



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:02 AM UTC

PDB ID : 4V4M / pdb_00004v4m
Title : 1.45 Angstrom Structure of STNV coat protein
Authors : Lane, S.W.; Dennis, C.A.; Lane, C.L.; Trinh, C.H.; Rizkallah, P.J.; Stockley, P.G.; Phillips, S.E.V.
Deposited on : 2011-04-28
Resolution : 1.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

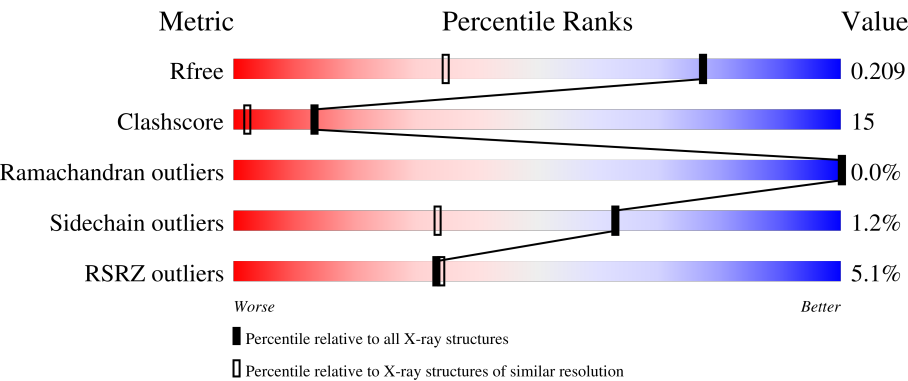
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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

Mol	Chain	Length	Quality of chain
1	0	196	6% 82% 11% 6%
1	1	196	5% 80% 13% 6%
1	2	196	6% 80% 13% 6%
1	3	196	5% 81% 12% 6%
1	4	196	4% 82% 11% 6%

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Mol	Chain	Length	Quality of chain
1	5	196	
1	6	196	
1	7	196	
1	A	196	
1	B	196	
1	C	196	
1	D	196	
1	E	196	
1	F	196	
1	G	196	
1	H	196	
1	I	196	
1	J	196	
1	K	196	
1	L	196	
1	M	196	
1	N	196	
1	O	196	
1	P	196	
1	Q	196	
1	R	196	
1	S	196	
1	T	196	
1	U	196	
1	V	196	

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Mol	Chain	Length	Quality of chain
1	W	196	
1	X	196	
1	Y	196	
1	Z	196	
1	a	196	
1	b	196	
1	c	196	
1	d	196	
1	e	196	
1	f	196	
1	g	196	
1	h	196	
1	i	196	
1	j	196	
1	k	196	
1	l	196	
1	m	196	
1	n	196	
1	o	196	
1	p	196	
1	q	196	
1	r	196	
1	s	196	
1	t	196	
1	u	196	

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Mol	Chain	Length	Quality of chain
1	v	196	5% 81% 12% 6%
1	w	196	4% 81% 13% 6%
1	x	196	6% 79% 15% 6%
1	y	196	6% 81% 12% 6%
1	z	196	5% 81% 12% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 102135 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 Coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	e	184	Total	C	N	O	S	0	2	0
			1439	898	261	273	7			
1	f	184	Total	C	N	O	S	0	4	0
			1450	908	263	272	7			
1	g	184	Total	C	N	O	S	0	2	0
			1437	898	260	272	7			
1	h	184	Total	C	N	O	S	0	4	0
			1451	906	265	274	6			
1	i	184	Total	C	N	O	S	0	3	0
			1448	902	265	274	7			
1	j	184	Total	C	N	O	S	0	2	0
			1441	898	264	273	6			
1	k	184	Total	C	N	O	S	0	2	0
			1440	897	264	273	6			
1	l	184	Total	C	N	O	S	0	1	0
			1432	893	260	272	7			
1	m	184	Total	C	N	O	S	0	2	0
			1440	898	263	272	7			
1	n	184	Total	C	N	O	S	0	4	0
			1450	906	264	273	7			
1	o	184	Total	C	N	O	S	0	1	0
			1433	893	261	273	6			
1	p	184	Total	C	N	O	S	0	1	0
			1432	893	260	272	7			
1	q	184	Total	C	N	O	S	0	1	0
			1432	893	260	272	7			
1	r	184	Total	C	N	O	S	0	3	0
			1448	903	266	272	7			
1	s	184	Total	C	N	O	S	0	2	0
			1436	897	260	272	7			
1	t	184	Total	C	N	O	S	0	7	0
			1472	919	272	274	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	u	184	Total	C	N	O	S	0	2	0
			1440	898	263	272	7			
1	v	184	Total	C	N	O	S	0	2	0
			1440	898	263	272	7			
1	w	184	Total	C	N	O	S	0	3	0
			1444	902	263	272	7			
1	x	184	Total	C	N	O	S	0	3	0
			1445	901	264	273	7			
1	y	184	Total	C	N	O	S	0	2	0
			1436	897	260	272	7			
1	z	184	Total	C	N	O	S	0	4	0
			1451	907	264	273	7			
1	0	184	Total	C	N	O	S	0	2	0
			1440	898	263	272	7			
1	1	184	Total	C	N	O	S	0	3	0
			1446	902	264	273	7			
1	2	184	Total	C	N	O	S	0	4	0
			1452	906	266	273	7			
1	3	184	Total	C	N	O	S	0	4	0
			1454	907	267	273	7			
1	4	184	Total	C	N	O	S	0	3	0
			1443	900	262	274	7			
1	5	184	Total	C	N	O	S	0	1	0
			1432	892	261	273	6			
1	6	184	Total	C	N	O	S	0	3	0
			1448	903	266	272	7			
1	7	184	Total	C	N	O	S	0	2	0
			1438	897	261	273	7			
1	A	184	Total	C	N	O	S	0	6	0
			1460	913	265	275	7			
1	B	184	Total	C	N	O	S	0	6	0
			1464	917	267	273	7			
1	C	184	Total	C	N	O	S	0	4	0
			1454	906	265	276	7			
1	D	184	Total	C	N	O	S	0	4	0
			1445	905	260	273	7			
1	E	184	Total	C	N	O	S	0	2	0
			1437	898	260	272	7			
1	F	184	Total	C	N	O	S	0	2	0
			1438	897	261	273	7			
1	G	184	Total	C	N	O	S	0	4	0
			1450	906	264	273	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	184	Total	C	N	O	S	0	2	0
			1440	898	263	272	7			
1	I	184	Total	C	N	O	S	0	3	0
			1443	902	260	274	7			
1	J	184	Total	C	N	O	S	0	2	0
			1440	898	263	272	7			
1	K	184	Total	C	N	O	S	0	7	0
			1470	919	269	275	7			
1	L	184	Total	C	N	O	S	0	5	0
			1458	913	266	272	7			
1	M	184	Total	C	N	O	S	0	3	0
			1442	901	261	273	7			
1	N	184	Total	C	N	O	S	0	3	0
			1445	901	264	273	7			
1	O	184	Total	C	N	O	S	0	2	0
			1440	898	263	272	7			
1	P	184	Total	C	N	O	S	0	6	0
			1465	917	268	273	7			
1	Q	184	Total	C	N	O	S	0	2	0
			1437	896	261	273	7			
1	R	184	Total	C	N	O	S	0	3	0
			1442	903	260	272	7			
1	S	184	Total	C	N	O	S	0	6	0
			1465	916	268	274	7			
1	T	184	Total	C	N	O	S	0	3	0
			1440	900	260	273	7			
1	U	184	Total	C	N	O	S	0	4	0
			1451	905	265	274	7			
1	V	184	Total	C	N	O	S	0	3	0
			1443	902	260	274	7			
1	W	184	Total	C	N	O	S	0	1	0
			1432	893	260	272	7			
1	X	184	Total	C	N	O	S	0	2	0
			1437	898	260	272	7			
1	Y	184	Total	C	N	O	S	0	3	0
			1445	901	264	273	7			
1	Z	184	Total	C	N	O	S	0	3	0
			1448	903	266	272	7			
1	a	184	Total	C	N	O	S	0	5	0
			1456	910	265	274	7			
1	b	184	Total	C	N	O	S	0	1	0
			1432	893	260	272	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	c	184	Total	C	N	O	S	0	3	0
			1448	903	266	272	7			
1	d	184	Total	C	N	O	S	0	2	0
			1439	898	261	273	7			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	e	1	Total	Ca	0	0
			1	1		
2	f	1	Total	Ca	0	0
			1	1		
2	g	1	Total	Ca	0	0
			1	1		
2	h	1	Total	Ca	0	0
			1	1		
2	i	2	Total	Ca	0	0
			2	2		
2	j	2	Total	Ca	0	0
			2	2		
2	k	1	Total	Ca	0	0
			1	1		
2	l	1	Total	Ca	0	0
			1	1		
2	m	1	Total	Ca	0	0
			1	1		
2	n	2	Total	Ca	0	0
			2	2		
2	o	2	Total	Ca	0	0
			2	2		
2	p	1	Total	Ca	0	0
			1	1		
2	q	2	Total	Ca	0	0
			2	2		
2	r	1	Total	Ca	0	0
			1	1		
2	s	1	Total	Ca	0	0
			1	1		
2	t	1	Total	Ca	0	0
			1	1		
2	u	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	v	1	Total 1	Ca 1	0	0
2	w	1	Total 1	Ca 1	0	0
2	x	1	Total 1	Ca 1	0	0
2	y	1	Total 1	Ca 1	0	0
2	z	1	Total 1	Ca 1	0	0
2	0	2	Total 2	Ca 2	0	0
2	1	3	Total 3	Ca 3	0	0
2	2	2	Total 2	Ca 2	0	0
2	3	2	Total 2	Ca 2	0	0
2	4	2	Total 2	Ca 2	0	0
2	5	2	Total 2	Ca 2	0	0
2	6	2	Total 2	Ca 2	0	0
2	7	1	Total 1	Ca 1	0	0
2	A	2	Total 2	Ca 2	0	0
2	B	3	Total 3	Ca 3	0	0
2	C	1	Total 1	Ca 1	0	0
2	D	1	Total 1	Ca 1	0	0
2	E	3	Total 3	Ca 3	0	0
2	F	1	Total 1	Ca 1	0	0
2	G	3	Total 3	Ca 3	0	0
2	H	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	2	Total 2	Ca 2	0	0
2	J	1	Total 1	Ca 1	0	0
2	K	2	Total 2	Ca 2	0	0
2	L	1	Total 1	Ca 1	0	0
2	M	1	Total 1	Ca 1	0	0
2	N	2	Total 2	Ca 2	0	0
2	O	1	Total 1	Ca 1	0	0
2	P	1	Total 1	Ca 1	0	0
2	Q	2	Total 2	Ca 2	0	0
2	R	2	Total 2	Ca 2	0	0
2	S	2	Total 2	Ca 2	0	0
2	T	2	Total 2	Ca 2	0	0
2	U	3	Total 3	Ca 3	0	0
2	V	2	Total 2	Ca 2	0	0
2	W	1	Total 1	Ca 1	0	0
2	X	1	Total 1	Ca 1	0	0
2	Y	1	Total 1	Ca 1	0	0
2	Z	1	Total 1	Ca 1	0	0
2	a	1	Total 1	Ca 1	0	0
2	b	2	Total 2	Ca 2	0	0
2	c	2	Total 2	Ca 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	d	1	Total 1	Ca 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	e	258	Total 258	O 258	0	0
3	f	231	Total 231	O 231	0	0
3	g	260	Total 260	O 260	0	0
3	h	281	Total 281	O 281	0	0
3	i	282	Total 282	O 282	0	0
3	j	267	Total 267	O 267	0	0
3	k	256	Total 256	O 256	0	0
3	l	257	Total 257	O 257	0	0
3	m	252	Total 252	O 252	0	0
3	n	251	Total 251	O 251	0	0
3	o	262	Total 262	O 262	0	0
3	p	238	Total 238	O 238	0	0
3	q	258	Total 258	O 258	0	0
3	r	287	Total 287	O 287	0	0
3	s	226	Total 226	O 226	0	0
3	t	236	Total 236	O 236	0	0
3	u	240	Total 240	O 240	0	0
3	v	249	Total 249	O 249	0	0

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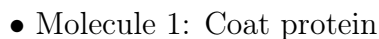
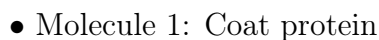
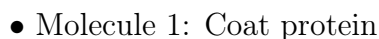
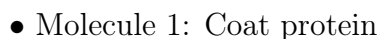
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	w	279	Total 279	O 279	0	0
3	x	260	Total 260	O 260	0	0
3	y	294	Total 294	O 294	0	0
3	z	264	Total 264	O 264	0	0
3	0	242	Total 242	O 242	0	0
3	1	256	Total 256	O 256	0	0
3	2	259	Total 259	O 259	0	0
3	3	245	Total 245	O 245	0	0
3	4	278	Total 278	O 278	0	0
3	5	247	Total 247	O 247	0	0
3	6	264	Total 264	O 264	0	0
3	7	249	Total 249	O 249	0	0
3	A	246	Total 246	O 246	0	0
3	B	235	Total 235	O 235	0	0
3	C	250	Total 250	O 250	0	0
3	D	255	Total 255	O 255	0	0
3	E	229	Total 229	O 229	0	0
3	F	217	Total 217	O 217	0	0
3	G	253	Total 253	O 253	0	0
3	H	248	Total 248	O 248	0	0
3	I	240	Total 240	O 240	0	0

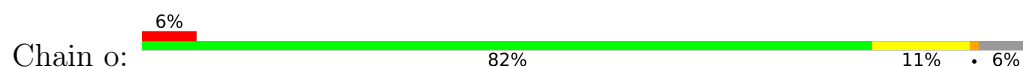
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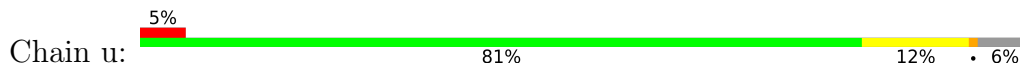
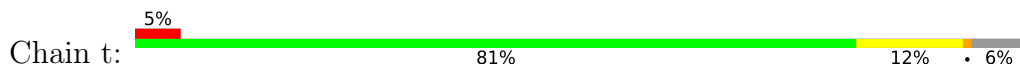
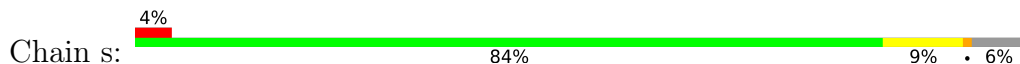
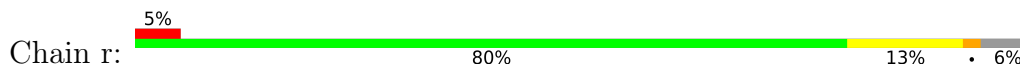
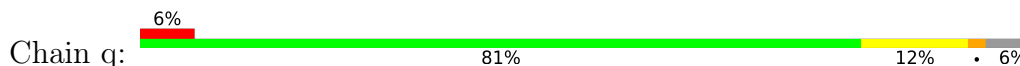
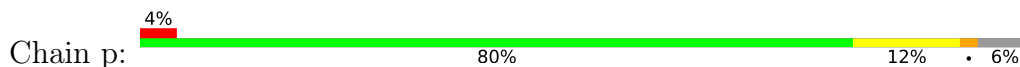
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	245	Total 245	O 245	0	0
3	K	273	Total 273	O 273	0	0
3	L	239	Total 239	O 239	0	0
3	M	253	Total 253	O 253	0	0
3	N	256	Total 256	O 256	0	0
3	O	250	Total 250	O 250	0	0
3	P	250	Total 250	O 250	0	0
3	Q	255	Total 255	O 255	0	0
3	R	286	Total 286	O 286	0	0
3	S	237	Total 237	O 237	0	0
3	T	295	Total 295	O 295	0	0
3	U	266	Total 266	O 266	0	0
3	V	258	Total 258	O 258	0	0
3	W	256	Total 256	O 256	0	0
3	X	256	Total 256	O 256	0	0
3	Y	262	Total 262	O 262	0	0
3	Z	285	Total 285	O 285	0	0
3	a	257	Total 257	O 257	0	0
3	b	254	Total 254	O 254	0	0
3	c	269	Total 269	O 269	0	0
3	d	244	Total 244	O 244	0	0

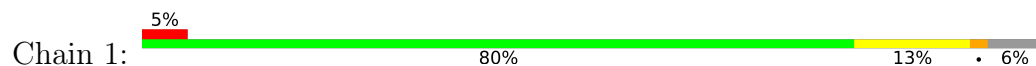
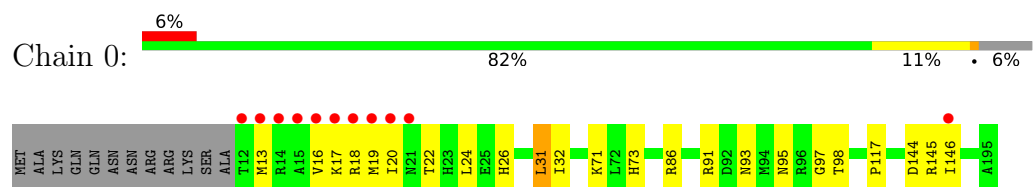
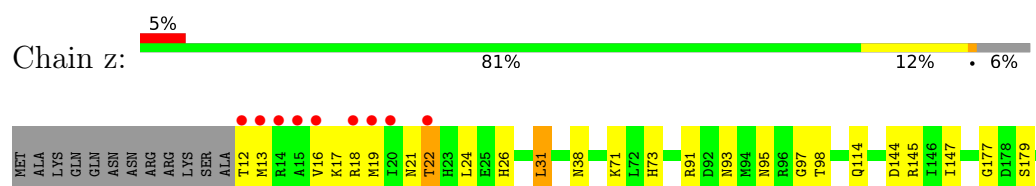
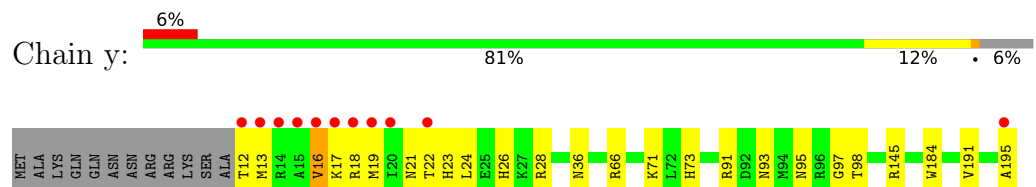
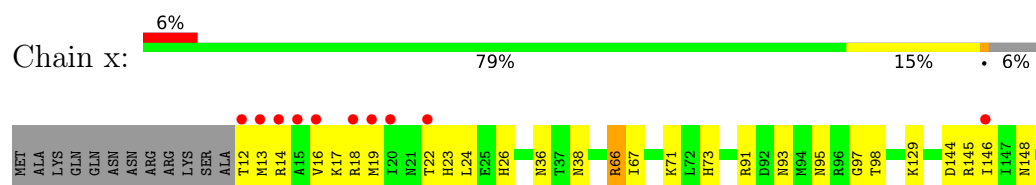
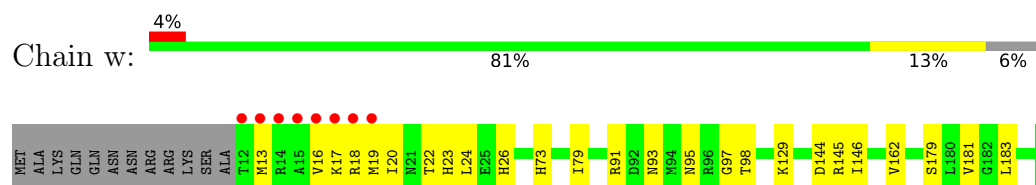
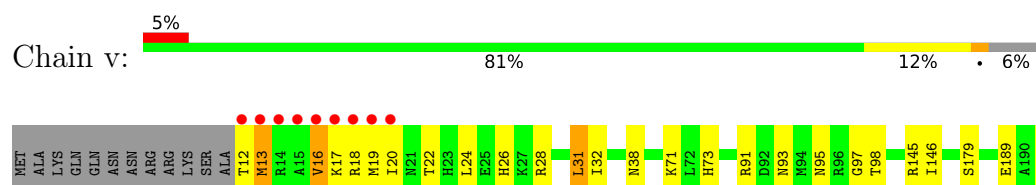
- Molecule 1: Coat protein

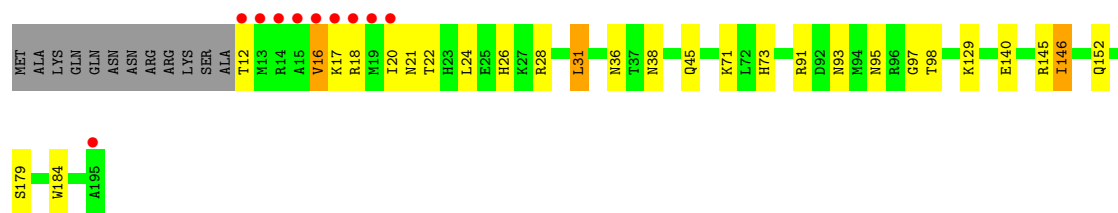




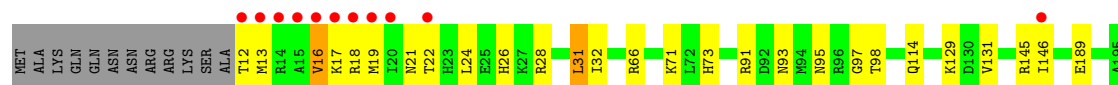
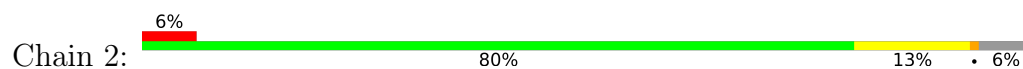


- Molecule 1: Coat protein

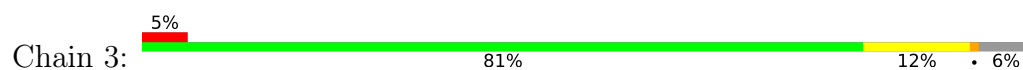




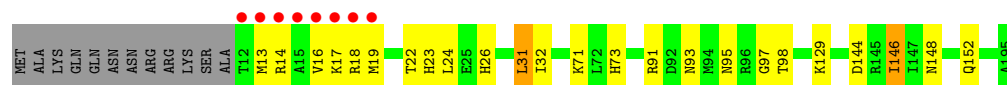
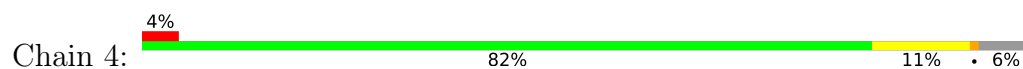
• Molecule 1: Coat protein



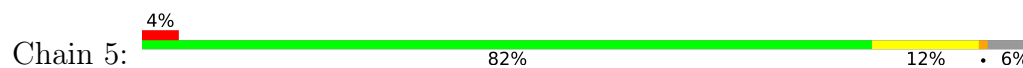
• Molecule 1: Coat protein



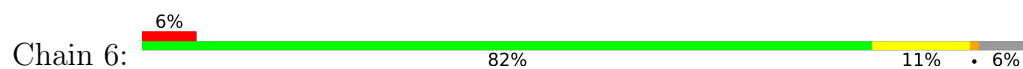
• Molecule 1: Coat protein



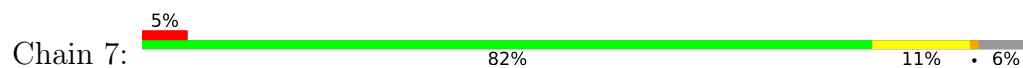
• Molecule 1: Coat protein

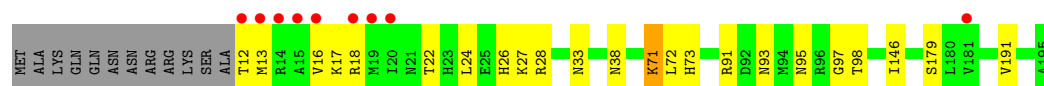


• Molecule 1: Coat protein

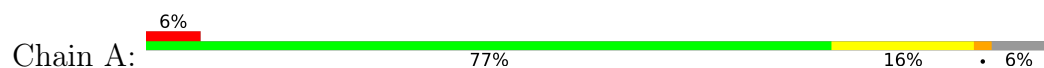


• Molecule 1: Coat protein

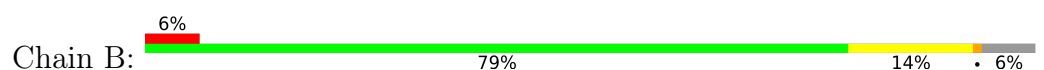




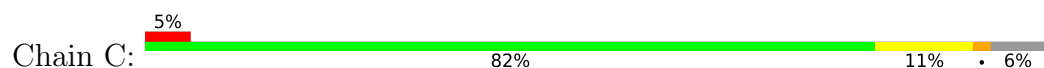
- Molecule 1: Coat protein



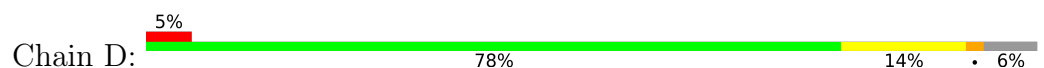
- Molecule 1: Coat protein



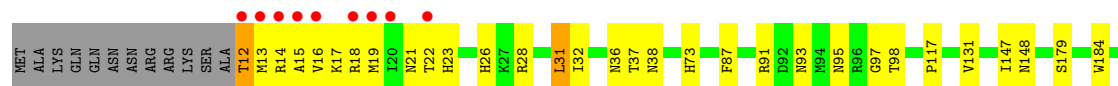
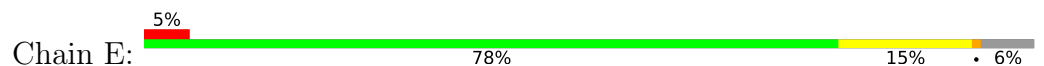
- Molecule 1: Coat protein



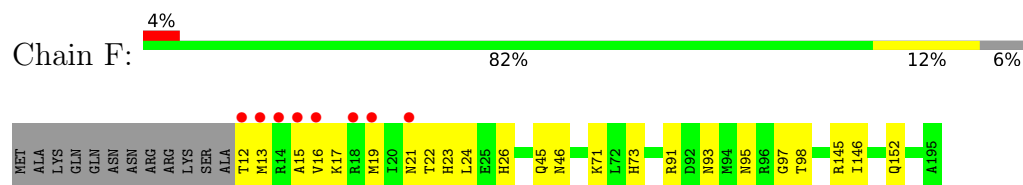
- Molecule 1: Coat protein



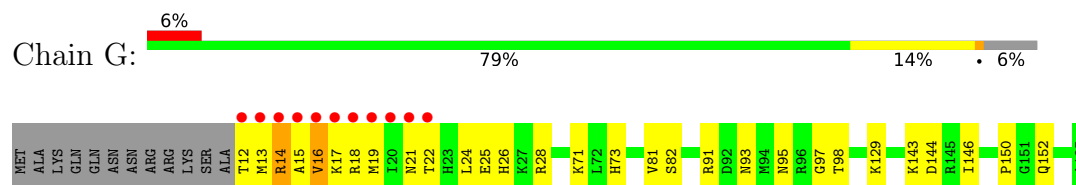
- Molecule 1: Coat protein



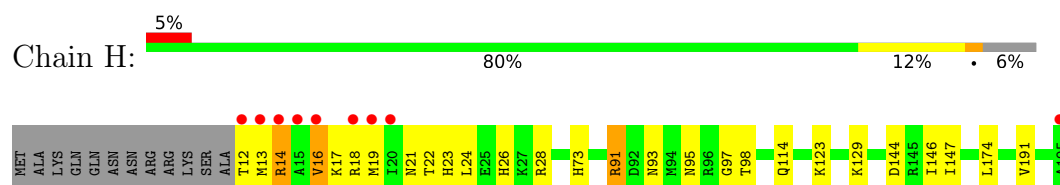
• Molecule 1: Coat protein



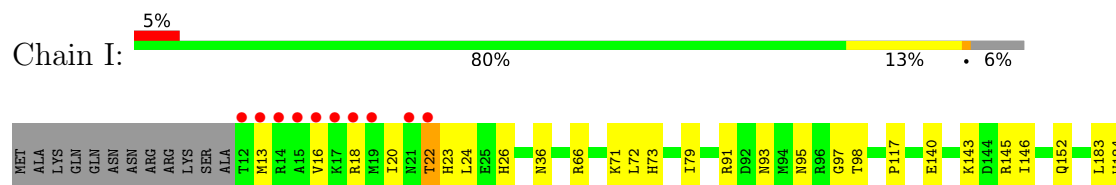
• Molecule 1: Coat protein



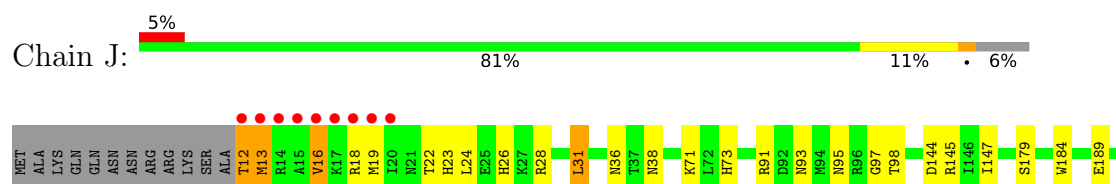
• Molecule 1: Coat protein



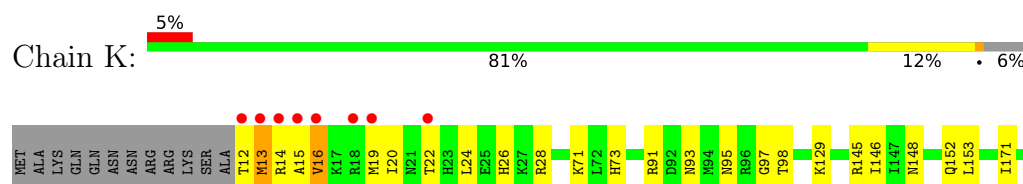
• Molecule 1: Coat protein



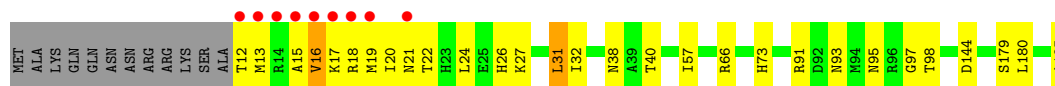
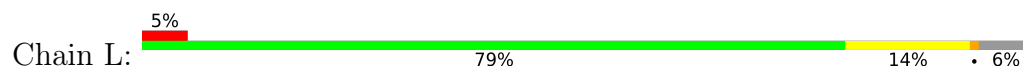
• Molecule 1: Coat protein



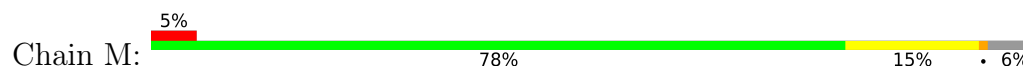
• Molecule 1: Coat protein



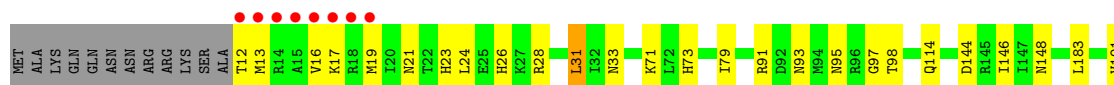
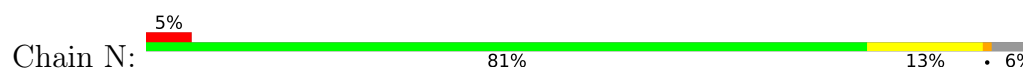
● Molecule 1: Coat protein



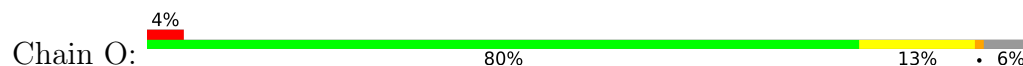
● Molecule 1: Coat protein



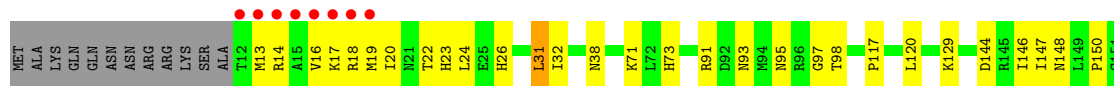
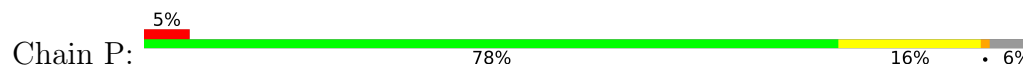
● Molecule 1: Coat protein



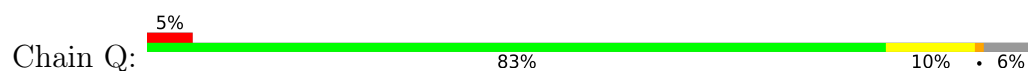
● Molecule 1: Coat protein



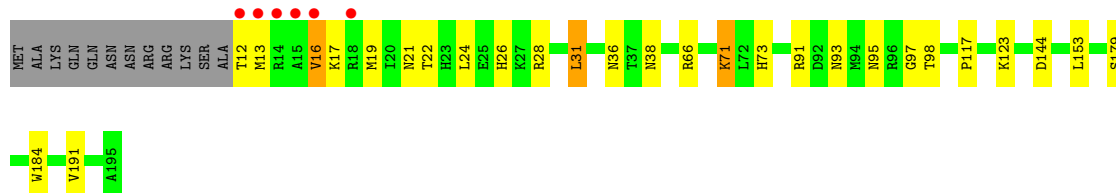
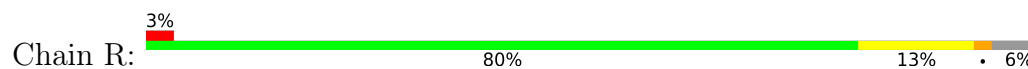
● Molecule 1: Coat protein



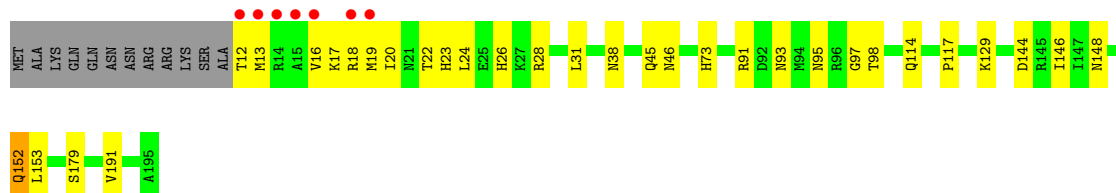
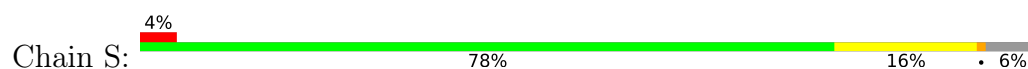
● Molecule 1: Coat protein



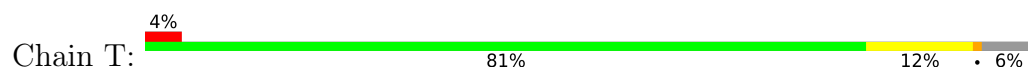
● Molecule 1: Coat protein



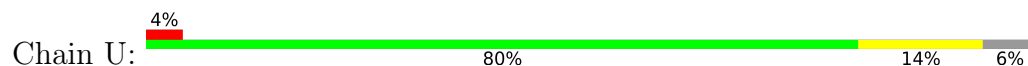
● Molecule 1: Coat protein



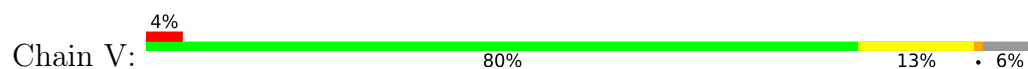
● Molecule 1: Coat protein



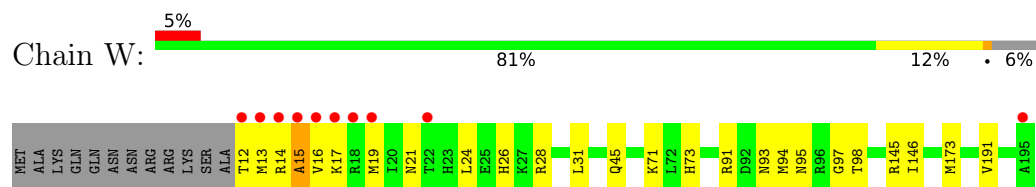
● Molecule 1: Coat protein



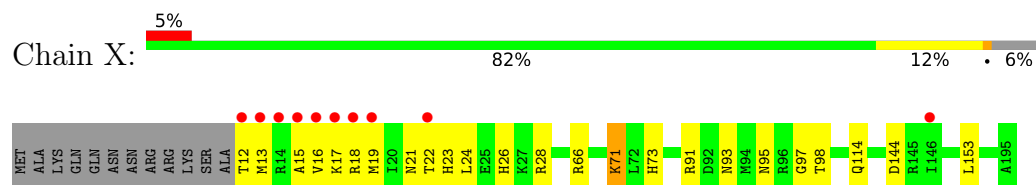
● Molecule 1: Coat protein



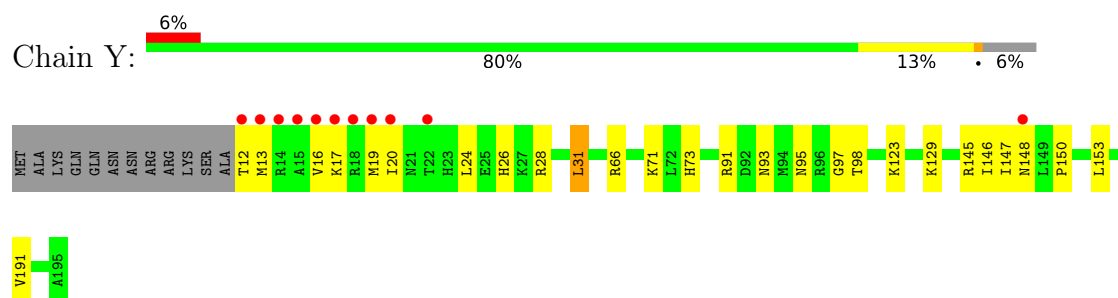
- Molecule 1: Coat protein



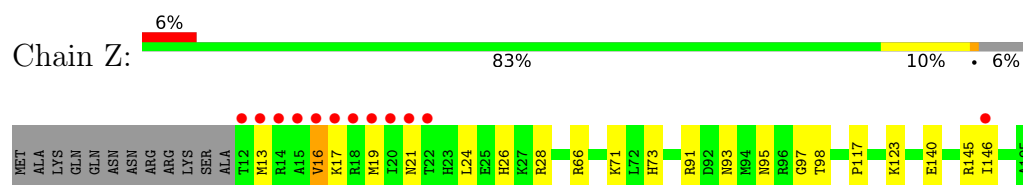
- Molecule 1: Coat protein



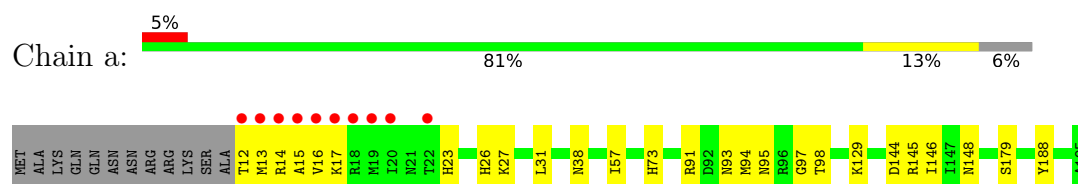
- Molecule 1: Coat protein



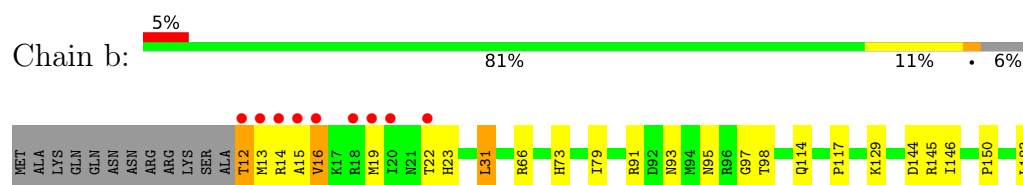
- Molecule 1: Coat protein



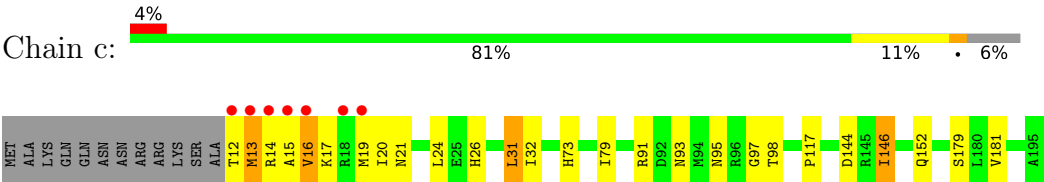
- Molecule 1: Coat protein



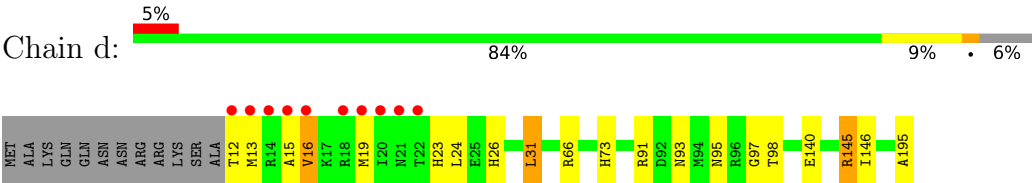
- Molecule 1: Coat protein



- Molecule 1: Coat protein



• Molecule 1: Coat protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	307.58Å 302.26Å 181.92Å 90.00° 92.77° 90.00°	Depositor
Resolution (Å)	12.00 – 1.45 12.00 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (12.00-1.45) 76.1 (12.00-1.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.175 , 0.208 0.185 , 0.209	Depositor DCC
R_{free} test set	111080 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	10.1	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 59.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for k,h,-l 0.009 for -k,-h,-l 0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	102135	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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

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

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	0	0.57	0/1468	0.75	0/1988
1	1	0.57	0/1477	0.72	0/2000
1	2	0.56	0/1486	0.74	0/2012
1	3	0.55	0/1488	0.73	0/2014
1	4	0.58	0/1474	0.73	0/1997
1	5	0.55	0/1457	0.74	0/1975
1	6	0.53	0/1479	0.75	0/2002
1	7	0.57	0/1466	0.74	0/1986
1	A	0.56	0/1500	0.75	0/2032
1	B	0.55	0/1504	0.75	0/2036
1	C	0.55	0/1485	0.75	0/2011
1	D	0.57	0/1479	0.72	0/2004
1	E	0.55	0/1465	0.72	0/1985
1	F	0.54	0/1466	0.73	0/1986
1	G	0.52	0/1484	0.76	0/2010
1	H	0.54	0/1468	0.75	0/1988
1	I	0.54	0/1474	0.73	0/1997
1	J	0.56	0/1468	0.75	0/1988
1	K	0.56	0/1513	0.74	0/2048
1	L	0.53	0/1495	0.72	0/2024
1	M	0.57	0/1473	0.72	0/1996
1	N	0.53	0/1476	0.74	0/1999
1	O	0.52	0/1468	0.74	0/1988
1	P	0.55	0/1505	0.74	0/2036
1	Q	0.56	0/1465	0.75	0/1985
1	R	0.57	0/1473	0.73	0/1996
1	S	0.56	0/1505	0.71	0/2037
1	T	0.58	0/1471	0.76	0/1993
1	U	0.56	0/1485	0.73	0/2011
1	V	0.57	0/1474	0.75	0/1997
1	W	0.57	0/1457	0.74	0/1974
1	X	0.56	0/1465	0.74	0/1985

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Y	0.58	0/1476	0.74	0/1999
1	Z	0.59	0/1479	0.75	0/2002
1	a	0.55	0/1493	0.74	0/2022
1	b	0.56	0/1457	0.76	0/1974
1	c	0.58	0/1479	0.73	0/2002
1	d	0.57	0/1464	0.77	0/1984
1	e	0.57	0/1464	0.74	0/1984
1	f	0.54	0/1484	0.72	0/2010
1	g	0.55	0/1465	0.73	0/1985
1	h	0.57	0/1485	0.75	0/2012
1	i	0.55	0/1476	0.73	0/1999
1	j	0.55	0/1469	0.75	0/1990
1	k	0.58	0/1468	0.76	0/1989
1	l	0.56	0/1457	0.73	0/1974
1	m	0.55	0/1468	0.73	0/1988
1	n	0.54	0/1484	0.71	0/2010
1	o	0.57	0/1458	0.76	0/1976
1	p	0.55	0/1457	0.72	0/1974
1	q	0.57	0/1457	0.74	0/1974
1	r	0.57	0/1479	0.77	0/2002
1	s	0.57	0/1464	0.77	0/1984
1	t	0.53	0/1515	0.72	0/2050
1	u	0.56	0/1468	0.75	0/1988
1	v	0.56	0/1468	0.74	0/1988
1	w	0.60	0/1475	0.76	0/1998
1	x	0.55	0/1476	0.74	0/1999
1	y	0.58	0/1464	0.76	0/1984
1	z	0.57	0/1485	0.72	0/2011
All	All	0.56	0/88547	0.74	0/119932

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	0	1440	0	1449	33	0
1	1	1446	0	1457	48	0
1	2	1452	0	1469	70	0
1	3	1454	0	1470	62	0
1	4	1443	0	1450	55	0
1	5	1432	0	1433	48	0
1	6	1448	0	1462	48	0
1	7	1438	0	1444	37	0
1	A	1460	0	1481	58	0
1	B	1464	0	1492	57	0
1	C	1454	0	1460	41	0
1	D	1445	0	1463	32	0
1	E	1437	0	1447	60	0
1	F	1438	0	1444	45	0
1	G	1450	0	1466	69	0
1	H	1440	0	1449	52	0
1	I	1443	0	1453	41	0
1	J	1440	0	1449	34	0
1	K	1470	0	1495	65	0
1	L	1458	0	1484	44	0
1	M	1442	0	1453	77	0
1	N	1445	0	1455	60	0
1	O	1440	0	1449	62	0
1	P	1465	0	1494	82	0
1	Q	1437	0	1442	50	0
1	R	1442	0	1458	60	0
1	S	1465	0	1487	49	0
1	T	1440	0	1452	51	0
1	U	1451	0	1463	48	0
1	V	1443	0	1453	65	0
1	W	1432	0	1436	45	0
1	X	1437	0	1447	42	0
1	Y	1445	0	1455	57	0
1	Z	1448	0	1462	43	0
1	a	1456	0	1474	36	0
1	b	1432	0	1436	53	0
1	c	1448	0	1462	50	0
1	d	1439	0	1444	37	0
1	e	1439	0	1444	57	0
1	f	1450	0	1471	44	0
1	g	1437	0	1447	34	0
1	h	1451	0	1465	49	0
1	i	1448	0	1454	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j	1441	0	1448	41	0
1	k	1440	0	1446	44	0
1	l	1432	0	1436	43	0
1	m	1440	0	1449	51	0
1	n	1450	0	1466	64	0
1	o	1433	0	1435	40	0
1	p	1432	0	1436	58	0
1	q	1432	0	1436	36	0
1	r	1448	0	1462	43	0
1	s	1436	0	1445	39	0
1	t	1472	0	1502	62	0
1	u	1440	0	1449	48	0
1	v	1440	0	1449	48	0
1	w	1444	0	1458	51	0
1	x	1445	0	1455	68	0
1	y	1436	0	1445	42	0
1	z	1451	0	1468	64	0
2	0	2	0	0	0	0
2	1	3	0	0	0	0
2	2	2	0	0	0	0
2	3	2	0	0	0	0
2	4	2	0	0	0	0
2	5	2	0	0	0	0
2	6	2	0	0	0	0
2	7	1	0	0	0	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	3	0	0	0	0
2	F	1	0	0	0	0
2	G	3	0	0	1	0
2	H	1	0	0	0	0
2	I	2	0	0	0	0
2	J	1	0	0	0	0
2	K	2	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	2	0	0	1	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	2	0	0	0	0
2	S	2	0	0	0	0
2	T	2	0	0	0	0
2	U	3	0	0	0	0
2	V	2	0	0	0	0
2	W	1	0	0	0	0
2	X	1	0	0	0	0
2	Y	1	0	0	0	0
2	Z	1	0	0	0	0
2	a	1	0	0	0	0
2	b	2	0	0	0	0
2	c	2	0	0	0	0
2	d	1	0	0	0	0
2	e	1	0	0	0	0
2	f	1	0	0	0	0
2	g	1	0	0	0	0
2	h	1	0	0	0	0
2	i	2	0	0	0	0
2	j	2	0	0	0	0
2	k	1	0	0	0	0
2	l	1	0	0	0	0
2	m	1	0	0	0	0
2	n	2	0	0	0	0
2	o	2	0	0	0	0
2	p	1	0	0	0	0
2	q	2	0	0	0	0
2	r	1	0	0	0	0
2	s	1	0	0	0	0
2	t	1	0	0	0	0
2	u	1	0	0	0	0
2	v	1	0	0	0	0
2	w	1	0	0	0	0
2	x	1	0	0	0	0
2	y	1	0	0	0	0
2	z	1	0	0	0	0
3	0	242	0	0	6	0
3	1	256	0	0	10	0
3	2	259	0	0	8	0
3	3	245	0	0	8	0
3	4	278	0	0	16	2
3	5	247	0	0	4	0
3	6	264	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	7	249	0	0	7	0
3	A	246	0	0	14	0
3	B	235	0	0	3	0
3	C	250	0	0	7	0
3	D	255	0	0	6	0
3	E	229	0	0	8	0
3	F	217	0	0	7	0
3	G	253	0	0	9	0
3	H	248	0	0	6	0
3	I	240	0	0	9	0
3	J	245	0	0	2	0
3	K	273	0	0	7	0
3	L	239	0	0	10	0
3	M	253	0	0	7	0
3	N	256	0	0	6	0
3	O	250	0	0	18	0
3	P	250	0	0	8	0
3	Q	255	0	0	9	0
3	R	286	0	0	7	0
3	S	237	0	0	5	0
3	T	295	0	0	11	1
3	U	266	0	0	7	0
3	V	258	0	0	12	0
3	W	256	0	0	6	0
3	X	256	0	0	6	0
3	Y	262	0	0	14	0
3	Z	285	0	0	11	0
3	a	257	0	0	5	0
3	b	254	0	0	14	0
3	c	269	0	0	5	0
3	d	244	0	0	7	0
3	e	258	0	0	10	0
3	f	231	0	0	4	0
3	g	260	0	0	7	0
3	h	281	0	0	9	2
3	i	282	0	0	7	0
3	j	267	0	0	6	0
3	k	256	0	0	13	0
3	l	257	0	0	11	0
3	m	252	0	0	8	0
3	n	251	0	0	9	0
3	o	262	0	0	5	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	p	238	0	0	4	0
3	q	258	0	0	5	0
3	r	287	0	0	6	4
3	s	226	0	0	3	0
3	t	236	0	0	13	0
3	u	240	0	0	8	1
3	v	249	0	0	3	0
3	w	279	0	0	10	0
3	x	260	0	0	8	0
3	y	294	0	0	6	0
3	z	264	0	0	8	0
All	All	102135	0	87405	2577	6

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 15.

All (2577) 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:i:19:MET:CE	1:Q:13:MET:CE	1.77	1.60
1:z:13:MET:HE3	1:S:19:MET:CE	1.32	1.56
1:G:19:MET:HE3	1:M:13:MET:CE	1.13	1.56
1:z:19:MET:HE1	1:Y:17:LYS:CB	1.32	1.56
1:G:19:MET:CE	1:M:13:MET:HE3	1.09	1.51
1:z:13:MET:CE	1:S:19:MET:HE3	1.45	1.46
1:X:66:ARG:NH2	1:X:153[B]:LEU:HD11	1.27	1.41
1:i:19:MET:CE	1:Q:13:MET:HE3	1.41	1.40
1:F:19:MET:CE	1:O:13:MET:HE3	1.48	1.40
1:P:120:LEU:HB3	1:S:28[B]:ARG:NH2	1.33	1.39
1:R:17:LYS:NZ	1:R:21:ASN:HD21	1.22	1.37
1:K:19:MET:HE3	1:d:13:MET:CE	1.53	1.36
1:n:19:MET:HE2	1:G:13:MET:CE	1.52	1.36
1:E:17:LYS:CB	1:J:19:MET:HE1	1.51	1.36
1:f:13:MET:HE3	1:m:19:MET:CE	1.57	1.32
1:g:19:MET:O	1:g:22:THR:HG22	1.29	1.29
1:h:13:MET:O	1:h:16:VAL:HG12	1.21	1.29
1:P:19:MET:HE1	1:W:13:MET:SD	1.73	1.29
1:e:23:HIS:ND1	1:i:66:ARG:NH1	1.79	1.28
1:M:13:MET:O	1:M:16:VAL:HG12	1.32	1.27
1:e:23:HIS:CG	1:i:66:ARG:HH12	1.52	1.27
1:N:19:MET:CE	1:P:13:MET:HE3	1.63	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:13:MET:O	1:7:16:VAL:HG12	1.21	1.25
1:i:19:MET:HE2	1:Q:13:MET:CE	1.45	1.25
1:K:19:MET:CE	1:d:13:MET:HE3	1.64	1.25
1:X:66:ARG:CZ	1:X:153[B]:LEU:HD11	1.67	1.25
1:z:19:MET:CE	1:Y:17:LYS:HB2	1.67	1.25
1:h:71:LYS:HG3	1:h:148[B]:ASN:OD1	1.07	1.24
1:2:129:LYS:NZ	1:2:145[A]:ARG:NH2	1.83	1.24
1:m:66:ARG:NH2	1:I:22:THR:O	1.70	1.24
1:v:17:LYS:CB	1:R:19:MET:HE1	1.66	1.24
1:E:17:LYS:HB2	1:J:19:MET:CE	1.65	1.24
1:z:19:MET:CE	1:Y:17:LYS:CB	2.15	1.24
1:C:129:LYS:NZ	1:C:147:ILE:HG21	1.50	1.24
1:K:19:MET:CE	1:d:13:MET:CE	2.16	1.24
1:u:13:MET:HE3	1:B:19:MET:CE	1.68	1.23
1:w:19:MET:CE	1:V:13:MET:HE3	1.66	1.23
1:W:13:MET:O	1:W:16:VAL:HG12	1.09	1.22
1:2:13:MET:O	1:2:16:VAL:HG13	1.40	1.21
1:M:129:LYS:NZ	1:M:147:ILE:HG21	1.56	1.20
1:2:129:LYS:HZ1	1:2:145[A]:ARG:NH2	1.33	1.20
1:n:23:HIS:CE1	1:G:17:LYS:HZ2	1.60	1.20
1:x:145:ARG:HD2	3:x:455:HOH:O	1.37	1.19
1:S:13:MET:O	1:S:16:VAL:HG12	1.41	1.19
1:F:145:ARG:HD2	3:F:333:HOH:O	1.06	1.19
1:n:23:HIS:HE1	1:G:17:LYS:NZ	1.39	1.19
1:M:13:MET:C	1:M:16:VAL:HG12	1.69	1.18
1:P:16:VAL:HG23	1:W:16:VAL:HG21	1.23	1.18
1:6:12:THR:HG21	1:F:12:THR:CG2	1.72	1.17
1:Q:71:LYS:HE2	1:Q:148[A]:ASN:OD1	1.42	1.16
1:v:13:MET:O	1:v:16:VAL:HG12	1.45	1.16
1:Z:146:ILE:HD11	3:Z:377:HOH:O	1.44	1.15
1:n:19:MET:HE2	1:G:13:MET:HE1	1.18	1.15
1:n:129:LYS:NZ	1:n:145[B]:ARG:NH2	1.96	1.14
1:l:13:MET:HE1	1:E:12:THR:HG22	1.28	1.14
1:i:13:MET:HA	1:i:16:VAL:HG12	1.14	1.14
1:n:23:HIS:CE1	1:G:17:LYS:NZ	2.15	1.14
1:I:22:THR:HG22	3:I:436:HOH:O	1.47	1.13
1:i:13:MET:HA	1:i:16:VAL:CG1	1.77	1.13
1:v:17:LYS:HB2	1:R:19:MET:HE1	1.13	1.13
1:6:13:MET:O	1:6:16:VAL:HG12	1.46	1.12
1:G:19:MET:HE3	1:M:13:MET:HE1	1.30	1.12
1:p:13:MET:HE2	1:p:13:MET:HA	1.14	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:91[A]:ARG:HD2	3:K:327:HOH:O	1.51	1.11
1:o:13:MET:HA	1:o:16:VAL:CG1	1.80	1.11
1:v:13:MET:HE2	1:v:13:MET:HA	1.27	1.11
1:R:22:THR:HG22	3:R:499:HOH:O	1.48	1.11
1:e:13:MET:SD	1:Q:19:MET:SD	2.49	1.10
1:k:71:LYS:HD3	1:k:148[B]:ASN:OD1	1.48	1.10
1:2:13:MET:HA	1:2:16:VAL:CG1	1.79	1.10
1:i:19:MET:CE	1:Q:13:MET:HE1	1.65	1.10
1:C:129:LYS:NZ	1:C:147:ILE:CG2	2.13	1.09
1:G:19:MET:CE	1:M:13:MET:CE	1.90	1.09
1:K:91[A]:ARG:HD3	1:K:171:ILE:HD11	1.34	1.09
1:b:19:MET:O	1:b:22:THR:HG22	1.50	1.09
1:t:15:ALA:HB3	1:C:13:MET:HE1	1.24	1.09
1:l:18:ARG:HB2	3:l:464:HOH:O	1.50	1.09
1:u:13:MET:HE3	1:B:19:MET:HE2	1.35	1.09
1:l:13:MET:HE1	1:E:12:THR:CG2	1.80	1.09
1:2:13:MET:O	1:2:16:VAL:CG1	2.00	1.09
1:6:19:MET:HE1	1:F:13:MET:SD	1.92	1.09
1:W:13:MET:O	1:W:16:VAL:CG1	1.99	1.09
1:K:71:LYS:HG3	1:K:148[B]:ASN:OD1	1.50	1.08
1:i:13:MET:CA	1:i:16:VAL:HG12	1.83	1.08
1:v:12:THR:HG23	1:v:13:MET:HE3	1.12	1.08
1:G:14:ARG:O	1:G:18:ARG:HG3	1.53	1.08
1:M:129:LYS:HZ2	1:M:147:ILE:HG21	0.92	1.08
1:N:19:MET:HE3	1:P:13:MET:CE	1.81	1.08
1:M:129:LYS:NZ	1:M:147:ILE:CG2	2.16	1.08
1:5:13:MET:O	1:5:16:VAL:CG1	2.02	1.08
1:F:19:MET:HE3	1:O:13:MET:HE3	1.31	1.08
1:N:19:MET:HE3	1:P:13:MET:HE3	1.19	1.08
1:i:19:MET:HE3	1:Q:13:MET:HE1	1.15	1.07
1:t:15:ALA:CB	1:C:13:MET:HE1	1.83	1.07
1:F:19:MET:HE2	1:O:13:MET:HE3	1.34	1.07
1:R:17:LYS:NZ	1:R:21:ASN:ND2	2.02	1.07
1:i:19:MET:HE3	1:Q:13:MET:CE	1.59	1.07
1:h:71:LYS:CG	1:h:148[B]:ASN:OD1	2.02	1.07
1:w:19:MET:HE2	1:V:13:MET:HE3	1.07	1.07
1:v:17:LYS:CA	1:R:19:MET:HE1	1.83	1.07
1:n:19:MET:HE2	1:G:13:MET:HE3	1.33	1.06
1:U:19:MET:HE3	1:Z:13:MET:CE	1.84	1.06
1:b:13:MET:HA	1:b:16:VAL:HG12	1.37	1.06
1:x:66:ARG:HG3	1:x:66:ARG:HH11	1.00	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:71:LYS:HD3	1:4:148[B]:ASN:HD21	1.19	1.06
1:5:19:MET:CE	1:H:13:MET:HE3	1.83	1.06
1:M:64[A]:GLN:HE21	1:M:153:LEU:HD13	1.14	1.06
1:x:12:THR:HB	3:x:394:HOH:O	1.55	1.06
1:6:13:MET:SD	1:O:12:THR:HG21	1.95	1.05
1:v:12:THR:HG23	1:v:13:MET:CE	1.85	1.05
1:M:64[A]:GLN:HE21	1:M:153:LEU:CD1	1.69	1.05
1:P:23:HIS:HE1	1:W:17:LYS:NZ	1.53	1.05
1:n:129:LYS:HZ1	1:n:145[B]:ARG:NH2	1.48	1.05
1:x:71:LYS:HD2	1:x:146:ILE:HD11	1.35	1.05
1:A:13:MET:N	1:A:13:MET:HE2	1.71	1.05
1:s:13:MET:CE	1:O:19:MET:HE3	1.86	1.05
1:w:129:LYS:HD3	3:w:449:HOH:O	1.55	1.05
1:3:16:VAL:HG21	1:C:16:VAL:HG23	1.10	1.04
1:P:120:LEU:CB	1:S:28[B]:ARG:NH2	2.20	1.04
1:v:17:LYS:HB2	1:R:19:MET:CE	1.88	1.04
1:2:91:ARG:HH11	1:2:93:ASN:HD22	1.04	1.04
1:s:16:VAL:HG21	1:O:16:VAL:HG23	1.34	1.03
1:Y:13:MET:HA	1:Y:16:VAL:CG1	1.88	1.03
1:e:23:HIS:CG	1:i:66:ARG:NH1	2.22	1.03
1:D:91:ARG:HH11	1:D:93:ASN:HD22	1.07	1.03
1:z:19:MET:HE2	1:Y:17:LYS:HA	1.39	1.03
1:X:66:ARG:CZ	1:X:153[B]:LEU:CD1	2.36	1.03
1:F:19:MET:HE3	1:O:13:MET:CE	1.89	1.02
1:G:19:MET:HE1	1:M:13:MET:HE3	1.05	1.02
1:w:19:MET:CE	1:V:13:MET:CE	2.36	1.02
1:z:91:ARG:HH11	1:z:93:ASN:HD22	1.06	1.02
1:f:13:MET:HE3	1:m:19:MET:HE3	1.35	1.02
1:v:17:LYS:HA	1:R:19:MET:CE	1.90	1.02
1:t:13:MET:HB3	1:3:19:MET:HE1	1.42	1.02
1:E:17:LYS:CA	1:J:19:MET:HE1	1.89	1.02
1:F:19:MET:CE	1:O:13:MET:CE	2.37	1.02
1:e:23:HIS:HA	1:i:66:ARG:HH11	1.21	1.01
1:n:16:VAL:HG23	1:G:16:VAL:HG21	1.38	1.01
1:t:13:MET:SD	1:3:12:THR:HG21	2.00	1.01
1:m:17:LYS:HZ2	1:I:23:HIS:HE1	1.02	1.01
1:z:13:MET:HE3	1:S:19:MET:HE1	1.42	1.01
1:K:145[B]:ARG:HH11	1:K:145[B]:ARG:CG	1.74	1.01
1:R:17:LYS:HZ1	1:R:21:ASN:HD21	1.08	1.01
1:X:66:ARG:NH2	1:X:153[B]:LEU:CD1	2.24	1.01
1:i:71:LYS:HD3	1:i:148[B]:ASN:OD1	1.60	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:19:MET:CE	1:G:13:MET:CE	2.39	1.01
1:O:91:ARG:HH11	1:O:93:ASN:HD22	1.08	1.01
1:f:91:ARG:HH11	1:f:93:ASN:HD22	1.06	1.01
1:G:91[B]:ARG:HE	1:G:93:ASN:HD21	1.05	1.00
1:K:19:MET:HE1	1:d:13:MET:HE3	1.39	1.00
1:i:91:ARG:HH11	1:i:93:ASN:HD22	1.03	1.00
1:3:133:LEU:HD21	1:3:145[B]:ARG:HD2	1.39	1.00
1:Q:71:LYS:CE	1:Q:148[A]:ASN:OD1	2.09	1.00
1:b:13:MET:HA	1:b:16:VAL:CG1	1.90	1.00
1:b:150:PRO:HG2	3:b:359:HOH:O	1.61	1.00
1:z:12:THR:HA	3:z:448:HOH:O	1.59	1.00
1:4:71:LYS:HD3	1:4:148[B]:ASN:ND2	1.73	1.00
1:a:13:MET:HE2	1:a:13:MET:HA	1.40	1.00
1:6:19:MET:CE	1:F:13:MET:SD	2.50	1.00
1:U:19:MET:HE3	1:Z:13:MET:HE2	1.40	1.00
1:o:91:ARG:HH11	1:o:93:ASN:HD22	1.06	0.99
1:U:91[A]:ARG:HH11	1:U:93:ASN:HD22	1.10	0.99
1:5:19:MET:HE3	1:H:13:MET:HE1	1.44	0.99
1:M:13:MET:CA	1:M:16:VAL:HG12	1.90	0.99
3:g:466:HOH:O	1:l:96:ARG:HG2	1.61	0.99
1:K:71:LYS:CG	1:K:148[B]:ASN:OD1	2.09	0.99
1:h:91:ARG:HH11	1:h:93:ASN:HD22	1.06	0.99
1:5:19:MET:CE	1:H:13:MET:CE	2.40	0.99
1:v:13:MET:O	1:v:16:VAL:CG1	2.10	0.99
1:M:13:MET:O	1:M:16:VAL:N	1.96	0.98
1:U:19:MET:CE	1:Z:13:MET:HE3	1.93	0.98
1:5:13:MET:O	1:5:16:VAL:HG13	1.60	0.98
1:T:23:HIS:HE1	1:c:17:LYS:HZ2	1.08	0.98
1:2:129:LYS:CE	1:2:145[A]:ARG:HH21	1.75	0.98
1:o:17:LYS:NZ	1:u:23:HIS:HE1	1.62	0.98
1:B:17:LYS:HE3	1:B:21:ASN:ND2	1.78	0.98
1:M:64[A]:GLN:NE2	1:M:153:LEU:CD1	2.26	0.98
1:N:16:VAL:HG23	1:P:16:VAL:HG21	1.44	0.98
1:x:66:ARG:HD2	1:x:66:ARG:C	1.87	0.98
1:6:12:THR:HG21	1:F:12:THR:HG23	1.45	0.98
1:M:13:MET:O	1:M:16:VAL:CG1	2.10	0.98
1:Q:91:ARG:HH11	1:Q:93:ASN:HD22	1.03	0.98
1:U:19:MET:CE	1:Z:13:MET:CE	2.41	0.98
1:q:91:ARG:HH11	1:q:93:ASN:HD22	1.02	0.97
1:V:71:LYS:HD3	1:V:146:ILE:HD11	1.45	0.97
1:f:13:MET:CE	1:m:19:MET:HE3	1.93	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:13:MET:CE	1:E:12:THR:HG22	1.94	0.97
1:2:17:LYS:HE3	1:2:21:ASN:HD21	1.28	0.97
1:f:13:MET:O	1:f:16:VAL:HG12	1.64	0.97
1:h:13:MET:O	1:h:16:VAL:CG1	2.11	0.97
1:w:19:MET:HE2	1:V:13:MET:CE	1.94	0.97
1:h:152:GLN:HG3	3:h:461:HOH:O	1.62	0.97
1:x:13:MET:O	1:x:16:VAL:HG12	1.63	0.97
1:3:91[A]:ARG:HH11	1:3:93:ASN:HD22	1.10	0.97
1:O:12:THR:HG23	1:O:12:THR:O	1.63	0.97
1:R:91:ARG:HH11	1:R:93:ASN:HD22	1.04	0.97
1:t:91[A]:ARG:HH11	1:t:93:ASN:HD22	1.09	0.97
1:N:13:MET:O	1:N:16:VAL:HG12	1.65	0.97
1:q:17:LYS:NZ	1:V:23:HIS:HE1	1.62	0.96
1:y:13:MET:O	1:y:16:VAL:HG13	1.63	0.96
1:2:17:LYS:HE3	1:2:21:ASN:ND2	1.80	0.96
1:M:64[A]:GLN:CG	1:M:153:LEU:HD11	1.95	0.96
1:T:91:ARG:HH11	1:T:93:ASN:HD22	1.13	0.96
1:p:91:ARG:HH11	1:p:93:ASN:HD22	1.12	0.96
1:3:16:VAL:HG21	1:C:16:VAL:CG2	1.95	0.96
1:b:13:MET:CA	1:b:16:VAL:HG12	1.96	0.96
1:f:146:ILE:HD12	3:F:420:HOH:O	1.65	0.96
1:v:13:MET:HE2	1:v:13:MET:CA	1.94	0.96
1:v:12:THR:CG2	1:v:13:MET:HE3	1.96	0.95
1:E:17:LYS:NZ	1:E:21:ASN:HD21	1.62	0.95
1:S:148:ASN:HB2	3:S:450:HOH:O	1.66	0.95
1:A:91[A]:ARG:HH11	1:A:93:ASN:HD22	1.07	0.95
1:n:23:HIS:HE1	1:G:17:LYS:HZ1	1.12	0.95
1:J:91:ARG:HH11	1:J:93:ASN:HD22	1.04	0.95
1:q:91:ARG:HH11	1:q:93:ASN:ND2	1.64	0.95
1:I:140[B]:GLU:OE1	1:I:143:LYS:HE2	1.63	0.95
1:2:129:LYS:NZ	1:2:145[A]:ARG:CZ	2.29	0.95
1:C:91:ARG:HH11	1:C:93:ASN:HD22	1.06	0.95
1:L:91[B]:ARG:HE	1:L:93:ASN:ND2	1.63	0.95
1:1:91[A]:ARG:NH1	1:1:152:GLN:HB2	1.81	0.95
1:A:13:MET:HA	1:A:16:VAL:CG1	1.95	0.95
1:R:17:LYS:HZ2	1:R:21:ASN:HD21	1.11	0.95
1:u:91:ARG:HH11	1:u:93:ASN:HD22	1.12	0.95
1:O:13:MET:HA	1:O:16:VAL:CG1	1.95	0.95
1:J:12:THR:O	1:J:16:VAL:HG12	1.67	0.95
1:f:13:MET:CE	1:m:19:MET:CE	2.45	0.94
1:Z:91[A]:ARG:HH11	1:Z:93:ASN:HD22	1.07	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:17:LYS:NZ	1:X:23:HIS:HE1	1.64	0.94
1:P:19:MET:CE	1:W:13:MET:SD	2.55	0.94
1:Y:13:MET:HA	1:Y:16:VAL:HG12	1.47	0.94
1:g:91:ARG:HH11	1:g:93:ASN:HD22	1.11	0.94
1:1:18:ARG:HD2	3:1:389:HOH:O	1.68	0.94
1:C:129:LYS:HZ2	1:C:147:ILE:HG21	1.15	0.94
1:a:91:ARG:HH11	1:a:93:ASN:HD22	1.10	0.94
1:k:91:ARG:HH11	1:k:93:ASN:HD22	1.12	0.94
1:t:13:MET:HA	1:t:16:VAL:HG12	1.50	0.94
1:O:13:MET:HA	1:O:16:VAL:HG12	1.47	0.94
1:X:91:ARG:HH11	1:X:93:ASN:HD22	1.15	0.94
1:b:13:MET:O	1:b:16:VAL:CG1	2.16	0.94
1:g:91:ARG:HH11	1:g:93:ASN:ND2	1.65	0.93
1:D:72:LEU:O	1:D:146[A]:ILE:HD12	1.68	0.93
1:K:152[A]:GLN:HG3	3:K:534:HOH:O	1.66	0.93
1:B:91[B]:ARG:HH11	1:B:93:ASN:HD22	1.11	0.93
1:W:91:ARG:HH11	1:W:93:ASN:HD22	1.04	0.93
1:i:91:ARG:HH11	1:i:93:ASN:ND2	1.66	0.93
1:5:23:HIS:HE1	1:H:17:LYS:HZ2	1.10	0.93
1:6:28[B]:ARG:HH12	1:I:117:PRO:HG3	1.29	0.93
1:f:13:MET:HE3	1:m:19:MET:HE1	1.50	0.93
1:s:13:MET:HE3	1:O:19:MET:CE	1.98	0.93
1:v:17:LYS:HA	1:R:19:MET:HE2	1.48	0.93
1:f:19:MET:HE3	1:I:13:MET:HE3	1.50	0.93
1:p:19:MET:HE3	1:y:13:MET:HE3	1.50	0.93
1:L:66:ARG:NH1	3:L:433:HOH:O	2.02	0.93
1:N:71:LYS:HD3	1:N:148[A]:ASN:OD1	1.69	0.93
1:p:19:MET:HE3	1:y:13:MET:CE	1.97	0.93
1:x:91[B]:ARG:HH11	1:x:93:ASN:HD22	1.08	0.93
1:K:91[B]:ARG:HH11	1:K:93:ASN:HD22	1.07	0.93
1:3:12:THR:OG1	1:3:15:ALA:HB3	1.68	0.93
1:G:91[B]:ARG:HE	1:G:93:ASN:ND2	1.66	0.93
1:o:17:LYS:HZ1	1:u:23:HIS:HE1	1.08	0.93
1:s:91:ARG:HH11	1:s:93:ASN:HD22	1.15	0.92
1:b:91:ARG:HH11	1:b:93:ASN:HD22	1.14	0.92
1:e:23:HIS:CE1	1:i:66:ARG:HH22	1.86	0.92
1:5:91:ARG:HH11	1:5:93:ASN:HD22	1.10	0.92
1:B:13:MET:HA	1:B:16:VAL:CG1	1.98	0.92
1:M:13:MET:HA	1:M:16:VAL:CG1	1.99	0.92
1:M:13:MET:HA	1:M:16:VAL:HG12	1.50	0.92
1:j:17:LYS:NZ	1:y:23:HIS:HE1	1.67	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:71:LYS:CD	1:N:148[A]:ASN:OD1	2.18	0.92
1:P:150:PRO:HG2	3:P:546:HOH:O	1.69	0.92
1:q:17:LYS:NZ	1:V:23:HIS:CE1	2.37	0.92
1:5:19:MET:HE3	1:H:13:MET:CE	2.00	0.92
1:E:91:ARG:HH11	1:E:93:ASN:HD22	1.16	0.92
1:P:14:ARG:HH11	1:P:14:ARG:HB2	1.31	0.92
1:m:17:LYS:NZ	1:I:23:HIS:HE1	1.66	0.92
1:x:71:LYS:HG3	1:x:148[B]:ASN:OD1	1.69	0.92
1:7:13:MET:O	1:7:16:VAL:CG1	2.15	0.92
1:7:91:ARG:HH11	1:7:93:ASN:HD22	1.14	0.92
1:o:17:LYS:NZ	1:u:23:HIS:CE1	2.38	0.92
1:W:17:LYS:HE3	1:W:21:ASN:HD21	1.34	0.92
1:s:13:MET:HE2	1:0:19:MET:HE3	1.47	0.91
1:y:91:ARG:HH11	1:y:93:ASN:HD22	1.16	0.91
1:j:13:MET:O	1:j:16:VAL:HG12	1.71	0.91
1:z:19:MET:CE	1:Y:17:LYS:CG	2.48	0.91
1:H:91[B]:ARG:HH21	1:H:93:ASN:HD22	1.11	0.91
1:v:17:LYS:CA	1:R:19:MET:CE	2.47	0.91
1:6:91:ARG:HH11	1:6:93:ASN:HD22	1.13	0.91
1:e:23:HIS:CE1	1:i:66:ARG:HH12	1.89	0.91
1:e:148:ASN:HB2	3:e:384:HOH:O	1.69	0.91
1:A:31[B]:LEU:HD11	3:A:533:HOH:O	1.69	0.91
1:p:13:MET:HA	1:p:13:MET:CE	2.00	0.91
1:H:13:MET:HA	1:H:16:VAL:CG1	2.00	0.91
1:d:12:THR:N	3:d:469:HOH:O	2.04	0.91
1:p:13:MET:HE2	1:p:13:MET:CA	2.01	0.91
1:P:129:LYS:HE3	1:P:147:ILE:HG21	1.50	0.91
1:z:19:MET:CE	1:Y:17:LYS:CA	2.48	0.90
1:H:18:ARG:O	1:H:22:THR:HG23	1.71	0.90
1:W:71:LYS:HD2	1:W:146:ILE:HD11	1.53	0.90
1:j:91:ARG:HH11	1:j:93:ASN:HD22	1.17	0.90
1:r:19:MET:CE	1:b:13:MET:HE3	2.00	0.90
1:r:66[A]:ARG:HG2	3:r:469:HOH:O	1.72	0.90
1:z:19:MET:HE3	1:Y:17:LYS:HG3	1.53	0.90
1:N:19:MET:CE	1:P:13:MET:CE	2.45	0.90
1:2:13:MET:HA	1:2:16:VAL:HG11	1.51	0.90
1:6:17:LYS:HB3	3:6:485:HOH:O	1.70	0.90
1:G:19:MET:HE3	1:M:13:MET:HE2	1.49	0.90
1:P:23:HIS:CE1	1:W:17:LYS:NZ	2.39	0.90
1:P:23:HIS:CE1	1:W:17:LYS:HZ3	1.89	0.90
1:1:129:LYS:NZ	1:1:145:ARG:HH12	1.69	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:91:ARG:HH11	1:Q:93:ASN:ND2	1.69	0.90
1:x:66:ARG:HG3	1:x:66:ARG:NH1	1.73	0.90
1:V:14:ARG:HB2	1:V:14:ARG:HH11	1.36	0.90
1:p:13:MET:HE2	1:p:16:VAL:HG11	1.52	0.90
1:q:17:LYS:HZ1	1:V:23:HIS:HE1	1.11	0.89
1:J:145:ARG:HD3	1:J:147:ILE:HD11	1.54	0.89
1:r:19:MET:HE3	1:b:13:MET:HE3	1.54	0.89
1:I:91:ARG:HH11	1:I:93:ASN:HD22	1.17	0.89
1:N:12:THR:HA	3:N:457:HOH:O	1.72	0.89
1:b:12:THR:HA	3:b:481:HOH:O	1.71	0.89
1:t:13:MET:HE3	1:t:16:VAL:HG11	1.54	0.89
1:6:37:THR:HG22	3:6:493:HOH:O	1.71	0.89
1:M:64[A]:GLN:HG3	1:M:153:LEU:HD11	1.53	0.89
1:N:71:LYS:HG3	1:N:148[A]:ASN:OD1	1.70	0.89
1:h:16:VAL:HG13	1:v:19:MET:SD	2.13	0.89
1:M:91:ARG:HH11	1:M:93:ASN:HD22	1.17	0.89
1:l:91:ARG:HH11	1:l:93:ASN:HD22	1.15	0.89
1:4:91:ARG:HH11	1:4:93:ASN:HD22	1.09	0.89
1:A:13:MET:HE2	1:A:13:MET:CA	2.02	0.89
1:I:71:LYS:HG2	1:I:146[B]:ILE:HD11	1.55	0.89
1:w:91:ARG:HH11	1:w:93:ASN:HD22	1.21	0.89
1:x:66:ARG:HD2	1:x:67:ILE:N	1.86	0.89
1:1:91[A]:ARG:NH1	3:1:443:HOH:O	2.06	0.89
1:t:13:MET:HA	1:t:16:VAL:CG1	2.03	0.89
1:f:16:VAL:HG23	1:I:16:VAL:HG21	1.54	0.88
1:B:91[B]:ARG:HH11	1:B:93:ASN:ND2	1.71	0.88
1:J:91:ARG:HH11	1:J:93:ASN:ND2	1.70	0.88
1:w:19:MET:HE1	1:V:16:VAL:CG1	2.03	0.88
1:z:19:MET:CE	1:Y:17:LYS:HG3	2.03	0.88
1:G:16:VAL:HG23	1:M:16:VAL:HG21	1.54	0.88
1:6:28[B]:ARG:NH1	1:I:117:PRO:HG3	1.86	0.88
1:s:12:THR:O	1:s:15:ALA:N	2.05	0.88
1:1:91[B]:ARG:HE	1:1:93:ASN:ND2	1.71	0.88
1:N:71:LYS:CG	1:N:148[A]:ASN:OD1	2.22	0.88
1:N:19:MET:HE1	1:P:13:MET:HE3	1.56	0.88
1:z:13:MET:CE	1:S:19:MET:CE	2.22	0.88
1:B:17:LYS:HE3	1:B:21:ASN:HD21	1.31	0.88
1:n:19:MET:CE	1:G:13:MET:HE3	2.00	0.88
1:n:91:ARG:HH11	1:n:93:ASN:HD22	1.22	0.88
1:V:91:ARG:HH11	1:V:93:ASN:HD22	1.14	0.88
1:p:23:HIS:HE1	1:y:17:LYS:NZ	1.71	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:131:VAL:CG1	1:3:145[B]:ARG:HD3	2.04	0.87
1:K:91[A]:ARG:HD3	1:K:171:ILE:CD1	2.04	0.87
1:5:23:HIS:HE1	1:H:17:LYS:NZ	1.71	0.87
1:A:84:THR:HG22	3:A:452:HOH:O	1.73	0.87
1:K:12:THR:HA	3:K:469:HOH:O	1.74	0.87
1:m:91:ARG:HH11	1:m:93:ASN:HD22	1.19	0.87
1:K:19:MET:HE3	1:d:13:MET:HE2	1.55	0.87
1:Y:13:MET:CA	1:Y:16:VAL:HG12	2.04	0.87
1:2:129:LYS:HZ1	1:2:145[A]:ARG:CZ	1.86	0.87
1:1:71:LYS:HD2	1:1:146:ILE:HD11	1.55	0.87
1:o:91:ARG:HH11	1:o:93:ASN:ND2	1.71	0.87
1:p:19:MET:CE	1:y:13:MET:HE3	2.05	0.87
1:5:13:MET:O	1:5:16:VAL:HG12	1.72	0.87
1:B:13:MET:HA	1:B:16:VAL:HG12	1.56	0.87
1:A:31[B]:LEU:HD12	3:A:426:HOH:O	1.75	0.87
1:s:13:MET:CE	1:0:19:MET:CE	2.53	0.86
1:z:19:MET:HE1	1:Y:17:LYS:CG	2.06	0.86
1:2:13:MET:CA	1:2:16:VAL:CG1	2.52	0.86
1:M:64[A]:GLN:NE2	1:M:153:LEU:HD13	1.86	0.86
1:v:71:LYS:HD3	1:v:146:ILE:HD11	1.57	0.86
1:w:162[A]:VAL:HG11	3:w:416:HOH:O	1.75	0.86
1:N:91[B]:ARG:HH11	1:N:93:ASN:HD22	1.22	0.86
1:X:13:MET:O	1:X:16:VAL:HG12	1.74	0.86
1:N:23:HIS:HE1	1:P:17:LYS:HZ2	1.17	0.86
1:d:91:ARG:HH11	1:d:93:ASN:HD22	1.16	0.86
1:k:81:VAL:HB	3:k:469:HOH:O	1.76	0.86
1:v:91:ARG:HH11	1:v:93:ASN:HD22	1.23	0.86
1:1:17:LYS:HZ2	1:X:23:HIS:HE1	1.16	0.86
1:C:12:THR:HG23	1:C:12:THR:O	1.76	0.86
1:C:91:ARG:HH11	1:C:93:ASN:ND2	1.72	0.86
1:G:14:ARG:O	1:G:18:ARG:CG	2.23	0.86
1:o:13:MET:HA	1:o:16:VAL:HG11	1.58	0.86
1:t:13:MET:SD	1:3:12:THR:CG2	2.64	0.86
1:P:23:HIS:HE1	1:W:17:LYS:HZ3	1.17	0.85
1:c:13:MET:HA	1:c:16:VAL:CG1	2.06	0.85
1:x:66:ARG:HH11	1:x:66:ARG:CG	1.89	0.85
1:3:16:VAL:CG2	1:C:16:VAL:HG23	2.01	0.85
1:D:91:ARG:HH11	1:D:93:ASN:ND2	1.74	0.85
1:E:17:LYS:HA	1:J:19:MET:CE	2.06	0.85
1:M:64[A]:GLN:CD	1:M:153:LEU:HD11	2.00	0.85
1:N:17:LYS:NZ	1:N:21:ASN:HD21	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:129:LYS:NZ	1:2:145[A]:ARG:HH21	1.64	0.85
1:4:91:ARG:HH11	1:4:93:ASN:ND2	1.74	0.85
1:K:19:MET:HE3	1:d:13:MET:HE1	1.53	0.85
1:u:13:MET:HE3	1:B:19:MET:HE3	1.57	0.85
1:M:64[A]:GLN:NE2	1:M:153:LEU:HD11	1.90	0.85
1:s:91:ARG:HH11	1:s:93:ASN:ND2	1.74	0.85
1:0:71:LYS:HD3	1:0:146:ILE:HD11	1.59	0.85
1:P:16:VAL:HG23	1:W:16:VAL:CG2	2.06	0.85
1:l:91:ARG:HH11	1:l:93:ASN:ND2	1.74	0.85
1:f:91:ARG:HH11	1:f:93:ASN:ND2	1.75	0.85
1:S:28[B]:ARG:HD2	1:S:191:VAL:HG22	1.60	0.84
1:U:16:VAL:HG23	1:Z:16:VAL:HG21	1.59	0.84
1:c:91[B]:ARG:HH11	1:c:93:ASN:ND2	1.75	0.84
1:p:26:HIS:HE1	3:p:455:HOH:O	1.60	0.84
1:a:14:ARG:HG2	3:a:457:HOH:O	1.77	0.84
1:w:145[B]:ARG:NH1	1:w:146:ILE:O	2.10	0.84
1:3:13:MET:O	1:3:16:VAL:CG1	2.26	0.84
1:T:23:HIS:HE1	1:c:17:LYS:NZ	1.75	0.84
1:X:66:ARG:HH22	1:X:153[B]:LEU:HD11	1.40	0.84
1:A:13:MET:N	1:A:13:MET:CE	2.41	0.84
1:G:143:LYS:HE2	3:G:439:HOH:O	1.75	0.84
1:S:28[B]:ARG:CD	1:S:191:VAL:HG22	2.06	0.84
1:6:13:MET:O	1:6:16:VAL:CG1	2.24	0.84
1:E:17:LYS:CA	1:J:19:MET:CE	2.54	0.84
1:p:91:ARG:HH11	1:p:93:ASN:ND2	1.75	0.84
1:A:12:THR:C	1:A:13:MET:HE2	2.02	0.84
1:V:14:ARG:NH1	1:V:14:ARG:CB	2.40	0.84
1:h:23:HIS:HE1	1:R:17:LYS:NZ	1.75	0.84
1:z:13:MET:HE1	1:S:19:MET:HE3	1.60	0.84
1:2:129:LYS:CE	1:2:145[A]:ARG:NH2	2.37	0.84
1:H:91[B]:ARG:HH21	1:H:93:ASN:ND2	1.76	0.84
1:4:13:MET:C	1:4:16:VAL:HG12	2.03	0.83
1:A:91[A]:ARG:HH11	1:A:93:ASN:ND2	1.75	0.83
1:r:91:ARG:HH11	1:r:93:ASN:HD22	1.26	0.83
1:2:19:MET:O	1:2:22[B]:THR:HG22	1.77	0.83
1:t:91[A]:ARG:HH11	1:t:93:ASN:ND2	1.73	0.83
1:D:19:MET:HG3	3:D:442:HOH:O	1.77	0.83
1:q:16:VAL:HG21	1:V:16:VAL:HG23	1.59	0.83
1:4:17:LYS:HG2	3:4:430:HOH:O	1.78	0.83
1:G:14:ARG:HB3	1:G:18:ARG:HH21	1.41	0.83
1:1:17:LYS:NZ	1:X:23:HIS:CE1	2.45	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:13:MET:O	1:3:16:VAL:HG13	1.77	0.83
1:Q:66:ARG:HG2	3:Q:553:HOH:O	1.76	0.83
1:Z:17:LYS:HE3	1:Z:21:ASN:ND2	1.94	0.83
1:q:17:LYS:HZ2	1:V:23:HIS:CE1	1.96	0.83
1:m:17:LYS:NZ	1:I:23:HIS:CE1	2.46	0.83
1:6:91:ARG:HH11	1:6:93:ASN:ND2	1.75	0.83
1:R:17:LYS:CE	1:R:21:ASN:ND2	2.42	0.83
1:d:91:ARG:HH11	1:d:93:ASN:ND2	1.77	0.83
1:m:17:LYS:HZ2	1:I:23:HIS:CE1	1.94	0.83
1:w:179:SER:OG	1:w:181:VAL:HG12	1.79	0.83
1:E:13:MET:O	1:E:16:VAL:HG12	1.79	0.83
1:P:152:GLN:HG3	3:P:416:HOH:O	1.77	0.83
1:j:13:MET:C	1:j:16:VAL:HG12	2.03	0.83
1:x:91[B]:ARG:HH11	1:x:93:ASN:ND2	1.76	0.83
1:z:19:MET:HE2	1:Y:17:LYS:CA	2.08	0.83
1:7:91:ARG:HH11	1:7:93:ASN:ND2	1.76	0.83
1:i:19:MET:CE	1:Q:13:MET:SD	2.66	0.82
1:s:23:HIS:HE1	1:2:17:LYS:NZ	1.77	0.82
1:2:91:ARG:HH11	1:2:93:ASN:ND2	1.77	0.82
1:R:91:ARG:HH11	1:R:93:ASN:ND2	1.77	0.82
1:n:13:MET:O	1:n:16:VAL:HG12	1.79	0.82
1:x:23:HIS:HE1	1:T:17:LYS:HZ2	1.25	0.82
1:y:91:ARG:HH11	1:y:93:ASN:ND2	1.76	0.82
1:P:120:LEU:HB3	1:S:28[B]:ARG:HH22	1.03	0.82
1:l:43:THR:OG1	1:l:45:GLN:NE2	2.13	0.82
1:z:91:ARG:HH11	1:z:93:ASN:ND2	1.77	0.82
1:6:12:THR:CG2	1:F:12:THR:CG2	2.57	0.82
1:C:129:LYS:HZ2	1:C:147:ILE:CG2	1.83	0.82
1:K:91[B]:ARG:HH11	1:K:93:ASN:ND2	1.78	0.82
1:z:13:MET:HE3	1:S:19:MET:HE3	0.84	0.82
1:E:17:LYS:CB	1:J:19:MET:CE	2.37	0.82
1:E:17:LYS:HB2	1:J:19:MET:HE1	0.85	0.82
1:x:23:HIS:HE1	1:T:17:LYS:NZ	1.76	0.82
1:1:45[B]:GLN:HG3	3:1:428:HOH:O	1.78	0.82
1:M:91:ARG:HH11	1:M:93:ASN:ND2	1.77	0.82
1:i:19:MET:HE2	1:Q:13:MET:HE3	0.82	0.82
1:3:13:MET:HA	1:3:16:VAL:CG1	2.10	0.81
1:j:91:ARG:HH11	1:j:93:ASN:ND2	1.77	0.81
1:o:13:MET:HE3	1:u:19:MET:HE3	1.62	0.81
1:q:17:LYS:HE3	1:q:21:ASN:ND2	1.95	0.81
1:u:91:ARG:HH11	1:u:93:ASN:ND2	1.76	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:16:VAL:HG21	1:W:16:VAL:HG23	1.63	0.81
1:O:91:ARG:HH11	1:O:93:ASN:ND2	1.76	0.81
1:P:19:MET:SD	1:W:16:VAL:HG13	2.20	0.81
1:W:91:ARG:HH11	1:W:93:ASN:ND2	1.78	0.81
1:Z:91[A]:ARG:HH11	1:Z:93:ASN:ND2	1.79	0.81
1:b:13:MET:O	1:b:16:VAL:HG12	1.79	0.81
1:b:13:MET:C	1:b:16:VAL:HG12	2.05	0.81
1:f:16:VAL:HG13	1:m:19:MET:SD	2.20	0.81
1:n:18:ARG:HD3	3:n:340:HOH:O	1.78	0.81
1:n:19:MET:CE	1:G:16:VAL:HG11	2.10	0.81
1:w:16:VAL:HG23	1:V:16:VAL:HG21	1.61	0.81
1:I:91:ARG:HH11	1:I:93:ASN:ND2	1.78	0.81
1:p:12:THR:O	1:p:16:VAL:HG12	1.77	0.81
1:u:13:MET:CE	1:B:19:MET:CE	2.57	0.81
1:5:91:ARG:HH11	1:5:93:ASN:ND2	1.78	0.81
1:A:13:MET:HA	1:A:16:VAL:HG12	1.60	0.81
1:e:13:MET:SD	1:Q:19:MET:CE	2.69	0.81
1:K:13:MET:HA	1:K:16:VAL:CG1	2.09	0.81
1:b:13:MET:O	1:b:16:VAL:HG13	1.79	0.81
1:n:19:MET:CE	1:G:13:MET:HE1	2.05	0.81
1:z:12:THR:CA	3:z:448:HOH:O	2.19	0.81
1:Q:31:LEU:CD2	3:Q:537:HOH:O	2.29	0.81
1:r:12:THR:HG23	1:r:13:MET:H	1.46	0.80
1:k:13:MET:HA	1:k:16:VAL:CG1	2.10	0.80
1:s:117:PRO:HA	1:B:28[B]:ARG:HD2	1.61	0.80
1:2:95:ASN:HD21	1:2:98:THR:H	1.29	0.80
1:2:129:LYS:HE3	1:2:145[A]:ARG:HH21	1.46	0.80
1:O:95:ASN:HD21	1:O:98:THR:H	1.28	0.80
1:g:17:LYS:NZ	1:b:23:HIS:HE1	1.78	0.80
1:n:16:VAL:CG2	1:G:16:VAL:HG21	2.11	0.80
1:r:66[B]:ARG:HG2	1:r:66[B]:ARG:HH11	1.46	0.80
1:3:95:ASN:HD21	1:3:98:THR:H	1.28	0.80
1:e:12:THR:HG23	1:e:12:THR:O	1.79	0.80
1:N:23:HIS:HE1	1:P:17:LYS:NZ	1.79	0.80
1:g:17:LYS:HZ2	1:b:23:HIS:HE1	1.27	0.80
1:s:22:THR:O	1:2:66:ARG:NH2	2.15	0.80
1:2:13:MET:C	1:2:16:VAL:CG1	2.55	0.80
1:y:17:LYS:HE3	1:y:21:ASN:ND2	1.97	0.80
1:1:129:LYS:HZ1	1:1:145:ARG:HH12	1.30	0.80
1:2:131:VAL:HG21	1:2:145[A]:ARG:HD3	1.62	0.80
1:X:28:ARG:HD3	3:X:481:HOH:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:19:MET:O	1:g:22:THR:CG2	2.22	0.80
1:F:71:LYS:HD2	1:F:146:ILE:HD11	1.62	0.80
1:n:19:MET:CE	1:G:16:VAL:CG1	2.60	0.79
1:5:19:MET:HE1	1:H:13:MET:HE3	1.62	0.79
1:G:71:LYS:HD2	1:G:146:ILE:HD11	1.62	0.79
1:w:91:ARG:HH11	1:w:93:ASN:ND2	1.79	0.79
1:K:145[B]:ARG:HH11	1:K:145[B]:ARG:HG3	1.45	0.79
1:r:18:ARG:O	1:r:22:THR:HG23	1.81	0.79
1:C:129:LYS:HZ1	1:C:147:ILE:HG21	1.46	0.79
1:0:91[A]:ARG:HH11	1:0:93:ASN:HD22	1.27	0.79
1:R:13:MET:HA	1:R:16:VAL:CG1	2.12	0.79
1:T:95:ASN:HD21	1:T:98:THR:H	1.29	0.79
1:r:19:MET:HE3	1:b:13:MET:CE	2.12	0.79
1:w:162[A]:VAL:HG12	3:w:541:HOH:O	1.82	0.79
1:i:91:ARG:NH1	1:i:93:ASN:HD22	1.77	0.79
1:r:26:HIS:HE1	3:r:441:HOH:O	1.65	0.79
1:6:12:THR:HG21	1:F:12:THR:HG21	1.61	0.79
1:F:15:ALA:HB1	1:O:13:MET:SD	2.21	0.79
1:R:117:PRO:HA	1:X:28:ARG:HD2	1.64	0.79
1:i:13:MET:C	1:i:16:VAL:HG12	2.07	0.79
1:0:91[A]:ARG:HH11	1:0:93:ASN:ND2	1.79	0.79
1:Y:71:LYS:HD3	1:Y:148[A]:ASN:OD1	1.83	0.79
1:i:95:ASN:HD21	1:i:98:THR:H	1.31	0.79
1:n:129:LYS:CE	1:n:145[B]:ARG:HH21	1.95	0.78
1:C:13:MET:O	1:C:16:VAL:HG12	1.82	0.78
1:C:95:ASN:HD21	1:C:98:THR:H	1.30	0.78
1:C:140[B]:GLU:HG3	3:C:376:HOH:O	1.82	0.78
1:E:91:ARG:HH11	1:E:93:ASN:ND2	1.80	0.78
1:R:95:ASN:HD21	1:R:98:THR:H	1.30	0.78
1:X:91:ARG:HH11	1:X:93:ASN:ND2	1.81	0.78
1:t:17:LYS:HE3	1:t:21:ASN:HD21	1.48	0.78
1:B:13:MET:CA	1:B:16:VAL:HG12	2.13	0.78
1:j:17:LYS:HZ3	1:y:23:HIS:HE1	1.30	0.78
1:y:17:LYS:HE3	1:y:21:ASN:HD21	1.47	0.78
1:6:28[A]:ARG:HD2	3:6:404:HOH:O	1.83	0.78
1:E:17:LYS:HZ1	1:E:21:ASN:HD21	1.29	0.78
1:p:23:HIS:HE1	1:y:17:LYS:HZ2	1.29	0.78
1:u:12:THR:HG23	1:u:15:ALA:HB3	1.63	0.78
1:B:13:MET:O	1:B:16:VAL:HG13	1.83	0.78
1:n:129:LYS:NZ	1:n:145[B]:ARG:HH21	1.82	0.78
1:B:12:THR:OG1	1:B:15:ALA:HB3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:71:LYS:CD	1:K:148[B]:ASN:OD1	2.30	0.78
1:h:91:ARG:HH11	1:h:93:ASN:ND2	1.79	0.78
1:3:13:MET:HA	1:3:16:VAL:HG12	1.65	0.78
1:A:13:MET:HE2	1:A:13:MET:HA	1.63	0.78
1:g:117:PRO:HA	1:E:28:ARG:HD2	1.64	0.78
1:N:19:MET:SD	1:P:16:VAL:HG13	2.24	0.78
1:d:12:THR:O	1:d:15:ALA:N	2.15	0.78
1:o:13:MET:HA	1:o:16:VAL:HG12	1.66	0.78
1:P:91[B]:ARG:HH21	1:P:93:ASN:HD22	1.32	0.78
1:j:13:MET:O	1:j:16:VAL:CG1	2.30	0.77
1:E:16:VAL:HG13	1:J:19:MET:SD	2.24	0.77
1:z:19:MET:HE1	1:Y:17:LYS:CA	2.08	0.77
1:3:133:LEU:CD2	1:3:145[B]:ARG:HD2	2.14	0.77
1:B:73:HIS:CG	1:B:146[A]:ILE:HG22	2.20	0.77
1:F:12:THR:O	1:F:15:ALA:HB3	1.83	0.77
1:m:91:ARG:HH11	1:m:93:ASN:ND2	1.83	0.77
1:a:26:HIS:HE1	3:a:325:HOH:O	1.67	0.77
1:b:91:ARG:HH11	1:b:93:ASN:ND2	1.81	0.77
1:o:26:HIS:HE1	3:o:548:HOH:O	1.67	0.77
1:c:91[B]:ARG:HH11	1:c:93:ASN:HD22	1.31	0.77
1:i:18:ARG:HB2	3:i:410:HOH:O	1.84	0.77
1:C:31:LEU:CD2	3:C:386:HOH:O	2.33	0.77
1:E:17:LYS:HA	1:J:19:MET:HE2	1.65	0.77
1:E:148:ASN:HB2	3:E:446:HOH:O	1.83	0.77
1:e:23:HIS:HA	1:i:66:ARG:NH1	1.98	0.77
1:V:91:ARG:HH11	1:V:93:ASN:ND2	1.82	0.77
1:v:17:LYS:CB	1:R:19:MET:CE	2.53	0.77
1:A:95:ASN:HD21	1:A:98:THR:H	1.33	0.77
1:K:145[B]:ARG:HH11	1:K:145[B]:ARG:HG2	1.48	0.77
1:i:19:MET:HE3	1:Q:13:MET:SD	2.24	0.77
1:V:14:ARG:HH11	1:V:14:ARG:CB	1.98	0.77
1:t:31:LEU:CD2	3:t:536:HOH:O	2.31	0.76
1:U:13:MET:O	1:U:16:VAL:HG12	1.86	0.76
1:4:13:MET:HA	1:4:16:VAL:CG1	2.15	0.76
1:X:153[B]:LEU:HD13	3:X:519:HOH:O	1.84	0.76
1:i:13:MET:O	1:i:16:VAL:N	2.17	0.76
1:Q:31:LEU:HD21	3:Q:537:HOH:O	1.85	0.76
1:q:91:ARG:NH1	1:q:93:ASN:HD22	1.80	0.76
1:x:16:VAL:HG23	1:T:16:VAL:HG21	1.65	0.76
1:z:12:THR:HG23	1:z:13:MET:N	2.01	0.76
1:3:91[A]:ARG:HH11	1:3:93:ASN:ND2	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:31:LEU:CD2	3:P:390:HOH:O	2.33	0.76
1:Y:13:MET:HA	1:Y:16:VAL:HG11	1.66	0.76
1:n:91:ARG:HH11	1:n:93:ASN:ND2	1.83	0.76
1:I:146[B]:ILE:HG23	3:I:536:HOH:O	1.86	0.76
1:f:16:VAL:HG21	1:m:16:VAL:HG23	1.67	0.76
1:R:17:LYS:HZ2	1:R:21:ASN:ND2	1.75	0.76
1:s:16:VAL:HG23	1:2:16:VAL:HG21	1.68	0.76
1:3:131:VAL:HG13	1:3:145[B]:ARG:HD3	1.66	0.76
1:4:95:ASN:HD21	1:4:98:THR:H	1.34	0.76
1:O:66:ARG:CG	3:O:456:HOH:O	2.33	0.76
1:7:16:VAL:HG13	1:7:17:LYS:N	2.01	0.76
1:I:72:LEU:O	1:I:146[B]:ILE:HD12	1.85	0.76
1:n:95:ASN:HD21	1:n:98:THR:H	1.33	0.75
1:6:129:LYS:NZ	1:6:145:ARG:HH21	1.84	0.75
1:A:12:THR:HG23	1:A:13:MET:CE	2.16	0.75
1:N:91[B]:ARG:HH11	1:N:93:ASN:ND2	1.84	0.75
1:O:13:MET:CA	1:O:16:VAL:HG12	2.15	0.75
1:i:13:MET:O	1:i:16:VAL:HG12	1.85	0.75
1:1:95:ASN:HD21	1:1:98:THR:H	1.34	0.75
1:4:31:LEU:CD2	3:4:319:HOH:O	2.33	0.75
1:5:23:HIS:CE1	1:H:17:LYS:NZ	2.53	0.75
1:6:129:LYS:NZ	1:6:145:ARG:NH2	2.34	0.75
1:2:129:LYS:HZ2	1:2:145[A]:ARG:CZ	1.98	0.75
1:N:16:VAL:CG2	1:W:16:VAL:HG23	2.16	0.75
1:W:26:HIS:HE1	3:W:549:HOH:O	1.70	0.75
1:j:17:LYS:NZ	1:y:23:HIS:CE1	2.53	0.75
1:p:23:HIS:CE1	1:y:17:LYS:NZ	2.55	0.75
1:M:71:LYS:NZ	1:M:189:GLU:OE2	2.19	0.75
1:b:95:ASN:HD21	1:b:98:THR:H	1.33	0.75
1:k:31:LEU:CD2	3:k:532:HOH:O	2.34	0.75
1:v:13:MET:HA	1:v:13:MET:CE	2.14	0.75
1:x:91[B]:ARG:HD3	1:x:93:ASN:ND2	2.02	0.75
1:o:13:MET:CA	1:o:16:VAL:CG1	2.64	0.75
1:p:13:MET:HE2	1:p:16:VAL:CG1	2.15	0.75
1:G:16:VAL:HG23	1:M:16:VAL:CG2	2.16	0.75
1:s:95:ASN:HD21	1:s:98:THR:H	1.34	0.75
1:e:152:GLN:HG3	3:e:327:HOH:O	1.86	0.75
1:g:91:ARG:NH1	1:g:93:ASN:HD22	1.84	0.75
1:t:15:ALA:CB	1:C:13:MET:CE	2.64	0.75
1:3:131:VAL:HG11	1:3:145[B]:ARG:HD3	1.69	0.75
1:G:95:ASN:HD21	1:G:98:THR:H	1.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:71:LYS:HG2	1:Q:146:ILE:HD11	1.67	0.75
1:V:14:ARG:HB2	1:V:14:ARG:NH1	2.02	0.75
1:Z:17:LYS:HE3	1:Z:21:ASN:HD21	1.50	0.75
1:e:91:ARG:HH11	1:e:93:ASN:HD22	1.32	0.74
1:n:33:ASN:OD1	1:n:45[B]:GLN:NE2	2.19	0.74
1:P:14:ARG:HB2	1:P:14:ARG:NH1	2.01	0.74
1:R:12:THR:HG23	1:R:13:MET:N	2.03	0.74
1:a:91:ARG:HH11	1:a:93:ASN:ND2	1.84	0.74
1:k:91:ARG:HH11	1:k:93:ASN:ND2	1.84	0.74
1:x:12:THR:HG21	1:T:13:MET:CE	2.17	0.74
1:M:71:LYS:HE2	1:N:114:GLN:OE1	1.86	0.74
1:c:13:MET:HA	1:c:16:VAL:HG12	1.69	0.74
1:o:16:VAL:HG22	1:u:19:MET:SD	2.26	0.74
1:p:13:MET:HA	1:p:16:VAL:CG1	2.17	0.74
1:y:13:MET:O	1:y:16:VAL:CG1	2.35	0.74
1:4:17:LYS:HB3	3:4:430:HOH:O	1.87	0.74
1:v:13:MET:CE	1:v:13:MET:CA	2.65	0.74
1:Q:91:ARG:NH1	1:Q:93:ASN:HD22	1.82	0.74
1:V:14:ARG:NH1	1:V:14:ARG:HB3	2.01	0.74
1:d:95:ASN:HD21	1:d:98:THR:H	1.35	0.74
1:p:95:ASN:HD21	1:p:98:THR:H	1.33	0.74
1:q:71:LYS:HD2	1:q:146:ILE:HD11	1.69	0.74
1:A:84:THR:CG2	3:A:452:HOH:O	2.33	0.74
1:B:13:MET:HE3	1:B:16:VAL:HG11	1.69	0.74
1:W:145:ARG:HD3	3:W:422:HOH:O	1.86	0.74
1:o:17:LYS:HZ2	1:u:23:HIS:CE1	2.04	0.74
1:x:23:HIS:CE1	1:T:17:LYS:NZ	2.55	0.74
1:F:95:ASN:HD21	1:F:98:THR:H	1.36	0.74
1:D:12:THR:O	1:D:16:VAL:HG12	1.88	0.74
1:L:95:ASN:HD21	1:L:98:THR:H	1.36	0.74
1:N:23:HIS:CE1	1:P:17:LYS:HZ2	2.05	0.74
1:P:91[B]:ARG:HH21	1:P:93:ASN:ND2	1.85	0.74
1:l:13:MET:O	1:l:16:VAL:HG12	1.87	0.74
1:n:19:MET:SD	1:G:16:VAL:CG1	2.76	0.74
1:p:13:MET:CE	1:p:16:VAL:HG11	2.17	0.74
1:y:95:ASN:HD21	1:y:98:THR:H	1.34	0.74
1:3:131:VAL:HG21	1:3:145[A]:ARG:HD3	1.70	0.74
1:6:19:MET:HE3	1:F:13:MET:SD	2.28	0.74
1:I:13:MET:HA	1:I:16:VAL:HG12	1.70	0.74
1:l:13:MET:CE	1:E:12:THR:CG2	2.61	0.73
1:0:95:ASN:HD21	1:0:98:THR:H	1.35	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:145:ARG:NH2	3:0:337:HOH:O	2.18	0.73
1:W:17:LYS:CE	1:W:21:ASN:HD21	2.01	0.73
1:g:26:HIS:HE1	3:g:306:HOH:O	1.69	0.73
1:o:17:LYS:HZ1	1:u:23:HIS:CE1	1.98	0.73
1:z:13:MET:C	1:z:16:VAL:HG12	2.12	0.73
1:z:19:MET:CE	1:Y:17:LYS:HA	2.09	0.73
1:3:133:LEU:HD21	1:3:145[B]:ARG:CD	2.16	0.73
1:5:71:LYS:CG	1:5:148[B]:ASN:OD1	2.36	0.73
1:K:91[A]:ARG:CD	1:K:171:ILE:HD11	2.14	0.73
1:f:16:VAL:CG1	1:m:19:MET:SD	2.76	0.73
1:h:129:LYS:HE3	1:h:147:ILE:HG21	1.70	0.73
1:5:95:ASN:HD21	1:5:98:THR:H	1.35	0.73
1:G:17:LYS:HE3	1:G:21:ASN:HD21	1.53	0.73
3:V:518:HOH:O	1:c:73:HIS:HD2	1.70	0.73
1:2:13:MET:C	1:2:16:VAL:HG13	2.13	0.73
1:M:95:ASN:HD21	1:M:98:THR:H	1.35	0.73
1:J:91:ARG:NH1	1:J:93:ASN:HD22	1.82	0.73
1:J:95:ASN:HD21	1:J:98:THR:H	1.32	0.73
1:U:71:LYS:HD3	1:U:148[A]:ASN:OD1	1.88	0.73
1:W:95:ASN:HD21	1:W:98:THR:H	1.36	0.73
1:h:152:GLN:CG	3:h:461:HOH:O	2.28	0.73
1:7:13:MET:SD	1:7:13:MET:C	2.72	0.73
1:H:95:ASN:HD21	1:H:98:THR:H	1.35	0.73
1:N:91[B]:ARG:HD3	1:N:93:ASN:ND2	2.04	0.73
1:x:95:ASN:HD21	1:x:98:THR:H	1.35	0.73
1:B:17:LYS:CE	1:B:21:ASN:HD21	2.00	0.73
1:E:95:ASN:HD21	1:E:98:THR:H	1.34	0.73
1:6:95:ASN:HD21	1:6:98:THR:H	1.36	0.73
1:b:13:MET:CA	1:b:16:VAL:CG1	2.63	0.73
1:E:87:PHE:HB2	1:E:131:VAL:CG2	2.18	0.73
1:I:95:ASN:HD21	1:I:98:THR:H	1.36	0.73
1:b:31:LEU:CD2	3:b:333:HOH:O	2.36	0.73
1:e:91:ARG:HH11	1:e:93:ASN:ND2	1.86	0.73
3:r:389:HOH:O	1:y:73:HIS:HD2	1.71	0.73
1:P:14:ARG:NH1	1:P:14:ARG:CB	2.52	0.73
1:Y:91:ARG:HH11	1:Y:93:ASN:ND2	1.86	0.73
1:n:129:LYS:NZ	1:n:145[B]:ARG:CZ	2.52	0.72
1:t:13:MET:CE	1:t:16:VAL:HG11	2.19	0.72
1:t:91[A]:ARG:NH1	1:t:93:ASN:HD22	1.86	0.72
1:z:13:MET:HA	1:z:16:VAL:HG12	1.71	0.72
1:D:73:HIS:CB	1:D:146[A]:ILE:HD13	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:12:THR:HG23	1:N:12:THR:O	1.88	0.72
1:P:95:ASN:HD21	1:P:98:THR:H	1.37	0.72
1:M:17:LYS:HD2	1:M:21:ASN:ND2	2.04	0.72
1:P:14:ARG:HH11	1:P:14:ARG:CB	2.03	0.72
1:R:123:LYS:HE2	3:R:429:HOH:O	1.90	0.72
1:Z:95:ASN:HD21	1:Z:98:THR:H	1.37	0.72
1:w:19:MET:HE1	1:V:16:VAL:HG11	1.70	0.72
1:1:17:LYS:HZ3	1:X:23:HIS:CE1	2.06	0.72
1:T:23:HIS:CE1	1:c:17:LYS:HZ2	2.00	0.72
1:U:91[A]:ARG:HH11	1:U:93:ASN:ND2	1.85	0.72
1:i:19:MET:HE1	1:Q:13:MET:HE3	1.65	0.72
1:i:26:HIS:HE1	3:i:503:HOH:O	1.71	0.72
1:u:17:LYS:HG3	3:u:439:HOH:O	1.89	0.72
1:3:13:MET:CA	1:3:16:VAL:HG12	2.19	0.72
1:6:26:HIS:HE1	3:6:559:HOH:O	1.71	0.72
1:r:91:ARG:HH11	1:r:93:ASN:ND2	1.86	0.72
1:K:71:LYS:HD3	1:K:148[B]:ASN:OD1	1.90	0.72
1:M:64[A]:GLN:CG	1:M:153:LEU:CD1	2.68	0.72
1:S:95:ASN:HD21	1:S:98:THR:H	1.35	0.72
1:U:95:ASN:HD21	1:U:98:THR:H	1.37	0.72
1:e:23:HIS:CE1	1:i:66:ARG:NH2	2.57	0.72
1:i:71:LYS:CD	1:i:148[B]:ASN:OD1	2.38	0.72
1:x:16:VAL:HG13	1:c:19:MET:SD	2.29	0.72
1:6:12:THR:CG2	1:F:12:THR:HG21	2.17	0.72
1:P:23:HIS:HE1	1:W:17:LYS:HZ2	1.37	0.72
3:k:446:HOH:O	1:r:146:ILE:HD11	1.90	0.72
1:s:23:HIS:HE1	1:2:17:LYS:HZ2	1.36	0.72
1:u:26:HIS:HE1	3:u:335:HOH:O	1.73	0.72
1:1:91[B]:ARG:HE	1:1:93:ASN:HD21	1.36	0.72
1:V:95:ASN:HD21	1:V:98:THR:H	1.36	0.72
1:k:26:HIS:HE1	3:k:397:HOH:O	1.70	0.72
1:B:91[B]:ARG:NH1	1:B:93:ASN:HD22	1.85	0.72
1:q:95:ASN:HD21	1:q:98:THR:H	1.38	0.72
1:r:95:ASN:HD21	1:r:98:THR:H	1.36	0.72
1:2:129:LYS:HZ2	1:2:145[A]:ARG:NE	1.88	0.72
1:P:120:LEU:HB3	1:S:28[B]:ARG:HH21	1.51	0.72
1:t:13:MET:CA	1:t:16:VAL:HG12	2.20	0.71
1:v:13:MET:C	1:v:16:VAL:HG12	2.15	0.71
1:x:129:LYS:HE3	3:x:398:HOH:O	1.90	0.71
1:z:13:MET:HA	1:z:16:VAL:CG1	2.20	0.71
1:c:95:ASN:HD21	1:c:98:THR:H	1.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:12:THR:HG21	1:T:13:MET:HE1	1.73	0.71
1:4:13:MET:O	1:4:16:VAL:CG1	2.39	0.71
1:T:91:ARG:HH11	1:T:93:ASN:ND2	1.87	0.71
1:g:95:ASN:HD21	1:g:98:THR:H	1.38	0.71
1:l:95:ASN:HD21	1:l:98:THR:H	1.39	0.71
1:o:91:ARG:NH1	1:o:93:ASN:HD22	1.83	0.71
1:K:95:ASN:HD21	1:K:98:THR:H	1.36	0.71
1:M:17:LYS:HE2	3:M:450:HOH:O	1.89	0.71
1:Y:13:MET:C	1:Y:16:VAL:HG12	2.16	0.71
1:v:13:MET:CE	1:v:13:MET:N	2.54	0.71
1:Y:146:ILE:O	1:Y:146:ILE:HD12	1.91	0.71
1:j:95:ASN:HD21	1:j:98:THR:H	1.37	0.71
1:z:95:ASN:HD21	1:z:98:THR:H	1.39	0.71
1:D:18:ARG:O	1:D:22:THR:HG23	1.91	0.71
1:N:19:MET:HE1	1:P:16:VAL:CG1	2.20	0.71
1:R:31[A]:LEU:CD2	3:R:564:HOH:O	2.37	0.71
1:M:71:LYS:CG	1:M:146:ILE:HD11	2.20	0.71
1:N:16:VAL:HG13	1:N:17:LYS:N	2.02	0.71
1:c:91[B]:ARG:NH1	1:c:93:ASN:HD22	1.88	0.71
1:l:14:ARG:NH2	3:l:459:HOH:O	2.22	0.71
1:1:91[A]:ARG:NH1	1:1:152:GLN:CB	2.53	0.71
1:V:14:ARG:HB3	1:V:14:ARG:CZ	2.20	0.71
1:Y:91:ARG:HH11	1:Y:93:ASN:HD22	1.38	0.71
1:Y:95:ASN:HD21	1:Y:98:THR:H	1.37	0.71
1:k:95:ASN:HD21	1:k:98:THR:H	1.38	0.71
1:4:13:MET:SD	1:a:15:ALA:HB1	2.30	0.71
1:M:13:MET:C	1:M:16:VAL:CG1	2.58	0.71
1:e:23:HIS:CA	1:i:66:ARG:HH11	2.02	0.71
1:r:13:MET:SD	1:r:13:MET:O	2.49	0.70
1:R:17:LYS:HE3	1:R:21:ASN:ND2	2.06	0.70
1:Z:13:MET:HA	1:Z:16:VAL:CG1	2.20	0.70
1:N:95:ASN:HD21	1:N:98:THR:H	1.35	0.70
1:v:95:ASN:HD21	1:v:98:THR:H	1.38	0.70
1:A:12:THR:HG23	1:A:13:MET:HE1	1.73	0.70
1:U:19:MET:HE1	1:Z:13:MET:HE3	1.72	0.70
1:7:95:ASN:HD21	1:7:98:THR:H	1.38	0.70
1:T:26:HIS:HE1	3:T:350:HOH:O	1.75	0.70
1:W:45:GLN:HG2	3:W:326:HOH:O	1.89	0.70
1:3:129:LYS:HE3	1:3:145[A]:ARG:HH21	1.55	0.70
1:B:12:THR:O	1:B:15:ALA:N	2.24	0.70
1:a:95:ASN:HD21	1:a:98:THR:H	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:152:GLN:CG	3:e:327:HOH:O	2.38	0.70
1:f:95:ASN:HD21	1:f:98:THR:H	1.40	0.70
1:g:17:LYS:NZ	1:b:23:HIS:CE1	2.59	0.70
1:w:95:ASN:HD21	1:w:98:THR:H	1.40	0.70
1:2:13:MET:HA	1:2:16:VAL:HG12	1.70	0.70
1:D:73:HIS:HB2	1:D:146[A]:ILE:HD13	1.72	0.70
1:H:12:THR:O	1:H:16:VAL:HG12	1.92	0.70
1:N:17:LYS:HZ2	1:N:21:ASN:HD21	1.39	0.70
1:i:13:MET:CA	1:i:16:VAL:CG1	2.55	0.70
1:x:12:THR:CG2	1:T:13:MET:HE1	2.22	0.70
1:U:71:LYS:HD2	1:U:146:ILE:HD11	1.74	0.70
1:i:23:HIS:HE1	1:Q:17:LYS:NZ	1.89	0.69
1:7:71:LYS:HG2	1:7:146:ILE:HD11	1.74	0.69
1:u:95:ASN:HD21	1:u:98:THR:H	1.39	0.69
1:d:145:ARG:NH2	3:d:426:HOH:O	2.25	0.69
1:f:91:ARG:NH1	1:f:93:ASN:HD22	1.85	0.69
1:i:13:MET:O	1:i:16:VAL:CG1	2.41	0.69
1:6:129:LYS:HZ2	1:6:145:ARG:HH21	1.39	0.69
1:D:95:ASN:HD21	1:D:98:THR:H	1.38	0.69
1:S:13:MET:O	1:S:16:VAL:CG1	2.32	0.69
1:n:19:MET:HE1	1:G:16:VAL:CG1	2.22	0.69
1:r:13:MET:O	1:r:16:VAL:HG13	1.92	0.69
1:s:16:VAL:HG21	1:0:16:VAL:CG2	2.17	0.69
1:H:23:HIS:HE1	1:L:17:LYS:NZ	1.90	0.69
1:O:66:ARG:HG3	3:O:456:HOH:O	1.92	0.69
3:n:497:HOH:O	2:G:203:CA:CA	1.69	0.69
1:B:71:LYS:CG	1:B:146[B]:ILE:HD11	2.23	0.69
1:0:146:ILE:HD13	3:0:374:HOH:O	1.93	0.69
1:A:91[A]:ARG:NH1	1:A:93:ASN:HD22	1.88	0.69
1:P:71[A]:LYS:HD3	1:P:146[A]:ILE:HD11	1.73	0.69
1:X:95:ASN:HD21	1:X:98:THR:H	1.40	0.69
1:e:95:ASN:HD21	1:e:98:THR:H	1.40	0.69
1:h:95:ASN:HD21	1:h:98:THR:H	1.40	0.69
1:v:91:ARG:HH11	1:v:93:ASN:ND2	1.90	0.69
1:w:16:VAL:O	1:w:20:ILE:HG13	1.93	0.69
1:B:13:MET:C	1:B:16:VAL:HG12	2.17	0.69
1:Q:12:THR:N	3:Q:317:HOH:O	2.24	0.69
1:T:31[A]:LEU:CD2	3:T:570:HOH:O	2.39	0.69
1:4:17:LYS:NZ	1:a:23:HIS:HE1	1.91	0.69
1:B:13:MET:O	1:B:16:VAL:CG1	2.40	0.69
1:j:17:LYS:HG3	3:j:373:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:r:129:LYS:HE3	1:r:145[A]:ARG:HH21	1.59	0.69
1:M:13:MET:CA	1:M:16:VAL:CG1	2.62	0.69
1:Z:91[A]:ARG:HD3	1:Z:93:ASN:ND2	2.08	0.69
1:d:13:MET:HA	1:d:16:VAL:CG1	2.23	0.69
1:n:129:LYS:CE	1:n:145[B]:ARG:NH2	2.53	0.68
1:A:71:LYS:HG2	1:A:146:ILE:HD11	1.75	0.68
1:L:91[B]:ARG:NE	1:L:93:ASN:ND2	2.40	0.68
1:O:12:THR:O	1:O:12:THR:CG2	2.35	0.68
1:t:14:ARG:HB3	3:t:455:HOH:O	1.93	0.68
1:U:14:ARG:HD2	3:U:458:HOH:O	1.92	0.68
1:j:17:LYS:HZ3	1:y:23:HIS:CE1	2.11	0.68
1:n:129:LYS:HE3	1:n:145[B]:ARG:HH21	1.56	0.68
1:p:12:THR:HG23	1:p:13:MET:N	2.08	0.68
1:w:19:MET:HE3	1:V:13:MET:CE	2.21	0.68
1:Q:95:ASN:HD21	1:Q:98:THR:H	1.38	0.68
1:X:13:MET:O	1:X:16:VAL:CG1	2.41	0.68
1:t:13:MET:HB3	1:3:19:MET:CE	2.21	0.68
1:t:28[A]:ARG:HD2	3:t:392:HOH:O	1.92	0.68
1:u:17:LYS:NZ	1:B:23:HIS:HE1	1.91	0.68
1:3:13:MET:C	1:3:16:VAL:HG12	2.19	0.68
1:L:31:LEU:CD2	3:L:530:HOH:O	2.41	0.68
1:X:66:ARG:NH1	1:X:153[B]:LEU:CD1	2.56	0.68
1:j:23:HIS:HE1	1:p:17:LYS:NZ	1.90	0.68
1:m:95:ASN:HD21	1:m:98:THR:H	1.39	0.68
1:q:17:LYS:HE3	1:q:21:ASN:HD21	1.57	0.68
1:r:19:MET:HE1	1:b:13:MET:HE3	1.76	0.68
1:3:131:VAL:HG13	1:3:145[B]:ARG:CD	2.23	0.68
1:4:91:ARG:NH1	1:4:93:ASN:HD22	1.87	0.68
1:k:13:MET:HA	1:k:16:VAL:HG12	1.75	0.68
1:e:23:HIS:ND1	1:i:66:ARG:CZ	2.56	0.68
3:p:488:HOH:O	1:3:73:HIS:HD2	1.75	0.68
1:5:16:VAL:O	1:5:20:ILE:HG13	1.93	0.68
1:C:129:LYS:HZ3	1:C:147:ILE:CG2	2.05	0.68
1:U:26:HIS:HE1	3:U:403:HOH:O	1.75	0.68
1:z:19:MET:HE1	1:Y:17:LYS:HB2	0.70	0.68
1:z:26:HIS:HE1	3:z:309:HOH:O	1.77	0.68
1:6:91:ARG:NH1	1:6:93:ASN:HD22	1.91	0.68
1:W:91:ARG:NH1	1:W:93:ASN:HD22	1.87	0.68
1:u:13:MET:CE	1:B:19:MET:HE3	2.20	0.68
1:w:145[A]:ARG:NH2	3:w:564:HOH:O	2.26	0.68
1:x:13:MET:HE3	1:c:19:MET:CE	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:23:HIS:HE1	1:7:17:LYS:NZ	1.90	0.68
1:H:23:HIS:CE1	1:L:17:LYS:NZ	2.62	0.67
1:L:91[B]:ARG:HE	1:L:93:ASN:HD21	1.39	0.67
1:x:16:VAL:HG23	1:T:16:VAL:CG2	2.24	0.67
1:J:26:HIS:HE1	3:J:358:HOH:O	1.77	0.67
1:2:13:MET:O	1:2:16:VAL:HG12	1.91	0.67
1:H:23:HIS:CE1	1:L:17:LYS:HZ2	2.12	0.67
1:e:13:MET:HE2	1:e:13:MET:HA	1.75	0.67
1:D:82:SER:HB3	3:Y:471:HOH:O	1.93	0.67
1:H:17:LYS:HE3	1:H:21:ASN:ND2	2.09	0.67
3:J:446:HOH:O	1:Q:73:HIS:HD2	1.77	0.67
1:o:13:MET:HE3	1:u:19:MET:CE	2.23	0.67
1:E:26:HIS:HE1	3:E:501:HOH:O	1.77	0.67
1:T:31[A]:LEU:HD21	3:T:570:HOH:O	1.94	0.67
1:j:13:MET:HA	1:j:16:VAL:HG12	1.76	0.67
1:j:13:MET:CA	1:j:16:VAL:HG12	2.25	0.67
1:w:162[A]:VAL:CG1	3:w:515:HOH:O	2.43	0.67
1:C:91:ARG:NH1	1:C:93:ASN:HD22	1.86	0.67
1:T:13:MET:HE2	3:T:499:HOH:O	1.94	0.67
1:U:16:VAL:HG23	1:Z:16:VAL:CG2	2.25	0.67
1:j:21:ASN:HB3	3:j:413:HOH:O	1.94	0.67
1:x:71:LYS:CD	1:x:146:ILE:HD11	2.19	0.67
1:z:17:LYS:HZ2	1:S:23:HIS:HE1	1.43	0.67
1:B:13:MET:HA	1:B:16:VAL:HG11	1.74	0.67
1:F:91:ARG:HE	1:F:93:ASN:ND2	1.92	0.67
1:L:18:ARG:CG	3:L:352:HOH:O	2.41	0.67
1:L:31:LEU:HD22	3:L:530:HOH:O	1.95	0.67
1:N:16:VAL:CG1	1:N:17:LYS:N	2.57	0.67
1:U:71:LYS:HG3	1:U:148[A]:ASN:OD1	1.94	0.67
1:m:12:THR:HG21	3:m:445:HOH:O	1.93	0.67
1:n:140:GLU:HG2	3:n:544:HOH:O	1.94	0.67
1:z:91:ARG:HD2	3:z:450:HOH:O	1.93	0.67
1:B:95:ASN:HD21	1:B:98:THR:H	1.43	0.67
1:K:71:LYS:HD3	1:K:148[B]:ASN:ND2	2.10	0.67
1:t:96[B]:ARG:CZ	3:t:415:HOH:O	2.42	0.67
3:2:477:HOH:O	1:R:73:HIS:HD2	1.78	0.67
1:5:71:LYS:CB	1:5:148[B]:ASN:OD1	2.43	0.67
1:L:180[B]:LEU:HD11	3:L:431:HOH:O	1.95	0.67
1:M:71:LYS:HG2	1:M:146:ILE:HD11	1.77	0.67
1:l:91:ARG:NH1	1:l:93:ASN:HD22	1.90	0.66
1:q:16:VAL:CG2	1:V:16:VAL:HG23	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:12:THR:C	1:v:13:MET:CE	2.67	0.66
1:v:20:ILE:HD12	1:R:19:MET:HE2	1.77	0.66
1:x:91[B]:ARG:HD3	1:x:93:ASN:HD21	1.60	0.66
1:A:13:MET:CA	1:A:16:VAL:HG12	2.26	0.66
1:1:91[B]:ARG:NE	1:1:93:ASN:HD21	1.92	0.66
1:2:95:ASN:ND2	1:2:97:GLY:H	1.93	0.66
1:L:13:MET:HA	1:L:16:VAL:HG12	1.78	0.66
1:N:19:MET:CE	1:P:16:VAL:CG1	2.73	0.66
1:t:95:ASN:HD21	1:t:98:THR:H	1.40	0.66
1:w:18:ARG:O	1:w:22:THR:HG23	1.93	0.66
1:H:91[A]:ARG:HD3	3:H:312:HOH:O	1.95	0.66
1:I:66:ARG:HG3	3:I:492:HOH:O	1.95	0.66
1:u:31:LEU:HD23	1:u:31:LEU:C	2.20	0.66
1:x:73:HIS:HD2	3:X:418:HOH:O	1.78	0.66
1:z:12:THR:HG23	1:z:13:MET:H	1.60	0.66
1:o:95:ASN:HD21	1:o:98:THR:H	1.41	0.66
1:1:91[A]:ARG:HG2	1:1:93:ASN:ND2	2.11	0.66
1:K:71:LYS:HD3	1:K:148[B]:ASN:CG	2.20	0.66
1:g:16:VAL:HG11	1:b:19:MET:HE1	1.76	0.66
1:t:17:LYS:HE3	1:t:21:ASN:ND2	2.09	0.66
1:4:13:MET:HA	1:4:16:VAL:HG11	1.77	0.66
1:T:22:THR:HG22	3:T:449:HOH:O	1.95	0.66
1:F:15:ALA:HB1	1:O:13:MET:CE	2.26	0.66
1:Q:26:HIS:HE1	3:Q:394:HOH:O	1.77	0.66
1:t:91[B]:ARG:NH2	3:t:464:HOH:O	2.27	0.66
1:x:12:THR:OG1	1:T:13:MET:HE1	1.96	0.66
1:R:26:HIS:HE1	3:R:386:HOH:O	1.79	0.66
1:y:91:ARG:NH1	1:y:93:ASN:HD22	1.90	0.66
1:6:129:LYS:HZ2	1:6:145:ARG:NH2	1.94	0.66
1:h:16:VAL:CG1	1:v:19:MET:SD	2.83	0.65
1:l:13:MET:HE1	1:E:12:THR:HG23	1.76	0.65
1:l:17:LYS:CG	3:l:459:HOH:O	2.44	0.65
1:r:66[B]:ARG:HG2	1:r:66[B]:ARG:NH1	2.11	0.65
1:H:91[B]:ARG:NH2	1:H:93:ASN:HD22	1.90	0.65
1:O:26:HIS:HE1	3:O:518:HOH:O	1.78	0.65
1:S:28[B]:ARG:HD3	1:S:191:VAL:HG22	1.77	0.65
3:e:520:HOH:O	1:l:73:HIS:HD2	1.78	0.65
1:j:26:HIS:HE1	3:j:355:HOH:O	1.79	0.65
1:o:23:HIS:HE1	1:B:17:LYS:NZ	1.94	0.65
1:c:12:THR:HG23	1:c:13:MET:N	2.12	0.65
1:d:91:ARG:NH1	1:d:93:ASN:HD22	1.92	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:129:LYS:HZ2	1:n:145[B]:ARG:NH2	1.94	0.65
1:s:13:MET:HE3	1:0:19:MET:HE1	1.77	0.65
1:f:19:MET:CE	1:I:13:MET:HE3	2.25	0.65
1:0:16:VAL:HG13	1:2:19:MET:SD	2.37	0.65
1:7:16:VAL:HG13	1:7:17:LYS:H	1.61	0.65
1:z:12:THR:CB	3:z:448:HOH:O	2.42	0.65
1:5:13:MET:C	1:5:16:VAL:HG12	2.22	0.65
1:h:23:HIS:HE1	1:R:17:LYS:HZ3	1.42	0.65
1:k:12:THR:O	1:k:16:VAL:HG12	1.96	0.65
1:5:140:GLU:HG2	3:5:478:HOH:O	1.97	0.65
1:U:31:LEU:HD13	3:U:562:HOH:O	1.96	0.65
1:D:91:ARG:NH1	1:D:93:ASN:HD22	1.87	0.65
1:K:13:MET:O	1:K:16:VAL:HG13	1.96	0.65
1:P:129:LYS:HE3	1:P:147:ILE:CG2	2.25	0.65
1:a:13:MET:HA	1:a:16:VAL:HG12	1.78	0.65
1:o:12:THR:O	1:o:16:VAL:HG12	1.97	0.65
1:q:19:MET:SD	1:w:16:VAL:HG13	2.37	0.65
1:s:13:MET:HA	1:s:16:VAL:HG12	1.78	0.65
1:6:28[B]:ARG:NH1	1:6:28[B]:ARG:HG2	2.10	0.65
1:O:91:ARG:NH1	1:O:93:ASN:HD22	1.88	0.65
1:y:66:ARG:CD	3:y:370:HOH:O	2.45	0.65
1:O:91:ARG:HD2	3:O:468:HOH:O	1.97	0.65
1:R:12:THR:CG2	1:R:13:MET:N	2.60	0.65
1:m:12:THR:O	1:m:15:ALA:N	2.30	0.65
1:P:13:MET:HA	1:P:16:VAL:HG12	1.78	0.65
1:P:95:ASN:ND2	1:P:97:GLY:H	1.93	0.65
1:b:146:ILE:HD11	3:b:422:HOH:O	1.96	0.65
1:f:21:ASN:ND2	3:f:518:HOH:O	2.31	0.64
1:2:13:MET:C	1:2:16:VAL:HG12	2.22	0.64
1:7:72:LEU:O	1:7:146:ILE:HD12	1.96	0.64
1:M:64[A]:GLN:HG3	1:M:153:LEU:CD1	2.26	0.64
1:e:145:ARG:HD2	3:e:441:HOH:O	1.96	0.64
1:g:19:MET:HE1	1:r:13:MET:HE1	1.79	0.64
1:n:16:VAL:HG13	1:n:17:LYS:N	2.12	0.64
1:P:91[A]:ARG:CZ	1:P:152:GLN:HE22	2.10	0.64
1:v:12:THR:C	1:v:13:MET:HE3	2.22	0.64
1:p:12:THR:HG23	1:p:13:MET:H	1.63	0.64
1:z:91:ARG:NH1	1:z:93:ASN:HD22	1.89	0.64
1:2:31:LEU:CD2	3:2:406:HOH:O	2.44	0.64
1:P:31:LEU:HD22	3:P:390:HOH:O	1.95	0.64
1:U:18:ARG:O	1:U:22:THR:HG23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:13:MET:CE	1:e:16:VAL:HG11	2.28	0.64
1:f:16:VAL:HG13	1:f:17:LYS:N	2.11	0.64
1:i:23:HIS:HE1	1:Q:17:LYS:HZ2	1.45	0.64
1:i:95:ASN:ND2	1:i:97:GLY:H	1.95	0.64
1:u:12:THR:CG2	1:u:15:ALA:HB3	2.27	0.64
1:l:16:VAL:CG1	1:X:19:MET:HE1	2.28	0.64
1:J:18:ARG:O	1:J:22:THR:HG23	1.97	0.64
1:Q:71:LYS:HE2	1:Q:148[A]:ASN:CG	2.20	0.64
1:T:73:HIS:HD2	3:U:364:HOH:O	1.80	0.64
3:Y:416:HOH:O	1:d:73:HIS:HD2	1.80	0.64
1:7:71:LYS:HE3	3:7:476:HOH:O	1.97	0.64
1:G:129:LYS:HE2	3:G:469:HOH:O	1.98	0.64
1:P:71[B]:LYS:HG3	1:P:148:ASN:OD1	1.98	0.64
1:W:17:LYS:HE3	1:W:21:ASN:ND2	2.09	0.64
1:z:13:MET:CA	1:z:16:VAL:HG12	2.26	0.64
1:R:95:ASN:ND2	1:R:97:GLY:H	1.95	0.64
3:g:513:HOH:O	1:E:73:HIS:HD2	1.80	0.64
1:h:23:HIS:HE1	1:R:17:LYS:HZ2	1.46	0.64
1:j:17:LYS:HZ2	1:y:23:HIS:HE1	1.46	0.64
1:s:23:HIS:CE1	1:2:17:LYS:NZ	2.63	0.64
1:1:26:HIS:HE1	3:1:464:HOH:O	1.81	0.64
1:2:13:MET:CA	1:2:16:VAL:HG12	2.26	0.64
1:L:91[B]:ARG:HE	1:L:93:ASN:HD22	1.44	0.64
1:M:95:ASN:ND2	1:M:97:GLY:H	1.96	0.64
1:V:31[B]:LEU:CD2	3:V:548:HOH:O	2.44	0.64
1:2:131:VAL:CG2	1:2:145[A]:ARG:HD3	2.28	0.64
1:4:17:LYS:CG	3:4:430:HOH:O	2.39	0.64
1:F:95:ASN:ND2	1:F:97:GLY:H	1.96	0.64
1:K:13:MET:HA	1:K:16:VAL:HG12	1.79	0.64
1:k:28[B]:ARG:HD3	1:k:191:VAL:HG22	1.79	0.64
1:4:13:MET:CA	1:4:16:VAL:HG12	2.28	0.64
1:4:71:LYS:CD	1:4:148[B]:ASN:HD21	2.03	0.64
1:F:13:MET:HE2	1:F:13:MET:HA	1.80	0.64
1:Z:73:HIS:HD2	3:b:382:HOH:O	1.81	0.64
1:u:17:LYS:HE3	1:u:21:ASN:ND2	2.12	0.63
1:A:13:MET:HA	1:A:16:VAL:HG11	1.80	0.63
1:N:33:ASN:ND2	3:N:358:HOH:O	2.31	0.63
1:U:14:ARG:HA	3:U:458:HOH:O	1.97	0.63
1:b:13:MET:HA	1:b:16:VAL:HG11	1.78	0.63
1:p:91:ARG:NH1	1:p:93:ASN:HD22	1.92	0.63
1:4:13:MET:HA	1:4:16:VAL:HG12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:13:MET:HA	1:H:16:VAL:HG11	1.80	0.63
1:M:91:ARG:NH1	1:M:93:ASN:HD22	1.93	0.63
1:f:145[A]:ARG:HD2	3:f:417:HOH:O	1.97	0.63
1:m:13:MET:O	1:m:16:VAL:HG12	1.97	0.63
1:n:19:MET:SD	1:G:16:VAL:HG13	2.38	0.63
1:t:95:ASN:ND2	1:t:97:GLY:H	1.97	0.63
1:x:13:MET:CE	1:c:19:MET:HE3	2.27	0.63
1:0:91[A]:ARG:NH1	1:0:93:ASN:HD22	1.96	0.63
1:G:17:LYS:HE3	1:G:21:ASN:ND2	2.13	0.63
1:R:31[A]:LEU:HD22	3:R:564:HOH:O	1.97	0.63
1:U:95:ASN:ND2	1:U:97:GLY:H	1.96	0.63
1:p:13:MET:CE	1:p:13:MET:CA	2.72	0.63
1:y:66:ARG:HD3	3:y:370:HOH:O	1.99	0.63
1:B:13:MET:CA	1:B:16:VAL:CG1	2.71	0.63
1:C:18:ARG:O	1:C:22:THR:HG23	1.98	0.63
1:K:73:HIS:HD2	3:Z:343:HOH:O	1.80	0.63
1:O:152:GLN:CD	3:O:464:HOH:O	2.41	0.63
1:n:28:ARG:HD2	3:n:399:HOH:O	1.97	0.63
1:s:95:ASN:ND2	1:s:97:GLY:H	1.97	0.63
1:F:91:ARG:HE	1:F:93:ASN:HD21	1.45	0.63
1:S:95:ASN:ND2	1:S:97:GLY:H	1.96	0.63
1:c:31:LEU:HD22	3:c:555:HOH:O	1.98	0.63
1:N:16:VAL:CG1	1:N:17:LYS:H	2.11	0.63
1:f:26:HIS:HE1	3:f:518:HOH:O	1.80	0.63
1:g:16:VAL:HG13	1:b:19:MET:SD	2.38	0.63
1:t:43[B]:THR:CG2	1:t:45:GLN:HE21	2.11	0.63
1:P:19:MET:SD	1:W:16:VAL:CG1	2.86	0.63
3:h:361:HOH:O	1:a:73:HIS:HD2	1.82	0.63
1:s:91:ARG:NH1	1:s:93:ASN:HD22	1.92	0.63
1:u:91:ARG:NH1	1:u:93:ASN:HD22	1.89	0.63
1:3:146:ILE:CD1	3:3:520:HOH:O	2.46	0.63
1:E:17:LYS:CE	1:E:21:ASN:HD21	2.12	0.63
1:6:13:MET:SD	1:O:12:THR:CG2	2.81	0.63
1:6:16:VAL:HG21	1:O:16:VAL:HG23	1.81	0.63
1:c:152:GLN:CD	3:c:330:HOH:O	2.41	0.63
1:n:19:MET:HE1	1:G:16:VAL:HG12	1.81	0.62
1:z:17:LYS:NZ	1:S:23:HIS:HE1	1.97	0.62
1:G:18:ARG:O	1:G:22:THR:HG23	1.99	0.62
1:L:18:ARG:HG3	3:L:352:HOH:O	1.97	0.62
1:N:16:VAL:HG23	1:P:16:VAL:CG2	2.26	0.62
1:N:16:VAL:HG13	1:W:19:MET:SD	2.39	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:12:THR:O	1:R:16:VAL:HG12	1.99	0.62
1:n:95:ASN:ND2	1:n:97:GLY:H	1.97	0.62
1:n:131:VAL:HG21	1:n:145[B]:ARG:HD3	1.81	0.62
1:E:31[A]:LEU:CD2	3:E:518:HOH:O	2.48	0.62
1:O:18:ARG:CD	3:O:461:HOH:O	2.45	0.62
1:o:79:ILE:HD12	1:o:183:LEU:HG	1.81	0.62
1:5:71:LYS:HB2	1:5:148[B]:ASN:OD1	1.98	0.62
1:D:13:MET:HG2	1:D:14:ARG:N	2.13	0.62
1:U:91[A]:ARG:HD3	1:U:93:ASN:ND2	2.13	0.62
1:w:91:ARG:NH1	1:w:93:ASN:HD22	1.96	0.62
1:2:19:MET:O	1:2:22[B]:THR:CG2	2.47	0.62
1:5:12:THR:HG23	1:5:13:MET:H	1.65	0.62
1:A:13:MET:CA	1:A:13:MET:CE	2.76	0.62
1:C:95:ASN:ND2	1:C:97:GLY:H	1.97	0.62
1:b:19:MET:O	1:b:22:THR:CG2	2.37	0.62
1:g:19:MET:CE	1:r:13:MET:HE1	2.30	0.62
1:k:31:LEU:HD21	3:k:532:HOH:O	1.95	0.62
1:z:13:MET:O	1:z:16:VAL:HG12	1.99	0.62
1:F:19:MET:HE1	1:O:16:VAL:CG1	2.29	0.62
1:N:26:HIS:HE1	3:N:437:HOH:O	1.81	0.62
1:V:95:ASN:ND2	1:V:97:GLY:H	1.97	0.62
1:e:73:HIS:HD2	3:K:352:HOH:O	1.83	0.62
1:p:95:ASN:ND2	1:p:97:GLY:H	1.98	0.62
1:6:95:ASN:ND2	1:6:97:GLY:H	1.98	0.62
1:7:95:ASN:ND2	1:7:97:GLY:H	1.98	0.62
1:C:12:THR:O	1:C:12:THR:CG2	2.46	0.62
1:M:13:MET:HA	1:M:16:VAL:HG11	1.79	0.62
1:V:71:LYS:CD	1:V:146:ILE:HD11	2.24	0.62
1:i:18:ARG:CD	3:i:410:HOH:O	2.47	0.62
1:z:18:ARG:O	1:z:22:THR:HG23	1.99	0.62
1:0:13:MET:HA	1:0:16:VAL:HG12	1.80	0.62
1:V:13:MET:HA	1:V:16:VAL:HG12	1.82	0.62
1:k:13:MET:HA	1:k:16:VAL:HG11	1.82	0.62
3:w:483:HOH:O	1:2:73:HIS:HD2	1.83	0.62
1:0:17:LYS:HE3	3:0:338:HOH:O	1.99	0.62
1:Q:148[A]:ASN:ND2	3:Q:427:HOH:O	2.32	0.62
1:h:91:ARG:NH1	1:h:93:ASN:HD22	1.89	0.62
1:i:19:MET:HE1	1:Q:13:MET:CE	2.15	0.62
1:l:14:ARG:HG2	1:l:14:ARG:O	1.99	0.62
1:n:129:LYS:HZ2	1:n:145[B]:ARG:CZ	2.12	0.62
1:x:91[A]:ARG:HE	1:x:93:ASN:ND2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:31:LEU:C	1:1:31:LEU:HD23	2.25	0.62
1:B:18:ARG:O	1:B:22:THR:HG23	1.99	0.62
1:H:13:MET:HA	1:H:16:VAL:HG12	1.79	0.62
1:I:91:ARG:NH1	1:I:93:ASN:HD22	1.94	0.62
1:P:91[A]:ARG:HE	1:P:93:ASN:ND2	1.98	0.62
1:t:31:LEU:HD22	3:t:536:HOH:O	1.96	0.61
1:3:95:ASN:ND2	1:3:97:GLY:H	1.98	0.61
1:4:13:MET:C	1:4:16:VAL:CG1	2.73	0.61
1:4:17:LYS:HZ3	1:a:23:HIS:CE1	2.18	0.61
1:G:91[B]:ARG:NE	1:G:93:ASN:HD21	1.89	0.61
1:T:71:LYS:HD3	1:T:148:ASN:HB2	1.82	0.61
1:a:17:LYS:HE3	3:a:318:HOH:O	2.00	0.61
1:v:31:LEU:HD23	1:v:31:LEU:C	2.24	0.61
1:x:95:ASN:ND2	1:x:97:GLY:H	1.98	0.61
1:4:23:HIS:HE1	1:7:17:LYS:HZ2	1.48	0.61
1:Z:95:ASN:ND2	1:Z:97:GLY:H	1.98	0.61
1:o:18:ARG:O	1:o:22:THR:HG23	2.00	0.61
1:3:131:VAL:CG1	1:3:145[B]:ARG:CD	2.77	0.61
1:N:23:HIS:CE1	1:P:17:LYS:NZ	2.66	0.61
1:O:31:LEU:HD22	3:O:347:HOH:O	1.98	0.61
1:j:17:LYS:HZ2	1:y:23:HIS:CE1	2.18	0.61
1:k:31:LEU:HD23	1:k:31:LEU:C	2.25	0.61
1:x:71:LYS:CG	1:x:148[B]:ASN:OD1	2.48	0.61
1:2:31:LEU:HD23	1:2:31:LEU:C	2.25	0.61
1:4:17:LYS:CB	3:4:430:HOH:O	2.47	0.61
1:I:16:VAL:O	1:I:20:ILE:HG13	2.01	0.61
1:S:91[A]:ARG:HE	1:S:93:ASN:HD21	1.47	0.61
1:T:95:ASN:ND2	1:T:97:GLY:H	1.96	0.61
1:h:17:LYS:HG3	1:h:18:ARG:N	2.15	0.61
1:i:18:ARG:O	1:i:22:THR:HG23	2.00	0.61
1:4:31:LEU:HD21	3:4:319:HOH:O	1.98	0.61
3:H:394:HOH:O	1:O:73:HIS:HD2	1.82	0.61
1:L:91[B]:ARG:NE	1:L:93:ASN:HD22	1.97	0.61
3:P:458:HOH:O	1:S:73:HIS:HD2	1.82	0.61
1:U:91[B]:ARG:HE	1:U:93:ASN:ND2	1.98	0.61
1:g:16:VAL:CG1	1:b:19:MET:HE1	2.29	0.61
1:k:71:LYS:CD	1:k:148[B]:ASN:OD1	2.37	0.61
1:p:73:HIS:HD2	3:q:376:HOH:O	1.82	0.61
1:s:18:ARG:O	1:s:22:THR:HG23	2.01	0.61
1:3:131:VAL:CG2	1:3:145[A]:ARG:HD3	2.30	0.61
1:4:23:HIS:CD2	3:4:338:HOH:O	2.53	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:91:ARG:NH1	1:5:93:ASN:HD22	1.91	0.61
1:j:91:ARG:NH1	1:j:93:ASN:HD22	1.93	0.61
1:3:146:ILE:HD11	3:3:520:HOH:O	2.01	0.61
1:4:13:MET:SD	1:a:15:ALA:CB	2.89	0.61
3:7:422:HOH:O	1:H:146:ILE:CD1	2.48	0.61
1:B:13:MET:C	1:B:16:VAL:CG1	2.74	0.61
1:G:16:VAL:CG1	1:G:17:LYS:N	2.63	0.61
1:Q:71:LYS:CG	1:Q:146:ILE:HD11	2.30	0.61
1:b:91:ARG:NH1	1:b:93:ASN:HD22	1.93	0.61
1:n:18:ARG:O	1:n:22:THR:HG23	2.00	0.61
1:u:95:ASN:ND2	1:u:97:GLY:H	1.98	0.61
1:n:19:MET:HE3	1:G:16:VAL:HG11	1.82	0.61
1:z:12:THR:CG2	1:z:13:MET:N	2.64	0.61
1:1:95:ASN:ND2	1:1:97:GLY:H	1.99	0.61
1:4:31:LEU:HD22	3:4:319:HOH:O	1.97	0.61
1:6:31:LEU:C	1:6:31:LEU:HD23	2.26	0.61
1:Y:13:MET:CA	1:Y:16:VAL:CG1	2.67	0.61
1:a:13:MET:HA	1:a:13:MET:CE	2.24	0.61
1:c:95:ASN:ND2	1:c:97:GLY:H	1.99	0.61
1:l:145:ARG:NH2	3:l:543:HOH:O	2.33	0.61
1:3:16:VAL:CG2	1:C:16:VAL:CG2	2.72	0.61
1:I:71:LYS:CG	1:I:146[B]:ILE:HD11	2.27	0.61
1:T:23:HIS:CE1	1:c:17:LYS:NZ	2.63	0.61
1:6:28[B]:ARG:NH1	1:I:117:PRO:CG	2.62	0.60
2:N:202:CA:CA	3:P:397:HOH:O	1.78	0.60
1:f:16:VAL:HG23	1:I:16:VAL:CG2	2.29	0.60
1:h:16:VAL:HG13	1:h:17:LYS:N	2.16	0.60
1:k:73:HIS:HD2	3:c:378:HOH:O	1.83	0.60
1:m:13:MET:C	1:m:16:VAL:HG12	2.27	0.60
1:K:91[B]:ARG:NH1	1:K:93:ASN:HD22	1.88	0.60
1:O:31:LEU:CD2	3:O:347:HOH:O	2.49	0.60
1:A:13:MET:HB3	1:d:19:MET:HE1	1.83	0.60
1:O:31:LEU:HD23	1:O:32:ILE:N	2.16	0.60
1:n:12:THR:N	3:n:400:HOH:O	2.33	0.60
1:7:73:HIS:HD2	3:W:371:HOH:O	1.84	0.60
1:5:23:HIS:CE1	1:H:17:LYS:HZ2	2.02	0.60
1:K:95:ASN:ND2	1:K:97:GLY:H	1.99	0.60
1:k:19:MET:SD	1:U:16:VAL:CG1	2.90	0.60
1:l:18:ARG:CB	3:l:464:HOH:O	2.26	0.60
1:s:23:HIS:CE1	1:2:17:LYS:HZ2	2.17	0.60
1:z:12:THR:CG2	1:z:13:MET:H	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:71:LYS:HD3	1:K:148[B]:ASN:HD21	1.66	0.60
1:l:16:VAL:HG21	1:E:16:VAL:HG23	1.84	0.60
1:p:23:HIS:CE1	1:y:17:LYS:HZ3	2.20	0.60
1:v:71:LYS:NZ	3:v:405:HOH:O	2.35	0.60
1:4:152:GLN:NE2	3:4:354:HOH:O	2.34	0.60
1:F:26:HIS:HE1	3:F:506:HOH:O	1.85	0.60
1:K:91[A]:ARG:HG3	1:K:171:ILE:HD13	1.84	0.60
1:N:19:MET:HE1	1:P:13:MET:HB3	1.84	0.60
1:n:73:HIS:HD2	3:O:375:HOH:O	1.83	0.60
1:Z:145[B]:ARG:NH1	3:Z:456:HOH:O	2.33	0.60
1:b:14:ARG:NE	3:b:486:HOH:O	2.34	0.60
1:t:96[B]:ARG:NE	3:t:415:HOH:O	2.35	0.60
1:5:95:ASN:ND2	1:5:97:GLY:H	2.00	0.60
1:G:129:LYS:CE	3:G:469:HOH:O	2.49	0.60
1:P:31:LEU:HD23	1:P:31:LEU:C	2.27	0.60
1:p:23:HIS:CE1	1:y:17:LYS:HZ2	2.15	0.59
1:w:23:HIS:HE1	1:V:17:LYS:NZ	2.01	0.59
1:x:18:ARG:O	1:x:22:THR:HG23	2.02	0.59
1:1:129:LYS:NZ	1:1:145:ARG:NH1	2.48	0.59
1:2:26:HIS:HE1	3:2:371:HOH:O	1.83	0.59
1:H:17:LYS:HE3	1:H:21:ASN:HD21	1.65	0.59
1:U:91[B]:ARG:HE	1:U:93:ASN:HD21	1.49	0.59
1:Z:146:ILE:HG13	3:Z:439:HOH:O	2.02	0.59
1:f:73:HIS:HD2	3:F:424:HOH:O	1.83	0.59
1:h:13:MET:C	1:h:16:VAL:HG12	2.21	0.59
1:w:19:MET:CE	1:V:16:VAL:CG1	2.78	0.59
1:w:95:ASN:ND2	1:w:97:GLY:H	2.00	0.59
1:A:95:ASN:ND2	1:A:97:GLY:H	2.00	0.59
1:E:95:ASN:ND2	1:E:97:GLY:H	2.00	0.59
1:G:21:ASN:ND2	3:G:467:HOH:O	2.34	0.59
1:k:13:MET:CA	1:k:16:VAL:HG12	2.32	0.59
1:6:66[A]:ARG:HG2	3:6:537:HOH:O	2.03	0.59
1:E:31[A]:LEU:HD22	3:E:518:HOH:O	2.00	0.59
1:P:13:MET:O	1:P:16:VAL:HG12	2.02	0.59
1:c:13:MET:CA	1:c:16:VAL:HG12	2.31	0.59
1:h:26:HIS:HE1	3:h:465:HOH:O	1.86	0.59
1:q:17:LYS:HZ1	1:V:23:HIS:CE1	2.02	0.59
1:a:12:THR:O	1:a:12:THR:HG23	2.02	0.59
1:0:95:ASN:ND2	1:0:97:GLY:H	1.99	0.59
1:7:91:ARG:NH1	1:7:93:ASN:HD22	1.93	0.59
1:M:129:LYS:NZ	1:M:147:ILE:HG23	2.12	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:95:ASN:ND2	1:O:97:GLY:H	1.99	0.59
1:P:23:HIS:CE1	1:W:17:LYS:HZ2	2.15	0.59
1:o:23:HIS:HE1	1:B:17:LYS:HZ2	1.50	0.59
1:v:13:MET:HE2	1:v:13:MET:N	2.14	0.59
1:A:13:MET:CA	1:A:16:VAL:CG1	2.78	0.59
1:J:95:ASN:ND2	1:J:97:GLY:H	2.01	0.59
1:K:145[B]:ARG:HG2	1:K:145[B]:ARG:NH1	2.14	0.59
1:4:13:MET:O	1:4:16:VAL:HG13	2.02	0.59
1:4:95:ASN:ND2	1:4:97:GLY:H	2.00	0.59
1:L:180[B]:LEU:HD13	3:L:367:HOH:O	2.01	0.59
1:U:71:LYS:NZ	3:U:456:HOH:O	2.36	0.59
1:e:13:MET:SD	1:Q:19:MET:HE1	2.42	0.59
1:x:91[B]:ARG:NH1	1:x:93:ASN:HD22	1.91	0.59
1:X:91:ARG:NH1	1:X:93:ASN:HD22	1.95	0.59
1:c:12:THR:O	1:c:15:ALA:N	2.36	0.59
1:i:13:MET:O	1:i:14:ARG:C	2.45	0.59
1:i:73:HIS:HD2	3:M:512:HOH:O	1.85	0.59
1:j:123:LYS:NZ	3:j:462:HOH:O	2.34	0.59
3:o:415:HOH:O	1:C:73:HIS:HD2	1.86	0.59
1:s:31:LEU:HD23	1:s:31:LEU:C	2.28	0.59
1:B:28[B]:ARG:HD3	3:B:466:HOH:O	2.03	0.59
1:L:31:LEU:C	1:L:31:LEU:HD23	2.28	0.59
1:M:79:ILE:HD11	3:M:370:HOH:O	2.01	0.59
1:N:91[B]:ARG:HD3	1:N:93:ASN:HD21	1.67	0.59
1:O:66:ARG:HG2	3:O:456:HOH:O	2.00	0.59
1:h:95:ASN:ND2	1:h:97:GLY:H	2.00	0.59
1:j:13:MET:HA	1:j:16:VAL:CG1	2.33	0.59
1:j:16:VAL:HG13	1:y:19:MET:SD	2.43	0.59
1:j:73:HIS:HD2	3:t:357:HOH:O	1.86	0.59
1:l:18:ARG:O	1:l:22:THR:HG23	2.02	0.59
1:p:31:LEU:HD23	1:p:31:LEU:C	2.28	0.59
1:0:31:LEU:HD23	1:0:31:LEU:C	2.27	0.59
1:1:73:HIS:HD2	3:S:432:HOH:O	1.86	0.59
1:5:12:THR:HG23	1:5:13:MET:N	2.18	0.59
1:L:13:MET:HA	1:L:16:VAL:CG1	2.33	0.59
1:c:91[B]:ARG:NH1	1:c:93:ASN:ND2	2.48	0.59
1:f:16:VAL:CG1	1:f:17:LYS:N	2.65	0.58
1:k:13:MET:HE1	1:Z:19:MET:HE3	1.83	0.58
1:3:13:MET:O	1:3:16:VAL:HG12	2.01	0.58
1:K:26:HIS:HE1	3:K:490:HOH:O	1.85	0.58
1:h:13:MET:SD	1:v:12:THR:OG1	2.61	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:16:VAL:HG23	1:p:16:VAL:HG21	1.83	0.58
1:w:19:MET:HE3	1:V:13:MET:HE1	1.84	0.58
1:3:152:GLN:NE2	3:3:448:HOH:O	2.35	0.58
1:E:28:ARG:HD3	3:E:478:HOH:O	2.02	0.58
1:S:148:ASN:CB	3:S:450:HOH:O	2.37	0.58
1:U:19:MET:CE	1:Z:13:MET:HE2	2.18	0.58
1:i:23:HIS:CE1	1:Q:17:LYS:NZ	2.69	0.58
1:x:13:MET:C	1:x:16:VAL:HG12	2.28	0.58
1:7:16:VAL:CG1	1:7:17:LYS:H	2.16	0.58
1:7:73:HIS:HB2	1:7:146:ILE:HD13	1.84	0.58
1:T:91:ARG:HD2	3:T:541:HOH:O	2.02	0.58
1:b:12:THR:CA	3:b:481:HOH:O	2.37	0.58
1:b:95:ASN:ND2	1:b:97:GLY:H	2.01	0.58
1:c:13:MET:HA	1:c:16:VAL:HG11	1.83	0.58
1:k:18:ARG:O	1:k:22:THR:HG23	2.03	0.58
1:x:91[A]:ARG:HE	1:x:93:ASN:HD21	1.49	0.58
1:2:91:ARG:NH1	1:2:93:ASN:HD22	1.88	0.58
1:K:13:MET:HA	1:K:16:VAL:HG11	1.82	0.58
1:g:95:ASN:ND2	1:g:97:GLY:H	2.01	0.58
1:x:23:HIS:CE1	1:T:17:LYS:HZ3	2.18	0.58
1:y:95:ASN:ND2	1:y:97:GLY:H	2.02	0.58
1:G:19:MET:HE1	1:M:13:MET:HB3	1.85	0.58
1:g:17:LYS:HZ3	1:b:23:HIS:CE1	2.21	0.58
1:k:95:ASN:ND2	1:k:97:GLY:H	2.01	0.58
1:L:95:ASN:ND2	1:L:97:GLY:H	2.02	0.58
1:X:13:MET:HA	1:X:16:VAL:HG12	1.84	0.58
1:X:66:ARG:CZ	1:X:153[B]:LEU:HD12	2.32	0.58
1:w:162[A]:VAL:HG12	3:w:515:HOH:O	2.03	0.58
1:U:16:VAL:CG1	1:U:17:LYS:N	2.67	0.58
1:b:13:MET:C	1:b:16:VAL:CG1	2.72	0.58
1:e:95:ASN:ND2	1:e:97:GLY:H	2.01	0.58
3:s:367:HOH:O	1:B:73:HIS:HD2	1.87	0.58
1:5:71:LYS:HG3	1:5:148[B]:ASN:OD1	2.03	0.58
1:6:28[B]:ARG:HG2	1:6:28[B]:ARG:HH11	1.68	0.58
1:7:16:VAL:CG1	1:7:17:LYS:N	2.66	0.58
1:Q:31:LEU:C	1:Q:31:LEU:HD23	2.29	0.58
1:U:71:LYS:CG	1:U:148[A]:ASN:OD1	2.52	0.58
1:U:145:ARG:HD3	3:U:545:HOH:O	2.03	0.58
1:W:71:LYS:NZ	3:W:390:HOH:O	2.36	0.58
1:m:28[A]:ARG:HD2	3:m:433:HOH:O	2.02	0.58
1:3:66:ARG:CG	3:3:526:HOH:O	2.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:7:402:HOH:O	1:H:73:HIS:HD2	1.87	0.58
1:R:13:MET:HA	1:R:16:VAL:HG11	1.86	0.58
1:l:16:VAL:HG13	1:l:17:LYS:H	1.69	0.57
1:r:19:MET:HE1	1:b:13:MET:HB3	1.86	0.57
1:r:95:ASN:ND2	1:r:97:GLY:H	2.02	0.57
1:F:19:MET:HE3	1:O:13:MET:HE1	1.84	0.57
1:T:71:LYS:HZ2	1:T:71:LYS:CB	2.15	0.57
1:V:91:ARG:NH1	1:V:93:ASN:HD22	1.96	0.57
1:q:73:HIS:HD2	3:0:347:HOH:O	1.86	0.57
1:t:15:ALA:HB1	1:C:13:MET:HE1	1.79	0.57
1:z:95:ASN:ND2	1:z:97:GLY:H	2.01	0.57
1:C:31:LEU:HD22	3:C:386:HOH:O	2.01	0.57
1:M:79:ILE:CD1	3:M:370:HOH:O	2.51	0.57
1:O:31:LEU:HD23	1:O:31:LEU:C	2.29	0.57
1:R:17:LYS:HE3	1:R:21:ASN:HD22	1.68	0.57
1:0:95:ASN:HD22	1:0:97:GLY:H	1.52	0.57
1:G:19:MET:SD	1:M:16:VAL:HG13	2.44	0.57
1:H:95:ASN:ND2	1:H:97:GLY:H	2.02	0.57
1:O:13:MET:C	1:O:16:VAL:HG12	2.29	0.57
1:q:18:ARG:O	1:q:22:THR:HG23	2.03	0.57
3:u:367:HOH:O	1:0:73:HIS:HD2	1.87	0.57
1:F:73:HIS:HD2	3:G:360:HOH:O	1.87	0.57
1:l:95:ASN:ND2	1:l:97:GLY:H	2.02	0.57
1:t:43[B]:THR:HG22	3:t:507:HOH:O	2.03	0.57
1:H:123:LYS:CE	3:H:458:HOH:O	2.52	0.57
1:K:19:MET:SD	1:d:16:VAL:HG22	2.44	0.57
1:N:95:ASN:ND2	1:N:97:GLY:H	2.03	0.57
1:T:13:MET:O	1:T:16:VAL:HG12	2.05	0.57
1:X:71:LYS:HB2	1:X:71:LYS:NZ	2.20	0.57
1:Y:95:ASN:ND2	1:Y:97:GLY:H	2.03	0.57
1:l:129:LYS:HE2	3:l:325:HOH:O	2.02	0.57
1:v:73:HIS:HD2	3:4:406:HOH:O	1.87	0.57
1:1:129:LYS:HZ2	1:1:145:ARG:HH12	1.48	0.57
1:C:31:LEU:HD21	3:C:386:HOH:O	2.00	0.57
1:C:129:LYS:NZ	1:C:147:ILE:HG23	2.16	0.57
1:Y:66[A]:ARG:HD3	3:Y:550:HOH:O	2.04	0.57
1:l:17:LYS:HG2	3:l:459:HOH:O	2.03	0.57
1:5:13:MET:HA	1:5:16:VAL:HG12	1.86	0.57
1:O:13:MET:HA	1:O:16:VAL:HG11	1.83	0.57
1:m:17:LYS:HZ3	1:I:23:HIS:CE1	2.22	0.57
1:w:19:MET:SD	1:V:16:VAL:HG13	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:95:ASN:ND2	1:o:97:GLY:H	2.02	0.57
1:t:43[B]:THR:CG2	3:t:507:HOH:O	2.53	0.57
1:2:31:LEU:HD21	3:2:406:HOH:O	2.04	0.57
1:G:95:ASN:ND2	1:G:97:GLY:H	2.02	0.57
1:K:19:MET:CE	1:d:13:MET:HE1	2.17	0.57
1:N:12:THR:CA	3:N:457:HOH:O	2.41	0.57
1:b:22:THR:HG23	1:b:23:HIS:CD2	2.39	0.57
1:y:13:MET:HA	1:y:16:VAL:CG1	2.35	0.56
1:B:146[B]:ILE:HG22	3:B:434:HOH:O	2.03	0.56
3:D:339:HOH:O	1:Y:73:HIS:HD2	1.88	0.56
1:n:131:VAL:CG2	1:n:145[B]:ARG:HD3	2.35	0.56
1:v:12:THR:C	1:v:13:MET:HE2	2.30	0.56
1:I:18:ARG:O	1:I:22:THR:HG23	2.05	0.56
1:S:18:ARG:O	1:S:22:THR:HG23	2.05	0.56
1:c:17:LYS:HE3	1:c:21:ASN:HD21	1.69	0.56
1:f:95:ASN:ND2	1:f:97:GLY:H	2.02	0.56
1:h:66:ARG:NH1	3:h:483:HOH:O	2.38	0.56
1:m:73:HIS:HD2	3:E:388:HOH:O	1.87	0.56
1:n:95:ASN:HD22	1:n:97:GLY:H	1.54	0.56
1:p:95:ASN:HD22	1:p:97:GLY:H	1.53	0.56
1:q:13:MET:HA	1:q:16:VAL:CG1	2.35	0.56
1:B:17:LYS:CE	1:B:21:ASN:ND2	2.62	0.56
1:I:13:MET:HA	1:I:16:VAL:CG1	2.34	0.56
1:N:17:LYS:CE	1:N:21:ASN:HD21	2.18	0.56
1:O:18:ARG:HD2	3:O:461:HOH:O	2.06	0.56
1:D:31[A]:LEU:HD23	1:D:32:ILE:N	2.20	0.56
1:G:81[A]:VAL:HG12	1:G:82:SER:O	2.06	0.56
1:c:12:THR:CG2	1:c:13:MET:N	2.68	0.56
1:s:73:HIS:HD2	3:v:374:HOH:O	1.88	0.56
1:O:152:GLN:HG3	3:O:455:HOH:O	2.05	0.56
1:O:152:GLN:NE2	3:O:464:HOH:O	2.38	0.56
1:T:13:MET:O	1:T:16:VAL:CG1	2.54	0.56
1:i:28[B]:ARG:HD2	1:M:117:PRO:HA	1.87	0.56
1:t:13:MET:CE	1:3:19:MET:HE3	2.35	0.56
1:2:17:LYS:CE	1:2:21:ASN:HD21	2.10	0.56
1:M:71:LYS:NZ	1:M:71:LYS:CB	2.68	0.56
1:c:31:LEU:CD2	3:c:555:HOH:O	2.52	0.56
1:z:16:VAL:HG13	1:S:19:MET:SD	2.46	0.56
1:4:17:LYS:HZ3	1:a:23:HIS:HE1	1.53	0.56
1:A:17:LYS:NZ	3:A:464:HOH:O	2.39	0.56
1:L:40:THR:HG23	1:L:180[B]:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:18:ARG:O	1:P:22:THR:HG23	2.05	0.56
1:a:95:ASN:ND2	1:a:97:GLY:H	2.02	0.56
1:d:95:ASN:ND2	1:d:97:GLY:H	2.03	0.56
1:h:18:ARG:O	1:h:22:THR:HG23	2.06	0.56
1:o:12:THR:O	1:o:12:THR:HG23	2.04	0.56
1:u:14:ARG:HG2	3:u:449:HOH:O	2.05	0.56
1:w:23:HIS:CE1	1:V:17:LYS:HZ3	2.24	0.56
1:K:73:HIS:CG	1:K:146[B]:ILE:HG22	2.41	0.56
1:S:91[A]:ARG:HE	1:S:93:ASN:ND2	2.03	0.56
1:V:14:ARG:CB	1:V:14:ARG:CZ	2.83	0.56
1:e:16:VAL:HG13	1:e:17:LYS:N	2.21	0.56
1:M:129:LYS:HZ3	1:M:147:ILE:CG2	2.16	0.56
1:T:14:ARG:NH2	1:T:18:ARG:NH1	2.54	0.56
1:m:17:LYS:HE3	1:m:21:ASN:HD21	1.71	0.56
1:B:95:ASN:ND2	1:B:97:GLY:H	2.03	0.56
1:D:95:ASN:ND2	1:D:97:GLY:H	2.04	0.56
1:Q:66:ARG:CG	3:Q:553:HOH:O	2.46	0.56
1:X:95:ASN:ND2	1:X:97:GLY:H	2.04	0.56
1:e:91:ARG:HD2	3:e:439:HOH:O	2.05	0.55
1:r:129:LYS:CE	1:r:145[A]:ARG:NH2	2.69	0.55
1:u:17:LYS:HZ2	1:B:23:HIS:HE1	1.52	0.55
1:z:73:HIS:HD2	3:A:399:HOH:O	1.88	0.55
1:2:66:ARG:NH2	3:2:348:HOH:O	2.39	0.55
1:R:12:THR:CG2	1:R:13:MET:H	2.18	0.55
1:h:73:HIS:HD2	3:1:340:HOH:O	1.89	0.55
1:j:12:THR:HG23	1:j:13:MET:N	2.21	0.55
1:6:14:ARG:N	3:6:480:HOH:O	2.39	0.55
1:I:95:ASN:ND2	1:I:97:GLY:H	2.05	0.55
1:Q:95:ASN:ND2	1:Q:97:GLY:H	2.04	0.55
1:V:31[B]:LEU:HD21	3:V:548:HOH:O	2.05	0.55
1:q:19:MET:CE	1:w:13:MET:CE	2.84	0.55
1:w:26:HIS:HE1	3:w:402:HOH:O	1.88	0.55
1:x:13:MET:HA	1:x:16:VAL:HG12	1.87	0.55
1:x:23:HIS:CE1	1:T:17:LYS:HZ2	2.14	0.55
1:4:13:MET:CA	1:4:16:VAL:CG1	2.83	0.55
1:R:91:ARG:NH1	1:R:93:ASN:HD22	1.88	0.55
1:U:71:LYS:CD	1:U:148[A]:ASN:OD1	2.53	0.55
1:Y:13:MET:O	1:Y:16:VAL:CG1	2.55	0.55
1:d:12:THR:CA	3:d:469:HOH:O	2.53	0.55
1:l:16:VAL:CG2	1:E:16:VAL:HG23	2.36	0.55
1:n:71:LYS:CG	1:n:146:ILE:HD11	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:p:19:MET:O	1:p:23:HIS:HD2	1.89	0.55
1:4:13:MET:O	1:4:16:VAL:HG12	2.04	0.55
1:K:19:MET:SD	1:d:13:MET:CE	2.95	0.55
1:O:18:ARG:HD3	3:O:461:HOH:O	2.04	0.55
1:Z:13:MET:HA	1:Z:16:VAL:HG12	1.86	0.55
1:1:16:VAL:HG11	1:X:19:MET:HE1	1.88	0.55
1:M:13:MET:O	1:M:14:ARG:C	2.49	0.55
1:n:91:ARG:NH1	1:n:93:ASN:HD22	2.00	0.55
1:x:129:LYS:CE	3:x:398:HOH:O	2.52	0.55
1:2:91:ARG:HD3	1:2:93:ASN:ND2	2.22	0.55
1:C:31:LEU:HD23	1:C:31:LEU:C	2.31	0.55
1:N:19:MET:CE	1:P:13:MET:HB3	2.36	0.55
1:P:91[A]:ARG:HE	1:P:93:ASN:HD21	1.55	0.55
1:V:123:LYS:HE3	3:V:480:HOH:O	2.06	0.55
1:b:31:LEU:HD23	1:b:31:LEU:C	2.31	0.55
1:e:23:HIS:HE1	1:i:66:ARG:HH22	1.52	0.55
1:M:26:HIS:HE1	3:M:483:HOH:O	1.89	0.55
1:Y:91:ARG:NH1	1:Y:93:ASN:HD22	2.04	0.55
1:Z:91[A]:ARG:NH1	1:Z:93:ASN:HD22	1.90	0.55
1:c:16:VAL:O	1:c:20:ILE:HG13	2.07	0.55
1:m:91:ARG:NH1	1:m:93:ASN:HD22	1.98	0.55
1:C:66[A]:ARG:HD3	3:C:372:HOH:O	2.06	0.55
1:K:22:THR:HG22	1:d:66:ARG:NH2	2.22	0.55
1:W:16:VAL:HG13	1:W:17:LYS:N	2.21	0.55
1:a:91:ARG:NH1	1:a:93:ASN:HD22	1.93	0.55
1:h:23:HIS:CE1	1:R:17:LYS:HZ2	2.23	0.55
1:h:23:HIS:CE1	1:R:17:LYS:NZ	2.67	0.55
1:l:31:LEU:C	1:l:31:LEU:HD23	2.32	0.55
1:E:13:MET:HA	1:E:16:VAL:HG12	1.89	0.55
1:I:146[A]:ILE:HD11	3:I:433:HOH:O	2.06	0.55
1:Q:71:LYS:HE3	1:Q:148[A]:ASN:OD1	2.03	0.55
1:U:19:MET:SD	1:Z:13:MET:HE3	2.46	0.55
1:e:150:PRO:HG2	3:e:480:HOH:O	2.07	0.54
1:t:13:MET:HE3	1:3:19:MET:HE3	1.89	0.54
1:t:17:LYS:CE	1:t:21:ASN:HD21	2.19	0.54
1:4:71:LYS:CD	1:4:148[B]:ASN:ND2	2.61	0.54
1:R:95:ASN:HD22	1:R:97:GLY:H	1.54	0.54
1:c:73:HIS:HE1	1:c:144:ASP:OD2	1.90	0.54
1:t:13:MET:C	1:t:16:VAL:HG12	2.32	0.54
3:7:422:HOH:O	1:H:146:ILE:HD11	2.05	0.54
1:C:95:ASN:HD22	1:C:97:GLY:H	1.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:16:VAL:HG13	1:S:17:LYS:N	2.22	0.54
1:i:95:ASN:HD22	1:i:97:GLY:H	1.54	0.54
1:n:16:VAL:CG1	1:n:17:LYS:N	2.70	0.54
1:3:13:MET:HA	1:3:16:VAL:HG11	1.86	0.54
1:E:91:ARG:NH1	1:E:93:ASN:HD22	1.95	0.54
1:j:16:VAL:HG13	1:j:17:LYS:N	2.22	0.54
1:t:13:MET:HA	1:t:16:VAL:HG11	1.86	0.54
1:x:12:THR:HG21	3:T:499:HOH:O	2.05	0.54
1:z:19:MET:HG2	1:Y:20:ILE:CD1	2.38	0.54
1:j:95:ASN:ND2	1:j:97:GLY:H	2.06	0.54
1:u:73:HIS:HD2	3:3:437:HOH:O	1.90	0.54
1:H:95:ASN:HD22	1:H:97:GLY:H	1.56	0.54
1:H:123:LYS:HE2	3:H:458:HOH:O	2.06	0.54
1:X:71:LYS:HB2	1:X:71:LYS:HZ2	1.72	0.54
1:c:17:LYS:HE3	1:c:21:ASN:ND2	2.23	0.54
1:r:73:HIS:HE1	1:r:144:ASP:OD2	1.90	0.54
1:s:16:VAL:HA	1:2:13:MET:HE1	1.89	0.54
1:v:13:MET:HE3	1:v:13:MET:N	2.21	0.54
1:2:18:ARG:O	1:2:22[A]:THR:HG23	2.08	0.54
1:6:73:HIS:HD2	3:I:496:HOH:O	1.88	0.54
1:X:13:MET:C	1:X:16:VAL:HG12	2.32	0.54
1:f:114:GLN:OE1	1:J:71:LYS:HE3	2.08	0.54
1:p:13:MET:HA	1:p:16:VAL:HG12	1.90	0.54
1:q:45:GLN:NE2	3:q:474:HOH:O	2.41	0.54
1:5:19:MET:HE2	1:H:13:MET:HE3	1.81	0.54
1:j:16:VAL:O	1:j:20:ILE:HG13	2.07	0.54
1:o:13:MET:CA	1:o:16:VAL:HG12	2.35	0.54
1:I:26:HIS:HE1	3:I:455:HOH:O	1.89	0.54
1:P:95:ASN:HD22	1:P:97:GLY:H	1.55	0.54
1:S:95:ASN:HD22	1:S:97:GLY:H	1.55	0.54
1:i:19:MET:HE1	1:Q:13:MET:SD	2.47	0.54
1:i:23:HIS:CE1	1:Q:17:LYS:HZ3	2.26	0.54
1:3:12:THR:O	1:3:16:VAL:HG12	2.08	0.54
1:a:129:LYS:NZ	1:a:145[B]:ARG:HH22	2.05	0.54
1:e:23:HIS:CE1	1:i:66:ARG:NH1	2.59	0.54
1:h:16:VAL:HG13	1:h:17:LYS:H	1.72	0.54
1:h:71:LYS:HB2	1:h:71:LYS:HZ2	1.73	0.54
1:F:15:ALA:CB	1:O:13:MET:SD	2.95	0.54
1:J:73:HIS:HE1	1:J:144:ASP:OD2	1.91	0.54
1:W:95:ASN:ND2	1:W:97:GLY:H	2.06	0.54
1:Y:146:ILE:HD12	1:Y:146:ILE:C	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:13:MET:HE1	1:m:19:MET:HE3	1.84	0.53
1:x:13:MET:HE3	1:c:19:MET:HE3	1.89	0.53
1:D:72:LEU:C	1:D:146[A]:ILE:HD12	2.33	0.53
1:E:17:LYS:NZ	1:J:23:HIS:HE1	2.06	0.53
1:T:91:ARG:HD3	1:T:93:ASN:ND2	2.23	0.53
1:e:13:MET:SD	1:e:16:VAL:CG1	2.96	0.53
1:e:26:HIS:HE1	3:e:379:HOH:O	1.90	0.53
1:e:148:ASN:CB	3:e:384:HOH:O	2.42	0.53
1:g:73:HIS:HD2	3:j:385:HOH:O	1.89	0.53
1:k:24:LEU:O	1:k:26:HIS:HD2	1.89	0.53
1:q:73:HIS:HE1	1:q:144:ASP:OD2	1.91	0.53
1:0:16:VAL:HG13	1:0:17:LYS:N	2.22	0.53
1:A:17:LYS:NZ	1:d:23:HIS:HE1	2.06	0.53
1:N:19:MET:CE	1:P:16:VAL:HG11	2.38	0.53
1:U:71:LYS:HD3	1:U:148[A]:ASN:CG	2.33	0.53
1:o:73:HIS:HD2	3:5:351:HOH:O	1.90	0.53
1:p:19:MET:HE1	1:y:13:MET:HE3	1.88	0.53
3:z:351:HOH:O	1:N:73:HIS:HD2	1.91	0.53
1:2:95:ASN:HD22	1:2:97:GLY:H	1.55	0.53
1:K:19:MET:SD	1:d:13:MET:HE1	2.48	0.53
1:R:13:MET:HA	1:R:16:VAL:HG12	1.89	0.53
1:c:31:LEU:HD23	1:c:31:LEU:C	2.34	0.53
1:u:31:LEU:HD23	1:u:32:ILE:N	2.23	0.53
1:V:21:ASN:HB3	3:V:469:HOH:O	2.07	0.53
1:c:13:MET:CA	1:c:16:VAL:CG1	2.84	0.53
1:d:145:ARG:HG3	3:d:333:HOH:O	2.08	0.53
1:v:145:ARG:NH2	3:v:529:HOH:O	2.42	0.53
1:3:13:MET:C	1:3:16:VAL:CG1	2.81	0.53
1:B:13:MET:CE	1:B:16:VAL:HG11	2.38	0.53
1:M:19:MET:HE3	1:M:23:HIS:NE2	2.23	0.53
1:R:13:MET:O	1:R:16:VAL:HG13	2.08	0.53
1:e:23:HIS:CA	1:i:66:ARG:NH1	2.67	0.53
3:l:352:HOH:O	1:b:73:HIS:HD2	1.90	0.53
1:m:18:ARG:O	1:m:22:THR:CG2	2.56	0.53
1:1:129:LYS:HZ2	1:1:145:ARG:NH1	2.07	0.53
1:F:16:VAL:HG13	1:F:17:LYS:N	2.23	0.53
1:P:73:HIS:HD2	3:a:415:HOH:O	1.92	0.53
1:Y:148[A]:ASN:CG	3:Y:545:HOH:O	2.51	0.53
1:m:18:ARG:O	1:m:22:THR:HG23	2.09	0.53
1:m:173[A]:MET:HE2	3:m:419:HOH:O	2.09	0.53
1:y:17:LYS:CE	1:y:21:ASN:HD21	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:95:ASN:HD22	1:1:97:GLY:H	1.57	0.53
1:G:73:HIS:HD2	3:Q:435:HOH:O	1.91	0.53
1:H:12:THR:C	1:H:14:ARG:H	2.17	0.53
1:I:152:GLN:HG3	3:I:465:HOH:O	2.09	0.53
1:P:71[B]:LYS:CG	1:P:148:ASN:OD1	2.57	0.53
1:T:18:ARG:O	1:T:22:THR:HG23	2.09	0.53
1:X:12:THR:O	1:X:15:ALA:HB3	2.09	0.53
3:k:446:HOH:O	1:r:146:ILE:CD1	2.54	0.53
1:q:23:HIS:HE1	1:w:17:LYS:HZ1	1.57	0.53
1:3:31:LEU:HD23	1:3:31:LEU:C	2.34	0.53
1:6:91:ARG:HD2	3:6:524:HOH:O	2.08	0.53
1:A:12:THR:O	1:A:16:VAL:HG12	2.08	0.53
1:N:148[A]:ASN:ND2	3:N:430:HOH:O	2.25	0.53
1:w:19:MET:HE1	1:V:16:VAL:HG13	1.90	0.53
1:L:31:LEU:HD23	1:L:32:ILE:N	2.23	0.53
1:d:31:LEU:C	1:d:31:LEU:HD23	2.34	0.53
1:s:16:VAL:HG23	1:2:16:VAL:CG2	2.36	0.52
1:s:145:ARG:NH2	3:s:313:HOH:O	2.41	0.52
1:w:19:MET:CE	1:V:16:VAL:HG11	2.37	0.52
1:y:71:LYS:NZ	3:y:430:HOH:O	2.42	0.52
1:7:12:THR:CG2	1:7:13:MET:N	2.72	0.52
1:e:91:ARG:HD3	1:e:93:ASN:ND2	2.25	0.52
1:j:23:HIS:HE1	1:p:17:LYS:HZ2	1.58	0.52
1:v:95:ASN:ND2	1:v:97:GLY:H	2.06	0.52
1:6:18:ARG:O	1:6:22:THR:HG23	2.09	0.52
1:H:91[B]:ARG:HD3	1:H:93:ASN:ND2	2.25	0.52
1:q:28:ARG:HG2	1:q:191:VAL:HG22	1.92	0.52
1:t:14:ARG:CB	3:t:455:HOH:O	2.52	0.52
1:2:13:MET:O	1:2:16:VAL:N	2.42	0.52
1:4:91:ARG:HD2	3:4:445:HOH:O	2.09	0.52
1:7:18:ARG:O	1:7:22:THR:HG23	2.10	0.52
1:A:73:HIS:HE1	1:A:144:ASP:OD2	1.91	0.52
1:E:95:ASN:HD22	1:E:97:GLY:H	1.57	0.52
1:K:91[A]:ARG:CD	1:K:171:ILE:CD1	2.80	0.52
1:M:73:HIS:HD2	3:N:501:HOH:O	1.92	0.52
1:c:26:HIS:HE1	3:c:387:HOH:O	1.92	0.52
1:m:31:LEU:HD23	1:m:31:LEU:C	2.35	0.52
1:p:17:LYS:CE	1:p:21:ASN:HD21	2.23	0.52
1:w:73:HIS:HD2	3:x:392:HOH:O	1.92	0.52
1:x:95:ASN:HD22	1:x:97:GLY:H	1.56	0.52
1:1:16:VAL:HG13	1:X:19:MET:HE1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:16:VAL:HG13	1:T:17:LYS:H	1.74	0.52
1:Z:145[A]:ARG:NH2	3:Z:338:HOH:O	2.06	0.52
1:7:16:VAL:HG23	1:a:16:VAL:HG21	1.91	0.52
3:C:364:HOH:O	1:I:73:HIS:HD2	1.92	0.52
1:K:12:THR:CA	3:K:469:HOH:O	2.44	0.52
1:K:13:MET:CA	1:K:16:VAL:HG12	2.39	0.52
1:R:91:ARG:HD3	1:R:93:ASN:ND2	2.25	0.52
1:U:73:HIS:HE1	1:U:144:ASP:OD2	1.92	0.52
1:a:13:MET:HE2	1:a:13:MET:CA	2.28	0.52
1:p:13:MET:O	1:p:16:VAL:HG13	2.10	0.52
1:4:23:HIS:CE1	1:7:17:LYS:NZ	2.76	0.52
1:J:28[B]:ARG:NH2	1:J:189:GLU:OE1	2.42	0.52
1:P:13:MET:HE3	1:P:16:VAL:HG11	1.92	0.52
1:P:91[A]:ARG:CZ	1:P:152:GLN:NE2	2.70	0.52
1:X:71:LYS:NZ	1:X:71:LYS:CB	2.72	0.52
1:j:16:VAL:HG13	1:j:17:LYS:H	1.75	0.52
1:u:12:THR:O	1:u:16:VAL:HG12	2.09	0.52
1:3:91[A]:ARG:HD3	1:3:93:ASN:ND2	2.25	0.52
1:D:73:HIS:HD2	3:T:405:HOH:O	1.92	0.52
1:J:31:LEU:HD23	1:J:31:LEU:C	2.35	0.52
1:M:64[A]:GLN:NE2	3:M:522:HOH:O	2.42	0.52
1:r:91:ARG:NH1	1:r:93:ASN:HD22	2.02	0.52
1:O:73:HIS:CG	1:O:146:ILE:HG12	2.44	0.52
3:m:388:HOH:O	1:t:73:HIS:HD2	1.92	0.52
1:K:13:MET:CA	1:K:16:VAL:CG1	2.85	0.52
1:R:71:LYS:HB2	1:R:71:LYS:NZ	2.25	0.52
1:V:26:HIS:HE1	3:V:484:HOH:O	1.91	0.52
1:g:71:LYS:NZ	3:g:336:HOH:O	2.42	0.52
1:i:13:MET:HA	1:i:16:VAL:HG11	1.79	0.52
1:m:16:VAL:O	1:m:20:ILE:HG13	2.10	0.52
3:y:466:HOH:O	1:V:73:HIS:HD2	1.92	0.52
1:1:17:LYS:HZ2	1:X:23:HIS:CE1	2.08	0.52
1:L:12:THR:OG1	1:L:15:ALA:HB3	2.11	0.52
1:V:19:MET:HE2	1:V:19:MET:HA	1.91	0.52
1:C:18:ARG:HD2	3:C:442:HOH:O	2.10	0.51
1:I:91:ARG:HD2	3:I:400:HOH:O	2.09	0.51
1:M:17:LYS:HD2	1:M:21:ASN:HD21	1.74	0.51
1:P:73:HIS:HE1	1:P:144:ASP:OD2	1.93	0.51
1:k:91:ARG:HD2	3:k:414:HOH:O	2.10	0.51
1:t:91[A]:ARG:HD3	1:t:93:ASN:ND2	2.26	0.51
1:1:24:LEU:O	1:1:26:HIS:HD2	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146[B]:ILE:HD12	3:T:491:HOH:O	2.10	0.51
1:F:15:ALA:C	1:O:13:MET:HE1	2.36	0.51
1:S:152[A]:GLN:HG3	1:S:153:LEU:O	2.10	0.51
1:Y:148[A]:ASN:ND2	3:Y:429:HOH:O	2.42	0.51
1:l:33:ASN:ND2	3:l:394:HOH:O	2.42	0.51
1:5:23:HIS:CE1	1:H:17:LYS:HZ3	2.27	0.51
1:5:73:HIS:HE1	1:5:144:ASP:OD2	1.93	0.51
1:V:24:LEU:O	1:V:26:HIS:HD2	1.94	0.51
1:m:95:ASN:ND2	1:m:97:GLY:H	2.08	0.51
1:7:72:LEU:C	1:7:146:ILE:HD12	2.35	0.51
1:k:31:LEU:HD23	1:k:32:ILE:N	2.25	0.51
1:y:18:ARG:O	1:y:22:THR:HG23	2.11	0.51
1:4:129:LYS:HE2	3:4:347:HOH:O	2.11	0.51
1:F:19:MET:HE1	1:O:16:VAL:HG13	1.92	0.51
1:S:17:LYS:HE3	1:Y:19:MET:HE2	1.93	0.51
1:U:16:VAL:HG13	1:U:17:LYS:N	2.26	0.51
1:r:91:ARG:HD2	3:r:420:HOH:O	2.10	0.51
1:t:15:ALA:HB1	1:C:13:MET:CE	2.36	0.51
1:Z:17:LYS:CE	1:Z:21:ASN:HD21	2.19	0.51
1:h:71:LYS:NZ	1:h:71:LYS:CB	2.74	0.51
1:w:95:ASN:HD22	1:w:97:GLY:H	1.58	0.51
1:B:73:HIS:CG	1:B:146[A]:ILE:CG2	2.93	0.51
1:H:23:HIS:HE1	1:L:17:LYS:HZ1	1.56	0.51
1:W:14:ARG:O	1:W:16:VAL:N	2.43	0.51
1:k:114:GLN:OE1	1:r:71:LYS:HE3	2.10	0.51
1:x:13:MET:O	1:x:16:VAL:CG1	2.48	0.51
1:A:17:LYS:HZ2	1:d:23:HIS:HE1	1.58	0.51
3:B:317:HOH:O	1:L:73:HIS:HD2	1.93	0.51
1:G:16:VAL:HG13	1:G:17:LYS:N	2.25	0.51
1:H:13:MET:CA	1:H:16:VAL:CG1	2.84	0.51
1:U:71:LYS:HD3	1:U:148[A]:ASN:ND2	2.26	0.51
1:q:95:ASN:ND2	1:q:97:GLY:H	2.09	0.51
1:s:23:HIS:HE1	1:2:17:LYS:HZ3	1.57	0.51
1:2:28[A]:ARG:HD2	3:2:380:HOH:O	2.11	0.51
1:4:26:HIS:HE1	3:4:385:HOH:O	1.92	0.51
1:4:73:HIS:HD2	3:L:382:HOH:O	1.93	0.51
1:5:71:LYS:HD3	1:5:148[B]:ASN:OD1	2.11	0.51
1:U:73:HIS:HD2	3:d:405:HOH:O	1.92	0.51
1:Y:31:LEU:C	1:Y:31:LEU:HD23	2.36	0.51
1:k:21:ASN:ND2	3:k:422:HOH:O	2.35	0.51
1:n:23:HIS:CE1	1:G:17:LYS:HZ1	2.04	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:z:13:MET:O	1:z:16:VAL:CG1	2.59	0.51
1:A:84:THR:CB	3:A:452:HOH:O	2.58	0.51
1:Y:66[B]:ARG:HG2	3:Y:457:HOH:O	2.11	0.51
1:o:91:ARG:HD2	3:o:452:HOH:O	2.11	0.50
1:v:28:ARG:HG2	1:v:191:VAL:HG22	1.93	0.50
1:w:162[A]:VAL:HG11	3:w:515:HOH:O	2.07	0.50
1:1:91[A]:ARG:CZ	1:1:152:GLN:HB2	2.41	0.50
1:A:71:LYS:CG	1:A:146:ILE:HD11	2.41	0.50
1:B:38:ASN:HB3	1:B:179:SER:O	2.11	0.50
1:E:37:THR:HG21	3:E:348:HOH:O	2.11	0.50
1:O:16:VAL:O	1:O:20:ILE:HG13	2.10	0.50
1:Y:123:LYS:CE	3:Y:437:HOH:O	2.59	0.50
1:Z:91[A]:ARG:HD3	1:Z:93:ASN:HD21	1.75	0.50
1:r:12:THR:C	1:r:14:ARG:N	2.69	0.50
1:y:95:ASN:HD22	1:y:97:GLY:H	1.57	0.50
1:4:18:ARG:O	1:4:22:THR:HG23	2.11	0.50
1:6:16:VAL:HG23	1:F:16:VAL:HG21	1.93	0.50
1:E:12:THR:HG23	1:E:15:ALA:HB3	1.91	0.50
1:Q:174:LEU:HD23	1:Q:174:LEU:C	2.35	0.50
1:U:91[A]:ARG:HD3	1:U:93:ASN:HD21	1.74	0.50
1:Y:71:LYS:CD	1:Y:148[A]:ASN:OD1	2.56	0.50
1:e:13:MET:HA	1:e:16:VAL:HG12	1.92	0.50
1:3:20:ILE:CD1	1:C:19:MET:HG3	2.42	0.50
1:5:73:HIS:HD2	3:6:406:HOH:O	1.94	0.50
1:U:71:LYS:HD3	1:U:148[A]:ASN:HD21	1.76	0.50
1:j:23:HIS:CE1	1:p:17:LYS:NZ	2.75	0.50
1:L:18:ARG:HG2	3:L:352:HOH:O	2.10	0.50
1:T:95:ASN:HD22	1:T:97:GLY:H	1.58	0.50
1:V:148:ASN:ND2	3:V:358:HOH:O	2.45	0.50
3:V:538:HOH:O	1:c:146:ILE:HD11	2.11	0.50
1:e:23:HIS:CB	1:i:66:ARG:NH1	2.73	0.50
1:i:18:ARG:CG	3:i:410:HOH:O	2.59	0.50
3:n:394:HOH:O	1:W:73:HIS:HD2	1.95	0.50
1:x:13:MET:O	1:x:16:VAL:N	2.44	0.50
1:E:17:LYS:CE	1:E:21:ASN:ND2	2.75	0.50
1:W:31:LEU:C	1:W:31:LEU:HD12	2.37	0.50
1:i:18:ARG:HD3	3:i:410:HOH:O	2.09	0.50
1:r:31:LEU:HD23	1:r:31:LEU:C	2.37	0.50
1:r:73:HIS:CG	1:r:146:ILE:HG12	2.46	0.50
1:t:31:LEU:HD21	3:t:536:HOH:O	2.07	0.50
1:t:43[B]:THR:HG21	1:t:45:GLN:HE21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:91[B]:ARG:NE	1:1:93:ASN:ND2	2.47	0.50
1:e:18:ARG:O	1:e:22:THR:HG23	2.11	0.50
1:r:129:LYS:CE	1:r:145[A]:ARG:HH21	2.23	0.50
1:u:95:ASN:HD22	1:u:97:GLY:H	1.60	0.50
1:B:71:LYS:HG2	1:B:146[B]:ILE:HD11	1.94	0.50
1:G:24:LEU:O	1:G:26:HIS:HD2	1.95	0.50
1:P:14:ARG:NH1	1:P:14:ARG:HB3	2.26	0.50
1:k:91:ARG:HD3	1:k:93:ASN:ND2	2.27	0.50
1:t:13:MET:HE1	1:3:16:VAL:HA	1.92	0.50
1:z:114:GLN:OE1	1:N:71:LYS:HE3	2.11	0.50
1:3:95:ASN:HD22	1:3:97:GLY:H	1.60	0.50
1:E:13:MET:O	1:E:16:VAL:N	2.45	0.50
1:T:14:ARG:HD2	3:T:494:HOH:O	2.12	0.50
1:W:14:ARG:C	1:W:16:VAL:N	2.69	0.50
1:k:95:ASN:HD22	1:k:97:GLY:H	1.60	0.50
1:3:91[A]:ARG:NH1	1:3:93:ASN:HD22	1.93	0.50
1:K:95:ASN:HD22	1:K:97:GLY:H	1.59	0.50
1:m:28[B]:ARG:HB3	1:E:117:PRO:HB3	1.94	0.49
1:n:13:MET:HA	1:n:16:VAL:HG12	1.93	0.49
1:q:16:VAL:O	1:q:20:ILE:HG13	2.12	0.49
1:4:19:MET:O	1:4:23:HIS:HD2	1.94	0.49
1:4:31:LEU:HD23	1:4:31:LEU:C	2.37	0.49
1:B:91[B]:ARG:HD3	1:B:93:ASN:ND2	2.27	0.49
1:c:24:LEU:O	1:c:26:HIS:HD2	1.95	0.49
1:x:16:VAL:CG1	1:c:19:MET:SD	2.99	0.49
1:W:26:HIS:CE1	3:W:549:HOH:O	2.55	0.49
1:g:91:ARG:NH1	1:g:93:ASN:ND2	2.48	0.49
1:o:79:ILE:CD1	1:o:183:LEU:HG	2.42	0.49
1:G:95:ASN:HD22	1:G:97:GLY:H	1.60	0.49
1:c:12:THR:C	1:c:14:ARG:N	2.70	0.49
3:k:370:HOH:O	1:r:73:HIS:HD2	1.95	0.49
1:n:71:LYS:HG2	1:n:146:ILE:HD11	1.93	0.49
1:s:95:ASN:HD22	1:s:97:GLY:H	1.60	0.49
1:3:66:ARG:HG2	3:3:526:HOH:O	2.11	0.49
1:6:31:LEU:HD23	1:6:32:ILE:N	2.27	0.49
1:M:71:LYS:HZ3	1:M:71:LYS:HB3	1.77	0.49
1:V:66:ARG:CG	3:V:526:HOH:O	2.59	0.49
1:V:123:LYS:NZ	3:V:435:HOH:O	2.45	0.49
1:v:91:ARG:HD3	1:v:93:ASN:ND2	2.28	0.49
1:G:91[B]:ARG:NH1	1:G:152:GLN:CD	2.70	0.49
1:e:71:LYS:HD2	1:e:146:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:13:MET:HA	1:m:16:VAL:HG12	1.94	0.49
1:q:19:MET:HE1	1:w:13:MET:HE3	1.95	0.49
1:t:16:VAL:HG13	1:t:17:LYS:H	1.78	0.49
1:z:13:MET:HB3	1:S:19:MET:HE1	1.95	0.49
1:R:73:HIS:HE1	1:R:144:ASP:OD2	1.95	0.49
1:e:12:THR:O	1:e:12:THR:CG2	2.52	0.49
1:e:38:ASN:HB3	1:e:179:SER:O	2.13	0.49
1:i:16:VAL:HG23	1:Q:16:VAL:HG21	1.95	0.49
1:n:24:LEU:O	1:n:26:HIS:HD2	1.95	0.49
1:1:91[A]:ARG:HH12	1:1:152:GLN:HB2	1.74	0.49
1:A:45[B]:GLN:HE21	1:A:173[B]:MET:HE3	1.77	0.49
1:O:66:ARG:CD	3:O:337:HOH:O	2.59	0.49
1:U:95:ASN:HD22	1:U:97:GLY:H	1.59	0.49
1:a:95:ASN:HD22	1:a:97:GLY:H	1.61	0.49
1:s:73:HIS:CG	1:s:146:ILE:HG12	2.47	0.49
1:c:12:THR:CG2	1:c:13:MET:H	2.26	0.49
1:k:19:MET:SD	1:U:16:VAL:HG13	2.52	0.49
1:n:146:ILE:HG23	1:n:146:ILE:O	2.11	0.49
1:4:23:HIS:CE1	1:7:17:LYS:HZ3	2.31	0.49
1:D:73:HIS:CA	1:D:146[A]:ILE:HD13	2.43	0.49
1:H:19:MET:HG2	1:L:20:ILE:CD1	2.41	0.49
1:J:24:LEU:O	1:J:26:HIS:HD2	1.96	0.49
1:Y:95:ASN:HD22	1:Y:97:GLY:H	1.60	0.49
1:h:73:HIS:CG	1:h:146:ILE:HG12	2.48	0.49
1:s:23:HIS:CE1	1:2:17:LYS:HZ3	2.31	0.49
1:V:95:ASN:HD22	1:V:97:GLY:H	1.59	0.49
1:v:16:VAL:HG13	1:v:17:LYS:H	1.77	0.48
1:1:28:ARG:HB3	1:S:117:PRO:HB3	1.95	0.48
1:2:12:THR:O	1:2:16:VAL:HG12	2.13	0.48
1:2:17:LYS:NZ	3:2:336:HOH:O	2.46	0.48
1:P:91[B]:ARG:HD3	1:P:93:ASN:ND2	2.27	0.48
1:g:73:HIS:HE1	1:g:144:ASP:OD2	1.95	0.48
1:2:129:LYS:HZ2	1:2:145[A]:ARG:HE	1.61	0.48
1:K:148[B]:ASN:ND2	3:K:487:HOH:O	2.46	0.48
1:W:14:ARG:O	1:W:15:ALA:C	2.57	0.48
1:Y:145:ARG:NH2	3:Y:506:HOH:O	2.40	0.48
1:Z:146:ILE:HD12	3:Z:578:HOH:O	2.13	0.48
1:b:31:LEU:HD22	3:b:333:HOH:O	2.07	0.48
1:h:91:ARG:HD2	3:h:399:HOH:O	2.14	0.48
1:p:12:THR:CG2	1:p:13:MET:N	2.76	0.48
1:q:23:HIS:CE1	1:w:17:LYS:NZ	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:71:LYS:CD	1:v:146:ILE:HD11	2.36	0.48
1:x:66:ARG:HD3	1:x:152:GLN:C	2.37	0.48
1:R:71:LYS:NZ	1:R:71:LYS:CB	2.76	0.48
1:Z:95:ASN:HD22	1:Z:97:GLY:H	1.59	0.48
1:e:73:HIS:HE1	1:e:144:ASP:OD2	1.97	0.48
1:o:27:LYS:HB3	1:o:57:ILE:O	2.13	0.48
1:t:16:VAL:HG13	1:t:17:LYS:N	2.29	0.48
1:u:31:LEU:CD2	3:u:515:HOH:O	2.61	0.48
1:z:31[B]:LEU:HD12	3:z:334:HOH:O	2.12	0.48
1:0:86:ARG:CZ	3:0:398:HOH:O	2.62	0.48
1:6:28[B]:ARG:HH11	1:6:28[B]:ARG:CG	2.25	0.48
1:P:13:MET:HA	1:P:16:VAL:CG1	2.43	0.48
1:S:16:VAL:HG13	1:S:17:LYS:H	1.78	0.48
1:Z:26:HIS:HE1	3:Z:369:HOH:O	1.96	0.48
1:k:31:LEU:HD22	3:k:532:HOH:O	2.10	0.48
1:w:16:VAL:HG23	1:V:16:VAL:CG2	2.39	0.48
1:5:91:ARG:HD2	3:5:428:HOH:O	2.14	0.48
1:7:12:THR:HG23	1:7:13:MET:N	2.28	0.48
1:G:81[A]:VAL:CG1	3:G:373:HOH:O	2.62	0.48
1:O:66:ARG:HD3	3:O:337:HOH:O	2.14	0.48
1:g:27:LYS:HE3	3:g:517:HOH:O	2.14	0.48
1:m:117:PRO:HB3	1:t:28[B]:ARG:HB3	1.96	0.48
1:n:73:HIS:HE1	1:n:144:ASP:OD2	1.96	0.48
1:p:17:LYS:NZ	1:p:21:ASN:HD21	2.12	0.48
1:p:71:LYS:HE3	1:q:114:GLN:OE1	2.13	0.48
1:s:12:THR:O	1:s:13:MET:C	2.57	0.48
1:s:13:MET:CE	1:s:16:VAL:HG11	2.43	0.48
1:5:13:MET:CA	1:5:16:VAL:HG12	2.43	0.48
1:5:18:ARG:O	1:5:22:THR:HG23	2.14	0.48
1:L:195:ALA:HA	3:L:534:HOH:O	2.12	0.48
1:a:16:VAL:HG13	1:a:17:LYS:N	2.28	0.48
1:n:18:ARG:O	1:n:21:ASN:OD1	2.31	0.48
1:o:95:ASN:HD22	1:o:97:GLY:H	1.60	0.48
1:u:27:LYS:HE3	3:u:495:HOH:O	2.13	0.48
1:0:18:ARG:O	1:0:22:THR:HG23	2.13	0.48
1:1:17:LYS:HE3	1:1:21:ASN:HD21	1.79	0.48
1:f:95:ASN:HD22	1:f:97:GLY:H	1.62	0.48
1:i:13:MET:O	1:i:15:ALA:N	2.46	0.48
1:l:13:MET:HE3	1:E:12:THR:N	2.29	0.48
1:A:12:THR:C	1:A:13:MET:CE	2.79	0.48
1:V:26:HIS:CE1	3:V:469:HOH:O	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:24:LEU:O	1:Z:26:HIS:HD2	1.96	0.48
1:a:38:ASN:HB3	1:a:179:SER:O	2.13	0.48
1:f:16:VAL:HG11	1:m:19:MET:CE	2.44	0.48
1:i:19:MET:HB2	1:Q:13:MET:HE1	1.96	0.48
1:w:79:ILE:HD12	1:w:183:LEU:HG	1.96	0.48
1:3:13:MET:CA	1:3:16:VAL:CG1	2.83	0.48
1:F:22:THR:O	1:F:22:THR:HG22	2.14	0.48
1:N:12:THR:O	1:N:12:THR:CG2	2.59	0.48
1:b:31:LEU:HD21	3:b:333:HOH:O	2.04	0.48
1:e:79:ILE:O	1:e:181[A]:VAL:HG23	2.14	0.48
1:e:179:SER:OG	1:e:181[A]:VAL:HG22	2.13	0.48
1:i:13:MET:C	1:i:15:ALA:N	2.71	0.48
1:k:81:VAL:HG12	3:k:444:HOH:O	2.14	0.48
1:r:13:MET:HA	1:r:16:VAL:CG1	2.43	0.48
1:7:95:ASN:HD22	1:7:97:GLY:H	1.60	0.48
1:A:84:THR:HB	3:A:452:HOH:O	2.12	0.48
1:G:14:ARG:HB3	1:G:18:ARG:NH2	2.21	0.48
1:L:91[B]:ARG:HH21	1:L:93:ASN:ND2	2.12	0.48
1:e:23:HIS:CE1	1:i:66:ARG:CZ	2.96	0.47
1:h:66:ARG:HD3	3:h:359:HOH:O	2.14	0.47
1:i:12:THR:HG23	1:i:13:MET:N	2.29	0.47
1:i:18:ARG:CB	3:i:410:HOH:O	2.52	0.47
1:d:13:MET:O	1:d:16:VAL:HG13	2.13	0.47
1:r:140:GLU:HG2	3:r:489:HOH:O	2.13	0.47
1:t:96[B]:ARG:NH1	3:t:415:HOH:O	2.46	0.47
1:K:24:LEU:O	1:K:26:HIS:HD2	1.97	0.47
1:L:12:THR:O	1:L:15:ALA:N	2.42	0.47
1:Y:13:MET:O	1:Y:16:VAL:HG12	2.13	0.47
1:t:16:VAL:HG23	1:C:16:VAL:HG21	1.96	0.47
1:z:17:LYS:HE3	1:z:21:ASN:ND2	2.29	0.47
1:5:12:THR:HG23	1:5:13:MET:HG2	1.95	0.47
1:7:38:ASN:HB3	1:7:179:SER:O	2.14	0.47
1:M:129:LYS:HZ1	1:M:147:ILE:CG2	2.18	0.47
1:c:17:LYS:CE	1:c:21:ASN:HD21	2.27	0.47
3:f:480:HOH:O	1:J:73:HIS:HD2	1.95	0.47
1:k:16:VAL:HG23	1:U:16:VAL:HG21	1.96	0.47
1:n:33:ASN:ND2	3:n:545:HOH:O	2.47	0.47
1:t:13:MET:CA	1:t:16:VAL:CG1	2.84	0.47
1:1:18:ARG:O	1:1:22:THR:HG23	2.14	0.47
1:5:24:LEU:O	1:5:26:HIS:HD2	1.96	0.47
1:A:179:SER:OG	1:A:181:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:THR:C	1:B:14:ARG:N	2.71	0.47
1:L:18:ARG:O	1:L:22:THR:HG23	2.14	0.47
1:P:120:LEU:C	1:S:28[B]:ARG:HH21	2.22	0.47
1:T:16:VAL:HG13	1:T:17:LYS:N	2.28	0.47
1:r:12:THR:C	1:r:14:ARG:H	2.21	0.47
1:t:129:LYS:HE3	1:t:145[A]:ARG:NH2	2.29	0.47
1:u:38:ASN:HB3	1:u:179:SER:O	2.14	0.47
1:x:13:MET:O	1:x:14:ARG:C	2.57	0.47
1:2:31:LEU:HD23	1:2:32:ILE:N	2.29	0.47
1:2:73:HIS:HB2	1:2:146:ILE:CD1	2.45	0.47
1:3:91[A]:ARG:HD3	1:3:93:ASN:HD21	1.79	0.47
1:A:72:LEU:O	1:A:146:ILE:HD12	2.14	0.47
1:K:13:MET:C	1:K:16:VAL:CG1	2.88	0.47
1:S:31[B]:LEU:HD12	3:S:370:HOH:O	2.15	0.47
1:u:91:ARG:HD3	1:u:93:ASN:ND2	2.29	0.47
1:y:24:LEU:O	1:y:26:HIS:HD2	1.97	0.47
1:0:73:HIS:HE1	1:0:144:ASP:OD2	1.98	0.47
1:1:91[A]:ARG:HH12	1:1:152:GLN:CB	2.25	0.47
1:3:133:LEU:HD21	1:3:145[B]:ARG:CG	2.44	0.47
1:6:28[B]:ARG:NH2	1:6:189:GLU:OE1	2.47	0.47
1:L:95:ASN:HD22	1:L:97:GLY:H	1.61	0.47
1:N:95:ASN:HD22	1:N:97:GLY:H	1.61	0.47
1:P:91[B]:ARG:NH2	1:P:93:ASN:HD22	2.06	0.47
1:b:73:HIS:HE1	1:b:144:ASP:OD2	1.98	0.47
1:e:66:ARG:NH1	3:e:427:HOH:O	2.47	0.47
1:h:31[B]:LEU:HD23	1:h:32:ILE:N	2.29	0.47
1:j:23:HIS:CE1	1:p:17:LYS:HZ2	2.32	0.47
1:n:16:VAL:CG1	1:n:17:LYS:H	2.27	0.47
1:o:152:GLN:NE2	3:o:453:HOH:O	2.48	0.47
1:t:24:LEU:O	1:t:26:HIS:HD2	1.97	0.47
1:v:18:ARG:O	1:v:22:THR:HG23	2.14	0.47
1:w:19:MET:CE	1:V:16:VAL:HG13	2.43	0.47
1:y:12:THR:HG23	1:y:12:THR:O	2.15	0.47
1:6:13:MET:HE3	1:O:19:MET:HE1	1.97	0.47
1:A:19:MET:HG2	1:K:20:ILE:CD1	2.44	0.47
1:E:87:PHE:HB2	1:E:131:VAL:HG23	1.97	0.47
1:H:73:HIS:CG	1:H:146:ILE:HG12	2.49	0.47
1:H:91[B]:ARG:HD3	1:H:93:ASN:HD21	1.79	0.47
1:L:91[B]:ARG:NH2	1:L:93:ASN:HD22	2.12	0.47
1:M:13:MET:O	1:M:15:ALA:N	2.47	0.47
1:N:73:HIS:CG	1:N:146:ILE:HG12	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:117:PRO:HB3	1:S:28[B]:ARG:HB3	1.96	0.47
1:T:140:GLU:HG3	3:T:472:HOH:O	2.13	0.47
1:z:13:MET:HA	1:z:16:VAL:HG11	1.93	0.47
1:4:95:ASN:HD22	1:4:97:GLY:H	1.61	0.47
1:G:13:MET:O	1:G:14:ARG:C	2.57	0.47
1:L:17:LYS:HE3	1:L:21:ASN:HD21	1.80	0.47
1:M:16:VAL:HG13	1:M:17:LYS:H	1.80	0.47
1:M:17:LYS:HG3	1:M:18:ARG:N	2.29	0.47
1:M:95:ASN:HD22	1:M:97:GLY:H	1.61	0.47
1:P:152:GLN:CG	3:P:416:HOH:O	2.49	0.47
1:R:13:MET:CA	1:R:16:VAL:CG1	2.89	0.47
1:V:18:ARG:O	1:V:22:THR:HG23	2.14	0.47
1:w:24:LEU:O	1:w:26:HIS:HD2	1.98	0.47
1:w:129:LYS:CD	3:w:449:HOH:O	2.34	0.47
1:z:95:ASN:HD22	1:z:97:GLY:H	1.63	0.47
1:A:13:MET:HA	1:A:13:MET:CE	2.37	0.47
1:T:14:ARG:NH2	1:T:18:ARG:HH12	2.12	0.47
1:T:24:LEU:O	1:T:26:HIS:HD2	1.98	0.47
1:A:95:ASN:HD22	1:A:97:GLY:H	1.62	0.47
1:D:146[A]:ILE:HG23	3:D:343:HOH:O	2.14	0.47
1:E:17:LYS:HE3	1:E:21:ASN:ND2	2.30	0.47
1:L:24:LEU:O	1:L:26:HIS:HD2	1.98	0.47
1:N:79:ILE:HD12	1:N:183:LEU:HG	1.96	0.47
1:f:16:VAL:CG1	1:f:17:LYS:H	2.28	0.46
1:k:28[B]:ARG:HG2	1:c:117:PRO:HA	1.97	0.46
1:x:19:MET:SD	1:T:16:VAL:HG13	2.55	0.46
1:z:145[B]:ARG:HG3	1:z:147:ILE:HD11	1.97	0.46
1:4:17:LYS:NZ	1:a:23:HIS:CE1	2.75	0.46
1:5:95:ASN:HD22	1:5:97:GLY:H	1.60	0.46
1:6:18:ARG:NH1	3:6:335:HOH:O	2.48	0.46
1:J:38:ASN:HB3	1:J:179:SER:O	2.15	0.46
3:R:426:HOH:O	1:X:73:HIS:HD2	1.98	0.46
1:T:31[A]:LEU:HD23	1:T:32:ILE:N	2.31	0.46
1:q:23:HIS:HE1	1:w:17:LYS:NZ	2.12	0.46
1:4:17:LYS:HZ2	1:a:23:HIS:HE1	1.62	0.46
1:5:71:LYS:CD	1:5:148[B]:ASN:OD1	2.63	0.46
1:E:19:MET:O	1:E:22:THR:OG1	2.29	0.46
1:P:31:LEU:HD23	1:P:32:ILE:N	2.30	0.46
1:V:16:VAL:O	1:V:20:ILE:HG13	2.15	0.46
1:X:66:ARG:HG2	3:X:530:HOH:O	2.15	0.46
1:Z:123:LYS:HE3	3:Z:329:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:26:HIS:HE1	3:x:401:HOH:O	1.98	0.46
1:3:133:LEU:HD21	1:3:145[B]:ARG:HG3	1.97	0.46
1:7:91:ARG:HD3	1:7:93:ASN:ND2	2.30	0.46
1:L:13:MET:O	1:L:16:VAL:HG13	2.15	0.46
1:V:79:ILE:HD12	1:V:183:LEU:HG	1.97	0.46
1:d:24:LEU:O	1:d:26:HIS:HD2	1.97	0.46
1:m:73:HIS:CG	1:m:146:ILE:HG12	2.50	0.46
1:p:12:THR:CG2	1:p:13:MET:H	2.27	0.46
1:z:16:VAL:HG13	1:z:17:LYS:N	2.30	0.46
1:B:19:MET:O	1:B:23:HIS:HD2	1.98	0.46
1:E:31[A]:LEU:HD23	1:E:32:ILE:N	2.30	0.46
1:N:28:ARG:HG2	1:N:191:VAL:HG22	1.97	0.46
1:Q:14:ARG:NH1	3:Q:455:HOH:O	2.48	0.46
1:b:146:ILE:CD1	3:b:422:HOH:O	2.59	0.46
1:l:13:MET:O	1:l:16:VAL:CG1	2.60	0.46
1:u:15:ALA:O	1:u:18:ARG:HB3	2.16	0.46
1:u:24:LEU:O	1:u:26:HIS:HD2	1.99	0.46
1:2:91:ARG:HD3	1:2:93:ASN:HD21	1.80	0.46
1:P:13:MET:C	1:P:16:VAL:HG12	2.41	0.46
1:W:12:THR:O	1:W:13:MET:C	2.59	0.46
1:X:13:MET:CA	1:X:16:VAL:HG12	2.44	0.46
1:Y:12:THR:O	1:Y:16:VAL:HG12	2.15	0.46
1:Y:13:MET:O	1:Y:16:VAL:HG13	2.16	0.46
1:b:73:HIS:CG	1:b:146:ILE:HG12	2.51	0.46
1:k:129:LYS:NZ	3:k:420:HOH:O	2.40	0.46
1:m:91:ARG:HD3	1:m:93:ASN:ND2	2.30	0.46
1:r:95:ASN:HD22	1:r:97:GLY:H	1.63	0.46
1:G:17:LYS:CE	1:G:21:ASN:HD21	2.25	0.46
1:I:24:LEU:O	1:I:26:HIS:HD2	1.99	0.46
1:M:16:VAL:HG13	1:M:17:LYS:N	2.31	0.46
1:a:73:HIS:HE1	1:a:144:ASP:OD2	1.99	0.46
1:e:13:MET:CG	1:Q:19:MET:HE1	2.46	0.46
1:e:16:VAL:HG23	1:i:16:VAL:HG21	1.98	0.46
1:k:28[B]:ARG:CD	1:k:191:VAL:HG22	2.46	0.46
1:z:147:ILE:N	1:z:147:ILE:HD12	2.30	0.46
1:L:38:ASN:HB3	1:L:179:SER:O	2.16	0.46
1:W:24:LEU:O	1:W:26:HIS:HD2	1.98	0.46
1:e:13:MET:HE1	1:e:16:VAL:HG11	1.96	0.46
1:x:12:THR:HG23	1:x:12:THR:O	2.15	0.46
1:x:146:ILE:HD13	3:X:369:HOH:O	2.16	0.46
1:z:12:THR:HB	3:z:448:HOH:O	2.09	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:22:THR:HG22	3:G:397:HOH:O	2.14	0.46
1:L:13:MET:CA	1:L:16:VAL:HG12	2.44	0.46
1:S:24:LEU:O	1:S:26:HIS:HD2	1.99	0.46
1:Y:26:HIS:HE1	3:Y:446:HOH:O	1.98	0.46
1:j:13:MET:SD	1:j:16:VAL:HG11	2.56	0.46
1:2:24:LEU:O	1:2:26:HIS:HD2	1.99	0.46
1:4:146:ILE:HG23	1:4:146:ILE:O	2.15	0.46
1:P:13:MET:CA	1:P:16:VAL:HG12	2.45	0.46
1:S:73:HIS:CG	1:S:146:ILE:HG12	2.51	0.46
1:W:94:MET:HG2	1:a:94:MET:HG2	1.98	0.46
1:c:95:ASN:HD22	1:c:97:GLY:H	1.61	0.46
1:d:95:ASN:HD22	1:d:97:GLY:H	1.63	0.46
1:e:79:ILE:O	1:e:181[A]:VAL:CG2	2.64	0.46
1:o:31:LEU:C	1:o:31:LEU:HD12	2.41	0.46
1:5:91:ARG:HD3	1:5:93:ASN:ND2	2.31	0.46
1:T:15:ALA:O	1:T:18:ARG:N	2.49	0.46
1:W:14:ARG:O	1:W:17:LYS:N	2.49	0.46
1:b:79:ILE:HD12	1:b:183:LEU:HG	1.98	0.46
1:i:28[A]:ARG:HG2	1:i:191:VAL:HG22	1.98	0.45
1:p:19:MET:HE3	1:y:13:MET:HE2	1.89	0.45
1:p:73:HIS:CG	1:p:146:ILE:HG12	2.51	0.45
1:x:13:MET:HE2	1:c:19:MET:HE3	1.97	0.45
1:z:24:LEU:O	1:z:26:HIS:HD2	2.00	0.45
1:7:24:LEU:O	1:7:26:HIS:HD2	1.99	0.45
1:A:73:HIS:HB2	1:A:146:ILE:HD13	1.98	0.45
1:D:14:ARG:HA	1:D:17:LYS:HB3	1.97	0.45
1:D:95:ASN:HD22	1:D:97:GLY:H	1.62	0.45
1:H:73:HIS:HE1	1:H:144:ASP:OD2	1.99	0.45
1:K:91[A]:ARG:CG	1:K:171:ILE:HD13	2.45	0.45
1:K:152[A]:GLN:CG	1:K:153:LEU:N	2.79	0.45
1:W:91:ARG:HD3	1:W:93:ASN:ND2	2.31	0.45
1:m:181:VAL:HG11	3:m:303:HOH:O	2.16	0.45
1:K:13:MET:C	1:K:16:VAL:HG12	2.41	0.45
1:N:24:LEU:O	1:N:26:HIS:HD2	1.99	0.45
1:Z:16:VAL:HG13	1:Z:17:LYS:H	1.81	0.45
1:k:13:MET:C	1:k:16:VAL:HG12	2.40	0.45
1:r:12:THR:HG23	1:r:13:MET:N	2.24	0.45
1:y:18:ARG:NH1	3:y:462:HOH:O	2.48	0.45
1:y:145:ARG:NH2	3:y:491:HOH:O	2.35	0.45
1:g:95:ASN:HD22	1:g:97:GLY:H	1.65	0.45
1:k:13:MET:CA	1:k:16:VAL:CG1	2.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:p:13:MET:CA	1:p:16:VAL:HG12	2.45	0.45
1:r:16:VAL:O	1:r:20:ILE:HG13	2.16	0.45
1:r:162:VAL:HG12	3:r:370:HOH:O	2.16	0.45
1:u:91:ARG:HD2	3:u:407:HOH:O	2.15	0.45
1:0:24:LEU:O	1:0:26:HIS:HD2	1.99	0.45
1:G:13:MET:O	1:G:15:ALA:N	2.49	0.45
1:S:129:LYS:NZ	3:S:366:HOH:O	2.48	0.45
1:X:17:LYS:HE3	1:X:21:ASN:ND2	2.31	0.45
1:Y:123:LYS:HE3	3:Y:437:HOH:O	2.15	0.45
1:h:20:ILE:CD1	1:v:19:MET:HG2	2.46	0.45
1:x:71:LYS:HE3	1:X:114:GLN:OE1	2.17	0.45
1:z:73:HIS:HE1	1:z:144:ASP:OD2	1.99	0.45
1:7:33:ASN:ND2	3:7:500:HOH:O	2.48	0.45
1:H:129:LYS:HE3	1:H:147:ILE:HG21	1.99	0.45
1:N:19:MET:O	1:N:23:HIS:HD2	2.00	0.45
1:b:95:ASN:HD22	1:b:97:GLY:H	1.64	0.45
1:z:16:VAL:CG1	1:S:19:MET:HE1	2.47	0.45
1:3:73:HIS:HE1	1:3:144:ASP:OD2	2.00	0.45
1:C:16:VAL:O	1:C:20:ILE:HG13	2.16	0.45
1:K:146[A]:ILE:HD13	3:Z:451:HOH:O	2.16	0.45
1:M:129:LYS:HZ3	1:M:147:ILE:HG23	1.75	0.45
1:U:24:LEU:O	1:U:26:HIS:HD2	2.00	0.45
1:V:73:HIS:HE1	1:V:144:ASP:OD2	2.00	0.45
1:X:24:LEU:O	1:X:26:HIS:HD2	2.00	0.45
1:f:28:ARG:HG2	1:f:191:VAL:HG22	1.99	0.45
1:g:91:ARG:HD2	3:g:527:HOH:O	2.16	0.45
1:q:31:LEU:HD23	1:q:31:LEU:C	2.41	0.45
1:A:91[A]:ARG:HD3	1:A:93:ASN:ND2	2.32	0.45
1:G:150:PRO:HB3	3:G:387:HOH:O	2.17	0.45
1:K:19:MET:HB2	1:d:13:MET:HE1	1.98	0.45
1:K:73:HIS:CG	1:K:146[A]:ILE:HG12	2.51	0.45
1:P:91[A]:ARG:NE	1:P:93:ASN:HD21	2.14	0.45
1:R:66:ARG:NH1	1:R:153[B]:LEU:HG	2.32	0.45
1:b:145:ARG:NH2	3:b:513:HOH:O	2.49	0.45
1:l:95:ASN:HD22	1:l:97:GLY:H	1.63	0.45
1:m:12:THR:CB	3:m:445:HOH:O	2.64	0.45
1:p:91:ARG:HD2	3:p:357:HOH:O	2.14	0.45
1:s:117:PRO:HB3	1:B:28[A]:ARG:HB3	1.99	0.45
1:1:71:LYS:HE3	1:S:114:GLN:OE1	2.17	0.45
1:4:14:ARG:HB3	3:4:449:HOH:O	2.16	0.45
1:A:17:LYS:HE3	1:A:21:ASN:ND2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:73:HIS:HE1	1:N:144:ASP:OD2	1.99	0.45
1:S:20:ILE:CD1	1:Y:19:MET:HG2	2.47	0.45
1:X:73:HIS:HE1	1:X:144:ASP:OD2	1.99	0.45
1:d:12:THR:O	1:d:13:MET:C	2.59	0.45
1:w:179:SER:HG	1:w:181:VAL:HG12	1.80	0.45
1:3:24:LEU:O	1:3:26:HIS:HD2	1.99	0.45
1:4:31:LEU:HD23	1:4:32:ILE:N	2.32	0.45
1:7:28:ARG:HG2	1:7:191:VAL:HG22	1.99	0.45
1:7:73:HIS:HB2	1:7:146:ILE:CD1	2.47	0.45
1:D:24:LEU:O	1:D:26:HIS:HD2	2.00	0.45
1:K:13:MET:O	1:K:16:VAL:CG1	2.63	0.45
1:f:117:PRO:HB3	1:J:28[B]:ARG:HB3	1.99	0.45
1:p:38:ASN:HB3	1:p:179:SER:O	2.16	0.45
1:A:66:ARG:HD3	3:A:464:HOH:O	2.17	0.45
1:E:16:VAL:HG13	1:E:17:LYS:N	2.31	0.45
1:N:17:LYS:CE	1:N:21:ASN:ND2	2.80	0.45
1:T:73:HIS:CG	1:T:146:ILE:HG12	2.52	0.45
1:c:13:MET:O	1:c:16:VAL:HG13	2.17	0.45
1:f:15:ALA:O	1:f:18:ARG:HB3	2.18	0.44
1:m:13:MET:HA	1:m:16:VAL:CG1	2.47	0.44
1:m:16:VAL:HG13	1:m:17:LYS:N	2.31	0.44
1:u:14:ARG:CG	3:u:449:HOH:O	2.64	0.44
1:w:16:VAL:HG13	1:w:17:LYS:N	2.32	0.44
1:z:19:MET:HE2	1:Y:20:ILE:HD12	1.99	0.44
1:2:129:LYS:HZ2	1:2:145[A]:ARG:NH2	1.90	0.44
1:H:114:GLN:OE1	1:O:71:LYS:HE3	2.17	0.44
1:J:13:MET:HE2	1:J:13:MET:HB3	1.83	0.44
1:M:24:LEU:O	1:M:26:HIS:HD2	1.99	0.44
1:P:31:LEU:HD21	3:P:390:HOH:O	2.07	0.44
1:j:12:THR:CG2	1:j:13:MET:N	2.81	0.44
1:k:91:ARG:NH1	1:k:93:ASN:HD22	1.96	0.44
1:s:15:ALA:O	1:s:18:ARG:HB3	2.16	0.44
1:t:73:HIS:CG	1:t:146:ILE:HG12	2.52	0.44
1:v:31:LEU:HD23	1:v:32:ILE:N	2.32	0.44
1:E:36:ASN:HB2	1:E:184:TRP:CE2	2.52	0.44
1:e:91:ARG:NH1	1:e:93:ASN:HD22	2.07	0.44
1:r:24:LEU:O	1:r:26:HIS:HD2	2.00	0.44
1:x:13:MET:CA	1:x:16:VAL:HG12	2.46	0.44
1:E:17:LYS:NZ	1:E:21:ASN:ND2	2.47	0.44
1:L:13:MET:O	1:L:16:VAL:CG1	2.65	0.44
1:N:31:LEU:HD23	1:N:31:LEU:C	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:91[A]:ARG:NH1	1:P:152:GLN:HE22	2.15	0.44
1:u:31:LEU:C	1:u:31:LEU:CD2	2.89	0.44
1:1:16:VAL:O	1:1:20:ILE:HG13	2.17	0.44
1:1:140:GLU:HG2	3:1:381:HOH:O	2.17	0.44
1:C:73:HIS:HE1	1:C:144:ASP:OD2	1.99	0.44
1:f:24:LEU:O	1:f:26:HIS:HD2	2.00	0.44
1:m:73:HIS:HE1	1:m:144:ASP:OD2	2.00	0.44
1:n:146:ILE:HG22	3:n:499:HOH:O	2.17	0.44
1:x:38:ASN:HB3	1:x:179:SER:O	2.18	0.44
1:2:19:MET:C	1:2:22[B]:THR:HG22	2.42	0.44
1:F:19:MET:SD	1:O:16:VAL:HG13	2.57	0.44
1:G:25:GLU:HG3	1:M:64[B]:GLN:OE1	2.17	0.44
1:L:91[B]:ARG:HH21	1:L:93:ASN:HD22	1.65	0.44
1:X:18:ARG:O	1:X:22:THR:HG23	2.18	0.44
1:e:91:ARG:HD3	1:e:93:ASN:HD21	1.80	0.44
1:i:71:LYS:CG	1:i:148[B]:ASN:OD1	2.66	0.44
1:i:73:HIS:HE1	1:i:144:ASP:OD2	2.01	0.44
1:l:152:GLN:CD	3:l:396:HOH:O	2.60	0.44
1:0:13:MET:C	1:0:16:VAL:HG12	2.43	0.44
1:1:12:THR:O	1:1:16:VAL:HG12	2.17	0.44
1:D:28:ARG:HG2	1:D:191:VAL:HG22	2.00	0.44
1:M:71:LYS:NZ	1:M:71:LYS:HB2	2.32	0.44
1:P:71[B]:LYS:HD3	1:P:189:GLU:OE2	2.17	0.44
1:Z:140:GLU:HG2	3:Z:502:HOH:O	2.17	0.44
1:n:129:LYS:HZ1	1:n:145[B]:ARG:CZ	2.15	0.44
1:p:152:GLN:HG3	3:p:400:HOH:O	2.18	0.44
1:t:13:MET:HE3	1:3:19:MET:CE	2.47	0.44
1:2:131:VAL:CG2	1:2:145[A]:ARG:CD	2.95	0.44
1:C:28:ARG:HG2	1:C:191:VAL:HG22	1.99	0.44
1:E:17:LYS:HZ2	1:J:23:HIS:CE1	2.36	0.44
1:X:66:ARG:CG	3:X:530:HOH:O	2.65	0.44
1:d:146:ILE:HD12	3:d:525:HOH:O	2.16	0.44
1:k:73:HIS:CG	1:k:146:ILE:HG12	2.53	0.44
1:B:28[A]:ARG:HG2	1:B:191:VAL:HG22	2.00	0.44
1:F:21:ASN:ND2	3:F:385:HOH:O	2.51	0.44
1:O:140:GLU:HG2	3:O:541:HOH:O	2.17	0.44
1:R:13:MET:CA	1:R:16:VAL:HG12	2.47	0.44
1:l:73:HIS:HE1	1:l:144:ASP:OD2	2.01	0.44
1:q:95:ASN:HD22	1:q:97:GLY:H	1.66	0.44
1:w:23:HIS:HE1	1:V:17:LYS:HZ2	1.65	0.44
1:2:71:LYS:NZ	3:2:408:HOH:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:114:GLN:OE1	1:R:71:LYS:HE2	2.18	0.44
1:H:174:LEU:HD23	1:H:174:LEU:C	2.43	0.44
1:N:19:MET:HE1	1:P:16:VAL:HG11	1.98	0.44
1:V:13:MET:O	1:V:16:VAL:HG12	2.18	0.44
1:Y:146:ILE:O	1:Y:146:ILE:CD1	2.64	0.44
1:f:16:VAL:CG1	1:m:19:MET:CE	2.96	0.43
1:h:129:LYS:HE3	1:h:147:ILE:CG2	2.44	0.43
1:m:12:THR:C	1:m:14:ARG:N	2.75	0.43
1:E:87:PHE:O	1:E:131:VAL:HG22	2.17	0.43
1:L:91[B]:ARG:CZ	1:L:93:ASN:HD22	2.30	0.43
1:T:36:ASN:HB2	1:T:184:TRP:CE2	2.53	0.43
1:T:73:HIS:HE1	1:T:144:ASP:OD2	2.01	0.43
1:Y:150:PRO:HB2	3:Y:434:HOH:O	2.18	0.43
1:h:95:ASN:HD22	1:h:97:GLY:H	1.66	0.43
1:w:73:HIS:HE1	1:w:144:ASP:OD2	2.01	0.43
1:J:36:ASN:HB2	1:J:184:TRP:CE2	2.53	0.43
1:W:28:ARG:HG2	1:W:191:VAL:HG22	2.00	0.43
1:d:24:LEU:HD22	1:d:195:ALA:HB2	2.00	0.43
1:l:31:LEU:C	1:l:31:LEU:CD2	2.91	0.43
1:q:12:THR:N	3:q:344:HOH:O	2.51	0.43
1:u:91:ARG:HD3	1:u:93:ASN:HD21	1.84	0.43
1:0:17:LYS:HG2	3:0:454:HOH:O	2.17	0.43
1:2:28[B]:ARG:NH2	1:2:189:GLU:OE1	2.48	0.43
1:D:27:LYS:HB3	1:D:57:ILE:O	2.18	0.43
1:G:28:ARG:HB2	1:Q:117:PRO:HB3	2.01	0.43
1:S:152[A]:GLN:HG3	1:S:153:LEU:N	2.29	0.43
1:T:91:ARG:HD3	1:T:93:ASN:HD21	1.83	0.43
1:l:12:THR:O	1:l:12:THR:HG23	2.19	0.43
1:x:16:VAL:HG13	1:x:17:LYS:N	2.34	0.43
1:3:31:LEU:HD23	1:3:32:ILE:N	2.33	0.43
1:B:91[A]:ARG:HG2	1:B:93:ASN:ND2	2.32	0.43
1:H:91[A]:ARG:NH2	3:H:522:HOH:O	2.52	0.43
1:J:95:ASN:HD22	1:J:97:GLY:H	1.66	0.43
1:K:16:VAL:O	1:K:20:ILE:HG13	2.19	0.43
1:P:16:VAL:O	1:P:20:ILE:HG13	2.17	0.43
1:U:23:HIS:HE1	1:Z:17:LYS:NZ	2.17	0.43
1:d:140:GLU:HG2	3:d:513:HOH:O	2.18	0.43
1:n:79:ILE:HD12	1:n:183:LEU:HG	2.01	0.43
1:0:13:MET:CA	1:0:16:VAL:HG12	2.45	0.43
1:O:129:LYS:HD3	3:O:495:HOH:O	2.19	0.43
1:T:13:MET:HA	1:T:16:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:146:ILE:HD11	3:m:463:HOH:O	2.18	0.43
1:0:31:LEU:HD23	1:0:32:ILE:N	2.34	0.43
1:4:146:ILE:HG22	3:4:398:HOH:O	2.18	0.43
1:b:12:THR:CG2	1:b:13:MET:N	2.81	0.43
1:i:129:LYS:HE3	1:i:147:ILE:HG21	2.00	0.43
1:j:91:ARG:HD2	3:j:524:HOH:O	2.17	0.43
1:o:13:MET:O	1:o:16:VAL:HG13	2.18	0.43
1:p:17:LYS:HE3	1:p:21:ASN:ND2	2.34	0.43
1:t:17:LYS:HZ1	1:3:23:HIS:HE1	1.66	0.43
1:u:17:LYS:CE	1:u:21:ASN:ND2	2.80	0.43
1:x:13:MET:HE3	1:c:19:MET:SD	2.58	0.43
1:x:148[A]:ASN:ND2	3:x:351:HOH:O	2.52	0.43
1:0:16:VAL:O	1:0:20:ILE:HG13	2.18	0.43
1:B:95:ASN:HD22	1:B:97:GLY:H	1.66	0.43
1:F:13:MET:HE2	1:F:13:MET:CA	2.47	0.43
1:F:95:ASN:HD22	1:F:97:GLY:H	1.62	0.43
1:H:123:LYS:HD2	3:H:458:HOH:O	2.17	0.43
1:M:71:LYS:CB	1:M:71:LYS:HZ3	2.32	0.43
1:R:17:LYS:CE	1:R:21:ASN:HD22	2.25	0.43
1:b:12:THR:O	1:b:15:ALA:N	2.50	0.43
1:f:36:ASN:HB2	1:f:184:TRP:CE2	2.54	0.43
1:g:66:ARG:HD3	3:g:328:HOH:O	2.19	0.43
1:v:38:ASN:HB3	1:v:179:SER:O	2.18	0.43
1:x:12:THR:CB	1:T:13:MET:HE1	2.49	0.43
1:H:24:LEU:O	1:H:26:HIS:HD2	2.01	0.43
1:I:79:ILE:HD12	1:I:183:LEU:HG	2.01	0.43
1:O:13:MET:O	1:O:16:VAL:CG1	2.67	0.43
1:S:17:LYS:HE3	1:Y:19:MET:CE	2.48	0.43
1:a:13:MET:HE2	1:a:16:VAL:CG1	2.49	0.43
1:h:174:LEU:HD23	1:h:174:LEU:C	2.44	0.43
1:1:31:LEU:C	1:1:31:LEU:CD2	2.92	0.43
1:2:146:ILE:HG23	1:2:146:ILE:O	2.18	0.43
1:5:66:ARG:HG3	1:5:66:ARG:HH11	1.84	0.43
1:E:12:THR:HG23	1:E:15:ALA:CB	2.49	0.43
1:H:28:ARG:HG2	1:H:191:VAL:HG22	2.01	0.43
1:K:28:ARG:HD3	1:Z:117:PRO:HA	1.99	0.43
1:Z:71:LYS:HE3	1:b:114:GLN:OE1	2.19	0.43
1:h:146:ILE:CD1	3:1:455:HOH:O	2.67	0.43
1:t:91[A]:ARG:HD3	1:t:93:ASN:HD21	1.83	0.43
1:u:73:HIS:HE1	1:u:144:ASP:OD2	2.02	0.43
1:4:146:ILE:HG23	3:4:470:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:95:ASN:HD22	1:6:97:GLY:H	1.63	0.43
1:A:145:ARG:HD2	3:A:357:HOH:O	2.18	0.43
1:C:16:VAL:O	1:C:19:MET:HB3	2.19	0.43
1:E:13:MET:C	1:E:16:VAL:HG12	2.42	0.43
1:G:19:MET:HE1	1:M:16:VAL:CG1	2.49	0.43
1:H:14:ARG:H	1:H:14:ARG:HG2	1.62	0.43
1:V:19:MET:HA	1:V:19:MET:CE	2.48	0.43
1:c:13:MET:C	1:c:16:VAL:HG12	2.44	0.43
1:u:73:HIS:CG	1:u:146:ILE:HG12	2.54	0.42
1:6:17:LYS:HE3	3:6:490:HOH:O	2.19	0.42
1:F:16:VAL:HG13	1:F:17:LYS:H	1.83	0.42
1:G:22:THR:CG2	3:G:397:HOH:O	2.67	0.42
1:K:12:THR:O	1:K:14:ARG:N	2.52	0.42
1:Q:72:LEU:O	1:Q:146:ILE:HD12	2.18	0.42
1:Q:73:HIS:HE1	1:Q:144:ASP:OD2	2.01	0.42
1:Q:95:ASN:HD22	1:Q:97:GLY:H	1.67	0.42
1:R:28:ARG:HG2	1:R:191:VAL:HG22	2.01	0.42
1:R:91:ARG:HD3	1:R:93:ASN:HD21	1.83	0.42
1:U:19:MET:HE1	1:Z:13:MET:HB3	2.00	0.42
1:Y:91:ARG:HD2	3:Y:384:HOH:O	2.19	0.42
1:c:12:THR:C	1:c:14:ARG:H	2.27	0.42
1:c:31:LEU:HD23	1:c:32:ILE:N	2.34	0.42
1:j:23:HIS:HE1	1:p:17:LYS:HZ3	1.61	0.42
1:j:94:MET:HB3	1:r:94:MET:HB3	2.01	0.42
1:l:14:ARG:O	1:l:14:ARG:NH1	2.52	0.42
1:l:16:VAL:HG13	1:l:17:LYS:N	2.34	0.42
1:m:13:MET:CA	1:m:16:VAL:HG12	2.50	0.42
1:o:13:MET:C	1:o:16:VAL:CG1	2.92	0.42
1:t:17:LYS:NZ	1:3:23:HIS:HE1	2.17	0.42
1:5:13:MET:HA	1:5:16:VAL:CG1	2.48	0.42
1:A:24:LEU:O	1:A:26:HIS:HD2	2.02	0.42
1:V:16:VAL:HG13	1:V:17:LYS:N	2.34	0.42
1:f:19:MET:HE1	1:I:13:MET:O	2.19	0.42
1:h:13:MET:HE2	1:h:13:MET:HB3	1.94	0.42
1:h:146:ILE:HD11	3:1:455:HOH:O	2.18	0.42
1:p:17:LYS:HE3	1:p:21:ASN:HD21	1.83	0.42
1:s:117:PRO:HB3	1:B:28[B]:ARG:HB3	2.00	0.42
1:7:91:ARG:HD3	1:7:93:ASN:HD21	1.84	0.42
1:I:36:ASN:HB2	1:I:184:TRP:CE2	2.53	0.42
1:K:129:LYS:NZ	1:K:145[B]:ARG:HH21	2.17	0.42
1:L:27:LYS:HB3	1:L:57:ILE:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:17:LYS:CD	1:M:21:ASN:ND2	2.80	0.42
1:W:173[B]:MET:HE3	1:W:173[B]:MET:HB3	1.85	0.42
1:h:73:HIS:HE1	1:h:144:ASP:OD2	2.03	0.42
1:n:17:LYS:HB2	1:M:19:MET:HE2	2.01	0.42
1:t:91[B]:ARG:HG2	1:t:93:ASN:ND2	2.34	0.42
1:E:91:ARG:HD2	3:E:463:HOH:O	2.19	0.42
1:O:95:ASN:HD22	1:O:97:GLY:H	1.64	0.42
1:R:38:ASN:HB3	1:R:179:SER:O	2.18	0.42
1:S:12:THR:O	1:S:13:MET:C	2.63	0.42
1:V:146:ILE:HD13	3:V:308:HOH:O	2.19	0.42
1:p:73:HIS:HE1	1:p:144:ASP:OD2	2.03	0.42
1:x:24:LEU:O	1:x:26:HIS:HD2	2.01	0.42
1:0:13:MET:HA	1:0:16:VAL:CG1	2.48	0.42
1:f:13:MET:HE3	1:m:19:MET:HE2	1.81	0.42
1:l:14:ARG:HG2	1:l:14:ARG:NH1	2.34	0.42
1:m:95:ASN:HD22	1:m:97:GLY:H	1.67	0.42
1:p:146:ILE:HD11	3:q:551:HOH:O	2.20	0.42
1:4:73:HIS:HE1	1:4:144:ASP:OD2	2.02	0.42
1:O:38:ASN:HB3	1:O:179:SER:O	2.19	0.42
1:f:12:THR:O	1:f:15:ALA:HB3	2.20	0.42
1:h:66:ARG:HG2	3:h:512:HOH:O	2.19	0.42
1:H:19:MET:O	1:H:23:HIS:HD2	2.03	0.42
1:L:73:HIS:HE1	1:L:144:ASP:OD2	2.03	0.42
1:N:19:MET:SD	1:P:16:VAL:CG1	3.03	0.42
1:V:13:MET:CA	1:V:16:VAL:HG12	2.48	0.42
3:Y:344:HOH:O	1:d:146:ILE:HD13	2.19	0.42
1:a:73:HIS:CG	1:a:146:ILE:HG12	2.54	0.42
1:c:179:SER:OG	1:c:181:VAL:HG22	2.19	0.42
1:f:47:LEU:HD11	1:f:173[B]:MET:HB2	2.02	0.42
1:g:24:LEU:O	1:g:26:HIS:HD2	2.03	0.42
1:h:71:LYS:HZ2	1:h:71:LYS:CB	2.31	0.42
1:j:24:LEU:O	1:j:26:HIS:HD2	2.03	0.42
1:x:71:LYS:HD3	1:x:148[B]:ASN:HD21	1.84	0.42
1:G:73:HIS:HE1	1:G:144:ASP:OD2	2.02	0.42
1:G:129:LYS:HD3	1:G:129:LYS:HA	1.88	0.42
1:U:19:MET:HE1	1:Z:13:MET:CE	2.37	0.42
1:e:95:ASN:HD22	1:e:97:GLY:H	1.66	0.42
1:h:148[B]:ASN:ND2	3:h:331:HOH:O	2.53	0.42
1:i:145:ARG:NH2	3:i:491:HOH:O	2.38	0.42
1:o:16:VAL:CG2	1:u:19:MET:SD	3.04	0.42
1:q:12:THR:O	1:q:16:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:148[B]:ASN:ND2	3:x:319:HOH:O	2.52	0.42
1:1:45[B]:GLN:NE2	3:1:383:HOH:O	2.51	0.42
1:1:71:LYS:CD	1:1:146:ILE:HD11	2.39	0.42
1:7:12:THR:HA	3:7:463:HOH:O	2.20	0.42
1:A:31[B]:LEU:CD1	3:A:426:HOH:O	2.50	0.42
1:D:71:LYS:HG2	1:D:146[A]:ILE:HD11	2.01	0.42
1:K:28:ARG:HB3	1:Z:117:PRO:HB3	2.01	0.42
1:N:91[B]:ARG:NH1	1:N:93:ASN:HD22	2.01	0.42
1:S:38:ASN:HB3	1:S:179:SER:O	2.20	0.42
1:a:27:LYS:HB3	1:a:57:ILE:O	2.20	0.42
1:a:31[B]:LEU:HD22	1:a:188:TYR:HB3	2.02	0.42
1:d:13:MET:C	1:d:15:ALA:H	2.28	0.42
1:f:13:MET:O	1:f:16:VAL:N	2.53	0.42
1:p:17:LYS:HZ2	1:p:21:ASN:HD21	1.66	0.42
1:p:24:LEU:O	1:p:26:HIS:HD2	2.02	0.42
1:s:13:MET:O	1:s:16:VAL:HG12	2.20	0.42
1:1:36:ASN:HB2	1:1:184:TRP:CE2	2.54	0.42
1:3:146:ILE:HD13	3:3:520:HOH:O	2.17	0.42
1:6:16:VAL:HG13	1:6:17:LYS:H	1.84	0.42
1:A:43[B]:THR:HG22	3:A:525:HOH:O	2.19	0.42
1:S:73:HIS:HE1	1:S:144:ASP:OD2	2.03	0.42
1:Y:129:LYS:HE3	1:Y:147:ILE:HG21	2.02	0.42
1:a:145[A]:ARG:NH2	3:a:340:HOH:O	2.44	0.42
1:u:12:THR:O	1:u:16:VAL:CG1	2.68	0.41
1:w:23:HIS:CE1	1:V:17:LYS:NZ	2.80	0.41
1:A:79:ILE:O	1:A:181:VAL:HG23	2.20	0.41
1:E:18:ARG:O	1:E:22:THR:HG23	2.19	0.41
1:O:174:LEU:C	1:O:174:LEU:HD23	2.46	0.41
1:c:12:THR:O	1:c:14:ARG:N	2.53	0.41
1:e:13:MET:SD	1:e:16:VAL:HG11	2.60	0.41
1:k:31:LEU:CD2	1:k:31:LEU:C	2.93	0.41
1:l:17:LYS:HG3	3:l:459:HOH:O	2.16	0.41
1:m:145:ARG:NH2	3:m:435:HOH:O	2.53	0.41
1:n:13:MET:C	1:n:16:VAL:HG12	2.45	0.41
1:p:146:ILE:CD1	3:q:551:HOH:O	2.68	0.41
1:u:13:MET:HB3	1:B:19:MET:HE1	2.02	0.41
1:u:17:LYS:CE	1:u:21:ASN:HD21	2.32	0.41
1:B:79:ILE:HD12	1:B:183:LEU:HG	2.01	0.41
1:B:91[B]:ARG:HD3	1:B:93:ASN:HD21	1.85	0.41
1:F:19:MET:O	1:F:23:HIS:HD2	2.03	0.41
1:Z:28:ARG:HB3	1:b:117:PRO:HB3	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:146:ILE:CD1	3:F:420:HOH:O	2.44	0.41
1:k:16:VAL:HG13	1:k:17:LYS:H	1.86	0.41
1:p:15:ALA:O	1:p:18:ARG:HB3	2.19	0.41
1:t:31:LEU:C	1:t:31:LEU:HD23	2.45	0.41
1:v:95:ASN:ND2	1:v:98:THR:H	2.13	0.41
1:y:13:MET:HA	1:y:16:VAL:HG12	2.02	0.41
1:z:19:MET:HG2	1:Y:20:ILE:HD12	2.02	0.41
1:E:13:MET:O	1:E:14:ARG:C	2.62	0.41
1:U:24:LEU:HD22	1:U:195:ALA:HB2	2.01	0.41
1:U:38:ASN:HB3	1:U:179:SER:O	2.20	0.41
1:h:16:VAL:CG1	1:h:17:LYS:N	2.82	0.41
1:o:13:MET:C	1:o:16:VAL:HG13	2.45	0.41
1:o:45[A]:GLN:NE2	3:o:523:HOH:O	2.54	0.41
1:t:13:MET:HE2	1:3:19:MET:HE3	2.02	0.41
1:z:38:ASN:HB3	1:z:179:SER:O	2.20	0.41
1:A:28:ARG:HD2	3:A:356:HOH:O	2.20	0.41
1:B:24:LEU:O	1:B:26:HIS:HD2	2.03	0.41
1:B:71:LYS:CD	1:B:146[B]:ILE:HD11	2.50	0.41
1:D:66:ARG:HD3	3:D:461:HOH:O	2.20	0.41
1:H:12:THR:C	1:H:14:ARG:N	2.76	0.41
1:P:38:ASN:HB3	1:P:179:SER:O	2.21	0.41
1:e:16:VAL:HG13	1:e:17:LYS:H	1.85	0.41
1:g:22:THR:HG23	1:g:23:HIS:CD2	2.55	0.41
1:k:91:ARG:HD3	1:k:93:ASN:HD21	1.86	0.41
1:o:24:LEU:O	1:o:26:HIS:HD2	2.02	0.41
1:1:17:LYS:HE3	1:1:21:ASN:ND2	2.36	0.41
1:4:24:LEU:O	1:4:26:HIS:HD2	2.02	0.41
1:6:129:LYS:HZ1	1:6:145:ARG:NH2	2.14	0.41
1:M:38:ASN:HB3	1:M:179:SER:O	2.20	0.41
1:O:13:MET:CA	1:O:16:VAL:CG1	2.80	0.41
1:q:28:ARG:HB3	1:O:117:PRO:HB3	2.02	0.41
1:3:91[B]:ARG:HD3	3:3:357:HOH:O	2.21	0.41
1:5:71:LYS:HD3	1:5:148[B]:ASN:ND2	2.35	0.41
1:A:13:MET:O	1:A:16:VAL:HG13	2.21	0.41
1:A:70:HIS:HD2	1:A:149:LEU:O	2.04	0.41
1:F:24:LEU:O	1:F:26:HIS:HD2	2.03	0.41
1:F:152:GLN:HG3	3:F:421:HOH:O	2.21	0.41
1:G:16:VAL:HG12	1:G:17:LYS:H	1.85	0.41
1:I:73:HIS:HB2	1:I:146[B]:ILE:HD13	2.00	0.41
1:M:36:ASN:HB2	1:M:184:TRP:CE2	2.55	0.41
1:P:24:LEU:O	1:P:26:HIS:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:66:ARG:HD3	3:R:498:HOH:O	2.19	0.41
1:f:13:MET:C	1:f:15:ALA:N	2.76	0.41
1:g:16:VAL:HG11	1:b:19:MET:CE	2.48	0.41
1:k:38:ASN:HB3	1:k:179:SER:O	2.21	0.41
1:m:117:PRO:O	1:t:28[A]:ARG:HD3	2.20	0.41
1:o:73:HIS:HE1	1:o:144:ASP:OD2	2.04	0.41
1:q:19:MET:HE3	1:w:13:MET:CE	2.50	0.41
1:y:36:ASN:HB2	1:y:184:TRP:CE2	2.56	0.41
1:1:45[B]:GLN:CG	3:1:428:HOH:O	2.51	0.41
1:D:18:ARG:NH2	3:D:458:HOH:O	2.53	0.41
1:O:24:LEU:O	1:O:26:HIS:HD2	2.04	0.41
1:Y:24:LEU:O	1:Y:26:HIS:HD2	2.04	0.41
1:j:36:ASN:HB2	1:j:184:TRP:CE2	2.56	0.41
1:n:129:LYS:HZ2	1:n:145[B]:ARG:NE	2.19	0.41
1:x:36:ASN:HB2	1:x:184:TRP:CE2	2.55	0.41
1:x:66:ARG:NE	1:x:67:ILE:O	2.53	0.41
1:5:12:THR:CG2	1:5:13:MET:H	2.32	0.41
1:5:173:MET:HE2	3:5:442:HOH:O	2.21	0.41
1:6:19:MET:SD	1:F:16:VAL:HG13	2.60	0.41
1:A:17:LYS:CE	1:A:21:ASN:HD21	2.34	0.41
1:b:14:ARG:HG3	3:b:486:HOH:O	2.21	0.41
1:b:129:LYS:NZ	3:b:330:HOH:O	2.44	0.41
1:c:79:ILE:O	1:c:181:VAL:HG23	2.20	0.41
1:e:24:LEU:O	1:e:26:HIS:HD2	2.04	0.41
1:i:95:ASN:ND2	1:i:98:THR:H	2.09	0.41
1:q:24:LEU:O	1:q:26:HIS:HD2	2.04	0.41
1:r:17:LYS:HE3	1:r:21:ASN:ND2	2.36	0.41
1:v:24:LEU:O	1:v:26:HIS:HD2	2.04	0.41
1:y:24:LEU:HD22	1:y:195:ALA:HB2	2.02	0.41
1:1:38:ASN:HB3	1:1:179:SER:O	2.20	0.41
1:2:12:THR:O	1:2:12:THR:HG23	2.20	0.41
1:7:73:HIS:CB	1:7:146:ILE:HD13	2.51	0.41
1:A:12:THR:CG2	1:A:13:MET:CE	2.94	0.41
1:A:79:ILE:HD12	1:A:183:LEU:HG	2.02	0.41
1:B:31[B]:LEU:HD23	1:B:32:ILE:N	2.35	0.41
1:E:16:VAL:CG1	1:J:19:MET:SD	3.01	0.41
1:E:19:MET:O	1:E:23:HIS:HD2	2.04	0.41
1:G:12:THR:HG23	1:G:12:THR:O	2.21	0.41
1:G:13:MET:C	1:G:15:ALA:N	2.79	0.41
1:I:95:ASN:HD22	1:I:97:GLY:H	1.68	0.41
1:J:145:ARG:HD3	1:J:147:ILE:CD1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:145[B]:ARG:HG3	1:K:145[B]:ARG:NH1	2.21	0.41
1:P:14:ARG:CB	1:P:14:ARG:CZ	2.99	0.41
1:Y:153:LEU:HD13	3:Y:550:HOH:O	2.21	0.41
1:c:91[A]:ARG:HG2	1:c:93:ASN:ND2	2.36	0.41
1:g:31[B]:LEU:HD23	1:g:32:ILE:N	2.35	0.41
1:j:73:HIS:CG	1:j:146:ILE:HG12	2.56	0.41
1:k:152:GLN:HG3	3:k:447:HOH:O	2.21	0.41
1:n:91:ARG:HD2	3:n:511:HOH:O	2.21	0.41
1:t:38:ASN:HB3	1:t:179:SER:O	2.21	0.41
1:z:71:LYS:HE3	1:A:114:GLN:OE1	2.21	0.41
1:5:66:ARG:HG3	1:5:66:ARG:NH1	2.35	0.41
1:5:79:ILE:HD12	1:5:183:LEU:HG	2.03	0.41
1:7:27:LYS:HE3	3:7:509:HOH:O	2.21	0.41
1:A:66:ARG:NH1	3:A:434:HOH:O	2.52	0.41
1:F:45[B]:GLN:HG2	1:F:46:ASN:N	2.34	0.41
1:J:145:ARG:HE	1:J:147:ILE:CG1	2.34	0.41
1:Z:146:ILE:HD13	3:b:411:HOH:O	2.20	0.41
1:j:95:ASN:HD22	1:j:97:GLY:H	1.68	0.40
1:l:14:ARG:HG2	1:l:14:ARG:HH11	1.87	0.40
1:t:95:ASN:HD22	1:t:97:GLY:H	1.66	0.40
1:3:24:LEU:HD22	1:3:195:ALA:HB2	2.03	0.40
1:4:73:HIS:HB2	1:4:146:ILE:HD12	2.03	0.40
1:A:13:MET:C	1:A:16:VAL:HG12	2.45	0.40
1:D:38:ASN:HB3	1:D:179:SER:O	2.20	0.40
1:D:66:ARG:NH2	3:D:404:HOH:O	2.40	0.40
1:O:31:LEU:CD2	1:O:31:LEU:C	2.94	0.40
1:W:13:MET:HE3	1:W:14:ARG:N	2.35	0.40
1:Z:66:ARG:HG2	3:Z:513:HOH:O	2.22	0.40
1:n:17:LYS:NZ	1:M:23:HIS:HE1	2.18	0.40
1:x:66:ARG:NH1	1:x:66:ARG:CG	2.55	0.40
1:5:71:LYS:HD3	1:5:148[B]:ASN:HD21	1.87	0.40
1:C:24:LEU:O	1:C:26:HIS:HD2	2.03	0.40
1:F:13:MET:O	1:F:16:VAL:HG12	2.20	0.40
1:H:12:THR:N	1:H:14:ARG:CZ	2.84	0.40
1:I:145:ARG:NH2	3:I:435:HOH:O	2.53	0.40
1:K:12:THR:O	1:K:15:ALA:N	2.53	0.40
1:M:131[A]:VAL:HG12	3:M:502:HOH:O	2.21	0.40
1:O:73:HIS:HE1	1:O:144:ASP:OD2	2.05	0.40
1:T:15:ALA:O	1:T:16:VAL:C	2.65	0.40
1:U:36:ASN:HB2	1:U:184:TRP:CE2	2.55	0.40
1:Y:28:ARG:HG2	1:Y:191:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:71:LYS:CG	1:Y:148[A]:ASN:OD1	2.69	0.40
1:o:17:LYS:HE3	1:o:21:ASN:ND2	2.37	0.40
1:y:28:ARG:HG2	1:y:191:VAL:HG22	2.03	0.40
1:F:19:MET:HE1	1:O:16:VAL:HG11	1.99	0.40
1:M:174:LEU:HD23	1:M:174:LEU:C	2.46	0.40
1:N:17:LYS:NZ	1:N:21:ASN:ND2	2.56	0.40
1:X:16:VAL:HG13	1:X:17:LYS:N	2.37	0.40
1:g:13:MET:HA	1:g:16:VAL:HG12	2.03	0.40
1:h:24:LEU:O	1:h:26:HIS:HD2	2.04	0.40
1:l:13:MET:HE2	1:l:13:MET:HB3	1.97	0.40
1:r:129:LYS:HE2	1:r:145[A]:ARG:NH2	2.36	0.40
1:s:31:LEU:HD23	1:s:32:ILE:N	2.37	0.40
1:z:38:ASN:OD1	1:z:177:GLY:HA3	2.22	0.40
1:D:73:HIS:HE1	1:D:144:ASP:OD2	2.04	0.40
1:E:38:ASN:HB3	1:E:179:SER:O	2.22	0.40
1:K:152[A]:GLN:CG	1:K:153:LEU:H	2.34	0.40
1:M:71:LYS:HD2	1:M:146:ILE:HD11	2.03	0.40
1:O:27:LYS:HB3	1:O:57:ILE:O	2.21	0.40
1:R:24:LEU:O	1:R:26:HIS:HD2	2.04	0.40
1:R:36:ASN:HB2	1:R:184:TRP:CE2	2.57	0.40
1:S:45[A]:GLN:HG2	1:S:46:ASN:N	2.36	0.40
1:e:16:VAL:CG1	1:e:17:LYS:N	2.84	0.40
1:g:174:LEU:C	1:g:174:LEU:HD23	2.46	0.40
1:l:79:ILE:O	1:l:80:THR:HB	2.22	0.40
1:p:27:LYS:HB3	1:p:57:ILE:O	2.22	0.40
1:s:66:ARG:HG2	3:s:492:HOH:O	2.21	0.40
1:t:18:ARG:O	1:t:22:THR:HG23	2.22	0.40
1:v:16:VAL:HG13	1:v:17:LYS:N	2.36	0.40
1:x:73:HIS:HE1	1:x:144:ASP:OD2	2.05	0.40
1:R:117:PRO:HB3	1:X:28:ARG:HB3	2.04	0.40
1:a:16:VAL:HG13	1:a:17:LYS:H	1.85	0.40

All (6) 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)
3:r:405:HOH:O	3:4:419:HOH:O[4_545]	1.23	0.97
3:h:501:HOH:O	3:r:544:HOH:O[4_555]	1.60	0.60
3:h:442:HOH:O	3:r:544:HOH:O[4_555]	1.78	0.42
3:T:434:HOH:O	3:T:585:HOH:O[2_655]	1.94	0.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o:317:HOH:O	3:u:479:HOH:O[2_555]	1.99	0.21
3:r:526:HOH:O	3:4:419:HOH:O[4_545]	2.03	0.17

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	184/196 (94%)	179 (97%)	5 (3%)	0	100	100
1	1	185/196 (94%)	178 (96%)	7 (4%)	0	100	100
1	2	186/196 (95%)	180 (97%)	6 (3%)	0	100	100
1	3	186/196 (95%)	181 (97%)	5 (3%)	0	100	100
1	4	185/196 (94%)	179 (97%)	6 (3%)	0	100	100
1	5	183/196 (93%)	179 (98%)	4 (2%)	0	100	100
1	6	185/196 (94%)	180 (97%)	5 (3%)	0	100	100
1	7	184/196 (94%)	179 (97%)	5 (3%)	0	100	100
1	A	188/196 (96%)	183 (97%)	5 (3%)	0	100	100
1	B	188/196 (96%)	183 (97%)	5 (3%)	0	100	100
1	C	186/196 (95%)	181 (97%)	5 (3%)	0	100	100
1	D	186/196 (95%)	181 (97%)	5 (3%)	0	100	100
1	E	184/196 (94%)	176 (96%)	8 (4%)	0	100	100
1	F	184/196 (94%)	176 (96%)	8 (4%)	0	100	100
1	G	186/196 (95%)	178 (96%)	7 (4%)	1 (0%)	24	7
1	H	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	I	185/196 (94%)	180 (97%)	5 (3%)	0	100	100
1	J	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	K	189/196 (96%)	184 (97%)	4 (2%)	1 (0%)	24	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	187/196 (95%)	182 (97%)	5 (3%)	0	100	100
1	M	185/196 (94%)	178 (96%)	7 (4%)	0	100	100
1	N	185/196 (94%)	180 (97%)	5 (3%)	0	100	100
1	O	184/196 (94%)	180 (98%)	4 (2%)	0	100	100
1	P	188/196 (96%)	182 (97%)	6 (3%)	0	100	100
1	Q	184/196 (94%)	179 (97%)	5 (3%)	0	100	100
1	R	185/196 (94%)	179 (97%)	6 (3%)	0	100	100
1	S	188/196 (96%)	182 (97%)	6 (3%)	0	100	100
1	T	185/196 (94%)	179 (97%)	6 (3%)	0	100	100
1	U	186/196 (95%)	181 (97%)	5 (3%)	0	100	100
1	V	185/196 (94%)	180 (97%)	5 (3%)	0	100	100
1	W	183/196 (93%)	176 (96%)	6 (3%)	1 (0%)	24	7
1	X	184/196 (94%)	180 (98%)	4 (2%)	0	100	100
1	Y	185/196 (94%)	180 (97%)	5 (3%)	0	100	100
1	Z	185/196 (94%)	179 (97%)	6 (3%)	0	100	100
1	a	187/196 (95%)	182 (97%)	5 (3%)	0	100	100
1	b	183/196 (93%)	179 (98%)	4 (2%)	0	100	100
1	c	185/196 (94%)	179 (97%)	5 (3%)	1 (0%)	24	7
1	d	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	e	184/196 (94%)	179 (97%)	5 (3%)	0	100	100
1	f	186/196 (95%)	178 (96%)	8 (4%)	0	100	100
1	g	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	h	186/196 (95%)	181 (97%)	5 (3%)	0	100	100
1	i	185/196 (94%)	179 (97%)	5 (3%)	1 (0%)	24	7
1	j	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	k	184/196 (94%)	179 (97%)	5 (3%)	0	100	100
1	l	183/196 (93%)	178 (97%)	5 (3%)	0	100	100
1	m	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	n	186/196 (95%)	180 (97%)	6 (3%)	0	100	100
1	o	183/196 (93%)	178 (97%)	5 (3%)	0	100	100
1	p	183/196 (93%)	178 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	q	183/196 (93%)	178 (97%)	5 (3%)	0	100	100
1	r	185/196 (94%)	179 (97%)	6 (3%)	0	100	100
1	s	184/196 (94%)	177 (96%)	7 (4%)	0	100	100
1	t	189/196 (96%)	183 (97%)	6 (3%)	0	100	100
1	u	184/196 (94%)	180 (98%)	4 (2%)	0	100	100
1	v	184/196 (94%)	179 (97%)	5 (3%)	0	100	100
1	w	185/196 (94%)	181 (98%)	4 (2%)	0	100	100
1	x	185/196 (94%)	178 (96%)	7 (4%)	0	100	100
1	y	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	z	186/196 (95%)	181 (97%)	5 (3%)	0	100	100
All	All	11101/11760 (94%)	10766 (97%)	330 (3%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	W	15	ALA
1	G	14	ARG
1	K	13	MET
1	i	14	ARG
1	c	13	MET

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	0	159/167 (95%)	158 (99%)	1 (1%)	78	58
1	1	160/167 (96%)	157 (98%)	3 (2%)	50	17
1	2	161/167 (96%)	159 (99%)	2 (1%)	63	33
1	3	161/167 (96%)	159 (99%)	2 (1%)	63	33
1	4	160/167 (96%)	158 (99%)	2 (1%)	61	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5	158/167 (95%)	157 (99%)	1 (1%)	78	58
1	6	160/167 (96%)	159 (99%)	1 (1%)	78	58
1	7	159/167 (95%)	158 (99%)	1 (1%)	78	58
1	A	163/167 (98%)	159 (98%)	4 (2%)	42	11
1	B	163/167 (98%)	160 (98%)	3 (2%)	51	19
1	C	161/167 (96%)	156 (97%)	5 (3%)	35	7
1	D	161/167 (96%)	154 (96%)	7 (4%)	26	3
1	E	159/167 (95%)	154 (97%)	5 (3%)	35	7
1	F	159/167 (95%)	159 (100%)	0	100	100
1	G	161/167 (96%)	160 (99%)	1 (1%)	78	58
1	H	159/167 (95%)	155 (98%)	4 (2%)	42	11
1	I	160/167 (96%)	159 (99%)	1 (1%)	78	58
1	J	159/167 (95%)	155 (98%)	4 (2%)	42	11
1	K	164/167 (98%)	163 (99%)	1 (1%)	78	58
1	L	162/167 (97%)	159 (98%)	3 (2%)	50	17
1	M	160/167 (96%)	158 (99%)	2 (1%)	61	31
1	N	160/167 (96%)	159 (99%)	1 (1%)	78	58
1	O	159/167 (95%)	157 (99%)	2 (1%)	61	31
1	P	163/167 (98%)	162 (99%)	1 (1%)	78	58
1	Q	159/167 (95%)	156 (98%)	3 (2%)	50	17
1	R	160/167 (96%)	156 (98%)	4 (2%)	42	11
1	S	163/167 (98%)	161 (99%)	2 (1%)	63	33
1	T	160/167 (96%)	157 (98%)	3 (2%)	50	17
1	U	161/167 (96%)	161 (100%)	0	100	100
1	V	160/167 (96%)	159 (99%)	1 (1%)	78	58
1	W	158/167 (95%)	158 (100%)	0	100	100
1	X	159/167 (95%)	158 (99%)	1 (1%)	78	58
1	Y	160/167 (96%)	159 (99%)	1 (1%)	78	58
1	Z	160/167 (96%)	159 (99%)	1 (1%)	78	58
1	a	162/167 (97%)	162 (100%)	0	100	100
1	b	158/167 (95%)	154 (98%)	4 (2%)	42	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	c	160/167 (96%)	157 (98%)	3 (2%)	50	17
1	d	159/167 (95%)	156 (98%)	3 (2%)	50	17
1	e	159/167 (95%)	157 (99%)	2 (1%)	61	31
1	f	161/167 (96%)	159 (99%)	2 (1%)	63	33
1	g	159/167 (95%)	159 (100%)	0	100	100
1	h	161/167 (96%)	160 (99%)	1 (1%)	78	58
1	i	160/167 (96%)	160 (100%)	0	100	100
1	j	159/167 (95%)	159 (100%)	0	100	100
1	k	159/167 (95%)	157 (99%)	2 (1%)	61	31
1	l	158/167 (95%)	156 (99%)	2 (1%)	61	31
1	m	159/167 (95%)	157 (99%)	2 (1%)	61	31
1	n	161/167 (96%)	159 (99%)	2 (1%)	63	33
1	o	158/167 (95%)	156 (99%)	2 (1%)	61	31
1	p	158/167 (95%)	154 (98%)	4 (2%)	42	11
1	q	158/167 (95%)	155 (98%)	3 (2%)	50	17
1	r	160/167 (96%)	157 (98%)	3 (2%)	50	17
1	s	159/167 (95%)	155 (98%)	4 (2%)	42	11
1	t	164/167 (98%)	162 (99%)	2 (1%)	63	33
1	u	159/167 (95%)	157 (99%)	2 (1%)	61	31
1	v	159/167 (95%)	155 (98%)	4 (2%)	42	11
1	w	160/167 (96%)	160 (100%)	0	100	100
1	x	160/167 (96%)	159 (99%)	1 (1%)	78	58
1	y	159/167 (95%)	158 (99%)	1 (1%)	78	58
1	z	161/167 (96%)	158 (98%)	3 (2%)	50	17
All	All	9601/10020 (96%)	9476 (99%)	125 (1%)	63	31

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	e	71	LYS
1	e	145	ARG
1	f	12	THR
1	f	22	THR
1	h	71	LYS

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Mol	Chain	Res	Type
1	k	16	VAL
1	k	31	LEU
1	l	16	VAL
1	l	31	LEU
1	m	22	THR
1	m	31	LEU
1	n	21	ASN
1	n	22	THR
1	o	16	VAL
1	o	31	LEU
1	p	13	MET
1	p	16	VAL
1	p	31	LEU
1	p	189	GLU
1	q	16	VAL
1	q	31	LEU
1	q	71	LYS
1	r	12	THR
1	r	16	VAL
1	r	31	LEU
1	s	22	THR
1	s	31	LEU
1	s	181[A]	VAL
1	s	181[B]	VAL
1	t	22	THR
1	t	31	LEU
1	u	16	VAL
1	u	31	LEU
1	v	13	MET
1	v	16	VAL
1	v	31	LEU
1	v	189	GLU
1	x	66	ARG
1	y	16	VAL
1	z	22	THR
1	z	31[A]	LEU
1	z	31[B]	LEU
1	0	31	LEU
1	1	16	VAL
1	1	31	LEU
1	1	146	ILE
1	2	16	VAL

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Mol	Chain	Res	Type
1	2	31	LEU
1	3	16	VAL
1	3	31	LEU
1	4	31	LEU
1	4	146	ILE
1	5	16	VAL
1	6	31	LEU
1	7	71	LYS
1	A	13	MET
1	A	16	VAL
1	A	22	THR
1	A	70	HIS
1	B	16	VAL
1	B	146[A]	ILE
1	B	146[B]	ILE
1	C	18	ARG
1	C	22	THR
1	C	31	LEU
1	C	148[A]	ASN
1	C	148[B]	ASN
1	D	16	VAL
1	D	31[A]	LEU
1	D	31[B]	LEU
1	D	34[A]	SER
1	D	34[B]	SER
1	D	146[A]	ILE
1	D	146[B]	ILE
1	E	12	THR
1	E	31[A]	LEU
1	E	31[B]	LEU
1	E	147	ILE
1	E	189	GLU
1	G	16	VAL
1	H	14	ARG
1	H	16	VAL
1	H	91[A]	ARG
1	H	91[B]	ARG
1	I	22	THR
1	J	12	THR
1	J	13	MET
1	J	16	VAL
1	J	31	LEU

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Mol	Chain	Res	Type
1	K	16	VAL
1	L	16	VAL
1	L	19	MET
1	L	31	LEU
1	M	71	LYS
1	M	146	ILE
1	N	31	LEU
1	O	12	THR
1	O	31	LEU
1	P	31	LEU
1	Q	31	LEU
1	Q	148[A]	ASN
1	Q	148[B]	ASN
1	R	16	VAL
1	R	31[A]	LEU
1	R	31[B]	LEU
1	R	71	LYS
1	S	152[A]	GLN
1	S	152[B]	GLN
1	T	31[A]	LEU
1	T	31[B]	LEU
1	T	71	LYS
1	V	22	THR
1	X	71	LYS
1	Y	31	LEU
1	Z	16	VAL
1	b	12	THR
1	b	16	VAL
1	b	31	LEU
1	b	66	ARG
1	c	16	VAL
1	c	31	LEU
1	c	146	ILE
1	d	16	VAL
1	d	31	LEU
1	d	145	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (587) such sidechains are listed below:

Mol	Chain	Res	Type
1	e	23	HIS
1	e	26	HIS

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Mol	Chain	Res	Type
1	e	33	ASN
1	e	36	ASN
1	e	64	GLN
1	e	73	HIS
1	e	93	ASN
1	e	95	ASN
1	e	107	ASN
1	e	148	ASN
1	f	23	HIS
1	f	26	HIS
1	f	33	ASN
1	f	36	ASN
1	f	73	HIS
1	f	93	ASN
1	f	95	ASN
1	f	107	ASN
1	f	148	ASN
1	g	23	HIS
1	g	26	HIS
1	g	33	ASN
1	g	36	ASN
1	g	49	ASN
1	g	64	GLN
1	g	73	HIS
1	g	93	ASN
1	g	95	ASN
1	g	107	ASN
1	g	134	ASN
1	g	152	GLN
1	g	155	ASN
1	h	23	HIS
1	h	26	HIS
1	h	49	ASN
1	h	64	GLN
1	h	73	HIS
1	h	93	ASN
1	h	95	ASN
1	h	107	ASN
1	i	23	HIS
1	i	26	HIS
1	i	33	ASN
1	i	36	ASN

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Mol	Chain	Res	Type
1	i	73	HIS
1	i	93	ASN
1	i	95	ASN
1	i	107	ASN
1	j	23	HIS
1	j	26	HIS
1	j	73	HIS
1	j	93	ASN
1	j	95	ASN
1	j	107	ASN
1	j	134	ASN
1	k	26	HIS
1	k	33	ASN
1	k	36	ASN
1	k	64	GLN
1	k	73	HIS
1	k	93	ASN
1	k	95	ASN
1	k	107	ASN
1	l	23	HIS
1	l	26	HIS
1	l	33	ASN
1	l	45	GLN
1	l	73	HIS
1	l	93	ASN
1	l	95	ASN
1	l	107	ASN
1	l	134	ASN
1	l	148	ASN
1	m	21	ASN
1	m	26	HIS
1	m	33	ASN
1	m	36	ASN
1	m	64	GLN
1	m	73	HIS
1	m	93	ASN
1	m	95	ASN
1	m	107	ASN
1	n	23	HIS
1	n	26	HIS
1	n	33	ASN
1	n	36	ASN

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Mol	Chain	Res	Type
1	n	64	GLN
1	n	73	HIS
1	n	93	ASN
1	n	95	ASN
1	n	107	ASN
1	o	21	ASN
1	o	23	HIS
1	o	26	HIS
1	o	49	ASN
1	o	73	HIS
1	o	93	ASN
1	o	95	ASN
1	o	107	ASN
1	o	152	GLN
1	p	21	ASN
1	p	23	HIS
1	p	26	HIS
1	p	33	ASN
1	p	36	ASN
1	p	64	GLN
1	p	73	HIS
1	p	93	ASN
1	p	95	ASN
1	p	107	ASN
1	p	134	ASN
1	q	21	ASN
1	q	23	HIS
1	q	26	HIS
1	q	33	ASN
1	q	36	ASN
1	q	64	GLN
1	q	73	HIS
1	q	93	ASN
1	q	95	ASN
1	q	107	ASN
1	q	148	ASN
1	r	21	ASN
1	r	23	HIS
1	r	26	HIS
1	r	33	ASN
1	r	36	ASN
1	r	73	HIS

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Mol	Chain	Res	Type
1	r	93	ASN
1	r	95	ASN
1	r	107	ASN
1	r	148	ASN
1	s	23	HIS
1	s	26	HIS
1	s	33	ASN
1	s	36	ASN
1	s	64	GLN
1	s	73	HIS
1	s	93	ASN
1	s	95	ASN
1	s	107	ASN
1	s	134	ASN
1	s	155	ASN
1	t	21	ASN
1	t	23	HIS
1	t	26	HIS
1	t	33	ASN
1	t	36	ASN
1	t	45	GLN
1	t	64	GLN
1	t	73	HIS
1	t	93	ASN
1	t	95	ASN
1	t	107	ASN
1	t	148	ASN
1	u	21	ASN
1	u	23	HIS
1	u	26	HIS
1	u	33	ASN
1	u	64	GLN
1	u	73	HIS
1	u	93	ASN
1	u	95	ASN
1	u	107	ASN
1	u	155	ASN
1	v	26	HIS
1	v	33	ASN
1	v	36	ASN
1	v	73	HIS
1	v	93	ASN

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Mol	Chain	Res	Type
1	v	95	ASN
1	v	107	ASN
1	v	134	ASN
1	v	148	ASN
1	v	152	GLN
1	w	23	HIS
1	w	26	HIS
1	w	33	ASN
1	w	49	ASN
1	w	64	GLN
1	w	73	HIS
1	w	93	ASN
1	w	95	ASN
1	w	107	ASN
1	w	148	ASN
1	x	21	ASN
1	x	23	HIS
1	x	26	HIS
1	x	33	ASN
1	x	36	ASN
1	x	64	GLN
1	x	73	HIS
1	x	93	ASN
1	x	95	ASN
1	x	107	ASN
1	x	134	ASN
1	x	152	GLN
1	y	21	ASN
1	y	23	HIS
1	y	26	HIS
1	y	33	ASN
1	y	36	ASN
1	y	49	ASN
1	y	64	GLN
1	y	73	HIS
1	y	93	ASN
1	y	95	ASN
1	y	107	ASN
1	y	148	ASN
1	y	175	GLN
1	z	21	ASN
1	z	26	HIS

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Mol	Chain	Res	Type
1	z	33	ASN
1	z	36	ASN
1	z	73	HIS
1	z	93	ASN
1	z	95	ASN
1	z	107	ASN
1	z	148	ASN
1	0	23	HIS
1	0	26	HIS
1	0	33	ASN
1	0	36	ASN
1	0	64	GLN
1	0	73	HIS
1	0	93	ASN
1	0	95	ASN
1	0	107	ASN
1	0	134	ASN
1	1	21	ASN
1	1	26	HIS
1	1	33	ASN
1	1	36	ASN
1	1	64	GLN
1	1	73	HIS
1	1	93	ASN
1	1	95	ASN
1	1	107	ASN
1	1	148	ASN
1	2	21	ASN
1	2	23	HIS
1	2	26	HIS
1	2	33	ASN
1	2	36	ASN
1	2	64	GLN
1	2	73	HIS
1	2	93	ASN
1	2	95	ASN
1	2	107	ASN
1	2	134	ASN
1	3	23	HIS
1	3	26	HIS
1	3	33	ASN
1	3	36	ASN

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Mol	Chain	Res	Type
1	3	64	GLN
1	3	73	HIS
1	3	93	ASN
1	3	95	ASN
1	3	107	ASN
1	3	148	ASN
1	4	23	HIS
1	4	26	HIS
1	4	73	HIS
1	4	93	ASN
1	4	95	ASN
1	4	107	ASN
1	5	23	HIS
1	5	26	HIS
1	5	33	ASN
1	5	64	GLN
1	5	73	HIS
1	5	93	ASN
1	5	95	ASN
1	5	107	ASN
1	6	21	ASN
1	6	23	HIS
1	6	26	HIS
1	6	33	ASN
1	6	36	ASN
1	6	49	ASN
1	6	64	GLN
1	6	73	HIS
1	6	93	ASN
1	6	95	ASN
1	6	134	ASN
1	7	26	HIS
1	7	33	ASN
1	7	36	ASN
1	7	73	HIS
1	7	93	ASN
1	7	95	ASN
1	7	107	ASN
1	A	21	ASN
1	A	26	HIS
1	A	33	ASN
1	A	36	ASN

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Mol	Chain	Res	Type
1	A	64	GLN
1	A	73	HIS
1	A	93	ASN
1	A	95	ASN
1	A	107	ASN
1	B	21	ASN
1	B	23	HIS
1	B	26	HIS
1	B	33	ASN
1	B	36	ASN
1	B	73	HIS
1	B	93	ASN
1	B	95	ASN
1	B	107	ASN
1	C	26	HIS
1	C	33	ASN
1	C	36	ASN
1	C	73	HIS
1	C	93	ASN
1	C	95	ASN
1	C	134	ASN
1	D	23	HIS
1	D	26	HIS
1	D	33	ASN
1	D	36	ASN
1	D	73	HIS
1	D	93	ASN
1	D	95	ASN
1	D	107	ASN
1	E	21	ASN
1	E	23	HIS
1	E	26	HIS
1	E	33	ASN
1	E	36	ASN
1	E	73	HIS
1	E	93	ASN
1	E	95	ASN
1	E	107	ASN
1	E	134	ASN
1	F	23	HIS
1	F	26	HIS
1	F	33	ASN

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Mol	Chain	Res	Type
1	F	36	ASN
1	F	64	GLN
1	F	73	HIS
1	F	93	ASN
1	F	95	ASN
1	F	107	ASN
1	F	134	ASN
1	G	21	ASN
1	G	26	HIS
1	G	33	ASN
1	G	36	ASN
1	G	64	GLN
1	G	73	HIS
1	G	93	ASN
1	G	95	ASN
1	G	107	ASN
1	H	21	ASN
1	H	23	HIS
1	H	26	HIS
1	H	33	ASN
1	H	36	ASN
1	H	73	HIS
1	H	93	ASN
1	H	95	ASN
1	H	107	ASN
1	H	148	ASN
1	I	21	ASN
1	I	23	HIS
1	I	26	HIS
1	I	33	ASN
1	I	36	ASN
1	I	49	ASN
1	I	73	HIS
1	I	93	ASN
1	I	95	ASN
1	I	107	ASN
1	J	21	ASN
1	J	23	HIS
1	J	26	HIS
1	J	33	ASN
1	J	36	ASN
1	J	73	HIS

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Mol	Chain	Res	Type
1	J	93	ASN
1	J	95	ASN
1	J	107	ASN
1	J	134	ASN
1	K	23	HIS
1	K	26	HIS
1	K	33	ASN
1	K	36	ASN
1	K	64	GLN
1	K	73	HIS
1	K	93	ASN
1	K	95	ASN
1	K	107	ASN
1	K	134	ASN
1	L	21	ASN
1	L	23	HIS
1	L	26	HIS
1	L	33	ASN
1	L	36	ASN
1	L	64	GLN
1	L	73	HIS
1	L	93	ASN
1	L	95	ASN
1	L	107	ASN
1	L	134	ASN
1	L	148	ASN
1	L	152	GLN
1	M	21	ASN
1	M	23	HIS
1	M	26	HIS
1	M	33	ASN
1	M	36	ASN
1	M	49	ASN
1	M	73	HIS
1	M	93	ASN
1	M	95	ASN
1	M	107	ASN
1	M	148	ASN
1	N	21	ASN
1	N	23	HIS
1	N	26	HIS
1	N	33	ASN

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Mol	Chain	Res	Type
1	N	36	ASN
1	N	64	GLN
1	N	73	HIS
1	N	93	ASN
1	N	95	ASN
1	N	107	ASN
1	N	134	ASN
1	N	152	GLN
1	O	23	HIS
1	O	26	HIS
1	O	33	ASN
1	O	36	ASN
1	O	73	HIS
1	O	93	ASN
1	O	95	ASN
1	O	107	ASN
1	O	148	ASN
1	P	23	HIS
1	P	26	HIS
1	P	33	ASN
1	P	36	ASN
1	P	73	HIS
1	P	93	ASN
1	P	95	ASN
1	P	107	ASN
1	Q	21	ASN
1	Q	23	HIS
1	Q	26	HIS
1	Q	33	ASN
1	Q	36	ASN
1	Q	64	GLN
1	Q	73	HIS
1	Q	93	ASN
1	Q	95	ASN
1	Q	107	ASN
1	R	21	ASN
1	R	26	HIS
1	R	33	ASN
1	R	36	ASN
1	R	73	HIS
1	R	93	ASN
1	R	95	ASN

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Mol	Chain	Res	Type
1	R	107	ASN
1	R	134	ASN
1	R	175	GLN
1	S	23	HIS
1	S	26	HIS
1	S	33	ASN
1	S	36	ASN
1	S	64	GLN
1	S	73	HIS
1	S	93	ASN
1	S	95	ASN
1	S	107	ASN
1	S	148	ASN
1	T	23	HIS
1	T	26	HIS
1	T	33	ASN
1	T	36	ASN
1	T	64	GLN
1	T	73	HIS
1	T	93	ASN
1	T	95	ASN
1	T	107	ASN
1	T	134	ASN
1	T	148	ASN
1	U	23	HIS
1	U	26	HIS
1	U	33	ASN
1	U	36	ASN
1	U	64	GLN
1	U	73	HIS
1	U	93	ASN
1	U	95	ASN
1	U	107	ASN
1	V	23	HIS
1	V	26	HIS
1	V	33	ASN
1	V	36	ASN
1	V	73	HIS
1	V	93	ASN
1	V	95	ASN
1	V	107	ASN
1	W	21	ASN

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Mol	Chain	Res	Type
1	W	23	HIS
1	W	26	HIS
1	W	33	ASN
1	W	36	ASN
1	W	73	HIS
1	W	93	ASN
1	W	95	ASN
1	W	107	ASN
1	W	134	ASN
1	X	21	ASN
1	X	23	HIS
1	X	26	HIS
1	X	33	ASN
1	X	36	ASN
1	X	73	HIS
1	X	93	ASN
1	X	95	ASN
1	X	107	ASN
1	X	152	GLN
1	Y	26	HIS
1	Y	33	ASN
1	Y	64	GLN
1	Y	73	HIS
1	Y	93	ASN
1	Y	95	ASN
1	Y	107	ASN
1	Z	21	ASN
1	Z	26	HIS
1	Z	33	ASN
1	Z	36	ASN
1	Z	49	ASN
1	Z	64	GLN
1	Z	73	HIS
1	Z	93	ASN
1	Z	95	ASN
1	Z	107	ASN
1	Z	148	ASN
1	a	23	HIS
1	a	26	HIS
1	a	33	ASN
1	a	36	ASN
1	a	64	GLN

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Mol	Chain	Res	Type
1	a	73	HIS
1	a	93	ASN
1	a	95	ASN
1	a	107	ASN
1	a	134	ASN
1	b	21	ASN
1	b	23	HIS
1	b	26	HIS
1	b	33	ASN
1	b	36	ASN
1	b	64	GLN
1	b	73	HIS
1	b	93	ASN
1	b	95	ASN
1	b	107	ASN
1	b	134	ASN
1	b	148	ASN
1	b	152	GLN
1	c	21	ASN
1	c	23	HIS
1	c	26	HIS
1	c	33	ASN
1	c	36	ASN
1	c	73	HIS
1	c	93	ASN
1	c	95	ASN
1	c	107	ASN
1	c	134	ASN
1	c	148	ASN
1	d	23	HIS
1	d	26	HIS
1	d	33	ASN
1	d	36	ASN
1	d	64	GLN
1	d	73	HIS
1	d	93	ASN
1	d	95	ASN
1	d	107	ASN
1	d	148	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 92 ligands modelled in this entry, 92 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	0	184/196 (93%)	-0.21	11 (5%)	27 27	5, 10, 27, 62	2 (1%)
1	1	184/196 (93%)	-0.15	10 (5%)	31 31	6, 10, 26, 63	3 (1%)
1	2	184/196 (93%)	-0.22	11 (5%)	27 27	6, 10, 21, 61	4 (2%)
1	3	184/196 (93%)	-0.17	9 (4%)	35 36	6, 11, 29, 61	4 (2%)
1	4	184/196 (93%)	-0.24	8 (4%)	40 42	6, 10, 25, 58	3 (1%)
1	5	184/196 (93%)	-0.19	8 (4%)	40 42	9, 11, 29, 64	1 (0%)
1	6	184/196 (93%)	-0.15	11 (5%)	27 27	7, 11, 29, 64	3 (1%)
1	7	184/196 (93%)	-0.13	9 (4%)	35 36	7, 11, 28, 61	2 (1%)
1	A	184/196 (93%)	-0.16	11 (5%)	27 27	6, 10, 29, 63	6 (3%)
1	B	184/196 (93%)	-0.13	11 (5%)	27 27	6, 11, 29, 62	6 (3%)
1	C	184/196 (93%)	-0.12	9 (4%)	35 36	7, 12, 28, 61	4 (2%)
1	D	184/196 (93%)	-0.22	9 (4%)	35 36	6, 10, 27, 64	4 (2%)
1	E	184/196 (93%)	-0.07	9 (4%)	35 36	7, 12, 27, 63	2 (1%)
1	F	184/196 (93%)	-0.13	8 (4%)	40 42	7, 12, 28, 63	2 (1%)
1	G	184/196 (93%)	-0.06	11 (5%)	27 27	6, 12, 29, 62	4 (2%)
1	H	184/196 (93%)	-0.13	9 (4%)	35 36	6, 11, 29, 64	2 (1%)
1	I	184/196 (93%)	-0.15	10 (5%)	31 31	7, 11, 29, 62	3 (1%)
1	J	184/196 (93%)	-0.13	9 (4%)	35 36	7, 11, 27, 60	2 (1%)
1	K	184/196 (93%)	-0.26	9 (4%)	35 36	5, 9, 27, 61	7 (3%)
1	L	184/196 (93%)	-0.19	9 (4%)	35 36	6, 10, 28, 62	5 (2%)
1	M	184/196 (93%)	-0.12	10 (5%)	31 31	6, 11, 28, 64	3 (1%)
1	N	184/196 (93%)	-0.02	9 (4%)	35 36	6, 12, 29, 63	3 (1%)
1	O	184/196 (93%)	-0.12	8 (4%)	40 42	7, 11, 29, 62	2 (1%)
1	P	184/196 (93%)	-0.14	9 (4%)	35 36	5, 11, 28, 62	6 (3%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	Q	184/196 (93%)	-0.10	10 (5%)	31 31	7, 11, 28, 62	2 (1%)
1	R	184/196 (93%)	-0.21	6 (3%)	49 52	6, 10, 27, 61	3 (1%)
1	S	184/196 (93%)	-0.19	7 (3%)	44 47	6, 10, 27, 62	6 (3%)
1	T	184/196 (93%)	-0.30	7 (3%)	44 47	6, 9, 27, 63	3 (1%)
1	U	184/196 (93%)	-0.24	8 (4%)	40 42	5, 9, 27, 64	4 (2%)
1	V	184/196 (93%)	-0.26	7 (3%)	44 47	6, 10, 26, 59	3 (1%)
1	W	184/196 (93%)	-0.07	10 (5%)	31 31	6, 11, 29, 65	1 (0%)
1	X	184/196 (93%)	-0.19	10 (5%)	31 31	6, 10, 28, 60	2 (1%)
1	Y	184/196 (93%)	-0.24	11 (5%)	27 27	6, 10, 28, 61	3 (1%)
1	Z	184/196 (93%)	-0.27	12 (6%)	25 24	5, 9, 28, 64	3 (1%)
1	a	184/196 (93%)	-0.18	10 (5%)	31 31	7, 11, 28, 59	5 (2%)
1	b	184/196 (93%)	-0.19	10 (5%)	31 31	6, 10, 27, 58	1 (0%)
1	c	184/196 (93%)	-0.21	7 (3%)	44 47	5, 10, 27, 64	3 (1%)
1	d	184/196 (93%)	-0.26	10 (5%)	31 31	5, 9, 27, 62	2 (1%)
1	e	184/196 (93%)	-0.12	11 (5%)	27 27	6, 10, 27, 63	2 (1%)
1	f	184/196 (93%)	-0.12	9 (4%)	35 36	7, 12, 29, 60	4 (2%)
1	g	184/196 (93%)	-0.12	11 (5%)	27 27	7, 11, 28, 63	2 (1%)
1	h	184/196 (93%)	-0.16	8 (4%)	40 42	5, 10, 25, 61	4 (2%)
1	i	184/196 (93%)	-0.15	9 (4%)	35 36	5, 10, 28, 60	3 (1%)
1	j	184/196 (93%)	-0.14	9 (4%)	35 36	7, 11, 26, 62	2 (1%)
1	k	184/196 (93%)	-0.21	8 (4%)	40 42	7, 10, 27, 61	2 (1%)
1	l	184/196 (93%)	-0.19	11 (5%)	27 27	7, 10, 27, 61	1 (0%)
1	m	184/196 (93%)	-0.06	11 (5%)	27 27	7, 12, 29, 64	2 (1%)
1	n	184/196 (93%)	0.02	10 (5%)	31 31	7, 12, 30, 63	4 (2%)
1	o	184/196 (93%)	-0.19	11 (5%)	27 27	7, 11, 29, 64	1 (0%)
1	p	184/196 (93%)	-0.16	7 (3%)	44 47	6, 11, 26, 61	1 (0%)
1	q	184/196 (93%)	-0.22	11 (5%)	27 27	6, 10, 26, 61	1 (0%)
1	r	184/196 (93%)	-0.22	10 (5%)	31 31	6, 9, 27, 62	3 (1%)
1	s	184/196 (93%)	-0.14	8 (4%)	40 42	6, 11, 28, 61	2 (1%)
1	t	184/196 (93%)	-0.15	10 (5%)	31 31	6, 11, 29, 61	7 (3%)
1	u	184/196 (93%)	-0.17	9 (4%)	35 36	6, 10, 29, 60	2 (1%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	v	184/196 (93%)	-0.19	10 (5%) 31 31	6, 10, 27, 61	2 (1%)
1	w	184/196 (93%)	-0.24	8 (4%) 40 42	5, 9, 25, 60	3 (1%)
1	x	184/196 (93%)	-0.24	11 (5%) 27 27	5, 10, 27, 62	3 (1%)
1	y	184/196 (93%)	-0.20	11 (5%) 27 27	6, 9, 26, 58	2 (1%)
1	z	184/196 (93%)	-0.13	9 (4%) 35 36	6, 11, 27, 61	4 (2%)
All	All	11040/11760 (93%)	-0.17	564 (5%) 33 34	5, 11, 34, 65	181 (1%)

All (564) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	h	12	THR	7.7
1	e	12	THR	7.5
1	7	16	VAL	7.0
1	A	12	THR	6.9
1	S	12	THR	6.8
1	k	12	THR	6.6
1	j	12	THR	6.6
1	U	15	ALA	6.5
1	s	16	VAL	6.3
1	3	12	THR	6.2
1	x	12	THR	6.2
1	X	16	VAL	6.1
1	Z	14	ARG	6.1
1	u	16	VAL	6.0
1	r	13	MET	5.9
1	W	15	ALA	5.9
1	Z	13	MET	5.7
1	y	16	VAL	5.6
1	4	15	ALA	5.5
1	Z	12	THR	5.4
1	w	16	VAL	5.4
1	U	16	VAL	5.4
1	M	15	ALA	5.4
1	m	16	VAL	5.3
1	v	16	VAL	5.3
1	E	16	VAL	5.3
1	v	12	THR	5.3
1	2	12	THR	5.3
1	v	15	ALA	5.3
1	4	13	MET	5.2

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Mol	Chain	Res	Type	RSRZ
1	p	16	VAL	5.2
1	j	19	MET	5.1
1	X	12	THR	5.1
1	D	13	MET	5.1
1	p	13	MET	5.1
1	e	16	VAL	5.1
1	i	16	VAL	5.1
1	H	16	VAL	5.1
1	p	12	THR	5.0
1	w	12	THR	5.0
1	G	12	THR	5.0
1	D	15	ALA	5.0
1	u	13	MET	5.0
1	F	13	MET	5.0
1	6	12	THR	5.0
1	h	13	MET	5.0
1	v	13	MET	5.0
1	l	12	THR	4.9
1	C	12	THR	4.9
1	W	12	THR	4.9
1	h	16	VAL	4.9
1	6	15	ALA	4.9
1	L	12	THR	4.9
1	t	12	THR	4.9
1	K	12	THR	4.9
1	a	12	THR	4.9
1	g	13	MET	4.9
1	i	14	ARG	4.9
1	H	15	ALA	4.9
1	c	12	THR	4.9
1	I	16	VAL	4.9
1	J	13	MET	4.9
1	X	14	ARG	4.8
1	z	15	ALA	4.8
1	6	16	VAL	4.8
1	z	14	ARG	4.8
1	Y	12	THR	4.8
1	g	15	ALA	4.8
1	J	15	ALA	4.8
1	5	16	VAL	4.7
1	0	14	ARG	4.7
1	K	14	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
1	H	18	ARG	4.7
1	Q	15	ALA	4.7
1	c	15	ALA	4.7
1	4	14	ARG	4.7
1	5	13	MET	4.6
1	7	13	MET	4.6
1	I	13	MET	4.6
1	W	16	VAL	4.6
1	e	15	ALA	4.6
1	p	18	ARG	4.6
1	w	14	ARG	4.6
1	M	13	MET	4.6
1	6	18	ARG	4.5
1	e	19	MET	4.5
1	x	13	MET	4.5
1	A	15	ALA	4.5
1	D	16	VAL	4.5
1	f	12	THR	4.5
1	l	12	THR	4.5
1	n	12	THR	4.5
1	N	14	ARG	4.5
1	w	15	ALA	4.5
1	1	13	MET	4.5
1	T	12	THR	4.4
1	A	16	VAL	4.4
1	3	13	MET	4.4
1	x	15	ALA	4.4
1	K	15	ALA	4.4
1	f	16	VAL	4.4
1	M	16	VAL	4.4
1	Q	13	MET	4.4
1	e	13	MET	4.4
1	0	19	MET	4.4
1	i	12	THR	4.4
1	5	15	ALA	4.4
1	Q	12	THR	4.4
1	d	18	ARG	4.3
1	C	13	MET	4.3
1	B	15	ALA	4.3
1	o	12	THR	4.3
1	P	12	THR	4.3
1	N	18	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	e	14	ARG	4.2
1	M	12	THR	4.2
1	R	18	ARG	4.2
1	q	13	MET	4.2
1	s	13	MET	4.2
1	W	17	LYS	4.2
1	b	16	VAL	4.2
1	c	16	VAL	4.2
1	7	12	THR	4.1
1	L	16	VAL	4.1
1	f	15	ALA	4.1
1	o	15	ALA	4.1
1	N	15	ALA	4.1
1	r	12	THR	4.1
1	q	14	ARG	4.1
1	i	13	MET	4.1
1	S	18	ARG	4.0
1	T	13	MET	4.0
1	U	14	ARG	4.0
1	b	18	ARG	4.0
1	O	12	THR	4.0
1	b	13	MET	4.0
1	J	18	ARG	4.0
1	I	15	ALA	4.0
1	0	12	THR	4.0
1	W	13	MET	4.0
1	i	18	ARG	4.0
1	4	19	MET	4.0
1	b	15	ALA	4.0
1	I	12	THR	4.0
1	O	18	ARG	3.9
1	2	13	MET	3.9
1	3	14	ARG	3.9
1	B	18	ARG	3.9
1	d	14	ARG	3.9
1	s	12	THR	3.9
1	F	16	VAL	3.9
1	N	16	VAL	3.9
1	V	16	VAL	3.9
1	j	15	ALA	3.9
1	n	15	ALA	3.9
1	t	13	MET	3.9

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Mol	Chain	Res	Type	RSRZ
1	a	13	MET	3.9
1	S	14	ARG	3.9
1	B	12	THR	3.9
1	C	16	VAL	3.9
1	S	13	MET	3.9
1	X	13	MET	3.9
1	5	14	ARG	3.8
1	k	17	LYS	3.8
1	d	13	MET	3.8
1	m	12	THR	3.8
1	o	18	ARG	3.8
1	g	16	VAL	3.8
1	l	15	ALA	3.8
1	A	19	MET	3.8
1	L	13	MET	3.8
1	K	16	VAL	3.8
1	P	16	VAL	3.8
1	d	16	VAL	3.8
1	c	19	MET	3.8
1	g	12	THR	3.8
1	6	13	MET	3.8
1	H	13	MET	3.8
1	Z	19	MET	3.8
1	V	14	ARG	3.8
1	0	16	VAL	3.7
1	y	17	LYS	3.7
1	q	12	THR	3.7
1	h	19	MET	3.7
1	b	19	MET	3.7
1	j	14	ARG	3.7
1	X	18	ARG	3.7
1	u	15	ALA	3.7
1	M	17	LYS	3.7
1	2	14	ARG	3.7
1	R	13	MET	3.7
1	y	12	THR	3.7
1	D	12	THR	3.7
1	h	14	ARG	3.7
1	Y	19	MET	3.7
1	Q	20	ILE	3.7
1	r	16	VAL	3.7
1	u	12	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	z	12	THR	3.7
1	4	12	THR	3.7
1	m	13	MET	3.7
1	M	14	ARG	3.7
1	c	18	ARG	3.7
1	U	12	THR	3.6
1	d	12	THR	3.6
1	x	16	VAL	3.6
1	p	14	ARG	3.6
1	O	19	MET	3.6
1	7	15	ALA	3.6
1	s	22	THR	3.6
1	v	17	LYS	3.6
1	f	14	ARG	3.6
1	x	18	ARG	3.6
1	Q	18	ARG	3.6
1	Y	18	ARG	3.6
1	P	19	MET	3.6
1	j	16	VAL	3.6
1	G	16	VAL	3.6
1	t	15	ALA	3.6
1	X	15	ALA	3.6
1	E	14	ARG	3.6
1	7	19	MET	3.6
1	R	16	VAL	3.6
1	s	14	ARG	3.6
1	v	14	ARG	3.6
1	l	19	MET	3.6
1	L	15	ALA	3.6
1	j	21	ASN	3.5
1	z	18	ARG	3.5
1	6	14	ARG	3.5
1	M	20	ILE	3.5
1	Z	20	ILE	3.5
1	a	16	VAL	3.5
1	0	18	ARG	3.5
1	j	13	MET	3.5
1	m	21	ASN	3.5
1	F	21	ASN	3.5
1	N	13	MET	3.5
1	4	16	VAL	3.5
1	P	14	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	W	14	ARG	3.5
1	g	19	MET	3.5
1	y	13	MET	3.5
1	A	17	LYS	3.5
1	P	13	MET	3.5
1	D	18	ARG	3.5
1	m	19	MET	3.5
1	r	19	MET	3.5
1	h	15	ALA	3.5
1	l	22	THR	3.5
1	0	15	ALA	3.5
1	C	15	ALA	3.5
1	N	12	THR	3.5
1	V	15	ALA	3.5
1	C	14	ARG	3.4
1	J	19	MET	3.4
1	q	15	ALA	3.4
1	2	20	ILE	3.4
1	G	20	ILE	3.4
1	w	18	ARG	3.4
1	7	18	ARG	3.4
1	B	14	ARG	3.4
1	F	14	ARG	3.4
1	G	14	ARG	3.4
1	o	16	VAL	3.4
1	J	16	VAL	3.4
1	q	19	MET	3.4
1	2	19	MET	3.4
1	G	19	MET	3.4
1	p	15	ALA	3.4
1	g	17	LYS	3.3
1	T	16	VAL	3.3
1	n	18	ARG	3.3
1	r	18	ARG	3.3
1	t	18	ARG	3.3
1	b	14	ARG	3.3
1	I	17	LYS	3.3
1	i	15	ALA	3.3
1	m	15	ALA	3.3
1	R	15	ALA	3.3
1	Z	15	ALA	3.3
1	m	14	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	c	13	MET	3.3
1	S	16	VAL	3.3
1	A	14	ARG	3.3
1	d	15	ALA	3.3
1	f	13	MET	3.3
1	D	19	MET	3.3
1	O	13	MET	3.3
1	W	19	MET	3.3
1	5	12	THR	3.3
1	E	12	THR	3.3
1	x	195	ALA	3.3
1	7	14	ARG	3.2
1	V	18	ARG	3.2
1	J	12	THR	3.2
1	t	16	VAL	3.2
1	r	15	ALA	3.2
1	y	15	ALA	3.2
1	u	18	ARG	3.2
1	K	19	MET	3.2
1	N	19	MET	3.2
1	f	22	THR	3.2
1	3	22	THR	3.2
1	Q	22	THR	3.2
1	R	12	THR	3.2
1	x	20	ILE	3.2
1	Y	16	VAL	3.2
1	R	14	ARG	3.2
1	V	12	THR	3.2
1	x	14	ARG	3.2
1	M	18	ARG	3.2
1	W	18	ARG	3.2
1	U	13	MET	3.2
1	j	18	ARG	3.1
1	u	14	ARG	3.1
1	6	22	THR	3.1
1	b	12	THR	3.1
1	3	19	MET	3.1
1	M	19	MET	3.1
1	l	16	VAL	3.1
1	k	14	ARG	3.1
1	l	14	ARG	3.1
1	E	18	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	k	13	MET	3.1
1	l	13	MET	3.1
1	p	19	MET	3.1
1	z	13	MET	3.1
1	4	18	ARG	3.1
1	Q	14	ARG	3.1
1	a	18	ARG	3.1
1	E	20	ILE	3.1
1	S	15	ALA	3.1
1	a	19	MET	3.1
1	H	14	ARG	3.1
1	P	18	ARG	3.1
1	o	13	MET	3.1
1	y	20	ILE	3.1
1	F	12	THR	3.0
1	k	16	VAL	3.0
1	B	16	VAL	3.0
1	G	13	MET	3.0
1	l	14	ARG	3.0
1	t	14	ARG	3.0
1	L	18	ARG	3.0
1	a	14	ARG	3.0
1	1	15	ALA	3.0
1	1	195	ALA	3.0
1	Z	22	THR	3.0
1	6	17	LYS	3.0
1	1	16	VAL	3.0
1	J	14	ARG	3.0
1	H	12	THR	3.0
1	k	15	ALA	3.0
1	n	19	MET	3.0
1	0	13	MET	3.0
1	D	14	ARG	3.0
1	F	18	ARG	3.0
1	O	14	ARG	3.0
1	L	21	ASN	3.0
1	Z	17	LYS	3.0
1	5	19	MET	3.0
1	A	13	MET	3.0
1	L	19	MET	3.0
1	y	22	THR	3.0
1	a	15	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	m	20	ILE	2.9
1	n	13	MET	2.9
1	B	19	MET	2.9
1	K	13	MET	2.9
1	y	14	ARG	2.9
1	C	22	THR	2.9
1	G	15	ALA	2.9
1	3	17	LYS	2.9
1	V	13	MET	2.9
1	V	19	MET	2.9
1	m	195	ALA	2.9
1	g	18	ARG	2.9
1	y	18	ARG	2.9
1	T	18	ARG	2.9
1	q	22	THR	2.9
1	A	22	THR	2.9
1	n	17	LYS	2.9
1	z	19	MET	2.9
1	B	17	LYS	2.9
1	l	18	ARG	2.8
1	6	19	MET	2.8
1	F	19	MET	2.8
1	n	22	THR	2.8
1	q	17	LYS	2.8
1	q	18	ARG	2.8
1	I	22	THR	2.8
1	z	16	VAL	2.8
1	T	15	ALA	2.8
1	T	19	MET	2.8
1	A	18	ARG	2.8
1	C	19	MET	2.8
1	e	21	ASN	2.8
1	o	21	ASN	2.8
1	r	21	ASN	2.8
1	o	14	ARG	2.8
1	k	19	MET	2.7
1	y	19	MET	2.7
1	g	14	ARG	2.7
1	i	20	ILE	2.7
1	a	20	ILE	2.7
1	l	17	LYS	2.7
1	E	19	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	22	THR	2.7
1	H	20	ILE	2.7
1	Q	19	MET	2.7
1	k	18	ARG	2.7
1	5	18	ARG	2.7
1	3	16	VAL	2.7
1	t	19	MET	2.7
1	S	19	MET	2.7
1	7	20	ILE	2.7
1	Y	15	ALA	2.6
1	o	33	ASN	2.6
1	B	22	THR	2.6
1	r	14	ARG	2.6
1	j	17	LYS	2.6
1	X	17	LYS	2.6
1	n	146	ILE	2.6
1	2	146	ILE	2.6
1	d	20	ILE	2.6
1	g	195	ALA	2.6
1	F	15	ALA	2.6
1	W	195	ALA	2.6
1	o	19	MET	2.6
1	I	18	ARG	2.6
1	L	14	ARG	2.6
1	Z	16	VAL	2.6
1	w	19	MET	2.6
1	y	195	ALA	2.6
1	6	20	ILE	2.6
1	C	20	ILE	2.6
1	D	20	ILE	2.6
1	I	19	MET	2.6
1	U	22	THR	2.6
1	l	19	MET	2.6
1	w	13	MET	2.6
1	E	13	MET	2.6
1	X	19	MET	2.6
1	s	18	ARG	2.5
1	T	14	ARG	2.5
1	U	18	ARG	2.5
1	Q	16	VAL	2.5
1	e	17	LYS	2.5
1	a	17	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	s	15	ALA	2.5
1	2	17	LYS	2.5
1	u	21	ASN	2.5
1	C	18	ARG	2.5
1	Y	14	ARG	2.5
1	g	20	ILE	2.5
1	v	20	ILE	2.5
1	X	146	ILE	2.5
1	4	17	LYS	2.5
1	l	45	GLN	2.5
1	e	18	ARG	2.5
1	B	13	MET	2.5
1	r	22	THR	2.5
1	M	22	THR	2.5
1	H	195	ALA	2.4
1	O	20	ILE	2.4
1	1	18	ARG	2.4
1	n	21	ASN	2.4
1	q	16	VAL	2.4
1	N	195	ALA	2.4
1	L	17	LYS	2.4
1	K	18	ARG	2.4
1	u	22	THR	2.4
1	m	18	ARG	2.4
1	P	15	ALA	2.4
1	2	16	VAL	2.4
1	d	21	ASN	2.4
1	l	20	ILE	2.4
1	D	22	THR	2.4
1	c	14	ARG	2.4
1	d	22	THR	2.4
1	v	19	MET	2.4
1	v	195	ALA	2.3
1	b	195	ALA	2.3
1	G	18	ARG	2.3
1	I	14	ARG	2.3
1	Y	17	LYS	2.3
1	u	19	MET	2.3
1	Y	22	THR	2.3
1	l	20	ILE	2.3
1	b	20	ILE	2.3
1	K	195	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	195	ALA	2.3
1	i	66	ARG	2.3
1	f	19	MET	2.3
1	O	16	VAL	2.3
1	a	22	THR	2.3
1	B	21	ASN	2.3
1	Z	146	ILE	2.3
1	0	17	LYS	2.3
1	i	19	MET	2.3
1	x	19	MET	2.3
1	6	195	ALA	2.3
1	E	15	ALA	2.3
1	Y	13	MET	2.3
1	o	22	THR	2.3
1	x	22	THR	2.3
1	2	22[A]	THR	2.3
1	b	22	THR	2.3
1	2	18	ARG	2.3
1	s	19	MET	2.3
1	H	19	MET	2.3
1	U	19	MET	2.3
1	q	20	ILE	2.3
1	h	195	ALA	2.2
1	2	15	ALA	2.2
1	O	15	ALA	2.2
1	l	17	LYS	2.2
1	J	17	LYS	2.2
1	0	146	ILE	2.2
1	f	21	ASN	2.2
1	w	17	LYS	2.2
1	N	17	LYS	2.2
1	n	16	VAL	2.2
1	q	21	ASN	2.2
1	3	18	ARG	2.2
1	G	21	ASN	2.2
1	I	21	ASN	2.2
1	f	20	ILE	2.2
1	g	146	ILE	2.2
1	B	20	ILE	2.2
1	e	22	THR	2.2
1	t	22	THR	2.2
1	E	22	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	Z	18	ARG	2.2
1	A	21	ASN	2.2
1	Y	148[A]	ASN	2.2
1	5	17	LYS	2.2
1	A	20	ILE	2.1
1	Y	20	ILE	2.1
1	z	22	THR	2.1
1	h	18	ARG	2.1
1	P	17	LYS	2.1
1	v	18	ARG	2.1
1	K	22	THR	2.1
1	0	20	ILE	2.1
1	0	21	ASN	2.1
1	7	181	VAL	2.1
1	t	195	ALA	2.1
1	W	22	THR	2.1
1	x	146	ILE	2.1
1	3	146	ILE	2.1
1	J	20	ILE	2.1
1	t	17	LYS	2.0
1	G	17	LYS	2.0
1	r	23	HIS	2.0
1	e	20	ILE	2.0
1	z	20	ILE	2.0
1	d	19	MET	2.0
1	Z	21	ASN	2.0
1	o	17	LYS	2.0
1	Q	17	LYS	2.0
1	m	145	ARG	2.0
1	X	22	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	N	202	1/1	0.97	0.05	10,10,10,10	0
2	CA	E	202	1/1	0.98	0.04	9,9,9,9	0
2	CA	N	201	1/1	0.98	0.03	11,11,11,11	0
2	CA	A	202	1/1	0.98	0.06	9,9,9,9	0
2	CA	n	202	1/1	0.99	0.03	11,11,11,11	0
2	CA	q	202	1/1	0.99	0.03	10,10,10,10	0
2	CA	x	201	1/1	0.99	0.01	8,8,8,8	0
2	CA	z	201	1/1	0.99	0.02	9,9,9,9	0
2	CA	0	201	1/1	0.99	0.04	8,8,8,8	0
2	CA	0	202	1/1	0.99	0.02	8,8,8,8	0
2	CA	1	202	1/1	0.99	0.05	8,8,8,8	0
2	CA	2	202	1/1	0.99	0.02	9,9,9,9	0
2	CA	3	202	1/1	0.99	0.04	9,9,9,9	0
2	CA	4	202	1/1	0.99	0.04	8,8,8,8	0
2	CA	5	201	1/1	0.99	0.02	10,10,10,10	0
2	CA	5	202	1/1	0.99	0.04	9,9,9,9	0
2	CA	6	202	1/1	0.99	0.06	9,9,9,9	0
2	CA	g	201	1/1	0.99	0.02	8,8,8,8	0
2	CA	B	203	1/1	0.99	0.07	9,9,9,9	0
2	CA	i	201	1/1	0.99	0.01	8,8,8,8	0
2	CA	E	203	1/1	0.99	0.03	11,11,11,11	0
2	CA	G	201	1/1	0.99	0.02	10,10,10,10	0
2	CA	G	202	1/1	0.99	0.04	12,12,12,12	0
2	CA	G	203	1/1	0.99	0.04	9,9,9,9	0
2	CA	I	201	1/1	0.99	0.06	10,10,10,10	0
2	CA	K	201	1/1	0.99	0.02	9,9,9,9	0
2	CA	M	201	1/1	0.99	0.02	9,9,9,9	0
2	CA	i	202	1/1	0.99	0.02	11,11,11,11	0
2	CA	m	201	1/1	0.99	0.02	11,11,11,11	0
2	CA	P	201	1/1	0.99	0.03	10,10,10,10	0
2	CA	Q	202	1/1	0.99	0.04	8,8,8,8	0
2	CA	R	201	1/1	0.99	0.03	8,8,8,8	0
2	CA	S	201	1/1	0.99	0.01	9,9,9,9	0
2	CA	S	202	1/1	0.99	0.07	8,8,8,8	0
2	CA	T	202	1/1	0.99	0.06	7,7,7,7	0
2	CA	U	203	1/1	0.99	0.07	8,8,8,8	0
2	CA	V	201	1/1	0.99	0.03	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	W	201	1/1	0.99	0.02	10,10,10,10	0
2	CA	Z	201	1/1	0.99	0.02	8,8,8,8	0
2	CA	b	201	1/1	0.99	0.02	9,9,9,9	0
2	CA	b	202	1/1	0.99	0.04	8,8,8,8	0
2	CA	q	201	1/1	1.00	0.01	7,7,7,7	0
2	CA	7	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	A	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	e	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	B	201	1/1	1.00	0.01	10,10,10,10	0
2	CA	B	202	1/1	1.00	0.03	10,10,10,10	0
2	CA	r	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	C	201	1/1	1.00	0.02	10,10,10,10	0
2	CA	D	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	E	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	s	201	1/1	1.00	0.02	8,8,8,8	0
2	CA	t	201	1/1	1.00	0.01	10,10,10,10	0
2	CA	F	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	u	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	v	201	1/1	1.00	0.01	8,8,8,8	0
2	CA	w	201	1/1	1.00	0.01	8,8,8,8	0
2	CA	H	201	1/1	1.00	0.01	10,10,10,10	0
2	CA	j	201	1/1	1.00	0.01	8,8,8,8	0
2	CA	I	202	1/1	1.00	0.01	10,10,10,10	0
2	CA	J	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	y	201	1/1	1.00	0.01	8,8,8,8	0
2	CA	K	202	1/1	1.00	0.01	9,9,9,9	0
2	CA	L	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	j	202	1/1	1.00	0.05	8,8,8,8	0
2	CA	k	201	1/1	1.00	0.01	8,8,8,8	0
2	CA	l	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	O	201	1/1	1.00	0.01	10,10,10,10	0
2	CA	1	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	Q	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	h	201	1/1	1.00	0.01	8,8,8,8	0
2	CA	1	203	1/1	1.00	0.03	10,10,10,10	0
2	CA	R	202	1/1	1.00	0.01	8,8,8,8	0
2	CA	2	201	1/1	1.00	0.04	10,10,10,10	0
2	CA	n	201	1/1	1.00	0.03	11,11,11,11	0
2	CA	T	201	1/1	1.00	0.01	8,8,8,8	0
2	CA	3	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	U	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	U	202	1/1	1.00	0.01	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	f	201	1/1	1.00	0.01	10,10,10,10	0
2	CA	4	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	V	202	1/1	1.00	0.01	8,8,8,8	0
2	CA	o	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	X	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	Y	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	o	202	1/1	1.00	0.03	12,12,12,12	0
2	CA	a	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	p	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	6	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	c	201	1/1	1.00	0.01	7,7,7,7	0
2	CA	c	202	1/1	1.00	0.02	10,10,10,10	0
2	CA	d	201	1/1	1.00	0.02	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.