



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:52 AM UTC

PDB ID : 8TUX / pdb_00008tux
EMDB ID : EMD-41632
Title : Capsid of mature PP7 virion with 3'end region of PP7 genomic RNA
Authors : Thongchol, J.; Zhang, J.; Zeng, L.
Deposited on : 2023-08-17
Resolution : 3.90 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

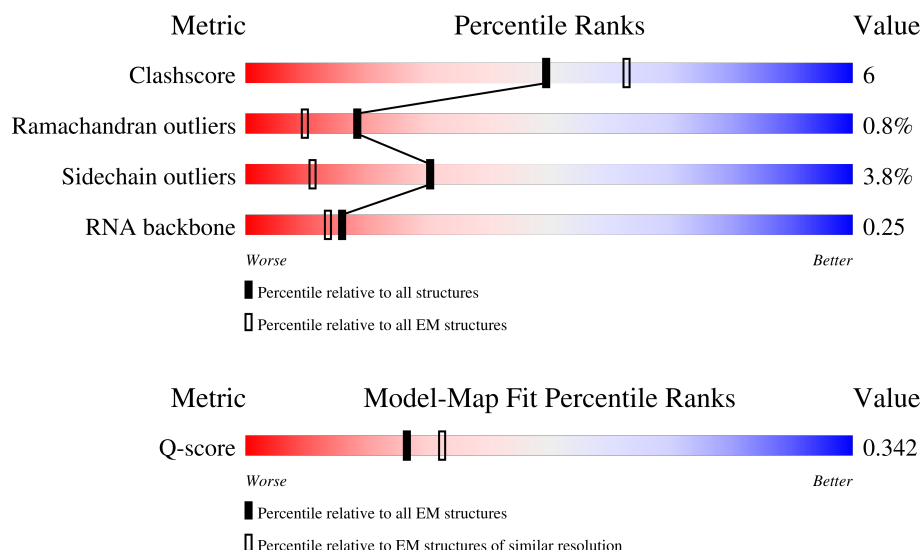
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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



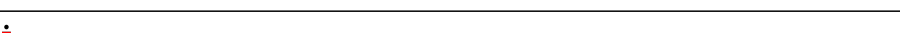
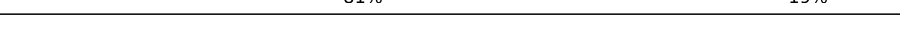
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8855 (3.40 - 4.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	95	
2	M	448	
2	m	448	

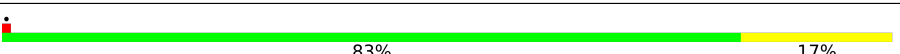
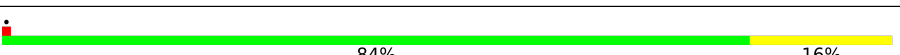
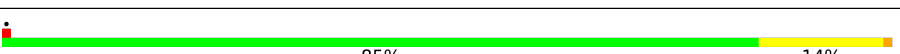
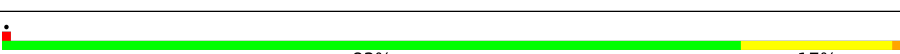
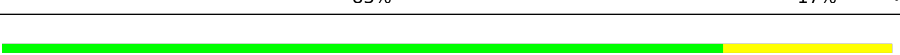
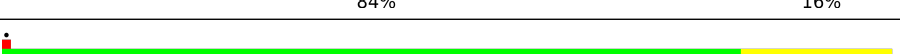
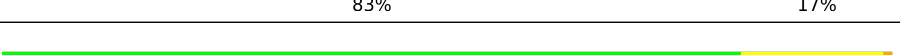
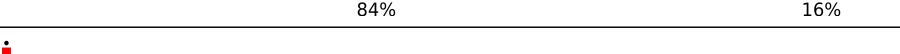
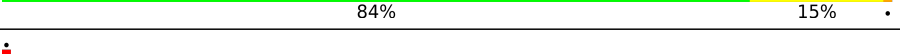
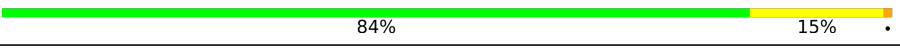
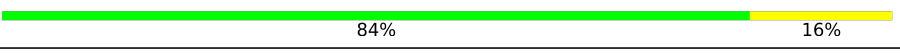
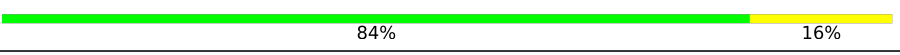
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Mol	Chain	Length	Quality of chain
3	01	127	
3	02	127	
3	11	127	
3	12	127	
3	21	127	
3	22	127	
3	2A	127	
3	2B	127	
3	2C	127	
3	2D	127	
3	2E	127	
3	2F	127	
3	2G	127	
3	2H	127	
3	2I	127	
3	2J	127	
3	2K	127	
3	2L	127	
3	2M	127	
3	2N	127	
3	2O	127	
3	2P	127	
3	2Q	127	
3	2R	127	
3	2S	127	

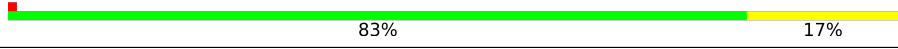
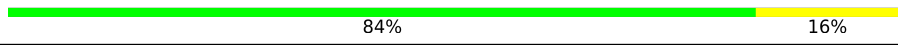
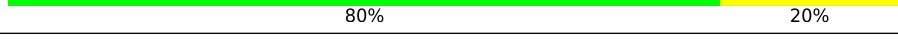
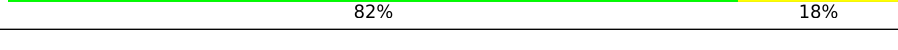
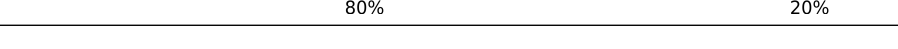
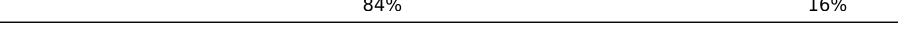
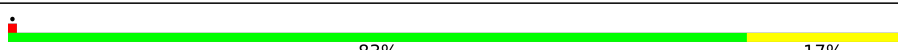
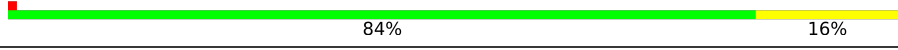
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Mol	Chain	Length	Quality of chain
3	2T	127	
3	2U	127	
3	2V	127	
3	2W	127	
3	2X	127	
3	2Y	127	
3	2Z	127	
3	2a	127	
3	2b	127	
3	2c	127	
3	2d	127	
3	2e	127	
3	2f	127	
3	2g	127	
3	2h	127	
3	2i	127	
3	2j	127	
3	2k	127	
3	2l	127	
3	2m	127	
3	2n	127	
3	2o	127	
3	2p	127	
3	2q	127	
3	2r	127	

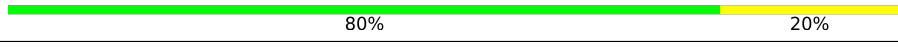
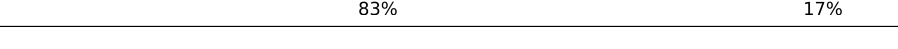
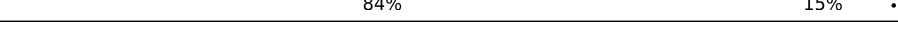
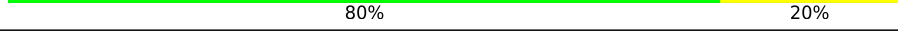
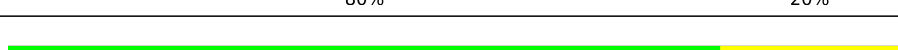
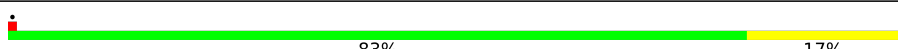
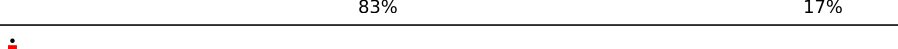
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Mol	Chain	Length	Quality of chain
3	2s	127	
3	2t	127	
3	2u	127	
3	2v	127	
3	2w	127	
3	2x	127	
3	2y	127	
3	2z	127	
3	31	127	
3	32	127	
3	41	127	
3	42	127	
3	51	127	
3	52	127	
3	61	127	
3	62	127	
3	71	127	
3	72	127	
3	82	127	
3	92	127	
3	A1	127	
3	A2	127	
3	B1	127	
3	B2	127	
3	C1	127	

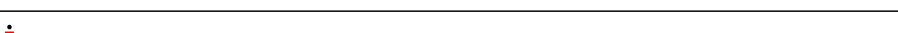
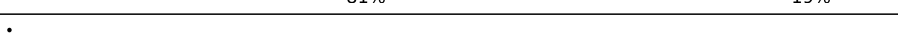
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Mol	Chain	Length	Quality of chain
3	C2	127	
3	D1	127	
3	D2	127	
3	E1	127	
3	E2	127	
3	F1	127	
3	F2	127	
3	G1	127	
3	G2	127	
3	H1	127	
3	H2	127	
3	I1	127	
3	I2	127	
3	J1	127	
3	J2	127	
3	K1	127	
3	K2	127	
3	L1	127	
3	L2	127	
3	M1	127	
3	M2	127	
3	N1	127	
3	N2	127	
3	O1	127	
3	O2	127	

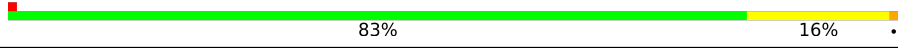
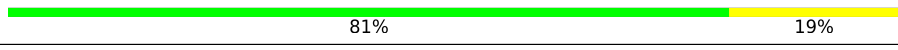
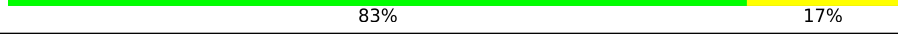
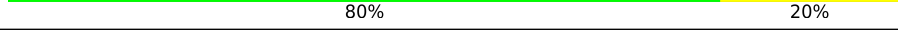
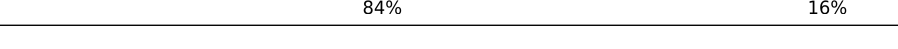
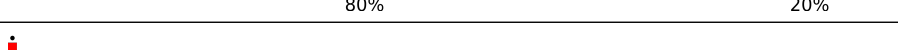
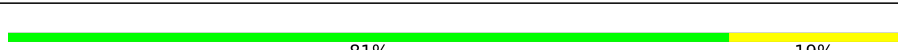
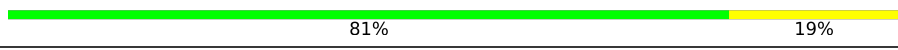
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Mol	Chain	Length	Quality of chain
3	P1	127	 80% 19%
3	P2	127	 82% 18%
3	Q1	127	 80% 20%
3	Q2	127	 84% 16%
3	R1	127	 82% 17%
3	R2	127	 84% 16%
3	S1	127	 81% 19%
3	S2	127	 84% 16%
3	T1	127	 79% 21%
3	T2	127	 83% 17%
3	U1	127	 80% 20%
3	U2	127	 83% 17%
3	V1	127	 80% 20%
3	V2	127	 84% 15%
3	W1	127	 81% 19%
3	W2	127	 83% 17%
3	X1	127	 80% 20%
3	X2	127	 83% 17%
3	Y1	127	 80% 20%
3	Y2	127	 84% 16%
3	Z1	127	 80% 19%
3	Z2	127	 84% 16%
3	a1	127	 80% 20%
3	a2	127	 84% 16%
3	aa	127	 82% 18%

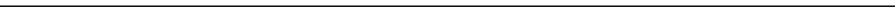
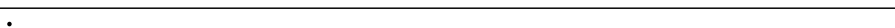
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Mol	Chain	Length	Quality of chain
3	ab	127	
3	ac	127	
3	ad	127	
3	b1	127	
3	b2	127	
3	c1	127	
3	c2	127	
3	d1	127	
3	d2	127	
3	e1	127	
3	e2	127	
3	f1	127	
3	f2	127	
3	g1	127	
3	g2	127	
3	h1	127	
3	h2	127	
3	i1	127	
3	i2	127	
3	j1	127	
3	j2	127	
3	k1	127	
3	k2	127	
3	l1	127	
3	l2	127	

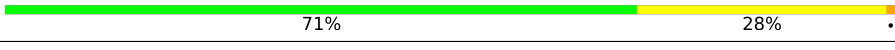
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Mol	Chain	Length	Quality of chain
3	m1	127	 82% 18%
3	m2	127	 80% 19% .
3	n1	127	 80% 20%
3	n2	127	 81% 18% .
3	o1	127	 80% 20%
3	o2	127	 83% 17%
3	p1	127	 81% 18% .
3	p2	127	 84% 16%
3	q1	127	 80% 19% .
3	q2	127	 81% 19%
3	r1	127	 80% 20%
3	r2	127	 84% 16%
3	s1	127	 82% 18%
3	s2	127	 83% 17%
3	t1	127	 80% 20%
3	t2	127	 81% 19%
3	u1	127	 81% 19%
3	u2	127	 83% 17%
3	v1	127	 82% 18%
3	v2	127	 84% 16%
3	w1	127	 80% 20%
3	w2	127	 84% 16%
3	x1	127	 82% 18%
3	x2	127	 84% 16%
3	y1	127	 80% 20%

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Mol	Chain	Length	Quality of chain
3	y2	127	
3	z1	127	
3	z2	127	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 188513 atoms, of which 7038 are hydrogens and 0 are deuteriums.

In the tables below, 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 RNA chain called 3'end of PP7 genomic RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	95	Total	C	N	O	P	0	0
			2011	899	353	665	94		

- Molecule 2 is a protein called Maturation protein A.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	m	448	Total	C	H	N	O	S	0	0
			7063	2275	3483	643	650	12		
2	M	448	Total	C	H	N	O	S	0	0
			7135	2275	3555	643	650	12		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	349	GLN	ARG	variant	UNP Q38061
m	360	CYS	SER	variant	UNP Q38061
M	349	GLN	ARG	variant	UNP Q38061
M	360	CYS	SER	variant	UNP Q38061

- Molecule 3 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a1	127	Total	C	N	O	S	0	0
			968	602	171	193	2		
3	b1	127	Total	C	N	O	S	0	0
			968	602	171	193	2		
3	c1	127	Total	C	N	O	S	0	0
			968	602	171	193	2		
3	d1	127	Total	C	N	O	S	0	0
			968	602	171	193	2		
3	e1	127	Total	C	N	O	S	0	0
			968	602	171	193	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	f1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	g1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	h1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	i1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	j1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	k1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	l1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	m1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	n1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	o1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	p1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	q1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	r1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	s1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	t1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	u1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	v1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	w1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	x1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	y1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	z1	127	Total 968	C 602	N 171	O 193	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	A1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	B1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	C1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	D1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	E1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	F1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	G1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	H1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	I1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	J1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	K1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	L1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	M1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	N1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	O1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	P1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	Q1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	R1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	S1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	T1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	U1	127	Total 968	C 602	N 171	O 193	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	V1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	W1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	X1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	Y1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	Z1	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	01	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	11	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	21	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	31	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	41	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	51	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	61	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	71	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	A2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	B2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	C2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	D2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	E2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	F2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	G2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	H2	127	Total 968	C 602	N 171	O 193	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	I2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	J2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	K2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	L2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	M2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	N2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	O2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	P2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	Q2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	R2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	S2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	T2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	U2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	V2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	W2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	X2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	Y2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	Z2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	a2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	b2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	c2	127	Total 968	C 602	N 171	O 193	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	d2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	e2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	f2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	g2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	h2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	i2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	j2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	k2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	l2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	m2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	n2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	o2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	p2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	q2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	r2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	s2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	t2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	u2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	v2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	w2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	x2	127	Total 968	C 602	N 171	O 193	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	y2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	z2	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	02	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	12	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	22	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	32	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	42	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	52	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	62	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	72	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	82	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	92	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2a	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2b	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2c	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2d	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2e	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2f	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2g	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2h	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2i	127	Total 968	C 602	N 171	O 193	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	2j	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2k	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2l	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2m	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2n	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2o	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2p	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2q	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2r	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2s	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2t	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2u	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2v	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2w	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2x	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2y	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2z	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2A	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2B	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2C	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2D	127	Total 968	C 602	N 171	O 193	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	2E	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2F	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2G	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2H	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2I	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2J	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2K	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2L	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2M	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2N	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2O	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2P	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2Q	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2R	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2S	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2T	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2U	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2V	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2W	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2X	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	2Y	127	Total 968	C 602	N 171	O 193	S 2	0	0

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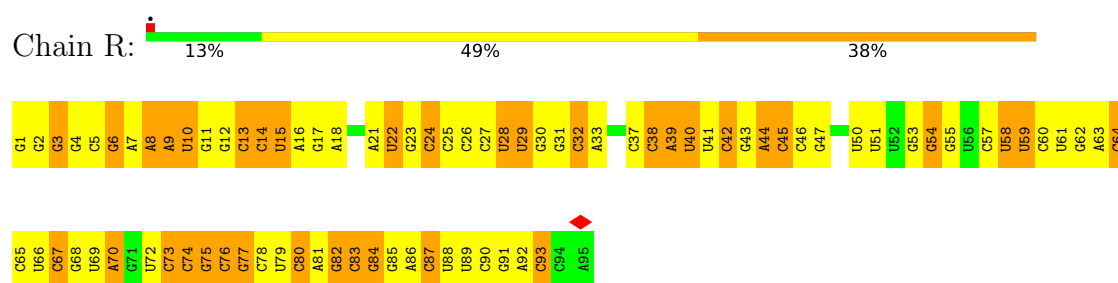
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Mol	Chain	Residues	Atoms					AltConf	Trace
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3	aa	127	Total 968	C 602	N 171	O 193	S 2	0	0
3	ab	127	Total 968	C 602	N 171	O 193	S 2	0	0
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3	ad	127	Total 968	C 602	N 171	O 193	S 2	0	0

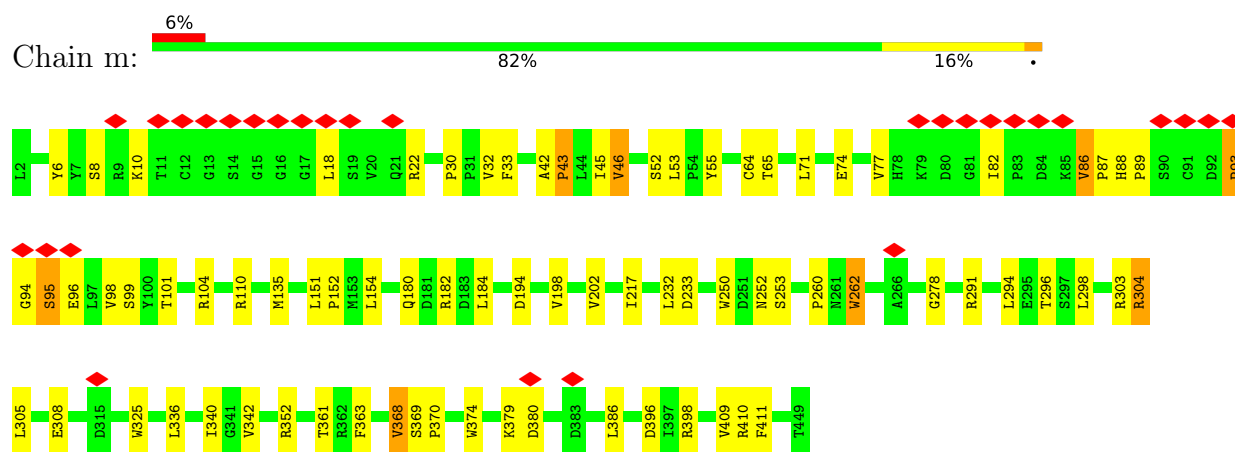
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

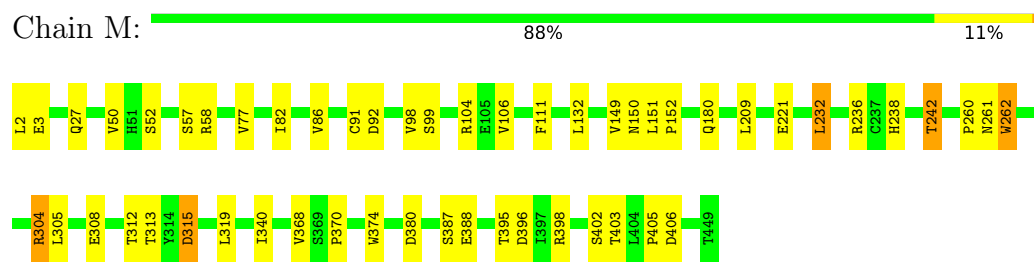
- Molecule 1: 3'end of PP7 genomic RNA



- Molecule 2: Maturation protein A

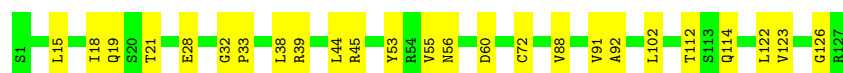


- Molecule 2: Maturation protein A



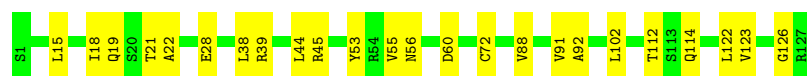
- Molecule 3: Capsid protein

Chain a1:  80% 20%



• Molecule 3: Capsid protein

Chain b1:  81% 19%



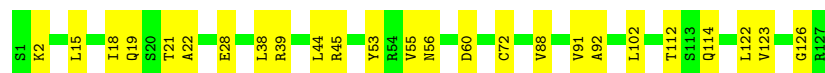
• Molecule 3: Capsid protein

Chain c1:  80% 20%



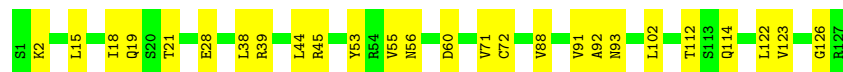
• Molecule 3: Capsid protein

Chain d1:  80% 20%



• Molecule 3: Capsid protein

Chain e1:  80% 20%



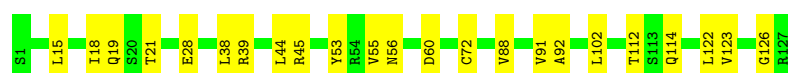
• Molecule 3: Capsid protein

Chain f1:  81% 18%



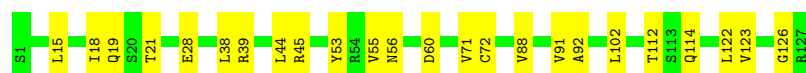
• Molecule 3: Capsid protein

Chain g1:  82% 18%



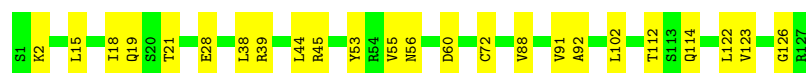
• Molecule 3: Capsid protein

Chain h1:  81% 19%



• Molecule 3: Capsid protein

Chain i1:  81% 19%



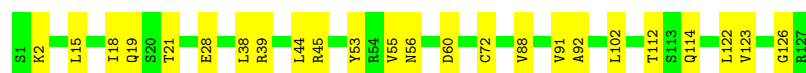
• Molecule 3: Capsid protein

Chain j1:  79% 21%



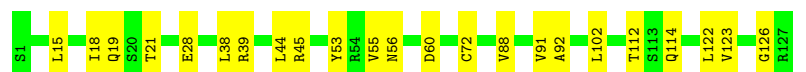
• Molecule 3: Capsid protein

Chain k1:  81% 19%



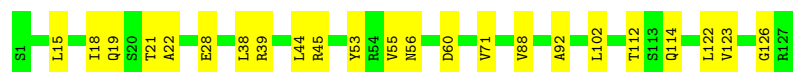
• Molecule 3: Capsid protein

Chain l1:  82% 18%



• Molecule 3: Capsid protein

Chain m1:  82% 18%



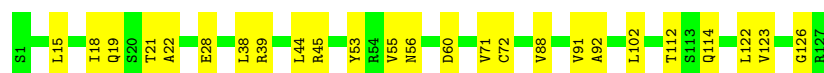
• Molecule 3: Capsid protein

Chain n1:  80% 20%



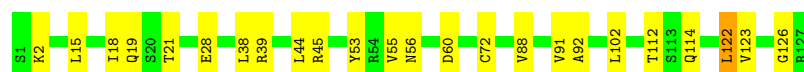
• Molecule 3: Capsid protein

Chain o1:  80% 20%



• Molecule 3: Capsid protein

Chain p1:  81% 18%



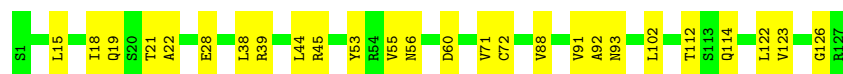
• Molecule 3: Capsid protein

Chain q1:  80% 19%



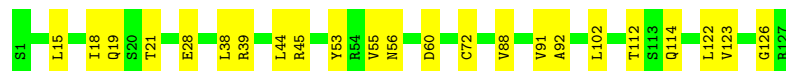
• Molecule 3: Capsid protein

Chain r1:  80% 20%



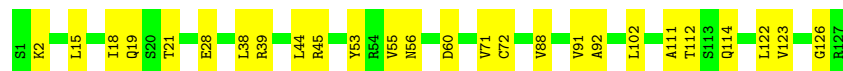
• Molecule 3: Capsid protein

Chain s1:  82% 18%



• Molecule 3: Capsid protein

Chain t1:  80% 20%



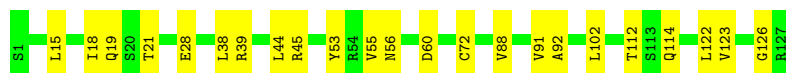
• Molecule 3: Capsid protein

Chain u1:  81% 19%



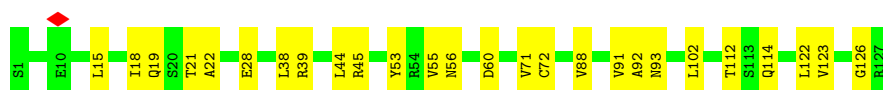
• Molecule 3: Capsid protein

Chain v1:  82% 18%



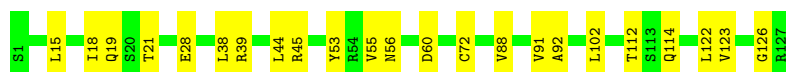
- Molecule 3: Capsid protein

Chain w1:  80% 20%



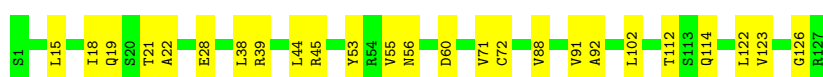
- Molecule 3: Capsid protein

Chain x1:  82% 18%



- Molecule 3: Capsid protein

Chain y1:  80% 20%



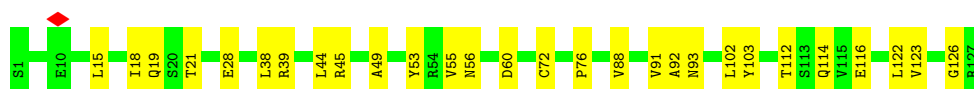
- Molecule 3: Capsid protein

Chain z1:  71% 28%



- Molecule 3: Capsid protein

Chain A1:  78% 22%

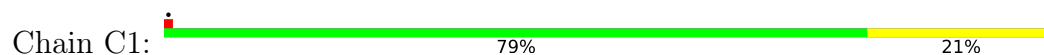


- Molecule 3: Capsid protein

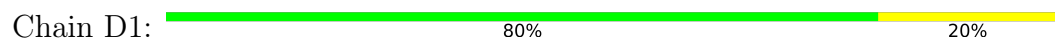
Chain B1:  80% 20%



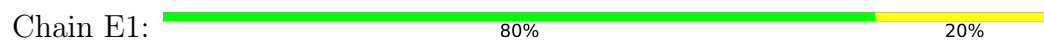
- Molecule 3: Capsid protein



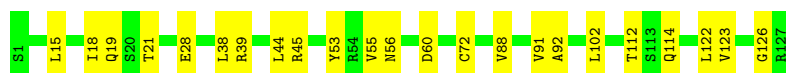
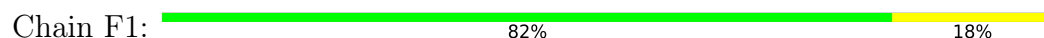
- Molecule 3: Capsid protein



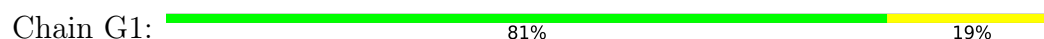
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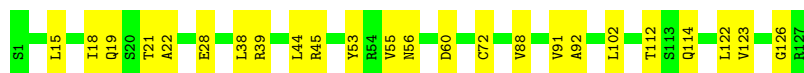
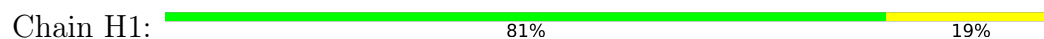
- Molecule 3: Capsid protein



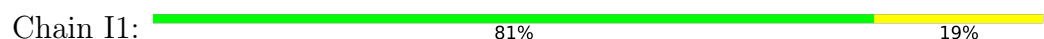
- Molecule 3: Capsid protein

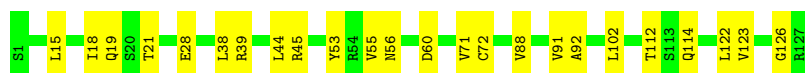


- Molecule 3: Capsid protein

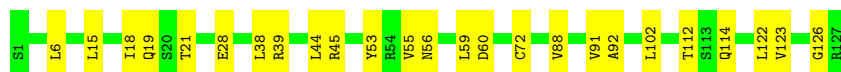
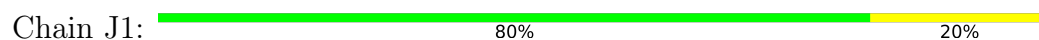


- Molecule 3: Capsid protein

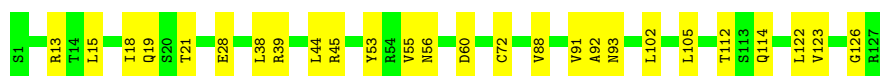
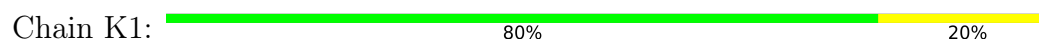




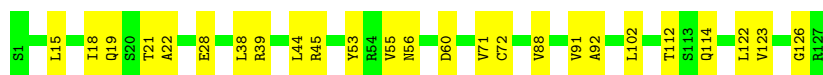
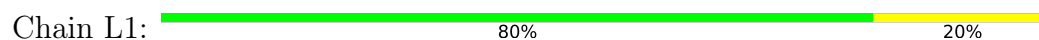
- Molecule 3: Capsid protein



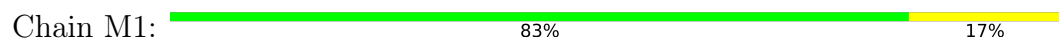
- Molecule 3: Capsid protein



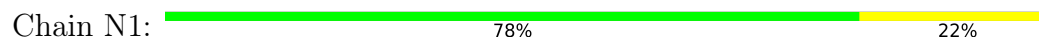
- Molecule 3: Capsid protein



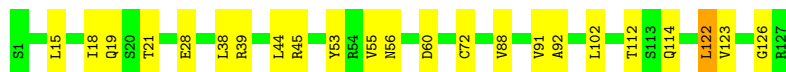
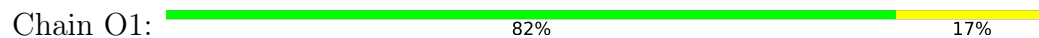
- Molecule 3: Capsid protein



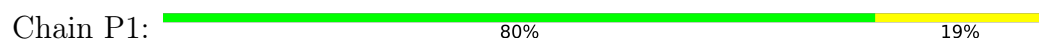
- Molecule 3: Capsid protein

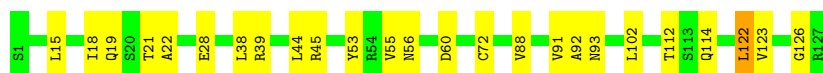


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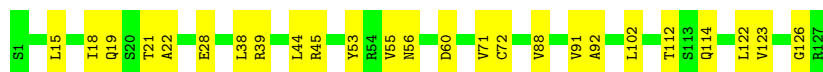
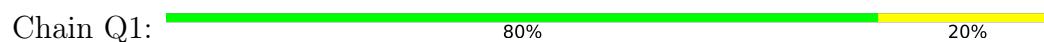


- Molecule 3: Capsid protein

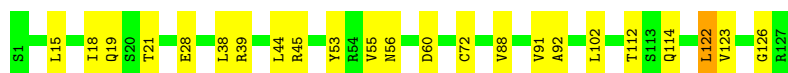
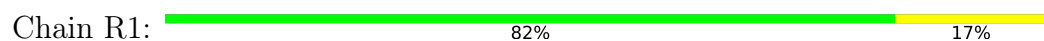




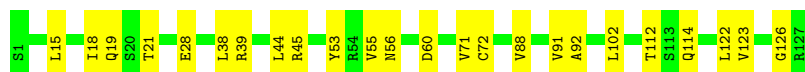
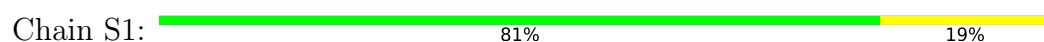
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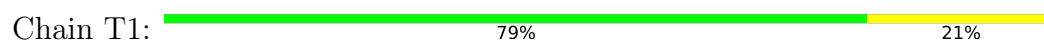
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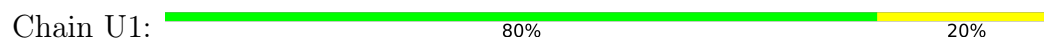
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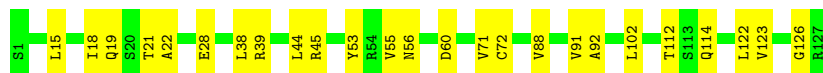
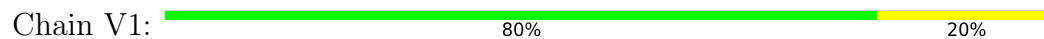
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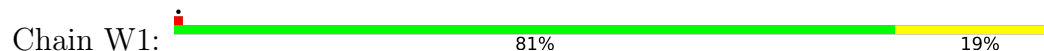
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- Molecule 3: Capsid protein

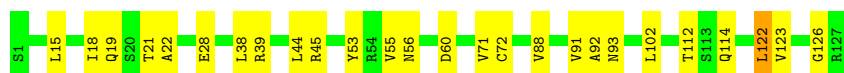
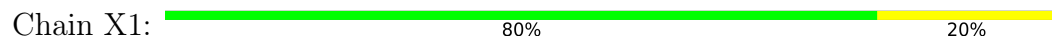


- Molecule 3: Capsid protein

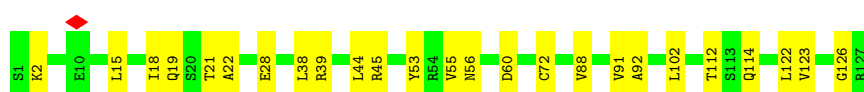
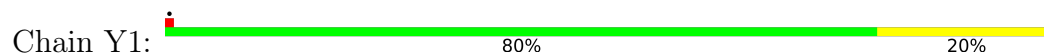




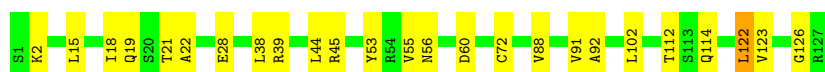
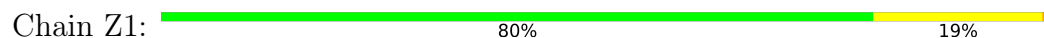
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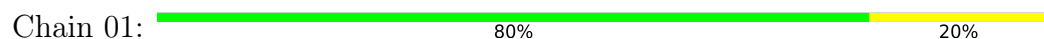
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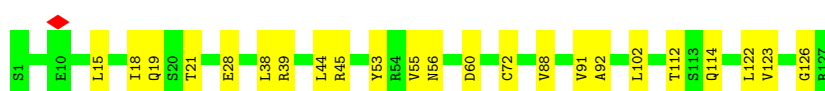
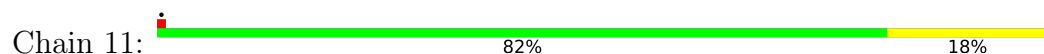
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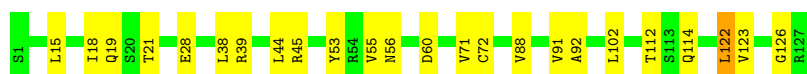
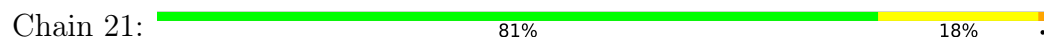
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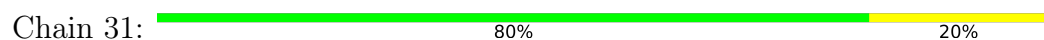
- Molecule 3: Capsid protein

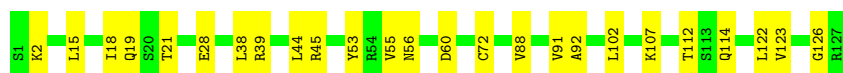


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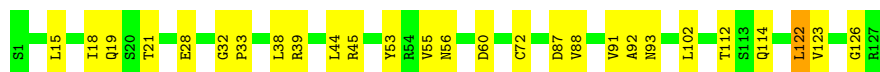
- Molecule 3: Capsid protein





- Molecule 3: Capsid protein

Chain 41: 79% 20%



- Molecule 3: Capsid protein

Chain 51: 81% 18%



- Molecule 3: Capsid protein

Chain 61: 73% 26%



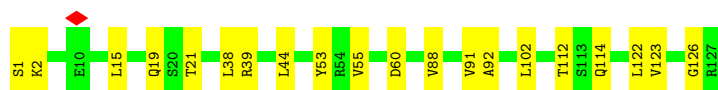
- Molecule 3: Capsid protein

Chain 71: 69% 31%



- Molecule 3: Capsid protein

Chain A2: 84% 16%



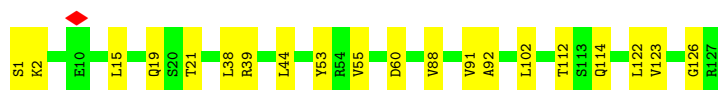
- Molecule 3: Capsid protein

Chain B2: 84% 16%



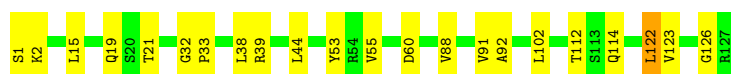
● Molecule 3: Capsid protein

Chain C2:  84% 16%



● Molecule 3: Capsid protein

Chain D2:  83% 17%



● Molecule 3: Capsid protein

Chain E2:  83% 17%



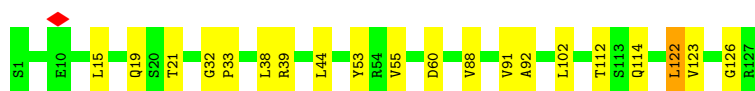
● Molecule 3: Capsid protein

Chain F2:  84% 16%



● Molecule 3: Capsid protein

Chain G2:  84% 15%



● Molecule 3: Capsid protein

Chain H2:  83% 17%



● Molecule 3: Capsid protein

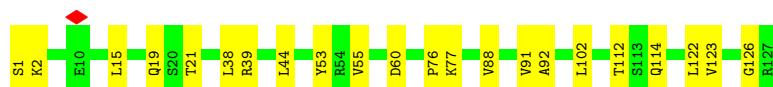
Chain I2:  75% 24%



● Molecule 3: Capsid protein

Chain J2:  80% 20%

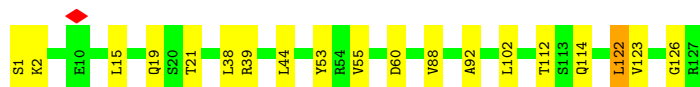
● Molecule 3: Capsid protein

Chain K2:  83% 17%

● Molecule 3: Capsid protein

Chain L2:  84% 16%

● Molecule 3: Capsid protein

Chain M2:  85% 14%

● Molecule 3: Capsid protein

Chain N2:  83% 17%

● Molecule 3: Capsid protein

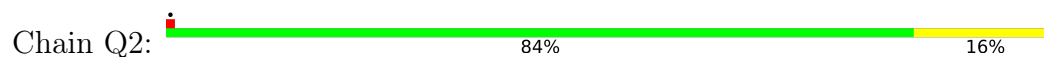
Chain O2:  83% 17%

● Molecule 3: Capsid protein

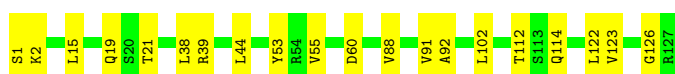
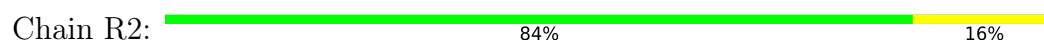
Chain P2:  82% 18%



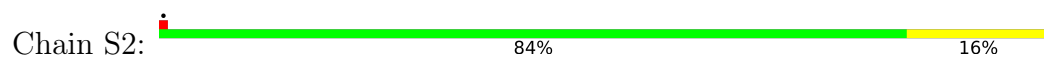
- Molecule 3: Capsid protein



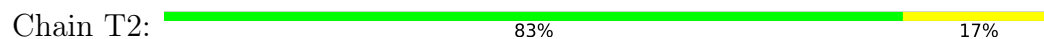
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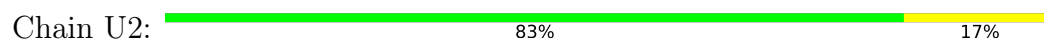
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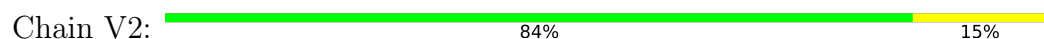
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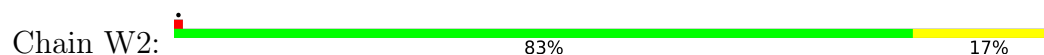
- Molecule 3: Capsid protein



- Molecule 3: Capsid protein

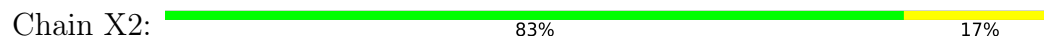


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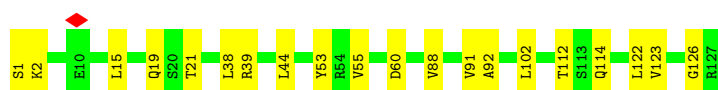
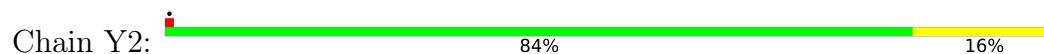




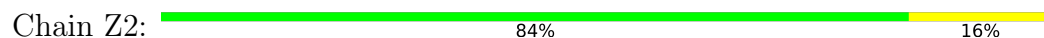
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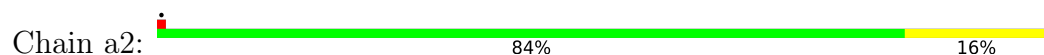
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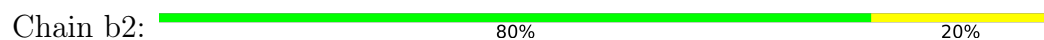
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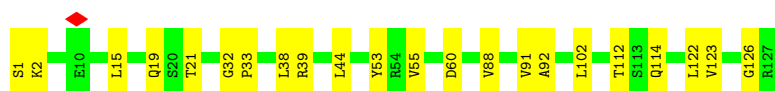
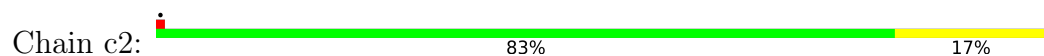
- Molecule 3: Capsid protein



- Molecule 3: Capsid protein



- Molecule 3: Capsid protein



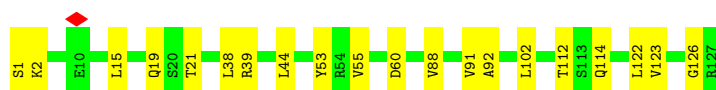
- Molecule 3: Capsid protein

Chain d2:  84% 16%



• Molecule 3: Capsid protein

Chain e2:  84% 16%



• Molecule 3: Capsid protein

Chain f2:  81% 19%



• Molecule 3: Capsid protein

Chain g2:  84% 16%



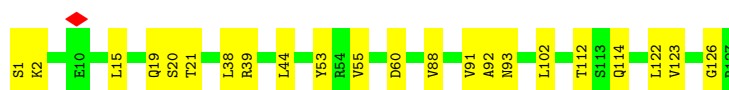
• Molecule 3: Capsid protein

Chain h2:  83% 17%



• Molecule 3: Capsid protein

Chain i2:  83% 17%

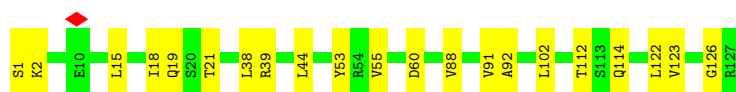
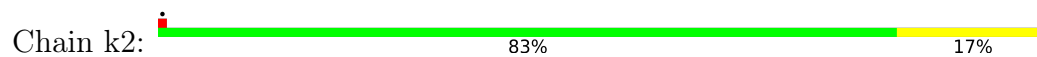


• Molecule 3: Capsid protein

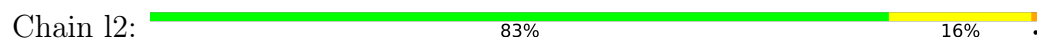
Chain j2:  84% 15%



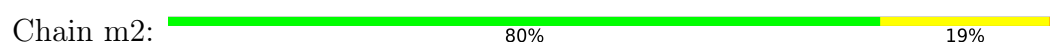
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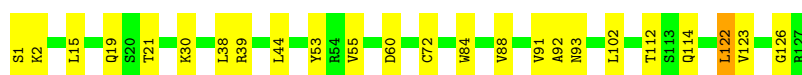
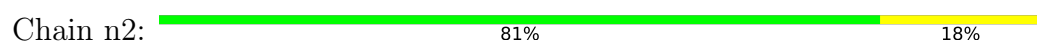
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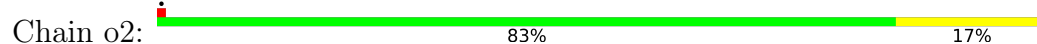
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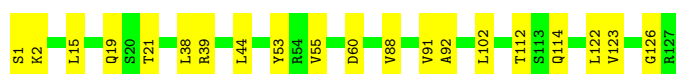
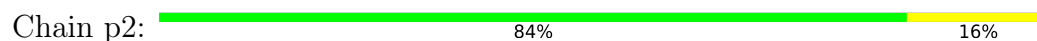
- Molecule 3: Capsid protein



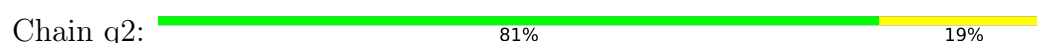
- Molecule 3: Capsid protein



- Molecule 3: Capsid protein



- Molecule 3: Capsid protein



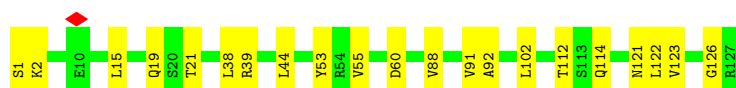
- Molecule 3: Capsid protein

Chain r2:  84% 16%



• Molecule 3: Capsid protein

Chain s2:  83% 17%



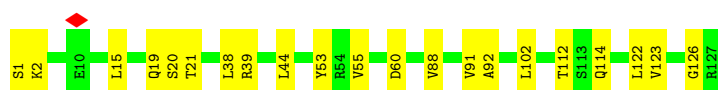
• Molecule 3: Capsid protein

Chain t2:  81% 19%



• Molecule 3: Capsid protein

Chain u2:  83% 17%



• Molecule 3: Capsid protein

Chain v2:  84% 16%



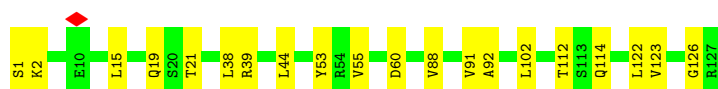
• Molecule 3: Capsid protein

Chain w2:  84% 16%



• Molecule 3: Capsid protein

Chain x2:  84% 16%



• Molecule 3: Capsid protein

Chain y2:  82% 17%



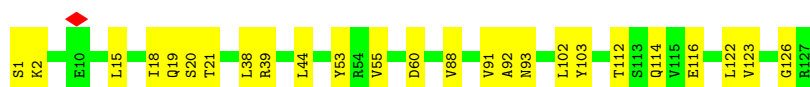
• Molecule 3: Capsid protein

Chain z2:  84% 15%



• Molecule 3: Capsid protein

Chain 02:  80% 20%



• Molecule 3: Capsid protein

Chain 12:  84% 16%



• Molecule 3: Capsid protein

Chain 22:  86% 13%



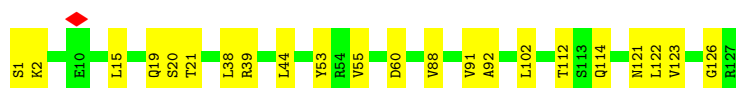
• Molecule 3: Capsid protein

Chain 32:  84% 16%

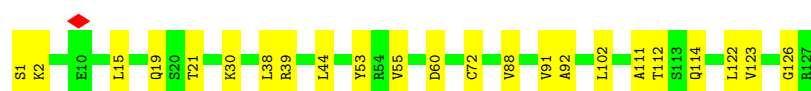
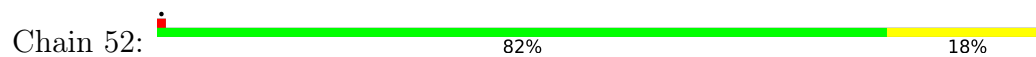


• Molecule 3: Capsid protein

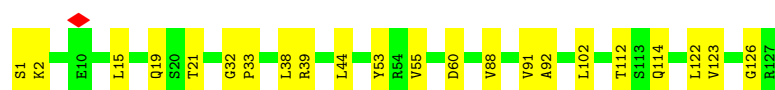
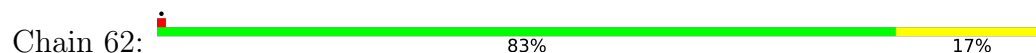
Chain 42:  83% 17%



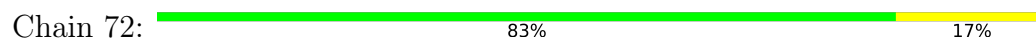
• Molecule 3: Capsid protein



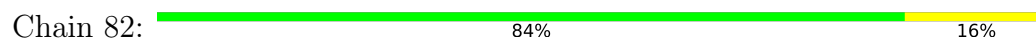
- Molecule 3: Capsid protein



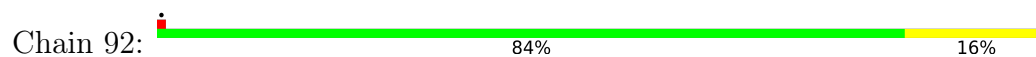
- Molecule 3: Capsid protein



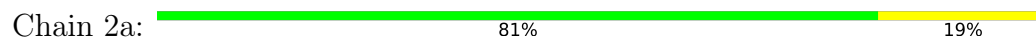
- Molecule 3: Capsid protein



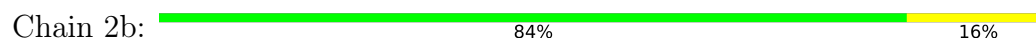
- Molecule 3: Capsid protein



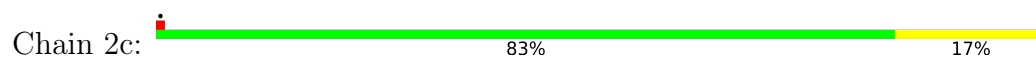
- Molecule 3: Capsid protein



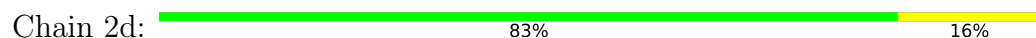
- Molecule 3: Capsid protein



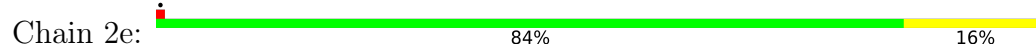
- Molecule 3: Capsid protein



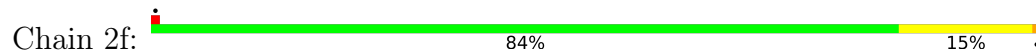
- Molecule 3: Capsid protein



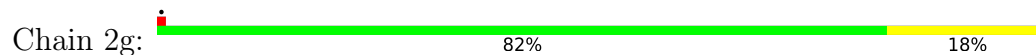
- Molecule 3: Capsid protein



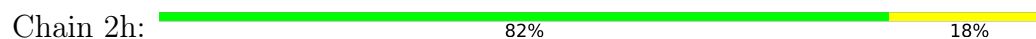
- Molecule 3: Capsid protein



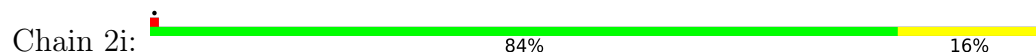
- Molecule 3: Capsid protein



- Molecule 3: Capsid protein



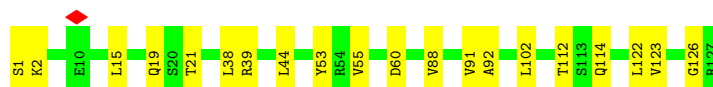
- Molecule 3: Capsid protein



● Molecule 3: Capsid protein

Chain 2j:  83% 17%

● Molecule 3: Capsid protein

Chain 2k:  84% 16%

● Molecule 3: Capsid protein

Chain 2l:  84% 15%

● Molecule 3: Capsid protein

Chain 2m:  84% 16%

● Molecule 3: Capsid protein

Chain 2n:  84% 16%

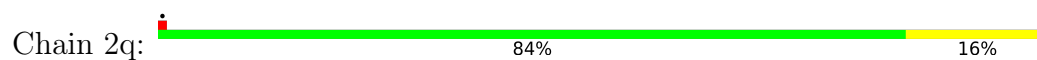
● Molecule 3: Capsid protein

Chain 2o:  86% 14%

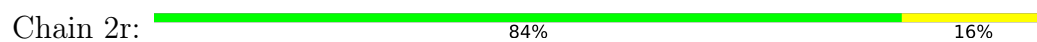
● Molecule 3: Capsid protein

Chain 2p:  83% 17%

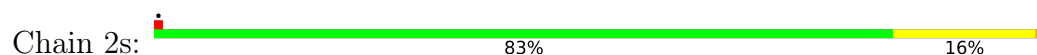
• Molecule 3: Capsid protein



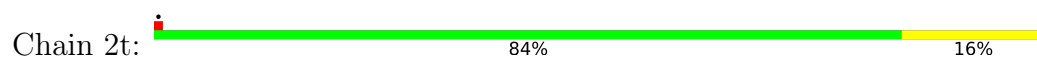
• Molecule 3: Capsid protein



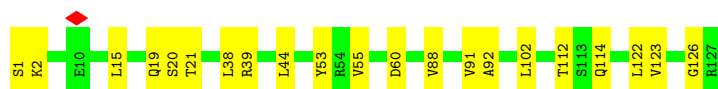
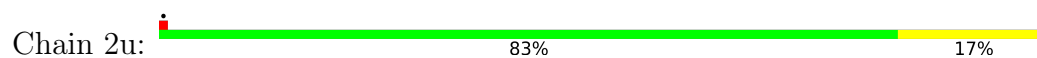
• Molecule 3: Capsid protein



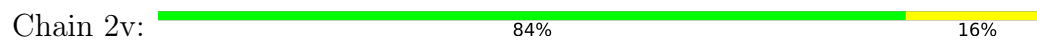
• Molecule 3: Capsid protein



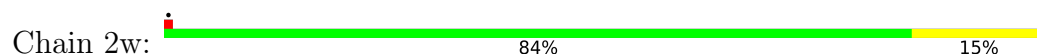
• Molecule 3: Capsid protein



• Molecule 3: Capsid protein

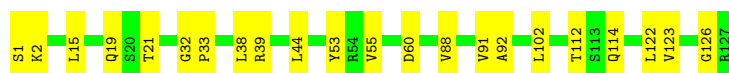
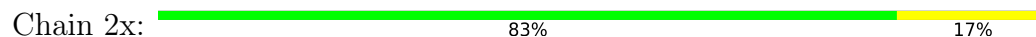


• Molecule 3: Capsid protein

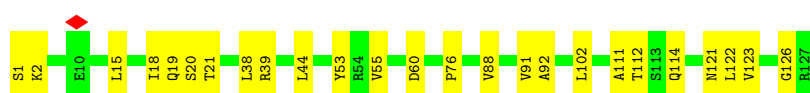
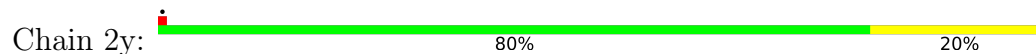




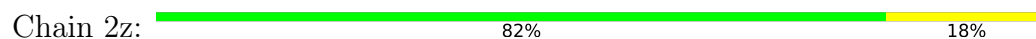
- Molecule 3: Capsid protein



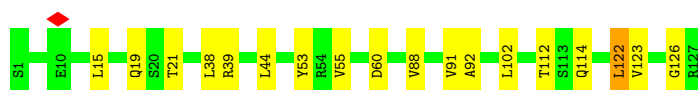
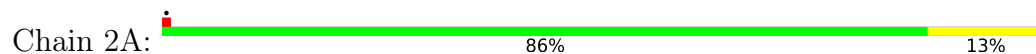
- Molecule 3: Capsid protein



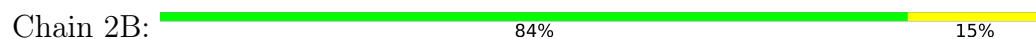
- Molecule 3: Capsid protein



- Molecule 3: Capsid protein



- Molecule 3: Capsid protein



- Molecule 3: Capsid protein

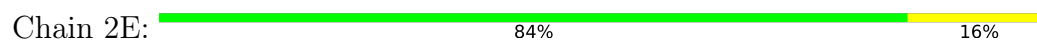


- Molecule 3: Capsid protein

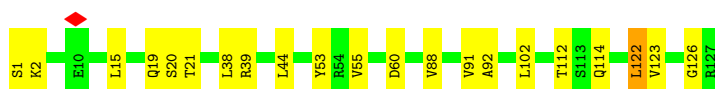
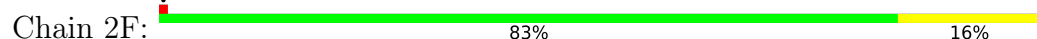




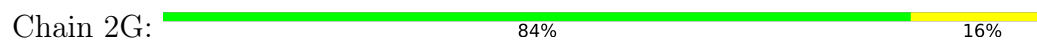
- Molecule 3: Capsid protein



- Molecule 3: Capsid protein



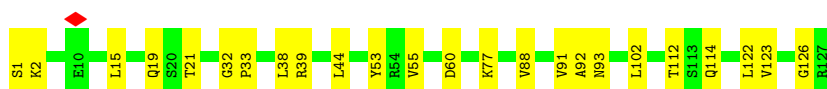
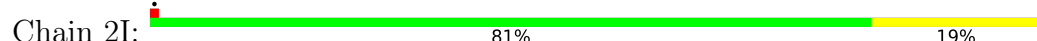
- Molecule 3: Capsid protein



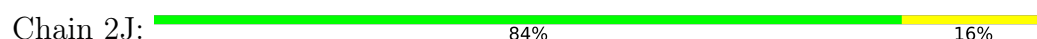
- Molecule 3: Capsid protein



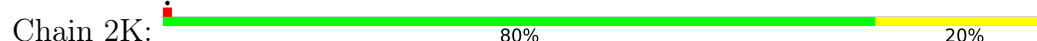
- Molecule 3: Capsid protein



- Molecule 3: Capsid protein



- Molecule 3: Capsid protein





- Molecule 3: Capsid protein

Chain 2L: 84% 16%



- Molecule 3: Capsid protein

Chain 2M: 83% 17%



- Molecule 3: Capsid protein

Chain 2N: 84% 16%



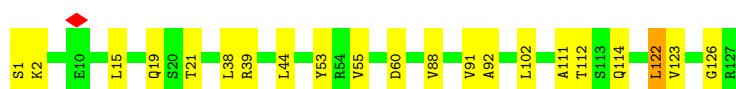
- Molecule 3: Capsid protein

Chain 2O: 84% 15%



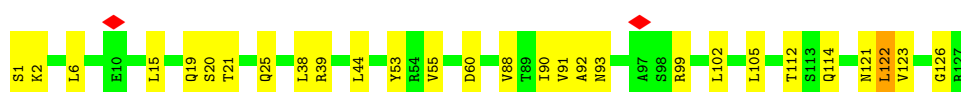
- Molecule 3: Capsid protein

Chain 2P: 83% 16%



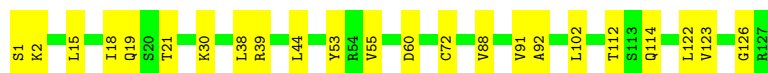
- Molecule 3: Capsid protein

Chain 2Q: 78% 21%



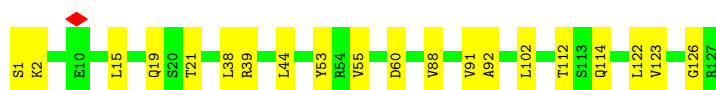
- Molecule 3: Capsid protein

Chain 2R:  82% 18%



• Molecule 3: Capsid protein

Chain 2S:  84% 16%



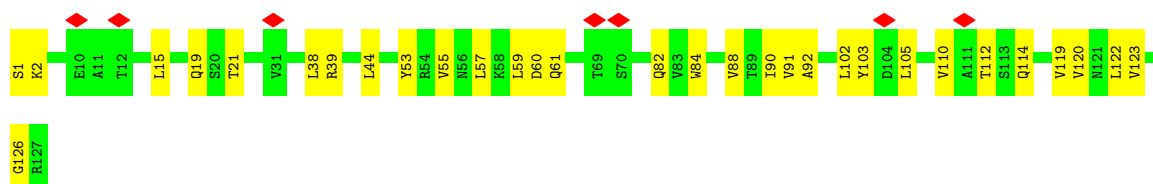
• Molecule 3: Capsid protein

Chain 2T:  84% 16%



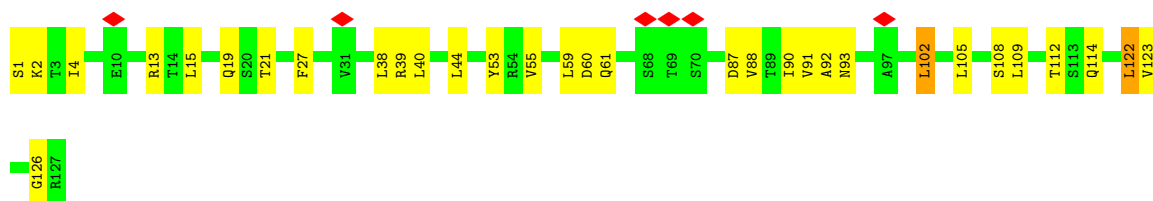
• Molecule 3: Capsid protein

Chain 2U:  76% 24% 6%



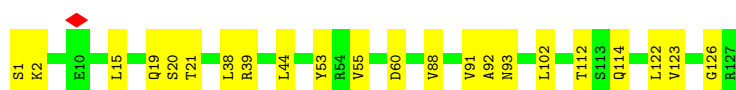
• Molecule 3: Capsid protein

Chain 2V:  75% 24% 5%



• Molecule 3: Capsid protein

Chain 2W:  83% 17%



• Molecule 3: Capsid protein

Chain 2X:  84% 16%



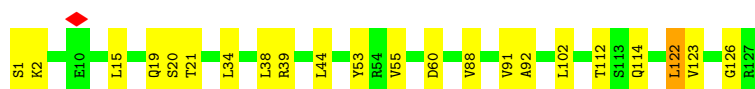
• Molecule 3: Capsid protein

Chain 2Y:  85% 14%



• Molecule 3: Capsid protein

Chain 2Z:  83% 17%



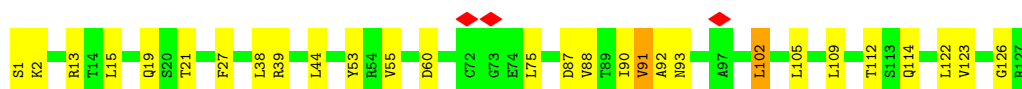
• Molecule 3: Capsid protein

Chain aa:  82% 18%



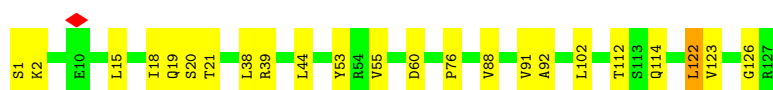
• Molecule 3: Capsid protein

Chain ab:  78% 20%



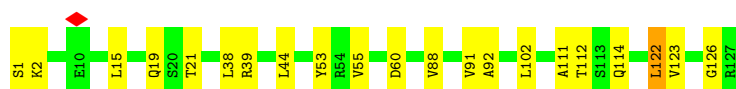
• Molecule 3: Capsid protein

Chain ac:  82% 17%



• Molecule 3: Capsid protein

Chain ad:  83% 16%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	644601	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.5	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.005	Depositor
Map size ($\text{\AA}$)	412.80002, 412.80002, 412.80002	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	R	0.09	0/2244	0.24	0/3495
2	M	0.09	0/3674	0.25	1/4983 (0.0%)
2	m	0.09	0/3674	0.22	0/4983
3	01	0.09	0/977	0.33	2/1328 (0.2%)
3	02	0.09	0/977	0.23	0/1328
3	11	0.09	0/977	0.33	0/1328
3	12	0.09	0/977	0.24	0/1328
3	21	0.09	0/977	0.34	2/1328 (0.2%)
3	22	0.09	0/977	0.23	0/1328
3	2A	0.09	0/977	0.23	0/1328
3	2B	0.11	0/977	0.27	0/1328
3	2C	0.10	0/977	0.24	0/1328
3	2D	0.09	0/977	0.22	0/1328
3	2E	0.08	0/977	0.25	0/1328
3	2F	0.09	0/977	0.23	0/1328
3	2G	0.09	0/977	0.24	0/1328
3	2H	0.09	0/977	0.22	0/1328
3	2I	0.08	0/977	0.22	0/1328
3	2J	0.09	0/977	0.24	0/1328
3	2K	0.09	0/977	0.23	0/1328
3	2L	0.09	0/977	0.24	0/1328
3	2M	0.08	0/977	0.23	0/1328
3	2N	0.09	0/977	0.24	0/1328
3	2O	0.08	0/977	0.22	0/1328
3	2P	0.08	0/977	0.24	0/1328
3	2Q	0.09	0/977	0.23	0/1328
3	2R	0.11	0/977	0.27	0/1328
3	2S	0.09	0/977	0.23	0/1328
3	2T	0.11	0/977	0.27	0/1328
3	2U	0.10	0/977	0.24	0/1328
3	2V	0.09	0/977	0.22	0/1328
3	2W	0.09	0/977	0.23	0/1328
3	2X	0.09	0/977	0.24	0/1328
3	2Y	0.09	0/977	0.22	0/1328

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	2Z	0.09	0/977	0.23	0/1328
3	2a	0.08	0/977	0.23	0/1328
3	2b	0.09	0/977	0.24	0/1328
3	2c	0.08	0/977	0.22	0/1328
3	2d	0.09	0/977	0.24	0/1328
3	2e	0.09	0/977	0.23	0/1328
3	2f	0.08	0/977	0.25	0/1328
3	2g	0.09	0/977	0.23	0/1328
3	2h	0.11	0/977	0.27	0/1328
3	2i	0.09	0/977	0.23	0/1328
3	2j	0.11	0/977	0.27	0/1328
3	2k	0.10	0/977	0.24	0/1328
3	2l	0.09	0/977	0.23	0/1328
3	2m	0.08	0/977	0.25	0/1328
3	2n	0.08	0/977	0.22	0/1328
3	2o	0.08	0/977	0.24	0/1328
3	2p	0.09	0/977	0.23	0/1328
3	2q	0.08	0/977	0.23	0/1328
3	2r	0.08	0/977	0.24	0/1328
3	2s	0.08	0/977	0.23	0/1328
3	2t	0.09	0/977	0.24	0/1328
3	2u	0.09	0/977	0.23	0/1328
3	2v	0.09	0/977	0.24	0/1328
3	2w	0.09	0/977	0.23	0/1328
3	2x	0.08	0/977	0.25	0/1328
3	2y	0.09	0/977	0.23	0/1328
3	2z	0.11	0/977	0.27	0/1328
3	31	0.09	0/977	0.32	0/1328
3	32	0.08	0/977	0.24	0/1328
3	41	0.09	0/977	0.32	0/1328
3	42	0.09	0/977	0.23	0/1328
3	51	0.09	0/977	0.33	2/1328 (0.2%)
3	52	0.11	0/977	0.27	0/1328
3	61	0.09	0/977	0.33	0/1328
3	62	0.09	0/977	0.23	0/1328
3	71	0.09	0/977	0.34	2/1328 (0.2%)
3	72	0.11	0/977	0.27	0/1328
3	82	0.09	0/977	0.22	0/1328
3	92	0.08	0/977	0.24	0/1328
3	A1	0.09	0/977	0.32	0/1328
3	A2	0.09	0/977	0.23	0/1328
3	B1	0.09	0/977	0.33	2/1328 (0.2%)
3	B2	0.09	0/977	0.24	0/1328

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	C1	0.09	0/977	0.33	0/1328
3	C2	0.09	0/977	0.23	0/1328
3	D1	0.09	0/977	0.34	2/1328 (0.2%)
3	D2	0.09	0/977	0.24	0/1328
3	E1	0.09	0/977	0.32	0/1328
3	E2	0.09	0/977	0.22	0/1328
3	F1	0.09	0/977	0.32	0/1328
3	F2	0.09	0/977	0.24	0/1328
3	G1	0.09	0/977	0.33	2/1328 (0.2%)
3	G2	0.09	0/977	0.23	0/1328
3	H1	0.09	0/977	0.33	0/1328
3	H2	0.08	0/977	0.24	0/1328
3	I1	0.09	0/977	0.34	2/1328 (0.2%)
3	I2	0.09	0/977	0.23	0/1328
3	J1	0.09	0/977	0.32	0/1328
3	J2	0.11	0/977	0.27	0/1328
3	K1	0.09	0/977	0.32	0/1328
3	K2	0.09	0/977	0.23	0/1328
3	L1	0.09	0/977	0.33	2/1328 (0.2%)
3	L2	0.11	0/977	0.27	0/1328
3	M1	0.09	0/977	0.33	0/1328
3	M2	0.09	0/977	0.23	0/1328
3	N1	0.09	0/977	0.34	2/1328 (0.2%)
3	N2	0.08	0/977	0.24	0/1328
3	O1	0.09	0/977	0.32	0/1328
3	O2	0.08	0/977	0.22	0/1328
3	P1	0.09	0/977	0.32	0/1328
3	P2	0.11	0/977	0.27	0/1328
3	Q1	0.09	0/977	0.33	2/1328 (0.2%)
3	Q2	0.09	0/977	0.23	0/1328
3	R1	0.09	0/977	0.32	0/1328
3	R2	0.11	0/977	0.27	0/1328
3	S1	0.09	0/977	0.34	2/1328 (0.2%)
3	S2	0.09	0/977	0.23	0/1328
3	T1	0.09	0/977	0.32	0/1328
3	T2	0.09	0/977	0.24	0/1328
3	U1	0.09	0/977	0.32	0/1328
3	U2	0.09	0/977	0.23	0/1328
3	V1	0.09	0/977	0.33	2/1328 (0.2%)
3	V2	0.09	0/977	0.24	0/1328
3	W1	0.09	0/977	0.33	0/1328
3	W2	0.09	0/977	0.23	0/1328
3	X1	0.09	0/977	0.34	2/1328 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	X2	0.09	0/977	0.24	0/1328
3	Y1	0.09	0/977	0.32	0/1328
3	Y2	0.09	0/977	0.23	0/1328
3	Z1	0.09	0/977	0.32	0/1328
3	Z2	0.08	0/977	0.24	0/1328
3	a1	0.09	0/977	0.32	0/1328
3	a2	0.09	0/977	0.23	0/1328
3	aa	0.08	0/977	0.24	0/1328
3	ab	0.09	0/977	0.23	0/1328
3	ac	0.09	0/977	0.23	0/1328
3	ad	0.11	0/977	0.27	0/1328
3	b1	0.09	0/977	0.32	0/1328
3	b2	0.11	0/977	0.27	0/1328
3	c1	0.09	0/977	0.33	2/1328 (0.2%)
3	c2	0.09	0/977	0.23	0/1328
3	d1	0.09	0/977	0.32	0/1328
3	d2	0.11	0/977	0.27	0/1328
3	e1	0.09	0/977	0.34	2/1328 (0.2%)
3	e2	0.09	0/977	0.23	0/1328
3	f1	0.09	0/977	0.32	0/1328
3	f2	0.09	0/977	0.24	0/1328
3	g1	0.09	0/977	0.32	0/1328
3	g2	0.09	0/977	0.23	0/1328
3	h1	0.09	0/977	0.33	2/1328 (0.2%)
3	h2	0.09	0/977	0.24	0/1328
3	i1	0.09	0/977	0.33	0/1328
3	i2	0.09	0/977	0.23	0/1328
3	j1	0.09	0/977	0.34	2/1328 (0.2%)
3	j2	0.09	0/977	0.24	0/1328
3	k1	0.09	0/977	0.32	0/1328
3	k2	0.09	0/977	0.23	0/1328
3	l1	0.09	0/977	0.32	0/1328
3	l2	0.08	0/977	0.25	0/1328
3	m1	0.09	0/977	0.33	2/1328 (0.2%)
3	m2	0.08	0/977	0.22	0/1328
3	n1	0.09	0/977	0.33	0/1328
3	n2	0.11	0/977	0.27	0/1328
3	o1	0.09	0/977	0.34	2/1328 (0.2%)
3	o2	0.09	0/977	0.23	0/1328
3	p1	0.09	0/977	0.32	0/1328
3	p2	0.11	0/977	0.27	0/1328
3	q1	0.09	0/977	0.32	0/1328
3	q2	0.09	0/977	0.23	0/1328

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	r1	0.09	0/977	0.33	2/1328 (0.2%)
3	r2	0.08	0/977	0.24	0/1328
3	s1	0.09	0/977	0.33	0/1328
3	s2	0.09	0/977	0.23	0/1328
3	t1	0.09	0/977	0.34	2/1328 (0.2%)
3	t2	0.11	0/977	0.27	0/1328
3	u1	0.09	0/977	0.32	0/1328
3	u2	0.09	0/977	0.22	0/1328
3	v1	0.09	0/977	0.32	0/1328
3	v2	0.11	0/977	0.27	0/1328
3	w1	0.09	0/977	0.33	2/1328 (0.2%)
3	w2	0.09	0/977	0.22	0/1328
3	x1	0.09	0/977	0.33	0/1328
3	x2	0.08	0/977	0.24	0/1328
3	y1	0.09	0/977	0.34	2/1328 (0.2%)
3	y2	0.09	0/977	0.23	0/1328
3	z1	0.09	0/977	0.32	0/1328
3	z2	0.09	0/977	0.24	0/1328
All	All	0.09	0/183498	0.27	49/249845 (0.0%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	o1	71	VAL	CA-C-N	5.55	127.98	120.38
3	o1	71	VAL	C-N-CA	5.55	127.98	120.38
3	71	71	VAL	CA-C-N	5.54	127.97	120.38
3	71	71	VAL	C-N-CA	5.54	127.97	120.38
3	t1	71	VAL	CA-C-N	5.53	127.96	120.38
3	t1	71	VAL	C-N-CA	5.53	127.96	120.38
3	D1	71	VAL	CA-C-N	5.53	127.96	120.38
3	D1	71	VAL	C-N-CA	5.53	127.96	120.38
3	X1	71	VAL	CA-C-N	5.52	127.95	120.38
3	X1	71	VAL	C-N-CA	5.52	127.95	120.38
3	21	71	VAL	CA-C-N	5.52	127.94	120.38
3	21	71	VAL	C-N-CA	5.52	127.94	120.38
3	y1	71	VAL	CA-C-N	5.51	127.94	120.38
3	y1	71	VAL	C-N-CA	5.51	127.94	120.38
3	e1	71	VAL	CA-C-N	5.51	127.93	120.38
3	e1	71	VAL	C-N-CA	5.51	127.93	120.38
3	N1	71	VAL	CA-C-N	5.51	127.93	120.38
3	N1	71	VAL	C-N-CA	5.51	127.93	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	232	LEU	N-CA-CB	5.50	123.58	111.87
3	j1	71	VAL	CA-C-N	5.50	127.91	120.38
3	j1	71	VAL	C-N-CA	5.50	127.91	120.38
3	I1	71	VAL	CA-C-N	5.50	127.91	120.38
3	I1	71	VAL	C-N-CA	5.50	127.91	120.38
3	S1	71	VAL	CA-C-N	5.50	127.91	120.38
3	S1	71	VAL	C-N-CA	5.50	127.91	120.38
3	r1	71	VAL	CA-C-N	5.15	127.44	120.38
3	r1	71	VAL	C-N-CA	5.15	127.44	120.38
3	G1	71	VAL	CA-C-N	5.15	127.44	120.38
3	G1	71	VAL	C-N-CA	5.15	127.44	120.38
3	w1	71	VAL	CA-C-N	5.15	127.43	120.38
3	w1	71	VAL	C-N-CA	5.15	127.43	120.38
3	51	71	VAL	CA-C-N	5.15	127.43	120.38
3	51	71	VAL	C-N-CA	5.15	127.43	120.38
3	c1	71	VAL	CA-C-N	5.14	127.43	120.38
3	c1	71	VAL	C-N-CA	5.14	127.43	120.38
3	01	71	VAL	CA-C-N	5.14	127.43	120.38
3	01	71	VAL	C-N-CA	5.14	127.43	120.38
3	h1	71	VAL	CA-C-N	5.12	127.39	120.38
3	h1	71	VAL	C-N-CA	5.12	127.39	120.38
3	Q1	71	VAL	CA-C-N	5.12	127.39	120.38
3	Q1	71	VAL	C-N-CA	5.12	127.39	120.38
3	V1	71	VAL	CA-C-N	5.12	127.39	120.38
3	V1	71	VAL	C-N-CA	5.12	127.39	120.38
3	L1	71	VAL	CA-C-N	5.11	127.39	120.38
3	L1	71	VAL	C-N-CA	5.11	127.39	120.38
3	m1	71	VAL	CA-C-N	5.11	127.38	120.38
3	m1	71	VAL	C-N-CA	5.11	127.38	120.38
3	B1	71	VAL	CA-C-N	5.10	127.37	120.38
3	B1	71	VAL	C-N-CA	5.10	127.37	120.38

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	R	2011	0	1024	145	0
2	M	3580	3555	3554	35	0
2	m	3580	3483	3554	59	0
3	01	968	0	1001	11	0
3	02	968	0	1000	15	0
3	11	968	0	1001	11	0
3	12	968	0	1000	9	0
3	21	968	0	1001	11	0
3	22	968	0	1000	8	0
3	2A	968	0	1000	8	0
3	2B	968	0	1000	9	0
3	2C	968	0	1000	9	0
3	2D	968	0	1000	8	0
3	2E	968	0	1000	9	0
3	2F	968	0	1000	11	0
3	2G	968	0	1000	8	0
3	2H	968	0	1000	8	0
3	2I	968	0	1000	11	0
3	2J	968	0	1000	8	0
3	2K	968	0	1000	13	0
3	2L	968	0	1000	9	0
3	2M	968	0	1000	9	0
3	2N	968	0	1000	9	0
3	2O	968	0	1000	9	0
3	2P	968	0	1000	10	0
3	2Q	968	0	1000	28	0
3	2R	968	0	1000	12	0
3	2S	968	0	1000	8	0
3	2T	968	0	1000	9	0
3	2U	968	0	1000	38	0
3	2V	968	0	1001	37	0
3	2W	968	0	1000	10	0
3	2X	968	0	1000	8	0
3	2Y	968	0	1000	9	0
3	2Z	968	0	1000	11	0
3	2a	968	0	1000	14	0
3	2b	968	0	1000	8	0
3	2c	968	0	1000	10	0
3	2d	968	0	1000	10	0
3	2e	968	0	1000	8	0
3	2f	968	0	1000	9	0
3	2g	968	0	1000	13	0
3	2h	968	0	1000	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2i	968	0	1000	8	0
3	2j	968	0	1000	10	0
3	2k	968	0	1000	9	0
3	2l	968	0	1000	10	0
3	2m	968	0	1000	9	0
3	2n	968	0	1000	9	0
3	2o	968	0	1000	7	0
3	2p	968	0	1000	10	0
3	2q	968	0	1000	8	0
3	2r	968	0	1000	8	0
3	2s	968	0	1000	10	0
3	2t	968	0	1000	8	0
3	2u	968	0	1000	11	0
3	2v	968	0	1000	9	0
3	2w	968	0	1000	9	0
3	2x	968	0	1000	9	0
3	2y	968	0	1000	15	0
3	2z	968	0	1000	11	0
3	31	968	0	1001	12	0
3	32	968	0	1000	8	0
3	41	968	0	1001	16	0
3	42	968	0	1000	11	0
3	51	968	0	1001	12	0
3	52	968	0	1000	11	0
3	61	968	0	1001	25	0
3	62	968	0	1000	9	0
3	71	968	0	1001	43	0
3	72	968	0	1000	10	0
3	82	968	0	1000	9	0
3	92	968	0	1000	8	0
3	A1	968	0	1001	30	0
3	A2	968	0	1000	8	0
3	B1	968	0	1001	12	0
3	B2	968	0	1000	8	0
3	C1	968	0	1001	14	0
3	C2	968	0	1000	8	0
3	D1	968	0	1001	13	0
3	D2	968	0	1000	12	0
3	E1	968	0	1001	14	0
3	E2	968	0	1000	9	0
3	F1	968	0	1001	10	0
3	F2	968	0	1000	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G1	968	0	1001	10	0
3	G2	968	0	1000	9	0
3	H1	968	0	1001	11	0
3	H2	968	0	1000	10	0
3	I1	968	0	1001	10	0
3	I2	968	0	1000	27	0
3	J1	968	0	1001	13	0
3	J2	968	0	1000	15	0
3	K1	968	0	1001	13	0
3	K2	968	0	1000	11	0
3	L1	968	0	1001	11	0
3	L2	968	0	1000	9	0
3	M1	968	0	1001	12	0
3	M2	968	0	1000	9	0
3	N1	968	0	1001	14	0
3	N2	968	0	1000	10	0
3	O1	968	0	1001	11	0
3	O2	968	0	1000	12	0
3	P1	968	0	1001	15	0
3	P2	968	0	1000	11	0
3	Q1	968	0	1001	11	0
3	Q2	968	0	1000	8	0
3	R1	968	0	1001	11	0
3	R2	968	0	1000	8	0
3	S1	968	0	1001	10	0
3	S2	968	0	1000	9	0
3	T1	968	0	1001	14	0
3	T2	968	0	1000	10	0
3	U1	968	0	1001	13	0
3	U2	968	0	1000	9	0
3	V1	968	0	1001	11	0
3	V2	968	0	1000	10	0
3	W1	968	0	1001	11	0
3	W2	968	0	1000	11	0
3	X1	968	0	1001	13	0
3	X2	968	0	1000	9	0
3	Y1	968	0	1001	12	0
3	Y2	968	0	1000	8	0
3	Z1	968	0	1001	15	0
3	Z2	968	0	1000	8	0
3	a1	968	0	1001	11	0
3	a2	968	0	1000	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	aa	968	0	1000	19	0
3	ab	968	0	1001	22	0
3	ac	968	0	1000	13	0
3	ad	968	0	1000	11	0
3	b1	968	0	1001	11	0
3	b2	968	0	1000	13	0
3	c1	968	0	1001	11	0
3	c2	968	0	1000	9	0
3	d1	968	0	1001	13	0
3	d2	968	0	1000	8	0
3	e1	968	0	1001	12	0
3	e2	968	0	1000	8	0
3	f1	968	0	998	12	0
3	f2	968	0	1000	12	0
3	g1	968	0	1001	10	0
3	g2	968	0	1000	9	0
3	h1	968	0	1001	10	0
3	h2	968	0	1000	10	0
3	i1	968	0	1001	11	0
3	i2	968	0	1000	10	0
3	j1	968	0	1001	12	0
3	j2	968	0	1000	9	0
3	k1	968	0	1001	11	0
3	k2	968	0	1000	10	0
3	l1	968	0	1001	10	0
3	l2	968	0	1000	11	0
3	m1	968	0	1001	12	0
3	m2	968	0	1000	17	0
3	n1	968	0	1001	12	0
3	n2	968	0	1000	13	0
3	o1	968	0	1001	11	0
3	o2	968	0	1000	11	0
3	p1	968	0	1001	13	0
3	p2	968	0	1000	9	0
3	q1	968	0	1001	12	0
3	q2	968	0	1000	11	0
3	r1	968	0	1001	13	0
3	r2	968	0	1000	9	0
3	s1	968	0	1001	10	0
3	s2	968	0	1000	10	0
3	t1	968	0	1001	12	0
3	t2	968	0	1000	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	u1	968	0	1001	11	0
3	u2	968	0	1000	10	0
3	v1	968	0	1001	10	0
3	v2	968	0	1000	9	0
3	w1	968	0	1001	13	0
3	w2	968	0	1000	8	0
3	x1	968	0	1001	10	0
3	x2	968	0	1000	8	0
3	y1	968	0	1001	11	0
3	y2	968	0	1000	13	0
3	z1	968	0	1001	39	0
3	z2	968	0	1000	9	0
All	All	181475	7038	186191	2095	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (2095) 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)
2:m:135:MET:CE	3:aa:121:ASN:ND2	1.90	1.34
2:m:135:MET:HE1	3:aa:121:ASN:ND2	1.48	1.21
1:R:55:G:C5'	3:A1:49:ALA:CB	2.18	1.21
1:R:55:G:H5'	3:A1:49:ALA:HB1	1.15	1.10
1:R:55:G:C5'	3:A1:49:ALA:HB1	1.78	1.09
1:R:55:G:H5'	3:A1:49:ALA:CB	1.82	1.07
3:71:110:VAL:HG11	3:2U:110:VAL:HG21	1.39	1.04
1:R:41:U:H3'	1:R:42:C:H5'	1.45	0.99
1:R:55:G:H5''	3:A1:49:ALA:CB	1.93	0.97
2:m:135:MET:HE1	3:aa:121:ASN:HD21	0.82	0.97
2:m:135:MET:CE	3:aa:121:ASN:HD21	1.58	0.96
1:R:73:C:H3'	1:R:74:C:H5''	1.53	0.90
1:R:7:A:N7	1:R:8:A:H2'	1.87	0.89
1:R:13:C:H2'	1:R:14:C:O4'	1.71	0.89
2:m:135:MET:HE2	3:aa:121:ASN:ND2	1.87	0.89
3:71:103:TYR:HB2	3:2U:119:VAL:HG11	1.56	0.87
3:71:106:THR:HG21	3:2U:84:TRP:CE2	2.09	0.86
2:m:135:MET:CE	3:aa:121:ASN:CG	2.50	0.84
1:R:39:A:O2'	1:R:40:U:O4'	1.96	0.82
1:R:83:C:H4'	1:R:83:C:OP1	1.80	0.81
1:R:8:A:H4'	2:M:242:THR:OG1	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:z1:114:GLN:OE1	3:2V:4:ILE:HG12	1.81	0.81
1:R:83:C:H2'	1:R:84:G:H4'	1.61	0.81
3:z1:22:ALA:HB2	3:2W:20:SER:H	1.47	0.80
3:71:118:LEU:HD21	3:2U:55:VAL:HG11	1.64	0.80
2:M:52:SER:OG	2:M:398:ARG:NH2	2.15	0.79
3:I2:119:VAL:HG13	3:2Q:90:ILE:HD12	1.63	0.79
3:z1:6:LEU:HD21	3:2V:109:LEU:HD13	1.64	0.78
1:R:8:A:H5'	2:M:242:THR:HG21	1.66	0.78
1:R:7:A:H3'	1:R:8:A:H5''	1.66	0.76
1:R:79:U:H2'	1:R:80:C:H5'	1.68	0.75
3:71:107:LYS:HG3	3:2U:110:VAL:HG12	1.68	0.74
1:R:55:G:C5'	3:A1:49:ALA:HB3	2.16	0.74
3:71:102:LEU:CD1	3:2U:84:TRP:HE3	2.01	0.73
3:I2:125:LEU:O	3:2Q:25:GLN:NE2	2.21	0.73
1:R:64:C:OP1	3:ab:75:LEU:HD11	1.88	0.73
3:I2:84:TRP:CZ2	3:2Q:88:VAL:HG22	2.23	0.73
3:71:103:TYR:CB	3:2U:119:VAL:HG11	2.18	0.72
1:R:8:A:N1	1:R:24:C:O2'	2.20	0.72
1:R:54:G:H1	1:R:65:C:H42	1.36	0.71
1:R:1:G:O2'	1:R:2:G:H5'	1.91	0.70
1:R:7:A:H3'	1:R:8:A:C5'	2.22	0.69
1:R:32:C:O2'	1:R:53:G:N2	2.25	0.69
1:R:80:C:H2'	1:R:81:A:H5'	1.74	0.69
2:M:221:GLU:OE2	2:M:304:ARG:NH1	2.25	0.69
3:N1:22:ALA:HB2	3:2c:20:SER:H	1.58	0.69
3:E1:53:TYR:OH	3:2Z:34:LEU:HD22	1.92	0.69
2:m:135:MET:HE3	3:aa:121:ASN:CG	2.16	0.68
3:A1:103:TYR:CZ	3:aa:116:GLU:HB2	2.29	0.68
3:71:96:GLU:OE2	3:2U:120:VAL:HG13	1.93	0.68
3:m1:22:ALA:HB2	3:2u:20:SER:H	1.58	0.68
1:R:53:G:H5''	1:R:55:G:OP1	1.94	0.67
1:R:5:C:H2'	1:R:6:G:C8	2.29	0.67
3:I2:84:TRP:CH2	3:2Q:88:VAL:HG22	2.30	0.67
1:R:6:G:H4'	1:R:7:A:O4'	1.94	0.67
1:R:13:C:H3'	1:R:13:C:OP2	1.95	0.67
1:R:59:U:H5'	1:R:62:G:O6	1.95	0.67
1:R:23:G:H2'	1:R:24:C:C6	2.30	0.66
1:R:14:C:H5'	1:R:15:U:OP1	1.94	0.66
1:R:24:C:O2	1:R:24:C:H2'	1.96	0.66
1:R:73:C:H3'	1:R:74:C:C5'	2.26	0.66
3:71:118:LEU:HD21	3:2U:55:VAL:CG1	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m2:84:TRP:HA	3:2a:87:ASP:O	1.96	0.65
1:R:55:G:H4'	3:A1:49:ALA:HB3	1.79	0.65
3:71:107:LYS:HG3	3:2U:110:VAL:CG1	2.26	0.65
2:M:180:GLN:OE1	2:M:180:GLN:N	2.30	0.65
1:R:55:G:H5''	3:A1:49:ALA:HB3	1.73	0.65
1:R:83:C:O2'	1:R:85:G:H5'	1.95	0.65
1:R:15:U:H5'	1:R:16:A:OP2	1.98	0.64
1:R:29:U:H2'	1:R:30:G:C8	2.32	0.64
3:z1:13:ARG:HD2	3:2V:105:LEU:HD11	1.80	0.64
3:z1:109:LEU:CD2	3:2V:59:LEU:HD12	2.26	0.64
3:61:84:TRP:HA	3:ab:87:ASP:O	1.98	0.64
3:61:105:LEU:HD11	3:ab:13:ARG:HH11	1.62	0.64
2:m:154:LEU:HD21	2:m:232:LEU:HD11	1.79	0.64
1:R:55:G:C4'	3:A1:49:ALA:CB	2.76	0.63
3:z1:105:LEU:HD13	3:2V:38:LEU:HD22	1.81	0.63
3:A1:116:GLU:HB2	3:aa:103:TYR:CZ	2.33	0.63
3:D1:22:ALA:HB2	3:2Q:20:SER:H	1.63	0.63
1:R:16:A:H2'	1:R:17:G:C8	2.34	0.63
1:R:83:C:HO2'	1:R:85:G:H5'	1.64	0.63
3:71:102:LEU:HG	3:2U:82:GLN:OE1	1.97	0.63
1:R:84:G:H5'	2:m:291:ARG:NH1	2.15	0.62
1:R:22:U:H2'	1:R:23:G:H5'	1.81	0.62
3:z1:126:GLY:HA2	3:2V:27:PHE:HZ	1.64	0.62
3:I2:122:LEU:HD12	3:2Q:44:LEU:HD11	1.83	0.61
3:71:106:THR:HG21	3:2U:84:TRP:CZ2	2.35	0.61
1:R:82:G:H3'	1:R:83:C:C5'	2.30	0.61
1:R:5:C:O2	1:R:7:A:H2	1.82	0.61
1:R:55:G:C4'	3:A1:49:ALA:HB1	2.30	0.61
2:m:8:SER:O	2:m:99:SER:HB3	2.00	0.61
1:R:63:A:H2'	1:R:64:C:C6	2.36	0.60
3:11:53:TYR:OH	3:2Y:34:LEU:HD22	2.01	0.60
3:41:93:ASN:CB	3:o2:76:PRO:HD2	2.31	0.60
2:M:387:SER:OG	2:M:388:GLU:N	2.35	0.60
3:b2:55:VAL:HB	3:b2:88:VAL:HB	1.84	0.60
3:j2:55:VAL:HB	3:j2:88:VAL:HB	1.84	0.60
3:w2:55:VAL:HB	3:w2:88:VAL:HB	1.84	0.60
3:82:55:VAL:HB	3:82:88:VAL:HB	1.84	0.60
3:2g:55:VAL:HB	3:2g:88:VAL:HB	1.84	0.60
3:2I:55:VAL:HB	3:2I:88:VAL:HB	1.84	0.60
2:M:132:LEU:HD23	2:M:286:VAL:HG23	1.82	0.60
3:D1:55:VAL:HB	3:D1:88:VAL:HB	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y1:55:VAL:HB	3:Y1:88:VAL:HB	1.84	0.60
3:31:55:VAL:HB	3:31:88:VAL:HB	1.84	0.60
3:41:55:VAL:HB	3:41:88:VAL:HB	1.84	0.60
3:z2:55:VAL:HB	3:z2:88:VAL:HB	1.84	0.60
3:2j:55:VAL:HB	3:2j:88:VAL:HB	1.84	0.60
3:2k:55:VAL:HB	3:2k:88:VAL:HB	1.84	0.60
3:2n:55:VAL:HB	3:2n:88:VAL:HB	1.84	0.60
3:2Z:55:VAL:HB	3:2Z:88:VAL:HB	1.84	0.60
3:d1:55:VAL:HB	3:d1:88:VAL:HB	1.84	0.59
3:B1:55:VAL:HB	3:B1:88:VAL:HB	1.84	0.59
3:L1:55:VAL:HB	3:L1:88:VAL:HB	1.84	0.59
3:M1:55:VAL:HB	3:M1:88:VAL:HB	1.84	0.59
3:N1:55:VAL:HB	3:N1:88:VAL:HB	1.84	0.59
3:61:55:VAL:HB	3:61:88:VAL:HB	1.84	0.59
3:B2:55:VAL:HB	3:B2:88:VAL:HB	1.84	0.59
3:Y2:55:VAL:HB	3:Y2:88:VAL:HB	1.84	0.59
3:a2:55:VAL:HB	3:a2:88:VAL:HB	1.84	0.59
3:d2:55:VAL:HB	3:d2:88:VAL:HB	1.84	0.59
3:e2:55:VAL:HB	3:e2:88:VAL:HB	1.84	0.59
3:f2:55:VAL:HB	3:f2:88:VAL:HB	1.84	0.59
3:g2:55:VAL:HB	3:g2:88:VAL:HB	1.84	0.59
3:h2:55:VAL:HB	3:h2:88:VAL:HB	1.84	0.59
3:22:55:VAL:HB	3:22:88:VAL:HB	1.84	0.59
3:2P:55:VAL:HB	3:2P:88:VAL:HB	1.84	0.59
3:i1:55:VAL:HB	3:i1:88:VAL:HB	1.84	0.59
3:m1:55:VAL:HB	3:m1:88:VAL:HB	1.84	0.59
3:s1:55:VAL:HB	3:s1:88:VAL:HB	1.84	0.59
3:I1:55:VAL:HB	3:I1:88:VAL:HB	1.84	0.59
3:Q1:55:VAL:HB	3:Q1:88:VAL:HB	1.84	0.59
3:01:55:VAL:HB	3:01:88:VAL:HB	1.84	0.59
3:71:55:VAL:HB	3:71:88:VAL:HB	1.84	0.59
3:i2:55:VAL:HB	3:i2:88:VAL:HB	1.84	0.59
3:m2:55:VAL:HB	3:m2:88:VAL:HB	1.84	0.59
3:2b:55:VAL:HB	3:2b:88:VAL:HB	1.84	0.59
3:2m:55:VAL:HB	3:2m:88:VAL:HB	1.84	0.59
3:2L:55:VAL:HB	3:2L:88:VAL:HB	1.84	0.59
3:2S:55:VAL:HB	3:2S:88:VAL:HB	1.84	0.59
3:ad:55:VAL:HB	3:ad:88:VAL:HB	1.84	0.59
3:j1:55:VAL:HB	3:j1:88:VAL:HB	1.84	0.59
3:o1:55:VAL:HB	3:o1:88:VAL:HB	1.84	0.59
3:r1:55:VAL:HB	3:r1:88:VAL:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:y1:55:VAL:HB	3:y1:88:VAL:HB	1.84	0.59
3:E1:55:VAL:HB	3:E1:88:VAL:HB	1.84	0.59
3:G1:55:VAL:HB	3:G1:88:VAL:HB	1.84	0.59
3:Z1:55:VAL:HB	3:Z1:88:VAL:HB	1.84	0.59
3:51:55:VAL:HB	3:51:88:VAL:HB	1.84	0.59
3:E2:55:VAL:HB	3:E2:88:VAL:HB	1.84	0.59
3:Z2:55:VAL:HB	3:Z2:88:VAL:HB	1.84	0.59
3:n2:55:VAL:HB	3:n2:88:VAL:HB	1.84	0.59
3:72:55:VAL:HB	3:72:88:VAL:HB	1.84	0.59
3:2M:55:VAL:HB	3:2M:88:VAL:HB	1.84	0.59
1:R:23:G:H2'	1:R:24:C:H6	1.65	0.59
3:b1:55:VAL:HB	3:b1:88:VAL:HB	1.84	0.59
3:K1:55:VAL:HB	3:K1:88:VAL:HB	1.84	0.59
3:71:76:PRO:HD2	3:ab:93:ASN:HB2	1.84	0.59
3:N2:55:VAL:HB	3:N2:88:VAL:HB	1.84	0.59
3:T2:55:VAL:HB	3:T2:88:VAL:HB	1.84	0.59
3:W2:55:VAL:HB	3:W2:88:VAL:HB	1.84	0.59
3:2p:55:VAL:HB	3:2p:88:VAL:HB	1.84	0.59
3:2J:55:VAL:HB	3:2J:88:VAL:HB	1.84	0.59
3:2Y:55:VAL:HB	3:2Y:88:VAL:HB	1.84	0.59
3:k1:55:VAL:HB	3:k1:88:VAL:HB	1.84	0.59
3:r1:22:ALA:HB2	3:2K:20:SER:H	1.67	0.59
3:S1:55:VAL:HB	3:S1:88:VAL:HB	1.84	0.59
3:71:8:VAL:HG23	3:2U:105:LEU:HG	1.83	0.59
3:71:119:VAL:HG13	3:2U:90:ILE:HD12	1.84	0.59
3:Q2:55:VAL:HB	3:Q2:88:VAL:HB	1.84	0.59
3:U2:55:VAL:HB	3:U2:88:VAL:HB	1.84	0.59
3:V2:55:VAL:HB	3:V2:88:VAL:HB	1.84	0.59
3:X2:55:VAL:HB	3:X2:88:VAL:HB	1.84	0.59
3:2U:55:VAL:HB	3:2U:88:VAL:HB	1.84	0.59
1:R:29:U:H2'	1:R:30:G:O4'	2.03	0.59
1:R:31:G:H2'	1:R:32:C:O4'	2.03	0.59
3:T1:55:VAL:HB	3:T1:88:VAL:HB	1.84	0.59
3:32:55:VAL:HB	3:32:88:VAL:HB	1.84	0.59
3:2x:55:VAL:HB	3:2x:88:VAL:HB	1.84	0.59
3:2V:55:VAL:HB	3:2V:88:VAL:HB	1.84	0.59
2:m:184:LEU:HD11	2:m:202:VAL:HG21	1.84	0.59
3:a1:55:VAL:HB	3:a1:88:VAL:HB	1.84	0.59
3:f1:309:VAL:HB	3:f1:342:VAL:HB	1.84	0.59
3:P1:55:VAL:HB	3:P1:88:VAL:HB	1.84	0.59
3:R1:55:VAL:HB	3:R1:88:VAL:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P2:55:VAL:HB	3:P2:88:VAL:HB	1.84	0.59
3:c2:55:VAL:HB	3:c2:88:VAL:HB	1.84	0.59
3:o2:55:VAL:HB	3:o2:88:VAL:HB	1.84	0.59
3:p2:55:VAL:HB	3:p2:88:VAL:HB	1.84	0.59
3:2z:55:VAL:HB	3:2z:88:VAL:HB	1.84	0.59
3:2F:55:VAL:HB	3:2F:88:VAL:HB	1.84	0.59
3:aa:55:VAL:HB	3:aa:88:VAL:HB	1.84	0.59
3:z1:55:VAL:HB	3:z1:88:VAL:HB	1.84	0.59
3:A2:55:VAL:HB	3:A2:88:VAL:HB	1.84	0.59
3:42:55:VAL:HB	3:42:88:VAL:HB	1.84	0.59
3:52:55:VAL:HB	3:52:88:VAL:HB	1.84	0.59
3:2C:55:VAL:HB	3:2C:88:VAL:HB	1.84	0.59
1:R:55:G:H5''	3:A1:49:ALA:HB2	1.84	0.59
3:A1:55:VAL:HB	3:A1:88:VAL:HB	1.84	0.59
3:H1:55:VAL:HB	3:H1:88:VAL:HB	1.84	0.59
3:M2:55:VAL:HB	3:M2:88:VAL:HB	1.84	0.59
3:O2:55:VAL:HB	3:O2:88:VAL:HB	1.84	0.59
3:R2:55:VAL:HB	3:R2:88:VAL:HB	1.84	0.59
3:2c:55:VAL:HB	3:2c:88:VAL:HB	1.84	0.59
3:2u:55:VAL:HB	3:2u:88:VAL:HB	1.84	0.59
3:ab:55:VAL:HB	3:ab:88:VAL:HB	1.84	0.59
3:t1:55:VAL:HB	3:t1:88:VAL:HB	1.84	0.59
3:J1:55:VAL:HB	3:J1:88:VAL:HB	1.84	0.59
3:U1:55:VAL:HB	3:U1:88:VAL:HB	1.84	0.59
3:k2:55:VAL:HB	3:k2:88:VAL:HB	1.84	0.59
3:s2:55:VAL:HB	3:s2:88:VAL:HB	1.84	0.59
3:92:55:VAL:HB	3:92:88:VAL:HB	1.84	0.59
3:2r:55:VAL:HB	3:2r:88:VAL:HB	1.84	0.59
3:2W:55:VAL:HB	3:2W:88:VAL:HB	1.84	0.59
3:w1:55:VAL:HB	3:w1:88:VAL:HB	1.84	0.58
3:A1:76:PRO:HD2	3:2V:93:ASN:HB2	1.84	0.58
3:11:55:VAL:HB	3:11:88:VAL:HB	1.84	0.58
3:71:109:LEU:HD22	3:2U:59:LEU:HD12	1.84	0.58
3:F2:55:VAL:HB	3:F2:88:VAL:HB	1.84	0.58
3:S2:55:VAL:HB	3:S2:88:VAL:HB	1.84	0.58
3:2v:55:VAL:HB	3:2v:88:VAL:HB	1.84	0.58
3:n1:55:VAL:HB	3:n1:88:VAL:HB	1.84	0.58
3:H2:55:VAL:HB	3:H2:88:VAL:HB	1.84	0.58
3:2s:55:VAL:HB	3:2s:88:VAL:HB	1.84	0.58
3:2B:55:VAL:HB	3:2B:88:VAL:HB	1.84	0.58
3:2E:55:VAL:HB	3:2E:88:VAL:HB	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:ac:55:VAL:HB	3:ac:88:VAL:HB	1.84	0.58
3:h1:55:VAL:HB	3:h1:88:VAL:HB	1.84	0.58
3:O1:55:VAL:HB	3:O1:88:VAL:HB	1.84	0.58
3:D2:55:VAL:HB	3:D2:88:VAL:HB	1.84	0.58
3:G2:55:VAL:HB	3:G2:88:VAL:HB	1.84	0.58
3:2H:55:VAL:HB	3:2H:88:VAL:HB	1.84	0.58
3:2K:55:VAL:HB	3:2K:88:VAL:HB	1.84	0.58
3:2N:55:VAL:HB	3:2N:88:VAL:HB	1.84	0.58
3:l1:55:VAL:HB	3:l1:88:VAL:HB	1.84	0.58
3:q1:55:VAL:HB	3:q1:88:VAL:HB	1.84	0.58
3:W1:55:VAL:HB	3:W1:88:VAL:HB	1.84	0.58
3:y2:55:VAL:HB	3:y2:88:VAL:HB	1.84	0.58
3:2l:55:VAL:HB	3:2l:88:VAL:HB	1.84	0.58
3:2o:55:VAL:HB	3:2o:88:VAL:HB	1.84	0.58
3:2q:55:VAL:HB	3:2q:88:VAL:HB	1.84	0.58
3:2t:55:VAL:HB	3:2t:88:VAL:HB	1.84	0.58
3:2A:55:VAL:HB	3:2A:88:VAL:HB	1.84	0.58
3:F1:55:VAL:HB	3:F1:88:VAL:HB	1.84	0.58
3:C2:55:VAL:HB	3:C2:88:VAL:HB	1.84	0.58
3:62:55:VAL:HB	3:62:88:VAL:HB	1.84	0.58
3:2w:55:VAL:HB	3:2w:88:VAL:HB	1.84	0.58
3:p1:55:VAL:HB	3:p1:88:VAL:HB	1.84	0.58
3:u1:55:VAL:HB	3:u1:88:VAL:HB	1.84	0.58
3:x1:55:VAL:HB	3:x1:88:VAL:HB	1.84	0.58
3:z1:109:LEU:HD22	3:2V:59:LEU:HD12	1.85	0.58
3:K2:55:VAL:HB	3:K2:88:VAL:HB	1.84	0.58
1:R:7:A:H61	1:R:9:A:H62	1.52	0.58
3:v1:55:VAL:HB	3:v1:88:VAL:HB	1.84	0.58
3:v2:55:VAL:HB	3:v2:88:VAL:HB	1.84	0.58
3:02:55:VAL:HB	3:02:88:VAL:HB	1.84	0.58
3:12:55:VAL:HB	3:12:88:VAL:HB	1.84	0.58
3:2a:55:VAL:HB	3:2a:88:VAL:HB	1.84	0.58
3:g1:55:VAL:HB	3:g1:88:VAL:HB	1.84	0.58
3:X1:55:VAL:HB	3:X1:88:VAL:HB	1.84	0.58
3:r2:55:VAL:HB	3:r2:88:VAL:HB	1.84	0.58
3:x2:55:VAL:HB	3:x2:88:VAL:HB	1.84	0.58
3:2d:55:VAL:HB	3:2d:88:VAL:HB	1.84	0.58
3:2i:55:VAL:HB	3:2i:88:VAL:HB	1.84	0.58
3:2T:55:VAL:HB	3:2T:88:VAL:HB	1.84	0.58
1:R:40:U:H2'	1:R:42:C:H4'	1.85	0.58
3:C1:55:VAL:HB	3:C1:88:VAL:HB	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:21:55:VAL:HB	3:21:88:VAL:HB	1.84	0.58
3:l2:55:VAL:HB	3:l2:88:VAL:HB	1.84	0.58
3:2y:55:VAL:HB	3:2y:88:VAL:HB	1.84	0.58
3:2G:55:VAL:HB	3:2G:88:VAL:HB	1.84	0.58
3:2X:55:VAL:HB	3:2X:88:VAL:HB	1.84	0.58
3:e1:55:VAL:HB	3:e1:88:VAL:HB	1.84	0.58
3:t2:55:VAL:HB	3:t2:88:VAL:HB	1.84	0.58
3:u2:55:VAL:HB	3:u2:88:VAL:HB	1.84	0.58
3:02:103:TYR:CZ	3:2K:116:GLU:HB2	2.39	0.58
3:2f:55:VAL:HB	3:2f:88:VAL:HB	1.84	0.58
3:2D:55:VAL:HB	3:2D:88:VAL:HB	1.84	0.58
1:R:46:C:H2'	1:R:47:G:O4'	2.04	0.57
1:R:57:C:H3'	1:R:58:U:C5'	2.34	0.57
3:J2:55:VAL:HB	3:J2:88:VAL:HB	1.84	0.57
3:2Q:55:VAL:HB	3:2Q:88:VAL:HB	1.84	0.57
3:V1:55:VAL:HB	3:V1:88:VAL:HB	1.84	0.57
3:2O:55:VAL:HB	3:2O:88:VAL:HB	1.84	0.57
3:61:82:GLN:OE1	3:ab:90:ILE:HG12	2.04	0.57
3:71:76:PRO:HD2	3:ab:93:ASN:CB	2.35	0.57
3:2e:55:VAL:HB	3:2e:88:VAL:HB	1.84	0.57
3:y1:22:ALA:HB2	3:2s:20:SER:H	1.70	0.57
3:q2:55:VAL:HB	3:q2:88:VAL:HB	1.84	0.57
3:2h:55:VAL:HB	3:2h:88:VAL:HB	1.84	0.57
2:m:18:LEU:HD22	2:m:88:HIS:HB3	1.86	0.57
3:l2:55:VAL:HB	3:l2:88:VAL:HB	1.84	0.57
1:R:55:G:H4'	3:A1:49:ALA:CB	2.33	0.57
3:c1:55:VAL:HB	3:c1:88:VAL:HB	1.84	0.57
3:L2:55:VAL:HB	3:L2:88:VAL:HB	1.84	0.57
3:2R:55:VAL:HB	3:2R:88:VAL:HB	1.84	0.57
3:61:6:LEU:HD21	3:ab:109:LEU:HD13	1.87	0.57
3:P1:19:GLN:OE1	3:P1:21:THR:OG1	2.23	0.57
3:2D:19:GLN:OE1	3:2D:21:THR:OG1	2.23	0.57
1:R:83:C:C2'	1:R:84:G:H4'	2.33	0.56
1:R:89:U:H2'	1:R:90:C:C6	2.40	0.56
2:m:250:TRP:O	2:m:278:GLY:N	2.38	0.56
3:A1:19:GLN:OE1	3:A1:21:THR:OG1	2.23	0.56
3:J1:59:LEU:CD2	3:l2:102:LEU:HD21	2.35	0.56
3:S1:19:GLN:OE1	3:S1:21:THR:OG1	2.23	0.56
3:S2:19:GLN:OE1	3:S2:21:THR:OG1	2.23	0.56
3:l2:19:GLN:OE1	3:l2:21:THR:OG1	2.23	0.56
3:h1:19:GLN:OE1	3:h1:21:THR:OG1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:k1:19:GLN:OE1	3:k1:21:THR:OG1	2.23	0.56
3:x1:19:GLN:OE1	3:x1:21:THR:OG1	2.23	0.56
3:E1:19:GLN:OE1	3:E1:21:THR:OG1	2.23	0.56
3:I1:19:GLN:OE1	3:I1:21:THR:OG1	2.23	0.56
3:11:19:GLN:OE1	3:11:21:THR:OG1	2.23	0.56
3:J2:19:GLN:OE1	3:J2:21:THR:OG1	2.23	0.56
3:X2:19:GLN:OE1	3:X2:21:THR:OG1	2.23	0.56
3:2h:19:GLN:OE1	3:2h:21:THR:OG1	2.23	0.56
3:2m:19:GLN:OE1	3:2m:21:THR:OG1	2.23	0.56
3:ac:19:GLN:OE1	3:ac:21:THR:OG1	2.23	0.56
1:R:15:U:H5''	1:R:16:A:N7	2.20	0.56
1:R:87:C:O2	1:R:87:C:H2'	2.05	0.56
3:p1:19:GLN:OE1	3:p1:21:THR:OG1	2.23	0.56
3:t1:19:GLN:OE1	3:t1:21:THR:OG1	2.23	0.56
3:w1:19:GLN:OE1	3:w1:21:THR:OG1	2.23	0.56
3:J1:53:TYR:OH	3:m2:34:LEU:HD22	2.05	0.56
3:Q1:19:GLN:OE1	3:Q1:21:THR:OG1	2.23	0.56
3:V1:19:GLN:OE1	3:V1:21:THR:OG1	2.23	0.56
3:H2:19:GLN:OE1	3:H2:21:THR:OG1	2.23	0.56
3:L2:19:GLN:OE1	3:L2:21:THR:OG1	2.23	0.56
3:M2:19:GLN:OE1	3:M2:21:THR:OG1	2.23	0.56
3:Y2:19:GLN:OE1	3:Y2:21:THR:OG1	2.23	0.56
3:n2:19:GLN:OE1	3:n2:21:THR:OG1	2.23	0.56
3:2t:19:GLN:OE1	3:2t:21:THR:OG1	2.23	0.56
3:2E:19:GLN:OE1	3:2E:21:THR:OG1	2.23	0.56
3:2G:19:GLN:OE1	3:2G:21:THR:OG1	2.23	0.56
3:2Y:19:GLN:OE1	3:2Y:21:THR:OG1	2.23	0.56
2:m:342:VAL:HG21	2:m:409:VAL:HG11	1.87	0.56
3:F1:19:GLN:OE1	3:F1:21:THR:OG1	2.23	0.56
3:W2:19:GLN:OE1	3:W2:21:THR:OG1	2.23	0.56
3:2i:19:GLN:OE1	3:2i:21:THR:OG1	2.23	0.56
3:2l:19:GLN:OE1	3:2l:21:THR:OG1	2.23	0.56
3:2x:19:GLN:OE1	3:2x:21:THR:OG1	2.23	0.56
3:2J:19:GLN:OE1	3:2J:21:THR:OG1	2.23	0.56
3:d1:19:GLN:OE1	3:d1:21:THR:OG1	2.23	0.56
3:K2:19:GLN:OE1	3:K2:21:THR:OG1	2.23	0.56
3:P2:19:GLN:OE1	3:P2:21:THR:OG1	2.23	0.56
3:U2:19:GLN:OE1	3:U2:21:THR:OG1	2.23	0.56
3:x2:19:GLN:OE1	3:x2:21:THR:OG1	2.23	0.56
3:2Z:19:GLN:OE1	3:2Z:21:THR:OG1	2.23	0.56
3:41:19:GLN:OE1	3:41:21:THR:OG1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:71:119:VAL:HG13	3:2U:90:ILE:CD1	2.35	0.56
3:R2:19:GLN:OE1	3:R2:21:THR:OG1	2.23	0.56
3:c2:19:GLN:OE1	3:c2:21:THR:OG1	2.23	0.56
3:ad:19:GLN:OE1	3:ad:21:THR:OG1	2.23	0.56
3:r1:19:GLN:OE1	3:r1:21:THR:OG1	2.23	0.56
3:O1:19:GLN:OE1	3:O1:21:THR:OG1	2.23	0.56
3:U1:19:GLN:OE1	3:U1:21:THR:OG1	2.23	0.56
3:X1:19:GLN:OE1	3:X1:21:THR:OG1	2.23	0.56
3:O2:19:GLN:OE1	3:O2:21:THR:OG1	2.23	0.56
3:v2:19:GLN:OE1	3:v2:21:THR:OG1	2.23	0.56
3:o2:19:GLN:OE1	3:o2:21:THR:OG1	2.23	0.56
3:2d:19:GLN:OE1	3:2d:21:THR:OG1	2.24	0.56
3:2e:19:GLN:OE1	3:2e:21:THR:OG1	2.23	0.56
3:2M:19:GLN:OE1	3:2M:21:THR:OG1	2.23	0.56
3:2P:19:GLN:OE1	3:2P:21:THR:OG1	2.23	0.56
3:2S:19:GLN:OE1	3:2S:21:THR:OG1	2.23	0.56
3:ab:19:GLN:OE1	3:ab:21:THR:OG1	2.23	0.56
3:i1:19:GLN:OE1	3:i1:21:THR:OG1	2.23	0.56
3:o2:19:GLN:OE1	3:o2:21:THR:OG1	2.23	0.56
3:q2:19:GLN:OE1	3:q2:21:THR:OG1	2.23	0.56
3:s2:19:GLN:OE1	3:s2:21:THR:OG1	2.23	0.56
3:y2:19:GLN:OE1	3:y2:21:THR:OG1	2.23	0.56
3:2p:19:GLN:OE1	3:2p:21:THR:OG1	2.23	0.56
3:f1:273:GLN:OE1	3:f1:275:THR:OG1	2.23	0.56
3:v1:19:GLN:OE1	3:v1:21:THR:OG1	2.23	0.56
3:z1:19:GLN:OE1	3:z1:21:THR:OG1	2.23	0.56
3:T1:19:GLN:OE1	3:T1:21:THR:OG1	2.23	0.56
3:Y1:19:GLN:OE1	3:Y1:21:THR:OG1	2.23	0.56
3:u2:19:GLN:OE1	3:u2:21:THR:OG1	2.23	0.56
3:z2:19:GLN:OE1	3:z2:21:THR:OG1	2.23	0.56
3:72:19:GLN:OE1	3:72:21:THR:OG1	2.23	0.56
3:2u:19:GLN:OE1	3:2u:21:THR:OG1	2.23	0.56
3:2v:19:GLN:OE1	3:2v:21:THR:OG1	2.23	0.56
3:o1:19:GLN:OE1	3:o1:21:THR:OG1	2.23	0.56
3:N2:19:GLN:OE1	3:N2:21:THR:OG1	2.23	0.56
3:Q2:19:GLN:OE1	3:Q2:21:THR:OG1	2.23	0.56
3:b2:19:GLN:OE1	3:b2:21:THR:OG1	2.23	0.56
3:r2:19:GLN:OE1	3:r2:21:THR:OG1	2.23	0.56
3:2b:19:GLN:OE1	3:2b:21:THR:OG1	2.23	0.56
3:2R:19:GLN:OE1	3:2R:21:THR:OG1	2.23	0.56
3:Z1:19:GLN:OE1	3:Z1:21:THR:OG1	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m2:19:GLN:OE1	3:m2:21:THR:OG1	2.23	0.55
3:n1:19:GLN:OE1	3:n1:21:THR:OG1	2.23	0.55
3:J1:6:LEU:HD13	3:I2:105:LEU:HD22	1.88	0.55
3:T2:19:GLN:OE1	3:T2:21:THR:OG1	2.23	0.55
3:h2:19:GLN:OE1	3:h2:21:THR:OG1	2.23	0.55
3:42:19:GLN:OE1	3:42:21:THR:OG1	2.23	0.55
3:2F:19:GLN:OE1	3:2F:21:THR:OG1	2.23	0.55
3:2I:19:GLN:OE1	3:2I:21:THR:OG1	2.23	0.55
3:a1:19:GLN:OE1	3:a1:21:THR:OG1	2.23	0.55
3:b1:19:GLN:OE1	3:b1:21:THR:OG1	2.23	0.55
3:e1:19:GLN:OE1	3:e1:21:THR:OG1	2.23	0.55
3:s1:19:GLN:OE1	3:s1:21:THR:OG1	2.23	0.55
3:K1:19:GLN:OE1	3:K1:21:THR:OG1	2.23	0.55
3:2j:19:GLN:OE1	3:2j:21:THR:OG1	2.23	0.55
3:aa:19:GLN:OE1	3:aa:21:THR:OG1	2.23	0.55
3:X1:22:ALA:HB2	3:42:20:SER:H	1.71	0.55
3:a2:19:GLN:OE1	3:a2:21:THR:OG1	2.23	0.55
3:52:19:GLN:OE1	3:52:21:THR:OG1	2.23	0.55
3:g1:19:GLN:OE1	3:g1:21:THR:OG1	2.23	0.55
3:R1:19:GLN:OE1	3:R1:21:THR:OG1	2.23	0.55
3:2I:19:GLN:OE1	3:2I:21:THR:OG1	2.23	0.55
3:I2:19:GLN:OE1	3:I2:21:THR:OG1	2.23	0.55
3:k2:19:GLN:OE1	3:k2:21:THR:OG1	2.23	0.55
3:2X:19:GLN:OE1	3:2X:21:THR:OG1	2.23	0.55
3:J1:19:GLN:OE1	3:J1:21:THR:OG1	2.23	0.55
3:F2:19:GLN:OE1	3:F2:21:THR:OG1	2.23	0.55
3:G2:19:GLN:OE1	3:G2:21:THR:OG1	2.23	0.55
3:w2:19:GLN:OE1	3:w2:21:THR:OG1	2.23	0.55
3:2g:19:GLN:OE1	3:2g:21:THR:OG1	2.23	0.55
3:2K:19:GLN:OE1	3:2K:21:THR:OG1	2.23	0.55
1:R:65:C:O2	1:R:65:C:H2'	2.06	0.55
2:m:232:LEU:HD13	2:m:296:THR:OG1	2.07	0.55
3:q1:19:GLN:OE1	3:q1:21:THR:OG1	2.23	0.55
3:Z1:22:ALA:HB2	3:02:20:SER:H	1.71	0.55
3:C2:19:GLN:OE1	3:C2:21:THR:OG1	2.23	0.55
3:p2:19:GLN:OE1	3:p2:21:THR:OG1	2.23	0.55
3:92:19:GLN:OE1	3:92:21:THR:OG1	2.23	0.55
3:2c:19:GLN:OE1	3:2c:21:THR:OG1	2.23	0.55
3:2s:19:GLN:OE1	3:2s:21:THR:OG1	2.23	0.55
3:2L:19:GLN:OE1	3:2L:21:THR:OG1	2.23	0.55
3:2Q:19:GLN:OE1	3:2Q:21:THR:OG1	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:j1:19:GLN:OE1	3:j1:21:THR:OG1	2.23	0.55
3:D1:19:GLN:OE1	3:D1:21:THR:OG1	2.23	0.55
3:71:103:TYR:CD1	3:2U:119:VAL:HG21	2.42	0.55
3:V2:19:GLN:OE1	3:V2:21:THR:OG1	2.23	0.55
3:2o:19:GLN:OE1	3:2o:21:THR:OG1	2.23	0.55
3:2A:19:GLN:OE1	3:2A:21:THR:OG1	2.23	0.55
3:2O:19:GLN:OE1	3:2O:21:THR:OG1	2.23	0.55
3:c1:19:GLN:OE1	3:c1:21:THR:OG1	2.23	0.55
3:C1:19:GLN:OE1	3:C1:21:THR:OG1	2.23	0.55
3:12:19:GLN:OE1	3:12:21:THR:OG1	2.23	0.55
3:2k:19:GLN:OE1	3:2k:21:THR:OG1	2.23	0.55
3:2n:19:GLN:OE1	3:2n:21:THR:OG1	2.23	0.55
1:R:13:C:O2'	1:R:14:C:P	2.64	0.55
2:M:77:VAL:HG12	2:M:374:TRP:CE2	2.42	0.55
3:l1:19:GLN:OE1	3:l1:21:THR:OG1	2.23	0.55
3:G1:19:GLN:OE1	3:G1:21:THR:OG1	2.23	0.55
3:N1:19:GLN:OE1	3:N1:21:THR:OG1	2.23	0.55
3:I2:105:LEU:HD22	3:2Q:6:LEU:HD13	1.89	0.55
3:22:19:GLN:OE1	3:22:21:THR:OG1	2.23	0.55
3:2w:19:GLN:OE1	3:2w:21:THR:OG1	2.23	0.55
3:2W:19:GLN:OE1	3:2W:21:THR:OG1	2.23	0.55
2:m:77:VAL:HG12	2:m:374:TRP:CD2	2.42	0.54
2:M:27:GLN:OE1	2:M:104:ARG:NH2	2.37	0.54
3:D2:19:GLN:OE1	3:D2:21:THR:OG1	2.23	0.54
3:2a:19:GLN:OE1	3:2a:21:THR:OG1	2.23	0.54
3:2U:19:GLN:OE1	3:2U:21:THR:OG1	2.23	0.54
3:L1:19:GLN:OE1	3:L1:21:THR:OG1	2.23	0.54
3:71:19:GLN:OE1	3:71:21:THR:OG1	2.23	0.54
3:A2:19:GLN:OE1	3:A2:21:THR:OG1	2.23	0.54
3:W1:19:GLN:OE1	3:W1:21:THR:OG1	2.23	0.54
3:31:19:GLN:OE1	3:31:21:THR:OG1	2.23	0.54
3:d2:19:GLN:OE1	3:d2:21:THR:OG1	2.23	0.54
3:2q:19:GLN:OE1	3:2q:21:THR:OG1	2.23	0.54
3:H1:19:GLN:OE1	3:H1:21:THR:OG1	2.23	0.54
3:e2:19:GLN:OE1	3:e2:21:THR:OG1	2.23	0.54
3:2T:19:GLN:OE1	3:2T:21:THR:OG1	2.23	0.54
1:R:27:C:H2'	1:R:28:U:N1	2.23	0.54
3:I2:120:VAL:HG13	3:2Q:99:ARG:HH21	1.70	0.54
3:t2:19:GLN:OE1	3:t2:21:THR:OG1	2.23	0.54
3:32:19:GLN:OE1	3:32:21:THR:OG1	2.23	0.54
3:2y:121:ASN:HB3	3:2z:30:LYS:NZ	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:25:C:OP1	2:m:182:ARG:NH1	2.40	0.54
3:N2:1:SER:OG	3:N2:2:LYS:N	2.41	0.54
3:2B:19:GLN:OE1	3:2B:21:THR:OG1	2.23	0.54
2:m:262:TRP:NE1	2:m:370:PRO:O	2.38	0.54
3:m1:19:GLN:OE1	3:m1:21:THR:OG1	2.23	0.54
3:g2:19:GLN:OE1	3:g2:21:THR:OG1	2.23	0.54
3:2b:1:SER:OG	3:2b:2:LYS:N	2.41	0.54
3:2Z:1:SER:OG	3:2Z:2:LYS:N	2.41	0.54
3:u1:19:GLN:OE1	3:u1:21:THR:OG1	2.23	0.54
3:B1:19:GLN:OE1	3:B1:21:THR:OG1	2.23	0.54
3:61:19:GLN:OE1	3:61:21:THR:OG1	2.23	0.54
3:i2:19:GLN:OE1	3:i2:21:THR:OG1	2.23	0.54
3:2k:1:SER:OG	3:2k:2:LYS:N	2.41	0.54
3:2m:1:SER:OG	3:2m:2:LYS:N	2.41	0.54
3:2s:1:SER:OG	3:2s:2:LYS:N	2.41	0.54
3:2y:19:GLN:OE1	3:2y:21:THR:OG1	2.23	0.54
3:2z:19:GLN:OE1	3:2z:21:THR:OG1	2.23	0.54
3:aa:1:SER:OG	3:aa:2:LYS:N	2.41	0.54
3:z1:13:ARG:CD	3:2V:105:LEU:HD11	2.37	0.54
3:z1:126:GLY:HA2	3:2V:27:PHE:CZ	2.42	0.54
3:E2:19:GLN:OE1	3:E2:21:THR:OG1	2.23	0.54
3:82:1:SER:OG	3:82:2:LYS:N	2.41	0.54
3:2f:19:GLN:OE1	3:2f:21:THR:OG1	2.23	0.54
3:2g:121:ASN:HB3	3:2h:30:LYS:NZ	2.23	0.54
3:2B:1:SER:OG	3:2B:2:LYS:N	2.41	0.54
3:C1:87:ASP:O	3:J2:84:TRP:HA	2.08	0.53
3:C2:1:SER:OG	3:C2:2:LYS:N	2.41	0.53
3:y2:1:SER:OG	3:y2:2:LYS:N	2.41	0.53
3:02:116:GLU:HB2	3:2K:103:TYR:CZ	2.43	0.53
3:42:121:ASN:HB3	3:52:30:LYS:NZ	2.23	0.53
3:2X:1:SER:OG	3:2X:2:LYS:N	2.41	0.53
2:m:368:VAL:HG22	2:m:369:SER:H	1.73	0.53
3:71:102:LEU:CD1	3:2U:84:TRP:CE3	2.88	0.53
3:Z2:19:GLN:OE1	3:Z2:21:THR:OG1	2.23	0.53
3:u2:1:SER:OG	3:u2:2:LYS:N	2.41	0.53
3:2I:1:SER:OG	3:2I:2:LYS:N	2.41	0.53
3:2N:19:GLN:OE1	3:2N:21:THR:OG1	2.23	0.53
3:2U:1:SER:OG	3:2U:2:LYS:N	2.41	0.53
1:R:83:C:O2'	1:R:84:G:O3'	2.25	0.53
2:M:296:THR:HG22	2:M:340:ILE:HG22	1.91	0.53
3:I2:1:SER:OG	3:I2:2:LYS:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m2:121:ASN:HB3	3:n2:30:LYS:NZ	2.23	0.53
3:2y:1:SER:OG	3:2y:2:LYS:N	2.41	0.53
3:2Q:121:ASN:HB3	3:2R:30:LYS:NZ	2.23	0.53
1:R:4:G:O2'	1:R:5:C:H5'	2.07	0.53
2:m:296:THR:HG22	2:m:340:ILE:HG22	1.89	0.53
3:z1:7:SER:O	3:2V:108:SER:HB2	2.08	0.53
3:01:19:GLN:OE1	3:01:21:THR:OG1	2.23	0.53
3:z2:1:SER:OG	3:z2:2:LYS:N	2.41	0.53
3:2n:1:SER:OG	3:2n:2:LYS:N	2.41	0.53
3:2w:1:SER:OG	3:2w:2:LYS:N	2.41	0.53
2:M:180:GLN:HB3	2:M:319:LEU:HD11	1.91	0.53
3:51:19:GLN:OE1	3:51:21:THR:OG1	2.23	0.53
3:j2:19:GLN:OE1	3:j2:21:THR:OG1	2.23	0.53
3:l2:1:SER:OG	3:l2:2:LYS:N	2.41	0.53
3:m2:105:LEU:HD11	3:2a:13:ARG:HH11	1.74	0.53
3:2F:1:SER:OG	3:2F:2:LYS:N	2.41	0.53
1:R:40:U:O2'	1:R:42:C:H4'	2.09	0.53
1:R:69:U:H2'	1:R:70:A:O4'	2.09	0.53
3:y1:19:GLN:OE1	3:y1:21:THR:OG1	2.24	0.53
3:41:93:ASN:HB2	3:o2:76:PRO:HD2	1.91	0.53
3:41:93:ASN:HB3	3:o2:76:PRO:HD2	1.91	0.53
3:B2:1:SER:OG	3:B2:2:LYS:N	2.41	0.53
3:E2:1:SER:OG	3:E2:2:LYS:N	2.41	0.53
3:I2:121:ASN:HB3	3:J2:30:LYS:NZ	2.23	0.53
3:O2:121:ASN:HB3	3:P2:30:LYS:NZ	2.23	0.53
3:R2:1:SER:OG	3:R2:2:LYS:N	2.41	0.53
3:s2:121:ASN:HB3	3:t2:30:LYS:NZ	2.23	0.53
3:w2:1:SER:OG	3:w2:2:LYS:N	2.41	0.53
1:R:60:C:H4'	2:M:266:ALA:HB3	1.90	0.53
3:71:8:VAL:HG23	3:2U:105:LEU:CD2	2.39	0.53
3:B2:19:GLN:OE1	3:B2:21:THR:OG1	2.23	0.53
3:L2:1:SER:OG	3:L2:2:LYS:N	2.41	0.53
3:t2:1:SER:OG	3:t2:2:LYS:N	2.42	0.53
3:62:19:GLN:OE1	3:62:21:THR:OG1	2.23	0.53
3:2r:1:SER:OG	3:2r:2:LYS:N	2.41	0.53
3:2r:19:GLN:OE1	3:2r:21:THR:OG1	2.23	0.53
3:H1:22:ALA:HB2	3:W2:20:SER:H	1.73	0.53
3:a2:121:ASN:HB3	3:b2:30:LYS:NZ	2.23	0.53
3:2a:1:SER:OG	3:2a:2:LYS:N	2.41	0.53
1:R:79:U:C2'	1:R:80:C:H5'	2.37	0.53
2:M:77:VAL:HG13	2:M:98:VAL:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P1:22:ALA:HB2	3:2y:20:SER:H	1.73	0.53
3:S2:1:SER:OG	3:S2:2:LYS:N	2.41	0.53
3:h2:1:SER:OG	3:h2:2:LYS:N	2.41	0.53
3:2c:1:SER:OG	3:2c:2:LYS:N	2.41	0.53
3:ab:1:SER:OG	3:ab:2:LYS:N	2.41	0.53
3:M2:1:SER:OG	3:M2:2:LYS:N	2.41	0.53
3:O2:1:SER:OG	3:O2:2:LYS:N	2.41	0.53
3:2C:19:GLN:OE1	3:2C:21:THR:OG1	2.23	0.53
3:M1:19:GLN:OE1	3:M1:21:THR:OG1	2.23	0.52
3:I2:121:ASN:HD22	3:J2:30:LYS:HD2	1.74	0.52
3:f2:19:GLN:OE1	3:f2:21:THR:OG1	2.23	0.52
3:82:19:GLN:OE1	3:82:21:THR:OG1	2.23	0.52
3:2D:1:SER:OG	3:2D:2:LYS:N	2.41	0.52
3:2R:1:SER:OG	3:2R:2:LYS:N	2.42	0.52
3:2T:1:SER:OG	3:2T:2:LYS:N	2.41	0.52
3:2V:19:GLN:OE1	3:2V:21:THR:OG1	2.23	0.52
1:R:21:A:H2'	1:R:22:U:C6	2.44	0.52
3:p2:1:SER:OG	3:p2:2:LYS:N	2.41	0.52
3:2g:121:ASN:HD22	3:2h:30:LYS:HD2	1.75	0.52
3:2v:1:SER:OG	3:2v:2:LYS:N	2.41	0.52
3:I2:84:TRP:CZ3	3:2Q:88:VAL:HG13	2.45	0.52
3:Y2:1:SER:OG	3:Y2:2:LYS:N	2.41	0.52
3:a2:121:ASN:HD22	3:b2:30:LYS:HD2	1.74	0.52
3:42:121:ASN:HD22	3:52:30:LYS:HD2	1.74	0.52
3:2H:19:GLN:OE1	3:2H:21:THR:OG1	2.23	0.52
1:R:74:C:H2'	1:R:74:C:O2	2.10	0.52
3:z1:13:ARG:HH11	3:2V:105:LEU:HD11	1.73	0.52
3:D2:1:SER:OG	3:D2:2:LYS:N	2.41	0.52
3:2z:1:SER:OG	3:2z:2:LYS:N	2.42	0.52
3:I2:127:ARG:C	3:2Q:2:LYS:HD2	2.34	0.52
3:v2:1:SER:OG	3:v2:2:LYS:N	2.41	0.52
1:R:31:G:N2	1:R:32:C:O2	2.43	0.52
2:M:180:GLN:HE21	2:M:209:LEU:HD13	1.75	0.52
3:2V:1:SER:OG	3:2V:2:LYS:N	2.41	0.52
1:R:69:U:H2'	1:R:70:A:C8	2.44	0.52
3:71:98:SER:OG	3:2U:82:GLN:NE2	2.42	0.52
3:s2:121:ASN:HD22	3:t2:30:LYS:HD2	1.75	0.52
1:R:32:C:C2'	1:R:53:G:H22	2.21	0.52
3:m2:121:ASN:HD22	3:n2:30:LYS:HD2	1.74	0.52
2:m:30:PRO:O	2:m:110:ARG:NE	2.41	0.52
3:W2:1:SER:OG	3:W2:2:LYS:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:12:1:SER:OG	3:12:2:LYS:N	2.41	0.52
1:R:40:U:C2'	1:R:42:C:H4'	2.39	0.51
3:O2:121:ASN:HD22	3:P2:30:LYS:HD2	1.74	0.51
3:2C:1:SER:OG	3:2C:2:LYS:N	2.41	0.51
3:02:1:SER:OG	3:02:2:LYS:N	2.41	0.51
1:R:29:U:H2'	1:R:30:G:H8	1.76	0.51
1:R:57:C:N4	1:R:59:U:O4'	2.43	0.51
3:2i:1:SER:OG	3:2i:2:LYS:N	2.41	0.51
3:2j:1:SER:OG	3:2j:2:LYS:N	2.41	0.51
1:R:59:U:H2'	1:R:59:U:O2	2.11	0.51
3:51:45:ARG:HH12	3:51:56:ASN:ND2	2.09	0.51
3:b2:1:SER:OG	3:b2:2:LYS:N	2.42	0.51
1:R:86:A:H2'	1:R:86:A:N3	2.24	0.51
3:a1:45:ARG:HH12	3:a1:56:ASN:ND2	2.09	0.51
3:i1:45:ARG:HH12	3:i1:56:ASN:ND2	2.09	0.51
3:K1:45:ARG:HH12	3:K1:56:ASN:ND2	2.09	0.51
3:M1:45:ARG:HH12	3:M1:56:ASN:ND2	2.09	0.51
3:J2:76:PRO:HD2	3:2Q:93:ASN:HD22	1.75	0.51
3:c2:1:SER:OG	3:c2:2:LYS:N	2.42	0.51
3:s2:1:SER:OG	3:s2:2:LYS:N	2.41	0.51
3:2J:1:SER:OG	3:2J:2:LYS:N	2.41	0.51
3:2Q:121:ASN:HD22	3:2R:30:LYS:HD2	1.74	0.51
3:E1:45:ARG:HH12	3:E1:56:ASN:ND2	2.09	0.51
3:F1:45:ARG:HH12	3:F1:56:ASN:ND2	2.09	0.51
3:L1:45:ARG:HH12	3:L1:56:ASN:ND2	2.09	0.51
3:41:45:ARG:HH12	3:41:56:ASN:ND2	2.09	0.51
3:X2:1:SER:OG	3:X2:2:LYS:N	2.41	0.51
3:x2:1:SER:OG	3:x2:2:LYS:N	2.41	0.51
3:h1:45:ARG:HH12	3:h1:56:ASN:ND2	2.09	0.51
3:p1:45:ARG:HH12	3:p1:56:ASN:ND2	2.09	0.51
3:w1:45:ARG:HH12	3:w1:56:ASN:ND2	2.09	0.51
3:H1:45:ARG:HH12	3:H1:56:ASN:ND2	2.09	0.51
3:W1:45:ARG:HH12	3:W1:56:ASN:ND2	2.09	0.51
3:31:45:ARG:HH12	3:31:56:ASN:ND2	2.09	0.51
1:R:11:G:C2	1:R:12:G:N7	2.78	0.51
2:M:149:VAL:HG13	2:M:150:ASN:OD1	2.10	0.51
3:j1:45:ARG:HH12	3:j1:56:ASN:ND2	2.09	0.51
3:q1:45:ARG:HH12	3:q1:56:ASN:ND2	2.09	0.51
3:A1:76:PRO:HD2	3:2V:93:ASN:CB	2.40	0.51
3:G1:45:ARG:HH12	3:G1:56:ASN:ND2	2.09	0.51
3:I1:45:ARG:HH12	3:I1:56:ASN:ND2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V1:45:ARG:HH12	3:V1:56:ASN:ND2	2.09	0.51
3:Z1:45:ARG:HH12	3:Z1:56:ASN:ND2	2.09	0.51
3:01:45:ARG:HH12	3:01:56:ASN:ND2	2.09	0.51
3:71:45:ARG:HH12	3:71:56:ASN:ND2	2.09	0.51
3:2y:121:ASN:HD22	3:2z:30:LYS:HD2	1.74	0.51
3:2L:1:SER:OG	3:2L:2:LYS:N	2.41	0.51
3:2P:1:SER:OG	3:2P:2:LYS:N	2.41	0.51
1:R:5:C:H2'	1:R:6:G:N9	2.24	0.51
2:m:361:THR:HG22	2:m:386:LEU:HD12	1.92	0.51
3:l1:45:ARG:HH12	3:l1:56:ASN:ND2	2.09	0.51
3:O1:45:ARG:HH12	3:O1:56:ASN:ND2	2.09	0.51
3:2H:1:SER:OG	3:2H:2:LYS:N	2.41	0.51
1:R:57:C:H2'	1:R:58:U:H5''	1.93	0.51
3:k1:45:ARG:HH12	3:k1:56:ASN:ND2	2.09	0.51
3:v1:45:ARG:HH12	3:v1:56:ASN:ND2	2.09	0.51
3:J1:45:ARG:HH12	3:J1:56:ASN:ND2	2.09	0.51
3:Q1:45:ARG:HH12	3:Q1:56:ASN:ND2	2.09	0.51
3:21:45:ARG:HH12	3:21:56:ASN:ND2	2.09	0.51
3:m2:1:SER:OG	3:m2:2:LYS:N	2.41	0.51
1:R:13:C:O2'	1:R:14:C:O5'	2.28	0.50
1:R:55:G:C5'	3:A1:49:ALA:HB2	2.30	0.50
1:R:55:G:C4'	3:A1:49:ALA:HB3	2.39	0.50
2:m:86:VAL:HG12	2:m:87:PRO:HD2	1.92	0.50
3:b1:45:ARG:HH12	3:b1:56:ASN:ND2	2.09	0.50
3:T1:45:ARG:HH12	3:T1:56:ASN:ND2	2.09	0.50
3:Y1:45:ARG:HH12	3:Y1:56:ASN:ND2	2.09	0.50
3:2t:1:SER:OG	3:2t:2:LYS:N	2.41	0.50
3:J2:1:SER:OG	3:J2:2:LYS:N	2.42	0.50
3:Z2:1:SER:OG	3:Z2:2:LYS:N	2.41	0.50
3:i2:1:SER:OG	3:i2:2:LYS:N	2.41	0.50
3:52:1:SER:OG	3:52:2:LYS:N	2.42	0.50
1:R:12:G:H3'	1:R:13:C:H5	1.75	0.50
3:f1:299:ARG:HH12	3:f1:310:ASN:ND2	2.09	0.50
3:o1:45:ARG:HH12	3:o1:56:ASN:ND2	2.09	0.50
3:D1:45:ARG:HH12	3:D1:56:ASN:ND2	2.09	0.50
3:P1:45:ARG:HH12	3:P1:56:ASN:ND2	2.09	0.50
3:n2:1:SER:OG	3:n2:2:LYS:N	2.42	0.50
3:t1:45:ARG:HH12	3:t1:56:ASN:ND2	2.09	0.50
3:N1:45:ARG:HH12	3:N1:56:ASN:ND2	2.09	0.50
3:11:45:ARG:HH12	3:11:56:ASN:ND2	2.09	0.50
1:R:27:C:H2'	1:R:28:U:C1'	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g1:45:ARG:HH12	3:g1:56:ASN:ND2	2.09	0.50
3:A1:45:ARG:HH12	3:A1:56:ASN:ND2	2.09	0.50
3:d1:45:ARG:HH12	3:d1:56:ASN:ND2	2.09	0.50
3:e1:45:ARG:HH12	3:e1:56:ASN:ND2	2.09	0.50
3:y1:45:ARG:HH12	3:y1:56:ASN:ND2	2.09	0.50
3:2W:1:SER:OG	3:2W:2:LYS:N	2.43	0.50
2:m:52:SER:C	2:m:53:LEU:HD22	2.36	0.50
3:x1:45:ARG:HH12	3:x1:56:ASN:ND2	2.09	0.50
3:B1:45:ARG:HH12	3:B1:56:ASN:ND2	2.09	0.50
3:61:45:ARG:HH12	3:61:56:ASN:ND2	2.09	0.50
3:2f:1:SER:OG	3:2f:2:LYS:N	2.41	0.50
1:R:80:C:N3	2:m:352:ARG:NH2	2.60	0.50
3:n1:45:ARG:HH12	3:n1:56:ASN:ND2	2.09	0.50
3:z1:45:ARG:HH12	3:z1:56:ASN:ND2	2.09	0.50
3:Y1:22:ALA:HB2	3:2M:20:SER:H	1.77	0.50
3:2e:1:SER:OG	3:2e:2:LYS:N	2.41	0.50
3:2l:1:SER:OG	3:2l:2:LYS:N	2.41	0.50
2:m:6:TYR:OH	2:m:22:ARG:NH1	2.45	0.50
3:c1:45:ARG:HH12	3:c1:56:ASN:ND2	2.09	0.50
3:U1:45:ARG:HH12	3:U1:56:ASN:ND2	2.09	0.50
3:V1:22:ALA:HB2	3:i2:20:SER:H	1.77	0.50
3:s1:45:ARG:HH12	3:s1:56:ASN:ND2	2.09	0.49
3:S1:45:ARG:HH12	3:S1:56:ASN:ND2	2.09	0.49
3:X1:45:ARG:HH12	3:X1:56:ASN:ND2	2.09	0.49
3:m1:45:ARG:HH12	3:m1:56:ASN:ND2	2.09	0.49
3:u1:45:ARG:HH12	3:u1:56:ASN:ND2	2.09	0.49
2:m:45:ILE:HG22	2:m:46:VAL:HG23	1.93	0.49
3:e2:1:SER:OG	3:e2:2:LYS:N	2.41	0.49
3:32:1:SER:OG	3:32:2:LYS:N	2.41	0.49
3:ac:1:SER:OG	3:ac:2:LYS:N	2.41	0.49
1:R:9:A:H2'	1:R:10:U:C6	2.47	0.49
1:R:22:U:C2'	1:R:23:G:H5'	2.43	0.49
3:z1:82:GLN:OE1	3:2V:90:ILE:HG12	2.12	0.49
3:R1:45:ARG:HH12	3:R1:56:ASN:ND2	2.09	0.49
3:r1:45:ARG:HH12	3:r1:56:ASN:ND2	2.09	0.49
3:C1:45:ARG:HH12	3:C1:56:ASN:ND2	2.09	0.49
1:R:11:G:C6	1:R:21:A:C6	3.00	0.49
1:R:8:A:N1	1:R:24:C:H1'	2.28	0.49
1:R:15:U:H5''	1:R:16:A:C8	2.48	0.49
3:N1:22:ALA:CB	3:2c:20:SER:H	2.25	0.49
3:r2:1:SER:OG	3:r2:2:LYS:N	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:42:1:SER:OG	3:42:2:LYS:N	2.43	0.49
3:71:125:LEU:HD13	3:2U:57:LEU:HD21	1.95	0.49
3:f2:1:SER:OG	3:f2:2:LYS:N	2.41	0.49
3:2x:1:SER:OG	3:2x:2:LYS:N	2.41	0.49
1:R:80:C:H4'	2:m:55:TYR:CE2	2.47	0.49
3:71:105:LEU:CD1	3:2U:61:GLN:OE1	2.61	0.49
3:2p:1:SER:OG	3:2p:2:LYS:N	2.41	0.49
3:2G:1:SER:OG	3:2G:2:LYS:N	2.41	0.49
2:m:298:LEU:HB3	2:m:336:LEU:HD11	1.94	0.48
3:2y:53:TYR:HE2	3:2y:92:ALA:HB2	1.79	0.48
1:R:75:G:H2'	1:R:76:C:O4'	2.13	0.48
2:m:363:PHE:HB2	2:m:386:LEU:HD11	1.96	0.48
3:51:53:TYR:HE2	3:51:92:ALA:HB2	1.79	0.48
3:61:126:GLY:O	3:ab:2:LYS:HD2	2.12	0.48
3:I2:6:LEU:HB3	3:2Q:105:LEU:HD22	1.94	0.48
1:R:24:C:O2	1:R:25:C:C5	2.66	0.48
3:b1:53:TYR:HE2	3:b1:92:ALA:HB2	1.79	0.48
3:F1:53:TYR:HE2	3:F1:92:ALA:HB2	1.79	0.48
3:Y1:53:TYR:HE2	3:Y1:92:ALA:HB2	1.79	0.48
3:41:53:TYR:HE2	3:41:92:ALA:HB2	1.79	0.48
3:61:80:TYR:CB	3:ab:91:VAL:HG21	2.43	0.48
3:P2:53:TYR:HE2	3:P2:92:ALA:HB2	1.79	0.48
3:T2:53:TYR:HE2	3:T2:92:ALA:HB2	1.79	0.48
3:z2:53:TYR:HE2	3:z2:92:ALA:HB2	1.79	0.48
3:02:53:TYR:HE2	3:02:92:ALA:HB2	1.79	0.48
3:2f:53:TYR:HE2	3:2f:92:ALA:HB2	1.79	0.48
3:2N:53:TYR:HE2	3:2N:92:ALA:HB2	1.79	0.48
3:2R:53:TYR:HE2	3:2R:92:ALA:HB2	1.79	0.48
3:2V:53:TYR:HE2	3:2V:92:ALA:HB2	1.79	0.48
1:R:3:G:H2'	1:R:4:G:H5'	1.94	0.48
1:R:37:C:H2'	1:R:38:C:C6	2.48	0.48
1:R:91:G:H2'	1:R:92:A:O4'	2.14	0.48
3:t1:53:TYR:HE2	3:t1:92:ALA:HB2	1.79	0.48
3:X1:53:TYR:HE2	3:X1:92:ALA:HB2	1.79	0.48
3:31:53:TYR:HE2	3:31:92:ALA:HB2	1.79	0.48
3:I2:119:VAL:HG13	3:2Q:90:ILE:CD1	2.40	0.48
3:e2:53:TYR:HE2	3:e2:92:ALA:HB2	1.79	0.48
3:h2:53:TYR:HE2	3:h2:92:ALA:HB2	1.79	0.48
3:o2:1:SER:OG	3:o2:2:LYS:N	2.41	0.48
3:p2:53:TYR:HE2	3:p2:92:ALA:HB2	1.79	0.48
3:12:53:TYR:HE2	3:12:92:ALA:HB2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:52:53:TYR:HE2	3:52:92:ALA:HB2	1.79	0.48
3:2r:53:TYR:HE2	3:2r:92:ALA:HB2	1.79	0.48
3:2Y:53:TYR:HE2	3:2Y:92:ALA:HB2	1.79	0.48
3:ac:53:TYR:HE2	3:ac:92:ALA:HB2	1.79	0.48
1:R:58:U:H4'	1:R:59:U:OP2	2.13	0.48
3:i1:53:TYR:HE2	3:i1:92:ALA:HB2	1.79	0.48
3:j1:53:TYR:HE2	3:j1:92:ALA:HB2	1.79	0.48
3:m1:53:TYR:HE2	3:m1:92:ALA:HB2	1.79	0.48
3:o1:53:TYR:HE2	3:o1:92:ALA:HB2	1.79	0.48
3:z1:53:TYR:HE2	3:z1:92:ALA:HB2	1.79	0.48
3:z1:109:LEU:HD21	3:2V:40:LEU:HD13	1.96	0.48
3:C1:53:TYR:HE2	3:C1:92:ALA:HB2	1.79	0.48
3:J1:53:TYR:HE2	3:J1:92:ALA:HB2	1.79	0.48
3:Q1:22:ALA:HB2	3:2F:20:SER:H	1.78	0.48
3:71:53:TYR:HE2	3:71:92:ALA:HB2	1.79	0.48
3:Q2:53:TYR:HE2	3:Q2:92:ALA:HB2	1.79	0.48
3:d2:53:TYR:HE2	3:d2:92:ALA:HB2	1.79	0.48
3:x2:53:TYR:HE2	3:x2:92:ALA:HB2	1.79	0.48
3:22:53:TYR:HE2	3:22:92:ALA:HB2	1.79	0.48
3:62:53:TYR:HE2	3:62:92:ALA:HB2	1.79	0.48
3:2q:53:TYR:HE2	3:2q:92:ALA:HB2	1.79	0.48
2:m:95:SER:OG	2:m:96:GLU:N	2.39	0.48
3:I1:53:TYR:HE2	3:I1:92:ALA:HB2	1.79	0.48
3:L1:53:TYR:HE2	3:L1:92:ALA:HB2	1.79	0.48
3:O1:53:TYR:HE2	3:O1:92:ALA:HB2	1.79	0.48
3:Z1:53:TYR:HE2	3:Z1:92:ALA:HB2	1.79	0.48
3:F2:53:TYR:HE2	3:F2:92:ALA:HB2	1.79	0.48
3:G2:53:TYR:HE2	3:G2:92:ALA:HB2	1.79	0.48
3:M2:53:TYR:HE2	3:M2:92:ALA:HB2	1.79	0.48
3:P2:1:SER:OG	3:P2:2:LYS:N	2.42	0.48
3:Q2:1:SER:OG	3:Q2:2:LYS:N	2.41	0.48
3:Y2:53:TYR:HE2	3:Y2:92:ALA:HB2	1.79	0.48
3:c2:53:TYR:HE2	3:c2:92:ALA:HB2	1.79	0.48
3:r2:53:TYR:HE2	3:r2:92:ALA:HB2	1.79	0.48
3:72:53:TYR:HE2	3:72:92:ALA:HB2	1.79	0.48
3:2a:53:TYR:HE2	3:2a:92:ALA:HB2	1.79	0.48
3:2c:53:TYR:HE2	3:2c:92:ALA:HB2	1.79	0.48
3:2j:53:TYR:HE2	3:2j:92:ALA:HB2	1.79	0.48
3:2P:53:TYR:HE2	3:2P:92:ALA:HB2	1.79	0.48
3:2T:53:TYR:HE2	3:2T:92:ALA:HB2	1.79	0.48
3:2W:53:TYR:HE2	3:2W:92:ALA:HB2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:aa:53:TYR:HE2	3:aa:92:ALA:HB2	1.79	0.48
2:m:232:LEU:HD23	2:m:294:LEU:C	2.39	0.48
3:W1:53:TYR:HE2	3:W1:92:ALA:HB2	1.79	0.48
3:61:53:TYR:HE2	3:61:92:ALA:HB2	1.79	0.48
3:B2:53:TYR:HE2	3:B2:92:ALA:HB2	1.79	0.48
3:E2:53:TYR:HE2	3:E2:92:ALA:HB2	1.79	0.48
3:H2:53:TYR:HE2	3:H2:92:ALA:HB2	1.79	0.48
3:V2:53:TYR:HE2	3:V2:92:ALA:HB2	1.79	0.48
3:m2:53:TYR:HE2	3:m2:92:ALA:HB2	1.79	0.48
3:s2:53:TYR:HE2	3:s2:92:ALA:HB2	1.79	0.48
3:2C:53:TYR:HE2	3:2C:92:ALA:HB2	1.79	0.48
3:2O:53:TYR:HE2	3:2O:92:ALA:HB2	1.79	0.48
3:c1:53:TYR:HE2	3:c1:92:ALA:HB2	1.79	0.48
3:f1:307:TYR:HE2	3:f1:346:ALA:HB2	1.79	0.48
3:q1:53:TYR:HE2	3:q1:92:ALA:HB2	1.79	0.48
3:A1:53:TYR:HE2	3:A1:92:ALA:HB2	1.79	0.48
3:01:53:TYR:HE2	3:01:92:ALA:HB2	1.79	0.48
3:a2:53:TYR:HE2	3:a2:92:ALA:HB2	1.79	0.48
3:f2:53:TYR:HE2	3:f2:92:ALA:HB2	1.79	0.48
3:o2:53:TYR:HE2	3:o2:92:ALA:HB2	1.79	0.48
3:32:53:TYR:HE2	3:32:92:ALA:HB2	1.79	0.48
3:72:1:SER:OG	3:72:2:LYS:N	2.41	0.48
3:92:53:TYR:HE2	3:92:92:ALA:HB2	1.79	0.48
3:2h:53:TYR:HE2	3:2h:92:ALA:HB2	1.79	0.48
3:2A:53:TYR:HE2	3:2A:92:ALA:HB2	1.79	0.48
3:2E:53:TYR:HE2	3:2E:92:ALA:HB2	1.79	0.48
3:2H:53:TYR:HE2	3:2H:92:ALA:HB2	1.79	0.48
1:R:74:C:H1'	1:R:85:G:H22	1.79	0.48
3:z1:105:LEU:HD12	3:2V:61:GLN:OE1	2.13	0.48
3:H1:53:TYR:HE2	3:H1:92:ALA:HB2	1.79	0.48
3:M1:53:TYR:HE2	3:M1:92:ALA:HB2	1.79	0.48
3:P1:53:TYR:HE2	3:P1:92:ALA:HB2	1.79	0.48
3:R2:53:TYR:HE2	3:R2:92:ALA:HB2	1.79	0.48
3:b2:53:TYR:HE2	3:b2:92:ALA:HB2	1.79	0.48
3:i2:53:TYR:HE2	3:i2:92:ALA:HB2	1.79	0.48
3:l2:53:TYR:HE2	3:l2:92:ALA:HB2	1.79	0.48
3:2b:53:TYR:HE2	3:2b:92:ALA:HB2	1.79	0.48
3:2X:53:TYR:HE2	3:2X:92:ALA:HB2	1.79	0.48
3:ab:53:TYR:HE2	3:ab:92:ALA:HB2	1.79	0.48
3:d1:53:TYR:HE2	3:d1:92:ALA:HB2	1.79	0.48
3:O2:53:TYR:HE2	3:O2:92:ALA:HB2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S2:53:TYR:HE2	3:S2:92:ALA:HB2	1.79	0.48
3:Z2:53:TYR:HE2	3:Z2:92:ALA:HB2	1.79	0.48
3:82:53:TYR:HE2	3:82:92:ALA:HB2	1.79	0.48
3:2n:53:TYR:HE2	3:2n:92:ALA:HB2	1.79	0.48
3:2o:53:TYR:HE2	3:2o:92:ALA:HB2	1.79	0.48
3:ad:53:TYR:HE2	3:ad:92:ALA:HB2	1.79	0.48
1:R:15:U:O5'	2:M:236:ARG:HG3	2.14	0.47
1:R:57:C:H3'	1:R:58:U:H5'	1.96	0.47
2:M:82:ILE:HG23	2:M:82:ILE:O	2.14	0.47
3:g1:53:TYR:HE2	3:g1:92:ALA:HB2	1.79	0.47
3:n1:53:TYR:HE2	3:n1:92:ALA:HB2	1.79	0.47
3:s1:53:TYR:HE2	3:s1:92:ALA:HB2	1.79	0.47
3:v1:53:TYR:HE2	3:v1:92:ALA:HB2	1.79	0.47
3:G1:53:TYR:HE2	3:G1:92:ALA:HB2	1.79	0.47
3:21:53:TYR:HE2	3:21:92:ALA:HB2	1.79	0.47
3:61:13:ARG:HD2	3:ab:105:LEU:HD11	1.96	0.47
3:A2:53:TYR:HE2	3:A2:92:ALA:HB2	1.79	0.47
3:j2:53:TYR:HE2	3:j2:92:ALA:HB2	1.79	0.47
3:42:53:TYR:HE2	3:42:92:ALA:HB2	1.79	0.47
3:2p:53:TYR:HE2	3:2p:92:ALA:HB2	1.79	0.47
1:R:75:G:H2'	1:R:76:C:C1'	2.45	0.47
3:l1:53:TYR:HE2	3:l1:92:ALA:HB2	1.79	0.47
3:p1:53:TYR:HE2	3:p1:92:ALA:HB2	1.79	0.47
3:u1:53:TYR:HE2	3:u1:92:ALA:HB2	1.79	0.47
3:V1:53:TYR:HE2	3:V1:92:ALA:HB2	1.79	0.47
3:11:53:TYR:HE2	3:11:92:ALA:HB2	1.79	0.47
3:K2:53:TYR:HE2	3:K2:92:ALA:HB2	1.79	0.47
3:k2:53:TYR:HE2	3:k2:92:ALA:HB2	1.79	0.47
3:u2:53:TYR:HE2	3:u2:92:ALA:HB2	1.79	0.47
3:2k:53:TYR:HE2	3:2k:92:ALA:HB2	1.79	0.47
3:2Q:53:TYR:HE2	3:2Q:92:ALA:HB2	1.79	0.47
3:ad:1:SER:OG	3:ad:2:LYS:N	2.41	0.47
3:D1:53:TYR:HE2	3:D1:92:ALA:HB2	1.79	0.47
3:E1:53:TYR:HE2	3:E1:92:ALA:HB2	1.79	0.47
3:U2:53:TYR:HE2	3:U2:92:ALA:HB2	1.79	0.47
3:2m:53:TYR:HE2	3:2m:92:ALA:HB2	1.79	0.47
3:2s:53:TYR:HE2	3:2s:92:ALA:HB2	1.79	0.47
3:2J:53:TYR:HE2	3:2J:92:ALA:HB2	1.79	0.47
3:2S:53:TYR:HE2	3:2S:92:ALA:HB2	1.79	0.47
3:h1:53:TYR:HE2	3:h1:92:ALA:HB2	1.79	0.47
3:K1:53:TYR:HE2	3:K1:92:ALA:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R1:53:TYR:HE2	3:R1:92:ALA:HB2	1.79	0.47
3:U1:53:TYR:HE2	3:U1:92:ALA:HB2	1.79	0.47
3:J2:53:TYR:HE2	3:J2:92:ALA:HB2	1.79	0.47
3:g2:53:TYR:HE2	3:g2:92:ALA:HB2	1.79	0.47
3:n2:53:TYR:HE2	3:n2:92:ALA:HB2	1.79	0.47
3:2e:53:TYR:HE2	3:2e:92:ALA:HB2	1.79	0.47
1:R:7:A:C8	1:R:8:A:H5''	2.47	0.47
2:M:261:ASN:OD1	2:M:262:TRP:N	2.47	0.47
3:k1:112:THR:HG23	3:k1:114:GLN:H	1.80	0.47
3:p1:53:TYR:OH	3:q2:34:LEU:HD22	2.14	0.47
3:r1:53:TYR:HE2	3:r1:92:ALA:HB2	1.79	0.47
3:r1:112:THR:HG23	3:r1:114:GLN:H	1.80	0.47
3:y1:53:TYR:HE2	3:y1:92:ALA:HB2	1.79	0.47
3:L1:22:ALA:HB2	3:2p:20:SER:H	1.78	0.47
3:S1:53:TYR:HE2	3:S1:92:ALA:HB2	1.79	0.47
3:U1:107:LYS:HD2	3:t2:111:ALA:HA	1.96	0.47
3:2l:53:TYR:HE2	3:2l:92:ALA:HB2	1.79	0.47
3:2F:53:TYR:HE2	3:2F:92:ALA:HB2	1.79	0.47
3:2G:112:THR:HG23	3:2G:114:GLN:H	1.80	0.47
3:a1:53:TYR:HE2	3:a1:92:ALA:HB2	1.79	0.47
3:e1:53:TYR:HE2	3:e1:92:ALA:HB2	1.79	0.47
3:n1:112:THR:HG23	3:n1:114:GLN:H	1.80	0.47
3:K1:112:THR:HG23	3:K1:114:GLN:H	1.80	0.47
3:G2:112:THR:HG23	3:G2:114:GLN:H	1.80	0.47
3:I2:112:THR:HG23	3:I2:114:GLN:H	1.80	0.47
3:K2:112:THR:HG23	3:K2:114:GLN:H	1.80	0.47
3:R2:112:THR:HG23	3:R2:114:GLN:H	1.80	0.47
3:c2:112:THR:HG23	3:c2:114:GLN:H	1.80	0.47
3:m2:112:THR:HG23	3:m2:114:GLN:H	1.80	0.47
3:62:112:THR:HG23	3:62:114:GLN:H	1.80	0.47
3:2a:112:THR:HG23	3:2a:114:GLN:H	1.80	0.47
3:2i:112:THR:HG23	3:2i:114:GLN:H	1.80	0.47
3:2t:53:TYR:HE2	3:2t:92:ALA:HB2	1.79	0.47
3:2t:112:THR:HG23	3:2t:114:GLN:H	1.80	0.47
3:2B:112:THR:HG23	3:2B:114:GLN:H	1.80	0.47
3:2I:53:TYR:HE2	3:2I:92:ALA:HB2	1.79	0.47
3:2M:53:TYR:HE2	3:2M:92:ALA:HB2	1.79	0.47
3:2U:53:TYR:HE2	3:2U:92:ALA:HB2	1.79	0.47
1:R:3:G:C2'	1:R:4:G:H5'	2.45	0.47
2:m:42:ALA:HB1	2:m:43:PRO:HD2	1.97	0.47
3:a1:112:THR:HG23	3:a1:114:GLN:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d1:112:THR:HG23	3:d1:114:GLN:H	1.80	0.47
3:m1:112:THR:HG23	3:m1:114:GLN:H	1.80	0.47
3:o1:112:THR:HG23	3:o1:114:GLN:H	1.80	0.47
3:p1:112:THR:HG23	3:p1:114:GLN:H	1.80	0.47
3:w1:53:TYR:HE2	3:w1:92:ALA:HB2	1.79	0.47
3:B1:112:THR:HG23	3:B1:114:GLN:H	1.80	0.47
3:T1:53:TYR:HE2	3:T1:92:ALA:HB2	1.79	0.47
3:U1:112:THR:HG23	3:U1:114:GLN:H	1.80	0.47
3:W1:112:THR:HG23	3:W1:114:GLN:H	1.80	0.47
3:41:112:THR:HG23	3:41:114:GLN:H	1.80	0.47
3:B2:112:THR:HG23	3:B2:114:GLN:H	1.80	0.47
3:C2:53:TYR:HE2	3:C2:92:ALA:HB2	1.79	0.47
3:F2:112:THR:HG23	3:F2:114:GLN:H	1.80	0.47
3:L2:53:TYR:HE2	3:L2:92:ALA:HB2	1.79	0.47
3:M2:112:THR:HG23	3:M2:114:GLN:H	1.80	0.47
3:N2:53:TYR:HE2	3:N2:92:ALA:HB2	1.79	0.47
3:T2:112:THR:HG23	3:T2:114:GLN:H	1.80	0.47
3:W2:53:TYR:HE2	3:W2:92:ALA:HB2	1.79	0.47
3:b2:112:THR:HG23	3:b2:114:GLN:H	1.80	0.47
3:r2:112:THR:HG23	3:r2:114:GLN:H	1.80	0.47
3:t2:53:TYR:HE2	3:t2:92:ALA:HB2	1.79	0.47
3:x2:112:THR:HG23	3:x2:114:GLN:H	1.80	0.47
3:02:112:THR:HG23	3:02:114:GLN:H	1.80	0.47
3:32:112:THR:HG23	3:32:114:GLN:H	1.80	0.47
3:52:112:THR:HG23	3:52:114:GLN:H	1.80	0.47
3:92:112:THR:HG23	3:92:114:GLN:H	1.80	0.47
3:2d:53:TYR:HE2	3:2d:92:ALA:HB2	1.79	0.47
3:2g:53:TYR:HE2	3:2g:92:ALA:HB2	1.79	0.47
3:2p:112:THR:HG23	3:2p:114:GLN:H	1.80	0.47
3:2s:112:THR:HG23	3:2s:114:GLN:H	1.80	0.47
3:2x:53:TYR:HE2	3:2x:92:ALA:HB2	1.79	0.47
3:2B:53:TYR:HE2	3:2B:92:ALA:HB2	1.79	0.47
3:2E:112:THR:HG23	3:2E:114:GLN:H	1.80	0.47
3:2K:53:TYR:HE2	3:2K:92:ALA:HB2	1.79	0.47
3:2N:112:THR:HG23	3:2N:114:GLN:H	1.80	0.47
3:2Q:112:THR:HG23	3:2Q:114:GLN:H	1.80	0.47
3:2U:112:THR:HG23	3:2U:114:GLN:H	1.80	0.47
3:ab:112:THR:HG23	3:ab:114:GLN:H	1.80	0.47
1:R:80:C:C2'	1:R:81:A:H5'	2.43	0.47
3:v1:112:THR:HG23	3:v1:114:GLN:H	1.80	0.47
3:N1:53:TYR:HE2	3:N1:92:ALA:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J2:112:THR:HG23	3:J2:114:GLN:H	1.80	0.47
3:U2:112:THR:HG23	3:U2:114:GLN:H	1.80	0.47
3:q2:112:THR:HG23	3:q2:114:GLN:H	1.80	0.47
3:2e:112:THR:HG23	3:2e:114:GLN:H	1.80	0.47
3:2m:112:THR:HG23	3:2m:114:GLN:H	1.80	0.47
3:2v:53:TYR:HE2	3:2v:92:ALA:HB2	1.79	0.47
3:2w:53:TYR:HE2	3:2w:92:ALA:HB2	1.79	0.47
3:2z:53:TYR:HE2	3:2z:92:ALA:HB2	1.79	0.47
3:2G:53:TYR:HE2	3:2G:92:ALA:HB2	1.79	0.47
3:2T:112:THR:HG23	3:2T:114:GLN:H	1.80	0.47
3:2Z:53:TYR:HE2	3:2Z:92:ALA:HB2	1.79	0.47
2:m:340:ILE:HD11	2:m:411:PHE:CB	2.45	0.47
3:e1:112:THR:HG23	3:e1:114:GLN:H	1.80	0.47
3:t1:112:THR:HG23	3:t1:114:GLN:H	1.80	0.47
3:H1:112:THR:HG23	3:H1:114:GLN:H	1.80	0.47
3:T1:22:ALA:HB2	3:y2:20:SER:H	1.80	0.47
3:V1:112:THR:HG23	3:V1:114:GLN:H	1.80	0.47
3:D2:112:THR:HG23	3:D2:114:GLN:H	1.80	0.47
3:H2:112:THR:HG23	3:H2:114:GLN:H	1.80	0.47
3:P2:112:THR:HG23	3:P2:114:GLN:H	1.80	0.47
3:W2:112:THR:HG23	3:W2:114:GLN:H	1.80	0.47
3:Y2:112:THR:HG23	3:Y2:114:GLN:H	1.80	0.47
3:n2:112:THR:HG23	3:n2:114:GLN:H	1.80	0.47
3:t2:112:THR:HG23	3:t2:114:GLN:H	1.80	0.47
3:u2:112:THR:HG23	3:u2:114:GLN:H	1.80	0.47
3:y2:53:TYR:HE2	3:y2:92:ALA:HB2	1.79	0.47
3:42:112:THR:HG23	3:42:114:GLN:H	1.80	0.47
3:2l:112:THR:HG23	3:2l:114:GLN:H	1.80	0.47
3:2y:112:THR:HG23	3:2y:114:GLN:H	1.80	0.47
3:2K:112:THR:HG23	3:2K:114:GLN:H	1.80	0.47
3:2L:53:TYR:HE2	3:2L:92:ALA:HB2	1.79	0.47
3:f1:366:THR:HG23	3:f1:368:GLN:H	1.80	0.47
3:k1:53:TYR:HE2	3:k1:92:ALA:HB2	1.79	0.47
3:u1:112:THR:HG23	3:u1:114:GLN:H	1.80	0.47
3:w1:112:THR:HG23	3:w1:114:GLN:H	1.80	0.47
3:z1:13:ARG:HH11	3:2V:105:LEU:CD1	2.28	0.47
3:G1:112:THR:HG23	3:G1:114:GLN:H	1.80	0.47
3:M1:112:THR:HG23	3:M1:114:GLN:H	1.80	0.47
3:P1:93:ASN:HB2	3:2y:76:PRO:HD2	1.96	0.47
3:11:112:THR:HG23	3:11:114:GLN:H	1.80	0.47
3:I2:13:ARG:HD2	3:2Q:105:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I2:53:TYR:HE2	3:I2:92:ALA:HB2	1.79	0.47
3:N2:112:THR:HG23	3:N2:114:GLN:H	1.80	0.47
3:X2:53:TYR:HE2	3:X2:92:ALA:HB2	1.79	0.47
3:s2:112:THR:HG23	3:s2:114:GLN:H	1.80	0.47
3:v2:53:TYR:HE2	3:v2:92:ALA:HB2	1.79	0.47
3:72:112:THR:HG23	3:72:114:GLN:H	1.80	0.47
3:2g:112:THR:HG23	3:2g:114:GLN:H	1.80	0.47
3:2h:112:THR:HG23	3:2h:114:GLN:H	1.80	0.47
3:2w:112:THR:HG23	3:2w:114:GLN:H	1.80	0.47
3:2L:112:THR:HG23	3:2L:114:GLN:H	1.80	0.47
3:2O:112:THR:HG23	3:2O:114:GLN:H	1.80	0.47
1:R:12:G:H3'	1:R:13:C:C5	2.49	0.46
3:z1:84:TRP:CZ2	3:2V:88:VAL:HG22	2.50	0.46
3:Q1:53:TYR:HE2	3:Q1:92:ALA:HB2	1.79	0.46
3:X2:112:THR:HG23	3:X2:114:GLN:H	1.80	0.46
3:2f:112:THR:HG23	3:2f:114:GLN:H	1.80	0.46
3:2i:53:TYR:HE2	3:2i:92:ALA:HB2	1.79	0.46
3:2u:53:TYR:HE2	3:2u:92:ALA:HB2	1.79	0.46
1:R:44:A:O2'	1:R:45:C:H5''	2.15	0.46
3:b1:112:THR:HG23	3:b1:114:GLN:H	1.80	0.46
3:g1:112:THR:HG23	3:g1:114:GLN:H	1.80	0.46
3:P1:112:THR:HG23	3:P1:114:GLN:H	1.80	0.46
3:21:112:THR:HG23	3:21:114:GLN:H	1.80	0.46
3:31:112:THR:HG23	3:31:114:GLN:H	1.80	0.46
3:61:22:ALA:HB2	3:ac:20:SER:H	1.79	0.46
3:71:112:THR:HG23	3:71:114:GLN:H	1.80	0.46
3:Q2:112:THR:HG23	3:Q2:114:GLN:H	1.80	0.46
3:S2:112:THR:HG23	3:S2:114:GLN:H	1.80	0.46
3:V2:1:SER:OG	3:V2:2:LYS:N	2.41	0.46
3:V2:112:THR:HG23	3:V2:114:GLN:H	1.80	0.46
3:y2:112:THR:HG23	3:y2:114:GLN:H	1.80	0.46
3:2I:112:THR:HG23	3:2I:114:GLN:H	1.80	0.46
3:2K:1:SER:OG	3:2K:2:LYS:N	2.41	0.46
3:aa:112:THR:HG23	3:aa:114:GLN:H	1.80	0.46
2:m:151:LEU:N	2:m:152:PRO:HD2	2.29	0.46
2:m:409:VAL:O	2:m:410:ARG:NE	2.48	0.46
3:j1:112:THR:HG23	3:j1:114:GLN:H	1.80	0.46
3:q1:112:THR:HG23	3:q1:114:GLN:H	1.80	0.46
3:C2:112:THR:HG23	3:C2:114:GLN:H	1.80	0.46
3:D2:53:TYR:HE2	3:D2:92:ALA:HB2	1.79	0.46
3:i2:112:THR:HG23	3:i2:114:GLN:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:j2:112:THR:HG23	3:j2:114:GLN:H	1.80	0.46
3:l2:112:THR:HG23	3:l2:114:GLN:H	1.80	0.46
3:q2:53:TYR:HE2	3:q2:92:ALA:HB2	1.79	0.46
3:2j:112:THR:HG23	3:2j:114:GLN:H	1.80	0.46
3:2o:112:THR:HG23	3:2o:114:GLN:H	1.80	0.46
3:2u:112:THR:HG23	3:2u:114:GLN:H	1.80	0.46
3:2A:112:THR:HG23	3:2A:114:GLN:H	1.80	0.46
3:2C:112:THR:HG23	3:2C:114:GLN:H	1.80	0.46
3:2D:53:TYR:HE2	3:2D:92:ALA:HB2	1.79	0.46
3:2H:112:THR:HG23	3:2H:114:GLN:H	1.80	0.46
3:2Z:112:THR:HG23	3:2Z:114:GLN:H	1.80	0.46
3:t1:111:ALA:HA	3:2z:107:LYS:HD2	1.96	0.46
3:B1:53:TYR:HE2	3:B1:92:ALA:HB2	1.79	0.46
3:C1:112:THR:HG23	3:C1:114:GLN:H	1.80	0.46
3:S1:112:THR:HG23	3:S1:114:GLN:H	1.80	0.46
3:L2:112:THR:HG23	3:L2:114:GLN:H	1.80	0.46
3:m2:83:VAL:H	3:2a:89:THR:HG1	1.62	0.46
3:2c:112:THR:HG23	3:2c:114:GLN:H	1.80	0.46
3:2P:112:THR:HG23	3:2P:114:GLN:H	1.80	0.46
3:x1:53:TYR:HE2	3:x1:92:ALA:HB2	1.79	0.46
3:z1:7:SER:O	3:2V:108:SER:CB	2.63	0.46
3:z1:84:TRP:HA	3:2V:87:ASP:O	2.16	0.46
3:B1:107:LYS:HD2	3:b2:111:ALA:HA	1.97	0.46
3:D1:112:THR:HG23	3:D1:114:GLN:H	1.80	0.46
3:L1:112:THR:HG23	3:L1:114:GLN:H	1.80	0.46
3:01:112:THR:HG23	3:01:114:GLN:H	1.80	0.46
3:a2:112:THR:HG23	3:a2:114:GLN:H	1.80	0.46
3:v2:112:THR:HG23	3:v2:114:GLN:H	1.80	0.46
3:w2:53:TYR:HE2	3:w2:92:ALA:HB2	1.79	0.46
3:2r:112:THR:HG23	3:2r:114:GLN:H	1.80	0.46
3:2M:1:SER:OG	3:2M:2:LYS:N	2.41	0.46
3:2S:1:SER:OG	3:2S:2:LYS:N	2.41	0.46
2:m:232:LEU:HD22	2:m:296:THR:N	2.31	0.46
2:M:312:THR:OG1	2:M:313:THR:N	2.49	0.46
3:e2:112:THR:HG23	3:e2:114:GLN:H	1.80	0.46
3:g2:112:THR:HG23	3:g2:114:GLN:H	1.80	0.46
1:R:30:G:H2'	1:R:31:G:H8	1.79	0.46
2:M:57:SER:OG	2:M:396:ASP:OD1	2.27	0.46
3:o1:22:ALA:HB2	3:O2:20:SER:H	1.81	0.46
3:N1:112:THR:HG23	3:N1:114:GLN:H	1.80	0.46
3:61:112:THR:HG23	3:61:114:GLN:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:w2:112:THR:HG23	3:w2:114:GLN:H	1.80	0.46
3:2d:112:THR:HG23	3:2d:114:GLN:H	1.80	0.46
3:2k:112:THR:HG23	3:2k:114:GLN:H	1.80	0.46
3:2q:112:THR:HG23	3:2q:114:GLN:H	1.80	0.46
3:2R:112:THR:HG23	3:2R:114:GLN:H	1.80	0.46
3:2Y:112:THR:HG23	3:2Y:114:GLN:H	1.80	0.46
1:R:81:A:OP1	2:m:398:ARG:NH1	2.49	0.46
3:i1:112:THR:HG23	3:i1:114:GLN:H	1.80	0.46
3:R1:112:THR:HG23	3:R1:114:GLN:H	1.80	0.46
3:Y1:112:THR:HG23	3:Y1:114:GLN:H	1.80	0.46
3:A2:112:THR:HG23	3:A2:114:GLN:H	1.80	0.46
3:f2:112:THR:HG23	3:f2:114:GLN:H	1.80	0.46
3:z2:112:THR:HG23	3:z2:114:GLN:H	1.80	0.46
3:12:112:THR:HG23	3:12:114:GLN:H	1.80	0.46
3:2b:112:THR:HG23	3:2b:114:GLN:H	1.80	0.46
3:2v:112:THR:HG23	3:2v:114:GLN:H	1.80	0.46
3:2z:112:THR:HG23	3:2z:114:GLN:H	1.80	0.46
3:2M:112:THR:HG23	3:2M:114:GLN:H	1.80	0.46
3:2S:112:THR:HG23	3:2S:114:GLN:H	1.80	0.46
3:z1:125:LEU:HD23	3:2V:27:PHE:CE1	2.51	0.46
3:X1:112:THR:HG23	3:X1:114:GLN:H	1.80	0.46
3:01:111:ALA:HA	3:72:107:LYS:HD2	1.98	0.46
3:E2:112:THR:HG23	3:E2:114:GLN:H	1.80	0.46
3:22:112:THR:HG23	3:22:114:GLN:H	1.80	0.46
3:2n:112:THR:HG23	3:2n:114:GLN:H	1.80	0.46
3:2q:1:SER:OG	3:2q:2:LYS:N	2.41	0.46
2:M:91:CYS:SG	2:M:92:ASP:N	2.89	0.46
3:F1:112:THR:HG23	3:F1:114:GLN:H	1.80	0.46
3:I1:112:THR:HG23	3:I1:114:GLN:H	1.80	0.46
3:Q1:112:THR:HG23	3:Q1:114:GLN:H	1.80	0.46
3:51:112:THR:HG23	3:51:114:GLN:H	1.80	0.46
3:61:105:LEU:HD11	3:ab:13:ARG:NH1	2.29	0.46
3:d2:112:THR:HG23	3:d2:114:GLN:H	1.80	0.46
3:q2:1:SER:OG	3:q2:2:LYS:N	2.41	0.46
3:2x:112:THR:HG23	3:2x:114:GLN:H	1.80	0.46
3:2V:112:THR:HG23	3:2V:114:GLN:H	1.80	0.46
3:ad:112:THR:HG23	3:ad:114:GLN:H	1.80	0.46
1:R:60:C:H5'	1:R:61:U:OP2	2.16	0.45
3:c1:112:THR:HG23	3:c1:114:GLN:H	1.80	0.45
3:Z2:112:THR:HG23	3:Z2:114:GLN:H	1.80	0.45
3:d2:1:SER:OG	3:d2:2:LYS:N	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2X:112:THR:HG23	3:2X:114:GLN:H	1.80	0.45
1:R:12:G:C5	1:R:13:C:C4	3.05	0.45
2:M:368:VAL:HG13	2:M:370:PRO:HD3	1.98	0.45
3:s1:112:THR:HG23	3:s1:114:GLN:H	1.80	0.45
3:y1:112:THR:HG23	3:y1:114:GLN:H	1.80	0.45
3:O1:112:THR:HG23	3:O1:114:GLN:H	1.80	0.45
3:l1:112:THR:HG23	3:l1:114:GLN:H	1.80	0.45
3:71:84:TRP:CZ2	3:2U:88:VAL:HG22	2.51	0.45
3:2E:1:SER:OG	3:2E:2:LYS:N	2.41	0.45
3:2W:112:THR:HG23	3:2W:114:GLN:H	1.80	0.45
1:R:67:C:H2'	1:R:68:G:H8	1.81	0.45
2:M:106:VAL:HG13	2:M:111:PHE:CE2	2.51	0.45
3:c1:111:ALA:HA	3:P2:107:LYS:HD2	1.98	0.45
3:x1:112:THR:HG23	3:x1:114:GLN:H	1.80	0.45
3:z1:84:TRP:CH2	3:2V:88:VAL:HG22	2.51	0.45
3:E1:112:THR:HG23	3:E1:114:GLN:H	1.80	0.45
3:k2:112:THR:HG23	3:k2:114:GLN:H	1.80	0.45
3:p2:112:THR:HG23	3:p2:114:GLN:H	1.80	0.45
3:2J:112:THR:HG23	3:2J:114:GLN:H	1.80	0.45
3:A1:112:THR:HG23	3:A1:114:GLN:H	1.80	0.45
3:T1:112:THR:HG23	3:T1:114:GLN:H	1.80	0.45
3:h2:112:THR:HG23	3:h2:114:GLN:H	1.80	0.45
3:m2:105:LEU:HD13	3:2a:38:LEU:HD22	1.98	0.45
3:o2:112:THR:HG23	3:o2:114:GLN:H	1.80	0.45
3:82:112:THR:HG23	3:82:114:GLN:H	1.80	0.45
3:ac:112:THR:HG23	3:ac:114:GLN:H	1.80	0.45
3:z1:112:THR:HG23	3:z1:114:GLN:H	1.80	0.45
3:C1:111:ALA:HA	3:J2:107:LYS:HD2	1.99	0.45
3:Z1:112:THR:HG23	3:Z1:114:GLN:H	1.80	0.45
3:2g:1:SER:OG	3:2g:2:LYS:N	2.41	0.45
3:2F:112:THR:HG23	3:2F:114:GLN:H	1.80	0.45
3:J1:112:THR:HG23	3:J1:114:GLN:H	1.80	0.45
3:O2:112:THR:HG23	3:O2:114:GLN:H	1.80	0.45
3:h1:18:ILE:HD12	3:h1:19:GLN:HB2	1.99	0.45
3:i1:18:ILE:HD12	3:i1:19:GLN:HB2	1.99	0.45
3:s1:18:ILE:HD12	3:s1:19:GLN:HB2	1.99	0.45
3:x1:18:ILE:HD12	3:x1:19:GLN:HB2	1.99	0.45
3:y1:18:ILE:HD12	3:y1:19:GLN:HB2	1.99	0.45
3:P1:22:ALA:HB1	3:2y:18:ILE:O	2.17	0.45
3:41:87:ASP:O	3:n2:84:TRP:HA	2.17	0.45
3:l1:18:ILE:HD12	3:l1:19:GLN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H1:18:ILE:HD12	3:H1:19:GLN:HB2	1.99	0.45
3:J1:18:ILE:HD12	3:J1:19:GLN:HB2	1.99	0.45
3:O1:18:ILE:HD12	3:O1:19:GLN:HB2	1.99	0.45
3:31:107:LYS:HD2	3:52:111:ALA:HA	1.98	0.45
2:M:58:ARG:HD2	2:M:395:THR:HG23	1.99	0.45
3:c1:18:ILE:HD12	3:c1:19:GLN:HB2	1.99	0.45
3:h1:112:THR:HG23	3:h1:114:GLN:H	1.80	0.45
3:A1:18:ILE:HD12	3:A1:19:GLN:HB2	1.99	0.45
3:F1:18:ILE:HD12	3:F1:19:GLN:HB2	1.99	0.45
3:Q1:18:ILE:HD12	3:Q1:19:GLN:HB2	1.99	0.45
3:31:18:ILE:HD12	3:31:19:GLN:HB2	1.99	0.45
3:2D:112:THR:HG23	3:2D:114:GLN:H	1.80	0.45
1:R:14:C:H2'	2:M:238:HIS:CE1	2.52	0.44
1:R:82:G:H5''	1:R:83:C:O5'	2.18	0.44
3:r1:18:ILE:HD12	3:r1:19:GLN:HB2	1.99	0.44
3:X1:18:ILE:HD12	3:X1:19:GLN:HB2	1.99	0.44
3:21:18:ILE:HD12	3:21:19:GLN:HB2	1.99	0.44
3:I2:118:LEU:HD21	3:2Q:55:VAL:CG1	2.47	0.44
3:g2:1:SER:OG	3:g2:2:LYS:N	2.41	0.44
1:R:77:G:H2'	1:R:78:C:C6	2.52	0.44
2:M:98:VAL:HG23	2:M:99:SER:N	2.32	0.44
3:m1:18:ILE:HD12	3:m1:19:GLN:HB2	1.99	0.44
3:n1:18:ILE:HD12	3:n1:19:GLN:HB2	1.99	0.44
3:q1:18:ILE:HD12	3:q1:19:GLN:HB2	1.99	0.44
3:11:18:ILE:HD12	3:11:19:GLN:HB2	1.99	0.44
3:t1:18:ILE:HD12	3:t1:19:GLN:HB2	1.99	0.44
3:B1:18:ILE:HD12	3:B1:19:GLN:HB2	1.99	0.44
3:G1:18:ILE:HD12	3:G1:19:GLN:HB2	1.99	0.44
3:K1:18:ILE:HD12	3:K1:19:GLN:HB2	1.99	0.44
3:M1:18:ILE:HD12	3:M1:19:GLN:HB2	1.99	0.44
3:2O:1:SER:OG	3:2O:2:LYS:N	2.41	0.44
1:R:23:G:C4	1:R:24:C:C5	3.05	0.44
3:a1:18:ILE:HD12	3:a1:19:GLN:HB2	1.99	0.44
3:b1:18:ILE:HD12	3:b1:19:GLN:HB2	1.99	0.44
3:k1:18:ILE:HD12	3:k1:19:GLN:HB2	1.99	0.44
3:p1:18:ILE:HD12	3:p1:19:GLN:HB2	1.99	0.44
3:V1:18:ILE:HD12	3:V1:19:GLN:HB2	1.99	0.44
3:61:22:ALA:HB1	3:ac:18:ILE:O	2.18	0.44
3:F2:1:SER:OG	3:F2:2:LYS:N	2.41	0.44
3:92:1:SER:OG	3:92:2:LYS:N	2.41	0.44
1:R:10:U:O2	1:R:10:U:H2'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:12:G:N7	1:R:13:C:N4	2.65	0.44
3:d1:18:ILE:HD12	3:d1:19:GLN:HB2	1.99	0.44
3:f1:272:ILE:HD12	3:f1:273:GLN:HB2	1.99	0.44
3:u1:18:ILE:HD12	3:u1:19:GLN:HB2	1.99	0.44
3:E1:18:ILE:HD12	3:E1:19:GLN:HB2	1.99	0.44
3:L1:39:ARG:HG2	3:L1:60:ASP:HB2	2.00	0.44
3:51:18:ILE:HD12	3:51:19:GLN:HB2	1.99	0.44
3:71:18:ILE:HD12	3:71:19:GLN:HB2	1.99	0.44
3:71:105:LEU:HD12	3:2U:61:GLN:OE1	2.17	0.44
3:P2:39:ARG:HG2	3:P2:60:ASP:HB2	2.00	0.44
3:g1:18:ILE:HD12	3:g1:19:GLN:HB2	1.99	0.44
3:w1:39:ARG:HG2	3:w1:60:ASP:HB2	2.00	0.44
3:z1:127:ARG:C	3:2V:2:LYS:HD2	2.43	0.44
3:L1:18:ILE:HD12	3:L1:19:GLN:HB2	1.99	0.44
3:R1:18:ILE:HD12	3:R1:19:GLN:HB2	1.99	0.44
3:T1:18:ILE:HD12	3:T1:19:GLN:HB2	1.99	0.44
3:Y1:39:ARG:HG2	3:Y1:60:ASP:HB2	2.00	0.44
3:Z1:39:ARG:HG2	3:Z1:60:ASP:HB2	2.00	0.44
3:B2:39:ARG:HG2	3:B2:60:ASP:HB2	2.00	0.44
3:s2:39:ARG:HG2	3:s2:60:ASP:HB2	2.00	0.44
3:x2:39:ARG:HG2	3:x2:60:ASP:HB2	2.00	0.44
3:2k:39:ARG:HG2	3:2k:60:ASP:HB2	2.00	0.44
3:2v:39:ARG:HG2	3:2v:60:ASP:HB2	2.00	0.44
3:2C:39:ARG:HG2	3:2C:60:ASP:HB2	2.00	0.44
3:2K:39:ARG:HG2	3:2K:60:ASP:HB2	2.00	0.44
1:R:7:A:N6	1:R:9:A:H62	2.13	0.44
3:b1:39:ARG:HG2	3:b1:60:ASP:HB2	2.00	0.44
3:d1:39:ARG:HG2	3:d1:60:ASP:HB2	2.00	0.44
3:k1:39:ARG:HG2	3:k1:60:ASP:HB2	2.00	0.44
3:q1:15:LEU:HD11	3:q1:38:LEU:HD23	2.00	0.44
3:w1:18:ILE:HD12	3:w1:19:GLN:HB2	1.99	0.44
3:x1:39:ARG:HG2	3:x1:60:ASP:HB2	2.00	0.44
3:z1:18:ILE:HD12	3:z1:19:GLN:HB2	1.99	0.44
3:E1:22:ALA:CB	3:2Z:20:SER:H	2.31	0.44
3:G1:39:ARG:HG2	3:G1:60:ASP:HB2	2.00	0.44
3:H1:15:LEU:HD11	3:H1:38:LEU:HD23	2.00	0.44
3:H1:39:ARG:HG2	3:H1:60:ASP:HB2	2.00	0.44
3:I1:15:LEU:HD11	3:I1:38:LEU:HD23	2.00	0.44
3:I1:18:ILE:HD12	3:I1:19:GLN:HB2	1.99	0.44
3:I1:39:ARG:HG2	3:I1:60:ASP:HB2	2.00	0.44
3:Y1:15:LEU:HD11	3:Y1:38:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y1:18:ILE:HD12	3:Y1:19:GLN:HB2	1.99	0.44
3:Z1:18:ILE:HD12	3:Z1:19:GLN:HB2	1.99	0.44
3:51:39:ARG:HG2	3:51:60:ASP:HB2	2.00	0.44
3:2g:39:ARG:HG2	3:2g:60:ASP:HB2	2.00	0.44
3:2F:15:LEU:HD11	3:2F:38:LEU:HD23	2.00	0.44
3:e1:18:ILE:HD12	3:e1:19:GLN:HB2	1.99	0.44
3:j1:18:ILE:HD12	3:j1:19:GLN:HB2	1.99	0.44
3:k1:15:LEU:HD11	3:k1:38:LEU:HD23	2.00	0.44
3:r1:39:ARG:HG2	3:r1:60:ASP:HB2	2.00	0.44
3:t1:39:ARG:HG2	3:t1:60:ASP:HB2	2.00	0.44
3:M1:15:LEU:HD11	3:M1:38:LEU:HD23	2.00	0.44
3:N1:18:ILE:HD12	3:N1:19:GLN:HB2	1.99	0.44
3:P1:18:ILE:HD12	3:P1:19:GLN:HB2	1.99	0.44
3:W1:18:ILE:HD12	3:W1:19:GLN:HB2	1.99	0.44
3:C2:15:LEU:HD11	3:C2:38:LEU:HD23	2.00	0.44
3:F2:39:ARG:HG2	3:F2:60:ASP:HB2	2.00	0.44
3:I2:39:ARG:HG2	3:I2:60:ASP:HB2	2.00	0.44
3:J2:39:ARG:HG2	3:J2:60:ASP:HB2	2.00	0.44
3:K2:39:ARG:HG2	3:K2:60:ASP:HB2	2.00	0.44
3:Q2:15:LEU:HD11	3:Q2:38:LEU:HD23	2.00	0.44
3:R2:39:ARG:HG2	3:R2:60:ASP:HB2	2.00	0.44
3:T2:39:ARG:HG2	3:T2:60:ASP:HB2	2.00	0.44
3:U2:39:ARG:HG2	3:U2:60:ASP:HB2	2.00	0.44
3:W2:15:LEU:HD11	3:W2:38:LEU:HD23	2.00	0.44
3:W2:39:ARG:HG2	3:W2:60:ASP:HB2	2.00	0.44
3:e2:39:ARG:HG2	3:e2:60:ASP:HB2	2.00	0.44
3:h2:39:ARG:HG2	3:h2:60:ASP:HB2	2.00	0.44
3:m2:15:LEU:HD11	3:m2:38:LEU:HD23	2.00	0.44
3:m2:82:GLN:OE1	3:2a:90:ILE:HG12	2.17	0.44
3:p2:15:LEU:HD11	3:p2:38:LEU:HD23	2.00	0.44
3:s2:15:LEU:HD11	3:s2:38:LEU:HD23	2.00	0.44
3:u2:39:ARG:HG2	3:u2:60:ASP:HB2	2.00	0.44
3:62:39:ARG:HG2	3:62:60:ASP:HB2	2.00	0.44
3:2e:15:LEU:HD11	3:2e:38:LEU:HD23	2.00	0.44
3:2N:39:ARG:HG2	3:2N:60:ASP:HB2	2.00	0.44
3:2O:15:LEU:HD11	3:2O:38:LEU:HD23	2.00	0.44
3:ab:15:LEU:HD11	3:ab:38:LEU:HD23	2.00	0.44
2:m:10:LYS:HE2	2:m:89:PRO:O	2.18	0.43
2:m:303:ARG:O	2:m:304:ARG:C	2.61	0.43
3:l1:39:ARG:HG2	3:l1:60:ASP:HB2	2.00	0.43
3:n1:15:LEU:HD11	3:n1:38:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o1:39:ARG:HG2	3:o1:60:ASP:HB2	2.00	0.43
3:v1:39:ARG:HG2	3:v1:60:ASP:HB2	2.00	0.43
3:B1:39:ARG:HG2	3:B1:60:ASP:HB2	2.00	0.43
3:C1:15:LEU:HD11	3:C1:38:LEU:HD23	2.00	0.43
3:K1:15:LEU:HD11	3:K1:38:LEU:HD23	2.00	0.43
3:N1:15:LEU:HD11	3:N1:38:LEU:HD23	2.00	0.43
3:Q1:15:LEU:HD11	3:Q1:38:LEU:HD23	2.00	0.43
3:O1:18:ILE:HD12	3:O1:19:GLN:HB2	1.99	0.43
3:51:15:LEU:HD11	3:51:38:LEU:HD23	2.00	0.43
3:61:39:ARG:HG2	3:61:60:ASP:HB2	2.00	0.43
3:71:15:LEU:HD11	3:71:38:LEU:HD23	2.00	0.43
3:B2:15:LEU:HD11	3:B2:38:LEU:HD23	2.00	0.43
3:M2:15:LEU:HD11	3:M2:38:LEU:HD23	2.00	0.43
3:Q2:39:ARG:HG2	3:Q2:60:ASP:HB2	2.00	0.43
3:f2:39:ARG:HG2	3:f2:60:ASP:HB2	2.00	0.43
3:g2:15:LEU:HD11	3:g2:38:LEU:HD23	2.00	0.43
3:q2:15:LEU:HD11	3:q2:38:LEU:HD23	2.00	0.43
3:02:15:LEU:HD11	3:02:38:LEU:HD23	2.00	0.43
3:2d:15:LEU:HD11	3:2d:38:LEU:HD23	2.00	0.43
3:2s:15:LEU:HD11	3:2s:38:LEU:HD23	2.00	0.43
3:2w:39:ARG:HG2	3:2w:60:ASP:HB2	2.00	0.43
3:2O:39:ARG:HG2	3:2O:60:ASP:HB2	2.00	0.43
3:2P:39:ARG:HG2	3:2P:60:ASP:HB2	2.00	0.43
3:2V:15:LEU:HD11	3:2V:38:LEU:HD23	2.00	0.43
3:ad:15:LEU:HD11	3:ad:38:LEU:HD23	2.00	0.43
3:a1:15:LEU:HD11	3:a1:38:LEU:HD23	2.00	0.43
3:e1:15:LEU:HD11	3:e1:38:LEU:HD23	2.00	0.43
3:m1:22:ALA:CB	3:2u:20:SER:H	2.30	0.43
3:y1:39:ARG:HG2	3:y1:60:ASP:HB2	2.00	0.43
3:z1:109:LEU:HD23	3:2V:59:LEU:HD12	1.98	0.43
3:E1:15:LEU:HD11	3:E1:38:LEU:HD23	2.00	0.43
3:P1:15:LEU:HD11	3:P1:38:LEU:HD23	2.00	0.43
3:S1:39:ARG:HG2	3:S1:60:ASP:HB2	2.00	0.43
3:T1:39:ARG:HG2	3:T1:60:ASP:HB2	2.00	0.43
3:U1:18:ILE:HD12	3:U1:19:GLN:HB2	1.99	0.43
3:V1:39:ARG:HG2	3:V1:60:ASP:HB2	2.00	0.43
3:31:15:LEU:HD11	3:31:38:LEU:HD23	2.00	0.43
3:A2:39:ARG:HG2	3:A2:60:ASP:HB2	2.00	0.43
3:D2:39:ARG:HG2	3:D2:60:ASP:HB2	2.00	0.43
3:G2:15:LEU:HD11	3:G2:38:LEU:HD23	2.00	0.43
3:L2:39:ARG:HG2	3:L2:60:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U2:15:LEU:HD11	3:U2:38:LEU:HD23	2.00	0.43
3:b2:39:ARG:HG2	3:b2:60:ASP:HB2	2.00	0.43
3:q2:39:ARG:HG2	3:q2:60:ASP:HB2	2.00	0.43
3:02:39:ARG:HG2	3:02:60:ASP:HB2	2.00	0.43
3:32:39:ARG:HG2	3:32:60:ASP:HB2	2.00	0.43
3:42:15:LEU:HD11	3:42:38:LEU:HD23	2.00	0.43
3:52:15:LEU:HD11	3:52:38:LEU:HD23	2.00	0.43
3:2a:39:ARG:HG2	3:2a:60:ASP:HB2	2.00	0.43
3:2e:39:ARG:HG2	3:2e:60:ASP:HB2	2.00	0.43
3:2i:15:LEU:HD11	3:2i:38:LEU:HD23	2.00	0.43
3:2i:39:ARG:HG2	3:2i:60:ASP:HB2	2.00	0.43
3:2l:15:LEU:HD11	3:2l:38:LEU:HD23	2.00	0.43
3:2x:15:LEU:HD11	3:2x:38:LEU:HD23	2.00	0.43
3:2z:39:ARG:HG2	3:2z:60:ASP:HB2	2.00	0.43
3:2S:39:ARG:HG2	3:2S:60:ASP:HB2	2.00	0.43
3:2X:15:LEU:HD11	3:2X:38:LEU:HD23	2.00	0.43
3:aa:15:LEU:HD11	3:aa:38:LEU:HD23	2.00	0.43
1:R:29:U:O2'	1:R:30:G:H5'	2.18	0.43
2:m:71:LEU:O	2:m:104:ARG:N	2.47	0.43
3:l1:15:LEU:HD11	3:l1:38:LEU:HD23	2.00	0.43
3:z1:15:LEU:HD11	3:z1:38:LEU:HD23	2.00	0.43
3:B1:116:GLU:HB2	3:b2:103:TYR:CZ	2.53	0.43
3:K1:13:ARG:HH11	3:f2:105:LEU:HD11	1.83	0.43
3:T1:22:ALA:CB	3:y2:20:SER:H	2.32	0.43
3:01:15:LEU:HD11	3:01:38:LEU:HD23	2.00	0.43
3:21:15:LEU:HD11	3:21:38:LEU:HD23	2.00	0.43
3:71:8:VAL:HG23	3:2U:105:LEU:CG	2.47	0.43
3:H2:15:LEU:HD11	3:H2:38:LEU:HD23	2.00	0.43
3:H2:39:ARG:HG2	3:H2:60:ASP:HB2	2.00	0.43
3:I2:15:LEU:HD11	3:I2:38:LEU:HD23	2.00	0.43
3:V2:39:ARG:HG2	3:V2:60:ASP:HB2	2.00	0.43
3:Y2:15:LEU:HD11	3:Y2:38:LEU:HD23	2.00	0.43
3:d2:39:ARG:HG2	3:d2:60:ASP:HB2	2.00	0.43
3:n2:15:LEU:HD11	3:n2:38:LEU:HD23	2.00	0.43
3:r2:15:LEU:HD11	3:r2:38:LEU:HD23	2.00	0.43
3:x2:15:LEU:HD11	3:x2:38:LEU:HD23	2.00	0.43
3:y2:39:ARG:HG2	3:y2:60:ASP:HB2	2.00	0.43
3:2n:15:LEU:HD11	3:2n:38:LEU:HD23	2.00	0.43
3:2r:39:ARG:HG2	3:2r:60:ASP:HB2	2.00	0.43
3:2u:15:LEU:HD11	3:2u:38:LEU:HD23	2.00	0.43
3:2z:15:LEU:HD11	3:2z:38:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:184:LEU:CD1	2:m:202:VAL:HG21	2.49	0.43
3:j1:39:ARG:HG2	3:j1:60:ASP:HB2	2.00	0.43
3:m1:39:ARG:HG2	3:m1:60:ASP:HB2	2.00	0.43
3:o1:15:LEU:HD11	3:o1:38:LEU:HD23	2.00	0.43
3:D1:39:ARG:HG2	3:D1:60:ASP:HB2	2.00	0.43
3:S1:15:LEU:HD11	3:S1:38:LEU:HD23	2.00	0.43
3:V1:15:LEU:HD11	3:V1:38:LEU:HD23	2.00	0.43
3:41:18:ILE:HD12	3:41:19:GLN:HB2	1.99	0.43
3:a2:39:ARG:HG2	3:a2:60:ASP:HB2	2.00	0.43
3:d2:15:LEU:HD11	3:d2:38:LEU:HD23	2.00	0.43
3:i2:15:LEU:HD11	3:i2:38:LEU:HD23	2.00	0.43
3:k2:1:SER:OG	3:k2:2:LYS:N	2.41	0.43
3:r2:39:ARG:HG2	3:r2:60:ASP:HB2	2.00	0.43
3:2f:39:ARG:HG2	3:2f:60:ASP:HB2	2.00	0.43
3:2t:39:ARG:HG2	3:2t:60:ASP:HB2	2.00	0.43
3:2F:39:ARG:HG2	3:2F:60:ASP:HB2	2.00	0.43
3:2L:15:LEU:HD11	3:2L:38:LEU:HD23	2.00	0.43
3:2Y:39:ARG:HG2	3:2Y:60:ASP:HB2	2.00	0.43
3:2Z:15:LEU:HD11	3:2Z:38:LEU:HD23	2.00	0.43
3:ac:39:ARG:HG2	3:ac:60:ASP:HB2	2.00	0.43
3:a1:39:ARG:HG2	3:a1:60:ASP:HB2	2.00	0.43
3:d1:15:LEU:HD11	3:d1:38:LEU:HD23	2.00	0.43
3:g1:39:ARG:HG2	3:g1:60:ASP:HB2	2.00	0.43
3:h1:39:ARG:HG2	3:h1:60:ASP:HB2	2.00	0.43
3:o1:18:ILE:HD12	3:o1:19:GLN:HB2	1.99	0.43
3:z1:39:ARG:HG2	3:z1:60:ASP:HB2	2.00	0.43
3:z1:105:LEU:HD11	3:2V:13:ARG:NH1	2.32	0.43
3:N1:39:ARG:HG2	3:N1:60:ASP:HB2	2.00	0.43
3:T1:15:LEU:HD11	3:T1:38:LEU:HD23	2.00	0.43
3:J2:15:LEU:HD11	3:J2:38:LEU:HD23	2.00	0.43
3:c2:39:ARG:HG2	3:c2:60:ASP:HB2	2.00	0.43
3:2j:39:ARG:HG2	3:2j:60:ASP:HB2	2.00	0.43
3:2m:15:LEU:HD11	3:2m:38:LEU:HD23	2.00	0.43
3:2p:15:LEU:HD11	3:2p:38:LEU:HD23	2.00	0.43
3:2B:39:ARG:HG2	3:2B:60:ASP:HB2	2.00	0.43
3:2D:39:ARG:HG2	3:2D:60:ASP:HB2	2.00	0.43
3:2G:39:ARG:HG2	3:2G:60:ASP:HB2	2.00	0.43
3:2H:15:LEU:HD11	3:2H:38:LEU:HD23	2.00	0.43
3:2J:39:ARG:HG2	3:2J:60:ASP:HB2	2.00	0.43
3:2M:15:LEU:HD11	3:2M:38:LEU:HD23	2.00	0.43
3:2Q:39:ARG:HG2	3:2Q:60:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2Y:15:LEU:HD11	3:2Y:38:LEU:HD23	2.00	0.43
3:aa:39:ARG:HG2	3:aa:60:ASP:HB2	2.00	0.43
3:ad:39:ARG:HG2	3:ad:60:ASP:HB2	2.00	0.43
1:R:80:C:H4'	2:m:55:TYR:HE2	1.84	0.43
2:m:294:LEU:HD23	2:m:342:VAL:HG12	1.99	0.43
2:M:232:LEU:HD22	2:M:296:THR:HG23	2.01	0.43
3:t1:15:LEU:HD11	3:t1:38:LEU:HD23	2.00	0.43
3:A1:15:LEU:HD11	3:A1:38:LEU:HD23	2.00	0.43
3:C1:39:ARG:HG2	3:C1:60:ASP:HB2	2.00	0.43
3:D1:18:ILE:HD12	3:D1:19:GLN:HB2	1.99	0.43
3:F1:39:ARG:HG2	3:F1:60:ASP:HB2	2.00	0.43
3:M1:87:ASP:O	3:2j:84:TRP:HA	2.18	0.43
3:R1:15:LEU:HD11	3:R1:38:LEU:HD23	2.00	0.43
3:11:15:LEU:HD11	3:11:38:LEU:HD23	2.00	0.43
3:11:39:ARG:HG2	3:11:60:ASP:HB2	2.00	0.43
3:G2:39:ARG:HG2	3:G2:60:ASP:HB2	2.00	0.43
3:O2:15:LEU:HD11	3:O2:38:LEU:HD23	2.00	0.43
3:P2:15:LEU:HD11	3:P2:38:LEU:HD23	2.00	0.43
3:u2:15:LEU:HD11	3:u2:38:LEU:HD23	2.00	0.43
3:z2:39:ARG:HG2	3:z2:60:ASP:HB2	2.00	0.43
3:12:15:LEU:HD11	3:12:38:LEU:HD23	2.00	0.43
3:82:39:ARG:HG2	3:82:60:ASP:HB2	2.00	0.43
3:2c:39:ARG:HG2	3:2c:60:ASP:HB2	2.00	0.43
3:2q:39:ARG:HG2	3:2q:60:ASP:HB2	2.00	0.43
3:2u:1:SER:OG	3:2u:2:LYS:N	2.41	0.43
3:2w:15:LEU:HD11	3:2w:38:LEU:HD23	2.00	0.43
3:2y:15:LEU:HD11	3:2y:38:LEU:HD23	2.00	0.43
2:m:98:VAL:HG23	2:m:99:SER:N	2.34	0.43
3:c1:39:ARG:HG2	3:c1:60:ASP:HB2	2.00	0.43
3:D1:15:LEU:HD11	3:D1:38:LEU:HD23	2.00	0.43
3:L1:15:LEU:HD11	3:L1:38:LEU:HD23	2.00	0.43
3:U1:39:ARG:HG2	3:U1:60:ASP:HB2	2.00	0.43
3:71:118:LEU:CD2	3:2U:55:VAL:HG11	2.42	0.43
3:N2:39:ARG:HG2	3:N2:60:ASP:HB2	2.00	0.43
3:o2:39:ARG:HG2	3:o2:60:ASP:HB2	2.00	0.43
3:22:39:ARG:HG2	3:22:60:ASP:HB2	2.00	0.43
3:32:15:LEU:HD11	3:32:38:LEU:HD23	2.00	0.43
3:2o:39:ARG:HG2	3:2o:60:ASP:HB2	2.00	0.43
3:2E:39:ARG:HG2	3:2E:60:ASP:HB2	2.00	0.43
3:2R:15:LEU:HD11	3:2R:38:LEU:HD23	2.00	0.43
2:m:101:THR:O	2:m:101:THR:OG1	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:q1:39:ARG:HG2	3:q1:60:ASP:HB2	2.00	0.43
3:s1:39:ARG:HG2	3:s1:60:ASP:HB2	2.00	0.43
3:v1:15:LEU:HD11	3:v1:38:LEU:HD23	2.00	0.43
3:v1:18:ILE:HD12	3:v1:19:GLN:HB2	1.99	0.43
3:J1:15:LEU:HD11	3:J1:38:LEU:HD23	2.00	0.43
3:P1:39:ARG:HG2	3:P1:60:ASP:HB2	2.00	0.43
3:S1:18:ILE:HD12	3:S1:19:GLN:HB2	1.99	0.43
3:W1:15:LEU:HD11	3:W1:38:LEU:HD23	2.00	0.43
3:H2:1:SER:OG	3:H2:2:LYS:N	2.41	0.43
3:l2:15:LEU:HD11	3:l2:38:LEU:HD23	2.00	0.43
3:p2:39:ARG:HG2	3:p2:60:ASP:HB2	2.00	0.43
3:72:44:LEU:HD13	3:72:55:VAL:HG22	2.01	0.43
3:82:2:LYS:HD3	3:82:2:LYS:HA	1.90	0.43
3:2f:15:LEU:HD11	3:2f:38:LEU:HD23	2.00	0.43
3:2h:15:LEU:HD11	3:2h:38:LEU:HD23	2.00	0.43
3:2D:15:LEU:HD11	3:2D:38:LEU:HD23	2.00	0.43
3:2F:44:LEU:HD13	3:2F:55:VAL:HG22	2.01	0.43
3:2M:39:ARG:HG2	3:2M:60:ASP:HB2	2.00	0.43
3:2N:44:LEU:HD13	3:2N:55:VAL:HG22	2.01	0.43
3:2T:15:LEU:HD11	3:2T:38:LEU:HD23	2.00	0.43
3:2U:39:ARG:HG2	3:2U:60:ASP:HB2	2.00	0.43
1:R:80:C:H2'	1:R:80:C:O2	2.19	0.43
2:m:82:ILE:HD11	2:m:93:PRO:HG3	1.99	0.43
3:f1:256:LYS:HD3	3:f1:256:LYS:HA	1.91	0.43
3:i1:44:LEU:HD13	3:i1:55:VAL:HG22	2.01	0.43
3:A1:39:ARG:HG2	3:A1:60:ASP:HB2	2.00	0.43
3:A1:44:LEU:HD13	3:A1:55:VAL:HG22	2.01	0.43
3:C1:18:ILE:HD12	3:C1:19:GLN:HB2	1.99	0.43
3:D1:44:LEU:HD13	3:D1:55:VAL:HG22	2.01	0.43
3:J1:44:LEU:HD13	3:J1:55:VAL:HG22	2.01	0.43
3:X1:15:LEU:HD11	3:X1:38:LEU:HD23	2.00	0.43
3:21:18:ILE:HG12	3:21:28:GLU:HG3	2.01	0.43
3:61:18:ILE:HD12	3:61:19:GLN:HB2	1.99	0.43
3:C2:39:ARG:HG2	3:C2:60:ASP:HB2	2.00	0.43
3:L2:15:LEU:HD11	3:L2:38:LEU:HD23	2.00	0.43
3:S2:15:LEU:HD11	3:S2:38:LEU:HD23	2.00	0.43
3:Z2:44:LEU:HD13	3:Z2:55:VAL:HG22	2.01	0.43
3:a2:15:LEU:HD11	3:a2:38:LEU:HD23	2.00	0.43
3:g2:39:ARG:HG2	3:g2:60:ASP:HB2	2.00	0.43
3:q2:44:LEU:HD13	3:q2:55:VAL:HG22	2.01	0.43
3:v2:44:LEU:HD13	3:v2:55:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:02:44:LEU:HD13	3:02:55:VAL:HG22	2.01	0.43
3:22:15:LEU:HD11	3:22:38:LEU:HD23	2.00	0.43
3:92:44:LEU:HD13	3:92:55:VAL:HG22	2.01	0.43
3:2k:44:LEU:HD13	3:2k:55:VAL:HG22	2.01	0.43
3:2p:39:ARG:HG2	3:2p:60:ASP:HB2	2.00	0.43
3:2v:15:LEU:HD11	3:2v:38:LEU:HD23	2.00	0.43
3:2C:2:LYS:HD3	3:2C:2:LYS:HA	1.90	0.43
3:2G:15:LEU:HD11	3:2G:38:LEU:HD23	2.00	0.43
3:2K:15:LEU:HD11	3:2K:38:LEU:HD23	2.00	0.43
3:2M:44:LEU:HD13	3:2M:55:VAL:HG22	2.01	0.43
3:2R:44:LEU:HD13	3:2R:55:VAL:HG22	2.01	0.43
3:ac:122:LEU:HD13	3:ac:122:LEU:HA	1.94	0.43
3:c1:44:LEU:HD13	3:c1:55:VAL:HG22	2.01	0.43
3:f1:269:LEU:HD11	3:f1:292:LEU:HD23	2.00	0.43
3:g1:18:ILE:HG12	3:g1:28:GLU:HG3	2.01	0.43
3:m1:15:LEU:HD11	3:m1:38:LEU:HD23	2.01	0.43
3:r1:18:ILE:HG12	3:r1:28:GLU:HG3	2.01	0.43
3:u1:2:LYS:HD3	3:u1:2:LYS:HA	1.91	0.43
3:z1:105:LEU:HD11	3:2V:13:ARG:HH11	1.84	0.43
3:K1:18:ILE:HG12	3:K1:28:GLU:HG3	2.01	0.43
3:M1:44:LEU:HD13	3:M1:55:VAL:HG22	2.01	0.43
3:O1:44:LEU:HD13	3:O1:55:VAL:HG22	2.01	0.43
3:P1:44:LEU:HD13	3:P1:55:VAL:HG22	2.01	0.43
3:X1:18:ILE:HG12	3:X1:28:GLU:HG3	2.01	0.43
3:21:44:LEU:HD13	3:21:55:VAL:HG22	2.01	0.43
3:71:116:GLU:HB2	3:2U:103:TYR:CE1	2.54	0.43
3:S2:44:LEU:HD13	3:S2:55:VAL:HG22	2.01	0.43
3:X2:15:LEU:HD11	3:X2:38:LEU:HD23	2.00	0.43
3:Y2:44:LEU:HD13	3:Y2:55:VAL:HG22	2.01	0.43
3:a2:2:LYS:HD3	3:a2:2:LYS:HA	1.91	0.43
3:b2:44:LEU:HD13	3:b2:55:VAL:HG22	2.01	0.43
3:f2:44:LEU:HD13	3:f2:55:VAL:HG22	2.01	0.43
3:k2:39:ARG:HG2	3:k2:60:ASP:HB2	2.00	0.43
3:t2:44:LEU:HD13	3:t2:55:VAL:HG22	2.01	0.43
3:y2:44:LEU:HD13	3:y2:55:VAL:HG22	2.01	0.43
3:52:44:LEU:HD13	3:52:55:VAL:HG22	2.01	0.43
3:2c:44:LEU:HD13	3:2c:55:VAL:HG22	2.01	0.43
3:2n:39:ARG:HG2	3:2n:60:ASP:HB2	2.00	0.43
3:2u:39:ARG:HG2	3:2u:60:ASP:HB2	2.00	0.43
3:2x:39:ARG:HG2	3:2x:60:ASP:HB2	2.00	0.43
3:2E:2:LYS:HD3	3:2E:2:LYS:HA	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2F:2:LYS:HD3	3:2F:2:LYS:HA	1.91	0.43
3:2H:39:ARG:HG2	3:2H:60:ASP:HB2	2.00	0.43
3:2K:44:LEU:HD13	3:2K:55:VAL:HG22	2.01	0.43
3:2P:44:LEU:HD13	3:2P:55:VAL:HG22	2.01	0.43
3:2R:39:ARG:HG2	3:2R:60:ASP:HB2	2.00	0.43
3:2U:15:LEU:HD11	3:2U:38:LEU:HD23	2.00	0.43
3:2W:15:LEU:HD11	3:2W:38:LEU:HD23	2.00	0.43
3:ad:44:LEU:HD13	3:ad:55:VAL:HG22	2.01	0.43
1:R:14:C:H5'	1:R:15:U:P	2.58	0.42
2:M:232:LEU:CD2	2:M:296:THR:HG23	2.49	0.42
2:M:315:ASP:N	2:M:315:ASP:OD1	2.48	0.42
3:e1:39:ARG:HG2	3:e1:60:ASP:HB2	2.00	0.42
3:i1:39:ARG:HG2	3:i1:60:ASP:HB2	2.00	0.42
3:p1:39:ARG:HG2	3:p1:60:ASP:HB2	2.00	0.42
3:s1:15:LEU:HD11	3:s1:38:LEU:HD23	2.00	0.42
3:t1:2:LYS:HD3	3:t1:2:LYS:HA	1.91	0.42
3:B1:18:ILE:HG12	3:B1:28:GLU:HG3	2.01	0.42
3:D1:18:ILE:HG12	3:D1:28:GLU:HG3	2.01	0.42
3:F1:44:LEU:HD13	3:F1:55:VAL:HG22	2.01	0.42
3:Z1:15:LEU:HD11	3:Z1:38:LEU:HD23	2.00	0.42
3:21:39:ARG:HG2	3:21:60:ASP:HB2	2.00	0.42
3:41:44:LEU:HD13	3:41:55:VAL:HG22	2.01	0.42
3:61:125:LEU:O	3:ab:27:PHE:HZ	2.01	0.42
3:C2:44:LEU:HD13	3:C2:55:VAL:HG22	2.01	0.42
3:E2:15:LEU:HD11	3:E2:38:LEU:HD23	2.00	0.42
3:N2:15:LEU:HD11	3:N2:38:LEU:HD23	2.00	0.42
3:b2:15:LEU:HD11	3:b2:38:LEU:HD23	2.00	0.42
3:i2:44:LEU:HD13	3:i2:55:VAL:HG22	2.01	0.42
3:t2:15:LEU:HD11	3:t2:38:LEU:HD23	2.00	0.42
3:v2:15:LEU:HD11	3:v2:38:LEU:HD23	2.00	0.42
3:w2:44:LEU:HD13	3:w2:55:VAL:HG22	2.01	0.42
3:42:44:LEU:HD13	3:42:55:VAL:HG22	2.01	0.42
3:2d:44:LEU:HD13	3:2d:55:VAL:HG22	2.01	0.42
3:2e:44:LEU:HD13	3:2e:55:VAL:HG22	2.01	0.42
3:2m:39:ARG:HG2	3:2m:60:ASP:HB2	2.00	0.42
3:2n:44:LEU:HD13	3:2n:55:VAL:HG22	2.01	0.42
3:2s:44:LEU:HD13	3:2s:55:VAL:HG22	2.01	0.42
3:2t:15:LEU:HD11	3:2t:38:LEU:HD23	2.00	0.42
3:2A:44:LEU:HD13	3:2A:55:VAL:HG22	2.01	0.42
3:2J:15:LEU:HD11	3:2J:38:LEU:HD23	2.00	0.42
3:2L:44:LEU:HD13	3:2L:55:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2P:15:LEU:HD11	3:2P:38:LEU:HD23	2.00	0.42
3:2U:44:LEU:HD13	3:2U:55:VAL:HG22	2.01	0.42
3:2X:44:LEU:HD13	3:2X:55:VAL:HG22	2.01	0.42
2:m:217:ILE:HG21	2:m:325:TRP:NE1	2.34	0.42
3:u1:15:LEU:HD11	3:u1:38:LEU:HD23	2.00	0.42
3:E1:44:LEU:HD13	3:E1:55:VAL:HG22	2.01	0.42
3:F1:15:LEU:HD11	3:F1:38:LEU:HD23	2.00	0.42
3:G1:18:ILE:HG12	3:G1:28:GLU:HG3	2.01	0.42
3:X1:44:LEU:HD13	3:X1:55:VAL:HG22	2.01	0.42
3:01:44:LEU:HD13	3:01:55:VAL:HG22	2.01	0.42
3:11:44:LEU:HD13	3:11:55:VAL:HG22	2.01	0.42
3:31:44:LEU:HD13	3:31:55:VAL:HG22	2.01	0.42
3:41:39:ARG:HG2	3:41:60:ASP:HB2	2.00	0.42
3:51:18:ILE:HG12	3:51:28:GLU:HG3	2.01	0.42
3:M2:39:ARG:HG2	3:M2:60:ASP:HB2	2.00	0.42
3:T2:15:LEU:HD11	3:T2:38:LEU:HD23	2.00	0.42
3:V2:15:LEU:HD11	3:V2:38:LEU:HD23	2.00	0.42
3:c2:15:LEU:HD11	3:c2:38:LEU:HD23	2.00	0.42
3:h2:15:LEU:HD11	3:h2:38:LEU:HD23	2.00	0.42
3:v2:39:ARG:HG2	3:v2:60:ASP:HB2	2.00	0.42
3:z2:44:LEU:HD13	3:z2:55:VAL:HG22	2.01	0.42
3:72:39:ARG:HG2	3:72:60:ASP:HB2	2.00	0.42
3:2b:15:LEU:HD11	3:2b:38:LEU:HD23	2.00	0.42
3:2c:15:LEU:HD11	3:2c:38:LEU:HD23	2.00	0.42
3:2g:15:LEU:HD11	3:2g:38:LEU:HD23	2.00	0.42
3:2j:15:LEU:HD11	3:2j:38:LEU:HD23	2.00	0.42
3:2q:15:LEU:HD11	3:2q:38:LEU:HD23	2.00	0.42
3:2r:15:LEU:HD11	3:2r:38:LEU:HD23	2.00	0.42
3:2x:44:LEU:HD13	3:2x:55:VAL:HG22	2.01	0.42
3:2A:15:LEU:HD11	3:2A:38:LEU:HD23	2.00	0.42
3:2B:15:LEU:HD11	3:2B:38:LEU:HD23	2.00	0.42
3:2C:15:LEU:HD11	3:2C:38:LEU:HD23	2.00	0.42
3:2E:15:LEU:HD11	3:2E:38:LEU:HD23	2.00	0.42
3:2R:2:LYS:HD3	3:2R:2:LYS:HA	1.91	0.42
1:R:1:G:C2'	1:R:2:G:H5'	2.49	0.42
2:m:232:LEU:HG	2:m:233:ASP:H	1.83	0.42
3:c1:18:ILE:HG12	3:c1:28:GLU:HG3	2.01	0.42
3:s1:18:ILE:HG12	3:s1:28:GLU:HG3	2.01	0.42
3:v1:18:ILE:HG12	3:v1:28:GLU:HG3	2.01	0.42
3:z1:18:ILE:HG12	3:z1:28:GLU:HG3	2.01	0.42
3:J1:18:ILE:HG12	3:J1:28:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O1:39:ARG:HG2	3:O1:60:ASP:HB2	2.00	0.42
3:R1:39:ARG:HG2	3:R1:60:ASP:HB2	2.00	0.42
3:W1:39:ARG:HG2	3:W1:60:ASP:HB2	2.00	0.42
3:O1:18:ILE:HG12	3:O1:28:GLU:HG3	2.01	0.42
3:O1:39:ARG:HG2	3:O1:60:ASP:HB2	2.00	0.42
3:31:39:ARG:HG2	3:31:60:ASP:HB2	2.00	0.42
3:E2:44:LEU:HD13	3:E2:55:VAL:HG22	2.01	0.42
3:F2:15:LEU:HD11	3:F2:38:LEU:HD23	2.00	0.42
3:F2:44:LEU:HD13	3:F2:55:VAL:HG22	2.01	0.42
3:I2:44:LEU:HD13	3:I2:55:VAL:HG22	2.01	0.42
3:O2:39:ARG:HG2	3:O2:60:ASP:HB2	2.00	0.42
3:U2:1:SER:OG	3:U2:2:LYS:N	2.41	0.42
3:m2:39:ARG:HG2	3:m2:60:ASP:HB2	2.00	0.42
3:m2:44:LEU:HD13	3:m2:55:VAL:HG22	2.01	0.42
3:r2:44:LEU:HD13	3:r2:55:VAL:HG22	2.01	0.42
3:t2:39:ARG:HG2	3:t2:60:ASP:HB2	2.00	0.42
3:w2:39:ARG:HG2	3:w2:60:ASP:HB2	2.00	0.42
3:12:44:LEU:HD13	3:12:55:VAL:HG22	2.01	0.42
3:2f:44:LEU:HD13	3:2f:55:VAL:HG22	2.01	0.42
3:2h:39:ARG:HG2	3:2h:60:ASP:HB2	2.00	0.42
3:2B:44:LEU:HD13	3:2B:55:VAL:HG22	2.01	0.42
3:2G:44:LEU:HD13	3:2G:55:VAL:HG22	2.01	0.42
3:2I:39:ARG:HG2	3:2I:60:ASP:HB2	2.00	0.42
3:2I:44:LEU:HD13	3:2I:55:VAL:HG22	2.01	0.42
3:2L:39:ARG:HG2	3:2L:60:ASP:HB2	2.00	0.42
3:2N:15:LEU:HD11	3:2N:38:LEU:HD23	2.00	0.42
3:aa:44:LEU:HD13	3:aa:55:VAL:HG22	2.01	0.42
1:R:54:G:C5'	1:R:93:C:H4'	2.50	0.42
3:a1:18:ILE:HG12	3:a1:28:GLU:HG3	2.01	0.42
3:b1:18:ILE:HG12	3:b1:28:GLU:HG3	2.01	0.42
3:c1:15:LEU:HD11	3:c1:38:LEU:HD23	2.00	0.42
3:h1:15:LEU:HD11	3:h1:38:LEU:HD23	2.00	0.42
3:h1:18:ILE:HG12	3:h1:28:GLU:HG3	2.01	0.42
3:p1:15:LEU:HD11	3:p1:38:LEU:HD23	2.00	0.42
3:r1:22:ALA:CB	3:2K:20:SER:H	2.31	0.42
3:u1:44:LEU:HD13	3:u1:55:VAL:HG22	2.01	0.42
3:x1:18:ILE:HG12	3:x1:28:GLU:HG3	2.01	0.42
3:B1:15:LEU:HD11	3:B1:38:LEU:HD23	2.00	0.42
3:C1:44:LEU:HD13	3:C1:55:VAL:HG22	2.01	0.42
3:E1:39:ARG:HG2	3:E1:60:ASP:HB2	2.00	0.42
3:P1:18:ILE:HG12	3:P1:28:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P1:93:ASN:CB	3:2y:76:PRO:HD2	2.50	0.42
3:Q1:18:ILE:HG12	3:Q1:28:GLU:HG3	2.01	0.42
3:Q1:39:ARG:HG2	3:Q1:60:ASP:HB2	2.00	0.42
3:U1:18:ILE:HG12	3:U1:28:GLU:HG3	2.01	0.42
3:U1:44:LEU:HD13	3:U1:55:VAL:HG22	2.01	0.42
3:X1:39:ARG:HG2	3:X1:60:ASP:HB2	2.00	0.42
3:51:44:LEU:HD13	3:51:55:VAL:HG22	2.01	0.42
3:61:15:LEU:HD11	3:61:38:LEU:HD23	2.00	0.42
3:61:44:LEU:HD13	3:61:55:VAL:HG22	2.01	0.42
3:M2:44:LEU:HD13	3:M2:55:VAL:HG22	2.01	0.42
3:V2:2:LYS:HD3	3:V2:2:LYS:HA	1.91	0.42
3:X2:39:ARG:HG2	3:X2:60:ASP:HB2	2.00	0.42
3:a2:44:LEU:HD13	3:a2:55:VAL:HG22	2.01	0.42
3:o2:15:LEU:HD11	3:o2:38:LEU:HD23	2.00	0.42
3:s2:44:LEU:HD13	3:s2:55:VAL:HG22	2.01	0.42
3:u2:44:LEU:HD13	3:u2:55:VAL:HG22	2.01	0.42
3:52:39:ARG:HG2	3:52:60:ASP:HB2	2.00	0.42
3:2h:1:SER:OG	3:2h:2:LYS:N	2.42	0.42
3:2h:44:LEU:HD13	3:2h:55:VAL:HG22	2.01	0.42
3:2j:44:LEU:HD13	3:2j:55:VAL:HG22	2.01	0.42
3:2o:15:LEU:HD11	3:2o:38:LEU:HD23	2.00	0.42
3:2y:44:LEU:HD13	3:2y:55:VAL:HG22	2.01	0.42
3:2Q:44:LEU:HD13	3:2Q:55:VAL:HG22	2.01	0.42
3:g1:15:LEU:HD11	3:g1:38:LEU:HD23	2.00	0.42
3:l1:44:LEU:HD13	3:l1:55:VAL:HG22	2.01	0.42
3:y1:15:LEU:HD11	3:y1:38:LEU:HD23	2.00	0.42
3:E1:18:ILE:HG12	3:E1:28:GLU:HG3	2.01	0.42
3:K1:39:ARG:HG2	3:K1:60:ASP:HB2	2.00	0.42
3:K1:44:LEU:HD13	3:K1:55:VAL:HG22	2.01	0.42
3:R1:44:LEU:HD13	3:R1:55:VAL:HG22	2.01	0.42
3:S1:18:ILE:HG12	3:S1:28:GLU:HG3	2.01	0.42
3:U1:15:LEU:HD11	3:U1:38:LEU:HD23	2.00	0.42
3:V1:18:ILE:HG12	3:V1:28:GLU:HG3	2.02	0.42
3:A2:15:LEU:HD11	3:A2:38:LEU:HD23	2.00	0.42
3:D2:122:LEU:HD13	3:D2:122:LEU:HA	1.94	0.42
3:n2:39:ARG:HG2	3:n2:60:ASP:HB2	2.00	0.42
3:w2:15:LEU:HD11	3:w2:38:LEU:HD23	2.00	0.42
3:42:39:ARG:HG2	3:42:60:ASP:HB2	2.00	0.42
3:92:39:ARG:HG2	3:92:60:ASP:HB2	2.00	0.42
3:2d:1:SER:OG	3:2d:2:LYS:N	2.41	0.42
3:2l:114:GLN:HE21	3:2l:114:GLN:HB3	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2u:44:LEU:HD13	3:2u:55:VAL:HG22	2.01	0.42
3:2T:44:LEU:HD13	3:2T:55:VAL:HG22	2.01	0.42
3:2W:39:ARG:HG2	3:2W:60:ASP:HB2	2.00	0.42
3:2X:39:ARG:HG2	3:2X:60:ASP:HB2	2.00	0.42
3:ab:39:ARG:HG2	3:ab:60:ASP:HB2	2.00	0.42
1:R:80:C:H1'	2:m:396:ASP:OD1	2.19	0.42
3:d1:44:LEU:HD13	3:d1:55:VAL:HG22	2.01	0.42
3:e1:18:ILE:HG12	3:e1:28:GLU:HG3	2.01	0.42
3:f1:293:ARG:HG2	3:f1:314:ASP:HB2	2.00	0.42
3:j1:15:LEU:HD11	3:j1:38:LEU:HD23	2.00	0.42
3:j1:44:LEU:HD13	3:j1:55:VAL:HG22	2.01	0.42
3:k1:44:LEU:HD13	3:k1:55:VAL:HG22	2.01	0.42
3:p1:18:ILE:HG12	3:p1:28:GLU:HG3	2.01	0.42
3:q1:44:LEU:HD13	3:q1:55:VAL:HG22	2.01	0.42
3:t1:18:ILE:HG12	3:t1:28:GLU:HG3	2.01	0.42
3:u1:39:ARG:HG2	3:u1:60:ASP:HB2	2.00	0.42
3:w1:44:LEU:HD13	3:w1:55:VAL:HG22	2.01	0.42
3:x1:15:LEU:HD11	3:x1:38:LEU:HD23	2.00	0.42
3:C1:2:LYS:HD3	3:C1:2:LYS:HA	1.90	0.42
3:J1:39:ARG:HG2	3:J1:60:ASP:HB2	2.00	0.42
3:L1:18:ILE:HG12	3:L1:28:GLU:HG3	2.01	0.42
3:41:18:ILE:HG12	3:41:28:GLU:HG3	2.01	0.42
3:41:122:LEU:HD13	3:41:122:LEU:HA	1.94	0.42
3:L2:44:LEU:HD13	3:L2:55:VAL:HG22	2.01	0.42
3:R2:15:LEU:HD11	3:R2:38:LEU:HD23	2.00	0.42
3:W2:44:LEU:HD13	3:W2:55:VAL:HG22	2.01	0.42
3:e2:15:LEU:HD11	3:e2:38:LEU:HD23	2.00	0.42
3:f2:15:LEU:HD11	3:f2:38:LEU:HD23	2.00	0.42
3:l2:2:LYS:HD3	3:l2:2:LYS:HA	1.91	0.42
3:o2:44:LEU:HD13	3:o2:55:VAL:HG22	2.01	0.42
3:62:15:LEU:HD11	3:62:38:LEU:HD23	2.00	0.42
3:82:15:LEU:HD11	3:82:38:LEU:HD23	2.00	0.42
3:2b:39:ARG:HG2	3:2b:60:ASP:HB2	2.00	0.42
3:2d:39:ARG:HG2	3:2d:60:ASP:HB2	2.00	0.42
3:2j:2:LYS:HD3	3:2j:2:LYS:HA	1.91	0.42
3:2y:39:ARG:HG2	3:2y:60:ASP:HB2	2.00	0.42
3:2z:44:LEU:HD13	3:2z:55:VAL:HG22	2.01	0.42
3:2N:2:LYS:HD3	3:2N:2:LYS:HA	1.91	0.42
3:2O:122:LEU:HD13	3:2O:122:LEU:HA	1.94	0.42
3:2Q:15:LEU:HD11	3:2Q:38:LEU:HD23	2.00	0.42
3:2V:122:LEU:HD13	3:2V:122:LEU:HA	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2Z:39:ARG:HG2	3:2Z:60:ASP:HB2	2.00	0.42
2:m:74:GLU:OE2	2:m:379:LYS:NZ	2.36	0.42
3:e1:44:LEU:HD13	3:e1:55:VAL:HG22	2.01	0.42
3:g1:44:LEU:HD13	3:g1:55:VAL:HG22	2.01	0.42
3:l1:18:ILE:HG12	3:l1:28:GLU:HG3	2.01	0.42
3:n1:44:LEU:HD13	3:n1:55:VAL:HG22	2.01	0.42
3:p1:44:LEU:HD13	3:p1:55:VAL:HG22	2.01	0.42
3:C1:18:ILE:HG12	3:C1:28:GLU:HG3	2.01	0.42
3:G1:15:LEU:HD11	3:G1:38:LEU:HD23	2.00	0.42
3:M1:39:ARG:HG2	3:M1:60:ASP:HB2	2.00	0.42
3:N1:18:ILE:HG12	3:N1:28:GLU:HG3	2.01	0.42
3:T1:2:LYS:HD3	3:T1:2:LYS:HA	1.91	0.42
3:31:18:ILE:HG12	3:31:28:GLU:HG3	2.01	0.42
3:D2:44:LEU:HD13	3:D2:55:VAL:HG22	2.01	0.42
3:E2:39:ARG:HG2	3:E2:60:ASP:HB2	2.00	0.42
3:i2:39:ARG:HG2	3:i2:60:ASP:HB2	2.00	0.42
3:p2:44:LEU:HD13	3:p2:55:VAL:HG22	2.01	0.42
3:u2:114:GLN:HE21	3:u2:114:GLN:HB3	1.68	0.42
3:2b:44:LEU:HD13	3:2b:55:VAL:HG22	2.01	0.42
3:2d:122:LEU:HD13	3:2d:122:LEU:HA	1.94	0.42
3:2k:15:LEU:HD11	3:2k:38:LEU:HD23	2.00	0.42
3:2l:39:ARG:HG2	3:2l:60:ASP:HB2	2.00	0.42
1:R:14:C:H4'	1:R:17:G:O6	2.19	0.42
3:i1:15:LEU:HD11	3:i1:38:LEU:HD23	2.00	0.42
3:t1:44:LEU:HD13	3:t1:55:VAL:HG22	2.01	0.42
3:u1:18:ILE:HG12	3:u1:28:GLU:HG3	2.01	0.42
3:A1:103:TYR:OH	3:aa:116:GLU:HB2	2.20	0.42
3:F1:18:ILE:HG12	3:F1:28:GLU:HG3	2.01	0.42
3:G1:44:LEU:HD13	3:G1:55:VAL:HG22	2.01	0.42
3:T1:44:LEU:HD13	3:T1:55:VAL:HG22	2.01	0.42
3:41:15:LEU:HD11	3:41:38:LEU:HD23	2.00	0.42
3:61:18:ILE:HG12	3:61:28:GLU:HG3	2.01	0.42
3:71:18:ILE:HG12	3:71:28:GLU:HG3	2.01	0.42
3:D2:15:LEU:HD11	3:D2:38:LEU:HD23	2.00	0.42
3:V2:44:LEU:HD13	3:V2:55:VAL:HG22	2.01	0.42
3:Y2:39:ARG:HG2	3:Y2:60:ASP:HB2	2.00	0.42
3:j2:122:LEU:HD13	3:j2:122:LEU:HA	1.94	0.42
3:k2:15:LEU:HD11	3:k2:38:LEU:HD23	2.00	0.42
3:22:44:LEU:HD13	3:22:55:VAL:HG22	2.01	0.42
3:62:44:LEU:HD13	3:62:55:VAL:HG22	2.01	0.42
3:82:44:LEU:HD13	3:82:55:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2a:15:LEU:HD11	3:2a:38:LEU:HD23	2.00	0.42
3:2a:44:LEU:HD13	3:2a:55:VAL:HG22	2.01	0.42
3:2S:15:LEU:HD11	3:2S:38:LEU:HD23	2.00	0.42
3:2T:39:ARG:HG2	3:2T:60:ASP:HB2	2.00	0.42
3:2V:44:LEU:HD13	3:2V:55:VAL:HG22	2.01	0.42
3:ac:15:LEU:HD11	3:ac:38:LEU:HD23	2.00	0.42
3:ac:44:LEU:HD13	3:ac:55:VAL:HG22	2.01	0.42
3:f1:298:LEU:HD13	3:f1:309:VAL:HG22	2.01	0.42
3:n1:39:ARG:HG2	3:n1:60:ASP:HB2	2.00	0.42
3:r1:15:LEU:HD11	3:r1:38:LEU:HD23	2.00	0.42
3:s1:44:LEU:HD13	3:s1:55:VAL:HG22	2.01	0.42
3:H1:44:LEU:HD13	3:H1:55:VAL:HG22	2.01	0.42
3:O1:15:LEU:HD11	3:O1:38:LEU:HD23	2.00	0.42
3:W1:22:ALA:HB1	3:k2:18:ILE:O	2.20	0.42
3:Y1:44:LEU:HD13	3:Y1:55:VAL:HG22	2.01	0.42
3:21:122:LEU:HD13	3:21:122:LEU:HA	1.94	0.42
3:G2:44:LEU:HD13	3:G2:55:VAL:HG22	2.01	0.42
3:I2:118:LEU:HD21	3:2Q:55:VAL:HG11	2.00	0.42
3:J2:44:LEU:HD13	3:J2:55:VAL:HG22	2.01	0.42
3:K2:15:LEU:HD11	3:K2:38:LEU:HD23	2.00	0.42
3:S2:39:ARG:HG2	3:S2:60:ASP:HB2	2.00	0.42
3:Z2:39:ARG:HG2	3:Z2:60:ASP:HB2	2.00	0.42
3:f2:114:GLN:HE21	3:f2:114:GLN:HB3	1.68	0.42
3:j2:15:LEU:HD11	3:j2:38:LEU:HD23	2.00	0.42
3:22:122:LEU:HD13	3:22:122:LEU:HA	1.94	0.42
3:72:15:LEU:HD11	3:72:38:LEU:HD23	2.00	0.42
3:2i:44:LEU:HD13	3:2i:55:VAL:HG22	2.01	0.42
3:2V:39:ARG:HG2	3:2V:60:ASP:HB2	2.00	0.42
3:ad:2:LYS:HD3	3:ad:2:LYS:HA	1.90	0.42
1:R:41:U:H3'	1:R:42:C:C5'	2.31	0.42
2:m:304:ARG:HG2	2:m:304:ARG:O	2.19	0.42
2:M:402:SER:O	2:M:403:THR:OG1	2.34	0.42
3:j1:18:ILE:HG12	3:j1:28:GLU:HG3	2.01	0.42
3:m1:18:ILE:HG12	3:m1:28:GLU:HG3	2.01	0.42
3:v1:44:LEU:HD13	3:v1:55:VAL:HG22	2.01	0.42
3:w1:15:LEU:HD11	3:w1:38:LEU:HD23	2.00	0.42
3:O1:18:ILE:HG12	3:O1:28:GLU:HG3	2.01	0.42
3:Y1:18:ILE:HG12	3:Y1:28:GLU:HG3	2.01	0.42
3:A2:44:LEU:HD13	3:A2:55:VAL:HG22	2.01	0.42
3:K2:44:LEU:HD13	3:K2:55:VAL:HG22	2.01	0.42
3:N2:44:LEU:HD13	3:N2:55:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P2:44:LEU:HD13	3:P2:55:VAL:HG22	2.01	0.42
3:Q2:44:LEU:HD13	3:Q2:55:VAL:HG22	2.01	0.42
3:X2:44:LEU:HD13	3:X2:55:VAL:HG22	2.01	0.42
3:k2:44:LEU:HD13	3:k2:55:VAL:HG22	2.01	0.42
3:n2:44:LEU:HD13	3:n2:55:VAL:HG22	2.01	0.42
3:p2:2:LYS:HD3	3:p2:2:LYS:HA	1.91	0.42
3:r2:2:LYS:HD3	3:r2:2:LYS:HA	1.91	0.42
3:z2:15:LEU:HD11	3:z2:38:LEU:HD23	2.00	0.42
3:z2:122:LEU:HD13	3:z2:122:LEU:HA	1.94	0.42
3:12:39:ARG:HG2	3:12:60:ASP:HB2	2.00	0.42
3:62:1:SER:OG	3:62:2:LYS:N	2.42	0.42
3:2l:44:LEU:HD13	3:2l:55:VAL:HG22	2.01	0.42
3:2m:44:LEU:HD13	3:2m:55:VAL:HG22	2.01	0.42
3:2I:15:LEU:HD11	3:2I:38:LEU:HD23	2.00	0.42
3:2W:44:LEU:HD13	3:2W:55:VAL:HG22	2.01	0.42
3:2Y:44:LEU:HD13	3:2Y:55:VAL:HG22	2.01	0.42
3:a1:44:LEU:HD13	3:a1:55:VAL:HG22	2.01	0.41
3:h1:44:LEU:HD13	3:h1:55:VAL:HG22	2.01	0.41
3:k1:18:ILE:HG12	3:k1:28:GLU:HG3	2.01	0.41
3:m1:44:LEU:HD13	3:m1:55:VAL:HG22	2.01	0.41
3:H1:18:ILE:HG12	3:H1:28:GLU:HG3	2.01	0.41
3:R1:18:ILE:HG12	3:R1:28:GLU:HG3	2.01	0.41
3:S1:44:LEU:HD13	3:S1:55:VAL:HG22	2.01	0.41
3:W1:18:ILE:HG12	3:W1:28:GLU:HG3	2.01	0.41
3:71:39:ARG:HG2	3:71:60:ASP:HB2	2.00	0.41
3:71:44:LEU:HD13	3:71:55:VAL:HG22	2.01	0.41
3:c2:32:GLY:HA3	3:c2:33:PRO:HD3	1.95	0.41
3:j2:39:ARG:HG2	3:j2:60:ASP:HB2	2.00	0.41
3:l2:39:ARG:HG2	3:l2:60:ASP:HB2	2.00	0.41
3:2r:44:LEU:HD13	3:2r:55:VAL:HG22	2.01	0.41
3:2u:2:LYS:HD3	3:2u:2:LYS:HA	1.91	0.41
3:2A:39:ARG:HG2	3:2A:60:ASP:HB2	2.00	0.41
3:2P:122:LEU:HD13	3:2P:122:LEU:HA	1.94	0.41
2:M:405:PRO:O	2:M:406:ASP:C	2.63	0.41
3:b1:15:LEU:HD11	3:b1:38:LEU:HD23	2.00	0.41
3:d1:18:ILE:HG12	3:d1:28:GLU:HG3	2.01	0.41
3:B1:44:LEU:HD13	3:B1:55:VAL:HG22	2.01	0.41
3:Q1:44:LEU:HD13	3:Q1:55:VAL:HG22	2.01	0.41
3:V1:44:LEU:HD13	3:V1:55:VAL:HG22	2.01	0.41
3:Z1:22:ALA:CB	3:02:20:SER:H	2.33	0.41
3:H2:44:LEU:HD13	3:H2:55:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:l2:44:LEU:HD13	3:l2:55:VAL:HG22	2.01	0.41
3:q2:107:LYS:HD2	3:2y:111:ALA:HA	2.01	0.41
3:92:15:LEU:HD11	3:92:38:LEU:HD23	2.00	0.41
3:2s:39:ARG:HG2	3:2s:60:ASP:HB2	2.00	0.41
3:2J:44:LEU:HD13	3:2J:55:VAL:HG22	2.01	0.41
3:2Y:122:LEU:HD13	3:2Y:122:LEU:HA	1.94	0.41
3:ab:44:LEU:HD13	3:ab:55:VAL:HG22	2.01	0.41
1:R:75:G:C2'	1:R:76:C:O4'	2.68	0.41
2:m:252:ASN:OD1	2:m:253:SER:N	2.53	0.41
3:n1:18:ILE:HG12	3:n1:28:GLU:HG3	2.01	0.41
3:o1:18:ILE:HG12	3:o1:28:GLU:HG3	2.01	0.41
3:w1:18:ILE:HG12	3:w1:28:GLU:HG3	2.01	0.41
3:w1:93:ASN:HB2	3:l2:76:PRO:HD2	2.03	0.41
3:y1:44:LEU:HD13	3:y1:55:VAL:HG22	2.01	0.41
3:z1:2:LYS:HD3	3:z1:2:LYS:HA	1.91	0.41
3:X1:122:LEU:HD13	3:X1:122:LEU:HA	1.94	0.41
3:B2:44:LEU:HD13	3:B2:55:VAL:HG22	2.01	0.41
3:K2:2:LYS:HD3	3:K2:2:LYS:HA	1.91	0.41
3:O2:44:LEU:HD13	3:O2:55:VAL:HG22	2.01	0.41
3:Z2:15:LEU:HD11	3:Z2:38:LEU:HD23	2.00	0.41
3:x2:44:LEU:HD13	3:x2:55:VAL:HG22	2.01	0.41
3:y2:15:LEU:HD11	3:y2:38:LEU:HD23	2.00	0.41
3:O2:114:GLN:HE21	3:O2:114:GLN:HB3	1.68	0.41
3:2H:44:LEU:HD13	3:2H:55:VAL:HG22	2.01	0.41
3:2K:32:GLY:HA3	3:2K:33:PRO:HD3	1.95	0.41
3:2Q:2:LYS:HD3	3:2Q:2:LYS:HA	1.90	0.41
3:2T:114:GLN:HE21	3:2T:114:GLN:HB3	1.68	0.41
1:R:37:C:O5'	1:R:37:C:H6	2.03	0.41
1:R:82:G:H3'	1:R:83:C:O4'	2.20	0.41
2:m:64:CYS:SG	2:m:65:THR:N	2.93	0.41
3:q1:18:ILE:HG12	3:q1:28:GLU:HG3	2.01	0.41
3:r1:44:LEU:HD13	3:r1:55:VAL:HG22	2.01	0.41
3:I1:18:ILE:HG12	3:I1:28:GLU:HG3	2.01	0.41
3:Z1:18:ILE:HG12	3:Z1:28:GLU:HG3	2.01	0.41
3:11:18:ILE:HG12	3:11:28:GLU:HG3	2.01	0.41
3:31:2:LYS:HD3	3:31:2:LYS:HA	1.91	0.41
3:J2:114:GLN:HE21	3:J2:114:GLN:HB3	1.68	0.41
3:O2:114:GLN:HE21	3:O2:114:GLN:HB3	1.68	0.41
3:U2:44:LEU:HD13	3:U2:55:VAL:HG22	2.01	0.41
3:e2:44:LEU:HD13	3:e2:55:VAL:HG22	2.01	0.41
3:g2:2:LYS:HD3	3:g2:2:LYS:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g2:44:LEU:HD13	3:g2:55:VAL:HG22	2.01	0.41
3:h2:44:LEU:HD13	3:h2:55:VAL:HG22	2.01	0.41
3:2m:2:LYS:HD3	3:2m:2:LYS:HA	1.91	0.41
3:2v:44:LEU:HD13	3:2v:55:VAL:HG22	2.01	0.41
3:2D:44:LEU:HD13	3:2D:55:VAL:HG22	2.01	0.41
3:2O:44:LEU:HD13	3:2O:55:VAL:HG22	2.01	0.41
3:2Q:1:SER:OG	3:2Q:2:LYS:N	2.44	0.41
3:2Z:122:LEU:HD13	3:2Z:122:LEU:HA	1.94	0.41
2:m:180:GLN:OE1	2:m:180:GLN:N	2.53	0.41
3:f1:272:ILE:HG12	3:f1:282:GLU:HG3	2.01	0.41
3:o1:44:LEU:HD13	3:o1:55:VAL:HG22	2.01	0.41
3:A1:18:ILE:HG12	3:A1:28:GLU:HG3	2.01	0.41
3:C1:93:ASN:CB	3:K2:76:PRO:HD2	2.51	0.41
3:T1:18:ILE:HG12	3:T1:28:GLU:HG3	2.01	0.41
3:Z1:122:LEU:HD13	3:Z1:122:LEU:HA	1.94	0.41
3:D2:2:LYS:HD3	3:D2:2:LYS:HA	1.91	0.41
3:S2:2:LYS:HA	3:S2:2:LYS:HD3	1.91	0.41
3:n2:122:LEU:HD13	3:n2:122:LEU:HA	1.94	0.41
3:2f:122:LEU:HD13	3:2f:122:LEU:HA	1.94	0.41
3:2g:2:LYS:HD3	3:2g:2:LYS:HA	1.91	0.41
3:2q:44:LEU:HD13	3:2q:55:VAL:HG22	2.01	0.41
3:2t:44:LEU:HD13	3:2t:55:VAL:HG22	2.01	0.41
3:2Q:122:LEU:HD13	3:2Q:122:LEU:HA	1.94	0.41
1:R:22:U:C4	1:R:23:G:HI'	2.56	0.41
3:j1:32:GLY:HA3	3:j1:33:PRO:HD3	1.95	0.41
3:k1:2:LYS:HD3	3:k1:2:LYS:HA	1.91	0.41
3:z1:44:LEU:HD13	3:z1:55:VAL:HG22	2.01	0.41
3:M1:18:ILE:HG12	3:M1:28:GLU:HG3	2.01	0.41
3:Y1:2:LYS:HD3	3:Y1:2:LYS:HA	1.91	0.41
3:Z1:44:LEU:HD13	3:Z1:55:VAL:HG22	2.01	0.41
3:G2:32:GLY:HA3	3:G2:33:PRO:HD3	1.95	0.41
3:L2:114:GLN:HE21	3:L2:114:GLN:HB3	1.68	0.41
3:R2:44:LEU:HD13	3:R2:55:VAL:HG22	2.01	0.41
3:T2:44:LEU:HD13	3:T2:55:VAL:HG22	2.01	0.41
3:c2:44:LEU:HD13	3:c2:55:VAL:HG22	2.01	0.41
3:d2:44:LEU:HD13	3:d2:55:VAL:HG22	2.01	0.41
3:j2:1:SER:OG	3:j2:2:LYS:N	2.41	0.41
3:y2:32:GLY:HA3	3:y2:33:PRO:HD3	1.95	0.41
3:y2:122:LEU:HD13	3:y2:122:LEU:HA	1.94	0.41
3:32:44:LEU:HD13	3:32:55:VAL:HG22	2.01	0.41
3:62:32:GLY:HA3	3:62:33:PRO:HD3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2p:44:LEU:HD13	3:2p:55:VAL:HG22	2.01	0.41
3:2v:2:LYS:HD3	3:2v:2:LYS:HA	1.91	0.41
3:2w:122:LEU:HD13	3:2w:122:LEU:HA	1.94	0.41
3:2C:44:LEU:HD13	3:2C:55:VAL:HG22	2.01	0.41
3:2Z:44:LEU:HD13	3:2Z:55:VAL:HG22	2.01	0.41
1:R:66:U:H5'	1:R:67:C:OP2	2.20	0.41
2:m:18:LEU:HD22	2:m:88:HIS:CB	2.49	0.41
3:a1:32:GLY:HA3	3:a1:33:PRO:HD3	1.95	0.41
3:i1:18:ILE:HG12	3:i1:28:GLU:HG3	2.01	0.41
3:W1:44:LEU:HD13	3:W1:55:VAL:HG22	2.01	0.41
3:K2:1:SER:OG	3:K2:2:LYS:N	2.41	0.41
3:W2:2:LYS:HA	3:W2:2:LYS:HD3	1.90	0.41
3:h2:114:GLN:HE21	3:h2:114:GLN:HB3	1.68	0.41
3:i1:2:LYS:HD3	3:i1:2:LYS:HA	1.90	0.41
3:p1:122:LEU:HD13	3:p1:122:LEU:HA	1.94	0.41
3:y1:18:ILE:HG12	3:y1:28:GLU:HG3	2.01	0.41
3:z1:61:GLN:OE1	3:2V:102:LEU:HD23	2.21	0.41
3:D1:107:LYS:HD2	3:2P:111:ALA:HA	2.03	0.41
3:M1:122:LEU:HD13	3:M1:122:LEU:HA	1.94	0.41
3:j2:44:LEU:HD13	3:j2:55:VAL:HG22	2.01	0.41
3:m2:122:LEU:HD13	3:m2:122:LEU:HA	1.94	0.41
3:2o:44:LEU:HD13	3:2o:55:VAL:HG22	2.01	0.41
3:2w:44:LEU:HD13	3:2w:55:VAL:HG22	2.01	0.41
3:2x:32:GLY:HA3	3:2x:33:PRO:HD3	1.95	0.41
3:2A:122:LEU:HD13	3:2A:122:LEU:HA	1.94	0.41
3:2L:2:LYS:HA	3:2L:2:LYS:HD3	1.90	0.41
3:2S:44:LEU:HD13	3:2S:55:VAL:HG22	2.01	0.41
3:aa:2:LYS:HD3	3:aa:2:LYS:HA	1.91	0.41
3:b1:44:LEU:HD13	3:b1:55:VAL:HG22	2.01	0.41
3:d1:22:ALA:HB2	3:E2:20:SER:H	1.86	0.41
3:p1:2:LYS:HD3	3:p1:2:LYS:HA	1.91	0.41
3:w1:22:ALA:HB1	3:I2:18:ILE:O	2.20	0.41
3:w1:93:ASN:CB	3:I2:76:PRO:HD2	2.51	0.41
3:z1:32:GLY:HA3	3:z1:33:PRO:HD3	1.95	0.41
3:I1:44:LEU:HD13	3:I1:55:VAL:HG22	2.01	0.41
3:N1:44:LEU:HD13	3:N1:55:VAL:HG22	2.01	0.41
3:O1:122:LEU:HD13	3:O1:122:LEU:HA	1.94	0.41
3:P1:122:LEU:HD13	3:P1:122:LEU:HA	1.94	0.41
3:51:122:LEU:HD13	3:51:122:LEU:HA	1.94	0.41
3:61:125:LEU:O	3:ab:27:PHE:CZ	2.74	0.41
3:71:110:VAL:HG11	3:2U:110:VAL:CG2	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J2:18:ILE:HD13	3:J2:18:ILE:HA	1.81	0.41
3:h2:32:GLY:HA3	3:h2:33:PRO:HD3	1.95	0.41
3:v2:114:GLN:HE21	3:v2:114:GLN:HB3	1.68	0.41
3:2a:2:LYS:HD3	3:2a:2:LYS:HA	1.91	0.41
3:2g:114:GLN:HE21	3:2g:114:GLN:HB3	1.68	0.41
3:2l:122:LEU:HD13	3:2l:122:LEU:HA	1.94	0.41
3:2s:122:LEU:HD13	3:2s:122:LEU:HA	1.94	0.41
3:2E:44:LEU:HD13	3:2E:55:VAL:HG22	2.01	0.41
3:2R:18:ILE:HD13	3:2R:18:ILE:HA	1.81	0.41
3:ac:114:GLN:HE21	3:ac:114:GLN:HB3	1.68	0.41
1:R:73:C:H5'	1:R:74:C:OP2	2.20	0.41
2:M:2:LEU:HD12	2:M:3:GLU:H	1.85	0.41
3:x1:44:LEU:HD13	3:x1:55:VAL:HG22	2.01	0.41
3:D1:122:LEU:HD13	3:D1:122:LEU:HA	1.94	0.41
3:N1:32:GLY:HA3	3:N1:33:PRO:HD3	1.95	0.41
3:R1:122:LEU:HD13	3:R1:122:LEU:HA	1.94	0.41
3:71:124:PRO:HG3	3:2U:44:LEU:HD23	2.02	0.41
3:f2:32:GLY:HA3	3:f2:33:PRO:HD3	1.95	0.41
3:12:2:LYS:HD3	3:12:2:LYS:HA	1.91	0.41
3:2g:44:LEU:HD13	3:2g:55:VAL:HG22	2.01	0.41
2:m:32:VAL:HG22	2:m:33:PHE:H	1.85	0.40
2:m:194:ASP:O	2:m:198:VAL:HG23	2.22	0.40
3:e1:2:LYS:HD3	3:e1:2:LYS:HA	1.91	0.40
3:f1:376:LEU:HD13	3:f1:376:LEU:HA	1.94	0.40
3:E1:107:LYS:HD2	3:ad:111:ALA:HA	2.03	0.40
3:61:2:LYS:HD3	3:61:2:LYS:HA	1.91	0.40
3:61:61:GLN:OE1	3:ab:102:LEU:HD23	2.21	0.40
3:A2:1:SER:OG	3:A2:2:LYS:N	2.41	0.40
3:D2:114:GLN:HE21	3:D2:114:GLN:HB3	1.68	0.40
3:M2:122:LEU:HD13	3:M2:122:LEU:HA	1.94	0.40
3:T2:2:LYS:HA	3:T2:2:LYS:HD3	1.91	0.40
3:t2:18:ILE:HD13	3:t2:18:ILE:HA	1.81	0.40
3:72:2:LYS:HD3	3:72:2:LYS:HA	1.90	0.40
3:2n:114:GLN:HE21	3:2n:114:GLN:HB3	1.68	0.40
3:2B:122:LEU:HD13	3:2B:122:LEU:HA	1.94	0.40
3:2I:77:LYS:HB3	3:2I:77:LYS:HE3	1.96	0.40
1:R:15:U:H3	2:M:50:VAL:CG2	2.34	0.40
1:R:27:C:C2'	1:R:28:U:O4'	2.69	0.40
2:m:86:VAL:HG12	2:m:87:PRO:CD	2.51	0.40
3:j1:2:LYS:HD3	3:j1:2:LYS:HA	1.91	0.40
3:n1:2:LYS:HD3	3:n1:2:LYS:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:q1:32:GLY:HA3	3:q1:33:PRO:HD3	1.95	0.40
3:E1:93:ASN:OD1	3:E1:93:ASN:N	2.55	0.40
3:K1:105:LEU:HD11	3:f2:13:ARG:HH11	1.86	0.40
3:Z1:22:ALA:HB1	3:02:18:ILE:O	2.21	0.40
3:51:114:GLN:HE21	3:51:114:GLN:HB3	1.68	0.40
3:D2:32:GLY:HA3	3:D2:33:PRO:HD3	1.95	0.40
3:T2:1:SER:OG	3:T2:2:LYS:N	2.41	0.40
3:V2:122:LEU:HD13	3:V2:122:LEU:HA	1.94	0.40
3:y2:114:GLN:HE21	3:y2:114:GLN:HB3	1.68	0.40
3:2I:32:GLY:HA3	3:2I:33:PRO:HD3	1.95	0.40
1:R:46:C:H2'	1:R:47:G:C8	2.56	0.40
1:R:85:G:C2	1:R:86:A:C8	3.09	0.40
2:M:151:LEU:N	2:M:152:PRO:CD	2.83	0.40
3:b1:22:ALA:HB1	3:U2:18:ILE:O	2.22	0.40
3:n1:32:GLY:HA3	3:n1:33:PRO:HD3	1.95	0.40
3:q1:122:LEU:HD13	3:q1:122:LEU:HA	1.94	0.40
3:L1:44:LEU:HD13	3:L1:55:VAL:HG22	2.01	0.40
3:H2:93:ASN:OD1	3:H2:93:ASN:N	2.55	0.40
1:R:12:G:C2'	1:R:13:C:O5'	2.69	0.40
1:R:45:C:H1'	1:R:46:C:C6	2.56	0.40
2:M:180:GLN:NE2	2:M:209:LEU:HD13	2.35	0.40
3:d1:2:LYS:HD3	3:d1:2:LYS:HA	1.91	0.40
3:e1:93:ASN:OD1	3:e1:93:ASN:N	2.55	0.40
3:r1:93:ASN:OD1	3:r1:93:ASN:N	2.55	0.40
3:z1:105:LEU:HD13	3:2V:38:LEU:CD2	2.48	0.40
3:K1:93:ASN:OD1	3:K1:93:ASN:N	2.55	0.40
3:T1:32:GLY:HA3	3:T1:33:PRO:HD3	1.95	0.40
3:U1:93:ASN:OD1	3:U1:93:ASN:N	2.55	0.40
3:X1:93:ASN:OD1	3:X1:93:ASN:N	2.55	0.40
3:Z1:2:LYS:HA	3:Z1:2:LYS:HD3	1.91	0.40
3:41:32:GLY:HA3	3:41:33:PRO:HD3	1.95	0.40
3:71:125:LEU:HD13	3:2U:57:LEU:CD2	2.51	0.40
3:K2:77:LYS:HB3	3:K2:77:LYS:HE3	1.96	0.40
3:N2:114:GLN:HE21	3:N2:114:GLN:HB3	1.68	0.40
3:T2:93:ASN:OD1	3:T2:93:ASN:N	2.55	0.40
3:X2:93:ASN:OD1	3:X2:93:ASN:N	2.55	0.40
3:n2:93:ASN:OD1	3:n2:93:ASN:N	2.55	0.40
3:2d:93:ASN:OD1	3:2d:93:ASN:N	2.55	0.40
3:2h:93:ASN:OD1	3:2h:93:ASN:N	2.55	0.40
3:2p:93:ASN:OD1	3:2p:93:ASN:N	2.55	0.40
3:2F:122:LEU:HD13	3:2F:122:LEU:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2W:93:ASN:OD1	3:2W:93:ASN:N	2.55	0.40
1:R:13:C:O2'	1:R:14:C:OP1	2.39	0.40
1:R:50:U:O2'	1:R:51:U:H5'	2.21	0.40
3:d1:114:GLN:HE21	3:d1:114:GLN:HB3	1.68	0.40
3:A1:93:ASN:OD1	3:A1:93:ASN:N	2.55	0.40
3:N1:93:ASN:OD1	3:N1:93:ASN:N	2.55	0.40
3:U1:22:ALA:HB2	3:u2:20:SER:H	1.86	0.40
3:61:93:ASN:HB2	3:ac:76:PRO:HD2	2.03	0.40
3:71:114:GLN:HE21	3:71:114:GLN:HB3	1.68	0.40
3:G2:122:LEU:HD13	3:G2:122:LEU:HA	1.94	0.40
3:H2:2:LYS:HA	3:H2:2:LYS:HD3	1.91	0.40
3:N2:93:ASN:OD1	3:N2:93:ASN:N	2.55	0.40
3:W2:77:LYS:HB3	3:W2:77:LYS:HE3	1.96	0.40
3:b2:93:ASN:OD1	3:b2:93:ASN:N	2.55	0.40
3:i2:93:ASN:OD1	3:i2:93:ASN:N	2.55	0.40
3:k2:2:LYS:HD3	3:k2:2:LYS:HA	1.91	0.40
3:q2:32:GLY:HA3	3:q2:33:PRO:HD3	1.95	0.40
3:02:93:ASN:OD1	3:02:93:ASN:N	2.55	0.40
3:2g:32:GLY:HA3	3:2g:33:PRO:HD3	1.95	0.40
3:2h:2:LYS:HD3	3:2h:2:LYS:HA	1.91	0.40
3:2k:114:GLN:HE21	3:2k:114:GLN:HB3	1.68	0.40
3:2I:93:ASN:OD1	3:2I:93:ASN:N	2.55	0.40
3:2N:93:ASN:OD1	3:2N:93:ASN:N	2.55	0.40
3:ad:122:LEU:HD13	3:ad:122:LEU:HA	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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
2	M	446/448 (100%)	386 (86%)	53 (12%)	7 (2%)	7 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	m	446/448 (100%)	382 (86%)	53 (12%)	11 (2%)	4	29
3	01	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	02	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	11	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	12	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	21	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	22	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2A	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2B	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2C	125/127 (98%)	108 (86%)	16 (13%)	1 (1%)	16	50
3	2D	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2E	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2F	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2G	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2H	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2I	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2J	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2K	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2L	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2M	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2N	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2O	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2P	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2Q	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2R	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2S	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2T	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2U	125/127 (98%)	108 (86%)	16 (13%)	1 (1%)	16	50
3	2V	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2W	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2X	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2Y	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2Z	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2a	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2b	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2c	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2d	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2e	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2f	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2g	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2h	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2i	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2j	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2k	125/127 (98%)	108 (86%)	16 (13%)	1 (1%)	16	50
3	2l	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2m	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2n	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2o	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2p	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2q	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2r	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2s	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2t	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2u	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2v	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2w	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2x	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	2y	125/127 (98%)	106 (85%)	18 (14%)	1 (1%)	16	50
3	2z	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	31	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	32	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	41	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	42	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	51	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	52	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	61	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	62	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	71	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	72	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	82	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	92	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	A1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	A2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	B1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	B2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	C1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	C2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	D1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	D2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	E1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	E2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	F1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	F2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	G1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	G2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	H1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	H2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	I1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	I2	125/127 (98%)	106 (85%)	18 (14%)	1 (1%)	16	50
3	J1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	J2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	K1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	K2	125/127 (98%)	106 (85%)	18 (14%)	1 (1%)	16	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	L2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	M1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	M2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	N1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	N2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	O1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	O2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	P1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	P2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	Q1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	Q2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	R1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	R2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	S1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	S2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	T1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	T2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	U1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	U2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	V1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	V2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	W1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	W2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	X1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	X2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	Y1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	Y2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	Z1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	Z2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	a1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	a2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	aa	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	ab	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	ac	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	ad	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	b1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	b2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	c1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	c2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	d1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	d2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	e1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	e2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	f1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	f2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	g1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	g2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	h1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	h2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	i1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	i2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	j1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	j2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	k1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	k2	125/127 (98%)	106 (85%)	18 (14%)	1 (1%)	16	50
3	l1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	l2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	m1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	m2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	n1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	n2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	o1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	o2	125/127 (98%)	106 (85%)	18 (14%)	1 (1%)	16	50
3	p1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	p2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	q1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	q2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	r1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	r2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	s1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	s2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	t1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	t2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	u1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	u2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	v1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	v2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	w1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	w2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	x1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	x2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	y1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	y2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	z1	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
3	z2	125/127 (98%)	107 (86%)	17 (14%)	1 (1%)	16	50
All	All	23142/23502 (98%)	19812 (86%)	3134 (14%)	196 (1%)	18	50

All (196) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	m	43	PRO
2	m	46	VAL
2	m	93	PRO
2	m	262	TRP
2	m	304	ARG

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Mol	Chain	Res	Type
2	m	305	LEU
2	m	368	VAL
2	m	380	ASP
2	M	262	TRP
2	M	304	ARG
2	M	305	LEU
2	M	380	ASP
2	M	260	PRO
2	M	315	ASP
2	m	94	GLY
2	m	260	PRO
2	m	308	GLU
3	a1	126	GLY
3	b1	126	GLY
3	c1	126	GLY
3	d1	126	GLY
3	e1	126	GLY
3	f1	380	GLY
3	g1	126	GLY
3	h1	126	GLY
3	i1	126	GLY
3	j1	126	GLY
3	k1	126	GLY
3	l1	126	GLY
3	m1	126	GLY
3	n1	126	GLY
3	o1	126	GLY
3	p1	126	GLY
3	q1	126	GLY
3	r1	126	GLY
3	s1	126	GLY
3	t1	126	GLY
3	u1	126	GLY
3	v1	126	GLY
3	w1	126	GLY
3	x1	126	GLY
3	y1	126	GLY
3	z1	126	GLY
3	A1	126	GLY
3	B1	126	GLY
3	C1	126	GLY
3	D1	126	GLY

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Mol	Chain	Res	Type
3	E1	126	GLY
3	F1	126	GLY
3	G1	126	GLY
3	H1	126	GLY
3	I1	126	GLY
3	J1	126	GLY
3	K1	126	GLY
3	L1	126	GLY
3	M1	126	GLY
3	N1	126	GLY
3	O1	126	GLY
3	P1	126	GLY
3	Q1	126	GLY
3	R1	126	GLY
3	S1	126	GLY
3	T1	126	GLY
3	U1	126	GLY
3	V1	126	GLY
3	W1	126	GLY
3	X1	126	GLY
3	Y1	126	GLY
3	Z1	126	GLY
3	01	126	GLY
3	11	126	GLY
3	21	126	GLY
3	31	126	GLY
3	41	126	GLY
3	51	126	GLY
3	61	126	GLY
3	71	126	GLY
3	A2	126	GLY
3	B2	126	GLY
3	C2	126	GLY
3	D2	126	GLY
3	E2	126	GLY
3	F2	126	GLY
3	G2	126	GLY
3	H2	126	GLY
3	I2	126	GLY
3	J2	126	GLY
3	K2	126	GLY
3	L2	126	GLY

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Mol	Chain	Res	Type
3	M2	126	GLY
3	N2	126	GLY
3	O2	126	GLY
3	P2	126	GLY
3	Q2	126	GLY
3	R2	126	GLY
3	S2	126	GLY
3	T2	126	GLY
3	U2	126	GLY
3	V2	126	GLY
3	W2	126	GLY
3	X2	126	GLY
3	Y2	126	GLY
3	Z2	126	GLY
3	a2	126	GLY
3	b2	126	GLY
3	c2	126	GLY
3	d2	126	GLY
3	e2	126	GLY
3	f2	126	GLY
3	g2	126	GLY
3	h2	126	GLY
3	i2	126	GLY
3	j2	126	GLY
3	k2	126	GLY
3	l2	126	GLY
3	m2	126	GLY
3	n2	126	GLY
3	o2	126	GLY
3	p2	126	GLY
3	q2	126	GLY
3	r2	126	GLY
3	s2	126	GLY
3	t2	126	GLY
3	u2	126	GLY
3	v2	126	GLY
3	w2	126	GLY
3	x2	126	GLY
3	y2	126	GLY
3	z2	126	GLY
3	02	126	GLY
3	12	126	GLY

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Mol	Chain	Res	Type
3	22	126	GLY
3	32	126	GLY
3	42	126	GLY
3	52	126	GLY
3	62	126	GLY
3	72	126	GLY
3	82	126	GLY
3	92	126	GLY
3	2a	126	GLY
3	2b	126	GLY
3	2c	126	GLY
3	2d	126	GLY
3	2e	126	GLY
3	2f	126	GLY
3	2g	126	GLY
3	2h	126	GLY
3	2i	126	GLY
3	2j	126	GLY
3	2k	126	GLY
3	2l	126	GLY
3	2m	126	GLY
3	2n	126	GLY
3	2o	126	GLY
3	2p	126	GLY
3	2q	126	GLY
3	2r	126	GLY
3	2s	126	GLY
3	2t	126	GLY
3	2u	126	GLY
3	2v	126	GLY
3	2w	126	GLY
3	2x	126	GLY
3	2y	126	GLY
3	2z	126	GLY
3	2A	126	GLY
3	2B	126	GLY
3	2C	126	GLY
3	2D	126	GLY
3	2E	126	GLY
3	2F	126	GLY
3	2G	126	GLY
3	2H	126	GLY

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Mol	Chain	Res	Type
3	2I	126	GLY
3	2J	126	GLY
3	2K	126	GLY
3	2L	126	GLY
3	2M	126	GLY
3	2N	126	GLY
3	2O	126	GLY
3	2P	126	GLY
3	2Q	126	GLY
3	2R	126	GLY
3	2S	126	GLY
3	2T	126	GLY
3	2U	126	GLY
3	2V	126	GLY
3	2W	126	GLY
3	2X	126	GLY
3	2Y	126	GLY
3	2Z	126	GLY
3	aa	126	GLY
3	ab	126	GLY
3	ac	126	GLY
3	ad	126	GLY
2	M	308	GLU

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 PDB entries followed by that with respect to all EM entries.

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	
2	M	389/389 (100%)	387 (100%)	2 (0%)	81	82
2	m	389/389 (100%)	387 (100%)	2 (0%)	81	82
3	01	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	02	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	11	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	12	111/112 (99%)	107 (96%)	4 (4%)	31	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	2I	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	22	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2A	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2B	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2C	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2D	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2E	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2F	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2G	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2H	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2I	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2J	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2K	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2L	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2M	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2N	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2O	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2P	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2Q	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2R	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	2S	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2T	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2U	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2V	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2W	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2X	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2Y	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2Z	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2a	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2b	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2c	111/112 (99%)	107 (96%)	4 (4%)	31	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	2d	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2e	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2f	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2g	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2h	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	2i	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2j	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2k	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2l	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2m	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2n	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2o	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2p	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2q	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2r	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2s	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2t	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2u	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2v	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2w	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2x	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2y	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	2z	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	31	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	32	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	41	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	42	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	51	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	52	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	61	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	62	111/112 (99%)	107 (96%)	4 (4%)	31	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	71	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	72	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	82	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	92	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	A1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	A2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	B1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	B2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	C1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	C2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	D1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	D2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	E1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	E2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	F1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	F2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	G1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	G2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	H1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	H2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	I1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	I2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	J1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	J2	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	K1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	K2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	L1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	L2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	M1	111/112 (99%)	108 (97%)	3 (3%)	39	60
3	M2	111/112 (99%)	108 (97%)	3 (3%)	39	60
3	N1	111/112 (99%)	106 (96%)	5 (4%)	24	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	N2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	O1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	O2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	P1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	P2	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	Q1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	Q2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	R1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	R2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	S1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	S2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	T1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	T2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	U1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	U2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	V1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	V2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	W1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	W2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	X1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	X2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	Y1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	Y2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	Z1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	Z2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	a1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	a2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	aa	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	ab	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	ac	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	ad	111/112 (99%)	107 (96%)	4 (4%)	31	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	b1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	b2	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	c1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	c2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	d1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	d2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	e1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	e2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	f1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	f2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	g1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	g2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	h1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	h2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	i1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	i2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	j1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	j2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	k1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	k2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	l1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	l2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	m1	111/112 (99%)	108 (97%)	3 (3%)	39	60
3	m2	111/112 (99%)	108 (97%)	3 (3%)	39	60
3	n1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	n2	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	o1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	o2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	p1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	p2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	q1	111/112 (99%)	106 (96%)	5 (4%)	24	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	q2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	r1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	r2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	s1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	s2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	t1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	t2	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	u1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	u2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	v1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	v2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	w1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	w2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	x1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	x2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	y1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	y2	111/112 (99%)	107 (96%)	4 (4%)	31	54
3	z1	111/112 (99%)	106 (96%)	5 (4%)	24	49
3	z2	111/112 (99%)	107 (96%)	4 (4%)	31	54
All	All	20536/20714 (99%)	19757 (96%)	779 (4%)	30	52

All (779) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	m	86	VAL
2	m	95	SER
2	M	86	VAL
2	M	242	THR
3	a1	72	CYS
3	a1	91	VAL
3	a1	102	LEU
3	a1	122	LEU
3	a1	123	VAL
3	b1	72	CYS
3	b1	91	VAL

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Mol	Chain	Res	Type
3	b1	102	LEU
3	b1	122	LEU
3	b1	123	VAL
3	c1	72	CYS
3	c1	91	VAL
3	c1	102	LEU
3	c1	122	LEU
3	c1	123	VAL
3	d1	72	CYS
3	d1	91	VAL
3	d1	102	LEU
3	d1	122	LEU
3	d1	123	VAL
3	e1	72	CYS
3	e1	91	VAL
3	e1	102	LEU
3	e1	122	LEU
3	e1	123	VAL
3	f1	326	CYS
3	f1	345	VAL
3	f1	356	LEU
3	f1	376	LEU
3	f1	377	VAL
3	g1	72	CYS
3	g1	91	VAL
3	g1	102	LEU
3	g1	122	LEU
3	g1	123	VAL
3	h1	72	CYS
3	h1	91	VAL
3	h1	102	LEU
3	h1	122	LEU
3	h1	123	VAL
3	i1	72	CYS
3	i1	91	VAL
3	i1	102	LEU
3	i1	122	LEU
3	i1	123	VAL
3	j1	72	CYS
3	j1	91	VAL
3	j1	102	LEU
3	j1	122	LEU

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Mol	Chain	Res	Type
3	j1	123	VAL
3	k1	72	CYS
3	k1	91	VAL
3	k1	102	LEU
3	k1	122	LEU
3	k1	123	VAL
3	l1	72	CYS
3	l1	91	VAL
3	l1	102	LEU
3	l1	122	LEU
3	l1	123	VAL
3	m1	102	LEU
3	m1	122	LEU
3	m1	123	VAL
3	n1	72	CYS
3	n1	91	VAL
3	n1	102	LEU
3	n1	122	LEU
3	n1	123	VAL
3	o1	72	CYS
3	o1	91	VAL
3	o1	102	LEU
3	o1	122	LEU
3	o1	123	VAL
3	p1	72	CYS
3	p1	91	VAL
3	p1	102	LEU
3	p1	122	LEU
3	p1	123	VAL
3	q1	72	CYS
3	q1	91	VAL
3	q1	102	LEU
3	q1	122	LEU
3	q1	123	VAL
3	r1	72	CYS
3	r1	91	VAL
3	r1	102	LEU
3	r1	122	LEU
3	r1	123	VAL
3	s1	72	CYS
3	s1	91	VAL
3	s1	102	LEU

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Mol	Chain	Res	Type
3	s1	122	LEU
3	s1	123	VAL
3	t1	72	CYS
3	t1	91	VAL
3	t1	102	LEU
3	t1	122	LEU
3	t1	123	VAL
3	u1	72	CYS
3	u1	91	VAL
3	u1	102	LEU
3	u1	122	LEU
3	u1	123	VAL
3	v1	72	CYS
3	v1	91	VAL
3	v1	102	LEU
3	v1	122	LEU
3	v1	123	VAL
3	w1	72	CYS
3	w1	91	VAL
3	w1	102	LEU
3	w1	122	LEU
3	w1	123	VAL
3	x1	72	CYS
3	x1	91	VAL
3	x1	102	LEU
3	x1	122	LEU
3	x1	123	VAL
3	y1	72	CYS
3	y1	91	VAL
3	y1	102	LEU
3	y1	122	LEU
3	y1	123	VAL
3	z1	72	CYS
3	z1	91	VAL
3	z1	102	LEU
3	z1	122	LEU
3	z1	123	VAL
3	A1	72	CYS
3	A1	91	VAL
3	A1	102	LEU
3	A1	122	LEU
3	A1	123	VAL

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Mol	Chain	Res	Type
3	B1	72	CYS
3	B1	91	VAL
3	B1	102	LEU
3	B1	122	LEU
3	B1	123	VAL
3	C1	72	CYS
3	C1	91	VAL
3	C1	102	LEU
3	C1	122	LEU
3	C1	123	VAL
3	D1	72	CYS
3	D1	91	VAL
3	D1	102	LEU
3	D1	122	LEU
3	D1	123	VAL
3	E1	72	CYS
3	E1	91	VAL
3	E1	102	LEU
3	E1	122	LEU
3	E1	123	VAL
3	F1	72	CYS
3	F1	91	VAL
3	F1	102	LEU
3	F1	122	LEU
3	F1	123	VAL
3	G1	72	CYS
3	G1	91	VAL
3	G1	102	LEU
3	G1	122	LEU
3	G1	123	VAL
3	H1	72	CYS
3	H1	91	VAL
3	H1	102	LEU
3	H1	122	LEU
3	H1	123	VAL
3	I1	72	CYS
3	I1	91	VAL
3	I1	102	LEU
3	I1	122	LEU
3	I1	123	VAL
3	J1	72	CYS
3	J1	91	VAL

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Mol	Chain	Res	Type
3	J1	102	LEU
3	J1	122	LEU
3	J1	123	VAL
3	K1	72	CYS
3	K1	91	VAL
3	K1	102	LEU
3	K1	122	LEU
3	K1	123	VAL
3	L1	72	CYS
3	L1	91	VAL
3	L1	102	LEU
3	L1	122	LEU
3	L1	123	VAL
3	M1	102	LEU
3	M1	122	LEU
3	M1	123	VAL
3	N1	72	CYS
3	N1	91	VAL
3	N1	102	LEU
3	N1	122	LEU
3	N1	123	VAL
3	O1	72	CYS
3	O1	91	VAL
3	O1	102	LEU
3	O1	122	LEU
3	O1	123	VAL
3	P1	72	CYS
3	P1	91	VAL
3	P1	102	LEU
3	P1	122	LEU
3	P1	123	VAL
3	Q1	72	CYS
3	Q1	91	VAL
3	Q1	102	LEU
3	Q1	122	LEU
3	Q1	123	VAL
3	R1	72	CYS
3	R1	91	VAL
3	R1	102	LEU
3	R1	122	LEU
3	R1	123	VAL
3	S1	72	CYS

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Mol	Chain	Res	Type
3	S1	91	VAL
3	S1	102	LEU
3	S1	122	LEU
3	S1	123	VAL
3	T1	72	CYS
3	T1	91	VAL
3	T1	102	LEU
3	T1	122	LEU
3	T1	123	VAL
3	U1	72	CYS
3	U1	91	VAL
3	U1	102	LEU
3	U1	122	LEU
3	U1	123	VAL
3	V1	72	CYS
3	V1	91	VAL
3	V1	102	LEU
3	V1	122	LEU
3	V1	123	VAL
3	W1	72	CYS
3	W1	91	VAL
3	W1	102	LEU
3	W1	122	LEU
3	W1	123	VAL
3	X1	72	CYS
3	X1	91	VAL
3	X1	102	LEU
3	X1	122	LEU
3	X1	123	VAL
3	Y1	72	CYS
3	Y1	91	VAL
3	Y1	102	LEU
3	Y1	122	LEU
3	Y1	123	VAL
3	Z1	72	CYS
3	Z1	91	VAL
3	Z1	102	LEU
3	Z1	122	LEU
3	Z1	123	VAL
3	01	72	CYS
3	01	91	VAL
3	01	102	LEU

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Mol	Chain	Res	Type
3	01	122	LEU
3	01	123	VAL
3	11	72	CYS
3	11	91	VAL
3	11	102	LEU
3	11	122	LEU
3	11	123	VAL
3	21	72	CYS
3	21	91	VAL
3	21	102	LEU
3	21	122	LEU
3	21	123	VAL
3	31	72	CYS
3	31	91	VAL
3	31	102	LEU
3	31	122	LEU
3	31	123	VAL
3	41	72	CYS
3	41	91	VAL
3	41	102	LEU
3	41	122	LEU
3	41	123	VAL
3	51	72	CYS
3	51	91	VAL
3	51	102	LEU
3	51	122	LEU
3	51	123	VAL
3	61	72	CYS
3	61	91	VAL
3	61	102	LEU
3	61	122	LEU
3	61	123	VAL
3	71	72	CYS
3	71	91	VAL
3	71	102	LEU
3	71	122	LEU
3	71	123	VAL
3	A2	91	VAL
3	A2	102	LEU
3	A2	122	LEU
3	A2	123	VAL
3	B2	91	VAL

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Mol	Chain	Res	Type
3	B2	102	LEU
3	B2	122	LEU
3	B2	123	VAL
3	C2	91	VAL
3	C2	102	LEU
3	C2	122	LEU
3	C2	123	VAL
3	D2	91	VAL
3	D2	102	LEU
3	D2	122	LEU
3	D2	123	VAL
3	E2	91	VAL
3	E2	102	LEU
3	E2	122	LEU
3	E2	123	VAL
3	F2	91	VAL
3	F2	102	LEU
3	F2	122	LEU
3	F2	123	VAL
3	G2	91	VAL
3	G2	102	LEU
3	G2	122	LEU
3	G2	123	VAL
3	H2	91	VAL
3	H2	102	LEU
3	H2	122	LEU
3	H2	123	VAL
3	I2	91	VAL
3	I2	102	LEU
3	I2	122	LEU
3	I2	123	VAL
3	J2	72	CYS
3	J2	91	VAL
3	J2	102	LEU
3	J2	122	LEU
3	J2	123	VAL
3	K2	91	VAL
3	K2	102	LEU
3	K2	122	LEU
3	K2	123	VAL
3	L2	91	VAL
3	L2	102	LEU

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Mol	Chain	Res	Type
3	L2	122	LEU
3	L2	123	VAL
3	M2	102	LEU
3	M2	122	LEU
3	M2	123	VAL
3	N2	91	VAL
3	N2	102	LEU
3	N2	122	LEU
3	N2	123	VAL
3	O2	91	VAL
3	O2	102	LEU
3	O2	122	LEU
3	O2	123	VAL
3	P2	72	CYS
3	P2	91	VAL
3	P2	102	LEU
3	P2	122	LEU
3	P2	123	VAL
3	Q2	91	VAL
3	Q2	102	LEU
3	Q2	122	LEU
3	Q2	123	VAL
3	R2	91	VAL
3	R2	102	LEU
3	R2	122	LEU
3	R2	123	VAL
3	S2	91	VAL
3	S2	102	LEU
3	S2	122	LEU
3	S2	123	VAL
3	T2	91	VAL
3	T2	102	LEU
3	T2	122	LEU
3	T2	123	VAL
3	U2	91	VAL
3	U2	102	LEU
3	U2	122	LEU
3	U2	123	VAL
3	V2	91	VAL
3	V2	102	LEU
3	V2	122	LEU
3	V2	123	VAL

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Mol	Chain	Res	Type
3	W2	91	VAL
3	W2	102	LEU
3	W2	122	LEU
3	W2	123	VAL
3	X2	91	VAL
3	X2	102	LEU
3	X2	122	LEU
3	X2	123	VAL
3	Y2	91	VAL
3	Y2	102	LEU
3	Y2	122	LEU
3	Y2	123	VAL
3	Z2	91	VAL
3	Z2	102	LEU
3	Z2	122	LEU
3	Z2	123	VAL
3	a2	91	VAL
3	a2	102	LEU
3	a2	122	LEU
3	a2	123	VAL
3	b2	72	CYS
3	b2	91	VAL
3	b2	102	LEU
3	b2	122	LEU
3	b2	123	VAL
3	c2	91	VAL
3	c2	102	LEU
3	c2	122	LEU
3	c2	123	VAL
3	d2	91	VAL
3	d2	102	LEU
3	d2	122	LEU
3	d2	123	VAL
3	e2	91	VAL
3	e2	102	LEU
3	e2	122	LEU
3	e2	123	VAL
3	f2	91	VAL
3	f2	102	LEU
3	f2	122	LEU
3	f2	123	VAL
3	g2	91	VAL

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Mol	Chain	Res	Type
3	g2	102	LEU
3	g2	122	LEU
3	g2	123	VAL
3	h2	91	VAL
3	h2	102	LEU
3	h2	122	LEU
3	h2	123	VAL
3	i2	91	VAL
3	i2	102	LEU
3	i2	122	LEU
3	i2	123	VAL
3	j2	91	VAL
3	j2	102	LEU
3	j2	122	LEU
3	j2	123	VAL
3	k2	91	VAL
3	k2	102	LEU
3	k2	122	LEU
3	k2	123	VAL
3	l2	91	VAL
3	l2	102	LEU
3	l2	122	LEU
3	l2	123	VAL
3	m2	102	LEU
3	m2	122	LEU
3	m2	123	VAL
3	n2	72	CYS
3	n2	91	VAL
3	n2	102	LEU
3	n2	122	LEU
3	n2	123	VAL
3	o2	91	VAL
3	o2	102	LEU
3	o2	122	LEU
3	o2	123	VAL
3	p2	91	VAL
3	p2	102	LEU
3	p2	122	LEU
3	p2	123	VAL
3	q2	91	VAL
3	q2	102	LEU
3	q2	122	LEU

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Mol	Chain	Res	Type
3	q2	123	VAL
3	r2	91	VAL
3	r2	102	LEU
3	r2	122	LEU
3	r2	123	VAL
3	s2	91	VAL
3	s2	102	LEU
3	s2	122	LEU
3	s2	123	VAL
3	t2	72	CYS
3	t2	91	VAL
3	t2	102	LEU
3	t2	122	LEU
3	t2	123	VAL
3	u2	91	VAL
3	u2	102	LEU
3	u2	122	LEU
3	u2	123	VAL
3	v2	91	VAL
3	v2	102	LEU
3	v2	122	LEU
3	v2	123	VAL
3	w2	91	VAL
3	w2	102	LEU
3	w2	122	LEU
3	w2	123	VAL
3	x2	91	VAL
3	x2	102	LEU
3	x2	122	LEU
3	x2	123	VAL
3	y2	91	VAL
3	y2	102	LEU
3	y2	122	LEU
3	y2	123	VAL
3	z2	91	VAL
3	z2	102	LEU
3	z2	122	LEU
3	z2	123	VAL
3	02	91	VAL
3	02	102	LEU
3	02	122	LEU
3	02	123	VAL

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Mol	Chain	Res	Type
3	12	91	VAL
3	12	102	LEU
3	12	122	LEU
3	12	123	VAL
3	22	91	VAL
3	22	102	LEU
3	22	122	LEU
3	22	123	VAL
3	32	91	VAL
3	32	102	LEU
3	32	122	LEU
3	32	123	VAL
3	42	91	VAL
3	42	102	LEU
3	42	122	LEU
3	42	123	VAL
3	52	72	CYS
3	52	91	VAL
3	52	102	LEU
3	52	122	LEU
3	52	123	VAL
3	62	91	VAL
3	62	102	LEU
3	62	122	LEU
3	62	123	VAL
3	72	91	VAL
3	72	102	LEU
3	72	122	LEU
3	72	123	VAL
3	82	91	VAL
3	82	102	LEU
3	82	122	LEU
3	82	123	VAL
3	92	91	VAL
3	92	102	LEU
3	92	122	LEU
3	92	123	VAL
3	2a	91	VAL
3	2a	102	LEU
3	2a	122	LEU
3	2a	123	VAL
3	2b	91	VAL

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Mol	Chain	Res	Type
3	2b	102	LEU
3	2b	122	LEU
3	2b	123	VAL
3	2c	91	VAL
3	2c	102	LEU
3	2c	122	LEU
3	2c	123	VAL
3	2d	91	VAL
3	2d	102	LEU
3	2d	122	LEU
3	2d	123	VAL
3	2e	91	VAL
3	2e	102	LEU
3	2e	122	LEU
3	2e	123	VAL
3	2f	91	VAL
3	2f	102	LEU
3	2f	122	LEU
3	2f	123	VAL
3	2g	91	VAL
3	2g	102	LEU
3	2g	122	LEU
3	2g	123	VAL
3	2h	72	CYS
3	2h	91	VAL
3	2h	102	LEU
3	2h	122	LEU
3	2h	123	VAL
3	2i	91	VAL
3	2i	102	LEU
3	2i	122	LEU
3	2i	123	VAL
3	2j	91	VAL
3	2j	102	LEU
3	2j	122	LEU
3	2j	123	VAL
3	2k	91	VAL
3	2k	102	LEU
3	2k	122	LEU
3	2k	123	VAL
3	2l	91	VAL
3	2l	102	LEU

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Mol	Chain	Res	Type
3	2l	122	LEU
3	2l	123	VAL
3	2m	91	VAL
3	2m	102	LEU
3	2m	122	LEU
3	2m	123	VAL
3	2n	91	VAL
3	2n	102	LEU
3	2n	122	LEU
3	2n	123	VAL
3	2o	91	VAL
3	2o	102	LEU
3	2o	122	LEU
3	2o	123	VAL
3	2p	91	VAL
3	2p	102	LEU
3	2p	122	LEU
3	2p	123	VAL
3	2q	91	VAL
3	2q	102	LEU
3	2q	122	LEU
3	2q	123	VAL
3	2r	91	VAL
3	2r	102	LEU
3	2r	122	LEU
3	2r	123	VAL
3	2s	91	VAL
3	2s	102	LEU
3	2s	122	LEU
3	2s	123	VAL
3	2t	91	VAL
3	2t	102	LEU
3	2t	122	LEU
3	2t	123	VAL
3	2u	91	VAL
3	2u	102	LEU
3	2u	122	LEU
3	2u	123	VAL
3	2v	91	VAL
3	2v	102	LEU
3	2v	122	LEU
3	2v	123	VAL

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Mol	Chain	Res	Type
3	2w	91	VAL
3	2w	102	LEU
3	2w	122	LEU
3	2w	123	VAL
3	2x	91	VAL
3	2x	102	LEU
3	2x	122	LEU
3	2x	123	VAL
3	2y	91	VAL
3	2y	102	LEU
3	2y	122	LEU
3	2y	123	VAL
3	2z	72	CYS
3	2z	91	VAL
3	2z	102	LEU
3	2z	122	LEU
3	2z	123	VAL
3	2A	91	VAL
3	2A	102	LEU
3	2A	122	LEU
3	2A	123	VAL
3	2B	91	VAL
3	2B	102	LEU
3	2B	122	LEU
3	2B	123	VAL
3	2C	91	VAL
3	2C	102	LEU
3	2C	122	LEU
3	2C	123	VAL
3	2D	91	VAL
3	2D	102	LEU
3	2D	122	LEU
3	2D	123	VAL
3	2E	91	VAL
3	2E	102	LEU
3	2E	122	LEU
3	2E	123	VAL
3	2F	91	VAL
3	2F	102	LEU
3	2F	122	LEU
3	2F	123	VAL
3	2G	91	VAL

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Mol	Chain	Res	Type
3	2G	102	LEU
3	2G	122	LEU
3	2G	123	VAL
3	2H	91	VAL
3	2H	102	LEU
3	2H	122	LEU
3	2H	123	VAL
3	2I	91	VAL
3	2I	102	LEU
3	2I	122	LEU
3	2I	123	VAL
3	2J	91	VAL
3	2J	102	LEU
3	2J	122	LEU
3	2J	123	VAL
3	2K	91	VAL
3	2K	102	LEU
3	2K	122	LEU
3	2K	123	VAL
3	2L	91	VAL
3	2L	102	LEU
3	2L	122	LEU
3	2L	123	VAL
3	2M	91	VAL
3	2M	102	LEU
3	2M	122	LEU
3	2M	123	VAL
3	2N	91	VAL
3	2N	102	LEU
3	2N	122	LEU
3	2N	123	VAL
3	2O	91	VAL
3	2O	102	LEU
3	2O	122	LEU
3	2O	123	VAL
3	2P	91	VAL
3	2P	102	LEU
3	2P	122	LEU
3	2P	123	VAL
3	2Q	91	VAL
3	2Q	102	LEU
3	2Q	122	LEU

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Mol	Chain	Res	Type
3	2Q	123	VAL
3	2R	72	CYS
3	2R	91	VAL
3	2R	102	LEU
3	2R	122	LEU
3	2R	123	VAL
3	2S	91	VAL
3	2S	102	LEU
3	2S	122	LEU
3	2S	123	VAL
3	2T	91	VAL
3	2T	102	LEU
3	2T	122	LEU
3	2T	123	VAL
3	2U	91	VAL
3	2U	102	LEU
3	2U	122	LEU
3	2U	123	VAL
3	2V	91	VAL
3	2V	102	LEU
3	2V	122	LEU
3	2V	123	VAL
3	2W	91	VAL
3	2W	102	LEU
3	2W	122	LEU
3	2W	123	VAL
3	2X	91	VAL
3	2X	102	LEU
3	2X	122	LEU
3	2X	123	VAL
3	2Y	91	VAL
3	2Y	102	LEU
3	2Y	122	LEU
3	2Y	123	VAL
3	2Z	91	VAL
3	2Z	102	LEU
3	2Z	122	LEU
3	2Z	123	VAL
3	aa	91	VAL
3	aa	102	LEU
3	aa	122	LEU
3	aa	123	VAL

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Mol	Chain	Res	Type
3	ab	91	VAL
3	ab	102	LEU
3	ab	122	LEU
3	ab	123	VAL
3	ac	91	VAL
3	ac	102	LEU
3	ac	122	LEU
3	ac	123	VAL
3	ad	91	VAL
3	ad	102	LEU
3	ad	122	LEU
3	ad	123	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (388) such sidechains are listed below:

Mol	Chain	Res	Type
2	m	49	HIS
2	m	350	ASN
2	M	167	ASN
2	M	204	ASN
2	M	241	HIS
3	a1	56	ASN
3	a1	114	GLN
3	a1	121	ASN
3	b1	56	ASN
3	b1	114	GLN
3	b1	121	ASN
3	c1	56	ASN
3	c1	114	GLN
3	d1	56	ASN
3	d1	114	GLN
3	d1	121	ASN
3	e1	56	ASN
3	e1	114	GLN
3	e1	121	ASN
3	f1	310	ASN
3	f1	368	GLN
3	f1	375	ASN
3	g1	56	ASN
3	g1	114	GLN
3	g1	121	ASN
3	h1	56	ASN

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Mol	Chain	Res	Type
3	h1	114	GLN
3	h1	121	ASN
3	i1	56	ASN
3	i1	114	GLN
3	i1	121	ASN
3	j1	56	ASN
3	j1	114	GLN
3	j1	121	ASN
3	k1	56	ASN
3	k1	114	GLN
3	k1	121	ASN
3	l1	56	ASN
3	l1	114	GLN
3	l1	121	ASN
3	m1	56	ASN
3	m1	114	GLN
3	n1	56	ASN
3	n1	114	GLN
3	n1	121	ASN
3	o1	56	ASN
3	o1	114	GLN
3	o1	121	ASN
3	p1	56	ASN
3	p1	114	GLN
3	q1	56	ASN
3	q1	114	GLN
3	q1	121	ASN
3	r1	56	ASN
3	r1	114	GLN
3	r1	121	ASN
3	s1	56	ASN
3	s1	114	GLN
3	t1	56	ASN
3	t1	114	GLN
3	t1	121	ASN
3	u1	56	ASN
3	u1	114	GLN
3	u1	121	ASN
3	v1	56	ASN
3	v1	114	GLN
3	w1	56	ASN
3	w1	114	GLN

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Mol	Chain	Res	Type
3	w1	121	ASN
3	x1	56	ASN
3	x1	114	GLN
3	x1	121	ASN
3	y1	56	ASN
3	y1	114	GLN
3	y1	121	ASN
3	z1	56	ASN
3	z1	121	ASN
3	A1	56	ASN
3	A1	114	GLN
3	A1	121	ASN
3	B1	56	ASN
3	B1	114	GLN
3	B1	121	ASN
3	C1	56	ASN
3	C1	114	GLN
3	C1	121	ASN
3	D1	56	ASN
3	D1	114	GLN
3	D1	121	ASN
3	E1	56	ASN
3	E1	114	GLN
3	E1	121	ASN
3	F1	56	ASN
3	F1	114	GLN
3	F1	121	ASN
3	G1	56	ASN
3	G1	114	GLN
3	G1	121	ASN
3	H1	56	ASN
3	H1	114	GLN
3	H1	121	ASN
3	I1	56	ASN
3	I1	114	GLN
3	I1	121	ASN
3	J1	56	ASN
3	J1	114	GLN
3	J1	121	ASN
3	K1	56	ASN
3	K1	114	GLN
3	K1	121	ASN

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Mol	Chain	Res	Type
3	L1	56	ASN
3	L1	114	GLN
3	L1	121	ASN
3	M1	56	ASN
3	M1	114	GLN
3	M1	121	ASN
3	N1	56	ASN
3	N1	114	GLN
3	N1	121	ASN
3	O1	56	ASN
3	O1	114	GLN
3	O1	121	ASN
3	P1	56	ASN
3	P1	114	GLN
3	P1	121	ASN
3	Q1	56	ASN
3	Q1	114	GLN
3	Q1	121	ASN
3	R1	56	ASN
3	R1	114	GLN
3	R1	121	ASN
3	S1	56	ASN
3	S1	114	GLN
3	S1	121	ASN
3	T1	56	ASN
3	T1	114	GLN
3	T1	121	ASN
3	U1	56	ASN
3	U1	114	GLN
3	U1	121	ASN
3	V1	56	ASN
3	V1	114	GLN
3	V1	121	ASN
3	W1	56	ASN
3	W1	114	GLN
3	W1	121	ASN
3	X1	56	ASN
3	X1	114	GLN
3	X1	121	ASN
3	Y1	56	ASN
3	Y1	114	GLN
3	Y1	121	ASN

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Mol	Chain	Res	Type
3	Z1	56	ASN
3	Z1	114	GLN
3	Z1	121	ASN
3	01	56	ASN
3	01	114	GLN
3	01	121	ASN
3	11	56	ASN
3	11	114	GLN
3	21	56	ASN
3	21	114	GLN
3	21	121	ASN
3	31	56	ASN
3	31	114	GLN
3	31	121	ASN
3	41	25	GLN
3	41	56	ASN
3	41	114	GLN
3	41	121	ASN
3	51	56	ASN
3	51	114	GLN
3	61	56	ASN
3	61	114	GLN
3	61	121	ASN
3	71	56	ASN
3	71	121	ASN
3	A2	114	GLN
3	B2	114	GLN
3	B2	121	ASN
3	C2	114	GLN
3	D2	114	GLN
3	D2	121	ASN
3	E2	114	GLN
3	F2	114	GLN
3	F2	121	ASN
3	G2	114	GLN
3	H2	114	GLN
3	H2	121	ASN
3	I2	114	GLN
3	I2	121	ASN
3	J2	56	ASN
3	J2	114	GLN
3	J2	121	ASN

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Mol	Chain	Res	Type
3	K2	25	GLN
3	K2	114	GLN
3	K2	121	ASN
3	L2	114	GLN
3	L2	121	ASN
3	M2	114	GLN
3	N2	114	GLN
3	N2	121	ASN
3	O2	114	GLN
3	O2	121	ASN
3	P2	114	GLN
3	P2	121	ASN
3	Q2	114	GLN
3	Q2	121	ASN
3	R2	114	GLN
3	R2	121	ASN
3	S2	56	ASN
3	S2	114	GLN
3	T2	114	GLN
3	T2	121	ASN
3	U2	114	GLN
3	V2	114	GLN
3	V2	121	ASN
3	W2	114	GLN
3	X2	114	GLN
3	X2	121	ASN
3	Y2	114	GLN
3	Z2	56	ASN
3	Z2	114	GLN
3	Z2	121	ASN
3	a2	114	GLN
3	a2	121	ASN
3	b2	56	ASN
3	b2	114	GLN
3	b2	121	ASN
3	c2	114	GLN
3	c2	121	ASN
3	d2	114	GLN
3	d2	121	ASN
3	e2	114	GLN
3	f2	114	GLN
3	f2	121	ASN

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Mol	Chain	Res	Type
3	g2	114	GLN
3	h2	114	GLN
3	h2	121	ASN
3	i2	114	GLN
3	j2	56	ASN
3	j2	114	GLN
3	j2	121	ASN
3	k2	114	GLN
3	l2	114	GLN
3	l2	121	ASN
3	m2	114	GLN
3	m2	121	ASN
3	n2	114	GLN
3	n2	121	ASN
3	o2	25	GLN
3	o2	114	GLN
3	o2	121	ASN
3	p2	114	GLN
3	p2	121	ASN
3	q2	25	GLN
3	q2	114	GLN
3	q2	121	ASN
3	r2	114	GLN
3	r2	121	ASN
3	s2	114	GLN
3	s2	121	ASN
3	t2	114	GLN
3	t2	121	ASN
3	u2	114	GLN
3	u2	121	ASN
3	v2	114	GLN
3	v2	121	ASN
3	w2	114	GLN
3	x2	114	GLN
3	x2	121	ASN
3	y2	114	GLN
3	z2	114	GLN
3	z2	121	ASN
3	02	114	GLN
3	12	114	GLN
3	12	121	ASN
3	22	114	GLN

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Mol	Chain	Res	Type
3	32	114	GLN
3	32	121	ASN
3	42	114	GLN
3	42	121	ASN
3	52	114	GLN
3	52	121	ASN
3	62	114	GLN
3	62	121	ASN
3	72	114	GLN
3	72	121	ASN
3	82	114	GLN
3	92	114	GLN
3	92	121	ASN
3	2a	114	GLN
3	2b	56	ASN
3	2b	114	GLN
3	2b	121	ASN
3	2c	114	GLN
3	2d	114	GLN
3	2e	114	GLN
3	2e	121	ASN
3	2f	114	GLN
3	2g	114	GLN
3	2g	121	ASN
3	2h	114	GLN
3	2h	121	ASN
3	2i	114	GLN
3	2i	121	ASN
3	2j	114	GLN
3	2j	121	ASN
3	2k	114	GLN
3	2k	121	ASN
3	2l	114	GLN
3	2m	114	GLN
3	2m	121	ASN
3	2n	114	GLN
3	2o	114	GLN
3	2o	121	ASN
3	2p	114	GLN
3	2q	114	GLN
3	2r	114	GLN
3	2r	121	ASN

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Mol	Chain	Res	Type
3	2s	114	GLN
3	2t	114	GLN
3	2t	121	ASN
3	2u	114	GLN
3	2v	114	GLN
3	2v	121	ASN
3	2w	56	ASN
3	2w	114	GLN
3	2x	114	GLN
3	2x	121	ASN
3	2y	25	GLN
3	2y	114	GLN
3	2y	121	ASN
3	2z	114	GLN
3	2z	121	ASN
3	2A	114	GLN
3	2A	121	ASN
3	2B	114	GLN
3	2B	121	ASN
3	2C	114	GLN
3	2C	121	ASN
3	2D	114	GLN
3	2E	114	GLN
3	2E	121	ASN
3	2F	114	GLN
3	2G	114	GLN
3	2G	121	ASN
3	2H	114	GLN
3	2I	114	GLN
3	2J	114	GLN
3	2J	121	ASN
3	2K	114	GLN
3	2L	114	GLN
3	2L	121	ASN
3	2M	114	GLN
3	2N	114	GLN
3	2N	121	ASN
3	2O	114	GLN
3	2P	56	ASN
3	2P	114	GLN
3	2P	121	ASN
3	2Q	114	GLN

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Mol	Chain	Res	Type
3	2Q	121	ASN
3	2R	114	GLN
3	2R	121	ASN
3	2S	114	GLN
3	2S	121	ASN
3	2T	114	GLN
3	2T	121	ASN
3	2U	25	GLN
3	2U	114	GLN
3	2U	121	ASN
3	2V	114	GLN
3	2V	121	ASN
3	2W	114	GLN
3	2X	114	GLN
3	2X	121	ASN
3	2Y	114	GLN
3	2Z	114	GLN
3	aa	25	GLN
3	aa	114	GLN
3	aa	121	ASN
3	ab	114	GLN
3	ab	121	ASN
3	ac	114	GLN
3	ac	121	ASN
3	ad	114	GLN
3	ad	121	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	94/95 (98%)	42 (44%)	1 (1%)

All (42) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	3	G
1	R	6	G
1	R	8	A
1	R	9	A
1	R	10	U
1	R	13	C

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Mol	Chain	Res	Type
1	R	14	C
1	R	15	U
1	R	18	A
1	R	22	U
1	R	24	C
1	R	26	C
1	R	28	U
1	R	29	U
1	R	32	C
1	R	33	A
1	R	38	C
1	R	39	A
1	R	40	U
1	R	42	C
1	R	43	G
1	R	44	A
1	R	45	C
1	R	54	G
1	R	58	U
1	R	59	U
1	R	64	C
1	R	67	C
1	R	70	A
1	R	72	U
1	R	73	C
1	R	74	C
1	R	75	G
1	R	76	C
1	R	77	G
1	R	80	C
1	R	82	G
1	R	83	C
1	R	84	G
1	R	87	C
1	R	88	U
1	R	93	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	13	C

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

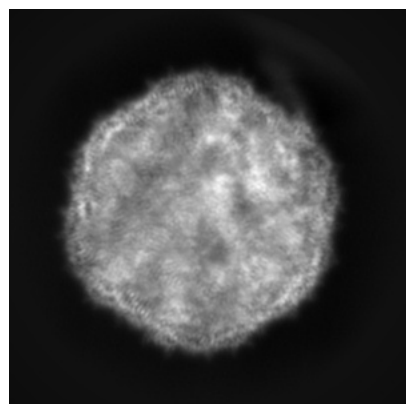
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41632. These allow visual inspection of the internal detail of the map and identification of artifacts.

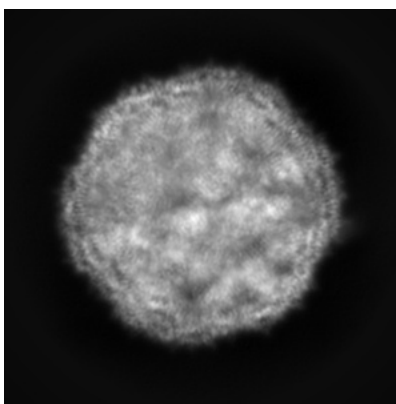
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

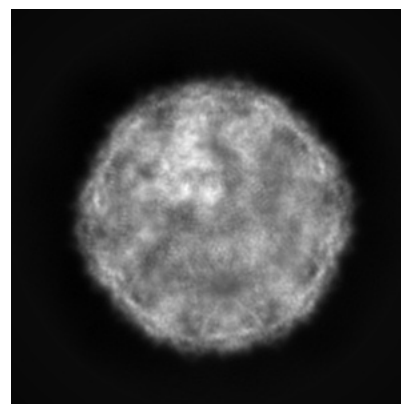
6.1.1 Primary map



X

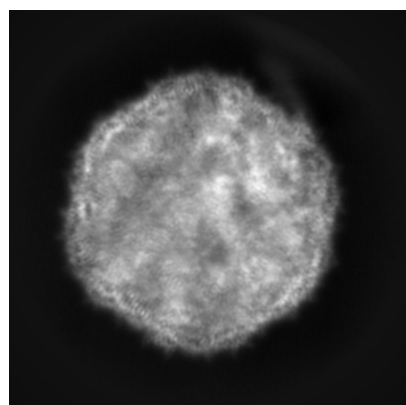


Y

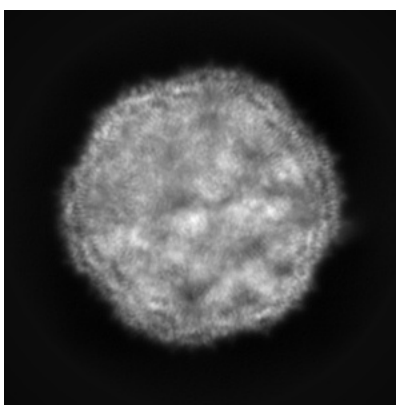


Z

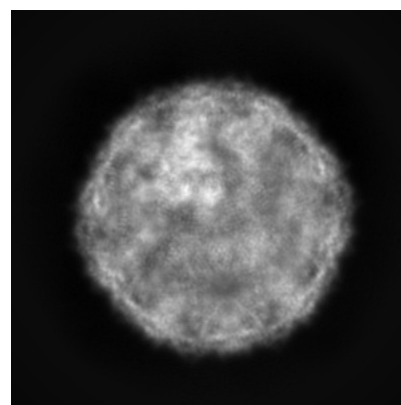
6.1.2 Raw map



X



Y

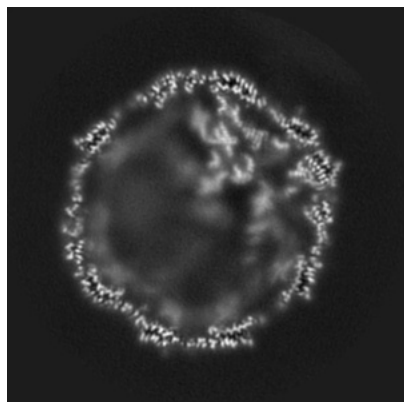


Z

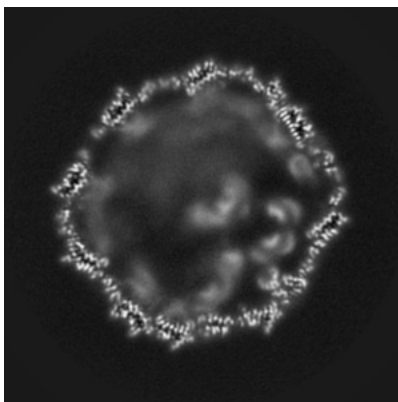
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

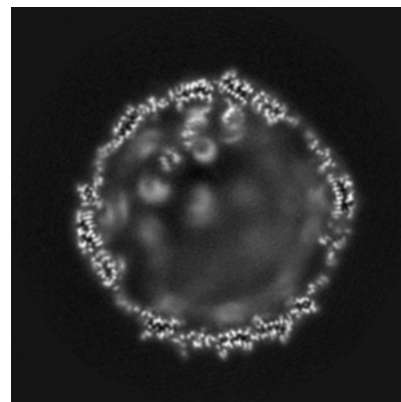
6.2.1 Primary map



X Index: 240

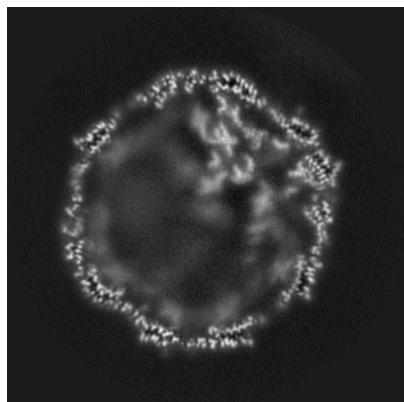


Y Index: 240

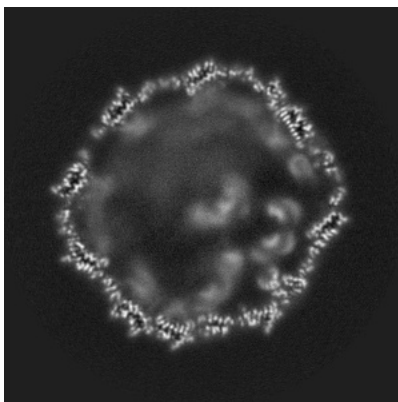


Z Index: 240

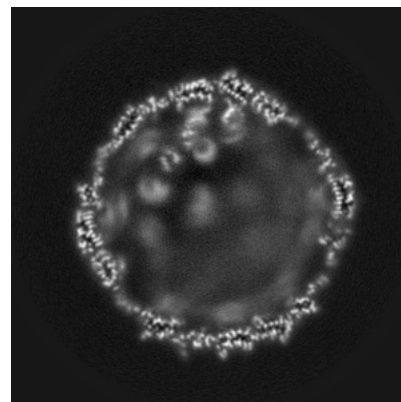
6.2.2 Raw map



X Index: 240



Y Index: 240

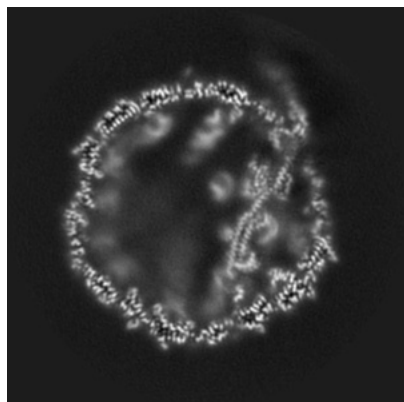


Z Index: 240

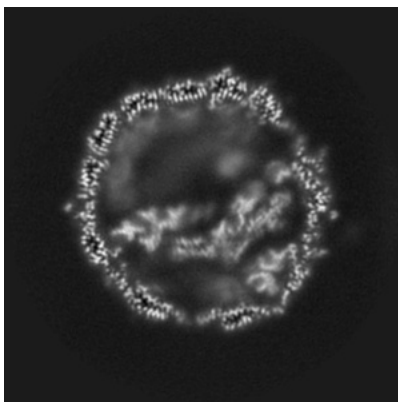
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

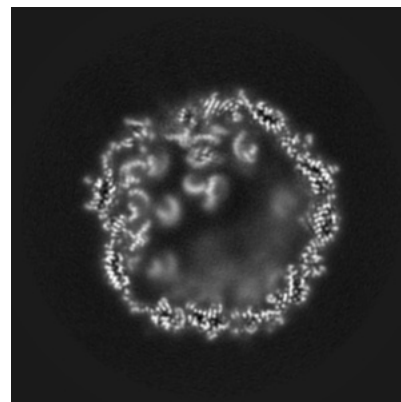
6.3.1 Primary map



X Index: 197

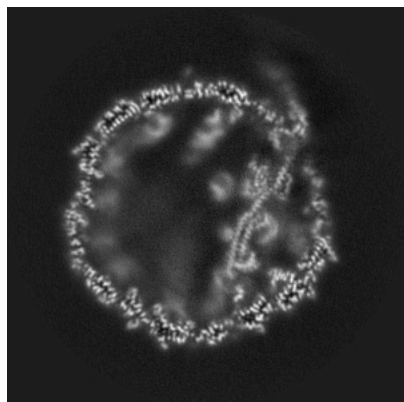


Y Index: 292

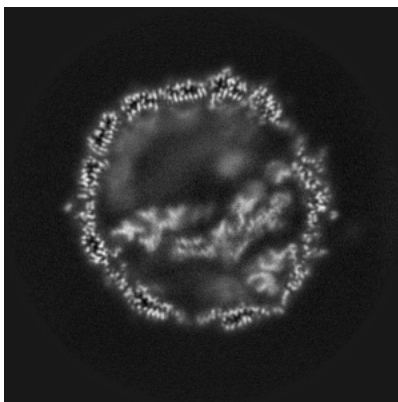


Z Index: 317

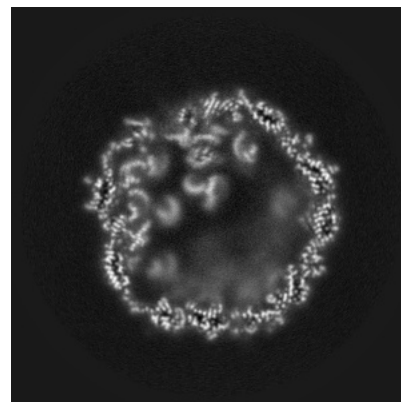
6.3.2 Raw map



X Index: 197



Y Index: 292

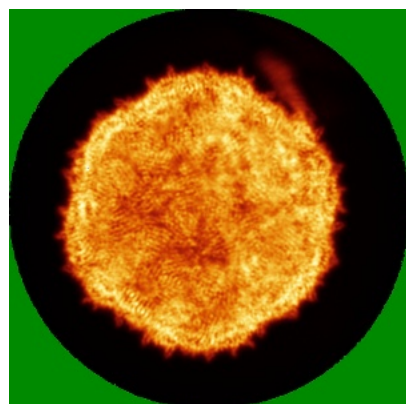


Z Index: 317

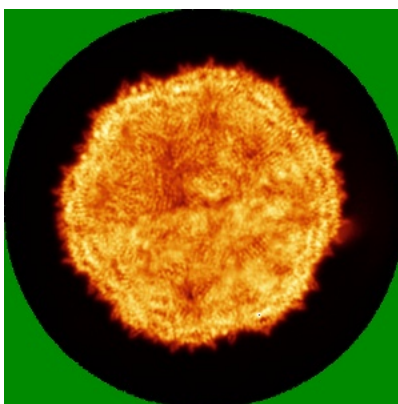
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

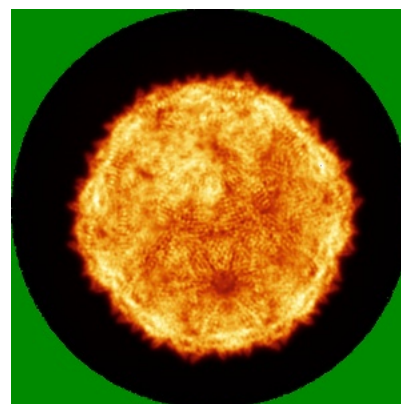
6.4.1 Primary map



X

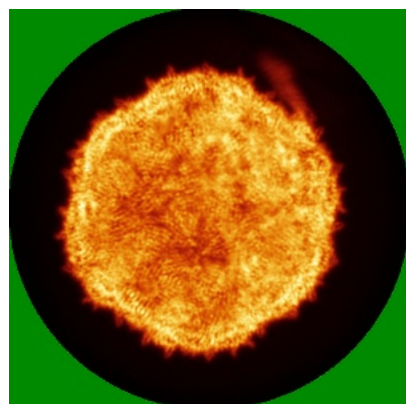


Y



Z

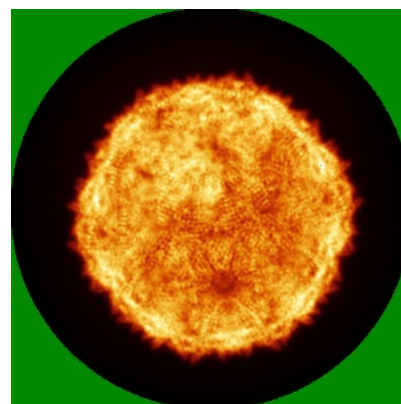
6.4.2 Raw map



X



Y

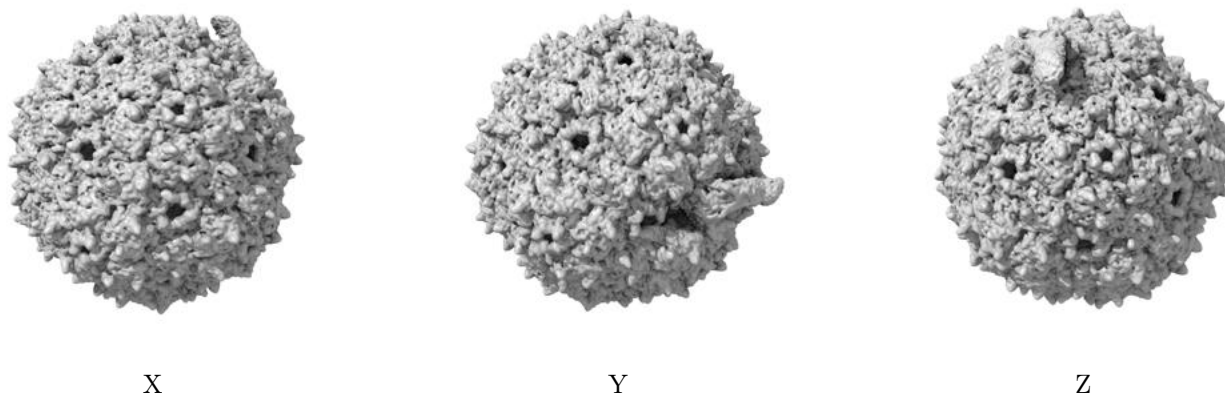


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

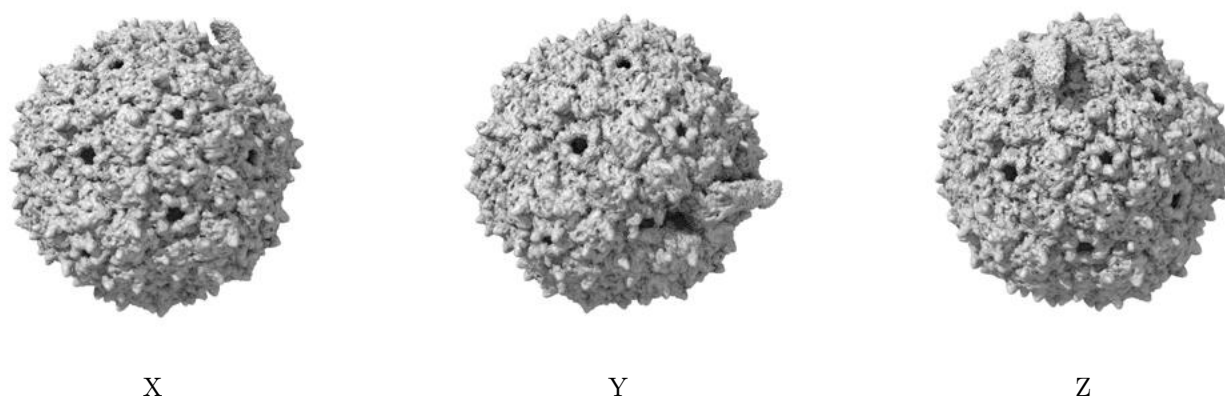
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

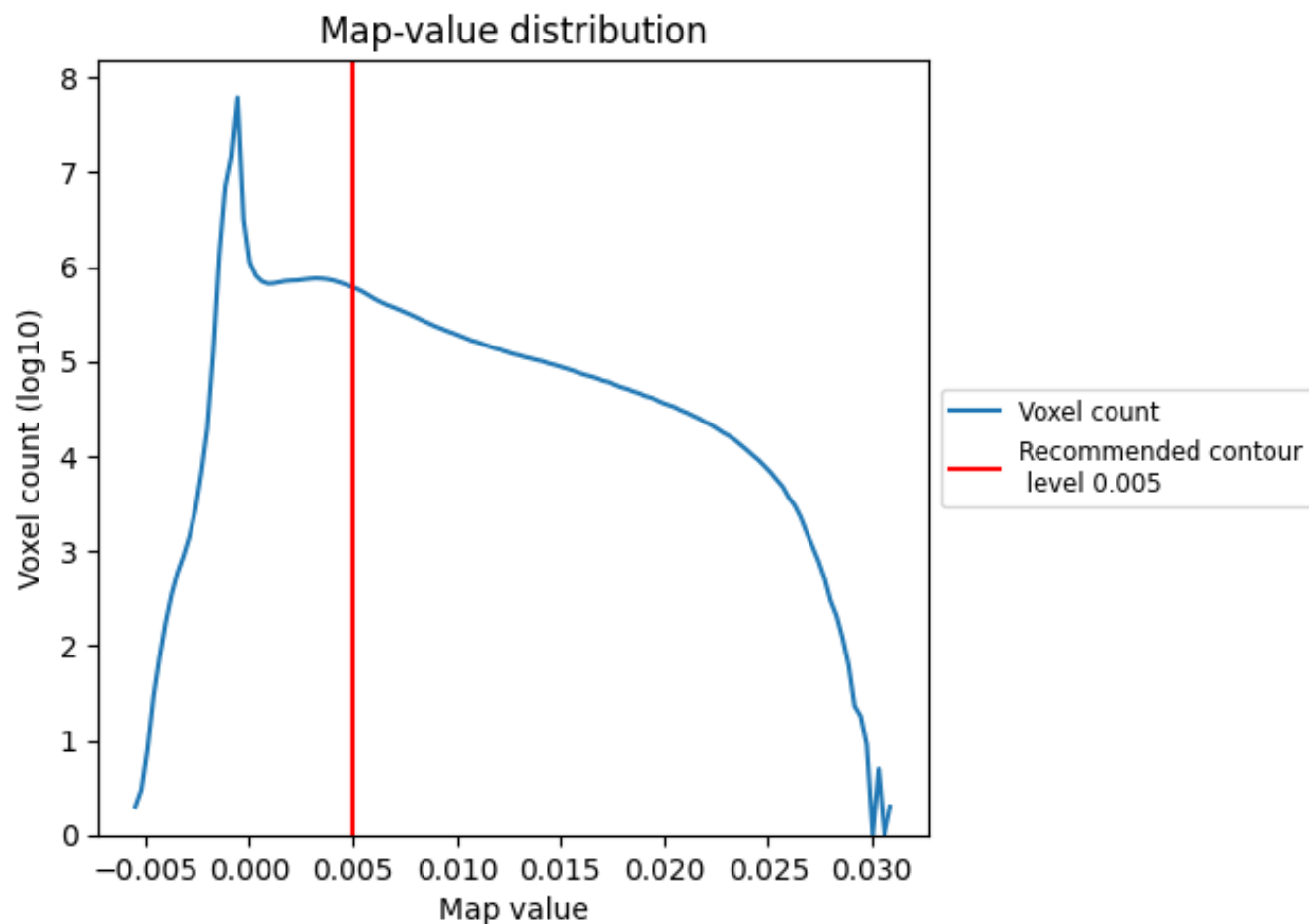
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

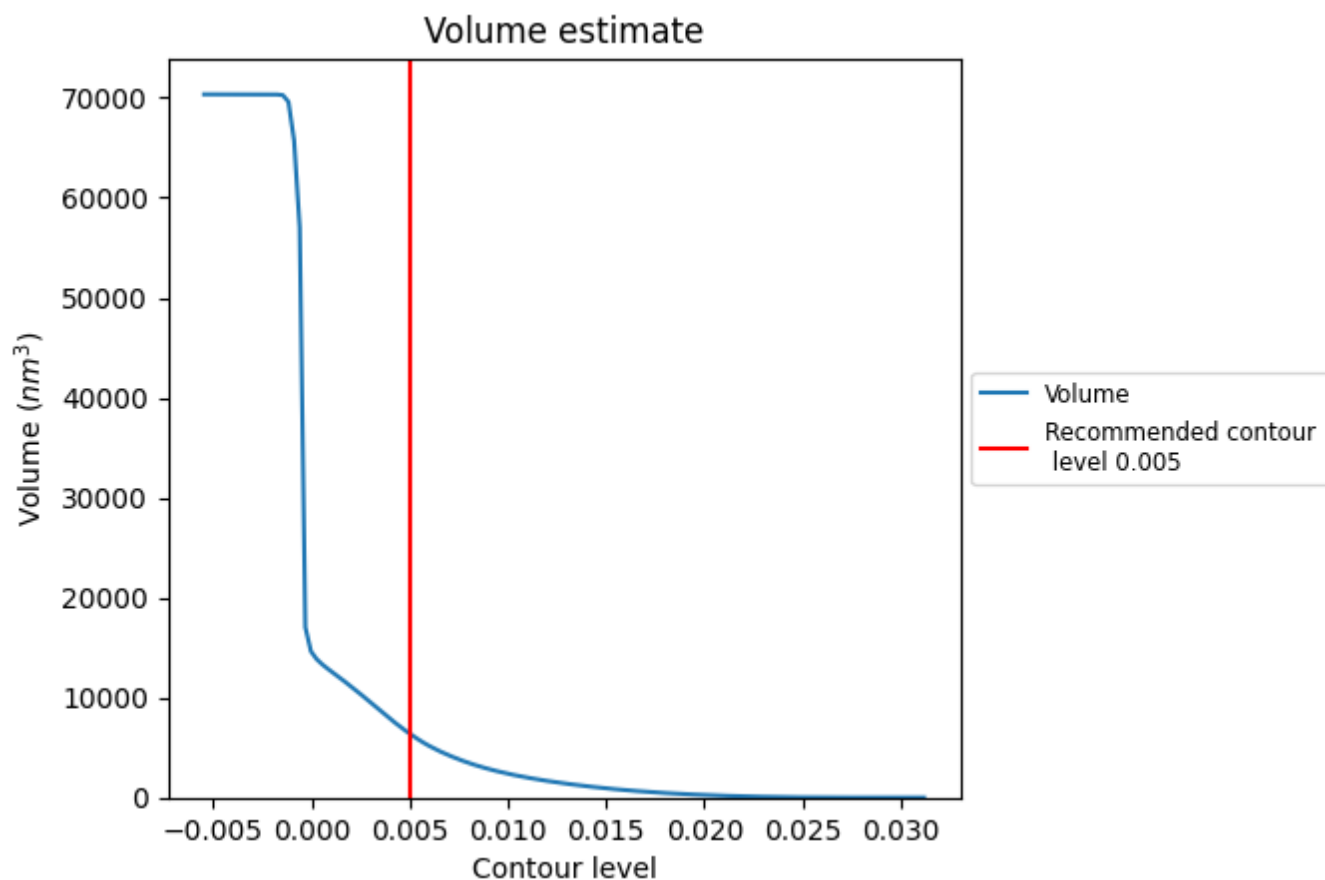
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

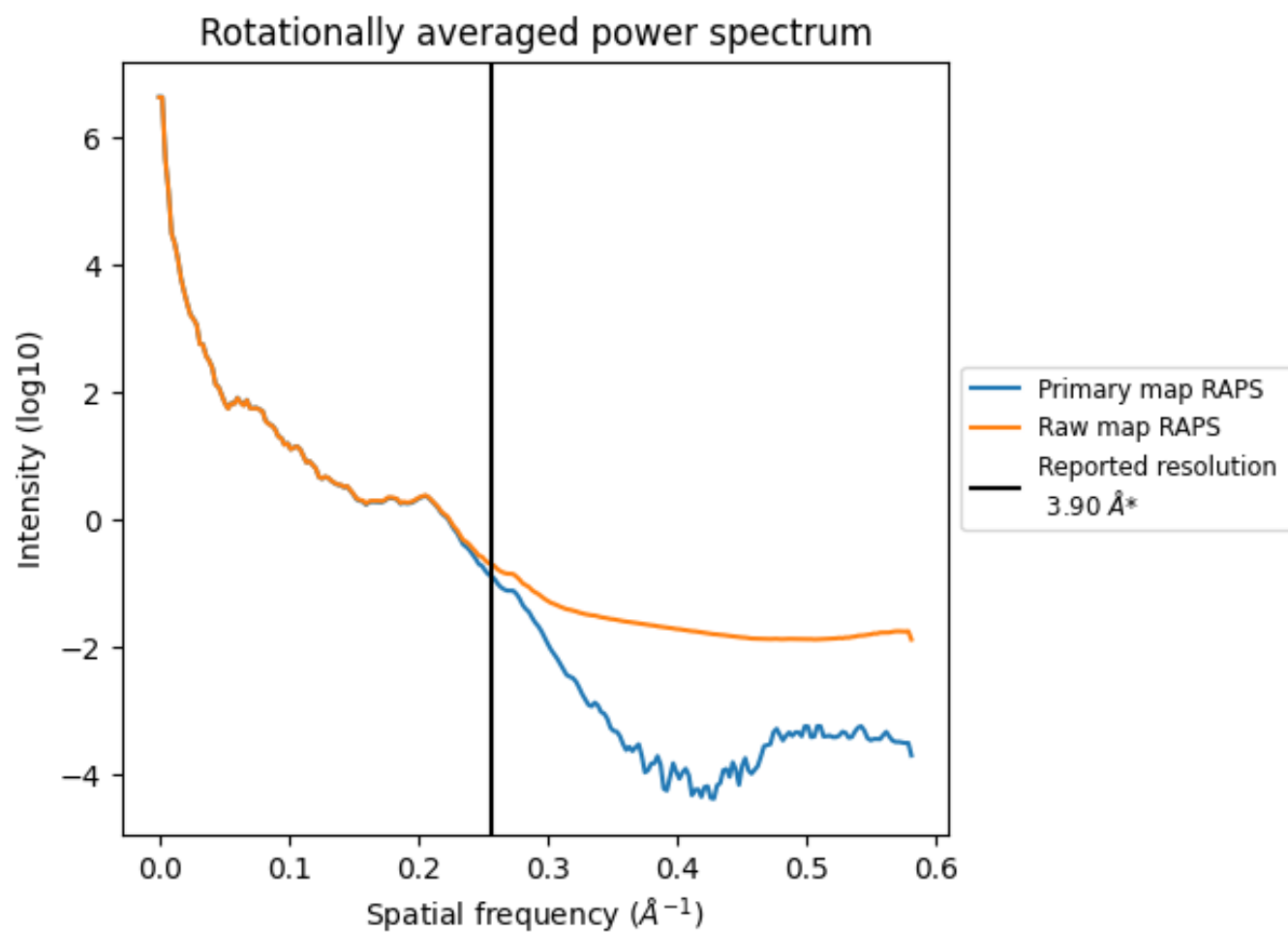
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6390 nm³; this corresponds to an approximate mass of 5772 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

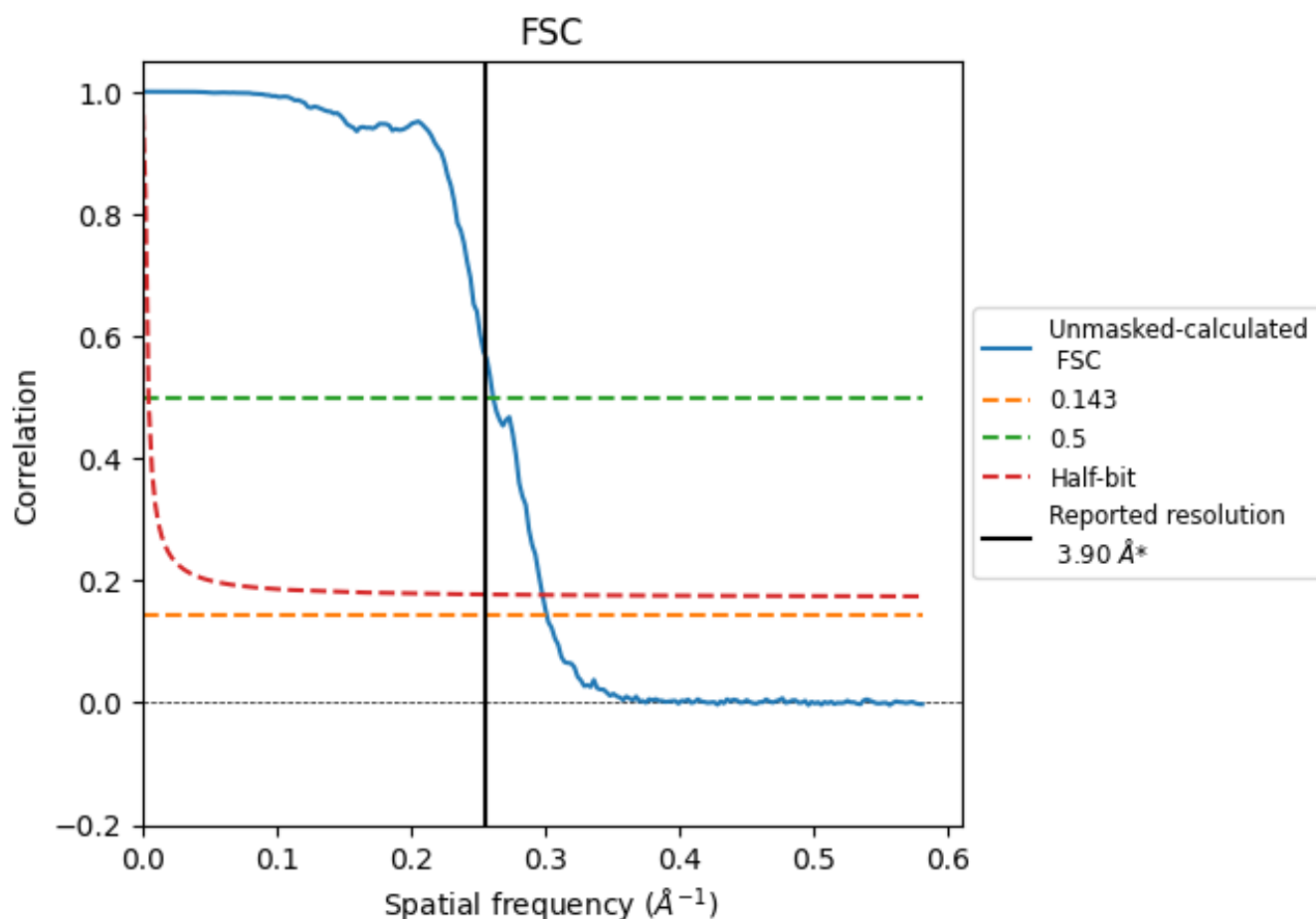


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

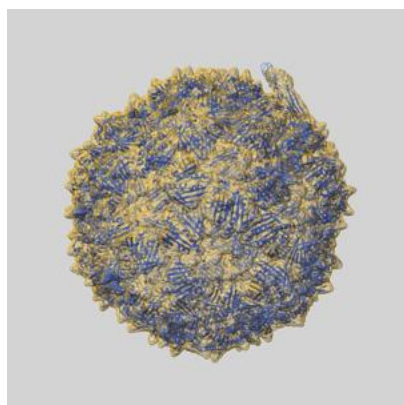
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	3.90	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.32	3.82	3.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

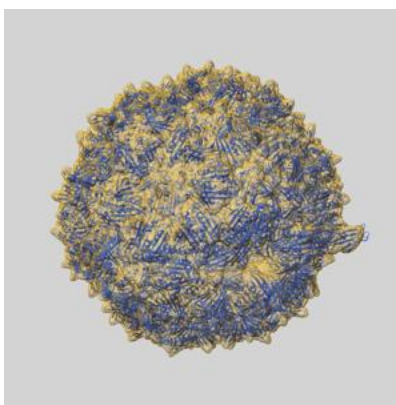
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41632 and PDB model 8TUX. Per-residue inclusion information can be found in section [3](#) on page [21](#).

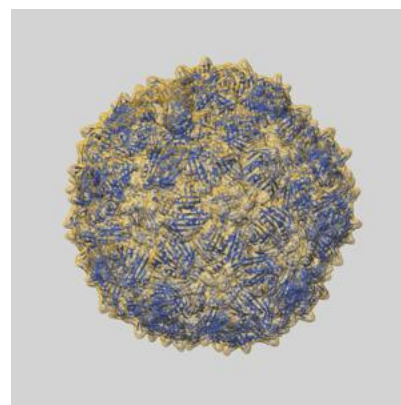
9.1 Map-model overlay [i](#)



X



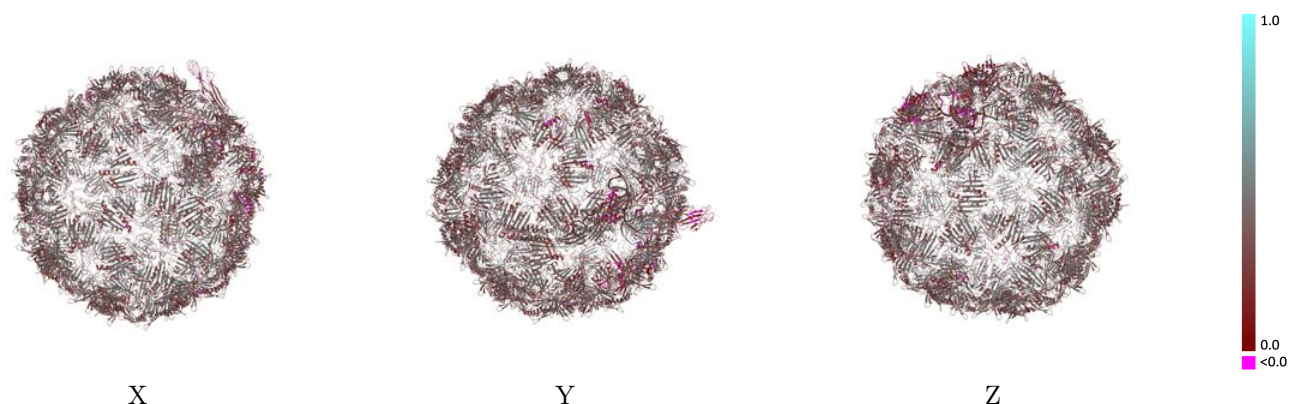
Y



Z

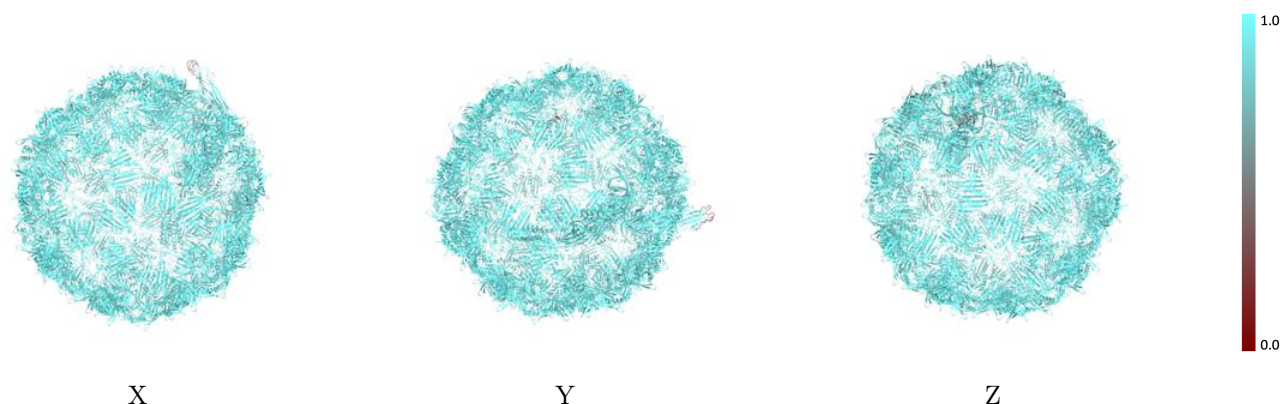
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



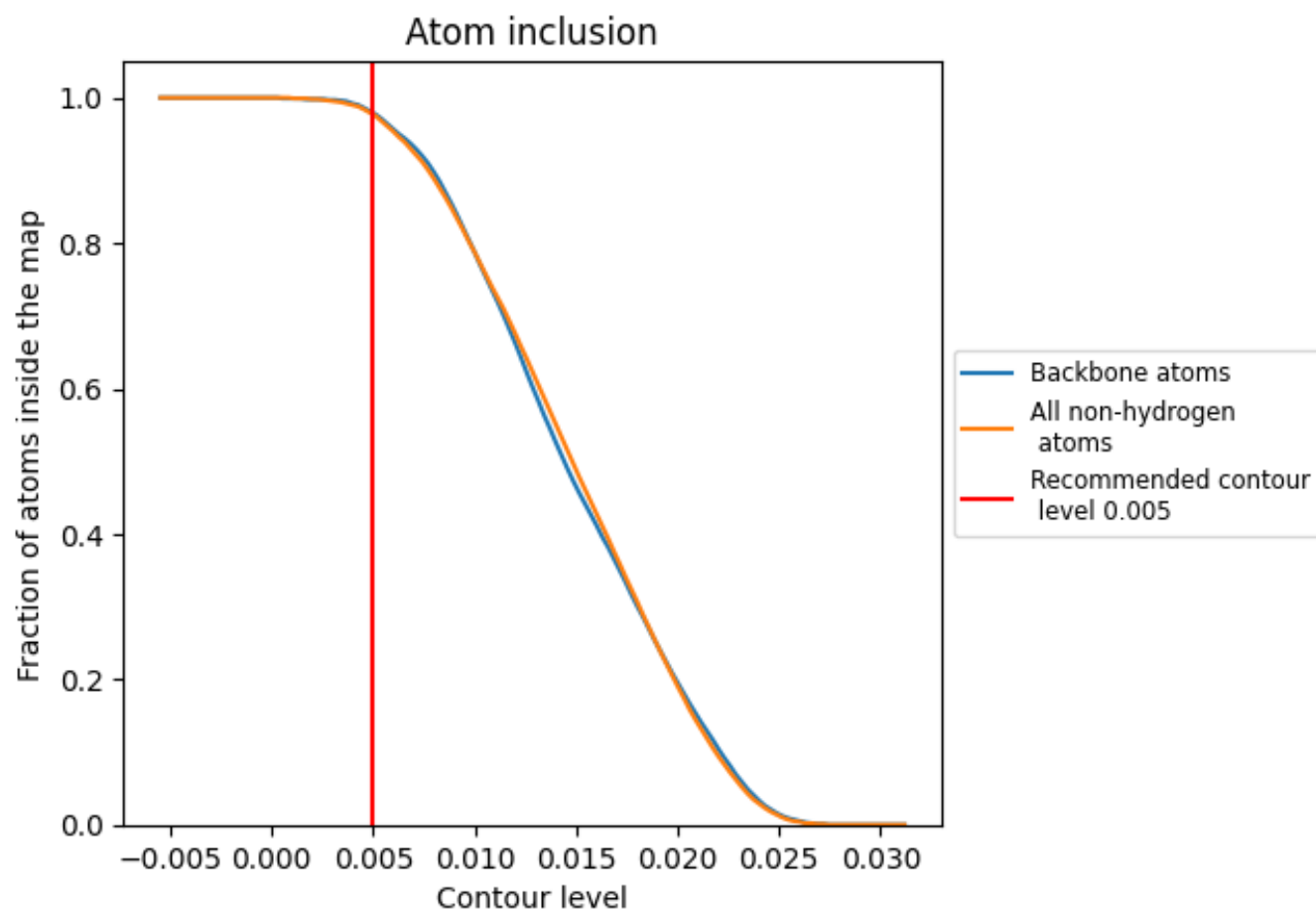
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9770	 0.3420
01	 0.9770	 0.3540
02	 0.9790	 0.3370
11	 0.9680	 0.3170
12	 0.9830	 0.3470
21	 0.9860	 0.3500
22	 0.9840	 0.3410
2A	 0.9860	 0.3590
2B	 0.9800	 0.3520
2C	 0.9900	 0.3560
2D	 0.9850	 0.3640
2E	 0.9780	 0.3550
2F	 0.9830	 0.3660
2G	 0.9840	 0.3570
2H	 0.9880	 0.3630
2I	 0.9800	 0.3640
2J	 0.9690	 0.3310
2K	 0.9800	 0.3360
2L	 0.9680	 0.3090
2M	 0.9780	 0.3460
2N	 0.9740	 0.3470
2O	 0.9800	 0.2950
2P	 0.9690	 0.2930
2Q	 0.9440	 0.2300
2R	 0.9760	 0.3140
2S	 0.9760	 0.3280
2T	 0.9770	 0.3270
2U	 0.8840	 0.1880
2V	 0.8940	 0.1540
2W	 0.9830	 0.3250
2X	 0.9810	 0.3130
2Y	 0.9690	 0.3300
2Z	 0.9760	 0.3560
2a	 0.9850	 0.3590
2b	 0.9760	 0.3410



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Chain	Atom inclusion	Q-score
2c	 0.9790	 0.3610
2d	 0.9740	 0.3570
2e	 0.9830	 0.3640
2f	 0.9800	 0.3470
2g	 0.9760	 0.3360
2h	 0.9790	 0.3350
2i	 0.9780	 0.3650
2j	 0.9720	 0.3470
2k	 0.9800	 0.3540
2l	 0.9880	 0.3680
2m	 0.9810	 0.3510
2n	 0.9870	 0.3670
2o	 0.9830	 0.3560
2p	 0.9850	 0.3670
2q	 0.9790	 0.3600
2r	 0.9710	 0.3400
2s	 0.9870	 0.3600
2t	 0.9780	 0.3410
2u	 0.9850	 0.3580
2v	 0.9840	 0.3580
2w	 0.9860	 0.3620
2x	 0.9800	 0.3410
2y	 0.9810	 0.3420
2z	 0.9790	 0.3320
31	 0.9830	 0.3530
32	 0.9750	 0.3410
41	 0.9660	 0.3350
42	 0.9740	 0.3140
51	 0.9760	 0.3320
52	 0.9770	 0.3090
61	 0.9850	 0.3460
62	 0.9710	 0.3200
71	 0.9670	 0.3070
72	 0.9780	 0.3260
82	 0.9840	 0.3520
92	 0.9640	 0.3140
A1	 0.9760	 0.3340
A2	 0.9850	 0.3680
B1	 0.9830	 0.3650
B2	 0.9820	 0.3550
C1	 0.9590	 0.2980
C2	 0.9850	 0.3610

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Chain	Atom inclusion	Q-score
D1	 0.9860	 0.3590
D2	 0.9820	 0.3540
E1	 0.9720	 0.3540
E2	 0.9880	 0.3680
F1	 0.9800	 0.3660
F2	 0.9800	 0.3530
G1	 0.9760	 0.3690
G2	 0.9820	 0.3640
H1	 0.9800	 0.3710
H2	 0.9830	 0.3570
I1	 0.9760	 0.3610
I2	 0.9830	 0.3680
J1	 0.9810	 0.3420
J2	 0.9800	 0.3470
K1	 0.9750	 0.3460
K2	 0.9860	 0.3640
L1	 0.9830	 0.3620
L2	 0.9790	 0.3560
M	 0.9950	 0.3530
M1	 0.9730	 0.3480
M2	 0.9840	 0.3590
N1	 0.9830	 0.3730
N2	 0.9820	 0.3400
O1	 0.9800	 0.3630
O2	 0.9750	 0.3290
P1	 0.9840	 0.3640
P2	 0.9770	 0.3260
Q1	 0.9810	 0.3670
Q2	 0.9810	 0.3490
R	 0.9840	 0.2500
R1	 0.9830	 0.3660
R2	 0.9780	 0.3470
S1	 0.9810	 0.3630
S2	 0.9860	 0.3610
T1	 0.9770	 0.3540
T2	 0.9770	 0.3450
U1	 0.9830	 0.3650
U2	 0.9850	 0.3630
V1	 0.9760	 0.3520
V2	 0.9780	 0.3470
W1	 0.9780	 0.3590
W2	 0.9790	 0.3650

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Chain	Atom inclusion	Q-score
X1	 0.9800	 0.3580
X2	 0.9840	 0.3570
Y1	 0.9690	 0.3290
Y2	 0.9830	 0.3620
Z1	 0.9840	 0.3640
Z2	 0.9780	 0.3380
a1	 0.9790	 0.3620
a2	 0.9690	 0.2940
aa	 0.9710	 0.3020
ab	 0.9520	 0.2070
ac	 0.9680	 0.2900
ad	 0.9560	 0.3020
b1	 0.9800	 0.3680
b2	 0.9670	 0.3090
c1	 0.9790	 0.3610
c2	 0.9820	 0.3570
d1	 0.9860	 0.3640
d2	 0.9750	 0.3540
e1	 0.9780	 0.3640
e2	 0.9780	 0.3600
f1	 0.9800	 0.3630
f2	 0.9740	 0.3460
g1	 0.9830	 0.3630
g2	 0.9750	 0.3550
h1	 0.9860	 0.3660
h2	 0.9670	 0.3350
i1	 0.9820	 0.3650
i2	 0.9860	 0.3660
j1	 0.9850	 0.3670
j2	 0.9860	 0.3570
k1	 0.9820	 0.3690
k2	 0.9770	 0.3390
l1	 0.9830	 0.3630
l2	 0.9720	 0.3220
m	 0.9160	 0.3010
m1	 0.9820	 0.3720
m2	 0.9760	 0.2860
n1	 0.9800	 0.3610
n2	 0.9720	 0.2710
o1	 0.9860	 0.3710
o2	 0.9840	 0.3430
p1	 0.9820	 0.3650

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Chain	Atom inclusion	Q-score
p2	 0.9810	 0.3350
q1	 0.9810	 0.3710
q2	 0.9860	 0.3550
r1	 0.9800	 0.3610
r2	 0.9790	 0.3280
s1	 0.9840	 0.3680
s2	 0.9780	 0.3070
t1	 0.9840	 0.3710
t2	 0.9710	 0.3100
u1	 0.9770	 0.3460
u2	 0.9790	 0.3390
v1	 0.9820	 0.3610
v2	 0.9800	 0.3430
w1	 0.9740	 0.3410
w2	 0.9830	 0.3560
x1	 0.9790	 0.3650
x2	 0.9720	 0.3170
y1	 0.9800	 0.3630
y2	 0.9870	 0.3490
z1	 0.9780	 0.3250
z2	 0.9850	 0.3300