:I:7:ARG:NH2	2.46	0.45
1:L:302:GLN:HB3	1:L:412:ILE:HD13	1.97	0.45
1:A:174:LEU:HD21	1:A:178:GLY:HA3	1.98	0.45
1:C:350:VAL:HG23	1:D:247:THR:HG21	1.99	0.45
1:G:206:LYS:HD2	1:G:206:LYS:HA	1.78	0.45
1:I:160:LEU:HD21	1:I:172:GLU:HB3	1.98	0.45
1:M:139:LEU:HD22	1:M:195:VAL:HG12	1.98	0.45
1:L:376:VAL:HG13	1:M:355:TYR:HA	1.99	0.45
1:O:147:THR:HG21	1:O:152:TYR:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:87:ASP:OD2	1:O:97:LYS:HG3	2.17	0.45
1:Q:194:ILE:O	1:Q:198:VAL:HG23	2.17	0.45
1:R:194:ILE:O	1:R:198:VAL:HG23	2.17	0.45
1:R:104:ILE:HG23	1:R:105:PHE:CD2	2.52	0.45
1:B:38:ILE:HD12	1:B:281:PHE:O	2.18	0.44
1:D:137:TYR:CZ	1:D:173:PRO:HD2	2.51	0.44
1:G:140:GLY:HA2	1:G:216:GLY:HA3	1.99	0.44
1:G:387:ARG:HB2	1:G:387:ARG:NH2	2.33	0.44
1:T:279:ILE:HD11	1:T:287:SER:HB2	1.98	0.44
1:F:176:PRO:O	1:F:179:ARG:HG2	2.17	0.44
1:H:230:THR:HG22	1:H:312:ARG:HH12	1.82	0.44
1:L:159:GLY:CA	1:L:163:GLN:H	2.30	0.44
1:M:147:THR:HG21	1:M:152:TYR:CE2	2.52	0.44
1:N:172:GLU:N	1:N:172:GLU:OE2	2.34	0.44
1:N:38:ILE:HD12	1:N:281:PHE:O	2.17	0.44
1:P:137:TYR:O	1:P:141:LEU:HD13	2.17	0.44
1:P:355:TYR:HA	1:O:376:VAL:HG13	1.99	0.44
1:P:77:LEU:C	1:P:80:ILE:HD11	2.37	0.44
1:Q:7:ARG:NH2	1:R:256:ASP:OD1	2.47	0.44
1:S:376:VAL:HG13	1:T:355:TYR:HA	1.99	0.44
1:B:88:TRP:CD2	1:B:95:ILE:HD11	2.51	0.44
1:O:223:LYS:HB3	1:O:279:ILE:HD11	1.99	0.44
1:P:313:ALA:HB1	1:P:412:ILE:HD11	1.98	0.44
1:S:51:LEU:HD23	1:S:54:TYR:HD2	1.81	0.44
1:E:77:LEU:HD12	1:E:80:ILE:HD11	2.00	0.44
1:F:160:LEU:HD11	1:F:172:GLU:HB3	1.99	0.44
1:G:195:VAL:HB	1:G:217:THR:HG22	2.00	0.44
1:H:84:LEU:HD23	1:H:205:PHE:HZ	1.82	0.44
1:H:381:TRP:O	1:H:385:GLN:HG2	2.18	0.44
1:I:155:LYS:O	1:I:158:ASP:HB3	2.17	0.44
1:J:214:ARG:HH21	1:J:218:ILE:HG13	1.82	0.44
1:K:148:GLN:OE1	1:K:148:GLN:N	2.49	0.44
1:L:80:ILE:HD11	1:L:104:ILE:HB	1.99	0.44
1:N:180:ASP:HA	1:N:183:ASP:HB2	2.00	0.44
1:N:45:THR:OG1	1:N:46:LYS:N	2.51	0.44
1:P:302:GLN:HB3	1:P:412:ILE:HD13	1.99	0.44
1:Q:381:TRP:O	1:Q:385:GLN:HG2	2.16	0.44
1:S:82:GLY:O	1:S:101:THR:HA	2.17	0.44
1:T:230:THR:HG21	1:T:298:HIS:ND1	2.33	0.44
1:D:88:TRP:CD2	1:D:95:ILE:HD11	2.53	0.44
1:E:324:TYR:O	1:E:328:THR:OG1	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:THR:HG21	1:G:152:TYR:HE2	1.82	0.44
1:A:147:THR:OG1	1:A:153:ARG:HG2	2.18	0.44
1:D:51:LEU:HB3	1:D:72:TYR:HB2	1.99	0.44
1:G:244:ASP:O	1:G:247:THR:OG1	2.33	0.44
1:H:138:LEU:O	1:H:191:TYR:OH	2.31	0.44
1:M:96:GLY:HA3	1:M:102:ILE:HD11	2.00	0.44
1:O:97:LYS:HE3	1:O:97:LYS:HB2	1.85	0.44
1:P:126:ARG:HD3	1:P:126:ARG:HA	1.68	0.44
1:R:226:ALA:O	1:R:230:THR:HG23	2.18	0.44
1:R:203:HIS:ND1	1:R:272:ASP:OD1	2.48	0.44
1:T:302:GLN:HB3	1:T:412:ILE:HD13	2.00	0.44
1:T:66:ILE:HD12	1:T:66:ILE:H	1.82	0.44
1:B:270:LYS:HE2	1:B:270:LYS:HB3	1.86	0.44
1:H:42:ILE:HD11	1:H:71:SER:N	2.33	0.44
1:M:243:GLU:N	1:M:243:GLU:OE1	2.50	0.44
1:E:59:LEU:HB3	1:E:173:PRO:O	2.17	0.44
1:G:27:TYR:CZ	1:G:263:LEU:HD22	2.52	0.44
1:J:104:ILE:HG23	1:J:105:PHE:CD2	2.53	0.44
1:J:122:SER:OG	1:J:123:ASP:N	2.50	0.44
1:J:177:GLU:O	1:J:179:ARG:N	2.50	0.44
1:T:51:LEU:HB3	1:T:72:TYR:HB2	2.00	0.44
1:B:154:LYS:HE3	1:B:157:MET:HG3	1.99	0.44
1:C:133:TRP:HB3	1:C:166:MET:HG3	1.98	0.44
1:C:381:TRP:O	1:C:385:GLN:HG2	2.18	0.44
1:D:257:GLU:O	1:D:261:MET:HG3	2.18	0.44
1:J:153:ARG:HE	1:J:179:ARG:HD2	1.83	0.44
1:M:143:ARG:HB2	1:M:216:GLY:HA2	1.99	0.44
1:N:52:ARG:NH1	1:N:128:SER:HA	2.33	0.44
1:N:355:TYR:HA	1:M:376:VAL:HG13	2.00	0.44
1:K:114:ASP:N	1:K:114:ASP:OD1	2.50	0.43
1:K:401:VAL:HG21	1:K:420:PHE:HB2	2.00	0.43
1:L:52:ARG:NH1	1:L:128:SER:HA	2.33	0.43
1:O:194:ILE:O	1:O:198:VAL:HG23	2.17	0.43
1:O:324:TYR:O	1:O:328:THR:HG23	2.18	0.43
1:R:142:TYR:O	1:R:146:ARG:HG3	2.18	0.43
1:S:124:ALA:C	1:S:126:ARG:H	2.21	0.43
1:C:227:ALA:HB1	1:C:261:MET:HE1	2.00	0.43
1:N:336:TYR:CG	1:N:393:MET:HG2	2.53	0.43
1:P:165:LYS:HA	1:O:184:VAL:HG21	2.00	0.43
1:P:269:ASP:OD1	1:P:269:ASP:N	2.50	0.43
1:Q:142:TYR:O	1:Q:146:ARG:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:87:ASP:OD1	1:R:98:ALA:N	2.51	0.43
1:A:117:LEU:HA	1:A:118:PRO:HD3	1.89	0.43
1:C:194:ILE:O	1:C:198:VAL:HG23	2.18	0.43
1:D:143:ARG:HB2	1:D:216:GLY:HA2	2.00	0.43
1:D:302:GLN:OE1	1:D:312:ARG:NH1	2.50	0.43
1:G:248:TRP:CE2	1:G:375:VAL:HG22	2.53	0.43
1:J:303:LEU:HD22	1:J:328:THR:HG22	1.99	0.43
1:S:302:GLN:OE1	1:S:312:ARG:NH1	2.51	0.43
1:T:52:ARG:NH1	1:T:128:SER:HA	2.33	0.43
1:T:177:GLU:HG2	1:T:177:GLU:O	2.18	0.43
1:B:21:ASN:N	1:B:21:ASN:OD1	2.52	0.43
1:E:143:ARG:CB	1:E:216:GLY:HA2	2.49	0.43
1:H:57:GLN:OE1	1:H:122:SER:N	2.50	0.43
1:K:126:ARG:HA	1:K:126:ARG:HD3	1.74	0.43
1:K:308:LEU:O	1:K:310:SER:N	2.50	0.43
1:L:155:LYS:HA	1:L:155:LYS:HD3	1.91	0.43
1:S:211:ALA:O	1:S:214:ARG:HG2	2.18	0.43
1:S:226:ALA:O	1:S:230:THR:HG23	2.18	0.43
1:A:123:ASP:OD1	1:A:124:ALA:N	2.52	0.43
1:A:27:TYR:CZ	1:A:263:LEU:HD22	2.53	0.43
1:C:66:ILE:HD12	1:C:66:ILE:H	1.83	0.43
1:C:88:TRP:CE2	1:C:95:ILE:HD11	2.53	0.43
1:F:359:ASP:N	1:F:359:ASP:OD1	2.49	0.43
1:K:86:LYS:HD3	1:K:86:LYS:HA	1.80	0.43
1:Q:277:TYR:O	1:Q:281:PHE:HB2	2.19	0.43
1:S:160:LEU:HD11	1:S:172:GLU:HB3	2.01	0.43
1:T:173:PRO:O	1:T:174:LEU:HD22	2.19	0.43
1:B:87:ASP:OD1	1:B:98:ALA:N	2.52	0.43
1:B:309:ARG:HB2	1:C:324:TYR:HB2	2.01	0.43
1:D:158:ASP:OD1	1:D:159:GLY:N	2.51	0.43
1:F:194:ILE:O	1:F:198:VAL:HG23	2.18	0.43
1:H:52:ARG:NH1	1:H:128:SER:HA	2.33	0.43
1:L:159:GLY:HA3	1:L:163:GLN:CD	2.38	0.43
1:L:143:ARG:HG3	1:L:219:VAL:HG11	1.99	0.43
1:P:39:PRO:O	1:P:193:LYS:NZ	2.51	0.43
1:A:164:CYS:HB3	1:A:170:GLN:HB3	2.00	0.43
1:C:126:ARG:NE	1:C:130:ASP:OD2	2.42	0.43
1:E:401:VAL:HG21	1:E:420:PHE:HB2	2.00	0.43
1:F:336:TYR:CG	1:F:393:MET:HG2	2.53	0.43
1:F:408:ARG:O	1:F:411:THR:OG1	2.28	0.43
1:G:158:ASP:O	1:G:162:ASN:CB	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:359:ASP:OD1	1:H:359:ASP:N	2.49	0.43
1:K:260:GLN:OE1	1:K:294:ASN:ND2	2.48	0.43
1:S:137:TYR:O	1:S:141:LEU:HD13	2.18	0.43
1:T:158:ASP:HB2	1:T:215:TYR:OH	2.18	0.43
1:T:140:GLY:HA2	1:T:216:GLY:HA3	2.01	0.43
1:A:104:ILE:HG23	1:A:105:PHE:CD2	2.54	0.43
1:C:308:LEU:HD11	1:C:335:ALA:HA	2.00	0.43
1:H:55:VAL:HG23	1:H:134:LEU:HD21	2.01	0.43
1:I:364:LEU:HG	1:I:366:THR:HG23	2.00	0.43
1:N:263:LEU:HA	1:N:264:PRO:HD3	1.86	0.43
1:P:293:LYS:O	1:P:294:ASN:ND2	2.52	0.43
1:T:126:ARG:HD3	1:T:126:ARG:HA	1.69	0.43
1:K:224:ASP:HB2	1:K:279:ILE:HG13	2.01	0.43
1:P:23:ASP:N	1:P:24:PRO:HD3	2.34	0.43
1:R:179:ARG:HA	1:R:182:PHE:CZ	2.54	0.43
1:A:80:ILE:O	1:A:81:ARG:NH1	2.44	0.43
1:C:278:LEU:HD12	1:C:284:SER:HB3	2.00	0.43
1:C:324:TYR:O	1:C:328:THR:OG1	2.24	0.43
1:F:139:LEU:HD22	1:F:195:VAL:HG12	2.01	0.43
1:H:172:GLU:N	1:H:172:GLU:OE2	2.31	0.43
1:J:328:THR:HG21	1:J:415:TYR:CE2	2.54	0.43
1:K:143:ARG:CB	1:K:216:GLY:HA2	2.47	0.43
1:K:83:LYS:HB3	1:K:83:LYS:HE2	1.79	0.43
1:M:21:ASN:OD1	1:M:21:ASN:N	2.52	0.43
1:O:230:THR:HG21	1:O:298:HIS:ND1	2.34	0.43
1:O:42:ILE:HG22	1:O:44:THR:HG23	2.00	0.43
1:B:158:ASP:HB3	1:B:215:TYR:OH	2.19	0.42
1:E:72:TYR:OH	1:E:131:ASP:OD1	2.29	0.42
1:F:147:THR:HG21	1:F:152:TYR:HE2	1.84	0.42
1:K:164:CYS:HA	1:K:167:ILE:O	2.18	0.42
1:L:336:TYR:OH	1:L:392:ASP:OD2	2.21	0.42
1:L:43:ASN:ND2	1:L:117:LEU:HD11	2.34	0.42
1:M:226:ALA:O	1:M:230:THR:HG23	2.19	0.42
1:N:143:ARG:HH11	1:N:216:GLY:H	1.67	0.42
1:R:184:VAL:HG13	1:S:165:LYS:HD2	2.00	0.42
1:T:328:THR:O	1:T:332:LEU:HB2	2.19	0.42
1:B:227:ALA:HB1	1:B:261:MET:HE1	2.00	0.42
1:E:241:SER:OG	1:E:243:GLU:HG2	2.19	0.42
1:O:223:LYS:HD3	1:O:279:ILE:CD1	2.49	0.42
1:B:89:SER:O	1:B:270:LYS:NZ	2.52	0.42
1:C:167:ILE:HG22	1:C:169:GLU:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:GLY:HA2	1:C:216:GLY:HA3	2.01	0.42
1:J:226:ALA:O	1:J:230:THR:HG23	2.19	0.42
1:K:130:ASP:O	1:K:134:LEU:HB2	2.19	0.42
1:N:202:PHE:HB2	1:N:214:ARG:HG3	2.01	0.42
1:N:51:LEU:HD23	1:N:54:TYR:HD2	1.84	0.42
1:R:162:ASN:HA	1:R:165:LYS:HD3	2.01	0.42
1:B:324:TYR:O	1:B:328:THR:OG1	2.22	0.42
1:C:137:TYR:CZ	1:C:173:PRO:HD2	2.54	0.42
1:C:74:TYR:O	1:C:78:LYS:N	2.52	0.42
1:D:88:TRP:CE2	1:D:95:ILE:HD11	2.54	0.42
1:L:304:THR:HG21	1:L:334:TYR:CD2	2.55	0.42
1:O:381:TRP:O	1:O:385:GLN:HG2	2.19	0.42
1:Q:66:ILE:HA	1:Q:69:VAL:HG22	2.01	0.42
1:I:354:LYS:HD3	1:A:8:ILE:HB	2.00	0.42
1:D:398:LYS:HG3	1:D:421:ASP:HA	2.01	0.42
1:F:172:GLU:N	1:F:172:GLU:OE2	2.27	0.42
1:F:244:ASP:O	1:F:247:THR:OG1	2.34	0.42
1:I:141:LEU:HD12	1:I:182:PHE:CE2	2.54	0.42
1:K:230:THR:HG21	1:K:298:HIS:ND1	2.35	0.42
1:R:309:ARG:HD2	1:R:309:ARG:N	2.34	0.42
1:S:263:LEU:HA	1:S:264:PRO:HD3	1.90	0.42
1:E:135:PRO:O	1:E:139:LEU:HG	2.20	0.42
1:F:242:THR:O	1:F:246:THR:OG1	2.29	0.42
1:F:381:TRP:O	1:F:385:GLN:HG2	2.20	0.42
1:H:248:TRP:CD1	1:H:375:VAL:HG22	2.54	0.42
1:B:194:ILE:O	1:B:198:VAL:HG23	2.19	0.42
1:B:298:HIS:O	1:B:302:GLN:HB2	2.20	0.42
1:I:52:ARG:HD2	1:I:130:ASP:HB2	2.01	0.42
1:R:159:GLY:CA	1:R:163:GLN:HB2	2.50	0.42
1:R:142:TYR:HB2	1:R:191:TYR:CE2	2.55	0.42
1:C:38:ILE:HD11	1:C:281:PHE:O	2.19	0.42
1:F:52:ARG:NH1	1:F:128:SER:HA	2.35	0.42
1:N:226:ALA:O	1:N:230:THR:HG23	2.20	0.42
1:N:242:THR:O	1:N:246:THR:OG1	2.25	0.42
1:P:359:ASP:N	1:P:359:ASP:OD1	2.49	0.42
1:T:143:ARG:HG3	1:T:219:VAL:HG11	2.02	0.42
1:B:56:TYR:O	1:B:60:LYS:HG2	2.20	0.42
1:H:141:LEU:HD12	1:H:182:PHE:CE2	2.54	0.42
1:O:404:LEU:HD23	1:O:404:LEU:HA	1.96	0.42
1:P:84:LEU:HD11	1:P:96:GLY:HA3	2.02	0.42
1:Q:230:THR:HG21	1:Q:298:HIS:ND1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:142:TYR:O	1:T:146:ARG:HG3	2.20	0.42
1:B:51:LEU:HB3	1:B:72:TYR:HB2	2.02	0.42
1:F:401:VAL:HG21	1:F:420:PHE:HB2	2.00	0.42
1:H:88:TRP:CD2	1:H:95:ILE:HD11	2.55	0.42
1:I:145:GLY:HA2	1:I:179:ARG:NH2	2.35	0.42
1:K:181:ILE:HD13	1:K:181:ILE:HA	1.90	0.42
1:M:104:ILE:HA	1:M:201:PHE:CD1	2.54	0.42
1:M:172:GLU:CD	1:M:172:GLU:H	2.22	0.42
1:M:278:LEU:HD12	1:M:284:SER:HB3	2.01	0.42
1:O:135:PRO:HB2	1:O:213:PHE:CE2	2.55	0.42
1:O:257:GLU:O	1:O:261:MET:HG3	2.19	0.42
1:P:153:ARG:HA	1:P:153:ARG:HD2	1.75	0.42
1:P:42:ILE:HD12	1:P:42:ILE:HA	1.88	0.42
1:R:97:LYS:HB2	1:R:97:LYS:HE3	1.81	0.42
1:A:65:SER:OG	1:A:118:PRO:HG2	2.19	0.41
1:A:88:TRP:CE2	1:A:95:ILE:HD11	2.55	0.41
1:F:277:TYR:O	1:F:281:PHE:HB2	2.20	0.41
1:G:268:ILE:HD11	1:H:17:LYS:HG3	2.01	0.41
1:I:70:ASN:ND2	1:I:188:ASP:OD2	2.39	0.41
1:J:52:ARG:NH1	1:J:128:SER:HA	2.35	0.41
1:K:287:SER:HA	1:K:288:PRO:HD3	1.93	0.41
1:L:175:VAL:HG23	1:L:178:GLY:HA3	2.01	0.41
1:E:350:VAL:HG23	1:F:247:THR:HG21	2.02	0.41
1:G:125:SER:O	1:G:126:ARG:NE	2.52	0.41
1:I:18:LEU:HA	1:I:18:LEU:HD23	1.93	0.41
1:J:228:LEU:HB2	1:J:289:TYR:HB3	2.02	0.41
1:O:140:GLY:HA2	1:O:216:GLY:HA3	2.02	0.41
1:P:135:PRO:O	1:P:139:LEU:HG	2.20	0.41
1:Q:148:GLN:OE1	1:Q:153:ARG:NH1	2.54	0.41
1:Q:52:ARG:NH1	1:Q:128:SER:HA	2.35	0.41
1:A:387:ARG:HB2	1:A:387:ARG:NH2	2.35	0.41
1:B:135:PRO:HB2	1:B:213:PHE:HE2	1.86	0.41
1:D:62:GLY:HA2	1:D:181:ILE:HD11	2.00	0.41
1:E:146:ARG:NH2	1:E:223:LYS:HE2	2.35	0.41
1:E:228:LEU:HB2	1:E:289:TYR:HB3	2.02	0.41
1:F:77:LEU:O	1:F:80:ILE:HG22	2.21	0.41
1:I:104:ILE:HG23	1:I:105:PHE:CD2	2.55	0.41
1:I:304:THR:HG21	1:I:334:TYR:CD2	2.55	0.41
1:I:66:ILE:H	1:I:66:ILE:HD12	1.85	0.41
1:M:39:PRO:O	1:M:193:LYS:NZ	2.34	0.41
1:T:137:TYR:CZ	1:T:173:PRO:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LYS:HE2	1:A:165:LYS:HB3	1.82	0.41
1:A:270:LYS:HB3	1:A:270:LYS:HE2	1.90	0.41
1:C:104:ILE:HG23	1:C:105:PHE:CD2	2.55	0.41
1:C:72:TYR:OH	1:C:131:ASP:OD1	2.24	0.41
1:C:328:THR:HG21	1:C:415:TYR:HE2	1.85	0.41
1:D:323:GLU:HB2	1:D:327:LEU:HD23	2.03	0.41
1:G:143:ARG:HE	1:G:155:LYS:HZ1	1.69	0.41
1:H:97:LYS:HB2	1:H:97:LYS:HE3	1.85	0.41
1:I:143:ARG:HB2	1:I:216:GLY:HA2	2.03	0.41
1:I:25:VAL:HG21	1:I:260:GLN:NE2	2.36	0.41
1:K:244:ASP:O	1:K:247:THR:OG1	2.36	0.41
1:L:174:LEU:HD21	1:L:178:GLY:O	2.21	0.41
1:L:230:THR:HG21	1:L:298:HIS:ND1	2.35	0.41
1:O:254:VAL:HG13	1:O:297:PHE:HD2	1.86	0.41
1:O:359:ASP:OD1	1:O:359:ASP:N	2.49	0.41
1:P:321:ASP:OD1	1:P:321:ASP:N	2.53	0.41
1:Q:412:ILE:HA	1:Q:415:TYR:HB3	2.02	0.41
1:S:104:ILE:HG23	1:S:105:PHE:CD2	2.55	0.41
1:T:220:SER:OG	1:T:280:ASP:OD2	2.25	0.41
1:T:42:ILE:CD1	1:T:74:TYR:HB2	2.50	0.41
1:C:21:ASN:OD1	1:C:21:ASN:N	2.54	0.41
1:F:153:ARG:HH22	1:F:183:ASP:CG	2.24	0.41
1:F:298:HIS:O	1:F:302:GLN:HB2	2.20	0.41
1:G:381:TRP:O	1:G:385:GLN:HG2	2.20	0.41
1:M:270:LYS:HB3	1:M:270:LYS:HE2	1.87	0.41
1:N:159:GLY:O	1:N:163:GLN:HG2	2.20	0.41
1:O:126:ARG:HH21	1:O:130:ASP:CG	2.23	0.41
1:O:42:ILE:HD11	1:O:194:ILE:HD11	2.01	0.41
1:Q:86:LYS:HA	1:Q:86:LYS:HD3	1.79	0.41
1:A:133:TRP:HB3	1:A:166:MET:SD	2.61	0.41
1:J:165:LYS:HZ2	1:A:184:VAL:CA	2.30	0.41
1:B:381:TRP:O	1:B:385:GLN:HG2	2.21	0.41
1:F:88:TRP:CE2	1:F:95:ILE:HD11	2.56	0.41
1:L:157:MET:HA	1:L:160:LEU:HB2	2.01	0.41
1:S:133:TRP:HB2	1:S:163:GLN:OE1	2.20	0.41
1:S:206:LYS:HD2	1:S:206:LYS:HA	1.83	0.41
1:S:401:VAL:HG23	1:S:421:ASP:HB2	2.03	0.41
1:A:153:ARG:NH1	1:A:179:ARG:O	2.54	0.41
1:D:155:LYS:NZ	1:D:155:LYS:HB3	2.35	0.41
1:D:86:LYS:HD3	1:D:86:LYS:HA	1.87	0.41
1:F:226:ALA:O	1:F:230:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:174:LEU:HD23	1:I:178:GLY:HA3	2.02	0.41
1:I:199:ASP:OD2	1:I:277:TYR:OH	2.34	0.41
1:I:51:LEU:HA	1:I:54:TYR:HB2	2.02	0.41
1:J:240:MET:HB2	1:J:245:VAL:HG23	2.03	0.41
1:K:157:MET:HA	1:K:160:LEU:HB2	2.03	0.41
1:K:254:VAL:HG21	1:K:327:LEU:HD11	2.03	0.41
1:L:178:GLY:C	1:L:180:ASP:H	2.24	0.41
1:M:110:LEU:HD13	1:M:110:LEU:HA	1.89	0.41
1:M:248:TRP:CD1	1:M:375:VAL:HG22	2.56	0.41
1:O:114:ASP:OD1	1:O:114:ASP:N	2.48	0.41
1:O:22:GLU:HB3	1:O:24:PRO:HD3	2.03	0.41
1:Q:226:ALA:O	1:Q:230:THR:HG23	2.21	0.41
1:A:104:ILE:O	1:A:107:LEU:HG	2.21	0.41
1:A:86:LYS:HD3	1:A:86:LYS:HA	1.89	0.41
1:B:67:ILE:HD12	1:B:67:ILE:H	1.86	0.41
1:C:87:ASP:OD2	1:C:97:LYS:HG3	2.21	0.41
1:H:199:ASP:OD1	1:H:277:TYR:OH	2.21	0.41
1:H:302:GLN:NE2	1:H:313:ALA:HA	2.36	0.41
1:K:66:ILE:H	1:K:66:ILE:HD12	1.84	0.41
1:L:172:GLU:CD	1:L:172:GLU:H	2.24	0.41
1:N:236:LYS:HB3	1:M:321:ASP:HB3	2.03	0.41
1:S:302:GLN:HB3	1:S:412:ILE:HD13	2.02	0.41
1:S:86:LYS:HD3	1:S:86:LYS:HA	1.90	0.41
1:B:419:GLU:OE2	1:A:309:ARG:NE	2.51	0.41
1:C:152:TYR:C	1:C:154:LYS:H	2.24	0.41
1:C:158:ASP:HB3	1:C:215:TYR:OH	2.20	0.41
1:C:336:TYR:CG	1:C:393:MET:HG2	2.56	0.41
1:F:327:LEU:HD13	1:F:327:LEU:HA	1.90	0.41
1:H:54:TYR:CE1	1:H:121:VAL:HG21	2.56	0.41
1:I:145:GLY:HA2	1:I:179:ARG:HH22	1.86	0.41
1:J:55:VAL:O	1:J:59:LEU:HG	2.20	0.41
1:P:73:LEU:HD23	1:P:73:LEU:HA	1.97	0.41
1:Q:68:HIS:NE2	1:Q:118:PRO:HG2	2.36	0.41
1:R:143:ARG:HB2	1:R:216:GLY:HA2	2.03	0.41
1:R:240:MET:HB2	1:R:245:VAL:HG23	2.03	0.41
1:T:153:ARG:HD2	1:T:179:ARG:HD2	2.03	0.41
1:B:175:VAL:HG23	1:B:177:GLU:H	1.86	0.41
1:C:27:TYR:CZ	1:C:263:LEU:HD22	2.56	0.41
1:G:143:ARG:HB3	1:G:216:GLY:HA2	2.03	0.41
1:L:6:LYS:HE2	1:L:6:LYS:HB3	1.87	0.41
1:M:52:ARG:NH1	1:M:128:SER:HA	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:6:LYS:NZ	1:O:11:ASN:O	2.50	0.41
1:S:126:ARG:HD3	1:S:126:ARG:HA	1.81	0.41
1:A:175:VAL:HB	1:A:177:GLU:O	2.21	0.41
1:D:304:THR:HG21	1:D:334:TYR:CD2	2.56	0.41
1:D:336:TYR:CG	1:D:393:MET:HG2	2.56	0.41
1:E:158:ASP:O	1:E:161:THR:HG22	2.20	0.41
1:F:117:LEU:HA	1:F:117:LEU:HD23	1.91	0.41
1:G:97:LYS:HE3	1:G:97:LYS:HB2	1.82	0.41
1:H:199:ASP:HB2	1:H:217:THR:HB	2.02	0.41
1:J:250:LEU:HD22	1:J:379:LEU:HD21	2.02	0.41
1:L:270:LYS:HB3	1:L:270:LYS:HE2	1.86	0.41
1:L:66:ILE:HA	1:L:69:VAL:HG22	2.02	0.41
1:P:166:MET:HB3	1:P:166:MET:HE2	1.90	0.41
1:S:323:GLU:O	1:S:327:LEU:HD23	2.21	0.41
1:T:80:ILE:HD12	1:T:80:ILE:HA	1.86	0.41
1:A:323:GLU:HB2	1:A:327:LEU:HD23	2.03	0.40
1:B:250:LEU:HD22	1:B:379:LEU:HD21	2.03	0.40
1:B:269:ASP:N	1:B:269:ASP:OD1	2.51	0.40
1:G:18:LEU:HA	1:G:18:LEU:HD23	1.96	0.40
1:H:344:LEU:HD22	1:I:330:ALA:HB2	2.03	0.40
1:H:81:ARG:HG2	1:H:103:GLY:HA2	2.02	0.40
1:N:130:ASP:O	1:N:134:LEU:HB2	2.21	0.40
1:N:89:SER:O	1:N:270:LYS:NZ	2.54	0.40
1:P:226:ALA:O	1:P:230:THR:HG23	2.21	0.40
1:R:135:PRO:O	1:R:139:LEU:HG	2.21	0.40
1:F:270:LYS:HB3	1:F:270:LYS:HE2	1.85	0.40
1:J:153:ARG:NE	1:J:179:ARG:HD2	2.37	0.40
1:K:167:ILE:HG12	1:K:169:GLU:H	1.85	0.40
1:M:143:ARG:CB	1:M:216:GLY:HA2	2.51	0.40
1:M:67:ILE:O	1:M:71:SER:HB2	2.20	0.40
1:P:260:GLN:OE1	1:P:294:ASN:ND2	2.46	0.40
1:Q:88:TRP:CE2	1:Q:95:ILE:HD11	2.57	0.40
1:B:147:THR:HG21	1:B:155:LYS:NZ	2.37	0.40
1:F:383:GLU:CD	1:F:387:ARG:HE	2.24	0.40
1:I:165:LYS:HD2	1:J:184:VAL:HA	2.03	0.40
1:K:41:TYR:HB2	1:K:190:ASN:HD21	1.86	0.40
1:K:79:ASP:HA	1:K:81:ARG:HE	1.85	0.40
1:L:287:SER:HA	1:L:288:PRO:HD3	1.98	0.40
1:L:75:GLY:HA2	1:L:78:LYS:HE3	2.03	0.40
1:M:327:LEU:HA	1:M:327:LEU:HD13	1.92	0.40
1:N:40:LEU:HD12	1:N:108:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:363:GLY:O	1:O:365:THR:N	2.54	0.40
1:O:88:TRP:CE2	1:O:95:ILE:HD11	2.56	0.40
1:A:141:LEU:HD12	1:A:182:PHE:CZ	2.56	0.40
1:C:287:SER:HA	1:C:288:PRO:HD3	1.95	0.40
1:G:153:ARG:NH1	1:G:183:ASP:OD1	2.55	0.40
1:J:172:GLU:N	1:J:172:GLU:OE2	2.38	0.40
1:N:270:LYS:HB3	1:N:270:LYS:HE2	1.93	0.40
1:T:401:VAL:HG21	1:T:420:PHE:HB2	2.03	0.40
1:A:111:LYS:HB3	1:A:112:ALA:H	1.62	0.40
1:C:41:TYR:HD1	1:C:111:LYS:HB2	1.85	0.40
1:H:299:PHE:HZ	1:H:415:TYR:CE2	2.40	0.40
1:J:135:PRO:O	1:J:139:LEU:HG	2.21	0.40
1:M:141:LEU:HD12	1:M:182:PHE:CD2	2.56	0.40
1:M:254:VAL:HG21	1:M:327:LEU:HD11	2.04	0.40
1:R:323:GLU:O	1:R:327:LEU:HD23	2.22	0.40
1:S:23:ASP:N	1:S:24:PRO:HD3	2.36	0.40
1:T:226:ALA:O	1:T:230:THR:HG23	2.22	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:Q:81:ARG:NH1	1:L:87:ASP:OD2[1_565]	2.15	0.05

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	410/422 (97%)	388 (95%)	22 (5%)	0	100	100
1	B	406/422 (96%)	372 (92%)	32 (8%)	2 (0%)	29	67
1	C	411/422 (97%)	384 (93%)	26 (6%)	1 (0%)	47	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	414/422 (98%)	383 (92%)	28 (7%)	3 (1%)	22	61
1	E	409/422 (97%)	379 (93%)	29 (7%)	1 (0%)	47	79
1	F	419/422 (99%)	387 (92%)	27 (6%)	5 (1%)	13	49
1	G	412/422 (98%)	379 (92%)	32 (8%)	1 (0%)	47	79
1	H	416/422 (99%)	384 (92%)	29 (7%)	3 (1%)	22	61
1	I	411/422 (97%)	385 (94%)	26 (6%)	0	100	100
1	J	416/422 (99%)	385 (92%)	28 (7%)	3 (1%)	22	61
1	K	419/422 (99%)	387 (92%)	30 (7%)	2 (0%)	29	67
1	L	419/422 (99%)	388 (93%)	28 (7%)	3 (1%)	22	61
1	M	412/422 (98%)	379 (92%)	33 (8%)	0	100	100
1	N	414/422 (98%)	386 (93%)	26 (6%)	2 (0%)	29	67
1	O	416/422 (99%)	389 (94%)	26 (6%)	1 (0%)	47	79
1	P	410/422 (97%)	388 (95%)	21 (5%)	1 (0%)	47	79
1	Q	415/422 (98%)	394 (95%)	20 (5%)	1 (0%)	47	79
1	R	415/422 (98%)	381 (92%)	34 (8%)	0	100	100
1	S	419/422 (99%)	389 (93%)	29 (7%)	1 (0%)	47	79
1	T	419/422 (99%)	392 (94%)	26 (6%)	1 (0%)	47	79
2	a	123/139 (88%)	115 (94%)	8 (6%)	0	100	100
2	b	123/139 (88%)	120 (98%)	3 (2%)	0	100	100
2	c	123/139 (88%)	119 (97%)	4 (3%)	0	100	100
2	d	123/139 (88%)	118 (96%)	4 (3%)	1 (1%)	19	58
2	e	123/139 (88%)	116 (94%)	7 (6%)	0	100	100
2	f	123/139 (88%)	119 (97%)	4 (3%)	0	100	100
2	g	123/139 (88%)	117 (95%)	6 (5%)	0	100	100
2	h	123/139 (88%)	117 (95%)	6 (5%)	0	100	100
2	i	123/139 (88%)	119 (97%)	4 (3%)	0	100	100
2	j	123/139 (88%)	119 (97%)	4 (3%)	0	100	100
2	k	123/139 (88%)	118 (96%)	5 (4%)	0	100	100
2	l	123/139 (88%)	116 (94%)	7 (6%)	0	100	100
2	m	123/139 (88%)	115 (94%)	8 (6%)	0	100	100
2	n	123/139 (88%)	117 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	o	123/139 (88%)	118 (96%)	5 (4%)	0	100	100
2	p	123/139 (88%)	118 (96%)	5 (4%)	0	100	100
2	q	123/139 (88%)	117 (95%)	6 (5%)	0	100	100
2	r	123/139 (88%)	119 (97%)	4 (3%)	0	100	100
2	s	123/139 (88%)	117 (95%)	6 (5%)	0	100	100
2	t	123/139 (88%)	118 (96%)	5 (4%)	0	100	100
All	All	10742/11220 (96%)	10051 (94%)	659 (6%)	32 (0%)	41	74

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	d	2	VAL
1	L	367	ASN
1	N	121	VAL
1	N	178	GLY
1	F	121	VAL
1	H	176	PRO
1	D	350	VAL
1	L	363	GLY
1	G	207	LYS
1	J	79	ASP
1	T	121	VAL
1	H	150	PRO
1	O	364	LEU
1	P	22	GLU
1	D	22	GLU
1	K	22	GLU
1	J	178	GLY
1	D	177	GLU
1	E	364	LEU
1	K	172	GLU
1	F	22	GLU
1	B	80	ILE
1	Q	74	TYR
1	L	121	VAL
1	F	178	GLY
1	F	323	GLU
1	S	150	PRO
1	J	350	VAL
1	B	150	PRO

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Mol	Chain	Res	Type
1	F	181	ILE
1	C	350	VAL
1	H	181	ILE

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	358/363 (99%)	351 (98%)	7 (2%)	55	80
1	B	356/363 (98%)	352 (99%)	4 (1%)	73	88
1	C	359/363 (99%)	356 (99%)	3 (1%)	81	93
1	D	360/363 (99%)	357 (99%)	3 (1%)	81	93
1	E	356/363 (98%)	351 (99%)	5 (1%)	67	86
1	F	362/363 (100%)	360 (99%)	2 (1%)	86	94
1	G	358/363 (99%)	353 (99%)	5 (1%)	67	86
1	H	361/363 (99%)	355 (98%)	6 (2%)	60	83
1	I	358/363 (99%)	352 (98%)	6 (2%)	60	83
1	J	362/363 (100%)	357 (99%)	5 (1%)	67	86
1	K	362/363 (100%)	357 (99%)	5 (1%)	67	86
1	L	362/363 (100%)	357 (99%)	5 (1%)	67	86
1	M	358/363 (99%)	354 (99%)	4 (1%)	73	88
1	N	360/363 (99%)	356 (99%)	4 (1%)	73	88
1	O	362/363 (100%)	361 (100%)	1 (0%)	92	96
1	P	357/363 (98%)	352 (99%)	5 (1%)	67	86
1	Q	361/363 (99%)	357 (99%)	4 (1%)	73	88
1	R	361/363 (99%)	357 (99%)	4 (1%)	73	88
1	S	362/363 (100%)	359 (99%)	3 (1%)	81	93
1	T	362/363 (100%)	360 (99%)	2 (1%)	86	94
2	a	101/111 (91%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	101/111 (91%)	98 (97%)	3 (3%)	41	73
2	c	101/111 (91%)	101 (100%)	0	100	100
2	d	101/111 (91%)	101 (100%)	0	100	100
2	e	101/111 (91%)	100 (99%)	1 (1%)	76	90
2	f	101/111 (91%)	101 (100%)	0	100	100
2	g	101/111 (91%)	100 (99%)	1 (1%)	76	90
2	h	101/111 (91%)	100 (99%)	1 (1%)	76	90
2	i	101/111 (91%)	100 (99%)	1 (1%)	76	90
2	j	101/111 (91%)	100 (99%)	1 (1%)	76	90
2	k	101/111 (91%)	101 (100%)	0	100	100
2	l	101/111 (91%)	101 (100%)	0	100	100
2	m	101/111 (91%)	101 (100%)	0	100	100
2	n	101/111 (91%)	101 (100%)	0	100	100
2	o	101/111 (91%)	101 (100%)	0	100	100
2	p	101/111 (91%)	99 (98%)	2 (2%)	55	80
2	q	101/111 (91%)	101 (100%)	0	100	100
2	r	101/111 (91%)	101 (100%)	0	100	100
2	s	101/111 (91%)	99 (98%)	2 (2%)	55	80
2	t	101/111 (91%)	101 (100%)	0	100	100
All	All	9217/9480 (97%)	9122 (99%)	95 (1%)	76	90

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	134	LEU
1	P	156	LEU
1	P	162	ASN
1	P	281	PHE
1	P	321	ASP
2	p	110	ARG
2	p	117	GLN
1	B	134	LEU
1	B	182	PHE
1	B	187	ASN
1	B	384	ASP

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Mol	Chain	Res	Type
2	b	11	LEU
2	b	52	SER
2	b	117	GLN
1	Q	208	HIS
1	Q	214	ARG
1	Q	252	ARG
1	Q	384	ASP
1	C	163	GLN
1	C	180	ASP
1	C	384	ASP
1	R	189	SER
1	R	215	TYR
1	R	312	ARG
1	R	384	ASP
1	D	134	LEU
1	D	215	TYR
1	D	291	SER
1	S	281	PHE
1	S	384	ASP
1	S	422	LYS
2	s	19	ARG
2	s	117	GLN
1	E	87	ASP
1	E	130	ASP
1	E	187	ASN
1	E	214	ARG
1	E	312	ARG
2	e	72	ARG
1	T	320	ASP
1	T	384	ASP
1	K	134	LEU
1	K	174	LEU
1	K	189	SER
1	K	281	PHE
1	K	384	ASP
1	L	60	LYS
1	L	174	LEU
1	L	189	SER
1	L	353	ASN
1	L	384	ASP
1	N	85	ASP
1	N	100	ASP

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Mol	Chain	Res	Type
1	N	291	SER
1	N	334	TYR
1	M	46	LYS
1	M	172	GLU
1	M	291	SER
1	M	312	ARG
1	F	281	PHE
1	F	312	ARG
1	G	134	LEU
1	G	155	LYS
1	G	189	SER
1	G	264	PRO
1	G	384	ASP
2	g	52	SER
1	H	79	ASP
1	H	214	ARG
1	H	291	SER
1	H	312	ARG
1	H	332	LEU
1	H	384	ASP
2	h	63	SER
1	I	87	ASP
1	I	134	LEU
1	I	152	TYR
1	I	169	GLU
1	I	312	ARG
1	I	334	TYR
2	i	117	GLN
1	O	252	ARG
1	J	87	ASP
1	J	126	ARG
1	J	143	ARG
1	J	281	PHE
1	J	312	ARG
2	j	17	SER
1	A	156	LEU
1	A	163	GLN
1	A	166	MET
1	A	252	ARG
1	A	291	SER
1	A	312	ARG
1	A	384	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	208	HIS
1	K	260	GLN
1	K	294	ASN
2	k	103	ASN
1	N	163	GLN
1	N	260	GLN
1	N	294	ASN
1	M	294	ASN
1	F	163	GLN
1	F	170	GLN
1	O	163	GLN
1	A	162	ASN
1	A	163	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	u	44/45 (97%)	15 (34%)	0
3	v	44/45 (97%)	14 (31%)	0
3	w	44/45 (97%)	15 (34%)	0
3	x	44/45 (97%)	13 (29%)	0
All	All	176/180 (97%)	57 (32%)	0

All (57) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	u	3	U
3	u	5	U
3	u	11	U
3	u	12	U
3	u	14	U
3	u	15	U
3	u	23	U
3	u	24	U
3	u	25	U
3	u	30	U
3	u	32	U
3	u	33	U
3	u	38	U
3	u	41	U

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Mol	Chain	Res	Type
3	u	42	U
3	v	2	U
3	v	3	U
3	v	5	U
3	v	11	U
3	v	12	U
3	v	14	U
3	v	15	U
3	v	24	U
3	v	25	U
3	v	30	U
3	v	32	U
3	v	33	U
3	v	38	U
3	v	41	U
3	w	3	U
3	w	5	U
3	w	12	U
3	w	14	U
3	w	15	U
3	w	21	U
3	w	23	U
3	w	24	U
3	w	25	U
3	w	30	U
3	w	32	U
3	w	33	U
3	w	38	U
3	w	41	U
3	w	42	U
3	x	3	U
3	x	5	U
3	x	11	U
3	x	12	U
3	x	14	U
3	x	15	U
3	x	16	U
3	x	24	U
3	x	25	U
3	x	32	U
3	x	33	U
3	x	39	U

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Mol	Chain	Res	Type
3	x	41	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	416/422 (98%)	-0.30	1 (0%) 95 94	35, 55, 77, 101	0
1	B	412/422 (97%)	-0.19	0 100 100	36, 64, 85, 93	0
1	C	417/422 (98%)	-0.16	4 (0%) 82 72	39, 63, 82, 99	0
1	D	418/422 (99%)	-0.27	0 100 100	35, 61, 79, 100	0
1	E	413/422 (97%)	-0.28	0 100 100	34, 56, 77, 89	0
1	F	421/422 (99%)	-0.20	3 (0%) 87 81	34, 54, 78, 91	0
1	G	416/422 (98%)	-0.22	4 (0%) 82 72	36, 60, 83, 97	0
1	H	420/422 (99%)	-0.06	5 (1%) 79 67	34, 64, 85, 93	0
1	I	415/422 (98%)	-0.32	0 100 100	35, 56, 76, 100	0
1	J	420/422 (99%)	-0.30	0 100 100	35, 56, 78, 91	0
1	K	421/422 (99%)	-0.25	2 (0%) 91 86	34, 55, 76, 85	0
1	L	421/422 (99%)	-0.26	0 100 100	35, 53, 73, 87	0
1	M	416/422 (98%)	-0.07	3 (0%) 87 81	36, 62, 85, 108	0
1	N	418/422 (99%)	-0.30	0 100 100	37, 60, 82, 96	0
1	O	420/422 (99%)	-0.31	2 (0%) 91 86	34, 51, 74, 94	0
1	P	414/422 (98%)	-0.32	1 (0%) 95 94	35, 57, 77, 99	0
1	Q	419/422 (99%)	-0.25	1 (0%) 95 94	35, 57, 75, 94	0
1	R	419/422 (99%)	-0.19	5 (1%) 79 67	36, 63, 82, 100	0
1	S	421/422 (99%)	-0.28	0 100 100	36, 61, 83, 101	0
1	T	421/422 (99%)	-0.31	0 100 100	34, 53, 75, 95	0
2	a	125/139 (89%)	-0.37	0 100 100	35, 51, 66, 75	0
2	b	125/139 (89%)	-0.33	0 100 100	40, 53, 69, 78	0
2	c	125/139 (89%)	-0.17	0 100 100	40, 55, 69, 76	0
2	d	125/139 (89%)	-0.43	0 100 100	39, 52, 65, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9		
2	e	125/139 (89%)	-0.46	0	100	100	38, 50, 65, 74	0
2	f	125/139 (89%)	-0.26	0	100	100	38, 52, 66, 73	0
2	g	125/139 (89%)	-0.36	0	100	100	40, 53, 67, 75	0
2	h	125/139 (89%)	-0.30	0	100	100	38, 50, 68, 74	0
2	i	125/139 (89%)	-0.48	0	100	100	37, 48, 67, 78	0
2	j	125/139 (89%)	-0.39	0	100	100	35, 49, 62, 70	0
2	k	125/139 (89%)	-0.42	0	100	100	37, 48, 66, 76	0
2	l	125/139 (89%)	-0.31	0	100	100	38, 51, 65, 79	0
2	m	125/139 (89%)	-0.28	0	100	100	39, 53, 68, 76	0
2	n	125/139 (89%)	-0.42	0	100	100	41, 54, 71, 79	0
2	o	125/139 (89%)	-0.42	0	100	100	37, 51, 64, 73	0
2	p	125/139 (89%)	-0.41	0	100	100	37, 51, 68, 76	0
2	q	125/139 (89%)	-0.36	0	100	100	37, 50, 70, 78	0
2	r	125/139 (89%)	-0.30	0	100	100	40, 53, 65, 83	0
2	s	125/139 (89%)	-0.36	0	100	100	35, 50, 66, 79	0
2	t	125/139 (89%)	-0.38	0	100	100	35, 47, 63, 69	0
3	u	45/45 (100%)	-0.39	0	100	100	44, 56, 68, 74	0
3	v	45/45 (100%)	-0.45	0	100	100	42, 54, 65, 76	0
3	w	45/45 (100%)	-0.41	0	100	100	44, 58, 71, 75	0
3	x	45/45 (100%)	-0.48	0	100	100	45, 52, 65, 71	0
All	All	11038/11400 (96%)	-0.27	31 (0%)	94	92	34, 55, 79, 108	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	180	ASP	4.4
1	G	53	GLY	3.7
1	R	43	ASN	3.6
1	G	178	GLY	3.2
1	C	363	GLY	3.1
1	F	362	GLY	3.0
1	O	179	ARG	3.0
1	H	363	GLY	2.8
1	M	363	GLY	2.7
1	R	365	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	119	ASP	2.6
1	H	364	LEU	2.5
1	F	178	GLY	2.3
1	O	178	GLY	2.3
1	G	166	MET	2.3
1	C	179	ARG	2.3
1	K	116	VAL	2.3
1	A	363	GLY	2.3
1	M	68	HIS	2.3
1	K	180	ASP	2.2
1	F	166	MET	2.2
1	G	51	LEU	2.2
1	Q	180	ASP	2.1
1	C	45	THR	2.1
1	R	363	GLY	2.1
1	H	54	TYR	2.1
1	M	102	ILE	2.1
1	H	55	VAL	2.1
1	C	57	GLN	2.1
1	R	178	GLY	2.0
1	R	44	THR	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.