



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 04:34 PM UTC

PDB ID : 6J6H / pdb_00006j6h
EMDB ID : EMD-0687
Title : Cryo-EM structure of the yeast B*-a1 complex at an average resolution of 3.6 angstrom
Authors : Wan, R.; Bai, R.; Yan, C.; Lei, J.; Shi, Y.
Deposited on : 2019-01-15
Resolution : 3.60 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:

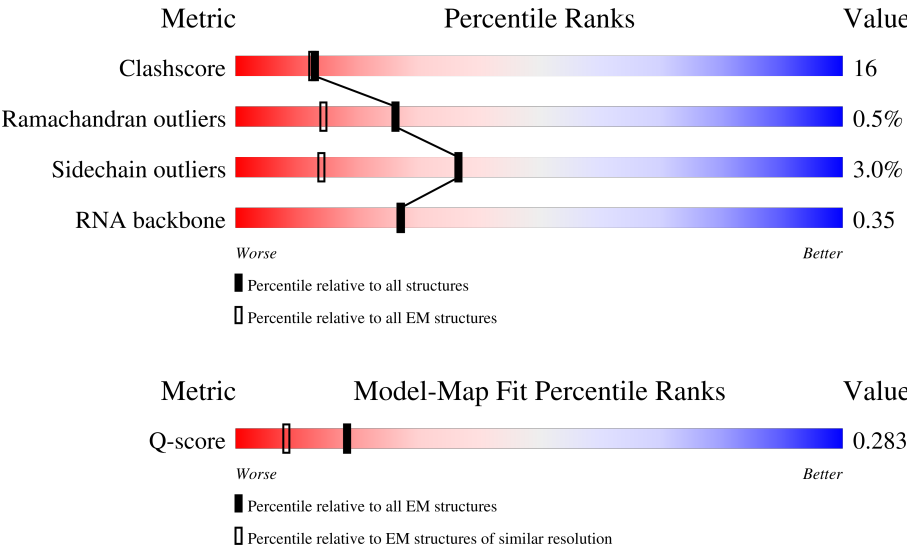
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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.



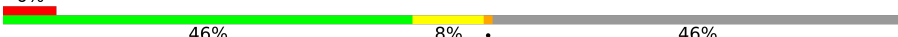
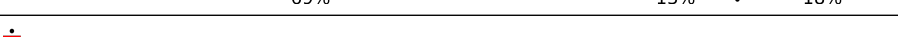
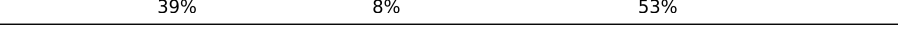
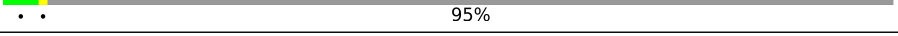
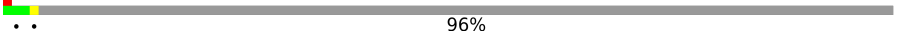
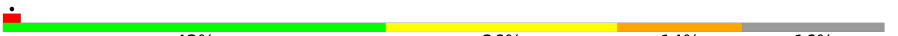
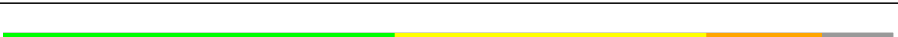
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	A	2413	
2	C	1008	
3	J	135	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	O	451	
5	P	379	
6	Q	364	
7	R	339	
8	S	175	
9	T	157	
10	Z	577	
11	c	590	
12	d	687	
13	I	215	
14	n	455	
15	H	235	
16	B	679	
17	D	214	
18	E	112	
19	L	1175	
20	v	859	
21	a	111	
22	b	238	
23	t	175	
24	i	94	
24	u	94	
25	m	146	
25	z	146	
26	j	77	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
26	x	77	
27	h	86	
27	w	86	
28	e	110	
28	g	110	
29	k	196	
29	s	196	
30	l	101	
30	y	101	
31	o	503	
31	p	503	
31	q	503	
31	r	503	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 76847 atoms, of which 0 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 protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1913	Total	C	N	O	S	0	0
			15793	10154	2714	2868	57		

- Molecule 2 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	920	Total	C	N	O	S	0	0
			7348	4733	1223	1362	30		

- Molecule 3 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	J	27	Total	C	N	O	0	0
			190	112	38	40		

- Molecule 4 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	357	Total	C	N	O	S	0	0
			2810	1777	493	530	10		

- Molecule 5 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	205	Total	C	N	O	S	0	0
			1608	1003	294	304	7		

- Molecule 6 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	292	Total	C	N	O	S	0	0
			2301	1461	399	426	15		

- Molecule 7 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	261	Total	C	N	O	S	0	0
			2089	1320	369	388	12		

- Molecule 8 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	70	Total	C	N	O	S	0	0
			567	355	113	98	1		

- Molecule 9 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	157	Total	C	N	O	S	0	0
			1291	808	240	232	11		

- Molecule 10 is a protein called Pre-mRNA-splicing factor CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Z	447	Total	C	N	O	S	0	0
			3651	2343	602	688	18		

- Molecule 11 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	436	Total	C	N	O	S	0	0
			2978	1843	552	575	8		

- Molecule 12 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	566	Total	C	N	O	S	0	0
			3881	2433	707	732	9		

- Molecule 13 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	102	Total	C	N	O	S	0	0
			822	504	152	165	1		

- Molecule 14 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	23	Total	C	N	O	P	0	0
			199	122	41	35	1		

- Molecule 15 is a protein called Pre-mRNA-splicing factor ISY1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	9	Total	C	N	O		0	0
			94	65	17	12			

- Molecule 16 is a RNA chain called ACT1 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	B	60	Total	C	N	O	P	0	0
			1266	567	213	426	60		

- Molecule 17 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	D	179	Total	C	N	O	P	0	0
			3795	1699	660	1258	178		

- Molecule 18 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	E	103	Total	C	N	O	P	0	0
			2192	982	391	716	103		

- Molecule 19 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	209	Total	C	N	O	P	0	0
			4405	1972	737	1487	209		

- Molecule 20 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	v	722	Total	C	N	O	S	0	0
			4625	2893	825	895	12		

- Molecule 21 is a protein called U2 small nuclear ribonucleoprotein B”.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	a	84	Total	C	N	O	0	0
			416	248	84	84		

- Molecule 22 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	b	169	Total	C	N	O	0	0
			841	503	169	169		

- Molecule 23 is a protein called Pre-mRNA-splicing factor SNT309.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	t	156	Total	C	N	O	S	0	0
			926	585	160	180	1		

- Molecule 24 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	u	74	Total	C	N	O	S	0	0
			526	346	87	90	3		
24	i	74	Total	C	N	O	S	0	0
			541	358	90	90	3		

- Molecule 25 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	m	119	Total	C	N	O	S	0	0
			917	575	163	176	3		
25	z	108	Total	C	N	O	S	0	0
			824	521	142	158	3		

- Molecule 26 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	j	75	Total	C	N	O	S	0	0
			552	350	98	103	1		
26	x	75	Total	C	N	O	S	0	0
			552	350	98	103	1		

- Molecule 27 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	h	68	Total	C	N	O	S	0	0
			518	337	96	84	1		
27	w	68	Total	C	N	O	S	0	0
			518	337	96	84	1		

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	g	101	Total	C	N	O	S	0	0
			785	504	149	128	4		
28	e	101	Total	C	N	O	S	0	0
			785	504	149	128	4		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	k	100	Total	C	N	O	S	0	0
			809	514	150	142	3		
29	s	93	Total	C	N	O	S	0	0
			749	476	138	132	3		

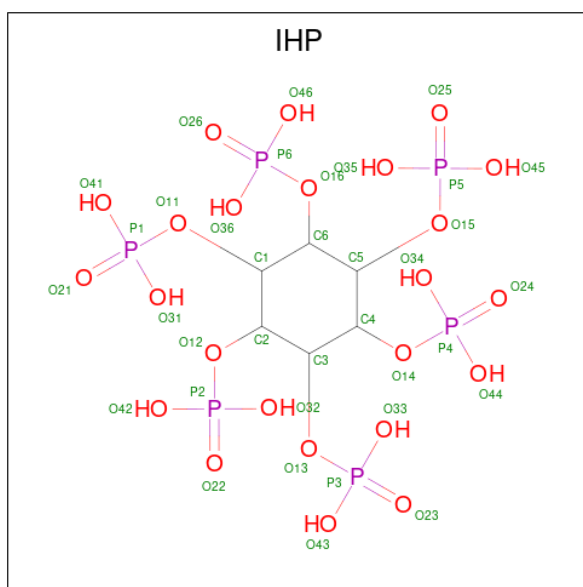
- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	l	83	Total	C	N	O	S	0	0
			641	408	111	120	2		
30	y	81	Total	C	N	O	S	0	0
			616	394	107	113	2		

- Molecule 31 is a protein called Pre-mRNA-processing factor 19.

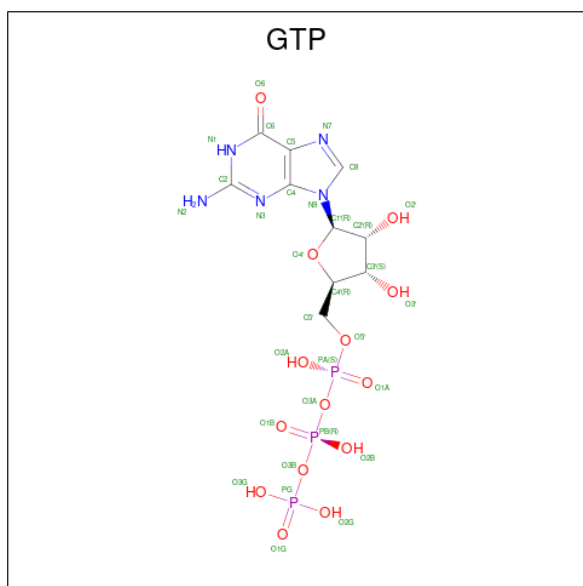
Mol	Chain	Residues	Atoms					AltConf	Trace
31	r	125	Total	C	N	O	S	0	0
			823	521	133	167	2		
31	p	128	Total	C	N	O	S	0	0
			843	532	136	173	2		
31	q	129	Total	C	N	O	S	0	0
			850	537	137	174	2		
31	o	126	Total	C	N	O	S	0	0
			830	525	134	169	2		

- Molecule 32 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 33 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms				AltConf
33	C	1	Total	C	N	O	P
			32	10	5	14	3
							0

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
34	C	1	Total 1	Mg 1	0
34	E	5	Total 5	Mg 5	0

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
35	Q	2	Total 2	Zn 2	0
35	R	1	Total 1	Zn 1	0
35	T	3	Total 3	Zn 3	0

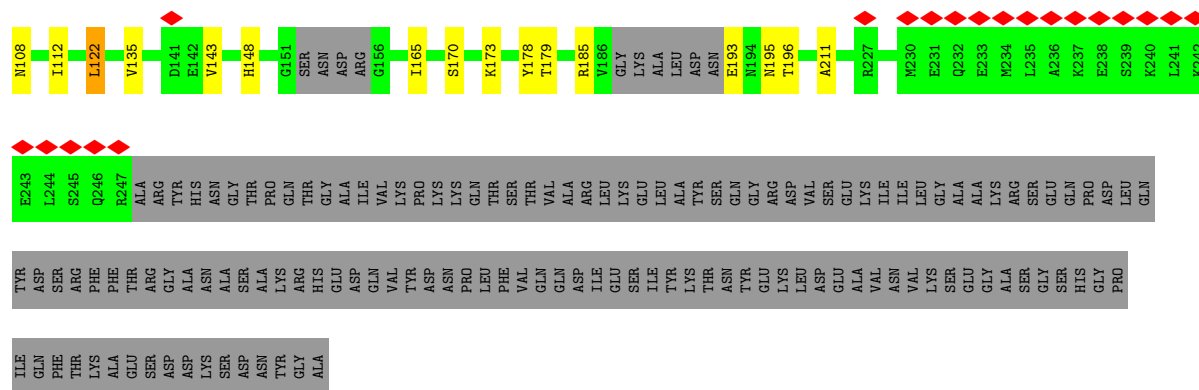


- Molecule 4: Pre-mRNA-splicing factor PRP46

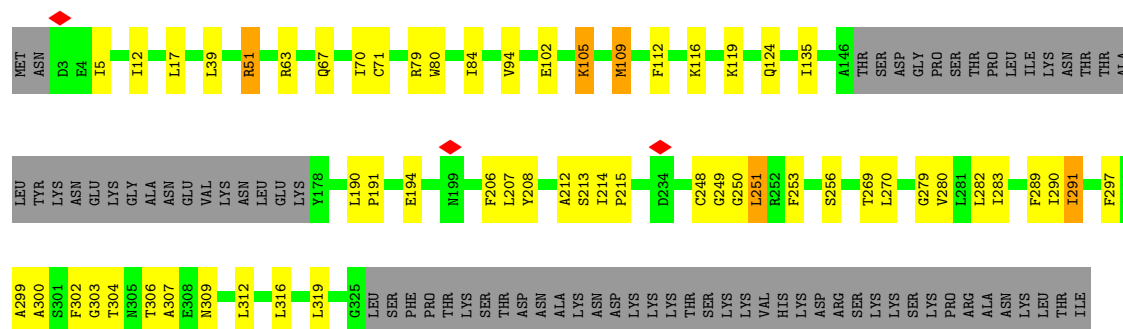
K424	P279	G158	PHE	MET
I425	Q280	S159	SER	ASP
W426	V281	GLY	GLY	GLY
		N160	ASN	ASN
T433		V182	GLY	ASP
K434	S285	M183	LYS	HIS
E435	T286		LYS	LYS
S436	D287	R186	VAL	VAL
E437			THR	GLU
	L292	L197	LEU	LEU
R450	W293	V200	GLN	GLN
F451	K302	S201	HIS	GLY
		E202	VAL	ASP
	H307	D203	PRO	VAL
	K308		THR	ASP
R309		V206	ASP	LYS
		K207	PHE	PHE
	T314	C208	SER	TYR
		W209	GLU	SER
	F321	D210	ALA	ARG
		L211	SER	ILE
			GLN	ARG
S325		N214	ALA	TRP
A326	S325		ASN	ASN
C327	C327	Q215	ILE	ASN
T328	T328	T216	GLN	GLN
		I217	LYS	PHE
		D218	LYS	SER
I331	I331	R219	ASP	TVR
R332	R332	Y220	ASP	TYR
			HIS	MET
T343	T343		ASP	ALA
N344	N344	L224	THR	THR
F345	F345		HIS	LEU
		T229	ALA	PRO
G351	G351	V230	S95	PRO
T352	T352	S231	A96	HIS
I353	I353		F97	LEU
		L236		GLN
L356	L356	D237	K100	SER
		L238	I101	GLU
L364	L364	T239	F102	MET
F365	F365	A240		GLU
		T241	E105	GLY
			V106	GLN
D369	D369		LYS	LYS
N370	N370	R244	SER	SER
G371	G371	L250	E109	LEU
V372	V372	W251	L110	LEU
L373	L373	D252	I111	MET
		M253		ARG
E391	E391		L118	TYR
N392	N392		Q121	ASP
		R256		THR
	R400		W125	TYR
			I135	ARG
	L414			LYS
	D420			GLU
		K421	V145	SER
S422	S422			SER
L423	L423	C274		SER
		T375		

- Molecule 5: Pre-mRNA-processing protein 45

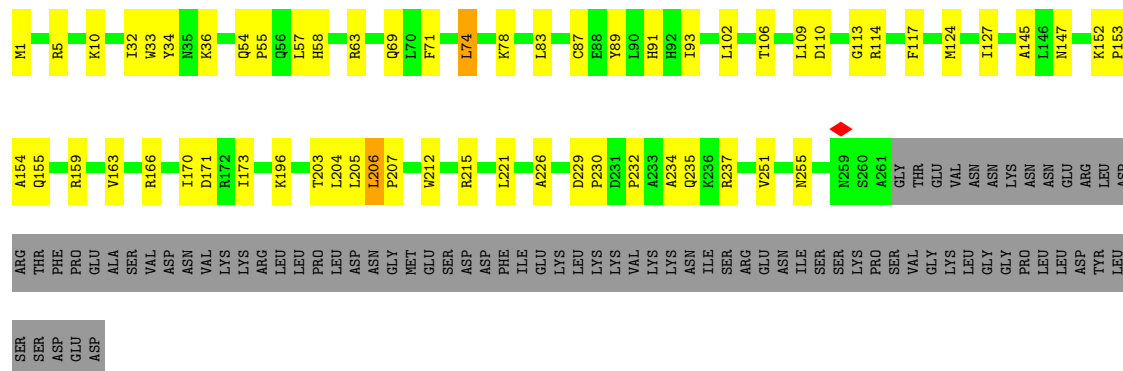
[illegible]



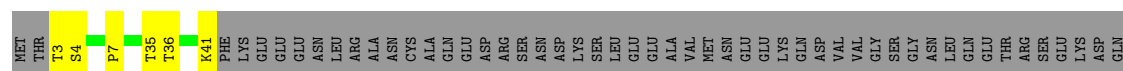
• Molecule 6: Pre-mRNA-splicing factor SLT11

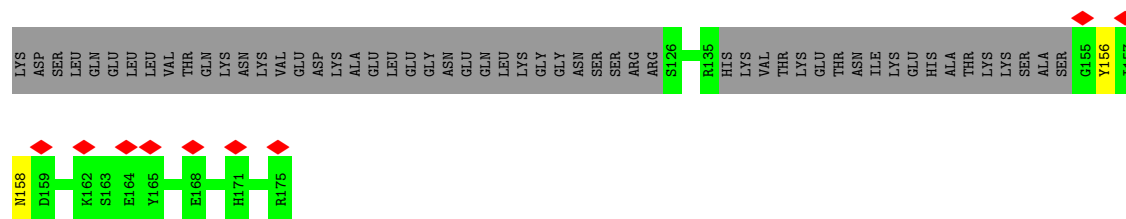


• Molecule 7: Pre-mRNA-splicing factor CWC2

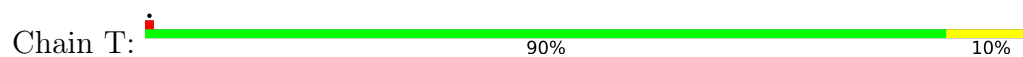


• Molecule 8: Pre-mRNA-splicing factor CWC15

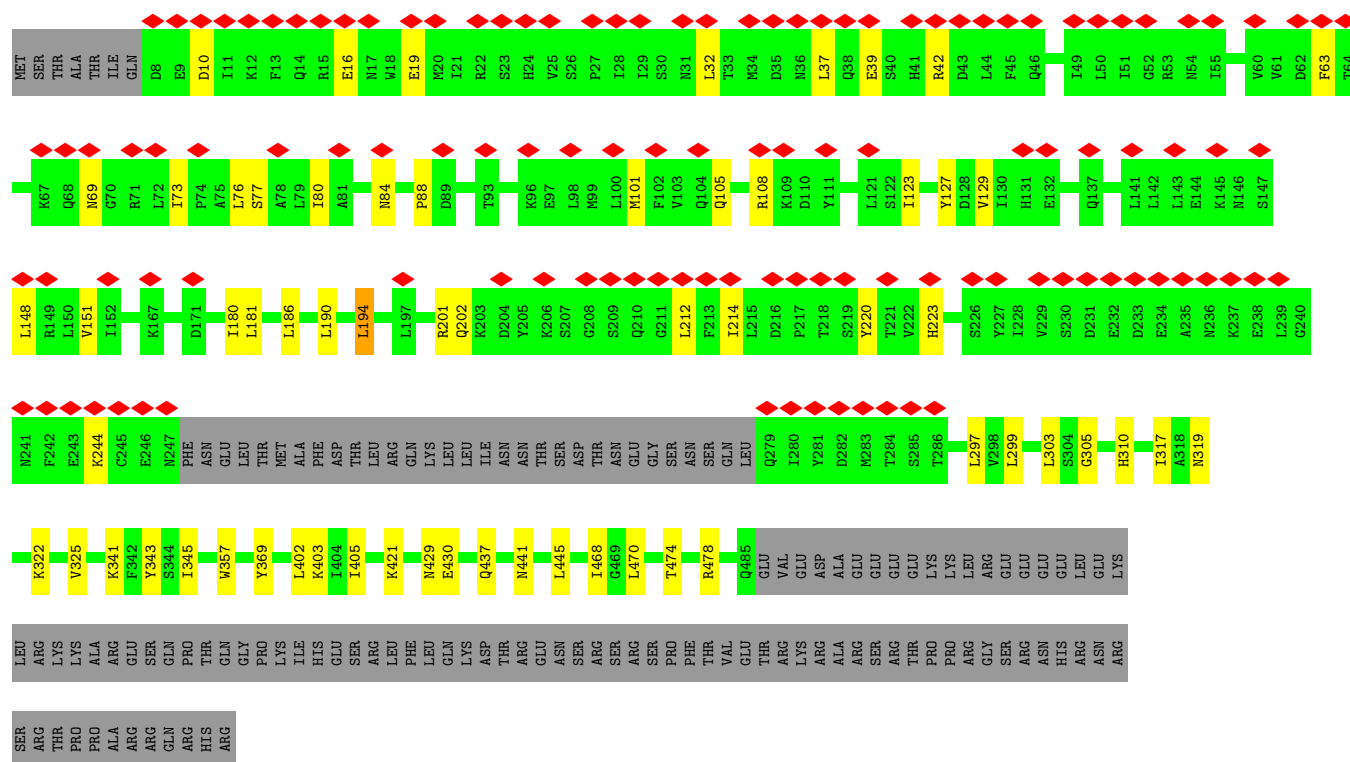




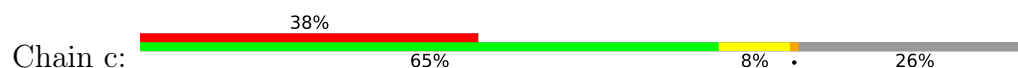
• Molecule 9: Pre-mRNA-splicing factor BUD31

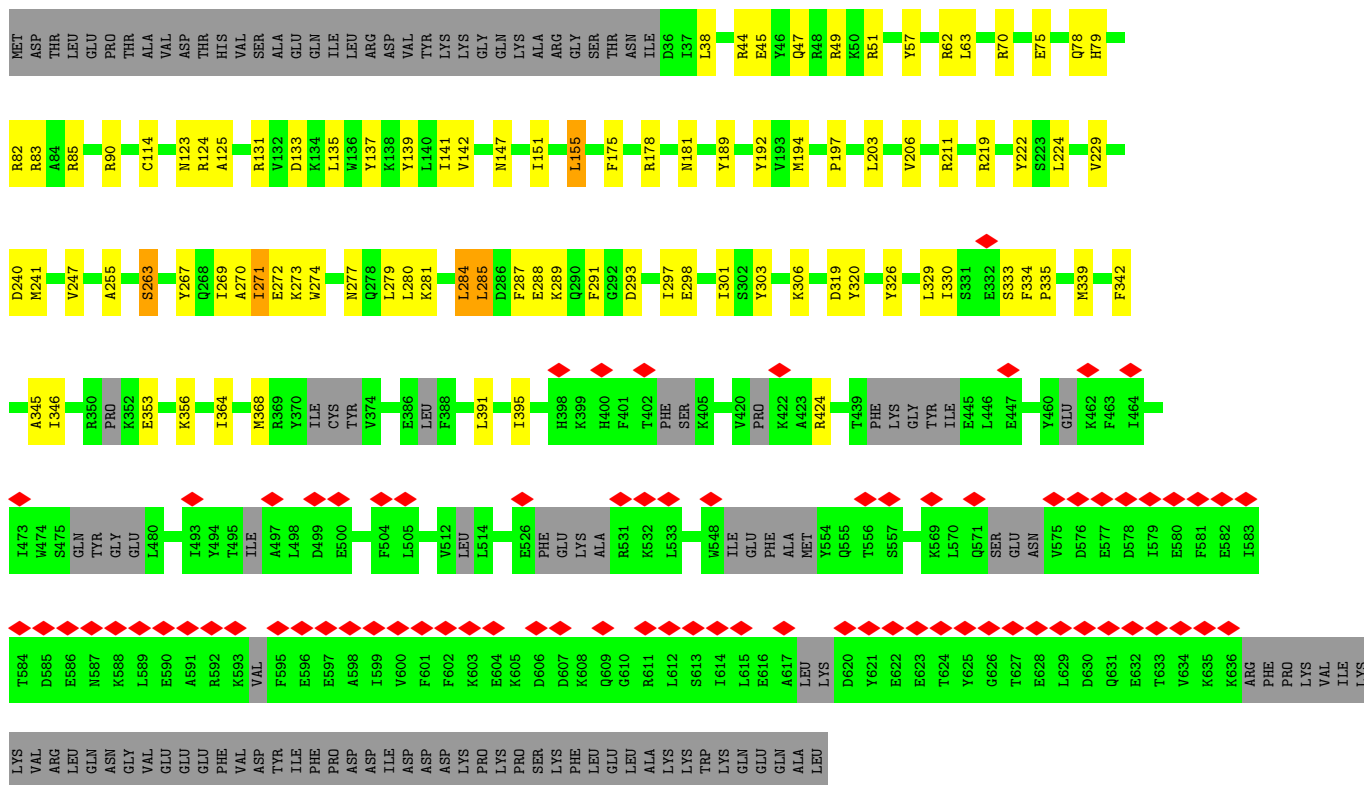


• Molecule 10: Pre-mRNA-splicing factor CWC22



• Molecule 11: Pre-mRNA-splicing factor CEF1

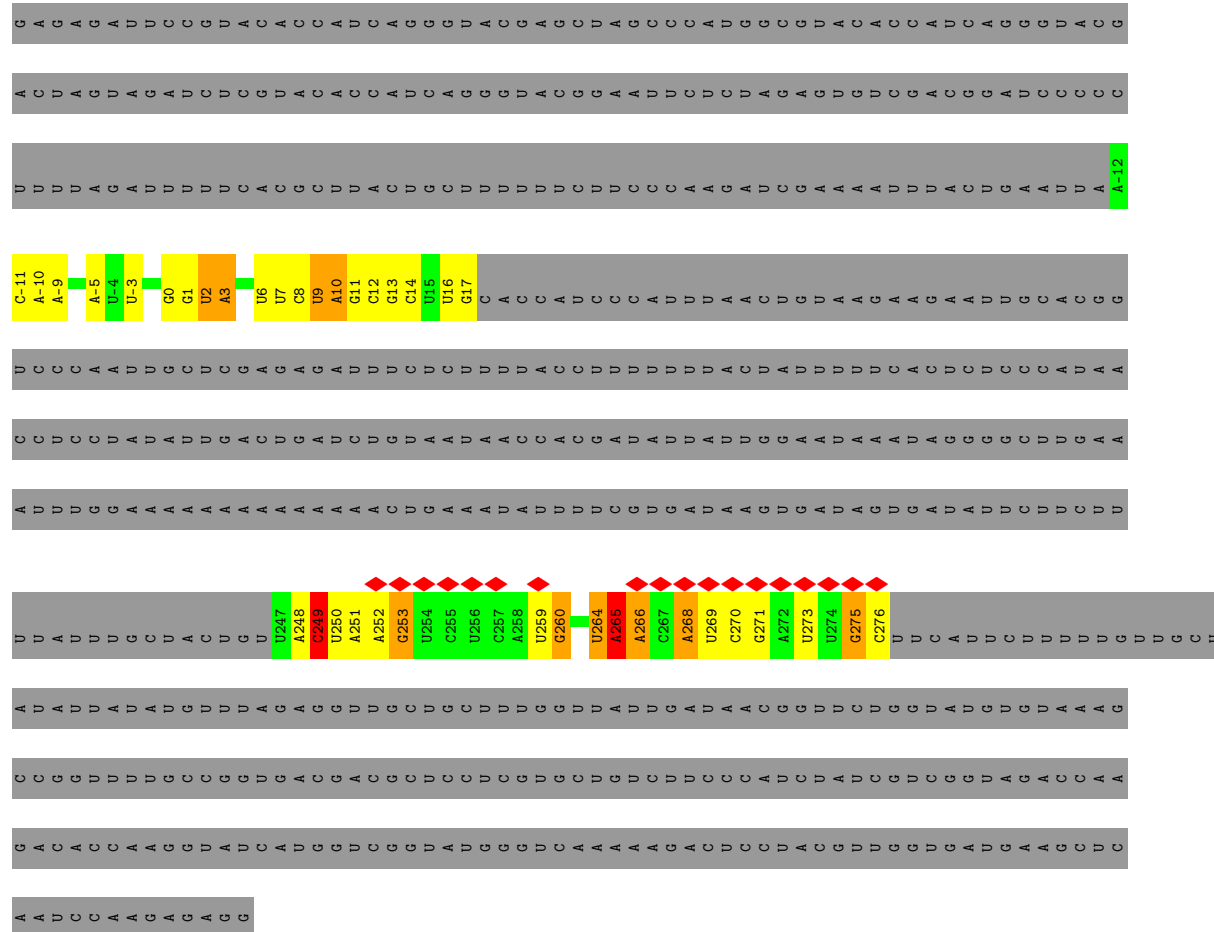




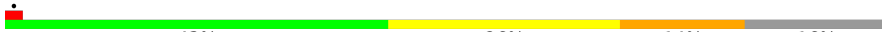
ALA ASN THR SER ILE LEU LYS ALA HIS TVR ASN VAL PRO VAL ASN ASP GLU GLU MET SER ARG GLN THR GLN GLU ILE HIS VAL PRO THR LEU ALA ASP MET GLU HIS TRP LEU VAL GLN ARG LYS LYS LEU MET ASP GLU ASN LEU

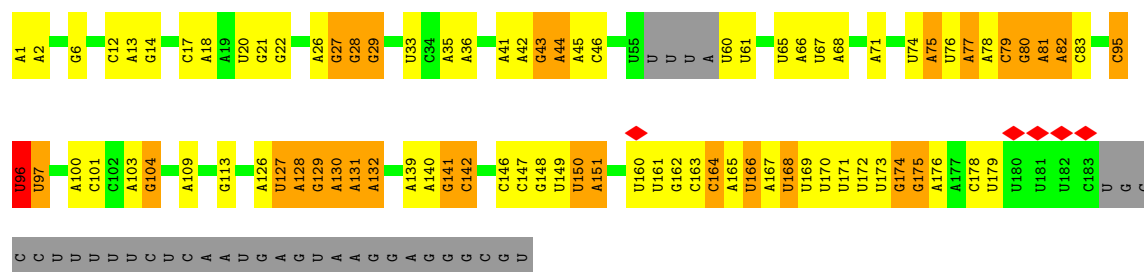
• Molecule 16: ACT1 pre-mRNA

Chain B:  91%

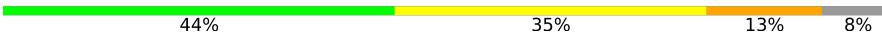


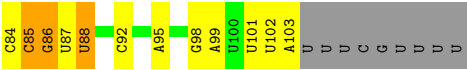
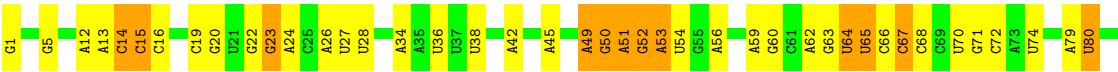
• Molecule 17: U5 snRNA

Chain D:  43% 26% 14% 16%

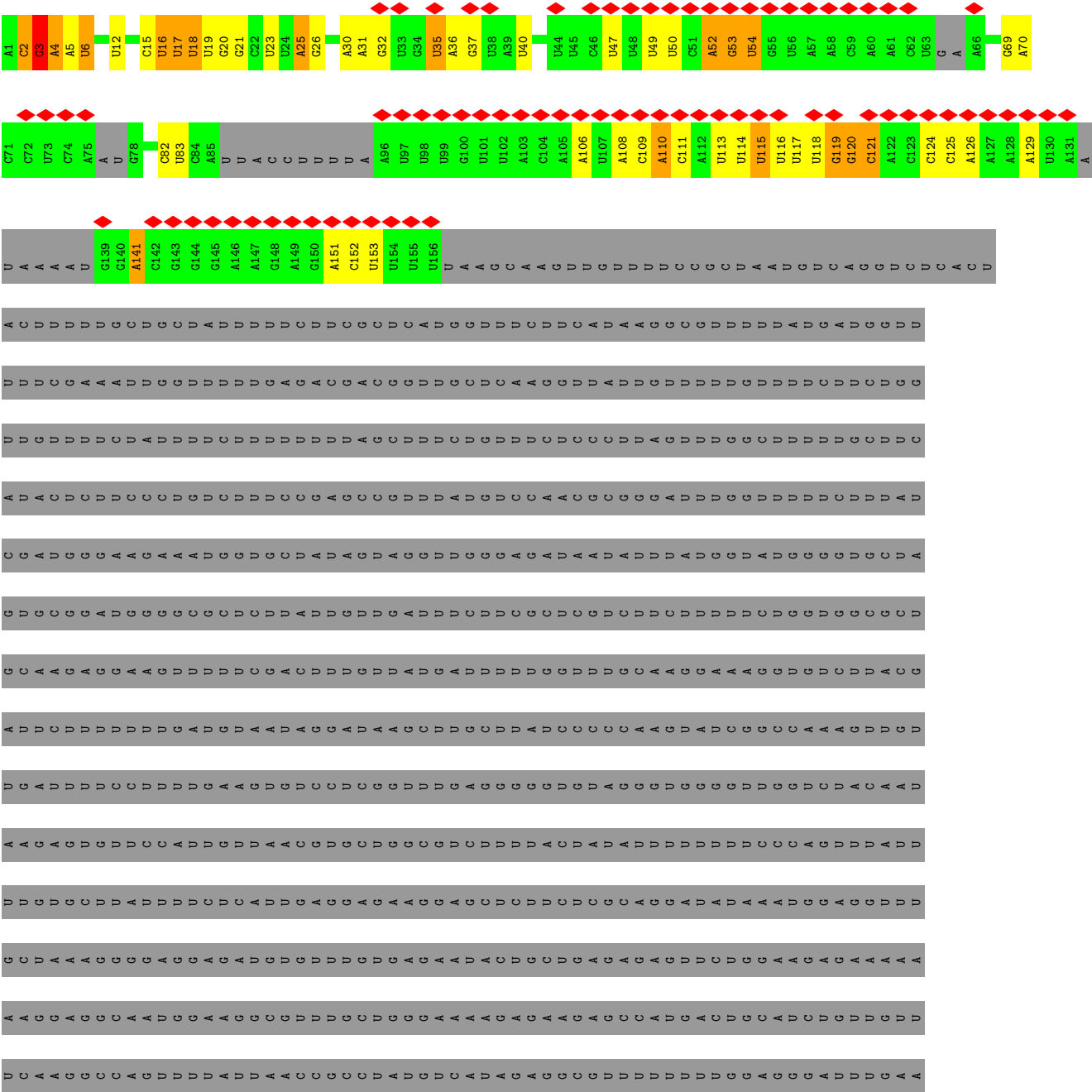


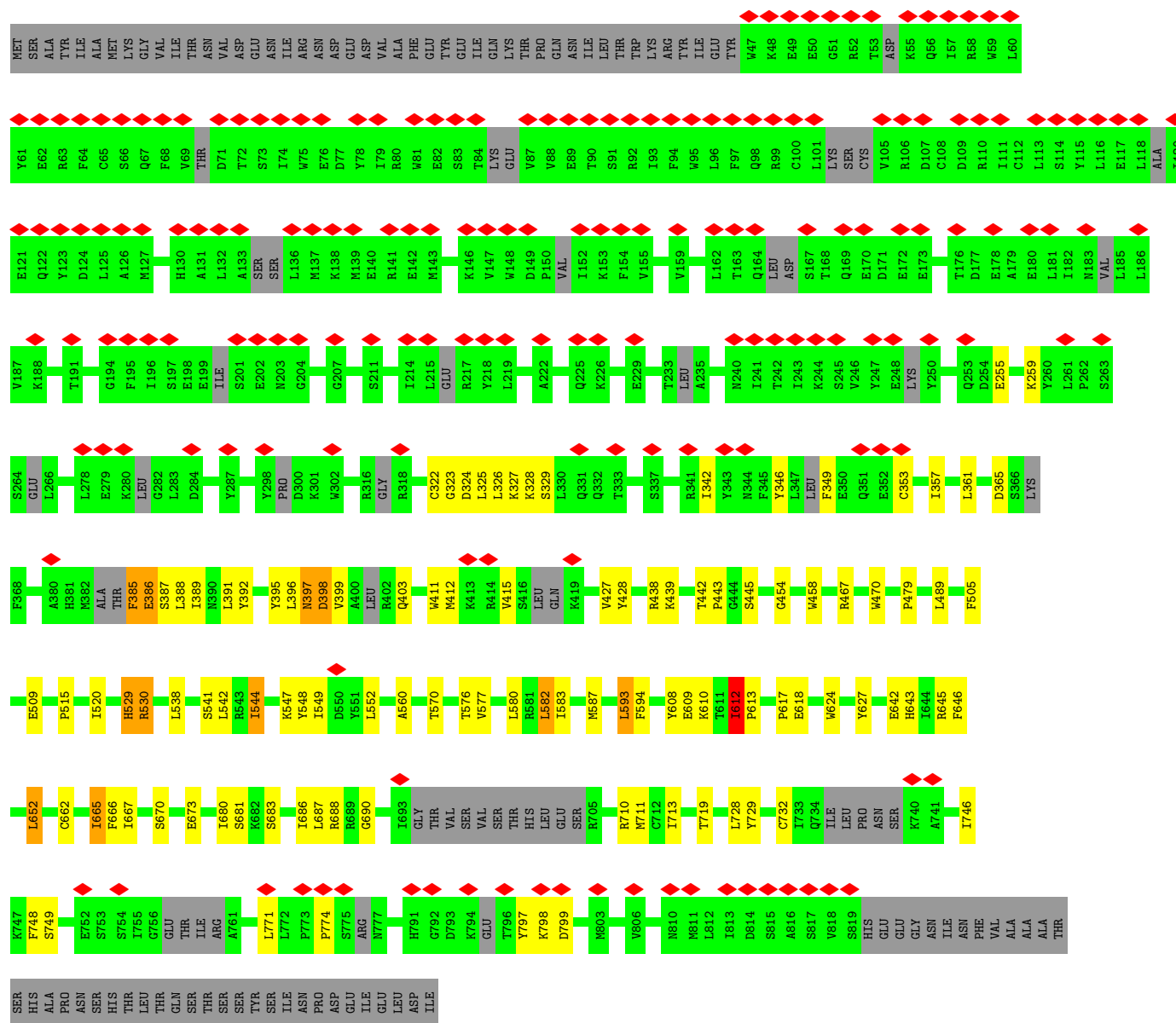
• Molecule 18: U6 snRNA

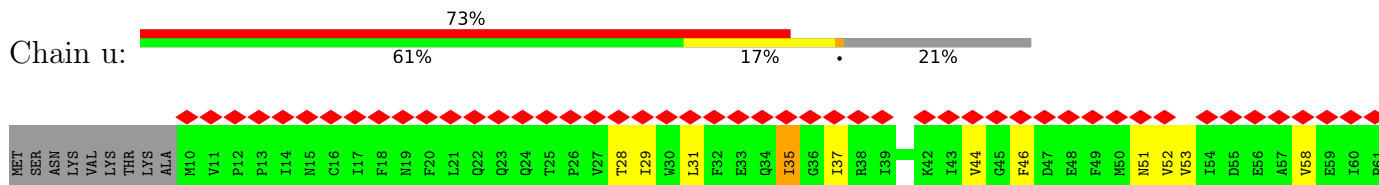
Chain E:  44% 35% 13% 8%

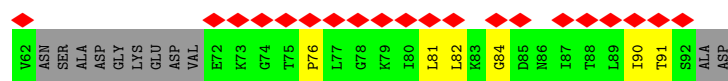


• Molecule 19: U2 snRNA

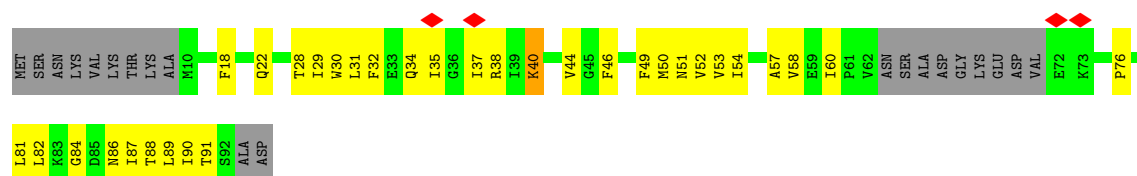




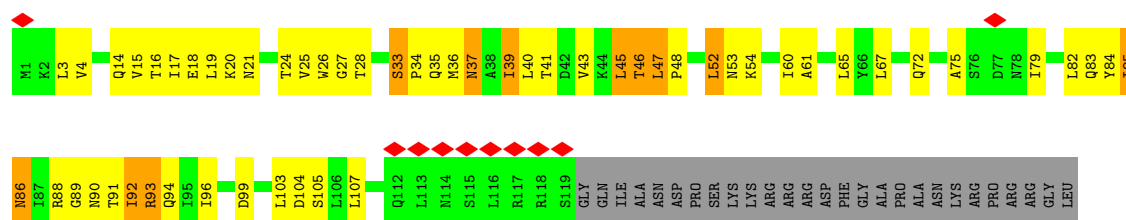
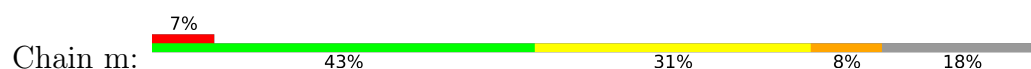




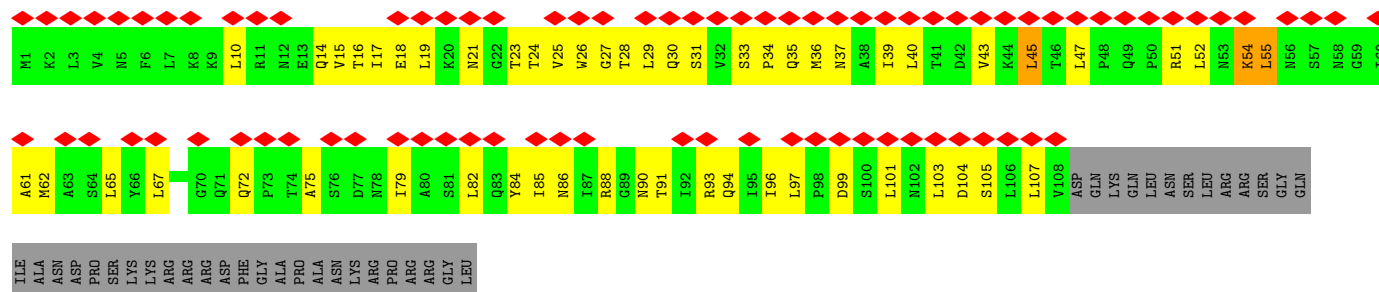
• Molecule 24: Small nuclear ribonucleoprotein E



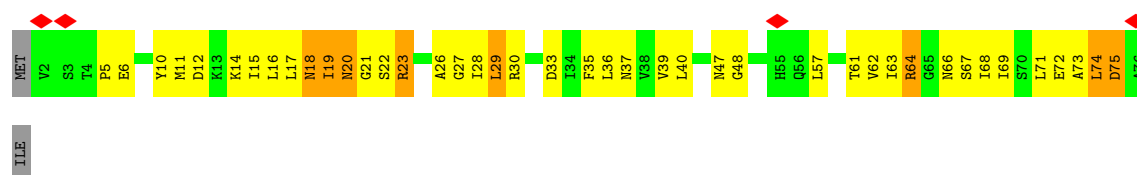
• Molecule 25: Small nuclear ribonucleoprotein Sm D1



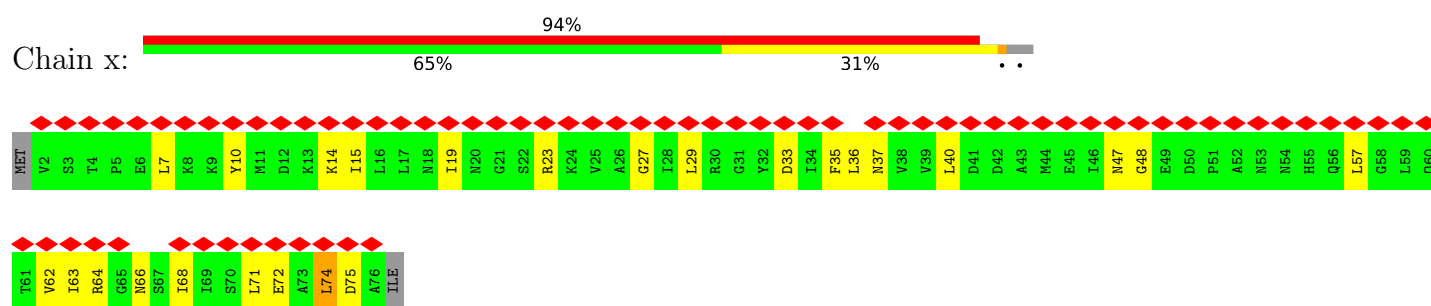
• Molecule 25: Small nuclear ribonucleoprotein Sm D1



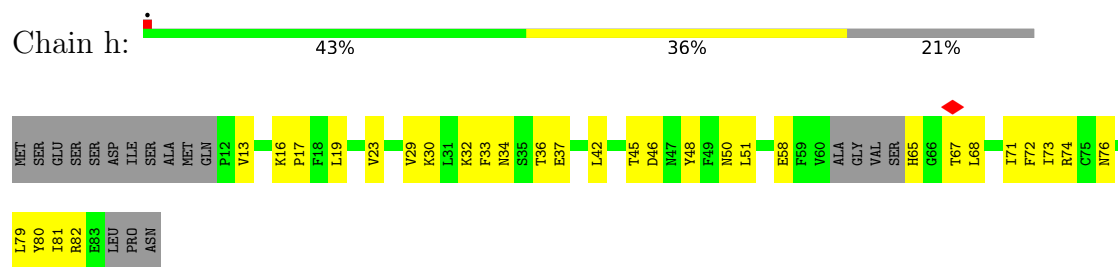
• Molecule 26: Small nuclear ribonucleoprotein G



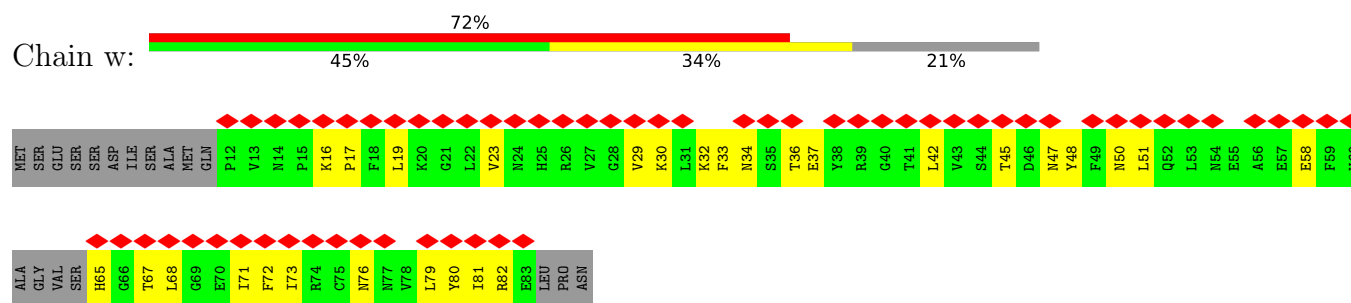
• Molecule 26: Small nuclear ribonucleoprotein G



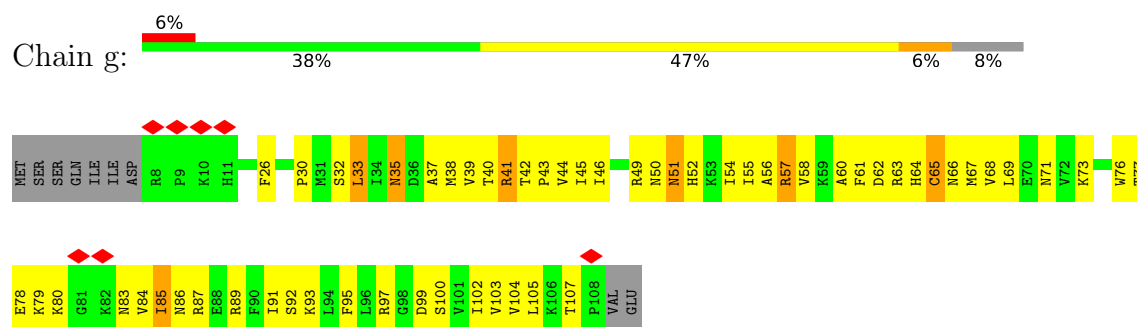
• Molecule 27: Small nuclear ribonucleoprotein F



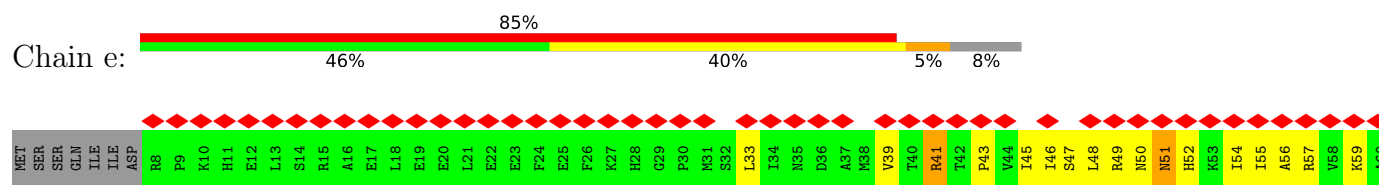
• Molecule 27: Small nuclear ribonucleoprotein F



• Molecule 28: Small nuclear ribonucleoprotein Sm D2

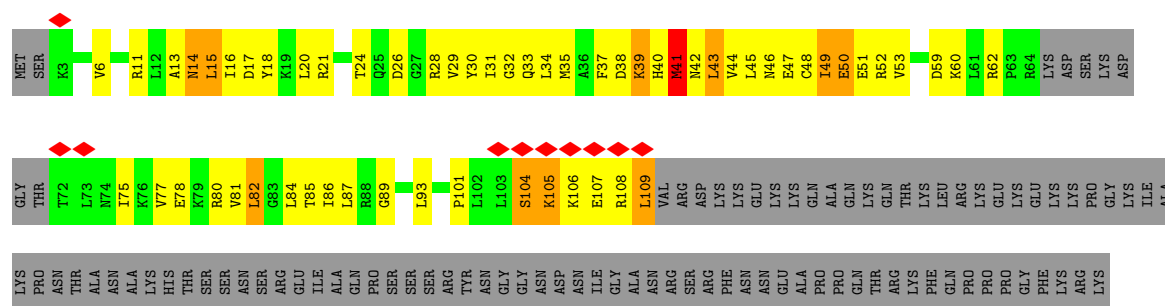


• Molecule 28: Small nuclear ribonucleoprotein Sm D2

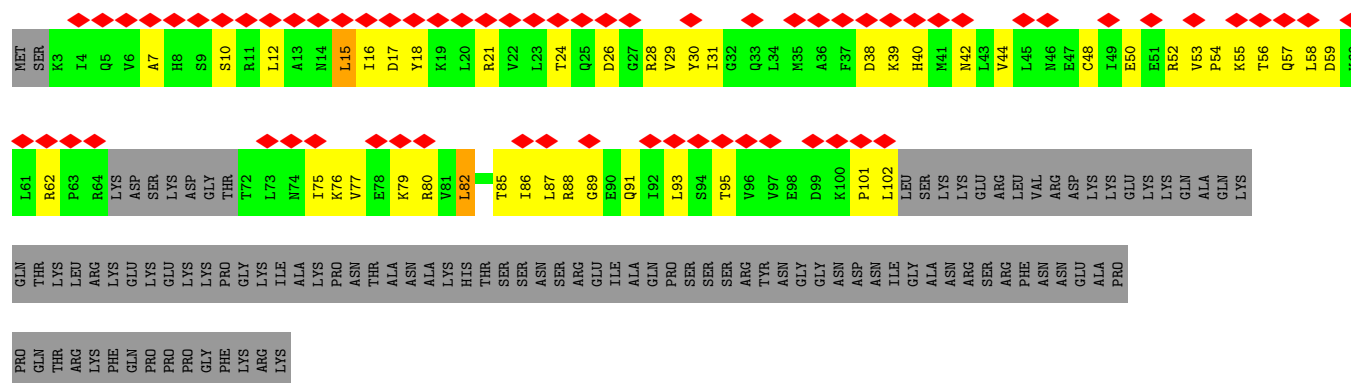




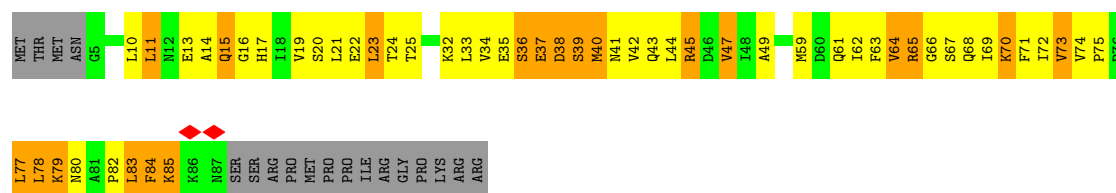
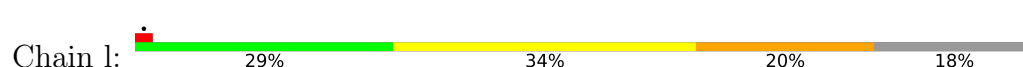
• Molecule 29: Small nuclear ribonucleoprotein-associated protein B



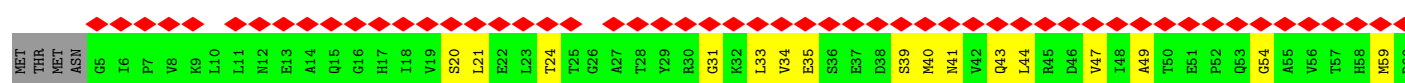
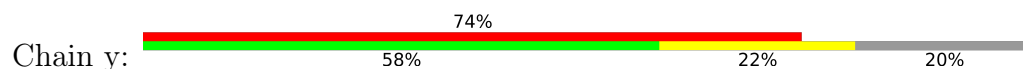
• Molecule 29: Small nuclear ribonucleoprotein-associated protein B

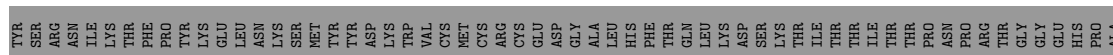


• Molecule 30: Small nuclear ribonucleoprotein Sm D3



• Molecule 30: Small nuclear ribonucleoprotein Sm D3





[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	555036	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.255	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	532.0, 532.0, 532.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, SEP, GTP, IHP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.47	0/16198	0.65	3/21958 (0.0%)
2	C	0.43	0/7503	0.60	1/10159 (0.0%)
3	J	0.36	0/191	0.58	0/254
4	O	0.51	0/2872	0.64	0/3902
5	P	0.34	0/1629	0.50	0/2194
6	Q	0.38	0/2339	0.72	0/3154
7	R	0.38	0/2135	0.61	0/2871
8	S	0.27	0/581	0.49	0/776
9	T	0.48	0/1315	0.58	0/1759
10	Z	0.25	0/3712	0.50	0/5004
11	c	0.27	0/2996	0.44	0/4033
12	d	0.35	0/3931	0.62	2/5356 (0.0%)
13	I	0.30	0/826	0.41	0/1097
14	n	0.38	0/194	0.53	0/256
15	H	0.35	0/98	0.58	0/130
16	B	0.34	0/1411	0.59	3/2191 (0.1%)
17	D	0.37	0/4239	0.45	1/6598 (0.0%)
18	E	0.41	0/2452	0.49	0/3817
19	L	0.33	0/4904	0.53	2/7607 (0.0%)
20	v	0.49	0/4662	0.76	4/6358 (0.1%)
21	a	0.63	0/415	1.15	0/577
22	b	1.07	0/839	1.44	8/1169 (0.7%)
23	t	0.29	0/924	0.54	0/1244
24	i	0.27	0/551	0.57	0/750
24	u	0.24	0/535	0.49	0/730
25	m	0.49	0/926	0.77	0/1257
25	z	0.31	0/833	0.61	0/1134
26	j	0.64	0/557	0.85	0/756
26	x	0.37	0/557	0.65	0/756
27	h	0.26	0/529	0.55	0/715
27	w	0.23	0/529	0.56	0/715
28	e	0.51	0/799	0.67	0/1078

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
28	g	0.56	0/799	0.78	0/1078
29	k	0.56	0/815	0.81	0/1092
29	s	0.43	0/755	0.72	0/1014
30	l	0.73	0/650	1.00	1/879 (0.1%)
30	y	0.30	0/625	0.59	0/847
31	o	0.23	0/835	0.56	2/1126 (0.2%)
31	p	0.18	0/848	0.44	0/1143
31	q	0.27	0/856	0.57	0/1155
31	r	0.30	0/828	0.57	0/1117
All	All	0.42	0/79193	0.63	27/109806 (0.0%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	43	MET	CA-C-N	8.57	128.71	119.28
22	b	43	MET	C-N-CA	8.57	128.71	119.28
16	B	265	A	C4'-C3'-O3'	7.98	121.38	109.40
22	b	4	THR	CA-C-N	7.87	127.43	118.85
22	b	4	THR	C-N-CA	7.87	127.43	118.85
17	D	96	U	C4'-C3'-O3'	-7.78	101.33	113.00
20	v	681	SER	N-CA-C	-6.52	105.08	113.16
22	b	11	ALA	CA-C-N	6.48	127.94	119.84
22	b	11	ALA	C-N-CA	6.48	127.94	119.84
19	L	1092	A	C2'-C3'-O3'	-6.43	104.05	113.70
20	v	612	ILE	O-C-N	6.24	124.50	120.07
16	B	249	C	C4'-C3'-O3'	6.12	118.58	109.40
31	o	37	ASN	CA-C-N	6.00	129.94	121.61
31	o	37	ASN	C-N-CA	6.00	129.94	121.61
12	d	424	ARG	CA-C-N	5.97	128.55	120.38
12	d	424	ARG	C-N-CA	5.97	128.55	120.38
1	A	1964	PRO	O-C-N	5.82	130.50	122.64
19	L	3	G	C2'-C3'-O3'	5.72	118.08	109.50
16	B	268	A	C4'-C3'-O3'	5.54	121.31	113.00
1	A	1488	ILE	O-C-N	5.42	123.92	120.07
1	A	1941	LEU	N-CA-C	5.39	117.16	111.28
2	C	90	LEU	N-CA-CB	-5.32	108.78	114.10
22	b	81	LEU	CA-C-N	5.20	124.91	119.92
22	b	81	LEU	C-N-CA	5.20	124.91	119.92
20	v	560	ALA	CA-C-N	5.05	130.49	122.61
20	v	560	ALA	C-N-CA	5.05	130.49	122.61
30	l	39	SER	N-CA-C	-5.03	105.92	111.71

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	A	15793	0	15768	482	0
2	C	7348	0	7520	138	0
3	J	190	0	186	4	0
4	O	2810	0	2804	102	0
5	P	1608	0	1631	44	0
6	Q	2301	0	2366	70	0
7	R	2089	0	2053	58	0
8	S	567	0	552	5	0
9	T	1291	0	1312	15	0
10	Z	3651	0	3707	39	0
11	c	2978	0	2459	55	0
12	d	3881	0	3041	139	0
13	I	822	0	845	27	0
14	n	199	0	197	6	0
15	H	94	0	92	4	0
16	B	1266	0	641	22	0
17	D	3795	0	1919	112	0
18	E	2192	0	1106	41	0
19	L	4405	0	2237	211	0
20	v	4625	0	3448	115	0
21	a	416	0	182	6	0
22	b	841	0	350	26	0
23	t	926	0	606	3	0
24	i	541	0	542	77	0
24	u	526	0	515	21	0
25	m	917	0	961	106	0
25	z	824	0	864	89	0
26	j	552	0	553	85	0
26	x	552	0	553	23	0
27	h	518	0	502	38	0
27	w	518	0	502	48	0
28	e	785	0	802	153	0
28	g	785	0	802	118	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	k	809	0	881	138	0
29	s	749	0	809	59	0
30	l	641	0	666	116	0
30	y	616	0	639	25	0
31	o	830	0	663	6	0
31	p	843	0	675	6	0
31	q	850	0	682	4	0
31	r	823	0	654	10	0
32	A	36	0	6	5	0
33	C	32	0	12	1	0
34	C	1	0	0	0	0
34	E	5	0	0	0	0
35	Q	2	0	0	0	0
35	R	1	0	0	0	0
35	T	3	0	0	0	0
All	All	76847	0	67305	2339	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 16.

All (2339) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1343:PHE:CD2	1:A:1440:ILE:HD11	1.34	1.59
1:A:1488:ILE:CG2	1:A:1489:PRO:HD3	1.43	1.48
26:j:17:LEU:CD1	26:j:19:ILE:HD11	1.43	1.47
29:k:31:ILE:CD1	29:k:49:ILE:HD11	1.45	1.45
28:g:35:ASN:HB2	28:g:61:PHE:CZ	1.52	1.43
1:A:2030:PRO:CG	28:e:73:LYS:HB2	1.54	1.35
5:P:34:ILE:HD13	12:d:155:LEU:CD1	1.57	1.34
19:L:1137:U:H2'	19:L:1138:G:C1'	1.58	1.34
1:A:763:MET:HE1	1:A:779:ALA:CB	1.56	1.33
12:d:255:ALA:HB1	12:d:291:PHE:CE2	1.63	1.33
20:v:612:ILE:HG13	20:v:613:PRO:CD	1.60	1.28
1:A:1343:PHE:HD2	1:A:1440:ILE:CD1	1.47	1.27
28:e:56:ALA:HB2	28:e:72:VAL:CG2	1.64	1.25
24:i:30:TRP:NE1	24:i:38:ARG:HD3	1.52	1.25
28:e:56:ALA:CB	28:e:69:LEU:HD23	1.66	1.25
1:A:1379:MET:CE	1:A:1620:TYR:H	1.49	1.24
12:d:241:MET:HG2	12:d:279:LEU:CD1	1.66	1.24
29:k:31:ILE:HD11	29:k:49:ILE:CD1	1.68	1.23

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:m:84:TYR:CD2	29:k:6:VAL:HG11	1.73	1.23
29:k:48:CYS:SG	29:k:82:LEU:HD12	1.79	1.23
19:L:1154:U:O2'	19:L:1155:C:H5'	1.07	1.22
1:A:1488:ILE:CG2	1:A:1489:PRO:CD	2.18	1.20
1:A:1379:MET:HE1	1:A:1620:TYR:N	1.57	1.20
1:A:1343:PHE:CD2	1:A:1440:ILE:CD1	2.22	1.19
26:j:64:ARG:NH2	24:i:50:MET:HB3	1.56	1.19
20:v:711:MET:HE1	20:v:748:PHE:CB	1.72	1.19
19:L:1154:U:O2'	19:L:1155:C:C5'	1.90	1.18
1:A:1889:LEU:CD2	1:A:1991:ILE:HG12	1.73	1.18
5:P:34:ILE:HD13	12:d:155:LEU:HD13	1.20	1.17
12:d:255:ALA:CB	12:d:291:PHE:CE2	2.27	1.17
7:R:74:LEU:HD11	7:R:78:LYS:NZ	1.60	1.15
25:m:19:LEU:HD22	25:m:91:THR:HG22	1.29	1.15
1:A:1035:LEU:CD1	1:A:1038:ILE:HB	1.76	1.15
26:j:28:ILE:O	26:j:40:LEU:HB2	1.44	1.15
1:A:2027:LEU:HD11	28:e:57:ARG:NE	1.60	1.15
26:j:64:ARG:HH22	24:i:50:MET:HB3	1.10	1.14
29:k:49:ILE:HG22	29:k:81:VAL:HA	1.26	1.14
1:A:1980:LYS:NZ	28:e:39:VAL:HG11	1.61	1.13
31:r:99:ARG:HG2	31:o:98:LEU:HD11	1.18	1.13
5:P:34:ILE:CD1	12:d:155:LEU:HD13	1.77	1.13
26:j:57:LEU:HB3	24:i:91:THR:HG21	1.22	1.13
20:v:612:ILE:HG13	20:v:613:PRO:HD3	1.16	1.12
28:e:56:ALA:HB3	28:e:69:LEU:HD23	1.23	1.12
1:A:763:MET:HE1	1:A:779:ALA:HB1	1.16	1.12
1:A:2033:THR:HG22	28:e:43:PRO:CG	1.78	1.12
19:L:1137:U:H2'	19:L:1138:G:H1'	1.26	1.12
29:k:105:LYS:HA	29:k:108:ARG:HH21	1.07	1.12
1:A:1992:TYR:HD2	1:A:1996:LEU:HG	1.11	1.12
26:j:17:LEU:HD12	26:j:19:ILE:HD11	1.24	1.11
1:A:1488:ILE:HG22	1:A:1489:PRO:CD	1.80	1.11
18:E:22:G:H3'	18:E:23:G:H5''	1.28	1.11
19:L:113:U:O4	27:w:48:TYR:HA	1.46	1.11
1:A:316:THR:HG23	1:A:317:PRO:CD	1.79	1.10
25:m:17:ILE:HG23	25:m:92:ILE:CG2	1.79	1.10
1:A:1275:MET:O	1:A:1276:GLU:HG3	1.50	1.10
29:k:86:ILE:HD11	30:l:11:LEU:HD12	1.33	1.10
29:k:31:ILE:CD1	29:k:49:ILE:CD1	2.27	1.10
30:l:21:LEU:HD23	30:l:72:ILE:HG12	1.32	1.09
1:A:2024:MET:HE2	28:e:93:LYS:CE	1.82	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2027:LEU:CD1	28:e:57:ARG:HE	1.64	1.09
20:v:385:PHE:HA	20:v:388:LEU:HD12	1.20	1.09
29:s:54:PRO:HB2	29:s:57:GLN:HG2	1.31	1.09
24:i:30:TRP:CD1	24:i:38:ARG:HD3	1.86	1.09
1:A:763:MET:CE	1:A:779:ALA:HB1	1.82	1.09
1:A:2030:PRO:HG3	28:e:73:LYS:HB2	1.13	1.09
12:d:271:ILE:HD13	12:d:281:LYS:HG3	1.12	1.09
4:O:238:LEU:HD11	5:P:74:ILE:CD1	1.82	1.08
28:g:35:ASN:CB	28:g:61:PHE:CZ	2.37	1.08
29:k:49:ILE:CG2	29:k:81:VAL:HA	1.84	1.07
30:l:47:VAL:HG23	30:l:59:MET:HG3	1.31	1.07
1:A:2027:LEU:HD11	28:e:57:ARG:HE	1.11	1.07
25:m:84:TYR:CE2	29:k:6:VAL:HG11	1.89	1.07
28:e:56:ALA:HB2	28:e:72:VAL:HG23	1.31	1.07
20:v:711:MET:CE	20:v:748:PHE:CB	2.34	1.06
1:A:2030:PRO:CG	28:e:73:LYS:CB	2.33	1.06
20:v:386:GLU:HA	20:v:389:ILE:HD12	1.38	1.06
19:L:1137:U:H2'	19:L:1138:G:O4'	1.55	1.06
26:j:17:LEU:HD13	26:j:19:ILE:HD11	1.32	1.06
1:A:1889:LEU:HD21	1:A:1991:ILE:HG12	1.10	1.05
25:m:17:ILE:HG23	25:m:92:ILE:HG22	1.36	1.05
12:d:247:VAL:HG21	12:d:280:LEU:HD11	1.36	1.05
17:D:175:G:O6	24:i:35:ILE:HD11	1.57	1.04
24:i:30:TRP:CD1	24:i:38:ARG:CD	2.40	1.04
1:A:1035:LEU:HD11	1:A:1038:ILE:CB	1.87	1.04
29:k:105:LYS:HA	29:k:108:ARG:NH2	1.73	1.03
30:y:21:LEU:CD1	30:y:44:LEU:HD11	1.87	1.03
29:k:31:ILE:CG1	29:k:49:ILE:CD1	2.36	1.03
26:j:27:GLY:HA3	26:j:40:LEU:HD12	1.36	1.03
25:m:17:ILE:CG2	25:m:92:ILE:CG2	2.36	1.02
1:A:2027:LEU:HB3	28:e:71:ASN:CB	1.88	1.02
19:L:113:U:C5	27:w:48:TYR:CD1	2.46	1.02
28:g:40:THR:O	28:g:41:ARG:HG2	1.60	1.02
1:A:1488:ILE:HG23	1:A:1489:PRO:CD	1.84	1.02
26:j:17:LEU:CD1	26:j:19:ILE:CD1	2.37	1.02
28:g:35:ASN:HA	28:g:61:PHE:CE2	1.93	1.02
6:Q:248:CYS:SG	6:Q:316:LEU:HD12	2.00	1.01
12:d:263:SER:HB3	12:d:287:PHE:CZ	1.93	1.01
4:O:238:LEU:HD11	5:P:74:ILE:HD13	1.41	1.01
19:L:1082:A:H2'	19:L:1083:A:H8	1.26	1.00
20:v:541:SER:O	20:v:544:ILE:HG22	1.61	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:34:ILE:HD13	12:d:155:LEU:HD12	1.41	1.00
1:A:316:THR:HG23	1:A:317:PRO:HD3	1.00	1.00
20:v:386:GLU:HA	20:v:389:ILE:CD1	1.92	1.00
1:A:2030:PRO:HG2	28:e:73:LYS:CB	1.89	1.00
12:d:267:TYR:CD2	12:d:284:LEU:HD23	1.97	0.99
29:k:48:CYS:SG	29:k:82:LEU:CD1	2.50	0.99
6:Q:303:GLY:HA3	6:Q:309:ASN:OD1	1.62	0.99
7:R:63:ARG:HD3	9:T:143:HIS:CD2	1.97	0.99
7:R:159:ARG:CZ	7:R:206:LEU:HD12	1.92	0.99
1:A:168:LEU:HD23	1:A:622:MET:HE2	1.44	0.99
24:u:35:ILE:CD1	27:w:79:LEU:CD1	2.40	0.99
1:A:2030:PRO:HG2	28:e:73:LYS:HB2	1.41	0.99
1:A:1161:TYR:OH	1:A:1168:ILE:HD11	1.63	0.98
12:d:241:MET:HG2	12:d:279:LEU:HD13	1.42	0.98
12:d:255:ALA:HB1	12:d:291:PHE:CD2	1.99	0.98
1:A:1972:ASP:CB	28:e:41:ARG:HD3	1.93	0.98
22:b:50:LEU:C	22:b:55:HIS:CB	2.36	0.98
1:A:2033:THR:CG2	28:e:43:PRO:HG3	1.93	0.98
19:L:1137:U:O2'	19:L:1138:G:H4'	1.63	0.97
1:A:2033:THR:HG22	28:e:43:PRO:HG3	0.99	0.97
12:d:271:ILE:CD1	12:d:281:LYS:HG3	1.93	0.97
24:i:28:THR:HG22	24:i:40:LYS:HD2	1.45	0.97
2:C:586:MET:HA	2:C:589:LEU:HD23	1.45	0.97
19:L:110:A:H61	25:z:35:GLN:NE2	1.61	0.97
1:A:316:THR:CG2	1:A:317:PRO:HD3	1.93	0.97
4:O:309:ARG:NH1	4:O:328:THR:HG21	1.79	0.97
25:m:96:ILE:HD11	28:g:89:ARG:HH22	1.29	0.97
18:E:49:A:O2'	18:E:50:G:OP1	1.82	0.96
1:A:1488:ILE:HG23	1:A:1489:PRO:HD3	0.97	0.96
22:b:110:ARG:HA	22:b:134:VAL:CB	1.95	0.96
29:s:59:ASP:HA	29:s:62:ARG:HH21	1.31	0.96
1:A:2024:MET:HE2	28:e:93:LYS:HE3	1.47	0.96
29:k:49:ILE:HG22	29:k:81:VAL:CA	1.94	0.96
6:Q:109:MET:CE	6:Q:112:PHE:CD2	2.48	0.96
1:A:2030:PRO:HG3	28:e:73:LYS:CB	1.95	0.96
19:L:1082:A:H2'	19:L:1083:A:C8	2.00	0.96
12:d:267:TYR:O	12:d:271:ILE:HG22	1.64	0.96
12:d:241:MET:CG	12:d:279:LEU:CD1	2.44	0.95
22:b:110:ARG:CA	22:b:134:VAL:CB	2.44	0.95
1:A:1889:LEU:HD21	1:A:1991:ILE:CG1	1.96	0.95
19:L:1085:G:C2	19:L:1086:U:C5	2.54	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:k:31:ILE:HG13	29:k:49:ILE:CD1	1.94	0.95
1:A:1035:LEU:HD11	1:A:1038:ILE:HB	0.97	0.95
1:A:1379:MET:HE1	1:A:1620:TYR:H	0.80	0.95
30:l:14:ALA:O	30:l:17:HIS:HB2	1.67	0.95
1:A:484:PHE:CE1	1:A:485:PRO:HB3	2.00	0.95
1:A:2027:LEU:HD11	28:e:57:ARG:CZ	1.96	0.94
19:L:121:C:H1'	28:e:49:ARG:HG2	1.48	0.94
1:A:1992:TYR:CD2	1:A:1996:LEU:HG	2.02	0.93
25:m:47:LEU:HD11	25:m:61:ALA:CB	1.98	0.93
12:d:241:MET:HG2	12:d:279:LEU:HD11	1.51	0.93
24:u:35:ILE:HD13	27:w:79:LEU:CD1	1.98	0.93
17:D:81:A:H4'	17:D:82:A:OP2	1.69	0.92
28:g:50:ASN:HD22	28:g:52:HIS:HE1	0.99	0.92
17:D:26:A:C6	17:D:141:G:H8	1.86	0.92
31:r:99:ARG:HG2	31:o:98:LEU:CD1	1.98	0.92
29:s:48:CYS:SG	29:s:82:LEU:O	2.27	0.92
6:Q:248:CYS:SG	6:Q:316:LEU:CD1	2.58	0.92
29:k:13:ALA:HB2	29:k:37:PHE:HZ	1.31	0.92
28:g:35:ASN:HB2	28:g:61:PHE:HZ	1.25	0.92
29:k:44:VAL:HG22	29:k:86:ILE:HG22	1.52	0.92
1:A:1889:LEU:HD11	1:A:1991:ILE:HG23	1.53	0.91
28:g:50:ASN:HD22	28:g:52:HIS:CE1	1.87	0.91
25:m:47:LEU:HD11	25:m:61:ALA:HB1	1.53	0.91
30:l:59:MET:SD	30:l:62:ILE:HD12	2.09	0.91
1:A:2027:LEU:HB2	28:e:71:ASN:CG	1.96	0.91
28:g:40:THR:C	28:g:41:ARG:HG2	1.94	0.91
29:k:35:MET:HB3	30:l:84:PHE:HE2	1.34	0.91
29:k:31:ILE:HG13	29:k:49:ILE:HD12	1.51	0.91
30:y:21:LEU:HD11	30:y:44:LEU:HD11	1.51	0.91
1:A:1980:LYS:HZ1	28:e:39:VAL:HG11	1.24	0.91
19:L:151:A:H61	19:L:1086:U:H3	1.11	0.91
27:w:32:LYS:HG3	27:w:33:PHE:CD1	2.06	0.91
19:L:113:U:C4	27:w:48:TYR:HA	2.05	0.91
17:D:168:U:H2'	24:i:49:PHE:CD1	2.06	0.90
17:D:173:U:H1'	28:g:99:ASP:HB3	1.48	0.90
1:A:2027:LEU:CB	28:e:71:ASN:CG	2.45	0.90
12:d:255:ALA:CB	12:d:291:PHE:HE2	1.81	0.90
26:j:17:LEU:HD13	26:j:19:ILE:CD1	2.01	0.90
29:k:86:ILE:HD11	30:l:11:LEU:CD1	2.02	0.90
6:Q:207:LEU:HD23	6:Q:290:ILE:HG22	1.51	0.90
17:D:95:C:H1'	17:D:96:U:OP2	1.71	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:g:76:TRP:CZ2	28:g:87:ARG:HD3	2.07	0.89
18:E:22:G:C3'	18:E:23:G:H5''	2.03	0.89
20:v:385:PHE:CA	20:v:388:LEU:HD12	2.03	0.89
30:l:21:LEU:CD2	30:l:72:ILE:HG12	2.02	0.89
4:O:309:ARG:HH12	4:O:328:THR:HG21	1.35	0.89
11:c:181:ARG:CZ	12:d:49:ARG:NH1	2.35	0.89
19:L:117:U:O2	25:z:35:GLN:HB3	1.72	0.89
29:k:40:HIS:O	29:k:41:MET:HB2	1.70	0.89
25:z:47:LEU:HD21	25:z:61:ALA:CB	2.02	0.89
1:A:2027:LEU:HB3	28:e:71:ASN:HB2	1.53	0.88
6:Q:109:MET:CE	6:Q:112:PHE:HD2	1.84	0.88
6:Q:207:LEU:CD2	6:Q:290:ILE:HG22	2.03	0.88
19:L:152:C:H42	19:L:1085:G:H1	1.20	0.88
30:l:17:HIS:CG	30:l:75:PRO:HG2	2.07	0.88
19:L:118:U:H3	28:e:66:ASN:HD22	1.17	0.88
30:l:65:ARG:HH11	30:l:65:ARG:HG3	1.36	0.88
1:A:1980:LYS:NZ	28:e:39:VAL:CG1	2.36	0.88
1:A:1993:ASP:OD2	1:A:2040:TRP:CD1	2.27	0.88
28:g:76:TRP:CH2	28:g:87:ARG:HD3	2.09	0.88
30:l:75:PRO:HB2	30:l:78:LEU:HD13	1.56	0.88
4:O:218:ARG:HD3	4:O:253:MET:O	1.74	0.88
12:d:289:LYS:HE2	20:v:643:HIS:HE1	1.36	0.88
24:u:35:ILE:HD11	27:w:79:LEU:CD1	2.03	0.88
30:y:33:LEU:HA	30:y:44:LEU:HD23	1.54	0.88
17:D:26:A:C5	17:D:141:G:C8	2.62	0.87
26:j:27:GLY:CA	26:j:40:LEU:HD12	2.05	0.87
26:j:61:THR:HG22	24:i:91:THR:HG23	1.55	0.87
19:L:1130:U:H2'	19:L:1131:U:O4'	1.73	0.87
1:A:1488:ILE:HG22	1:A:1489:PRO:HD3	1.38	0.87
28:g:50:ASN:HB3	28:g:52:HIS:ND1	1.90	0.87
2:C:248:VAL:HA	2:C:933:TRP:HH2	1.39	0.87
11:c:227:ILE:O	13:I:152:ILE:HG22	1.74	0.87
19:L:151:A:N6	19:L:1086:U:H3	1.72	0.87
1:A:1488:ILE:HG22	1:A:1489:PRO:HD2	1.54	0.87
28:g:45:ILE:HD12	28:g:55:ILE:HG12	1.57	0.87
1:A:763:MET:HE1	1:A:779:ALA:HB2	1.54	0.87
30:l:82:PRO:O	30:l:85:LYS:HD2	1.73	0.87
20:v:386:GLU:CA	20:v:389:ILE:HD12	2.04	0.86
1:A:1987:VAL:HG11	1:A:1989:PHE:HE2	1.39	0.86
1:A:1987:VAL:CG1	1:A:1989:PHE:HE2	1.89	0.86
19:L:1146:G:H2'	19:L:1147:A:C8	2.11	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:LYS:HE3	32:A:3000:IHP:O45	1.75	0.86
29:k:29:VAL:O	29:k:50:GLU:HA	1.76	0.86
7:R:74:LEU:O	7:R:74:LEU:HD12	1.76	0.85
1:A:1961:LEU:HD21	1:A:2084:LEU:HD13	1.56	0.85
19:L:1154:U:HO2'	19:L:1155:C:H5'	1.37	0.85
28:e:56:ALA:HB2	28:e:72:VAL:HG21	1.56	0.85
30:y:21:LEU:HD12	30:y:44:LEU:HD11	1.56	0.85
11:c:200:ILE:HG21	12:d:45:GLU:HG3	1.56	0.85
25:m:52:LEU:HD21	28:g:79:LYS:C	2.00	0.85
28:e:56:ALA:HB1	28:e:69:LEU:HD23	1.57	0.85
12:d:229:VAL:HG12	12:d:274:TRP:CZ2	2.12	0.85
28:g:50:ASN:ND2	28:g:52:HIS:HE1	1.75	0.85
17:D:26:A:C6	17:D:141:G:C8	2.65	0.85
19:L:1137:U:C2'	19:L:1138:G:H1'	2.05	0.84
30:l:49:ALA:HB2	30:l:59:MET:HE3	1.59	0.84
1:A:1990:ASN:ND2	1:A:1993:ASP:H	1.73	0.84
19:L:1154:U:H2'	19:L:1155:C:C6	2.11	0.84
7:R:159:ARG:NH1	7:R:206:LEU:HD12	1.91	0.84
1:A:1527:TRP:CE3	1:A:1528:THR:HG22	2.12	0.84
4:O:238:LEU:HD11	5:P:74:ILE:HD11	1.60	0.84
28:e:56:ALA:CB	28:e:72:VAL:HG23	2.08	0.84
1:A:1987:VAL:CG1	1:A:1989:PHE:CE2	2.61	0.84
5:P:34:ILE:CD1	12:d:155:LEU:CD1	2.42	0.84
25:m:39:ILE:HD11	25:m:84:TYR:CE1	2.13	0.84
28:g:43:PRO:O	28:g:107:THR:CB	2.26	0.84
7:R:74:LEU:HD11	7:R:78:LYS:HZ2	1.39	0.83
11:c:227:ILE:HD12	13:I:151:LYS:HA	1.59	0.83
12:d:289:LYS:HG3	20:v:609:GLU:HG2	1.58	0.83
16:B:2:U:O2'	16:B:3:A:OP2	1.94	0.83
20:v:385:PHE:HA	20:v:388:LEU:CD1	2.05	0.83
29:s:54:PRO:CB	29:s:57:GLN:HG2	2.08	0.83
7:R:74:LEU:HD11	7:R:78:LYS:HZ3	1.41	0.83
29:k:35:MET:HB3	30:l:84:PHE:CE2	2.13	0.83
17:D:26:A:N6	17:D:141:G:H8	1.76	0.83
22:b:14:TYR:O	29:s:102:LEU:CD1	2.26	0.83
12:d:255:ALA:CB	12:d:291:PHE:CD2	2.60	0.83
19:L:110:A:N6	25:z:35:GLN:NE2	2.26	0.83
12:d:247:VAL:HG21	12:d:280:LEU:CD1	2.07	0.82
1:A:2024:MET:HE2	28:e:93:LYS:HE2	1.61	0.82
12:d:284:LEU:O	12:d:284:LEU:HD22	1.79	0.82
24:i:30:TRP:NE1	24:i:38:ARG:CD	2.39	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:x:19:ILE:O	26:x:23:ARG:HB2	1.78	0.82
12:d:334:PHE:N	12:d:335:PRO:HD3	1.94	0.82
25:m:52:LEU:HD21	28:g:80:LYS:N	1.94	0.82
30:l:47:VAL:HG23	30:l:59:MET:CG	2.10	0.82
24:u:35:ILE:CD1	27:w:79:LEU:HD12	2.09	0.81
26:j:6:GLU:HG2	30:l:37:GLU:OE2	1.80	0.81
26:j:64:ARG:HG3	24:i:50:MET:SD	2.20	0.81
29:k:42:ASN:HB3	29:k:89:GLY:H	1.45	0.81
29:k:49:ILE:CG2	29:k:81:VAL:CA	2.57	0.81
11:c:181:ARG:NH2	12:d:49:ARG:HH12	1.78	0.81
30:l:15:GLN:C	30:l:15:GLN:HE21	1.89	0.81
1:A:428:LEU:HD22	2:C:896:GLY:O	1.80	0.81
25:m:3:LEU:CD2	28:g:95:PHE:HE1	1.94	0.81
2:C:501:ILE:HD13	2:C:567:ILE:HG23	1.61	0.81
19:L:1085:G:C2	19:L:1086:U:C4	2.68	0.81
29:k:13:ALA:HA	29:k:37:PHE:CE2	2.16	0.81
29:k:42:ASN:HB3	29:k:89:GLY:N	1.95	0.81
1:A:1889:LEU:CG	1:A:1991:ILE:HG12	2.10	0.81
19:L:1085:G:N2	19:L:1086:U:C4	2.49	0.81
20:v:612:ILE:CG1	20:v:613:PRO:HD3	2.07	0.81
29:k:84:LEU:HD23	30:l:75:PRO:O	1.81	0.81
28:e:56:ALA:CB	28:e:72:VAL:CG2	2.55	0.81
25:m:4:VAL:HG22	25:m:36:MET:HE2	1.63	0.81
26:j:27:GLY:HA3	26:j:40:LEU:CD1	2.09	0.81
1:A:665:GLY:HA2	1:A:667:TYR:CE1	2.16	0.80
1:A:769:MET:HE2	4:O:352:ILE:HD12	1.63	0.80
1:A:1980:LYS:HZ2	28:e:39:VAL:CG1	1.91	0.80
25:m:96:ILE:CD1	28:g:89:ARG:HH22	1.92	0.80
28:g:35:ASN:HB2	28:g:61:PHE:CE2	2.15	0.80
1:A:140:ARG:HD3	1:A:252:GLU:CD	2.06	0.80
25:z:47:LEU:HD21	25:z:61:ALA:HB3	1.62	0.80
12:d:263:SER:HB3	12:d:287:PHE:HZ	1.42	0.80
19:L:1137:U:C2'	19:L:1138:G:C4'	2.60	0.80
30:l:17:HIS:ND1	30:l:75:PRO:HG2	1.96	0.80
26:j:17:LEU:HD12	26:j:19:ILE:CD1	2.07	0.80
1:A:2027:LEU:O	28:e:71:ASN:HB3	1.82	0.80
12:d:267:TYR:HE2	12:d:287:PHE:HB3	1.47	0.80
19:L:109:C:OP1	25:z:34:PRO:HG3	1.81	0.80
5:P:148:HIS:HB2	12:d:131:ARG:HG3	1.62	0.80
19:L:109:C:OP1	25:z:34:PRO:CG	2.30	0.80
1:A:1527:TRP:CE3	1:A:1528:THR:CG2	2.64	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2024:MET:HA	28:e:71:ASN:HD21	1.47	0.79
20:v:662:CYS:SG	20:v:665:ILE:HD11	2.22	0.79
29:k:86:ILE:CD1	30:l:11:LEU:HD12	2.11	0.79
29:k:105:LYS:CA	29:k:108:ARG:HH21	1.91	0.79
1:A:1379:MET:HE3	1:A:1620:TYR:HB2	1.64	0.79
25:z:72:GLN:HE22	25:z:79:ILE:HD11	1.46	0.79
27:h:71:ILE:HG23	28:g:103:VAL:HG23	1.64	0.79
6:Q:206:PHE:HD2	6:Q:291:ILE:CD1	1.96	0.79
19:L:1085:G:N2	19:L:1086:U:C5	2.51	0.79
1:A:2027:LEU:HD11	28:e:57:ARG:NH2	1.96	0.79
28:g:35:ASN:O	28:g:39:VAL:HG23	1.83	0.79
4:O:200:VAL:CG2	4:O:230:VAL:CG2	2.60	0.79
25:m:72:GLN:HE22	25:m:79:ILE:HD11	1.47	0.79
1:A:168:LEU:CD2	1:A:622:MET:HE2	2.13	0.79
6:Q:214:ILE:HD11	6:Q:283:ILE:HG12	1.65	0.79
17:D:167:A:H2'	27:h:48:TYR:CE2	2.18	0.79
25:m:17:ILE:CG2	25:m:92:ILE:HG22	2.07	0.78
11:c:227:ILE:CD1	13:I:151:LYS:HA	2.13	0.78
19:L:113:U:O4	27:w:48:TYR:CA	2.31	0.78
22:b:14:TYR:O	29:s:102:LEU:HD12	1.84	0.78
1:A:1961:LEU:HD21	1:A:2084:LEU:CD1	2.12	0.78
19:L:113:U:C5	27:w:48:TYR:CE1	2.71	0.78
30:l:11:LEU:HD11	30:l:72:ILE:CD1	2.13	0.78
24:i:40:LYS:HG3	24:i:60:ILE:CD1	2.13	0.78
19:L:52:A:C3'	19:L:53:G:H5''	2.13	0.78
25:m:19:LEU:HD22	25:m:91:THR:CG2	2.10	0.78
2:C:248:VAL:HA	2:C:933:TRP:CH2	2.19	0.78
4:O:200:VAL:HG22	4:O:230:VAL:CG2	2.13	0.78
30:l:21:LEU:HD23	30:l:72:ILE:CG1	2.13	0.78
30:y:21:LEU:CD2	30:y:72:ILE:HG12	2.14	0.78
19:L:1136:U:O3'	19:L:1137:U:H4'	1.82	0.78
30:y:21:LEU:HD12	30:y:44:LEU:CD1	2.12	0.78
1:A:1980:LYS:HZ2	28:e:39:VAL:HG11	1.44	0.77
19:L:1137:U:H2'	19:L:1138:G:C4'	2.13	0.77
28:e:68:VAL:C	28:e:69:LEU:HD12	2.09	0.77
29:s:59:ASP:HA	29:s:62:ARG:NH2	1.99	0.77
29:k:13:ALA:CB	29:k:37:PHE:HZ	1.97	0.77
12:d:267:TYR:CE2	12:d:287:PHE:HB3	2.20	0.77
1:A:404:ASN:ND2	2:C:927:MET:SD	2.57	0.77
1:A:1092:PHE:CE2	1:A:1093:LYS:HD3	2.19	0.77
17:D:129:G:H1'	17:D:131:A:H2'	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:MET:SD	1:A:779:ALA:HB1	2.24	0.77
16:B:2:U:O2'	16:B:3:A:P	2.42	0.77
25:m:93:ARG:HH11	25:m:93:ARG:HG3	1.50	0.77
1:A:814:ARG:HH22	4:O:369:ASP:CG	1.93	0.77
25:m:39:ILE:HD11	25:m:84:TYR:HE1	1.49	0.77
29:k:35:MET:CB	30:l:84:PHE:HE2	1.97	0.77
1:A:1379:MET:CE	1:A:1620:TYR:CB	2.62	0.77
29:s:57:GLN:HB3	29:s:75:ILE:HG23	1.67	0.77
24:i:32:PHE:HD1	24:i:86:ASN:O	1.68	0.77
11:c:227:ILE:HD11	13:I:150:GLY:O	1.84	0.76
19:L:1101:C:H5'	19:L:1102:C:OP2	1.84	0.76
1:A:1972:ASP:HB2	28:e:41:ARG:HD3	1.65	0.76
12:d:329:LEU:HD23	20:v:642:GLU:HG3	1.67	0.76
19:L:1137:U:C2'	19:L:1138:G:H4'	2.15	0.76
28:e:59:LYS:CG	28:e:70:GLU:HG2	2.13	0.76
30:l:33:LEU:HD21	30:l:35:GLU:O	1.85	0.76
19:L:125:C:H5''	28:e:80:LYS:HA	1.67	0.76
29:s:54:PRO:HB2	29:s:57:GLN:CG	2.15	0.76
20:v:612:ILE:HG13	20:v:613:PRO:HD2	1.67	0.76
30:y:35:GLU:HB2	30:y:43:GLN:HG2	1.68	0.76
20:v:617:PRO:O	20:v:618:GLU:HB2	1.84	0.76
4:O:200:VAL:CG2	4:O:230:VAL:HG23	2.16	0.76
20:v:612:ILE:CG1	20:v:613:PRO:CD	2.55	0.76
25:m:86:ASN:HD21	29:k:41:MET:CE	1.99	0.76
12:d:70:ARG:NH1	18:E:88:U:H1'	2.02	0.75
26:j:61:THR:CG2	24:i:91:THR:HG23	2.16	0.75
1:A:1375:LEU:N	1:A:1375:LEU:HD23	2.01	0.75
24:i:30:TRP:CG	24:i:38:ARG:NE	2.54	0.75
6:Q:109:MET:HE2	6:Q:112:PHE:CD2	2.21	0.75
12:d:255:ALA:HB3	12:d:291:PHE:HE2	1.51	0.75
19:L:1114:G:H2'	19:L:1115:G:O4'	1.87	0.75
1:A:1992:TYR:HD2	1:A:1996:LEU:CG	1.96	0.75
1:A:2030:PRO:HG2	28:e:73:LYS:HB3	1.68	0.75
24:u:35:ILE:HD13	27:w:79:LEU:HD11	1.67	0.75
1:A:1379:MET:HE3	1:A:1620:TYR:CB	2.16	0.75
1:A:2021:SER:HA	1:A:2024:MET:SD	2.27	0.75
24:u:35:ILE:HD13	27:w:79:LEU:HD12	1.64	0.75
30:l:17:HIS:ND1	30:l:75:PRO:CG	2.50	0.75
30:y:31:GLY:HA3	30:y:47:VAL:HG12	1.68	0.75
25:m:41:THR:O	25:m:83:GLN:HG2	1.86	0.75
26:j:14:LYS:HG2	26:j:74:LEU:HD11	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:k:13:ALA:HB2	29:k:37:PHE:CZ	2.21	0.74
29:k:49:ILE:HD12	29:k:49:ILE:H	1.52	0.74
1:A:352:PHE:CE1	1:A:527:LYS:HG3	2.23	0.74
1:A:2027:LEU:HB3	28:e:71:ASN:CG	2.10	0.74
12:d:267:TYR:CD2	12:d:284:LEU:CD2	2.69	0.74
2:C:153:LEU:HD13	2:C:212:PHE:CZ	2.22	0.74
12:d:267:TYR:HE2	12:d:287:PHE:CD2	2.05	0.74
29:k:15:LEU:HB2	29:k:18:TYR:CD2	2.22	0.74
29:s:28:ARG:HD3	29:s:52:ARG:HE	1.51	0.74
25:z:23:THR:HG22	25:z:47:LEU:HD11	1.68	0.74
1:A:1972:ASP:HB3	28:e:41:ARG:HD3	1.68	0.74
27:w:32:LYS:HG3	27:w:33:PHE:HD1	1.53	0.74
16:B:260:G:H1	19:L:40:U:H3	1.35	0.74
19:L:1085:G:N3	19:L:1086:U:C5	2.55	0.74
1:A:503:LYS:HA	1:A:506:PHE:CE1	2.22	0.74
30:l:24:THR:HA	30:l:70:LYS:NZ	2.03	0.74
1:A:1093:LYS:HB3	1:A:1093:LYS:NZ	2.03	0.74
17:D:167:A:H2'	27:h:48:TYR:HE2	1.51	0.74
26:j:29:LEU:HD23	26:j:29:LEU:C	2.13	0.74
26:j:57:LEU:HB3	24:i:91:THR:CG2	2.11	0.74
28:e:59:LYS:HG2	28:e:70:GLU:CG	2.18	0.74
1:A:316:THR:CG2	1:A:317:PRO:CD	2.59	0.73
25:z:45:LEU:HD11	25:z:65:LEU:HD13	1.68	0.73
1:A:659:HIS:HE1	32:A:3000:IHP:O42	1.72	0.73
29:s:52:ARG:O	29:s:77:VAL:HG13	1.87	0.73
4:O:200:VAL:HG22	4:O:230:VAL:HG23	1.68	0.73
19:L:117:U:C2	25:z:35:GLN:HB3	2.21	0.73
19:L:1129:U:H2'	19:L:1130:U:H5'	1.71	0.73
1:A:1035:LEU:O	1:A:1035:LEU:HD12	1.87	0.73
26:j:23:ARG:H	26:j:23:ARG:HD3	1.52	0.73
16:B:9:U:H1'	16:B:10:A:OP2	1.88	0.73
1:A:2021:SER:HA	1:A:2024:MET:HB2	1.70	0.73
19:L:1105:C:H1'	19:L:1106:G:C1'	2.19	0.73
28:g:78:GLU:HG2	28:g:85:ILE:CG2	2.19	0.73
19:L:1137:U:C2'	19:L:1138:G:O4'	2.35	0.73
1:A:1990:ASN:HD21	1:A:1993:ASP:H	1.35	0.73
2:C:625:ILE:HG21	2:C:655:LEU:HD21	1.70	0.73
4:O:111:ILE:HG22	12:d:194:MET:O	1.88	0.73
30:l:24:THR:HA	30:l:70:LYS:HZ2	1.54	0.73
5:P:34:ILE:HD11	12:d:155:LEU:HD13	1.69	0.73
17:D:173:U:C2	28:g:97:ARG:CZ	2.72	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:m:82:LEU:HD11	25:m:85:ILE:HB	1.70	0.72
1:A:1961:LEU:HD23	1:A:2084:LEU:HB2	1.69	0.72
1:A:1991:ILE:HD12	1:A:1992:TYR:CE1	2.25	0.72
25:m:45:LEU:HD11	25:m:65:LEU:HD13	1.69	0.72
26:j:18:ASN:C	26:j:19:ILE:HD13	2.14	0.72
29:k:109:LEU:C	29:k:109:LEU:HD12	2.15	0.72
1:A:404:ASN:HB3	2:C:919:ARG:NH1	2.03	0.72
1:A:912:LEU:HD13	1:A:912:LEU:C	2.13	0.72
1:A:1025:VAL:HG22	1:A:1262:MET:CG	2.20	0.72
1:A:1035:LEU:HD12	1:A:1035:LEU:C	2.13	0.72
25:z:47:LEU:HD21	25:z:61:ALA:HB1	1.70	0.72
1:A:1393:GLU:C	1:A:1575:TRP:HE1	1.97	0.72
29:k:15:LEU:C	29:k:15:LEU:HD12	2.14	0.72
1:A:659:HIS:CE1	32:A:3000:IHP:O42	2.41	0.72
28:e:41:ARG:O	28:e:57:ARG:NH1	2.23	0.72
1:A:1343:PHE:CE2	1:A:1440:ILE:HD11	2.15	0.72
11:c:214:ASN:ND2	12:d:44:ARG:O	2.22	0.72
1:A:1527:TRP:CD2	1:A:1528:THR:HG23	2.25	0.72
2:C:187:ARG:NH2	2:C:654:CYS:SG	2.63	0.72
12:d:263:SER:CB	12:d:287:PHE:CZ	2.71	0.72
28:e:59:LYS:HG2	28:e:70:GLU:HG2	1.69	0.72
27:w:34:ASN:HB3	27:w:36:THR:HG23	1.72	0.72
28:g:50:ASN:HB3	28:g:52:HIS:HD1	1.53	0.72
29:k:109:LEU:HD12	29:k:109:LEU:O	1.90	0.72
24:i:30:TRP:CD2	24:i:38:ARG:NE	2.58	0.72
12:d:330:ILE:HA	12:d:334:PHE:HB2	1.70	0.71
20:v:608:TYR:O	20:v:612:ILE:HG23	1.90	0.71
24:u:35:ILE:CD1	27:w:79:LEU:HD11	2.20	0.71
27:h:34:ASN:HB3	27:h:36:THR:HG23	1.72	0.71
6:Q:102:GLU:OE2	12:d:82:ARG:NH2	2.24	0.71
12:d:267:TYR:OH	12:d:287:PHE:HB2	1.90	0.71
27:w:32:LYS:HG3	27:w:33:PHE:CE1	2.25	0.71
25:m:19:LEU:CD2	25:m:91:THR:HG22	2.16	0.71
30:l:70:LYS:HZ2	30:l:70:LYS:HB2	1.55	0.71
12:d:267:TYR:CE2	12:d:287:PHE:CD2	2.79	0.71
20:v:388:LEU:HA	20:v:391:LEU:HD12	1.72	0.71
28:g:33:LEU:C	28:g:33:LEU:HD12	2.15	0.71
28:g:50:ASN:CB	28:g:52:HIS:CE1	2.73	0.71
28:e:48:LEU:HD22	28:e:52:HIS:NE2	2.05	0.71
17:D:103:A:O2'	17:D:104:G:O5'	2.09	0.71
24:i:30:TRP:CD2	24:i:38:ARG:CZ	2.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2027:LEU:CD1	28:e:57:ARG:HH21	2.02	0.71
17:D:166:U:O2	28:g:63:ARG:NH1	2.23	0.71
25:m:47:LEU:HD11	25:m:61:ALA:HB3	1.73	0.71
1:A:1379:MET:CE	1:A:1620:TYR:N	2.31	0.71
5:P:143:VAL:HG11	12:d:124:ARG:HG3	1.72	0.71
15:H:91:ARG:NE	16:B:249:C:H5''	2.06	0.71
19:L:3:G:O2'	19:L:4:A:OP1	2.07	0.71
19:L:117:U:C5	25:z:88:ARG:NH1	2.59	0.71
20:v:365:ASP:HA	20:v:399:VAL:HG22	1.72	0.71
1:A:1993:ASP:OD2	1:A:2040:TRP:CG	2.44	0.71
27:h:68:LEU:HD23	27:h:71:ILE:HD11	1.73	0.71
30:l:65:ARG:HG3	30:l:65:ARG:NH1	1.99	0.71
25:m:3:LEU:HG	28:g:95:PHE:HE1	1.55	0.70
25:m:84:TYR:CD2	29:k:6:VAL:CG1	2.64	0.70
1:A:1889:LEU:CD2	1:A:1991:ILE:CG1	2.64	0.70
24:i:40:LYS:HG3	24:i:60:ILE:HD11	1.74	0.70
30:y:21:LEU:HD23	30:y:72:ILE:HG12	1.73	0.70
11:c:252:GLY:HA2	12:d:38:LEU:O	1.91	0.70
19:L:110:A:H61	25:z:35:GLN:CD	1.98	0.70
29:k:52:ARG:NH2	29:k:78:GLU:OE2	2.24	0.70
1:A:2032:ILE:HD11	1:A:2043:PHE:CD1	2.26	0.70
20:v:385:PHE:O	20:v:389:ILE:HD12	1.92	0.70
1:A:1992:TYR:HB3	1:A:1996:LEU:HB2	1.74	0.70
29:k:40:HIS:O	29:k:41:MET:CB	2.40	0.70
30:l:11:LEU:HD11	30:l:72:ILE:HD12	1.73	0.70
26:x:14:LYS:HG2	26:x:74:LEU:HD11	1.74	0.70
31:r:99:ARG:CG	31:o:98:LEU:HD11	2.12	0.70
11:c:181:ARG:NH2	12:d:49:ARG:NH1	2.40	0.70
28:g:105:LEU:C	28:g:105:LEU:HD12	2.16	0.70
29:k:31:ILE:HD11	29:k:49:ILE:HD11	0.73	0.70
20:v:388:LEU:HB3	20:v:392:TYR:OH	1.92	0.69
20:v:797:TYR:C	20:v:799:ASP:H	1.99	0.69
19:L:1146:G:H3'	19:L:1147:A:H5''	1.74	0.69
22:b:54:THR:HA	22:b:77:HIS:CB	2.22	0.69
25:z:39:ILE:HD11	25:z:84:TYR:HE1	1.56	0.69
25:m:20:LYS:HG2	25:m:91:THR:O	1.92	0.69
12:d:267:TYR:HE2	12:d:287:PHE:CB	2.06	0.69
27:w:68:LEU:HD23	27:w:71:ILE:HD11	1.73	0.69
4:O:331:ILE:HD11	4:O:353:ILE:CD1	2.23	0.69
19:L:1137:U:C2'	19:L:1138:G:C1'	2.53	0.69
25:m:3:LEU:CG	28:g:95:PHE:HE1	2.06	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:e:59:LYS:HD3	28:e:70:GLU:OE1	1.93	0.69
12:d:147:ASN:HD22	13:l:160:LEU:HD21	1.57	0.69
20:v:396:LEU:HD23	20:v:396:LEU:C	2.18	0.69
22:b:14:TYR:C	29:s:102:LEU:HD12	2.17	0.69
1:A:267:PRO:O	1:A:268:LEU:HB2	1.91	0.69
18:E:84:C:H3'	18:E:85:C:H5''	1.74	0.69
18:E:84:C:O2'	18:E:85:C:OP1	2.10	0.69
28:g:35:ASN:CA	28:g:61:PHE:CE2	2.72	0.69
29:k:82:LEU:HD13	29:k:85:THR:HG21	1.75	0.69
12:d:289:LYS:HE2	20:v:643:HIS:CE1	2.25	0.68
17:D:128:A:H3'	17:D:128:A:N3	2.07	0.68
30:l:82:PRO:O	30:l:85:LYS:CD	2.41	0.68
24:i:29:ILE:HG22	24:i:90:ILE:HA	1.76	0.68
24:i:30:TRP:CD1	24:i:38:ARG:CG	2.76	0.68
1:A:2024:MET:CA	28:e:71:ASN:HD21	2.05	0.68
12:d:284:LEU:HD13	12:d:284:LEU:C	2.18	0.68
20:v:530:ARG:CA	20:v:530:ARG:HH11	2.06	0.68
29:k:49:ILE:HG23	29:k:81:VAL:HA	1.75	0.68
4:O:370:ASN:O	4:O:372:VAL:N	2.21	0.68
6:Q:109:MET:HE2	6:Q:112:PHE:HB3	1.74	0.68
7:R:205:LEU:O	7:R:206:LEU:O	2.10	0.68
17:D:174:G:H3'	28:g:49:ARG:HH12	1.58	0.68
28:e:89:ARG:NH2	28:e:91:ILE:HD11	2.07	0.68
24:i:54:ILE:HG13	24:i:57:ALA:HB2	1.73	0.68
1:A:2027:LEU:HB2	28:e:71:ASN:OD1	1.93	0.68
16:B:8:C:H42	18:E:45:A:H61	1.40	0.68
1:A:404:ASN:HB3	2:C:919:ARG:CZ	2.23	0.68
17:D:141:G:OP2	17:D:142:C:H5	1.76	0.68
19:L:1118:U:H2'	19:L:1119:C:C6	2.28	0.68
2:C:168:VAL:HG11	2:C:175:LEU:HD12	1.75	0.68
4:O:206:VAL:HB	4:O:220:TYR:HB2	1.76	0.68
7:R:74:LEU:HD12	7:R:74:LEU:C	2.19	0.68
17:D:176:A:H1'	27:h:33:PHE:HE1	1.59	0.68
26:j:20:ASN:HD22	26:j:21:GLY:N	1.90	0.68
30:y:20:SER:HB2	30:y:73:VAL:HB	1.75	0.68
4:O:238:LEU:CD1	5:P:74:ILE:CD1	2.68	0.68
25:m:103:LEU:HD13	28:g:93:LYS:HD3	1.76	0.68
26:j:28:ILE:O	26:j:40:LEU:CB	2.33	0.68
29:s:50:GLU:OE2	29:s:80:ARG:NE	2.23	0.68
17:D:130:A:H5''	17:D:131:A:H3'	1.75	0.68
25:m:88:ARG:HH11	25:m:90:ASN:ND2	1.92	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ARG:HD3	1:A:252:GLU:HG2	1.75	0.68
2:C:175:LEU:HD23	2:C:175:LEU:C	2.19	0.68
19:L:1093:C:H6	19:L:1093:C:C5'	2.06	0.68
26:j:23:ARG:HD3	26:j:23:ARG:N	2.08	0.68
28:g:33:LEU:HD12	28:g:33:LEU:O	1.94	0.68
17:D:95:C:C1'	17:D:96:U:OP2	2.41	0.68
24:u:29:ILE:HG22	24:u:90:ILE:HA	1.75	0.68
28:g:50:ASN:ND2	28:g:52:HIS:CE1	2.54	0.68
1:A:1961:LEU:CD2	1:A:2084:LEU:HB2	2.24	0.67
28:e:49:ARG:NH2	27:w:76:ASN:OD1	2.27	0.67
28:e:93:LYS:HB3	25:z:97:LEU:HD11	1.76	0.67
1:A:854:ARG:HH21	1:A:1093:LYS:HG3	1.60	0.67
12:d:229:VAL:HG12	12:d:274:TRP:HZ2	1.60	0.67
19:L:114:U:O4'	26:x:64:ARG:NH1	2.26	0.67
19:L:1117:G:O2'	19:L:1118:U:H5'	1.94	0.67
25:m:86:ASN:HD21	29:k:41:MET:HE1	1.59	0.67
26:j:57:LEU:CB	24:i:91:THR:HG21	2.14	0.67
26:j:27:GLY:CA	26:j:40:LEU:CD1	2.69	0.67
30:l:70:LYS:NZ	30:l:70:LYS:HB2	2.07	0.67
1:A:770:MET:HG3	1:A:774:ILE:HG13	1.76	0.67
7:R:234:ALA:HA	7:R:237:ARG:HE	1.59	0.67
17:D:141:G:N3	17:D:141:G:H3'	2.10	0.67
19:L:125:C:OP1	25:z:55:LEU:HD11	1.94	0.67
19:L:1119:C:O5'	19:L:1119:C:H6	1.78	0.67
19:L:1125:U:H2'	19:L:1126:G:C8	2.30	0.67
29:k:50:GLU:HG3	29:k:50:GLU:O	1.94	0.67
29:k:52:ARG:HG2	29:k:52:ARG:HH11	1.60	0.67
29:s:28:ARG:HG2	29:s:52:ARG:HG2	1.75	0.67
7:R:159:ARG:NH1	7:R:206:LEU:CD1	2.57	0.67
12:d:267:TYR:CG	12:d:284:LEU:HD23	2.29	0.67
29:k:15:LEU:HB2	29:k:18:TYR:CE2	2.29	0.67
30:l:20:SER:OG	30:l:73:VAL:CG2	2.43	0.67
1:A:2033:THR:CG2	28:e:43:PRO:CG	2.64	0.67
19:L:52:A:H3'	19:L:53:G:H5''	1.76	0.67
19:L:1168:U:O5'	19:L:1168:U:H6	1.78	0.67
25:m:43:VAL:HG21	25:m:85:ILE:CG2	2.25	0.67
7:R:226:ALA:HA	16:B:13:G:N7	2.08	0.67
19:L:117:U:C5	25:z:88:ARG:CZ	2.78	0.67
19:L:1146:G:H2'	19:L:1147:A:N9	2.10	0.67
20:v:395:TYR:O	20:v:398:ASP:HB3	1.95	0.67
25:m:103:LEU:CD1	28:g:93:LYS:HD3	2.25	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:l:47:VAL:CG2	30:l:59:MET:HG3	2.19	0.67
25:m:21:ASN:HD21	29:k:93:LEU:HD11	1.60	0.66
29:s:82:LEU:HD13	29:s:85:THR:HG21	1.75	0.66
1:A:1573:LEU:HD12	1:A:1825:ILE:HG22	1.77	0.66
6:Q:248:CYS:SG	6:Q:316:LEU:HD11	2.34	0.66
12:d:241:MET:CG	12:d:279:LEU:HD11	2.17	0.66
24:i:40:LYS:CG	24:i:60:ILE:CD1	2.73	0.66
1:A:1999:ILE:HD11	1:A:2045:ASP:OD2	1.95	0.66
28:e:78:GLU:CG	25:z:52:LEU:HD22	2.25	0.66
4:O:197:LEU:HB3	4:O:209:TRP:HB2	1.76	0.66
25:m:17:ILE:CG2	25:m:92:ILE:HG23	2.26	0.66
29:s:44:VAL:HG22	29:s:86:ILE:HG22	1.77	0.66
17:D:168:U:C6	24:i:49:PHE:CE1	2.83	0.66
19:L:125:C:H4'	28:e:81:GLY:N	2.09	0.66
28:e:56:ALA:HB3	28:e:69:LEU:CD2	2.14	0.66
9:T:150:CYS:SG	9:T:151:ARG:N	2.68	0.66
20:v:711:MET:HE1	20:v:748:PHE:CA	2.26	0.66
22:b:32:ARG:HA	22:b:60:THR:O	1.96	0.66
30:l:21:LEU:HD22	30:l:69:ILE:HD13	1.77	0.66
25:z:45:LEU:HD11	25:z:65:LEU:CD1	2.26	0.66
1:A:2023:LYS:O	28:e:71:ASN:ND2	2.29	0.66
12:d:137:TYR:CD1	13:I:105:TYR:CD2	2.83	0.66
23:t:111:VAL:O	23:t:114:LEU:N	2.29	0.66
1:A:2013:ARG:NH1	1:A:2082:ILE:O	2.29	0.66
1:A:2024:MET:CE	28:e:93:LYS:CE	2.68	0.66
20:v:746:ILE:CB	20:v:771:LEU:CB	2.73	0.66
30:l:43:GLN:C	30:l:44:LEU:HD23	2.20	0.66
19:L:114:U:H1'	26:x:66:ASN:HB2	1.76	0.66
19:L:125:C:OP1	25:z:55:LEU:CD1	2.42	0.66
28:g:40:THR:C	28:g:41:ARG:CG	2.69	0.66
1:A:1260:PHE:HE1	1:A:1269:ILE:HD11	1.60	0.66
4:O:370:ASN:OD1	4:O:372:VAL:HB	1.95	0.66
19:L:1093:C:H6	19:L:1093:C:O5'	1.78	0.66
25:m:3:LEU:HG	28:g:95:PHE:CE1	2.31	0.66
29:s:93:LEU:HD11	25:z:21:ASN:HD21	1.60	0.66
4:O:309:ARG:NH1	4:O:309:ARG:HG3	2.11	0.65
1:A:996:ASP:OD2	1:A:1511:ARG:NH2	2.29	0.65
1:A:1987:VAL:HG12	1:A:1989:PHE:CE2	2.31	0.65
19:L:1129:U:H2'	19:L:1130:U:C5'	2.26	0.65
25:m:88:ARG:HH11	25:m:90:ASN:HD22	1.42	0.65
29:k:86:ILE:CG2	30:l:10:LEU:HD23	2.26	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:e:89:ARG:CZ	28:e:91:ILE:HD11	2.26	0.65
12:d:267:TYR:CE2	12:d:287:PHE:CB	2.79	0.65
18:E:22:G:H3'	18:E:23:G:C5'	2.18	0.65
19:L:121:C:H1'	28:e:49:ARG:CG	2.24	0.65
19:L:1150:U:OP1	29:s:55:LYS:HG3	1.95	0.65
25:m:43:VAL:HG21	25:m:85:ILE:HG21	1.78	0.65
24:i:58:VAL:HG12	24:i:76:PRO:HA	1.79	0.65
2:C:168:VAL:HG13	2:C:175:LEU:HB2	1.79	0.65
28:g:38:MET:HA	28:g:58:VAL:O	1.96	0.65
29:k:48:CYS:HG	29:k:82:LEU:HD12	1.60	0.65
28:e:93:LYS:HZ2	25:z:103:LEU:CD1	2.09	0.65
25:z:51:ARG:O	25:z:54:LYS:N	2.29	0.65
6:Q:109:MET:HE1	6:Q:112:PHE:HD2	1.59	0.65
2:C:251:GLN:HE21	2:C:255:GLN:HE21	1.44	0.65
28:g:50:ASN:HB3	28:g:52:HIS:CE1	2.32	0.65
9:T:151:ARG:NH2	14:n:71:SER:HB3	2.11	0.65
17:D:176:A:N3	27:h:33:PHE:HD1	1.94	0.65
19:L:1137:U:C4	21:a:67:LYS:O	2.50	0.65
27:h:71:ILE:HG23	28:g:103:VAL:CG2	2.25	0.65
1:A:2027:LEU:CB	28:e:71:ASN:CB	2.69	0.65
2:C:391:MET:HE2	2:C:395:LYS:HG3	1.79	0.65
13:I:209:ARG:NH1	19:L:15:C:N3	2.44	0.65
26:j:63:ILE:HG13	24:i:89:LEU:CD2	2.26	0.65
26:j:64:ARG:HH22	24:i:50:MET:CB	2.00	0.65
30:y:34:VAL:HG12	30:y:35:GLU:HG2	1.77	0.65
1:A:1379:MET:HE1	1:A:1620:TYR:CB	2.26	0.65
12:d:147:ASN:ND2	13:I:160:LEU:HD21	2.12	0.65
19:L:121:C:C1'	28:e:49:ARG:HG2	2.24	0.65
24:i:30:TRP:CE2	24:i:38:ARG:CZ	2.80	0.65
1:A:140:ARG:HD3	1:A:252:GLU:CG	2.26	0.64
12:d:334:PHE:N	12:d:335:PRO:CD	2.60	0.64
25:m:3:LEU:CD2	28:g:95:PHE:CE1	2.79	0.64
29:k:30:TYR:CD1	29:k:50:GLU:HB3	2.32	0.64
28:e:48:LEU:HD22	28:e:52:HIS:CE1	2.33	0.64
1:A:1093:LYS:O	19:L:25:A:N1	2.30	0.64
11:c:72:GLN:NE2	11:c:91:MET:SD	2.70	0.64
19:L:114:U:O2	26:x:64:ARG:HG2	1.97	0.64
22:b:110:ARG:CB	22:b:134:VAL:CB	2.74	0.64
29:s:88:ARG:NH1	30:y:40:MET:SD	2.70	0.64
25:z:45:LEU:CD1	25:z:65:LEU:HD13	2.26	0.64
17:D:131:A:H4'	17:D:132:A:OP2	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:e:93:LYS:HB3	25:z:97:LEU:CD1	2.27	0.64
1:A:705:GLN:HB3	1:A:706:PRO:HD3	1.78	0.64
12:d:270:ALA:CB	12:d:280:LEU:HD21	2.27	0.64
25:m:45:LEU:CD1	25:m:65:LEU:HD13	2.27	0.64
26:j:11:MET:O	26:j:12:ASP:HB2	1.97	0.64
24:i:32:PHE:CD1	24:i:86:ASN:O	2.50	0.64
27:w:32:LYS:CG	27:w:33:PHE:CE1	2.81	0.64
12:d:284:LEU:HD13	12:d:285:LEU:N	2.12	0.64
1:A:2027:LEU:HD11	28:e:57:ARG:HH21	1.61	0.64
1:A:697:LYS:CE	32:A:3000:IHP:O45	2.46	0.64
1:A:2027:LEU:C	28:e:71:ASN:HB3	2.22	0.64
19:L:1105:C:H1'	19:L:1106:G:H1'	1.78	0.64
25:m:15:VAL:HG23	25:m:96:ILE:O	1.96	0.64
25:m:45:LEU:HD11	25:m:65:LEU:CD1	2.27	0.64
29:k:60:LYS:HD2	29:k:75:ILE:HD13	1.78	0.64
29:k:84:LEU:HG	30:l:74:VAL:HG23	1.80	0.64
1:A:342:LEU:HD13	1:A:392:ASN:HD21	1.62	0.64
1:A:1379:MET:HE1	1:A:1620:TYR:CA	2.28	0.64
22:b:110:ARG:N	22:b:134:VAL:CB	2.60	0.64
19:L:1086:U:O5'	19:L:1086:U:H6	1.81	0.64
5:P:76:ARG:HE	6:Q:5:ILE:HD12	1.62	0.64
12:d:303:TYR:CD1	12:d:334:PHE:HZ	2.16	0.64
17:D:6:G:H4'	29:k:11:ARG:NH2	2.12	0.64
17:D:81:A:OP1	17:D:81:A:H2'	1.97	0.64
17:D:130:A:H5'	17:D:132:A:H5'	1.80	0.64
4:O:327:CYS:SG	4:O:328:THR:N	2.71	0.63
26:j:69:ILE:HA	30:l:68:GLN:HG3	1.80	0.63
28:e:93:LYS:HD2	25:z:97:LEU:CD1	2.27	0.63
2:C:187:ARG:NH1	2:C:653:ASP:OD2	2.31	0.63
19:L:141:A:C2	19:L:1168:U:O2	2.51	0.63
25:m:67:LEU:HB3	29:k:29:VAL:HG21	1.80	0.63
1:A:1032:ILE:O	1:A:1035:LEU:HG	1.97	0.63
4:O:200:VAL:HG21	4:O:230:VAL:CG2	2.27	0.63
29:k:28:ARG:HG2	29:k:52:ARG:HG2	1.81	0.63
1:A:1896:THR:HA	1:A:1899:TRP:HD1	1.63	0.63
6:Q:206:PHE:HD2	6:Q:291:ILE:HD11	1.63	0.63
26:j:63:ILE:HG13	24:i:89:LEU:HD23	1.79	0.63
4:O:239:ILE:HG13	4:O:251:TRP:HB2	1.81	0.63
17:D:167:A:H3'	27:h:48:TYR:OH	1.98	0.63
25:m:83:GLN:NE2	25:m:84:TYR:HB2	2.13	0.63
1:A:1991:ILE:HD12	1:A:1992:TYR:HE1	1.62	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:152:LYS:HB3	7:R:155:GLN:H	1.62	0.63
12:d:270:ALA:HB3	12:d:280:LEU:HD21	1.80	0.63
24:u:58:VAL:HG12	24:u:76:PRO:HA	1.79	0.63
25:m:89:GLY:O	25:m:92:ILE:HG13	1.99	0.63
29:s:29:VAL:HG21	25:z:67:LEU:HB3	1.80	0.63
19:L:4:A:H2'	19:L:5:A:H8	1.63	0.63
29:k:11:ARG:O	29:k:14:ASN:N	2.31	0.63
30:l:17:HIS:O	30:l:19:VAL:HG13	1.98	0.63
2:C:607:LEU:HD12	2:C:607:LEU:O	1.98	0.63
25:m:17:ILE:HG23	25:m:92:ILE:HG21	1.76	0.63
24:i:30:TRP:CD1	24:i:38:ARG:NE	2.66	0.63
26:x:27:GLY:HA3	26:x:40:LEU:HD13	1.80	0.63
1:A:1889:LEU:HB2	1:A:1989:PHE:O	1.98	0.62
2:C:804:LYS:HD3	2:C:805:GLU:HG3	1.80	0.62
17:D:174:G:C3'	28:g:49:ARG:HH12	2.12	0.62
18:E:49:A:HO2'	18:E:50:G:P	2.20	0.62
29:k:13:ALA:HA	29:k:37:PHE:HE2	1.64	0.62
10:Z:101:MET:O	10:Z:105:GLN:NE2	2.33	0.62
17:D:141:G:N3	17:D:141:G:H5''	2.14	0.62
26:j:63:ILE:HG21	26:j:68:ILE:HD11	1.80	0.62
29:k:105:LYS:HA	29:k:108:ARG:CZ	2.30	0.62
1:A:404:ASN:HB3	2:C:919:ARG:NH2	2.14	0.62
19:L:1090:A:O2'	19:L:1091:G:H5'	2.00	0.62
25:m:86:ASN:ND2	29:k:41:MET:HE1	2.15	0.62
25:m:93:ARG:HG3	25:m:93:ARG:NH1	2.14	0.62
28:g:76:TRP:CZ2	28:g:87:ARG:CD	2.79	0.62
30:l:77:LEU:HD23	30:l:77:LEU:H	1.64	0.62
1:A:1990:ASN:HD21	1:A:1993:ASP:N	1.98	0.62
20:v:612:ILE:N	20:v:613:PRO:HD2	2.15	0.62
26:j:64:ARG:NH2	24:i:50:MET:CB	2.47	0.62
29:s:54:PRO:HG2	29:s:76:LYS:O	1.98	0.62
1:A:687:ILE:HD11	1:A:706:PRO:HG2	1.81	0.62
1:A:1379:MET:CE	1:A:1620:TYR:HB3	2.30	0.62
26:j:19:ILE:CG2	24:i:88:THR:HG23	2.29	0.62
28:g:38:MET:SD	28:g:60:ALA:HA	2.38	0.62
1:A:426:PRO:HG3	10:Z:201:ARG:HH11	1.64	0.62
1:A:518:VAL:O	1:A:521:SER:N	2.32	0.62
1:A:518:VAL:HG11	1:A:689:TYR:CD2	2.35	0.62
1:A:2024:MET:HA	28:e:71:ASN:ND2	2.15	0.62
11:c:218:VAL:HG12	11:c:219:TYR:CE2	2.35	0.62
20:v:385:PHE:O	20:v:388:LEU:HB2	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:115:U:C2	30:y:39:SER:OG	2.53	0.61
20:v:322:CYS:O	20:v:326:LEU:N	2.28	0.61
20:v:580:LEU:HB3	20:v:582:LEU:HD23	1.82	0.61
28:g:78:GLU:CD	28:g:85:ILE:HG23	2.25	0.61
1:A:1286:TRP:HB2	1:A:1300:ALA:HB3	1.82	0.61
19:L:1154:U:H2'	19:L:1155:C:H6	1.63	0.61
2:C:866:ILE:HB	2:C:902:VAL:HB	1.81	0.61
17:D:173:U:O2	28:g:97:ARG:NE	2.32	0.61
29:s:42:ASN:HB3	29:s:89:GLY:H	1.65	0.61
24:i:30:TRP:HA	24:i:38:ARG:HG3	1.82	0.61
2:C:139:ILE:HD12	2:C:252:LEU:HD22	1.82	0.61
30:l:41:ASN:HB3	30:l:66:GLY:H	1.65	0.61
2:C:498:THR:HG22	2:C:538:GLU:HG2	1.82	0.61
20:v:582:LEU:HD12	20:v:582:LEU:O	2.00	0.61
22:b:65:ILE:HA	22:b:85:ASN:O	2.01	0.61
1:A:319:ARG:NH1	1:A:321:GLU:OE2	2.33	0.61
1:A:1197:ASN:ND2	1:A:1221:ASN:OD1	2.34	0.61
1:A:1343:PHE:HD2	1:A:1440:ILE:CG1	2.10	0.61
4:O:102:PHE:CZ	12:d:224:LEU:HD21	2.36	0.61
4:O:238:LEU:CD1	5:P:74:ILE:HD11	2.31	0.61
17:D:173:U:C2	28:g:97:ARG:NH1	2.68	0.61
29:k:13:ALA:CA	29:k:37:PHE:CZ	2.83	0.61
30:l:13:GLU:OE1	30:l:13:GLU:HA	2.01	0.61
4:O:231:SER:HG	4:O:274:CYS:HG	1.47	0.61
4:O:309:ARG:HH11	4:O:309:ARG:CG	2.14	0.61
19:L:119:G:H2'	19:L:120:G:H5'	1.82	0.61
19:L:1137:U:C5	21:a:67:LYS:O	2.54	0.61
20:v:396:LEU:HD23	20:v:396:LEU:O	1.99	0.61
30:l:39:SER:O	30:l:40:MET:HB3	2.01	0.61
4:O:309:ARG:HG3	4:O:309:ARG:HH11	1.65	0.61
11:c:181:ARG:NE	12:d:49:ARG:NH1	2.49	0.61
19:L:1083:A:H2'	19:L:1084:A:H8	1.65	0.61
28:g:62:ASP:OD1	28:g:63:ARG:N	2.26	0.61
29:k:13:ALA:HA	29:k:37:PHE:CZ	2.34	0.61
1:A:255:ILE:HG23	1:A:640:ARG:HG2	1.83	0.61
12:d:267:TYR:HE2	12:d:287:PHE:CG	2.18	0.61
19:L:1095:U:H2'	19:L:1096:C:C6	2.35	0.61
1:A:1283:GLU:HB3	10:Z:341:LYS:HB2	1.83	0.61
1:A:1393:GLU:O	1:A:1575:TRP:NE1	2.34	0.61
1:A:2040:TRP:HA	1:A:2040:TRP:CE3	2.36	0.61
1:A:2047:GLN:O	1:A:2051:ILE:N	2.31	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:133:ILE:HG22	2:C:209:MET:HB3	1.83	0.61
1:A:1527:TRP:CD2	1:A:1528:THR:CG2	2.84	0.60
19:L:117:U:C6	25:z:88:ARG:NH1	2.69	0.60
19:L:126:A:P	28:e:80:LYS:CB	2.89	0.60
29:k:43:LEU:CD1	29:k:87:LEU:HD22	2.31	0.60
29:k:105:LYS:O	29:k:108:ARG:HG2	2.01	0.60
18:E:49:A:O2'	18:E:50:G:P	2.58	0.60
20:v:387:SER:O	20:v:391:LEU:HG	2.01	0.60
30:l:42:VAL:HG22	30:l:64:VAL:HG22	1.83	0.60
1:A:312:TYR:O	1:A:319:ARG:NH2	2.32	0.60
1:A:745:THR:HG21	4:O:203:ASP:HB2	1.82	0.60
19:L:1125:U:H2'	19:L:1126:G:H8	1.64	0.60
2:C:99:LYS:NZ	17:D:43:G:OP2	2.33	0.60
19:L:1085:G:N3	19:L:1085:G:H2'	2.16	0.60
28:e:62:ASP:OD1	28:e:63:ARG:N	2.32	0.60
1:A:1992:TYR:HB3	1:A:1996:LEU:CB	2.31	0.60
19:L:35:U:O5'	19:L:35:U:H6	1.85	0.60
25:m:67:LEU:HD11	29:k:53:VAL:HG23	1.82	0.60
1:A:1011:ASN:O	1:A:1014:LYS:HE3	2.02	0.60
1:A:1990:ASN:ND2	1:A:1993:ASP:N	2.48	0.60
19:L:1107:C:H2'	19:L:1108:A:OP2	2.00	0.60
4:O:309:ARG:NH1	4:O:328:THR:CG2	2.61	0.60
19:L:1106:G:H4'	19:L:1107:C:OP1	2.00	0.60
25:m:52:LEU:O	25:m:52:LEU:HD12	2.01	0.60
1:A:661:GLY:O	1:A:667:TYR:HE1	1.85	0.60
4:O:186:ARG:NH1	4:O:202:GLU:OE2	2.34	0.60
25:m:41:THR:O	25:m:83:GLN:HA	2.02	0.60
13:I:190:TYR:O	13:I:201:LYS:NZ	2.35	0.60
16:B:2:U:HO2'	16:B:3:A:P	2.21	0.60
20:v:680:ILE:O	20:v:680:ILE:HG22	2.00	0.60
26:j:20:ASN:OD1	24:i:32:PHE:CE2	2.55	0.60
6:Q:105:LYS:HD3	11:c:215:GLU:CG	2.31	0.60
6:Q:213:SER:O	6:Q:214:ILE:HG22	2.02	0.60
1:A:1800:ASN:OD1	1:A:1803:ARG:NH2	2.34	0.59
12:d:342:PHE:O	12:d:346:ILE:N	2.31	0.59
20:v:530:ARG:NH1	20:v:530:ARG:HB2	2.17	0.59
20:v:797:TYR:O	20:v:799:ASP:N	2.34	0.59
30:l:20:SER:OG	30:l:73:VAL:HG23	2.01	0.59
6:Q:109:MET:HG2	11:c:218:VAL:O	2.02	0.59
19:L:69:G:H1	19:L:83:U:H3	1.49	0.59
19:L:1117:G:C2'	19:L:1118:U:H5'	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:ARG:HH22	19:L:25:A:H5''	1.66	0.59
1:A:2023:LYS:O	1:A:2027:LEU:HB2	2.03	0.59
5:P:196:THR:HA	11:c:90:MET:HE1	1.85	0.59
28:e:46:ILE:HD12	28:e:54:ILE:HD11	1.84	0.59
29:s:12:LEU:HD12	29:s:15:LEU:HD11	1.84	0.59
1:A:372:ARG:HB3	2:C:973:ARG:HH11	1.67	0.59
2:C:231:ALA:O	2:C:487:ARG:NH1	2.35	0.59
7:R:10:LYS:NZ	7:R:57:LEU:O	2.36	0.59
7:R:145:ALA:HB2	7:R:221:LEU:HB3	1.84	0.59
25:m:39:ILE:CD1	25:m:84:TYR:CE1	2.85	0.59
1:A:1527:TRP:CZ3	1:A:1528:THR:CG2	2.85	0.59
6:Q:251:LEU:HG	6:Q:251:LEU:O	2.02	0.59
18:E:53:A:C5'	18:E:53:A:H8	2.15	0.59
24:u:35:ILE:HD11	27:w:79:LEU:HD13	1.82	0.59
4:O:236:LEU:HD11	5:P:74:ILE:HD12	1.85	0.59
19:L:1142:G:C2'	19:L:1143:C:H5'	2.32	0.59
27:h:33:PHE:CZ	28:g:49:ARG:CD	2.86	0.59
28:e:78:GLU:HG2	25:z:52:LEU:HD22	1.85	0.59
28:g:46:ILE:HD12	28:g:54:ILE:HD11	1.84	0.59
24:i:40:LYS:CD	24:i:60:ILE:HD13	2.32	0.59
1:A:1296:ARG:NH1	10:Z:430:GLU:OE2	2.35	0.59
1:A:2043:PHE:HE2	1:A:2047:GLN:H	1.50	0.59
2:C:220:ASN:HB3	2:C:651:TYR:HB2	1.84	0.59
17:D:167:A:O4'	28:g:64:HIS:NE2	2.25	0.59
19:L:1142:G:H2'	19:L:1143:C:H5'	1.84	0.59
25:m:16:THR:OG1	25:m:96:ILE:HB	2.03	0.59
29:k:43:LEU:HD11	29:k:87:LEU:HD22	1.85	0.59
30:l:17:HIS:HE1	30:l:77:LEU:HD11	1.66	0.59
26:j:6:GLU:OE2	30:l:35:GLU:HB3	2.03	0.59
1:A:724:ARG:HH21	1:A:725:TYR:HE1	1.50	0.59
6:Q:109:MET:CG	11:c:218:VAL:O	2.51	0.59
6:Q:213:SER:C	6:Q:214:ILE:HG22	2.28	0.59
12:d:284:LEU:HD22	12:d:284:LEU:C	2.28	0.59
17:D:167:A:C5	27:h:48:TYR:CE1	2.91	0.59
2:C:269:LYS:HG2	33:C:1500:GTP:C6	2.38	0.58
6:Q:212:ALA:O	7:R:237:ARG:NH1	2.34	0.58
16:B:9:U:C1'	16:B:10:A:OP2	2.51	0.58
19:L:113:U:O4	27:w:47:ASN:O	2.21	0.58
19:L:1107:C:C2'	19:L:1108:A:OP2	2.51	0.58
19:L:1146:G:C2'	19:L:1147:A:C8	2.85	0.58
25:m:18:GLU:OE1	25:m:94:GLN:OE1	2.20	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:g:50:ASN:O	28:g:51:ASN:HB3	2.03	0.58
28:e:73:LYS:NZ	28:e:75:LEU:HD21	2.17	0.58
28:e:91:ILE:HD13	25:z:96:ILE:HD11	1.84	0.58
1:A:1092:PHE:HB3	1:A:1095:MET:HG3	1.83	0.58
28:g:37:ALA:HB1	28:g:44:VAL:HG11	1.83	0.58
28:g:105:LEU:HD12	28:g:105:LEU:O	2.04	0.58
29:k:52:ARG:HH11	29:k:52:ARG:CG	2.15	0.58
26:j:61:THR:HG22	24:i:91:THR:CG2	2.31	0.58
1:A:484:PHE:CD1	1:A:485:PRO:HB3	2.38	0.58
4:O:259:VAL:HG12	4:O:260:ILE:HG13	1.85	0.58
17:D:128:A:O2'	17:D:129:G:C8	2.56	0.58
17:D:141:G:OP2	17:D:142:C:C5	2.56	0.58
1:A:1192:ASP:OD2	1:A:1197:ASN:ND2	2.36	0.58
1:A:1275:MET:C	1:A:1276:GLU:HG3	2.27	0.58
1:A:1852:VAL:HB	1:A:1935:VAL:HG22	1.85	0.58
4:O:111:ILE:HG21	12:d:197:PRO:HD3	1.85	0.58
19:L:1093:C:C5'	19:L:1093:C:C6	2.85	0.58
26:j:23:ARG:HH21	26:j:23:ARG:HB2	1.68	0.58
30:l:11:LEU:CD1	30:l:72:ILE:HD12	2.33	0.58
25:z:16:THR:OG1	25:z:96:ILE:HB	2.03	0.58
1:A:1201:TYR:OH	1:A:1248:VAL:O	2.21	0.58
11:c:227:ILE:O	11:c:227:ILE:HD12	2.02	0.58
19:L:4:A:OP1	20:v:530:ARG:NH2	2.37	0.58
4:O:105:GLU:HG2	4:O:106:VAL:HG23	1.86	0.58
5:P:135:VAL:HG21	11:c:219:TYR:HE1	1.68	0.58
10:Z:10:ASP:OD2	10:Z:244:LYS:NZ	2.36	0.58
1:A:168:LEU:N	1:A:169:PRO:CD	2.66	0.58
1:A:1092:PHE:CE2	1:A:1093:LYS:CD	2.86	0.58
1:A:2023:LYS:O	28:e:71:ASN:OD1	2.21	0.58
1:A:2035:LYS:HB2	1:A:2038:HIS:HB2	1.85	0.58
2:C:634:ILE:HG12	2:C:644:ILE:HG12	1.83	0.58
4:O:145:VAL:HG22	4:O:157:THR:HG22	1.86	0.58
11:c:237:ILE:HD11	12:d:114:CYS:SG	2.43	0.58
20:v:323:GLY:O	20:v:327:LYS:N	2.29	0.58
25:m:17:ILE:HG21	25:m:92:ILE:CG2	2.33	0.58
2:C:270:LEU:HD11	2:C:313:PHE:HB3	1.86	0.58
4:O:414:LEU:HB3	4:O:426:TRP:HB2	1.86	0.58
6:Q:109:MET:HE2	6:Q:112:PHE:HD2	1.62	0.58
19:L:1118:U:O2'	19:L:1119:C:H5'	2.04	0.58
28:g:40:THR:O	28:g:40:THR:HG22	2.04	0.58
1:A:404:ASN:HB3	2:C:919:ARG:HH12	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1093:LYS:HB3	1:A:1093:LYS:HZ3	1.67	0.57
1:A:1921:VAL:O	1:A:1929:GLN:NE2	2.36	0.57
7:R:63:ARG:HD3	9:T:143:HIS:HD2	1.66	0.57
25:m:52:LEU:HD12	25:m:52:LEU:C	2.28	0.57
25:m:82:LEU:C	25:m:82:LEU:HD12	2.29	0.57
1:A:1210:ASP:OD1	1:A:1214:ARG:NH2	2.38	0.57
2:C:153:LEU:CD1	2:C:212:PHE:CZ	2.87	0.57
12:d:303:TYR:HD1	12:d:334:PHE:HZ	1.50	0.57
12:d:330:ILE:CG2	12:d:339:MET:HA	2.34	0.57
16:B:275:G:N3	16:B:275:G:H2'	2.19	0.57
29:k:15:LEU:HD12	29:k:15:LEU:O	2.03	0.57
1:A:493:MET:N	1:A:493:MET:SD	2.78	0.57
2:C:788:LEU:HD11	2:C:823:ILE:HG21	1.85	0.57
17:D:95:C:O2'	17:D:96:U:OP2	2.21	0.57
25:m:84:TYR:HD2	29:k:6:VAL:HG21	1.68	0.57
24:i:30:TRP:CE3	24:i:38:ARG:NH2	2.72	0.57
1:A:1855:THR:HG22	1:A:1937:ARG:HH21	1.69	0.57
17:D:173:U:O2'	27:h:74:ARG:NH2	2.37	0.57
4:O:121:GLN:NE2	5:P:49:SER:O	2.36	0.57
19:L:1137:U:O2'	19:L:1138:G:C4'	2.43	0.57
20:v:690:GLY:HA3	20:v:710:ARG:HE	1.68	0.57
25:m:52:LEU:HD21	28:g:79:LYS:CA	2.34	0.57
29:s:91:GLN:HG3	30:y:70:LYS:HG3	1.87	0.57
1:A:1014:LYS:NZ	1:A:1019:GLU:OE2	2.37	0.57
4:O:292:LEU:HD12	4:O:302:LYS:HB3	1.86	0.57
7:R:229:ASP:O	7:R:235:GLN:NE2	2.35	0.57
18:E:53:A:H8	18:E:53:A:H5''	1.68	0.57
1:A:742:VAL:HB	4:O:224:LEU:HD23	1.87	0.57
1:A:1843:LEU:HA	1:A:1849:LYS:HZ3	1.69	0.57
1:A:1987:VAL:HG12	1:A:1989:PHE:CD2	2.39	0.57
4:O:391:GLU:OE2	4:O:400:ARG:NH1	2.38	0.57
12:d:70:ARG:HH11	18:E:88:U:H1'	1.69	0.57
28:g:46:ILE:HG12	28:g:104:VAL:HG22	1.87	0.57
28:e:56:ALA:HB2	28:e:72:VAL:CB	2.32	0.57
29:s:29:VAL:O	29:s:50:GLU:HA	2.05	0.57
2:C:67:GLU:HG2	2:C:68:HIS:ND1	2.19	0.57
4:O:331:ILE:HD11	4:O:353:ILE:HD13	1.85	0.57
11:c:21:LEU:HD22	11:c:56:LEU:HD22	1.86	0.57
11:c:229:ASP:HB2	13:I:151:LYS:HB3	1.87	0.57
12:d:142:VAL:HG13	13:I:164:LEU:HD21	1.87	0.57
17:D:95:C:C2'	17:D:96:U:OP2	2.52	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:m:90:ASN:OD1	25:m:91:THR:N	2.38	0.57
30:l:44:LEU:HD12	30:l:47:VAL:CG1	2.35	0.57
22:b:14:TYR:C	29:s:102:LEU:CD1	2.76	0.57
28:e:46:ILE:HG12	28:e:104:VAL:HG22	1.86	0.57
1:A:1914:ALA:HA	1:A:1944:LEU:HD23	1.87	0.57
2:C:94:VAL:HG21	8:S:41:LYS:HB2	1.85	0.57
17:D:147:C:H2'	17:D:148:G:H8	1.70	0.57
26:j:16:LEU:HD22	26:j:72:GLU:OE2	2.05	0.57
29:k:30:TYR:HD1	29:k:50:GLU:HB3	1.69	0.57
29:k:49:ILE:CG2	29:k:81:VAL:CB	2.83	0.57
4:O:280:GLN:NE2	5:P:66:CYS:SG	2.77	0.56
7:R:196:LYS:NZ	18:E:38:U:O2	2.36	0.56
12:d:289:LYS:CG	20:v:609:GLU:HG2	2.32	0.56
19:L:1106:G:H5'	19:L:1107:C:OP1	2.05	0.56
27:h:58:GLU:O	27:h:65:HIS:N	2.38	0.56
9:T:3:ARG:NH2	9:T:85:LYS:O	2.39	0.56
11:c:513:ILE:O	11:c:517:VAL:N	2.38	0.56
18:E:64:U:O2'	18:E:65:U:P	2.63	0.56
19:L:4:A:P	19:L:4:A:H8	2.28	0.56
19:L:110:A:H61	25:z:35:GLN:HE21	1.50	0.56
20:v:530:ARG:HB2	20:v:530:ARG:CZ	2.34	0.56
20:v:610:LYS:O	20:v:613:PRO:HG2	2.05	0.56
1:A:194:HIS:CD2	5:P:122:LEU:HD22	2.40	0.56
1:A:1214:ARG:HE	2:C:981:PHE:HB2	1.71	0.56
2:C:780:PRO:HA	2:C:783:ILE:HB	1.87	0.56
6:Q:299:ALA:O	6:Q:300:ALA:HB3	2.05	0.56
29:k:11:ARG:H	29:k:14:ASN:HB2	1.69	0.56
28:e:68:VAL:O	28:e:69:LEU:HD12	2.06	0.56
29:s:53:VAL:HG23	25:z:67:LEU:HD11	1.86	0.56
26:x:47:ASN:OD1	26:x:48:GLY:N	2.31	0.56
2:C:168:VAL:CG1	2:C:175:LEU:HB2	2.35	0.56
4:O:285:SER:OG	4:O:287:ASP:OD1	2.22	0.56
10:Z:148:LEU:HB2	10:Z:190:LEU:HD11	1.88	0.56
20:v:349:PHE:O	20:v:353:CYS:N	2.37	0.56
30:l:17:HIS:HB3	30:l:75:PRO:CG	2.35	0.56
5:P:30:LEU:HD21	12:d:151:ILE:HG12	1.87	0.56
9:T:118:SER:HB3	18:E:28:U:H5''	1.88	0.56
22:b:14:TYR:O	29:s:102:LEU:HD13	2.03	0.56
1:A:484:PHE:CG	1:A:485:PRO:HA	2.40	0.56
1:A:1328:PHE:HE2	1:A:1375:LEU:HD21	1.71	0.56
18:E:88:U:O2'	19:L:17:U:OP2	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:g:38:MET:HB2	28:g:58:VAL:HG12	1.88	0.56
29:k:35:MET:HE2	29:k:46:ASN:HB2	1.87	0.56
29:k:86:ILE:CD1	30:l:11:LEU:CD1	2.78	0.56
28:e:54:ILE:HD13	28:e:72:VAL:HG21	1.88	0.56
2:C:573:LYS:NZ	2:C:630:PRO:O	2.33	0.56
2:C:644:ILE:HG21	2:C:655:LEU:CD1	2.36	0.56
5:P:29:ILE:HG23	5:P:30:LEU:HD23	1.87	0.56
12:d:267:TYR:CE2	12:d:287:PHE:CG	2.94	0.56
19:L:125:C:H5''	28:e:80:LYS:CA	2.34	0.56
20:v:392:TYR:HA	20:v:395:TYR:HD2	1.70	0.56
26:j:19:ILE:HD12	26:j:68:ILE:HD13	1.87	0.56
24:i:40:LYS:CG	24:i:60:ILE:HD13	2.36	0.56
1:A:2023:LYS:O	28:e:71:ASN:CG	2.49	0.56
5:P:170:SER:OG	5:P:173:LYS:O	2.24	0.56
27:w:58:GLU:O	27:w:65:HIS:N	2.38	0.56
26:x:7:LEU:HD23	26:x:29:LEU:HD11	1.87	0.56
1:A:1440:ILE:O	1:A:1443:TYR:N	2.37	0.56
16:B:264:U:HO2'	16:B:265:A:P	2.28	0.56
30:l:10:LEU:HD12	30:l:10:LEU:O	2.04	0.56
24:i:30:TRP:CG	24:i:38:ARG:HE	2.24	0.56
25:z:23:THR:HG22	25:z:47:LEU:CD1	2.34	0.56
1:A:265:ASN:OD1	9:T:7:ARG:NH2	2.36	0.56
6:Q:270:LEU:HD12	6:Q:289:PHE:HE1	1.71	0.56
17:D:26:A:N7	17:D:141:G:C8	2.73	0.56
20:v:530:ARG:HH11	20:v:530:ARG:HA	1.70	0.56
26:j:14:LYS:CG	26:j:74:LEU:HD11	2.34	0.56
28:g:78:GLU:HG2	28:g:85:ILE:HG22	1.88	0.56
28:g:102:ILE:HG13	28:g:103:VAL:H	1.70	0.56
30:l:21:LEU:CD2	30:l:69:ILE:HD13	2.36	0.55
1:A:1748:ILE:HD13	1:A:1785:ASP:HB2	1.88	0.55
20:v:542:LEU:HD23	20:v:582:LEU:HD12	1.88	0.55
25:z:39:ILE:HD11	25:z:84:TYR:CE1	2.40	0.55
17:D:130:A:H4'	17:D:131:A:O5'	2.04	0.55
26:j:19:ILE:HG21	24:i:88:THR:HG23	1.88	0.55
29:k:49:ILE:HD12	29:k:49:ILE:N	2.16	0.55
28:e:93:LYS:NZ	25:z:103:LEU:HD13	2.21	0.55
1:A:416:GLU:HB3	1:A:419:THR:HG23	1.87	0.55
2:C:232:SER:OG	2:C:234:LEU:O	2.24	0.55
4:O:332:ARG:HG2	4:O:344:ASN:HD22	1.71	0.55
6:Q:194:GLU:O	6:Q:291:ILE:HG21	2.05	0.55
19:L:116:U:N3	29:s:40:HIS:CD2	2.74	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:v:385:PHE:N	20:v:385:PHE:CD1	2.73	0.55
1:A:305:LEU:N	1:A:306:PRO:CD	2.70	0.55
1:A:2040:TRP:HA	1:A:2040:TRP:HE3	1.71	0.55
19:L:1129:U:C2'	19:L:1130:U:C5'	2.85	0.55
20:v:386:GLU:HA	20:v:389:ILE:HD13	1.84	0.55
28:g:35:ASN:CB	28:g:61:PHE:CE2	2.81	0.55
28:e:56:ALA:CA	28:e:72:VAL:HG23	2.36	0.55
28:e:97:ARG:NH2	25:z:36:MET:SD	2.79	0.55
28:e:102:ILE:HG13	28:e:103:VAL:H	1.70	0.55
4:O:182:VAL:HG23	4:O:183:MET:HG3	1.89	0.55
7:R:69:GLN:HG2	7:R:89:TYR:HA	1.88	0.55
10:Z:39:GLU:OE2	10:Z:42:ARG:NH1	2.39	0.55
10:Z:63:PHE:O	10:Z:69:ASN:ND2	2.33	0.55
28:g:37:ALA:CB	28:g:44:VAL:HG11	2.37	0.55
28:e:56:ALA:HB1	28:e:69:LEU:HB3	1.88	0.55
28:e:73:LYS:HG3	28:e:90:PHE:CD2	2.41	0.55
24:i:30:TRP:O	24:i:88:THR:HB	2.07	0.55
1:A:988:GLU:OE1	1:A:1085:LYS:NZ	2.39	0.55
1:A:1889:LEU:HG	1:A:1991:ILE:HG12	1.89	0.55
1:A:2056:ARG:O	1:A:2060:LEU:N	2.35	0.55
19:L:120:G:H4'	19:L:121:C:O5'	2.06	0.55
15:H:88:GLU:HA	15:H:91:ARG:HG3	1.89	0.55
19:L:152:C:N4	19:L:1085:G:H1	1.97	0.55
29:k:49:ILE:HG23	29:k:81:VAL:HG23	1.88	0.55
1:A:1443:TYR:CE2	1:A:1542:TYR:HA	2.42	0.55
2:C:181:LEU:HB2	2:C:184:GLU:HG3	1.89	0.55
20:v:325:LEU:O	20:v:329:SER:N	2.38	0.55
1:A:2024:MET:CE	25:z:99:ASP:O	2.55	0.55
29:k:44:VAL:HG13	29:k:85:THR:O	2.06	0.55
24:i:30:TRP:CE2	24:i:38:ARG:NE	2.75	0.55
26:x:74:LEU:O	26:x:74:LEU:HD12	2.07	0.55
1:A:291:LYS:HE3	1:A:292:LYS:HE2	1.88	0.54
1:A:1025:VAL:HG22	1:A:1262:MET:HG2	1.89	0.54
2:C:233:ASP:OD1	2:C:487:ARG:NH2	2.37	0.54
2:C:586:MET:CA	2:C:589:LEU:HD23	2.30	0.54
4:O:229:THR:HG21	4:O:271:GLN:HA	1.89	0.54
4:O:230:VAL:HG13	4:O:241:THR:HG22	1.89	0.54
16:B:264:U:O2'	16:B:265:A:OP1	2.22	0.54
29:s:53:VAL:HG23	25:z:67:LEU:CD1	2.37	0.54
1:A:676:GLN:HG2	1:A:714:PHE:HB2	1.87	0.54
1:A:2018:ASN:ND2	1:A:2058:LEU:HD22	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:113:U:C6	27:w:48:TYR:CE1	2.96	0.54
29:k:49:ILE:HG22	29:k:80:ARG:C	2.32	0.54
1:A:765:ASP:OD2	1:A:815:TYR:OH	2.22	0.54
20:v:255:GLU:O	20:v:259:LYS:N	2.40	0.54
24:u:44:VAL:HB	24:u:53:VAL:HG23	1.89	0.54
26:j:35:PHE:HB2	26:j:37:ASN:ND2	2.23	0.54
26:j:47:ASN:OD1	26:j:48:GLY:N	2.31	0.54
2:C:500:ARG:NH1	2:C:536:SER:OG	2.41	0.54
17:D:172:U:N3	25:m:37:ASN:OD1	2.41	0.54
29:k:39:LYS:HG3	29:k:40:HIS:N	2.23	0.54
1:A:308:MET:HG2	1:A:489:THR:HG22	1.88	0.54
1:A:1934:ILE:HG12	1:A:1957:ARG:HB2	1.89	0.54
12:d:211:ARG:HG2	20:v:520:ILE:CG1	2.38	0.54
26:j:63:ILE:CG1	24:i:89:LEU:CD2	2.86	0.54
24:i:44:VAL:HB	24:i:53:VAL:HG23	1.89	0.54
1:A:1403:SER:OG	1:A:1429:MET:SD	2.59	0.54
20:v:711:MET:HE2	20:v:748:PHE:CB	2.33	0.54
30:l:21:LEU:HD12	30:l:44:LEU:HD11	1.90	0.54
6:Q:304:THR:HG22	7:R:153:PRO:HG2	1.90	0.54
8:S:3:THR:OG1	8:S:4:SER:N	2.40	0.54
26:x:71:LEU:N	30:y:63:PHE:O	2.28	0.54
1:A:185:GLN:HE21	1:A:263:PRO:HD3	1.73	0.54
1:A:895:PHE:CE2	1:A:1073:ILE:HG12	2.43	0.54
2:C:947:LYS:NZ	2:C:984:ASN:O	2.40	0.54
12:d:319:ASP:OD1	12:d:319:ASP:N	2.40	0.54
17:D:132:A:N6	17:D:146:C:O2	2.41	0.54
25:m:86:ASN:ND2	29:k:41:MET:CE	2.70	0.54
28:e:56:ALA:CB	28:e:72:VAL:HB	2.37	0.54
1:A:2020:GLU:CG	1:A:2024:MET:HE1	2.38	0.54
12:d:298:GLU:HA	12:d:301:ILE:HG22	1.88	0.54
1:A:208:VAL:HG11	1:A:213:TYR:CD1	2.43	0.54
4:O:159:SER:OG	4:O:160:ASN:N	2.39	0.54
11:c:157:ALA:O	11:c:161:ASN:ND2	2.41	0.54
19:L:1155:C:H6	19:L:1155:C:O5'	1.90	0.54
27:h:71:ILE:CG2	28:g:103:VAL:HG23	2.37	0.54
29:k:51:GLU:OE1	29:k:77:VAL:HG11	2.07	0.54
1:A:484:PHE:CD1	1:A:484:PHE:C	2.86	0.53
1:A:1328:PHE:CE2	1:A:1375:LEU:HD21	2.44	0.53
4:O:97:PHE:HA	4:O:100:LYS:HG2	1.89	0.53
12:d:267:TYR:HD2	12:d:284:LEU:HD23	1.70	0.53
17:D:22:G:H1	17:D:149:U:H3	1.57	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:E:53:A:H5''	18:E:53:A:C8	2.42	0.53
20:v:686:ILE:HG12	20:v:713:ILE:HG21	1.89	0.53
22:b:125:LYS:O	22:b:152:GLU:CB	2.55	0.53
28:g:79:LYS:HA	28:g:83:ASN:O	2.08	0.53
29:k:52:ARG:HB3	29:k:52:ARG:NH1	2.23	0.53
29:s:16:ILE:O	29:s:17:ASP:HB2	2.09	0.53
25:z:27:GLY:HA3	25:z:43:VAL:HG12	1.90	0.53
1:A:1348:GLU:OE2	1:A:1446:THR:HB	2.09	0.53
2:C:89:PRO:O	2:C:90:LEU:CB	2.56	0.53
2:C:232:SER:O	2:C:452:LYS:NZ	2.38	0.53
5:P:34:ILE:HG21	12:d:155:LEU:HD12	1.90	0.53
12:d:137:TYR:CE1	13:I:105:TYR:HD2	2.26	0.53
26:j:71:LEU:HB3	30:l:63:PHE:HB3	1.90	0.53
28:e:50:ASN:O	28:e:51:ASN:CB	2.57	0.53
30:l:63:PHE:CD1	30:l:63:PHE:C	2.85	0.53
2:C:173:LYS:NZ	17:D:75:A:OP1	2.41	0.53
4:O:370:ASN:C	4:O:372:VAL:H	2.12	0.53
17:D:149:U:H2'	17:D:150:U:O4'	2.08	0.53
19:L:1129:U:C2'	19:L:1130:U:H5'	2.38	0.53
22:b:160:THR:O	22:b:163:GLU:N	2.42	0.53
29:k:31:ILE:CG1	29:k:49:ILE:HD13	2.37	0.53
29:k:31:ILE:O	29:k:48:CYS:HA	2.09	0.53
30:l:11:LEU:HD23	30:l:36:SER:HB3	1.90	0.53
26:x:63:ILE:HG21	26:x:68:ILE:HD11	1.90	0.53
1:A:874:ILE:HD12	1:A:879:ALA:HB2	1.90	0.53
19:L:1137:U:H5'	21:a:66:LYS:O	2.09	0.53
26:j:23:ARG:HH21	26:j:23:ARG:CG	2.22	0.53
30:l:71:PHE:C	30:l:71:PHE:CD1	2.85	0.53
1:A:400:ILE:HD12	2:C:187:ARG:HE	1.74	0.53
24:i:30:TRP:HE1	24:i:38:ARG:HD3	1.62	0.53
1:A:1458:TRP:CZ2	1:A:1489:PRO:HB2	2.44	0.53
1:A:1494:LEU:O	1:A:1499:ARG:NH2	2.42	0.53
1:A:1850:LEU:HD13	1:A:1930:PRO:HG3	1.89	0.53
12:d:137:TYR:CE1	13:I:105:TYR:CD2	2.97	0.53
17:D:28:G:O2'	17:D:29:G:OP1	2.26	0.53
19:L:53:G:H4'	19:L:54:U:OP1	2.07	0.53
29:s:58:LEU:HD11	25:z:62:MET:HE3	1.91	0.53
1:A:966:PRO:HB3	1:A:1089:VAL:HB	1.89	0.53
1:A:1093:LYS:O	19:L:25:A:C2	2.62	0.53
1:A:1843:LEU:HD22	1:A:1851:PHE:HZ	1.74	0.53
6:Q:303:GLY:CA	6:Q:309:ASN:OD1	2.48	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:v:391:LEU:HB3	20:v:395:TYR:CE2	2.43	0.53
25:m:27:GLY:HA3	25:m:43:VAL:HG12	1.90	0.53
26:x:35:PHE:HB2	26:x:37:ASN:ND2	2.23	0.53
1:A:1626:GLN:HE21	1:A:1631:GLY:HA2	1.73	0.53
1:A:2057:ASP:HA	1:A:2060:LEU:HB2	1.89	0.53
2:C:625:ILE:HD13	2:C:655:LEU:CD2	2.38	0.53
7:R:159:ARG:NH1	7:R:204:LEU:O	2.41	0.53
19:L:1107:C:H6	19:L:1107:C:H5'	1.74	0.53
20:v:357:ILE:O	20:v:361:LEU:N	2.35	0.53
26:j:10:TYR:HB3	26:j:15:ILE:HD11	1.90	0.53
1:A:2027:LEU:CB	28:e:71:ASN:OD1	2.52	0.53
2:C:176:ARG:NH2	2:C:179:ASP:OD2	2.40	0.53
2:C:398:ASN:OD1	2:C:401:ARG:NH2	2.42	0.53
4:O:200:VAL:HG12	4:O:206:VAL:HG22	1.90	0.53
20:v:489:LEU:HD22	20:v:547:LYS:HD3	1.89	0.53
26:x:14:LYS:CG	26:x:74:LEU:HD11	2.39	0.53
1:A:1159:ARG:HE	1:A:1173:HIS:HB3	1.74	0.53
4:O:275:THR:OG1	4:O:279:PRO:O	2.26	0.53
4:O:343:THR:HA	5:P:45:PRO:HB3	1.90	0.53
7:R:205:LEU:O	7:R:206:LEU:HB2	2.08	0.53
12:d:211:ARG:HG2	20:v:520:ILE:HG13	1.91	0.53
17:D:130:A:H4'	17:D:131:A:C5'	2.39	0.53
26:j:27:GLY:C	26:j:40:LEU:HD12	2.34	0.53
26:j:29:LEU:HD23	26:j:29:LEU:O	2.09	0.53
28:e:54:ILE:HB	28:e:72:VAL:CG2	2.38	0.53
1:A:1056:GLU:HB2	1:A:1059:GLU:HB3	1.91	0.52
1:A:1161:TYR:CZ	1:A:1168:ILE:HD11	2.44	0.52
2:C:138:VAL:HG21	2:C:150:MET:HE3	1.90	0.52
5:P:105:LEU:HD13	5:P:112:ILE:HD12	1.91	0.52
6:Q:109:MET:HE1	6:Q:112:PHE:CD2	2.38	0.52
7:R:159:ARG:HG2	7:R:206:LEU:HD11	1.90	0.52
12:d:342:PHE:O	12:d:345:ALA:N	2.42	0.52
19:L:114:U:O2	26:x:64:ARG:CG	2.57	0.52
28:g:35:ASN:HA	28:g:61:PHE:CD2	2.40	0.52
1:A:2020:GLU:HG3	1:A:2024:MET:HE1	1.90	0.52
11:c:509:LEU:O	11:c:513:ILE:N	2.39	0.52
17:D:167:A:C6	27:h:48:TYR:CD1	2.98	0.52
25:m:84:TYR:CD2	29:k:6:VAL:HG21	2.44	0.52
29:k:18:TYR:CE1	29:k:101:PRO:HD3	2.44	0.52
28:e:45:ILE:HB	28:e:105:LEU:HG	1.91	0.52
28:e:93:LYS:NZ	25:z:103:LEU:CD1	2.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:l:10:LEU:O	30:l:13:GLU:HB2	2.09	0.52
1:A:581:LEU:HD12	7:R:33:TRP:HE3	1.74	0.52
2:C:880:MET:HE3	2:C:886:SER:HB3	1.91	0.52
4:O:236:LEU:O	4:O:236:LEU:HD13	2.09	0.52
17:D:28:G:H2'	17:D:29:G:H8	1.74	0.52
19:L:1125:U:H6	19:L:1125:U:H5''	1.74	0.52
29:s:42:ASN:HB3	29:s:89:GLY:N	2.23	0.52
1:A:864:GLN:HE22	1:A:1101:TYR:H	1.58	0.52
1:A:1294:LYS:O	10:Z:429:ASN:ND2	2.40	0.52
1:A:1390:THR:HB	1:A:1396:GLY:HA3	1.92	0.52
4:O:371:GLY:O	4:O:373:LEU:N	2.42	0.52
12:d:330:ILE:HG22	12:d:339:MET:HA	1.90	0.52
19:L:1101:C:H2'	19:L:1101:C:O2	2.09	0.52
1:A:709:ARG:NH2	17:D:82:A:O3'	2.40	0.52
1:A:1489:PRO:O	1:A:1490:ARG:HB2	2.08	0.52
2:C:88:THR:O	4:O:214:ASN:ND2	2.42	0.52
20:v:683:SER:O	20:v:687:LEU:N	2.40	0.52
26:j:19:ILE:HG21	24:i:88:THR:CG2	2.40	0.52
28:g:68:VAL:C	28:g:69:LEU:HD12	2.35	0.52
30:l:79:LYS:HG3	30:l:80:ASN:N	2.25	0.52
25:z:52:LEU:HD23	25:z:55:LEU:HD22	1.92	0.52
1:A:1017:ASP:OD1	1:A:1508:HIS:N	2.42	0.52
1:A:1711:VAL:HG12	1:A:1791:PHE:HB3	1.90	0.52
20:v:467:ARG:HA	20:v:470:TRP:HD1	1.75	0.52
20:v:612:ILE:HD13	20:v:624:TRP:CZ2	2.44	0.52
26:j:64:ARG:HH21	24:i:50:MET:HB3	1.64	0.52
28:e:93:LYS:CB	25:z:97:LEU:CD1	2.87	0.52
1:A:1093:LYS:NZ	1:A:1093:LYS:CB	2.73	0.52
1:A:1980:LYS:HZ1	28:e:39:VAL:CG1	2.06	0.52
5:P:112:ILE:HD11	6:Q:17:LEU:HD21	1.92	0.52
10:Z:32:LEU:HD23	10:Z:76:LEU:HD23	1.92	0.52
18:E:65:U:O2'	18:E:67:C:OP2	2.26	0.52
28:g:50:ASN:O	28:g:51:ASN:CB	2.57	0.52
30:l:17:HIS:CG	30:l:75:PRO:CG	2.88	0.52
2:C:557:HIS:H	2:C:560:GLN:HE21	1.58	0.52
20:v:530:ARG:NH1	20:v:530:ARG:CB	2.73	0.52
25:m:99:ASP:OD1	28:g:92:SER:HB3	2.09	0.52
27:h:13:VAL:HG12	24:i:44:VAL:HG11	1.92	0.52
27:h:29:VAL:HG12	27:h:81:ILE:HG12	1.91	0.52
28:g:32:SER:O	28:g:35:ASN:ND2	2.37	0.52
28:g:41:ARG:HG3	28:g:41:ARG:NH2	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:l:44:LEU:HD12	30:l:47:VAL:HG11	1.91	0.52
1:A:168:LEU:CG	1:A:622:MET:HE2	2.39	0.52
1:A:982:TYR:HB2	1:A:1106:GLY:HA3	1.92	0.52
17:D:27:G:OP2	17:D:141:G:O5'	2.28	0.52
19:L:1154:U:C2'	19:L:1155:C:C5'	2.88	0.52
25:m:17:ILE:HD12	25:m:40:LEU:HD11	1.92	0.52
28:g:37:ALA:HB1	28:g:44:VAL:CG1	2.39	0.52
30:l:22:GLU:HB3	30:l:71:PHE:CE1	2.44	0.52
27:w:23:VAL:HA	27:w:42:LEU:HD22	1.92	0.52
27:w:32:LYS:CG	27:w:33:PHE:CD1	2.88	0.52
4:O:125:TRP:NE1	4:O:437:GLU:O	2.43	0.52
4:O:236:LEU:HD23	5:P:67:THR:HG23	1.92	0.52
6:Q:109:MET:HE3	6:Q:112:PHE:CD2	2.44	0.52
6:Q:213:SER:O	6:Q:214:ILE:CG2	2.58	0.52
7:R:152:LYS:HD2	7:R:155:GLN:HG3	1.92	0.52
7:R:159:ARG:NH1	7:R:206:LEU:CG	2.73	0.52
30:l:21:LEU:HD22	30:l:42:VAL:HG21	1.92	0.52
27:w:29:VAL:HG12	27:w:81:ILE:HG12	1.91	0.52
27:w:32:LYS:HA	27:w:79:LEU:HD12	1.92	0.52
1:A:1527:TRP:CZ3	1:A:1528:THR:HG22	2.45	0.51
1:A:1716:LEU:O	1:A:1795:LYS:NZ	2.42	0.51
7:R:203:THR:HB	7:R:205:LEU:HD23	1.91	0.51
17:D:128:A:N3	17:D:128:A:C3'	2.73	0.51
19:L:113:U:C6	27:w:48:TYR:CD1	2.96	0.51
27:h:32:LYS:HA	27:h:79:LEU:HD12	1.92	0.51
1:A:770:MET:O	4:O:309:ARG:NH2	2.44	0.51
4:O:309:ARG:C	4:O:327:CYS:HG	2.17	0.51
17:D:28:G:H2'	17:D:29:G:C8	2.45	0.51
19:L:119:G:N7	28:e:49:ARG:HD2	2.24	0.51
1:A:1047:ALA:HB3	1:A:1251:TYR:HB3	1.92	0.51
2:C:586:MET:HG3	2:C:589:LEU:HD21	1.92	0.51
4:O:200:VAL:HG21	4:O:230:VAL:HG23	1.91	0.51
4:O:201:SER:OG	4:O:202:GLU:N	2.43	0.51
6:Q:51:ARG:NH1	6:Q:51:ARG:HA	2.25	0.51
6:Q:306:THR:HG23	6:Q:307:ALA:N	2.26	0.51
11:c:226:GLY:O	13:I:151:LYS:NZ	2.40	0.51
28:g:76:TRP:CH2	28:g:87:ARG:CD	2.86	0.51
29:s:18:TYR:CE1	29:s:101:PRO:HD3	2.44	0.51
1:A:722:LEU:HA	1:A:725:TYR:HB2	1.92	0.51
19:L:1127:A:C2'	19:L:1128:C:O5'	2.58	0.51
27:h:23:VAL:HA	27:h:42:LEU:HD22	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:s:24:THR:OG1	29:s:26:ASP:OD1	2.25	0.51
17:D:179:U:OP1	28:g:79:LYS:O	2.27	0.51
1:A:342:LEU:HD13	1:A:392:ASN:ND2	2.23	0.51
6:Q:67:GLN:NE2	6:Q:116:LYS:O	2.43	0.51
17:D:141:G:N3	17:D:141:G:C5'	2.73	0.51
18:E:14:C:H4'	18:E:15:C:O5'	2.09	0.51
26:j:19:ILE:HD13	26:j:19:ILE:N	2.23	0.51
27:h:74:ARG:HE	27:h:76:ASN:ND2	2.08	0.51
28:g:78:GLU:CG	28:g:85:ILE:CG2	2.88	0.51
30:y:21:LEU:CD1	30:y:44:LEU:CD1	2.71	0.51
31:r:8:LYS:CG	31:o:88:TRP:HH2	2.24	0.51
10:Z:84:ASN:ND2	10:Z:220:TYR:OH	2.44	0.51
12:d:269:ILE:O	12:d:273:LYS:HB2	2.11	0.51
17:D:141:G:N3	17:D:141:G:C3'	2.73	0.51
28:g:76:TRP:CZ2	28:g:87:ARG:NE	2.79	0.51
28:e:70:GLU:OE2	28:e:71:ASN:OD1	2.28	0.51
24:i:28:THR:CG2	24:i:40:LYS:HD2	2.31	0.51
24:i:30:TRP:CE2	24:i:38:ARG:HD3	2.38	0.51
1:A:857:ILE:HB	1:A:1095:MET:HE2	1.93	0.51
1:A:1048:VAL:HG22	1:A:1250:VAL:HG22	1.91	0.51
2:C:234:LEU:HD21	2:C:439:ILE:HG23	1.93	0.51
12:d:301:ILE:HD11	20:v:646:PHE:CG	2.46	0.51
19:L:1154:U:C2'	19:L:1155:C:O5'	2.58	0.51
20:v:365:ASP:CA	20:v:399:VAL:HG22	2.39	0.51
20:v:729:TYR:CE1	20:v:749:SER:CB	2.94	0.51
25:m:4:VAL:HG11	25:m:34:PRO:O	2.11	0.51
25:m:47:LEU:HD23	25:m:48:PRO:HD2	1.92	0.51
1:A:1207:TRP:O	1:A:1212:ARG:NH2	2.44	0.51
1:A:1458:TRP:HZ2	1:A:1489:PRO:HB2	1.76	0.51
1:A:1701:ILE:HB	1:A:1734:PHE:HB2	1.93	0.51
1:A:2044:THR:O	1:A:2045:ASP:HB2	2.11	0.51
2:C:968:MET:HE1	2:C:986:GLY:HA2	1.93	0.51
16:B:253:G:H1	19:L:47:U:H3	1.59	0.51
29:k:13:ALA:CB	29:k:37:PHE:CZ	2.85	0.51
29:k:24:THR:OG1	29:k:26:ASP:OD1	2.25	0.51
28:e:59:LYS:HG3	28:e:70:GLU:HG2	1.90	0.51
1:A:661:GLY:O	1:A:667:TYR:CE1	2.64	0.51
1:A:1092:PHE:CD2	1:A:1093:LYS:HG2	2.46	0.51
1:A:1991:ILE:O	1:A:2040:TRP:NE1	2.44	0.51
17:D:140:A:O2'	17:D:142:C:OP1	2.23	0.51
1:A:213:TYR:CE2	1:A:217:TRP:CD1	2.99	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ASP:OD1	1:A:508:GLN:NE2	2.44	0.50
2:C:607:LEU:CD2	2:C:644:ILE:HD12	2.41	0.50
2:C:683:ASN:HD22	2:C:854:ILE:HG13	1.75	0.50
7:R:159:ARG:CZ	7:R:206:LEU:CD1	2.80	0.50
19:L:1146:G:C6	19:L:1147:A:C6	3.00	0.50
1:A:905:TYR:HB3	1:A:908:ASP:HB2	1.93	0.50
4:O:345:PHE:HE2	4:O:364:LEU:HD13	1.76	0.50
11:c:30:THR:O	11:c:33:TRP:NE1	2.44	0.50
11:c:60:LEU:HD22	11:c:94:PRO:HG3	1.93	0.50
19:L:1090:A:C2'	19:L:1091:G:H5'	2.41	0.50
26:j:71:LEU:HD23	26:j:71:LEU:C	2.36	0.50
1:A:1567:PHE:CE2	1:A:1573:LEU:HD11	2.47	0.50
2:C:348:LEU:HD12	2:C:372:THR:HG22	1.92	0.50
17:D:128:A:N3	17:D:128:A:C2'	2.74	0.50
19:L:5:A:C2'	19:L:6:U:OP1	2.59	0.50
29:k:38:ASP:OD1	29:k:39:LYS:N	2.41	0.50
28:e:89:ARG:NH2	28:e:91:ILE:CD1	2.72	0.50
30:l:41:ASN:HB3	30:l:66:GLY:N	2.26	0.50
25:z:17:ILE:HD12	25:z:40:LEU:HD11	1.92	0.50
1:A:1379:MET:CE	1:A:1620:TYR:HB2	2.30	0.50
1:A:2021:SER:O	1:A:2025:ILE:N	2.43	0.50
12:d:175:PHE:HA	12:d:178:ARG:NH2	2.27	0.50
16:B:2:U:O4	18:E:51:A:OP2	2.30	0.50
19:L:117:U:H5'	25:z:90:ASN:HB3	1.93	0.50
20:v:530:ARG:CA	20:v:530:ARG:NH1	2.73	0.50
26:j:62:VAL:CG1	24:i:90:ILE:HB	2.41	0.50
26:x:10:TYR:HB3	26:x:15:ILE:HD11	1.94	0.50
6:Q:214:ILE:HG23	6:Q:214:ILE:O	2.12	0.50
13:I:206:LYS:HA	13:I:209:ARG:HE	1.75	0.50
17:D:79:C:H5''	17:D:80:G:H2'	1.93	0.50
19:L:3:G:O2'	19:L:4:A:N7	2.44	0.50
30:y:33:LEU:HA	30:y:44:LEU:CD2	2.35	0.50
25:z:16:THR:HA	25:z:25:VAL:O	2.11	0.50
1:A:503:LYS:HA	1:A:506:PHE:HE1	1.75	0.50
2:C:105:ILE:O	2:C:105:ILE:HG13	2.11	0.50
4:O:207:LYS:HD3	4:O:216:ILE:HG21	1.92	0.50
11:c:218:VAL:HG12	11:c:219:TYR:CD2	2.45	0.50
17:D:6:G:H4'	29:k:11:ARG:HH22	1.76	0.50
19:L:1106:G:C4'	19:L:1107:C:OP1	2.60	0.50
29:s:85:THR:HG22	30:y:73:VAL:HG22	1.93	0.50
25:z:30:GLN:HB2	25:z:39:ILE:HG23	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2021:SER:CA	1:A:2024:MET:HB2	2.40	0.50
2:C:514:GLN:HE22	2:C:589:LEU:HG	1.77	0.50
6:Q:207:LEU:HD22	6:Q:290:ILE:HG22	1.93	0.50
7:R:1:MET:HA	7:R:5:ARG:HB2	1.93	0.50
10:Z:421:LYS:HG3	10:Z:468:ILE:HG23	1.92	0.50
24:u:35:ILE:HG23	24:u:37:ILE:H	1.77	0.50
28:g:41:ARG:HG3	28:g:41:ARG:HH21	1.75	0.50
30:l:61:GLN:HG3	30:l:62:ILE:N	2.25	0.50
6:Q:207:LEU:CD2	6:Q:290:ILE:CG2	2.83	0.50
9:T:82:ILE:HG21	9:T:89:LYS:HD3	1.94	0.50
14:n:57:LYS:NZ	18:E:1:G:OP2	2.45	0.50
17:D:175:G:O5'	28:g:49:ARG:NH1	2.45	0.50
18:E:22:G:C3'	18:E:23:G:C5'	2.83	0.50
19:L:1127:A:H8	19:L:1127:A:O5'	1.95	0.50
22:b:67:ILE:CB	22:b:89:VAL:CB	2.90	0.50
11:c:62:PHE:HE1	11:c:94:PRO:HG2	1.77	0.50
18:E:53:A:C5'	18:E:53:A:C8	2.94	0.50
19:L:1105:C:H1'	19:L:1106:G:O4'	2.12	0.50
20:v:530:ARG:NH1	20:v:530:ARG:N	2.60	0.50
28:g:71:ASN:N	28:g:92:SER:O	2.41	0.50
29:k:52:ARG:CG	29:k:52:ARG:NH1	2.74	0.50
29:s:38:ASP:OD1	29:s:39:LYS:N	2.39	0.50
30:l:21:LEU:CD1	30:l:44:LEU:HD11	2.42	0.50
24:i:46:PHE:HB3	24:i:52:VAL:HG12	1.94	0.50
25:z:19:LEU:HD22	25:z:91:THR:HG22	1.94	0.50
6:Q:250:GLY:C	6:Q:297:PHE:CZ	2.90	0.49
7:R:55:PRO:HB3	7:R:93:ILE:HD11	1.92	0.49
15:H:87:LYS:O	15:H:91:ARG:HG3	2.12	0.49
25:m:16:THR:HA	25:m:25:VAL:O	2.11	0.49
28:e:63:ARG:HH11	28:e:64:HIS:HE1	1.59	0.49
1:A:1993:ASP:CG	1:A:2040:TRP:H	2.19	0.49
1:A:2027:LEU:CD1	28:e:57:ARG:NE	2.38	0.49
2:C:175:LEU:C	2:C:175:LEU:CD2	2.85	0.49
7:R:159:ARG:NH1	7:R:206:LEU:HG	2.27	0.49
19:L:1168:U:H2'	19:L:1169:C:C6	2.46	0.49
20:v:396:LEU:C	20:v:396:LEU:CD2	2.86	0.49
24:i:54:ILE:CG1	24:i:57:ALA:HB2	2.41	0.49
1:A:1214:ARG:HH12	1:A:1256:PRO:HD2	1.77	0.49
6:Q:215:PRO:HB3	7:R:171:ASP:OD1	2.12	0.49
10:Z:180:ILE:HG22	10:Z:186:LEU:HD11	1.95	0.49
20:v:667:ILE:HA	20:v:670:SER:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:e:73:LYS:HE3	28:e:90:PHE:HE2	1.78	0.49
30:y:24:THR:HA	30:y:70:LYS:HE3	1.93	0.49
1:A:1769:SER:O	1:A:1771:THR:N	2.41	0.49
2:C:405:ARG:NH2	17:D:1:A:O5'	2.45	0.49
6:Q:12:ILE:HA	6:Q:71:CYS:HB2	1.95	0.49
6:Q:206:PHE:CD2	6:Q:291:ILE:CD1	2.87	0.49
10:Z:73:ILE:HG22	10:Z:123:ILE:HD12	1.94	0.49
17:D:131:A:H5''	17:D:132:A:C8	2.47	0.49
19:L:1084:A:O3'	19:L:1085:G:H8	1.95	0.49
29:k:49:ILE:HG22	29:k:81:VAL:N	2.27	0.49
29:k:84:LEU:O	30:l:74:VAL:HG22	2.12	0.49
1:A:1382:ARG:NH2	1:A:1635:HIS:O	2.44	0.49
6:Q:39:LEU:HD23	6:Q:63:ARG:HH12	1.78	0.49
6:Q:283:ILE:HD12	6:Q:283:ILE:N	2.26	0.49
17:D:130:A:H4'	17:D:131:A:H5''	1.94	0.49
28:e:59:LYS:HG3	25:z:103:LEU:HD22	1.94	0.49
1:A:621:LEU:HD13	1:A:722:LEU:HD21	1.94	0.49
1:A:1964:PRO:HG2	1:A:2013:ARG:HA	1.93	0.49
30:l:44:LEU:HB2	30:l:47:VAL:CG1	2.43	0.49
2:C:138:VAL:HG22	2:C:236:LEU:HB3	1.95	0.49
4:O:422:SER:OG	4:O:424:LYS:NZ	2.46	0.49
9:T:13:PRO:HG2	9:T:77:LEU:HA	1.95	0.49
17:D:176:A:H1'	27:h:33:PHE:CE1	2.43	0.49
19:L:1095:U:H3'	19:L:1096:C:C6	2.48	0.49
19:L:1107:C:H3'	19:L:1107:C:OP2	2.12	0.49
20:v:365:ASP:CB	20:v:399:VAL:HG22	2.42	0.49
26:j:19:ILE:HG22	24:i:88:THR:HG23	1.94	0.49
1:A:168:LEU:HD21	1:A:626:LEU:HD21	1.95	0.49
1:A:388:PRO:O	1:A:392:ASN:OD1	2.30	0.49
2:C:675:THR:HG22	2:C:909:ILE:HD13	1.94	0.49
10:Z:105:GLN:OE1	10:Z:108:ARG:NH2	2.46	0.49
17:D:65:U:H2'	17:D:66:A:H8	1.77	0.49
19:L:109:C:OP1	25:z:34:PRO:HG2	2.12	0.49
24:u:35:ILE:HD12	27:w:32:LYS:O	2.12	0.49
25:m:14:GLN:HB3	25:m:26:TRP:CH2	2.48	0.49
26:j:63:ILE:CG1	24:i:89:LEU:HD23	2.43	0.49
27:h:72:PHE:O	28:g:103:VAL:HA	2.13	0.49
28:g:77:THR:HB	28:g:86:ASN:HD22	1.78	0.49
28:e:93:LYS:CD	25:z:97:LEU:HD11	2.43	0.49
29:s:93:LEU:HD11	25:z:21:ASN:ND2	2.28	0.49
27:w:32:LYS:HD2	27:w:33:PHE:HE1	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1153:GLU:O	1:A:1159:ARG:NH1	2.46	0.49
1:A:1549:ALA:HA	10:Z:297:LEU:HD21	1.95	0.49
2:C:247:PHE:CD2	2:C:933:TRP:HZ3	2.30	0.49
4:O:231:SER:OG	4:O:274:CYS:SG	2.64	0.49
22:b:49:HIS:O	22:b:50:LEU:CB	2.61	0.49
28:e:56:ALA:HB1	28:e:69:LEU:CD2	2.37	0.49
1:A:1487:GLY:O	1:A:1490:ARG:NH2	2.39	0.49
10:Z:77:SER:HA	10:Z:80:ILE:HD12	1.95	0.49
18:E:64:U:O2'	18:E:65:U:OP1	2.30	0.49
19:L:1114:G:H2'	19:L:1115:G:C1'	2.42	0.49
19:L:1150:U:OP1	29:s:55:LYS:CG	2.61	0.49
29:k:35:MET:CB	30:l:84:PHE:CE2	2.85	0.49
28:e:91:ILE:HG21	25:z:96:ILE:HG12	1.95	0.49
30:l:65:ARG:HD3	30:l:67:SER:HB3	1.94	0.49
1:A:769:MET:HE2	4:O:352:ILE:CD1	2.40	0.48
1:A:1526:TRP:O	1:A:1526:TRP:HE3	1.95	0.48
6:Q:194:GLU:O	6:Q:291:ILE:CG2	2.61	0.48
6:Q:280:VAL:HG23	6:Q:280:VAL:O	2.13	0.48
19:L:1106:G:N2	21:a:69:ARG:O	2.46	0.48
25:m:46:THR:HB	25:m:79:ILE:HA	1.95	0.48
30:l:15:GLN:HE21	30:l:16:GLY:N	2.11	0.48
30:l:21:LEU:CD2	30:l:72:ILE:CG1	2.81	0.48
30:l:39:SER:O	30:l:40:MET:CB	2.60	0.48
24:i:40:LYS:O	24:i:57:ALA:HA	2.13	0.48
25:z:14:GLN:HB3	25:z:26:TRP:CH2	2.48	0.48
1:A:182:PRO:HB3	1:A:264:ILE:HD12	1.95	0.48
1:A:1405:ILE:HD13	10:Z:303:LEU:HB2	1.93	0.48
1:A:2032:ILE:HD11	1:A:2043:PHE:HD1	1.77	0.48
1:A:2043:PHE:HE2	1:A:2047:GLN:N	2.11	0.48
20:v:617:PRO:O	20:v:618:GLU:CB	2.60	0.48
28:g:64:HIS:O	28:g:65:CYS:CB	2.61	0.48
30:l:44:LEU:CB	30:l:47:VAL:HG13	2.43	0.48
1:A:1961:LEU:CD2	1:A:2084:LEU:CD1	2.89	0.48
4:O:321:PHE:HB2	5:P:57:LEU:HD23	1.95	0.48
31:r:8:LYS:CG	31:o:88:TRP:CH2	2.96	0.48
24:u:46:PHE:HB3	24:u:52:VAL:HG12	1.94	0.48
25:m:19:LEU:HD23	25:m:92:ILE:HA	1.94	0.48
28:g:41:ARG:HB2	28:g:57:ARG:HD3	1.95	0.48
31:r:137:LEU:HD23	31:o:137:LEU:HD23	1.95	0.48
7:R:83:LEU:HB2	7:R:87:CYS:HB2	1.95	0.48
24:u:35:ILE:HD11	27:w:79:LEU:HD12	1.86	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:j:64:ARG:HD2	24:i:87:ILE:HB	1.95	0.48
28:g:38:MET:HG3	28:g:58:VAL:O	2.13	0.48
28:e:59:LYS:HG2	28:e:70:GLU:HG3	1.95	0.48
31:r:14:VAL:HG12	31:r:52:GLU:HA	1.95	0.48
4:O:239:ILE:HG13	4:O:239:ILE:O	2.13	0.48
4:O:239:ILE:CG1	4:O:251:TRP:HB2	2.42	0.48
17:D:127:U:H6	17:D:127:U:OP2	1.96	0.48
17:D:147:C:H2'	17:D:148:G:C8	2.49	0.48
1:A:654:HIS:O	1:A:658:ASN:ND2	2.47	0.48
1:A:1014:LYS:O	1:A:1164:TYR:O	2.31	0.48
2:C:89:PRO:O	2:C:90:LEU:HB2	2.13	0.48
2:C:567:ILE:O	2:C:567:ILE:HG22	2.12	0.48
10:Z:474:THR:OG1	10:Z:478:ARG:NH1	2.46	0.48
17:D:130:A:C5'	17:D:131:A:H3'	2.42	0.48
17:D:168:U:C4	24:i:49:PHE:CZ	3.02	0.48
19:L:110:A:N6	25:z:35:GLN:CD	2.68	0.48
20:v:652:LEU:HD11	20:v:666:PHE:CZ	2.49	0.48
28:e:45:ILE:HD12	28:e:55:ILE:HG12	1.96	0.48
30:l:17:HIS:CB	30:l:75:PRO:HG2	2.44	0.48
1:A:1276:GLU:O	1:A:1277:GLU:HB2	2.13	0.48
2:C:117:ARG:HE	2:C:159:LYS:HA	1.78	0.48
19:L:16:U:OP2	19:L:18:U:O2'	2.25	0.48
19:L:1085:G:P	19:L:1085:G:C8	3.06	0.48
20:v:608:TYR:CD2	20:v:627:TYR:HD1	2.32	0.48
26:j:11:MET:HA	26:j:29:LEU:HD22	1.96	0.48
29:s:28:ARG:CG	29:s:52:ARG:HG2	2.42	0.48
29:s:53:VAL:CG2	25:z:67:LEU:CD1	2.91	0.48
31:r:20:ARG:CB	31:q:51:VAL:HG13	2.44	0.48
26:x:35:PHE:O	26:x:36:LEU:HB3	2.14	0.48
1:A:770:MET:CE	5:P:165:ILE:HD11	2.44	0.48
1:A:860:GLU:OE2	1:A:863:ARG:NH2	2.45	0.48
7:R:87:CYS:HB3	7:R:91:HIS:HE1	1.77	0.48
15:H:91:ARG:HE	16:B:249:C:H5''	1.77	0.48
27:h:29:VAL:O	27:h:37:GLU:HA	2.14	0.48
28:e:56:ALA:CB	28:e:72:VAL:CB	2.91	0.48
1:A:826:ALA:O	1:A:830:ASN:ND2	2.47	0.47
1:A:1343:PHE:CD2	1:A:1440:ILE:CG1	2.91	0.47
4:O:95:SER:OG	4:O:96:ALA:N	2.46	0.47
25:z:82:LEU:HD11	25:z:85:ILE:HB	1.96	0.47
1:A:1993:ASP:HB2	1:A:2040:TRP:HB2	1.96	0.47
2:C:90:LEU:O	2:C:90:LEU:HD22	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:493:LEU:HD21	2:C:539:VAL:HG21	1.96	0.47
10:Z:319:ASN:HA	10:Z:322:LYS:HD3	1.95	0.47
12:d:241:MET:CG	12:d:279:LEU:HD12	2.41	0.47
17:D:41:A:N1	17:D:78:A:O2'	2.42	0.47
28:g:67:MET:HG3	28:g:69:LEU:CD1	2.44	0.47
29:k:33:GLN:O	29:k:45:LEU:HA	2.14	0.47
29:k:49:ILE:CG2	29:k:81:VAL:HB	2.43	0.47
29:s:48:CYS:SG	29:s:82:LEU:HD12	2.54	0.47
1:A:950:THR:OG1	1:A:953:ARG:NH2	2.48	0.47
4:O:372:VAL:O	4:O:372:VAL:HG12	2.14	0.47
6:Q:70:ILE:HD13	6:Q:84:ILE:HD11	1.95	0.47
10:Z:299:LEU:HD21	10:Z:343:TYR:HE1	1.78	0.47
11:c:81:PRO:HA	11:c:82:ASN:HA	1.70	0.47
19:L:1107:C:HO2'	19:L:1108:A:P	2.37	0.47
20:v:403:GLN:HG2	20:v:439:LYS:HB2	1.95	0.47
25:m:21:ASN:ND2	29:k:93:LEU:HD11	2.28	0.47
25:m:25:VAL:HG22	25:m:45:LEU:HB2	1.96	0.47
27:w:29:VAL:O	27:w:37:GLU:HA	2.14	0.47
1:A:304:ASP:C	1:A:306:PRO:HD2	2.40	0.47
1:A:1183:THR:HB	1:A:1222:LEU:HD23	1.96	0.47
10:Z:317:ILE:HD13	10:Z:325:VAL:HG21	1.95	0.47
20:v:365:ASP:O	20:v:399:VAL:HG13	2.14	0.47
20:v:385:PHE:HA	20:v:388:LEU:HB2	1.95	0.47
26:j:23:ARG:HH21	26:j:23:ARG:CB	2.27	0.47
30:l:77:LEU:O	30:l:79:LYS:N	2.47	0.47
1:A:1992:TYR:N	1:A:1992:TYR:HD1	2.12	0.47
2:C:629:TYR:HE2	2:C:655:LEU:HA	1.78	0.47
27:h:19:LEU:HD11	24:i:81:LEU:HD22	1.96	0.47
28:e:102:ILE:HG13	28:e:103:VAL:N	2.30	0.47
1:A:1863:HIS:CD2	1:A:1873:LYS:HD2	2.49	0.47
2:C:153:LEU:CD1	2:C:212:PHE:CE1	2.98	0.47
6:Q:208:TYR:HB2	6:Q:316:LEU:HD13	1.95	0.47
7:R:232:PRO:HA	7:R:235:GLN:HB2	1.95	0.47
19:L:120:G:H4'	19:L:121:C:C5'	2.45	0.47
22:b:60:THR:HA	22:b:82:GLY:O	2.15	0.47
25:m:92:ILE:HG13	25:m:92:ILE:H	1.45	0.47
28:g:89:ARG:NH2	28:g:91:ILE:HD11	2.29	0.47
30:l:11:LEU:HD23	30:l:36:SER:CB	2.45	0.47
25:z:25:VAL:HG22	25:z:45:LEU:HB2	1.97	0.47
1:A:484:PHE:CD1	1:A:485:PRO:CA	2.97	0.47
1:A:1260:PHE:CE1	1:A:1269:ILE:HD11	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1992:TYR:N	1:A:1992:TYR:CD1	2.83	0.47
3:J:24:LEU:H	10:Z:310:HIS:HD2	1.63	0.47
4:O:111:ILE:CG2	12:d:194:MET:O	2.61	0.47
7:R:230:PRO:HD2	16:B:14:C:H2'	1.96	0.47
8:S:7:PRO:HD2	19:L:20:G:H1'	1.97	0.47
10:Z:127:TYR:OH	10:Z:212:LEU:N	2.47	0.47
11:c:55:TYR:HD2	11:c:56:LEU:HD12	1.80	0.47
22:b:65:ILE:O	22:b:86:ILE:HA	2.14	0.47
25:m:86:ASN:ND2	25:m:86:ASN:C	2.73	0.47
26:j:63:ILE:CG2	26:j:68:ILE:HD11	2.45	0.47
29:s:7:ALA:HB3	29:s:10:SER:HB2	1.96	0.47
19:L:1083:A:H2'	19:L:1084:A:C8	2.47	0.47
20:v:577:VAL:HG12	20:v:583:ILE:HB	1.97	0.47
26:j:37:ASN:OD1	26:j:64:ARG:HA	2.14	0.47
29:k:45:LEU:O	29:k:84:LEU:HA	2.13	0.47
29:s:54:PRO:HG2	29:s:57:GLN:HG3	1.96	0.47
29:s:95:THR:OG1	25:z:86:ASN:HB3	2.15	0.47
1:A:342:LEU:HD22	1:A:392:ASN:ND2	2.30	0.47
1:A:1673:LEU:HB2	1:A:1678:ILE:HD11	1.97	0.47
6:Q:105:LYS:HD3	11:c:215:GLU:HG3	1.96	0.47
19:L:54:U:C4	19:L:106:A:N1	2.82	0.47
28:e:49:ARG:NH2	27:w:76:ASN:CG	2.73	0.47
28:e:93:LYS:CB	25:z:97:LEU:HD12	2.45	0.47
30:l:42:VAL:HG22	30:l:64:VAL:CG2	2.44	0.47
1:A:905:TYR:OH	1:A:1002:GLU:OE2	2.27	0.47
1:A:1369:ASN:O	1:A:1373:LEU:N	2.46	0.47
6:Q:214:ILE:HD12	6:Q:283:ILE:HG21	1.96	0.47
6:Q:304:THR:HG23	7:R:154:ALA:CB	2.45	0.47
17:D:130:A:OP1	17:D:130:A:H2'	2.14	0.47
19:L:1127:A:H2'	19:L:1128:C:O5'	2.14	0.47
20:v:389:ILE:HA	20:v:392:TYR:CD2	2.50	0.47
1:A:416:GLU:HG2	1:A:418:ASP:H	1.80	0.46
1:A:467:GLU:O	2:C:387:TYR:OH	2.32	0.46
1:A:737:ARG:NH1	18:E:70:U:OP2	2.46	0.46
1:A:816:ILE:O	1:A:820:ALA:N	2.44	0.46
1:A:1201:TYR:OH	1:A:1213:MET:SD	2.62	0.46
10:Z:84:ASN:HD22	10:Z:129:VAL:HG13	1.80	0.46
19:L:118:U:N3	28:e:66:ASN:ND2	2.58	0.46
20:v:397:ASN:HB3	20:v:411:TRP:HD1	1.79	0.46
22:b:137:LEU:O	22:b:140:TYR:CB	2.63	0.46
28:g:54:ILE:HA	28:g:73:LYS:O	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:l:63:PHE:C	30:l:63:PHE:HD1	2.24	0.46
25:z:33:SER:HB2	25:z:37:ASN:HB2	1.97	0.46
1:A:1379:MET:HE1	1:A:1620:TYR:HB3	1.93	0.46
4:O:433:THR:OG1	4:O:435:GLU:O	2.32	0.46
11:c:41:GLN:O	11:c:42:LYS:HB2	2.14	0.46
12:d:219:ARG:HA	12:d:222:TYR:HB2	1.98	0.46
12:d:269:ILE:HA	12:d:272:GLU:HG2	1.96	0.46
19:L:113:U:O4	27:w:47:ASN:C	2.58	0.46
24:u:81:LEU:HD22	27:w:19:LEU:HD11	1.97	0.46
26:j:30:ARG:HE	26:j:30:ARG:HB2	1.60	0.46
28:g:102:ILE:HG13	28:g:103:VAL:N	2.30	0.46
29:k:30:TYR:CE1	29:k:50:GLU:HB3	2.50	0.46
1:A:1426:ARG:HD2	3:J:8:LEU:HD11	1.97	0.46
4:O:121:GLN:HE22	5:P:50:ASN:HA	1.80	0.46
19:L:1146:G:H5'	19:L:1147:A:OP2	2.15	0.46
20:v:442:THR:HG1	20:v:445:SER:HG	1.57	0.46
20:v:479:PRO:HB3	20:v:530:ARG:HD3	1.97	0.46
20:v:505:PHE:O	20:v:509:GLU:N	2.46	0.46
20:v:797:TYR:C	20:v:799:ASP:N	2.66	0.46
23:t:111:VAL:O	23:t:112:SER:C	2.58	0.46
28:g:78:GLU:HG2	28:g:85:ILE:HG23	1.94	0.46
29:k:11:ARG:H	29:k:14:ASN:CB	2.27	0.46
1:A:306:PRO:CD	1:A:307:GLU:H	2.27	0.46
2:C:153:LEU:HD13	2:C:212:PHE:CE2	2.51	0.46
2:C:164:MET:HG3	2:C:168:VAL:CG1	2.45	0.46
2:C:625:ILE:HD13	2:C:655:LEU:HD21	1.96	0.46
9:T:151:ARG:HD3	14:n:71:SER:HA	1.97	0.46
12:d:281:LYS:O	12:d:284:LEU:HB3	2.15	0.46
20:v:385:PHE:O	20:v:389:ILE:CD1	2.63	0.46
20:v:729:TYR:HE1	20:v:749:SER:CB	2.28	0.46
25:m:53:ASN:O	25:m:54:LYS:HB3	2.15	0.46
26:j:74:LEU:O	26:j:75:ASP:CB	2.64	0.46
28:g:26:PHE:HE1	28:g:63:ARG:HA	1.80	0.46
31:p:19:SER:OG	31:p:38:ASP:OD2	2.26	0.46
1:A:427:SER:HA	10:Z:202:GLN:HB3	1.97	0.46
1:A:1125:LEU:O	1:A:1233:ARG:NH1	2.48	0.46
11:c:14:THR:HG23	11:c:17:GLU:H	1.81	0.46
19:L:1095:U:C3'	19:L:1096:C:C6	2.99	0.46
29:s:53:VAL:CG2	25:z:67:LEU:HD11	2.45	0.46
30:l:21:LEU:HD21	30:l:72:ILE:CD1	2.45	0.46
30:y:44:LEU:CB	30:y:47:VAL:HG11	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ASN:HB3	9:T:36:ASP:HB2	1.97	0.46
1:A:428:LEU:HD23	2:C:897:THR:C	2.39	0.46
1:A:618:SER:OG	18:E:72:C:OP1	2.31	0.46
1:A:1093:LYS:HG2	1:A:1093:LYS:H	1.57	0.46
12:d:57:TYR:CE2	18:E:86:G:C2	3.04	0.46
28:g:67:MET:HG3	28:g:69:LEU:HD11	1.97	0.46
1:A:732:ARG:NH2	18:E:71:G:OP2	2.46	0.46
1:A:1054:LEU:N	1:A:1166:ASP:O	2.45	0.46
1:A:1889:LEU:HG	1:A:1991:ILE:CG1	2.45	0.46
1:A:1910:LYS:HB3	1:A:1940:MET:HG2	1.97	0.46
10:Z:181:LEU:HG	10:Z:194:LEU:HD12	1.97	0.46
18:E:50:G:C2'	18:E:51:A:OP2	2.63	0.46
19:L:1117:G:H2'	19:L:1118:U:H5'	1.98	0.46
24:u:51:ASN:HB3	24:u:84:GLY:H	1.81	0.46
28:g:41:ARG:CB	28:g:57:ARG:HD3	2.45	0.46
30:l:77:LEU:C	30:l:79:LYS:H	2.24	0.46
24:i:51:ASN:HB3	24:i:84:GLY:H	1.81	0.46
1:A:1711:VAL:HA	1:A:1791:PHE:HA	1.96	0.46
1:A:1748:ILE:H	1:A:1748:ILE:HG13	1.44	0.46
2:C:67:GLU:HG2	2:C:68:HIS:CE1	2.51	0.46
4:O:106:VAL:HG11	4:O:109:GLU:HG2	1.98	0.46
19:L:1105:C:O3'	19:L:1106:G:O4'	2.34	0.46
19:L:1107:C:O2'	19:L:1108:A:P	2.74	0.46
19:L:1137:U:O4	21:a:67:LYS:O	2.33	0.46
21:a:67:LYS:O	21:a:68:GLN:CB	2.64	0.46
1:A:148:ASP:OD1	1:A:148:ASP:N	2.47	0.46
1:A:617:ASN:O	1:A:621:LEU:HB2	2.16	0.46
1:A:631:LEU:HD21	1:A:663:LEU:HD13	1.97	0.46
1:A:1961:LEU:HD21	1:A:2084:LEU:HD12	1.96	0.46
12:d:320:TYR:CD1	12:d:356:LYS:HA	2.50	0.46
19:L:121:C:N4	27:w:33:PHE:CG	2.84	0.46
29:k:16:ILE:O	29:k:17:ASP:HB2	2.16	0.46
28:e:93:LYS:CD	25:z:97:LEU:CD1	2.94	0.46
30:l:11:LEU:HD11	30:l:72:ILE:HD13	1.94	0.46
1:A:1099:ASN:HD22	1:A:1104:ILE:HG13	1.81	0.46
2:C:500:ARG:HD2	2:C:534:THR:HB	1.97	0.46
2:C:803:VAL:HA	2:C:813:ILE:HD12	1.97	0.46
4:O:236:LEU:CD1	5:P:74:ILE:HD12	2.46	0.46
12:d:306:LYS:NZ	12:d:326:TYR:OH	2.40	0.46
26:j:23:ARG:CG	26:j:23:ARG:NH2	2.79	0.46
29:k:84:LEU:HD21	30:l:78:LEU:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:p:105:LEU:O	31:p:109:LEU:N	2.47	0.46
1:A:814:ARG:NH2	4:O:369:ASP:OD2	2.48	0.45
1:A:2013:ARG:NH2	1:A:2083:ILE:O	2.49	0.45
10:Z:403:LYS:HG2	10:Z:445:LEU:HB3	1.98	0.45
17:D:168:U:C6	24:i:49:PHE:HE1	2.33	0.45
17:D:173:U:C5	28:g:64:HIS:CE1	3.04	0.45
25:m:82:LEU:HD12	25:m:83:GLN:N	2.31	0.45
28:e:33:LEU:HD23	27:w:72:PHE:HB2	1.99	0.45
28:e:48:LEU:HD22	28:e:52:HIS:HE2	1.77	0.45
1:A:893:ARG:NH1	1:A:1136:GLY:O	2.47	0.45
1:A:1035:LEU:CD1	1:A:1035:LEU:C	2.85	0.45
1:A:1961:LEU:CD2	1:A:2084:LEU:HD13	2.37	0.45
12:d:333:SER:C	12:d:335:PRO:HD3	2.41	0.45
26:x:37:ASN:OD1	26:x:64:ARG:HA	2.16	0.45
1:A:1056:GLU:HG2	1:A:1060:LYS:HG3	1.99	0.45
1:A:1965:PHE:O	1:A:1966:SER:HB3	2.16	0.45
11:c:152:LEU:HD21	11:c:156:ARG:HH21	1.81	0.45
17:D:167:A:C1'	28:g:64:HIS:HE2	2.27	0.45
19:L:117:U:C5	25:z:88:ARG:NH2	2.84	0.45
19:L:1146:G:H3'	19:L:1147:A:C5'	2.44	0.45
25:m:18:GLU:HG3	25:m:24:THR:HG22	1.98	0.45
26:j:18:ASN:ND2	26:j:18:ASN:N	2.60	0.45
30:l:44:LEU:HB2	30:l:47:VAL:HG13	1.98	0.45
4:O:308:LYS:HA	5:P:148:HIS:CE1	2.50	0.45
12:d:263:SER:CB	12:d:287:PHE:HZ	2.17	0.45
17:D:65:U:H2'	17:D:66:A:C8	2.52	0.45
17:D:168:U:C4	24:i:49:PHE:HZ	2.35	0.45
19:L:1129:U:H2'	19:L:1130:U:O5'	2.16	0.45
20:v:509:GLU:OE2	20:v:548:TYR:OH	2.23	0.45
20:v:771:LEU:O	20:v:774:PRO:CB	2.64	0.45
26:j:20:ASN:OD1	24:i:32:PHE:CD2	2.70	0.45
27:h:46:ASP:N	28:g:30:PRO:HG2	2.31	0.45
28:e:91:ILE:HG21	25:z:96:ILE:HD13	1.97	0.45
29:s:50:GLU:O	29:s:79:LYS:HA	2.17	0.45
30:l:23:LEU:HB3	30:l:25:THR:HG22	1.98	0.45
27:w:33:PHE:CD1	27:w:33:PHE:N	2.84	0.45
1:A:376:ARG:HG3	2:C:909:ILE:HG13	1.98	0.45
1:A:770:MET:HE2	5:P:165:ILE:HD11	1.98	0.45
2:C:564:ILE:HG22	2:C:567:ILE:CD1	2.46	0.45
12:d:267:TYR:OH	12:d:287:PHE:CB	2.61	0.45
16:B:265:A:OP2	16:B:266:A:H4'	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:g:62:ASP:HB3	28:g:66:ASN:OD1	2.17	0.45
28:e:62:ASP:HB3	28:e:66:ASN:OD1	2.17	0.45
30:l:65:ARG:HH11	30:l:65:ARG:CG	2.14	0.45
26:x:15:ILE:HG23	26:x:72:GLU:O	2.16	0.45
31:p:14:VAL:HG12	31:p:52:GLU:HA	1.97	0.45
1:A:1801:SER:O	1:A:1804:THR:OG1	2.31	0.45
2:C:84:GLN:HE21	2:C:88:THR:HG21	1.82	0.45
2:C:135:ASN:O	2:C:233:ASP:N	2.44	0.45
2:C:802:ALA:HB2	2:C:843:LYS:HA	1.99	0.45
7:R:170:ILE:HD13	7:R:173:ILE:HD11	1.98	0.45
12:d:272:GLU:HG3	12:d:273:LYS:N	2.30	0.45
17:D:96:U:C2'	17:D:97:U:OP1	2.65	0.45
17:D:128:A:O2'	17:D:129:G:O5'	2.34	0.45
28:g:78:GLU:CG	28:g:85:ILE:HG23	2.47	0.45
29:s:54:PRO:CG	29:s:57:GLN:CG	2.94	0.45
1:A:834:ILE:HG12	1:A:840:VAL:HG11	1.98	0.45
1:A:1608:LEU:HD11	1:A:1648:ILE:HD11	1.99	0.45
1:A:2032:ILE:HG21	1:A:2041:PRO:HB2	1.97	0.45
6:Q:109:MET:HG3	11:c:218:VAL:HA	1.99	0.45
17:D:173:U:C2	28:g:97:ARG:NE	2.84	0.45
24:u:91:THR:HG21	26:x:57:LEU:HB3	1.99	0.45
25:m:17:ILE:CG2	25:m:92:ILE:HG21	2.38	0.45
26:j:19:ILE:HG22	26:j:67:SER:HB2	1.98	0.45
29:k:45:LEU:HD12	29:k:87:LEU:CD1	2.47	0.45
28:e:91:ILE:HG21	25:z:96:ILE:CG1	2.47	0.45
25:z:18:GLU:HG3	25:z:24:THR:HG22	1.98	0.45
1:A:1211:SER:O	1:A:1257:ASN:ND2	2.50	0.45
1:A:1286:TRP:CE2	1:A:1302:LEU:HD11	2.52	0.45
2:C:416:ASP:HB2	2:C:419:PRO:HD2	1.98	0.45
4:O:392:MET:HG2	8:S:158:ASN:HB2	1.99	0.45
17:D:21:G:N2	17:D:150:U:O2'	2.45	0.45
20:v:570:THR:HG21	20:v:594:PHE:CZ	2.51	0.45
20:v:645:ARG:NH2	20:v:673:GLU:OE2	2.43	0.45
29:s:54:PRO:CG	29:s:76:LYS:O	2.65	0.45
30:l:14:ALA:HB1	30:l:19:VAL:HG11	1.98	0.45
1:A:857:ILE:HB	1:A:1095:MET:CE	2.47	0.45
6:Q:283:ILE:N	6:Q:283:ILE:CD1	2.79	0.45
20:v:324:ASP:O	20:v:328:LYS:N	2.47	0.45
26:j:35:PHE:O	26:j:36:LEU:CB	2.64	0.45
29:k:45:LEU:HD12	29:k:87:LEU:HD13	1.98	0.45
29:k:86:ILE:HG22	30:l:10:LEU:HD23	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:l:33:LEU:CD2	30:l:35:GLU:O	2.63	0.45
2:C:229:LEU:HD23	2:C:235:VAL:HG11	1.99	0.45
12:d:47:GLN:NE2	12:d:78:GLN:OE1	2.39	0.45
18:E:19:C:O2'	18:E:20:G:H5''	2.17	0.45
19:L:1095:U:H2'	19:L:1096:C:N1	2.32	0.45
20:v:412:MET:HE2	20:v:428:TYR:HA	1.99	0.45
20:v:415:VAL:HG21	20:v:427:VAL:HG21	1.98	0.45
22:b:54:THR:CA	22:b:77:HIS:CB	2.94	0.45
22:b:148:VAL:O	22:b:149:PRO:CB	2.64	0.45
28:e:66:ASN:HB3	28:e:98:GLY:H	1.81	0.45
30:l:21:LEU:CD2	30:l:42:VAL:HG21	2.46	0.45
1:A:402:TRP:CD1	1:A:403:TYR:O	2.70	0.44
1:A:763:MET:CE	1:A:779:ALA:CB	2.48	0.44
1:A:1192:ASP:N	1:A:1192:ASP:OD1	2.50	0.44
1:A:1687:HIS:HD2	1:A:1688:PRO:HD2	1.82	0.44
2:C:713:GLU:HB3	2:C:817:GLN:HB3	1.98	0.44
11:c:41:GLN:O	11:c:42:LYS:CB	2.64	0.44
17:D:150:U:O2'	17:D:151:A:OP1	2.24	0.44
19:L:116:U:C2	29:s:40:HIS:CD2	3.04	0.44
25:m:14:GLN:NE2	25:m:28:THR:OG1	2.50	0.44
29:k:15:LEU:HD13	29:k:18:TYR:HB2	1.99	0.44
28:e:52:HIS:CD2	28:e:52:HIS:O	2.70	0.44
25:z:14:GLN:NE2	25:z:28:THR:OG1	2.50	0.44
1:A:831:ARG:CD	1:A:852:LEU:HD11	2.47	0.44
1:A:1964:PRO:O	1:A:1965:PHE:HB2	2.17	0.44
2:C:644:ILE:HG21	2:C:655:LEU:HD11	1.99	0.44
4:O:118:LEU:HD21	5:P:48:GLN:HB2	1.98	0.44
6:Q:302:PHE:O	6:Q:312:LEU:HD13	2.18	0.44
12:d:267:TYR:CB	12:d:284:LEU:HD23	2.47	0.44
18:E:22:G:H5'	18:E:23:G:OP2	2.15	0.44
18:E:23:G:C5'	18:E:23:G:C8	3.01	0.44
22:b:97:ASN:O	22:b:98:VAL:CB	2.64	0.44
25:m:39:ILE:CD1	25:m:84:TYR:HE1	2.22	0.44
30:l:34:VAL:HG12	30:l:35:GLU:HG2	1.98	0.44
30:l:38:ASP:OD1	30:l:38:ASP:N	2.43	0.44
1:A:140:ARG:CD	1:A:252:GLU:OE2	2.66	0.44
1:A:392:ASN:OD1	1:A:392:ASN:N	2.48	0.44
1:A:1093:LYS:O	19:L:25:A:C6	2.70	0.44
2:C:655:LEU:HD23	2:C:655:LEU:O	2.18	0.44
2:C:697:ARG:O	2:C:709:SER:OG	2.27	0.44
2:C:869:HIS:HA	2:C:899:LEU:HA	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:30:LEU:O	5:P:30:LEU:HD12	2.17	0.44
6:Q:190:LEU:HD11	6:Q:312:LEU:HD11	1.99	0.44
11:c:227:ILE:CD1	13:I:150:GLY:O	2.60	0.44
12:d:293:ASP:OD1	12:d:293:ASP:N	2.46	0.44
19:L:1093:C:C5	19:L:1093:C:OP2	2.70	0.44
25:m:72:GLN:NE2	25:m:75:ALA:HB2	2.33	0.44
27:h:33:PHE:CZ	28:g:49:ARG:NE	2.85	0.44
27:h:80:TYR:HE1	27:h:82:ARG:HD2	1.82	0.44
28:g:63:ARG:HE	28:g:63:ARG:HB3	1.60	0.44
28:e:49:ARG:N	28:e:100:SER:O	2.49	0.44
28:e:73:LYS:HG3	28:e:90:PHE:HD2	1.83	0.44
30:l:70:LYS:NZ	30:l:70:LYS:CB	2.79	0.44
25:z:72:GLN:NE2	25:z:75:ALA:HB2	2.33	0.44
1:A:134:MET:HE1	9:T:107:ARG:HB2	1.99	0.44
2:C:778:THR:HG23	2:C:781:ASP:H	1.81	0.44
6:Q:94:VAL:HG11	6:Q:135:ILE:HG23	1.99	0.44
13:I:195:PHE:HE1	13:I:204:ASN:HB2	1.82	0.44
16:B:6:U:H2'	16:B:7:U:C6	2.53	0.44
19:L:4:A:H2'	19:L:5:A:C8	2.49	0.44
19:L:1107:C:OP2	19:L:1107:C:C6	2.70	0.44
26:j:5:PRO:HA	30:l:37:GLU:OE1	2.17	0.44
27:h:16:LYS:HB3	27:h:17:PRO:HD3	2.00	0.44
29:k:30:TYR:CD1	29:k:50:GLU:CB	2.98	0.44
1:A:654:HIS:CE1	1:A:658:ASN:HD21	2.34	0.44
2:C:905:GLN:OE1	2:C:938:ARG:NH2	2.50	0.44
7:R:110:ASP:OD1	7:R:114:ARG:N	2.51	0.44
10:Z:88:PRO:HB3	10:Z:223:HIS:CG	2.53	0.44
12:d:271:ILE:HD13	12:d:281:LYS:CG	2.08	0.44
16:B:8:C:H42	18:E:45:A:N6	2.13	0.44
17:D:26:A:H5'	17:D:131:A:OP1	2.17	0.44
19:L:117:U:H5'	25:z:90:ASN:CB	2.48	0.44
20:v:479:PRO:HB3	20:v:530:ARG:CD	2.47	0.44
28:g:56:ALA:HB3	28:g:69:LEU:HD23	2.00	0.44
1:A:428:LEU:HD22	2:C:896:GLY:C	2.42	0.44
1:A:1972:ASP:HB3	28:e:41:ARG:HH21	1.82	0.44
1:A:2019:GLU:HB3	1:A:2020:GLU:OE1	2.18	0.44
1:A:2030:PRO:HB3	28:e:71:ASN:O	2.17	0.44
2:C:599:THR:OG1	2:C:647:ASN:ND2	2.51	0.44
12:d:298:GLU:O	12:d:301:ILE:HG22	2.17	0.44
19:L:114:U:C2	26:x:64:ARG:HG3	2.52	0.44
19:L:1129:U:O2'	19:L:1130:U:C5'	2.65	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:v:549:ILE:HD12	20:v:587:MET:HE3	1.99	0.44
25:m:36:MET:HE3	25:m:36:MET:HB2	1.90	0.44
29:k:49:ILE:HG22	29:k:80:ARG:O	2.17	0.44
29:k:105:LYS:HA	29:k:108:ARG:NE	2.32	0.44
26:x:33:ASP:OD1	26:x:37:ASN:N	2.51	0.44
31:q:14:VAL:HG12	31:q:52:GLU:HA	2.00	0.44
1:A:140:ARG:NE	1:A:252:GLU:OE2	2.51	0.44
1:A:1406:LEU:HB3	1:A:1425:PHE:HB3	2.00	0.44
1:A:1689:ARG:NH1	1:A:1692:TYR:OH	2.51	0.44
2:C:234:LEU:HD23	2:C:443:TYR:HB2	1.98	0.44
6:Q:79:ARG:HG2	6:Q:80:TRP:CD1	2.53	0.44
6:Q:304:THR:HG23	7:R:154:ALA:HB2	1.99	0.44
10:Z:305:GLY:HA3	10:Z:345:ILE:HG23	1.98	0.44
10:Z:437:GLN:HE21	10:Z:441:ASN:HD21	1.65	0.44
13:I:105:TYR:O	13:I:105:TYR:CD1	2.70	0.44
18:E:64:U:O2'	18:E:65:U:O5'	2.35	0.44
19:L:1085:G:C8	19:L:1085:G:OP2	2.70	0.44
19:L:1093:C:OP2	19:L:1093:C:H5	2.00	0.44
19:L:1136:U:OP1	19:L:1136:U:C6	2.70	0.44
19:L:1154:U:H2'	19:L:1155:C:C5	2.49	0.44
20:v:391:LEU:O	20:v:395:TYR:CD2	2.70	0.44
25:m:43:VAL:HG21	25:m:85:ILE:HG22	1.96	0.44
27:h:13:VAL:O	24:i:53:VAL:HG21	2.17	0.44
29:k:15:LEU:C	29:k:15:LEU:CD1	2.86	0.44
29:s:54:PRO:HG2	29:s:57:GLN:CG	2.48	0.44
27:w:16:LYS:HB3	27:w:17:PRO:HD3	2.00	0.44
1:A:484:PHE:CD1	1:A:485:PRO:CB	3.01	0.44
1:A:849:LEU:HD13	1:A:973:GLU:HB2	1.99	0.44
1:A:1216:ILE:HG13	1:A:1254:ASN:HB3	2.00	0.44
1:A:1995:TRP:O	1:A:1999:ILE:HD12	2.17	0.44
2:C:655:LEU:CD2	2:C:655:LEU:C	2.91	0.44
17:D:176:A:N3	27:h:33:PHE:CD1	2.81	0.44
20:v:549:ILE:HD12	20:v:587:MET:CE	2.48	0.44
26:j:33:ASP:OD1	26:j:37:ASN:N	2.51	0.44
30:y:44:LEU:HB3	30:y:47:VAL:HG11	2.00	0.44
1:A:488:ARG:HA	1:A:488:ARG:HD3	1.81	0.44
1:A:1574:PHE:O	1:A:1575:TRP:HB2	2.17	0.44
1:A:1990:ASN:O	1:A:1993:ASP:OD1	2.35	0.44
1:A:2024:MET:HE1	25:z:99:ASP:O	2.17	0.44
2:C:576:THR:HG21	2:C:591:PHE:HD1	1.83	0.44
4:O:309:ARG:O	4:O:327:CYS:SG	2.71	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:320:TYR:CE1	12:d:356:LYS:HA	2.53	0.44
17:D:169:U:O2	26:j:66:ASN:N	2.51	0.44
19:L:2:C:H3'	19:L:2:C:OP2	2.17	0.44
19:L:1093:C:C6	19:L:1093:C:H5''	2.52	0.44
24:u:31:LEU:HD21	24:u:82:LEU:HD21	2.00	0.44
28:e:93:LYS:NZ	25:z:101:LEU:O	2.51	0.44
24:i:31:LEU:HD21	24:i:82:LEU:HD21	2.00	0.44
1:A:1991:ILE:H	1:A:1991:ILE:HG13	1.40	0.43
1:A:2027:LEU:CG	28:e:57:ARG:HE	2.26	0.43
1:A:2043:PHE:CE2	1:A:2047:GLN:HB3	2.53	0.43
2:C:68:HIS:CD2	2:C:68:HIS:O	2.71	0.43
2:C:205:SER:O	30:l:83:LEU:HD23	2.17	0.43
2:C:274:ILE:HD13	2:C:385:PHE:HD2	1.83	0.43
4:O:250:LEU:HD12	4:O:260:ILE:HB	2.00	0.43
17:D:60:U:C6	17:D:61:U:C6	3.05	0.43
19:L:4:A:OP1	19:L:4:A:C8	2.70	0.43
19:L:116:U:C4	29:s:40:HIS:NE2	2.86	0.43
20:v:385:PHE:C	20:v:389:ILE:HD12	2.43	0.43
24:i:30:TRP:CE2	24:i:38:ARG:CD	2.99	0.43
1:A:158:LYS:NZ	7:R:32:ILE:O	2.40	0.43
1:A:1158:ILE:HG12	1:A:1172:PHE:CE1	2.52	0.43
1:A:1526:TRP:O	1:A:1526:TRP:CE3	2.70	0.43
1:A:1995:TRP:CZ3	1:A:2040:TRP:CD1	3.06	0.43
6:Q:51:ARG:HA	6:Q:51:ARG:CZ	2.49	0.43
7:R:69:GLN:HG3	7:R:71:PHE:H	1.82	0.43
11:c:65:PHE:HE2	11:c:73:LEU:HD22	1.83	0.43
19:L:1126:G:H8	19:L:1126:G:O5'	2.01	0.43
20:v:612:ILE:N	20:v:613:PRO:CD	2.81	0.43
25:m:26:TRP:O	25:m:43:VAL:HA	2.17	0.43
25:m:103:LEU:HD23	25:m:107:LEU:HD11	2.01	0.43
29:k:32:GLY:HA3	29:k:47:GLU:O	2.18	0.43
1:A:1889:LEU:HD21	1:A:1991:ILE:CD1	2.47	0.43
2:C:90:LEU:HD13	4:O:211:LEU:HD22	2.00	0.43
2:C:680:SER:OG	2:C:681:CYS:N	2.51	0.43
4:O:135:ILE:HB	4:O:423:ILE:HB	2.01	0.43
7:R:74:LEU:CD1	7:R:78:LYS:HZ3	2.21	0.43
11:c:181:ARG:CZ	12:d:49:ARG:CZ	2.94	0.43
17:D:74:U:O2'	17:D:77:A:N3	2.46	0.43
17:D:167:A:C8	27:h:48:TYR:CZ	3.06	0.43
19:L:70:A:H61	19:L:82:C:H42	1.64	0.43
25:m:47:LEU:CD1	25:m:61:ALA:HB1	2.38	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:j:62:VAL:HG12	24:i:90:ILE:HB	2.00	0.43
29:k:28:ARG:CD	29:k:52:ARG:HG2	2.48	0.43
29:k:52:ARG:HB3	29:k:52:ARG:CZ	2.48	0.43
28:e:91:ILE:HG21	25:z:96:ILE:CD1	2.48	0.43
28:e:93:LYS:HZ3	25:z:103:LEU:HD13	1.82	0.43
30:l:33:LEU:HD23	30:l:33:LEU:C	2.43	0.43
1:A:1347:ARG:HB2	1:A:1447:TRP:CD1	2.54	0.43
1:A:1361:VAL:HG22	1:A:1403:SER:HB2	1.99	0.43
12:d:139:TYR:CG	12:d:155:LEU:HD21	2.53	0.43
19:L:1097:G:C2	19:L:1146:G:C4	3.07	0.43
28:g:105:LEU:C	28:g:105:LEU:CD1	2.88	0.43
29:k:35:MET:CE	29:k:46:ASN:HB2	2.49	0.43
29:s:54:PRO:CG	29:s:57:GLN:HG2	2.47	0.43
25:z:15:VAL:HG11	25:z:29:LEU:HD12	2.00	0.43
1:A:1348:GLU:CD	1:A:1446:THR:HB	2.43	0.43
3:J:23:SER:HA	10:Z:310:HIS:HD2	1.84	0.43
5:P:178:TYR:O	5:P:185:ARG:NH1	2.51	0.43
10:Z:369:TYR:CZ	10:Z:405:ILE:HG23	2.54	0.43
10:Z:402:LEU:HD12	10:Z:405:ILE:HD13	2.01	0.43
11:c:214:ASN:HD21	12:d:44:ARG:HG3	1.83	0.43
16:B:8:C:N4	18:E:45:A:H61	2.14	0.43
18:E:79:A:H3'	18:E:80:U:H5'	2.01	0.43
19:L:1146:G:H2'	19:L:1147:A:C1'	2.48	0.43
29:k:104:SER:O	29:k:107:GLU:HB3	2.17	0.43
28:e:79:LYS:HA	28:e:83:ASN:O	2.19	0.43
25:z:26:TRP:O	25:z:43:VAL:HA	2.17	0.43
1:A:165:LEU:HD13	1:A:578:MET:HB3	2.00	0.43
1:A:1040:ASP:O	1:A:1045:GLN:NE2	2.52	0.43
1:A:1093:LYS:HB3	1:A:1093:LYS:HZ2	1.81	0.43
12:d:364:ILE:O	12:d:368:MET:N	2.48	0.43
19:L:1086:U:OP2	19:L:1086:U:C6	2.71	0.43
26:j:15:ILE:HG12	26:j:73:ALA:HA	2.00	0.43
30:l:36:SER:C	30:l:37:GLU:HG2	2.44	0.43
25:z:31:SER:O	25:z:39:ILE:HG22	2.18	0.43
5:P:179:THR:H	13:I:200:ASN:ND2	2.17	0.43
7:R:124:MET:HB2	16:B:13:G:O6	2.18	0.43
17:D:128:A:N3	17:D:128:A:H2'	2.34	0.43
20:v:728:LEU:O	20:v:732:CYS:N	2.48	0.43
22:b:77:HIS:HA	22:b:98:VAL:HA	1.99	0.43
28:e:77:THR:HB	28:e:86:ASN:HD22	1.84	0.43
24:i:32:PHE:HB3	24:i:34:GLN:OE1	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:721:GLN:O	2:C:724:SER:OG	2.34	0.43
2:C:863:GLU:OE2	2:C:934:HIS:ND1	2.52	0.43
20:v:454:GLY:O	20:v:458:TRP:N	2.52	0.43
25:m:84:TYR:CG	25:m:84:TYR:O	2.71	0.43
29:k:86:ILE:HG21	30:l:10:LEU:HD23	1.99	0.43
29:k:105:LYS:O	29:k:108:ARG:NE	2.52	0.43
29:s:21:ARG:HD3	25:z:67:LEU:O	2.19	0.43
30:y:49:ALA:HB2	30:y:59:MET:HE3	2.01	0.43
1:A:139:LEU:HD13	1:A:193:TYR:CG	2.52	0.43
1:A:864:GLN:HE22	1:A:1101:TYR:N	2.17	0.43
1:A:1991:ILE:O	1:A:1993:ASP:OD2	2.36	0.43
2:C:110:LYS:HD2	2:C:113:ILE:HD12	1.99	0.43
2:C:478:TYR:CE2	2:C:550:VAL:HG23	2.54	0.43
7:R:54:GLN:H	7:R:58:HIS:HD2	1.66	0.43
7:R:102:LEU:O	7:R:106:THR:OG1	2.30	0.43
7:R:163:VAL:HG13	7:R:166:ARG:HH21	1.84	0.43
10:Z:16:GLU:HA	10:Z:19:GLU:HB3	2.01	0.43
12:d:203:LEU:HA	12:d:206:VAL:HG22	2.01	0.43
14:n:67:GLY:HA2	14:n:70:GLY:H	1.84	0.43
17:D:129:G:H1'	17:D:131:A:C2'	2.43	0.43
25:m:17:ILE:HG21	25:m:92:ILE:HG23	1.98	0.43
27:h:67:THR:C	27:h:68:LEU:HD12	2.44	0.43
27:w:80:TYR:HE1	27:w:82:ARG:HD2	1.83	0.43
1:A:964:PHE:O	11:c:85:ARG:NH1	2.42	0.43
4:O:237:ASP:O	4:O:238:LEU:HD23	2.19	0.43
6:Q:119:LYS:O	6:Q:124:GLN:NE2	2.52	0.43
11:c:189:ARG:CZ	12:d:38:LEU:HD13	2.49	0.43
17:D:26:A:N1	17:D:141:G:H1'	2.34	0.43
17:D:67:U:H2'	17:D:68:A:C8	2.54	0.43
19:L:113:U:H5	27:w:48:TYR:CE1	2.30	0.43
25:m:33:SER:HB2	25:m:37:ASN:HB2	2.01	0.43
25:m:96:ILE:CD1	28:g:89:ARG:NH2	2.73	0.43
29:s:54:PRO:CB	29:s:57:GLN:CG	2.88	0.43
1:A:168:LEU:HD21	1:A:626:LEU:HD11	2.01	0.42
1:A:1879:ILE:HG12	1:A:1913:THR:HG22	2.00	0.42
2:C:644:ILE:HG22	2:C:652:MET:HE1	2.00	0.42
6:Q:206:PHE:HB3	6:Q:291:ILE:HD12	2.00	0.42
6:Q:208:TYR:HB2	6:Q:316:LEU:CD1	2.48	0.42
12:d:289:LYS:HD3	12:d:289:LYS:HA	1.90	0.42
12:d:298:GLU:HA	12:d:301:ILE:CG2	2.49	0.42
19:L:119:G:OP2	27:w:76:ASN:ND2	2.39	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:1147:A:O2'	19:L:1148:U:H5'	2.19	0.42
20:v:593:LEU:HD22	20:v:593:LEU:HA	1.84	0.42
25:m:15:VAL:HG22	25:m:16:THR:N	2.33	0.42
25:m:67:LEU:O	29:k:21:ARG:HD3	2.19	0.42
30:l:21:LEU:HD13	30:l:42:VAL:HG21	2.00	0.42
27:w:67:THR:C	27:w:68:LEU:HD12	2.44	0.42
1:A:484:PHE:CD1	1:A:485:PRO:N	2.87	0.42
1:A:591:LEU:HD11	1:A:613:SER:HB2	2.02	0.42
1:A:1048:VAL:HB	1:A:1172:PHE:HB2	2.02	0.42
4:O:307:HIS:HB3	4:O:327:CYS:HB2	2.01	0.42
7:R:87:CYS:HB3	7:R:91:HIS:CE1	2.54	0.42
7:R:234:ALA:HB2	7:R:237:ARG:HH21	1.84	0.42
11:c:213:TYR:CD1	11:c:218:VAL:HG21	2.54	0.42
13:I:105:TYR:O	13:I:105:TYR:HD1	2.02	0.42
17:D:175:G:P	28:g:49:ARG:HH12	2.42	0.42
19:L:120:G:H4'	19:L:121:C:H5'	2.01	0.42
19:L:125:C:H4'	28:e:81:GLY:H	1.83	0.42
20:v:385:PHE:CD1	20:v:388:LEU:HD12	2.54	0.42
28:e:91:ILE:HD12	28:e:94:LEU:CD1	2.48	0.42
1:A:306:PRO:HD2	1:A:307:GLU:H	1.83	0.42
1:A:1991:ILE:O	1:A:2040:TRP:CD1	2.73	0.42
1:A:2080:LYS:HB2	1:A:2084:LEU:HD21	2.00	0.42
11:c:82:ASN:OD1	11:c:82:ASN:N	2.51	0.42
11:c:217:ILE:HG12	12:d:83:ARG:HG2	2.02	0.42
13:I:105:TYR:CD1	13:I:105:TYR:C	2.95	0.42
17:D:173:U:C1'	28:g:99:ASP:HB3	2.34	0.42
20:v:397:ASN:HD22	20:v:397:ASN:HA	1.66	0.42
20:v:529:HIS:O	20:v:529:HIS:CG	2.71	0.42
26:j:23:ARG:NH2	26:j:23:ARG:HG2	2.34	0.42
29:k:51:GLU:HB3	29:k:77:VAL:HG11	2.02	0.42
30:l:77:LEU:C	30:l:79:LYS:N	2.76	0.42
25:z:45:LEU:HG	25:z:45:LEU:O	2.20	0.42
1:A:372:ARG:HD2	2:C:973:ARG:HD2	2.00	0.42
1:A:1012:TRP:HB2	1:A:1162:THR:HA	2.01	0.42
1:A:1573:LEU:HD12	1:A:1825:ILE:CG2	2.46	0.42
1:A:1910:LYS:HE2	1:A:1940:MET:HG2	2.01	0.42
2:C:106:PHE:O	17:D:44:A:H3'	2.19	0.42
2:C:184:GLU:HG2	2:C:191:ILE:HD12	2.00	0.42
2:C:222:MET:HE3	2:C:933:TRP:HZ2	1.83	0.42
6:Q:306:THR:CG2	6:Q:307:ALA:N	2.82	0.42
11:c:237:ILE:HD11	12:d:85:ARG:HH22	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:s:31:ILE:O	29:s:48:CYS:HA	2.19	0.42
1:A:140:ARG:HD3	1:A:252:GLU:OE2	2.18	0.42
1:A:1010:PRO:HD2	1:A:1013:ILE:HD12	2.01	0.42
1:A:1365:THR:HG21	3:J:15:SER:HB3	2.01	0.42
2:C:944:VAL:HG13	2:C:945:LEU:HD12	2.01	0.42
4:O:370:ASN:C	4:O:372:VAL:N	2.73	0.42
7:R:34:TYR:O	7:R:36:LYS:N	2.52	0.42
17:D:129:G:C2'	17:D:129:G:N3	2.82	0.42
17:D:169:U:H1'	26:j:66:ASN:HB2	2.01	0.42
19:L:1084:A:H2'	19:L:1084:A:N3	2.34	0.42
20:v:342:ILE:O	20:v:346:TYR:N	2.45	0.42
24:u:28:THR:N	24:u:91:THR:O	2.49	0.42
25:m:84:TYR:CG	29:k:6:VAL:HG11	2.41	0.42
26:j:74:LEU:H	26:j:74:LEU:HG	1.65	0.42
29:k:35:MET:HE2	29:k:46:ASN:CA	2.50	0.42
28:e:78:GLU:HG3	25:z:52:LEU:HD22	2.00	0.42
30:y:41:ASN:HB3	30:y:66:GLY:H	1.83	0.42
1:A:140:ARG:CD	1:A:252:GLU:HG2	2.45	0.42
1:A:275:TYR:HB3	1:A:307:GLU:HG2	2.00	0.42
1:A:404:ASN:CB	2:C:919:ARG:NH2	2.83	0.42
1:A:428:LEU:CD2	2:C:896:GLY:O	2.59	0.42
1:A:470:LEU:HB2	1:A:473:THR:HG23	2.01	0.42
1:A:1972:ASP:HB3	28:e:41:ARG:NH2	2.35	0.42
1:A:2024:MET:CE	28:e:93:LYS:HE3	2.35	0.42
4:O:326:ALA:HB2	4:O:356:LEU:HD11	2.02	0.42
18:E:23:G:C5'	18:E:23:G:H8	2.33	0.42
28:g:50:ASN:CB	28:g:52:HIS:ND1	2.69	0.42
29:k:35:MET:SD	30:l:84:PHE:CE2	3.13	0.42
25:z:103:LEU:HD23	25:z:107:LEU:HD11	2.01	0.42
1:A:168:LEU:HD23	1:A:622:MET:CE	2.30	0.42
1:A:709:ARG:HH22	17:D:83:C:P	2.42	0.42
1:A:1624:LEU:HD21	1:A:1635:HIS:CE1	2.54	0.42
2:C:607:LEU:HD21	2:C:644:ILE:CD1	2.50	0.42
12:d:241:MET:HG3	12:d:279:LEU:CD1	2.45	0.42
17:D:35:A:H2'	17:D:36:A:C8	2.55	0.42
19:L:1146:G:C4	19:L:1147:A:C5	3.07	0.42
23:t:105:PRO:O	23:t:109:SER:OG	2.37	0.42
26:j:74:LEU:O	26:j:74:LEU:HD12	2.20	0.42
28:e:54:ILE:HB	28:e:72:VAL:HG22	2.01	0.42
1:A:261:LEU:HD12	1:A:261:LEU:HA	1.91	0.42
1:A:1268:ARG:HB3	1:A:1301:TYR:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1660:SER:OG	1:A:1809:ASN:OD1	2.29	0.42
2:C:495:ARG:HE	2:C:554:HIS:HA	1.83	0.42
7:R:251:VAL:O	7:R:255:ASN:ND2	2.53	0.42
19:L:1082:A:C2	19:L:1083:A:C5	3.07	0.42
28:e:91:ILE:CG2	25:z:96:ILE:CG2	2.98	0.42
1:A:342:LEU:CD1	1:A:392:ASN:HD21	2.31	0.42
1:A:426:PRO:HG3	10:Z:201:ARG:NH1	2.31	0.42
1:A:898:ILE:N	1:A:1073:ILE:O	2.45	0.42
1:A:1711:VAL:HB	1:A:1789:ASN:HB3	2.02	0.42
1:A:1967:ALA:O	1:A:1971:ILE:N	2.39	0.42
1:A:2047:GLN:HG2	1:A:2051:ILE:HG13	2.01	0.42
4:O:345:PHE:O	4:O:450:ARG:NH2	2.53	0.42
12:d:270:ALA:HB1	12:d:280:LEU:HD11	2.02	0.42
12:d:271:ILE:O	12:d:274:TRP:C	2.63	0.42
16:B:264:U:H2'	16:B:265:A:O5'	2.19	0.42
17:D:67:U:H2'	17:D:68:A:H8	1.85	0.42
30:l:41:ASN:ND2	30:l:63:PHE:CZ	2.88	0.42
1:A:269:ASP:HB3	1:A:272:ASP:HB2	2.02	0.42
1:A:1035:LEU:HD11	1:A:1038:ILE:CG1	2.48	0.42
1:A:1748:ILE:HG12	1:A:1783:MET:HB3	2.01	0.42
1:A:1993:ASP:HB3	1:A:2038:HIS:HB3	2.00	0.42
2:C:161:ILE:HG22	2:C:163:ASP:H	1.85	0.42
2:C:352:VAL:O	2:C:372:THR:OG1	2.23	0.42
7:R:159:ARG:NH2	7:R:206:LEU:HD12	2.30	0.42
12:d:269:ILE:O	12:d:273:LYS:CB	2.68	0.42
17:D:168:U:H2'	24:i:49:PHE:CE1	2.53	0.42
19:L:1097:G:H21	19:L:1146:G:H1'	1.84	0.42
1:A:814:ARG:NH2	4:O:369:ASP:OD1	2.46	0.41
7:R:117:PHE:HE2	7:R:127:ILE:HD12	1.85	0.41
9:T:151:ARG:CZ	14:n:71:SER:HB3	2.50	0.41
11:c:252:GLY:CA	12:d:38:LEU:O	2.64	0.41
25:m:104:ASP:OD1	25:m:105:SER:N	2.53	0.41
29:k:44:VAL:CG2	29:k:86:ILE:HG22	2.36	0.41
30:l:44:LEU:HD23	30:l:44:LEU:N	2.32	0.41
24:i:28:THR:N	24:i:91:THR:O	2.49	0.41
27:w:45:THR:HA	27:w:50:ASN:O	2.20	0.41
1:A:146:HIS:HB3	1:A:149:MET:HE3	2.02	0.41
1:A:1896:THR:HA	1:A:1899:TRP:CD1	2.49	0.41
4:O:420:ASP:OD1	4:O:422:SER:OG	2.36	0.41
10:Z:37:LEU:HD23	10:Z:214:ILE:HG13	2.01	0.41
10:Z:148:LEU:HA	10:Z:151:VAL:HG12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Z:322:LYS:HE3	10:Z:357:TRP:CE2	2.55	0.41
17:D:174:G:H2'	28:g:49:ARG:NH1	2.35	0.41
25:m:52:LEU:CD2	28:g:79:LYS:CA	2.98	0.41
26:j:14:LYS:CD	26:j:74:LEU:HD11	2.49	0.41
26:j:15:ILE:O	26:j:26:ALA:HA	2.19	0.41
28:e:89:ARG:NH1	28:e:91:ILE:HD11	2.35	0.41
1:A:383:TYR:OH	2:C:917:ASP:OD2	2.37	0.41
2:C:607:LEU:HD23	2:C:644:ILE:HD12	2.01	0.41
2:C:711:ALA:HB2	2:C:821:LEU:HD11	2.02	0.41
2:C:780:PRO:O	2:C:784:SER:N	2.35	0.41
4:O:307:HIS:NE2	4:O:325:SER:OG	2.45	0.41
5:P:104:LEU:HD12	5:P:108:ASN:HB2	2.01	0.41
12:d:125:ALA:HB1	12:d:135:LEU:HD22	2.02	0.41
19:L:1093:C:O2'	30:y:54:GLY:HA3	2.20	0.41
19:L:1095:U:C2'	19:L:1096:C:C6	3.03	0.41
19:L:1137:U:H6	19:L:1137:U:H3'	1.85	0.41
22:b:84:ASN:O	22:b:106:ASN:HA	2.21	0.41
25:m:45:LEU:HG	25:m:45:LEU:O	2.20	0.41
27:h:45:THR:HA	27:h:50:ASN:O	2.20	0.41
27:h:74:ARG:NE	28:g:99:ASP:HA	2.35	0.41
31:p:98:LEU:HG	31:q:99:ARG:HE	1.84	0.41
1:A:737:ARG:NH2	18:E:70:U:OP2	2.51	0.41
1:A:880:THR:HG23	5:P:211:ALA:HB2	2.02	0.41
1:A:1154:LYS:HA	1:A:1159:ARG:HH12	1.85	0.41
1:A:1408:PRO:HB3	1:A:1422:ILE:HG23	2.02	0.41
5:P:35:ALA:H	12:d:123:ASN:HD21	1.66	0.41
20:v:442:THR:HA	20:v:443:PRO:HD3	1.91	0.41
20:v:552:LEU:HD13	20:v:570:THR:HA	2.02	0.41
20:v:686:ILE:HG21	20:v:713:ILE:HG21	2.03	0.41
30:l:44:LEU:HB2	30:l:62:ILE:HG22	2.02	0.41
30:l:44:LEU:CB	30:l:47:VAL:CG1	2.97	0.41
24:i:35:ILE:HG22	24:i:37:ILE:HG12	2.02	0.41
4:O:218:ARG:HG3	4:O:256:ARG:HD3	2.02	0.41
5:P:76:ARG:NE	6:Q:5:ILE:HD12	2.32	0.41
6:Q:304:THR:CG2	7:R:153:PRO:HG2	2.50	0.41
6:Q:316:LEU:O	6:Q:319:LEU:N	2.53	0.41
9:T:123:ARG:NH2	18:E:26:A:O2'	2.47	0.41
11:c:16:VAL:HG13	11:c:152:LEU:HD12	2.01	0.41
11:c:544:LEU:HA	11:c:547:HIS:HB2	2.02	0.41
19:L:1085:G:N2	19:L:1086:U:C6	2.87	0.41
29:k:86:ILE:CG1	30:l:72:ILE:HB	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:l:34:VAL:CG2	30:l:45:ARG:HB2	2.51	0.41
30:l:83:LEU:HD12	30:l:84:PHE:N	2.35	0.41
26:x:35:PHE:O	26:x:36:LEU:CB	2.68	0.41
1:A:500:ALA:HB1	1:A:503:LYS:HB2	2.03	0.41
1:A:796:ASN:ND2	1:A:861:GLN:OE1	2.54	0.41
1:A:1015:PRO:HD2	1:A:1510:ILE:HD13	2.03	0.41
1:A:1287:ASP:HB3	1:A:1296:ARG:HG2	2.03	0.41
1:A:1361:VAL:HG21	1:A:1407:ILE:HD11	2.02	0.41
1:A:1709:TRP:N	1:A:1729:THR:O	2.54	0.41
6:Q:207:LEU:O	6:Q:249:GLY:N	2.50	0.41
7:R:109:LEU:HD13	7:R:113:GLY:HA2	2.01	0.41
7:R:147:ASN:HD21	7:R:215:ARG:HA	1.85	0.41
12:d:133:ASP:OD2	13:I:98:ASP:HB2	2.20	0.41
17:D:2:A:N1	17:D:164:C:N4	2.67	0.41
26:j:72:GLU:O	26:j:72:GLU:HG3	2.19	0.41
29:k:28:ARG:HD2	29:k:50:GLU:OE1	2.21	0.41
1:A:1312:PHE:CE2	1:A:1316:ILE:HD11	2.56	0.41
1:A:1965:PHE:HE1	1:A:2012:LEU:HD13	1.85	0.41
1:A:2075:THR:O	1:A:2079:ILE:N	2.44	0.41
32:A:3000:IHP:O12	32:A:3000:IHP:P1	2.79	0.41
5:P:179:THR:H	13:I:200:ASN:HD21	1.66	0.41
11:c:166:LYS:HG2	18:E:52:G:H4'	2.03	0.41
11:c:219:TYR:O	12:d:90:ARG:HD2	2.21	0.41
19:L:4:A:OP1	19:L:4:A:H8	2.03	0.41
19:L:1082:A:O2'	19:L:1083:A:H5'	2.21	0.41
29:k:59:ASP:HA	29:k:62:ARG:HH21	1.86	0.41
27:w:30:LYS:HD2	27:w:80:TYR:CE2	2.55	0.41
1:A:982:TYR:HD2	1:A:1106:GLY:H	1.68	0.41
1:A:1212:ARG:HA	1:A:1259:LEU:HD11	2.02	0.41
1:A:1271:PRO:HG2	1:A:1274:ARG:HB2	2.01	0.41
1:A:1654:TRP:CD1	1:A:1692:TYR:HB3	2.55	0.41
2:C:722:ASP:OD2	2:C:755:TYR:OH	2.37	0.41
2:C:808:LEU:O	2:C:971:ARG:NH1	2.46	0.41
25:m:3:LEU:HD21	28:g:95:PHE:HE1	1.83	0.41
27:h:33:PHE:HZ	28:g:49:ARG:NE	2.19	0.41
28:e:50:ASN:O	28:e:51:ASN:HB3	2.21	0.41
29:s:15:LEU:O	29:s:16:ILE:HD13	2.20	0.41
29:s:48:CYS:SG	29:s:85:THR:HG23	2.60	0.41
27:w:79:LEU:HD22	27:w:80:TYR:HD2	1.86	0.41
1:A:305:LEU:N	1:A:306:PRO:HD3	2.36	0.41
2:C:586:MET:CG	2:C:589:LEU:HD21	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:271:GLN:HG2	4:O:314:THR:H	1.84	0.41
4:O:309:ARG:HH11	4:O:328:THR:HG21	1.75	0.41
4:O:365:PHE:CE1	4:O:373:LEU:HB2	2.56	0.41
5:P:193:GLU:OE1	5:P:195:ASN:N	2.51	0.41
6:Q:269:THR:HG22	6:Q:279:GLY:HA2	2.02	0.41
11:c:241:PHE:CD1	12:d:79:HIS:O	2.74	0.41
17:D:168:U:C5	24:i:49:PHE:CE1	3.08	0.41
19:L:114:U:O2'	30:y:65:ARG:NH2	2.53	0.41
19:L:1085:G:N3	19:L:1086:U:H5	2.12	0.41
19:L:1097:G:N2	19:L:1146:G:HI'	2.36	0.41
20:v:687:LEU:HD22	20:v:688:ARG:HH21	1.85	0.41
22:b:68:PRO:O	22:b:69:ASP:CB	2.69	0.41
25:m:3:LEU:HD23	28:g:95:PHE:CE1	2.53	0.41
29:k:18:TYR:HE1	29:k:101:PRO:HD3	1.84	0.41
29:k:84:LEU:O	30:l:74:VAL:CG2	2.68	0.41
28:e:67:MET:HG3	28:e:69:LEU:CD1	2.50	0.41
29:s:30:TYR:HD2	29:s:87:LEU:HD21	1.86	0.41
30:l:71:PHE:C	30:l:71:PHE:HD1	2.27	0.41
31:p:98:LEU:HD12	31:q:98:LEU:HG	2.03	0.41
1:A:1576:GLU:HG3	1:A:1826:TYR:HE2	1.86	0.41
1:A:2043:PHE:CG	1:A:2044:THR:N	2.89	0.41
1:A:2056:ARG:O	1:A:2060:LEU:HG	2.20	0.41
2:C:607:LEU:HD12	2:C:607:LEU:C	2.45	0.41
12:d:270:ALA:HB1	12:d:280:LEU:HD21	2.01	0.41
12:d:391:LEU:O	12:d:395:ILE:N	2.53	0.41
17:D:28:G:O2'	17:D:29:G:P	2.79	0.41
20:v:711:MET:HE1	20:v:748:PHE:HA	1.99	0.41
25:m:33:SER:HB2	25:m:37:ASN:CB	2.50	0.41
25:m:67:LEU:HB3	29:k:29:VAL:CG2	2.49	0.41
28:g:26:PHE:CE1	28:g:63:ARG:HA	2.56	0.41
28:g:49:ARG:N	28:g:100:SER:O	2.49	0.41
29:k:20:LEU:HD12	29:k:34:LEU:HB2	2.03	0.41
30:l:17:HIS:CE1	30:l:77:LEU:HD11	2.52	0.41
30:l:21:LEU:CD2	30:l:72:ILE:CD1	2.99	0.41
1:A:305:LEU:C	1:A:305:LEU:HD13	2.46	0.40
1:A:394:ARG:HD3	2:C:610:LEU:HD13	2.02	0.40
1:A:1526:TRP:CE3	1:A:1526:TRP:C	2.98	0.40
7:R:207:PRO:HA	7:R:212:TRP:CD2	2.55	0.40
11:c:160:LEU:HD23	13:I:196:ILE:HG12	2.02	0.40
12:d:255:ALA:HB2	12:d:291:PHE:CD2	2.48	0.40
19:L:1129:U:C2'	19:L:1130:U:O5'	2.69	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:j:29:LEU:C	26:j:29:LEU:CD2	2.86	0.40
29:k:29:VAL:O	29:k:50:GLU:CA	2.58	0.40
29:k:85:THR:HG22	30:l:73:VAL:HG13	2.03	0.40
25:z:93:ARG:HG2	25:z:94:GLN:HG3	2.03	0.40
25:z:104:ASP:OD1	25:z:105:SER:N	2.53	0.40
1:A:484:PHE:CZ	1:A:485:PRO:HB3	2.50	0.40
1:A:760:ASN:OD1	4:O:244:ARG:NE	2.40	0.40
1:A:804:MET:HE3	1:A:805:PRO:HD2	2.04	0.40
1:A:982:TYR:CD2	1:A:1104:ILE:HG23	2.56	0.40
2:C:385:PHE:HE1	2:C:425:LEU:HD11	1.87	0.40
4:O:200:VAL:HG21	4:O:230:VAL:HG22	2.00	0.40
12:d:240:ASP:CG	12:d:277:ASN:HB3	2.46	0.40
14:n:63:ARG:HD2	14:n:72:TRP:CH2	2.56	0.40
19:L:35:U:H6	19:L:35:U:C5'	2.34	0.40
19:L:117:U:O2	25:z:35:GLN:O	2.39	0.40
27:h:51:LEU:HB2	27:h:73:ILE:HB	2.04	0.40
29:k:28:ARG:CG	29:k:52:ARG:HG2	2.48	0.40
29:k:30:TYR:HH	30:l:71:PHE:HD2	1.69	0.40
1:A:231:ARG:HD2	1:A:231:ARG:HA	1.96	0.40
1:A:1095:MET:H	1:A:1095:MET:HG2	1.55	0.40
2:C:152:LEU:HD23	2:C:152:LEU:HA	1.89	0.40
4:O:281:VAL:HB	4:O:293:TRP:HB2	2.03	0.40
4:O:392:MET:HE2	8:S:156:TYR:HD2	1.85	0.40
9:T:150:CYS:SG	9:T:152:GLY:N	2.90	0.40
12:d:51:ARG:NE	12:d:75:GLU:OE2	2.51	0.40
12:d:141:ILE:CG2	13:I:105:TYR:CD1	3.05	0.40
12:d:189:TYR:HA	12:d:192:TYR:HB3	2.03	0.40
13:I:205:GLU:O	13:I:208:SER:OG	2.31	0.40
17:D:131:A:H5''	17:D:132:A:H8	1.86	0.40
17:D:169:U:C6	26:j:35:PHE:CD1	3.10	0.40
28:g:77:THR:CB	28:g:86:ASN:HD22	2.34	0.40
29:k:30:TYR:CE1	29:k:50:GLU:CB	3.04	0.40
29:k:105:LYS:HA	29:k:108:ARG:HE	1.86	0.40
28:e:69:LEU:HD12	28:e:69:LEU:N	2.36	0.40
28:e:70:GLU:HG3	28:e:70:GLU:H	1.73	0.40
28:e:92:SER:CB	25:z:99:ASP:OD1	2.70	0.40
24:i:31:LEU:HD12	24:i:37:ILE:HG13	2.04	0.40
24:i:54:ILE:CD1	24:i:57:ALA:CB	3.00	0.40
1:A:312:TYR:HE1	1:A:482:SER:OG	2.05	0.40
1:A:997:GLN:OE1	1:A:1511:ARG:NH2	2.54	0.40
1:A:1794:LEU:O	1:A:1798:ILE:N	2.45	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1810:PRO:HB3	1:A:1911:TRP:CE2	2.56	0.40
1:A:2021:SER:O	1:A:2024:MET:HB2	2.21	0.40
2:C:299:THR:HG22	2:C:302:ASN:H	1.86	0.40
6:Q:251:LEU:HD11	6:Q:253:PHE:CZ	2.56	0.40
12:d:137:TYR:CE2	13:I:102:LYS:HA	2.56	0.40
12:d:288:GLU:HB3	12:d:297:ILE:HG13	2.03	0.40
12:d:330:ILE:HG21	12:d:339:MET:HA	2.02	0.40
17:D:103:A:HO2'	17:D:104:G:P	2.39	0.40
19:L:121:C:N4	27:w:33:PHE:CD1	2.90	0.40
25:m:83:GLN:HE22	25:m:84:TYR:HB2	1.82	0.40
27:h:30:LYS:HD2	27:h:80:TYR:CE2	2.56	0.40
28:e:47:SER:HB2	28:e:103:VAL:HG12	2.04	0.40
28:e:73:LYS:HE3	28:e:90:PHE:CE2	2.56	0.40
25:z:10:LEU:O	25:z:10:LEU:HD23	2.22	0.40
31:r:19:SER:OG	31:r:38:ASP:OD2	2.34	0.40
31:r:85:GLN:HG2	31:p:80:LEU:HD21	2.03	0.40
19:L:1106:G:C5'	19:L:1107:C:OP1	2.70	0.40
20:v:385:PHE:HD1	20:v:388:LEU:HD12	1.85	0.40
24:u:90:ILE:HB	26:x:62:VAL:CG1	2.52	0.40
25:m:4:VAL:CG2	25:m:36:MET:HE2	2.45	0.40
26:j:15:ILE:HG12	26:j:73:ALA:CB	2.51	0.40
27:h:79:LEU:HD22	27:h:80:TYR:HD2	1.86	0.40
28:g:50:ASN:HB2	28:g:52:HIS:CE1	2.55	0.40
28:e:89:ARG:HH22	28:e:91:ILE:CD1	2.33	0.40
27:w:51:LEU:HB2	27:w:73:ILE:HB	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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
1	A	1905/2413 (79%)	1826 (96%)	68 (4%)	11 (1%)	21 54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	914/1008 (91%)	881 (96%)	33 (4%)	0	100	100
3	J	25/135 (18%)	23 (92%)	2 (8%)	0	100	100
4	O	355/451 (79%)	315 (89%)	36 (10%)	4 (1%)	11	43
5	P	197/379 (52%)	192 (98%)	5 (2%)	0	100	100
6	Q	288/364 (79%)	264 (92%)	22 (8%)	2 (1%)	18	51
7	R	259/339 (76%)	248 (96%)	10 (4%)	1 (0%)	30	61
8	S	64/175 (37%)	63 (98%)	1 (2%)	0	100	100
9	T	155/157 (99%)	147 (95%)	8 (5%)	0	100	100
10	Z	443/577 (77%)	427 (96%)	16 (4%)	0	100	100
11	c	418/590 (71%)	396 (95%)	19 (4%)	3 (1%)	18	51
12	d	534/687 (78%)	513 (96%)	18 (3%)	3 (1%)	21	54
13	I	98/215 (46%)	97 (99%)	1 (1%)	0	100	100
14	n	21/455 (5%)	21 (100%)	0	0	100	100
15	H	7/235 (3%)	7 (100%)	0	0	100	100
20	v	666/859 (78%)	642 (96%)	22 (3%)	2 (0%)	36	65
21	a	82/111 (74%)	78 (95%)	3 (4%)	1 (1%)	10	41
22	b	165/238 (69%)	138 (84%)	20 (12%)	7 (4%)	2	19
23	t	150/175 (86%)	145 (97%)	4 (3%)	1 (1%)	18	51
24	i	70/94 (74%)	67 (96%)	3 (4%)	0	100	100
24	u	70/94 (74%)	67 (96%)	3 (4%)	0	100	100
25	m	117/146 (80%)	111 (95%)	6 (5%)	0	100	100
25	z	106/146 (73%)	100 (94%)	6 (6%)	0	100	100
26	j	73/77 (95%)	67 (92%)	5 (7%)	1 (1%)	9	38
26	x	73/77 (95%)	65 (89%)	7 (10%)	1 (1%)	9	38
27	h	64/86 (74%)	60 (94%)	4 (6%)	0	100	100
27	w	64/86 (74%)	61 (95%)	3 (5%)	0	100	100
28	e	99/110 (90%)	95 (96%)	3 (3%)	1 (1%)	12	45
28	g	99/110 (90%)	93 (94%)	4 (4%)	2 (2%)	6	32
29	k	96/196 (49%)	90 (94%)	5 (5%)	1 (1%)	12	45
29	s	89/196 (45%)	83 (93%)	6 (7%)	0	100	100
30	l	81/101 (80%)	79 (98%)	0	2 (2%)	4	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	y	79/101 (78%)	75 (95%)	4 (5%)	0	100	100
31	o	120/503 (24%)	115 (96%)	5 (4%)	0	100	100
31	p	122/503 (24%)	118 (97%)	4 (3%)	0	100	100
31	q	125/503 (25%)	116 (93%)	9 (7%)	0	100	100
31	r	119/503 (24%)	112 (94%)	7 (6%)	0	100	100
All	All	8412/13195 (64%)	7997 (95%)	372 (4%)	43 (0%)	26	57

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1575	TRP
1	A	1965	PHE
4	O	372	VAL
12	d	181	ASN
12	d	353	GLU
21	a	68	GLN
22	b	68	PRO
22	b	95	PRO
22	b	125	LYS
22	b	149	PRO
26	j	75	ASP
1	A	260	PRO
1	A	1277	GLU
1	A	1491	ILE
1	A	1964	PRO
4	O	351	GLY
4	O	371	GLY
11	c	43	LYS
20	v	798	LYS
22	b	98	VAL
23	t	112	SER
28	g	51	ASN
28	g	65	CYS
29	k	41	MET
28	e	51	ASN
30	l	78	LEU
1	A	510	PRO
1	A	1490	ARG
7	R	206	LEU
11	c	42	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	d	63	LEU
20	v	515	PRO
22	b	67	ILE
22	b	94	LEU
1	A	1522	ASN
30	l	40	MET
26	x	75	ASP
4	O	352	ILE
6	Q	256	SER
1	A	1156	HIS
1	A	1157	PRO
6	Q	191	PRO
11	c	418	PRO

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	
1	A	1737/2182 (80%)	1706 (98%)	31 (2%)	51	68
2	C	830/910 (91%)	824 (99%)	6 (1%)	76	78
3	J	21/121 (17%)	21 (100%)	0	100	100
4	O	312/397 (79%)	309 (99%)	3 (1%)	68	75
5	P	175/328 (53%)	173 (99%)	2 (1%)	65	74
6	Q	265/332 (80%)	259 (98%)	6 (2%)	44	64
7	R	224/296 (76%)	223 (100%)	1 (0%)	84	81
8	S	57/151 (38%)	55 (96%)	2 (4%)	32	57
9	T	141/141 (100%)	140 (99%)	1 (1%)	76	78
10	Z	417/538 (78%)	415 (100%)	2 (0%)	81	80
11	c	214/525 (41%)	204 (95%)	10 (5%)	23	50
12	d	274/633 (43%)	268 (98%)	6 (2%)	45	65
13	I	92/193 (48%)	92 (100%)	0	100	100
14	n	19/412 (5%)	19 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	H	9/216 (4%)	9 (100%)	0	100	100
20	v	294/786 (37%)	278 (95%)	16 (5%)	20	47
23	t	39/165 (24%)	26 (67%)	13 (33%)	0	2
24	i	55/83 (66%)	52 (94%)	3 (6%)	19	47
24	u	52/83 (63%)	51 (98%)	1 (2%)	50	67
25	m	106/129 (82%)	93 (88%)	13 (12%)	4	23
25	z	95/129 (74%)	92 (97%)	3 (3%)	34	58
26	j	56/66 (85%)	47 (84%)	9 (16%)	2	15
26	x	56/66 (85%)	55 (98%)	1 (2%)	51	68
27	h	51/77 (66%)	51 (100%)	0	100	100
27	w	51/77 (66%)	51 (100%)	0	100	100
28	e	82/103 (80%)	76 (93%)	6 (7%)	13	40
28	g	82/103 (80%)	75 (92%)	7 (8%)	10	35
29	k	92/176 (52%)	80 (87%)	12 (13%)	4	21
29	s	85/176 (48%)	82 (96%)	3 (4%)	32	57
30	l	72/89 (81%)	54 (75%)	18 (25%)	0	4
30	y	68/89 (76%)	68 (100%)	0	100	100
31	o	60/451 (13%)	57 (95%)	3 (5%)	22	49
31	p	62/451 (14%)	58 (94%)	4 (6%)	15	43
31	q	62/451 (14%)	59 (95%)	3 (5%)	23	50
31	r	60/451 (13%)	57 (95%)	3 (5%)	22	49
All	All	6367/11576 (55%)	6179 (97%)	188 (3%)	37	59

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	249	LEU
1	A	316	THR
1	A	317	PRO
1	A	331	PHE
1	A	462	LEU
1	A	518	VAL
1	A	621	LEU
1	A	667	TYR
1	A	742	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	770	MET
1	A	912	LEU
1	A	1093	LYS
1	A	1094	ASP
1	A	1095	MET
1	A	1182	LEU
1	A	1222	LEU
1	A	1262	MET
1	A	1270	LEU
1	A	1375	LEU
1	A	1379	MET
1	A	1488	ILE
1	A	1489	PRO
1	A	1523	SER
1	A	1661	ILE
1	A	1748	ILE
1	A	1961	LEU
1	A	1965	PHE
1	A	1991	ILE
1	A	1992	TYR
1	A	1993	ASP
1	A	2084	LEU
2	C	90	LEU
2	C	267	ILE
2	C	545	LEU
2	C	655	LEU
2	C	841	LEU
2	C	879	LEU
4	O	230	VAL
4	O	236	LEU
4	O	309	ARG
5	P	30	LEU
5	P	122	LEU
6	Q	51	ARG
6	Q	105	LYS
6	Q	109	MET
6	Q	251	LEU
6	Q	282	LEU
6	Q	291	ILE
7	R	74	LEU
8	S	35	THR
8	S	36	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	T	153	CYS
10	Z	194	LEU
10	Z	470	LEU
11	c	41	GLN
11	c	42	LYS
11	c	43	LYS
11	c	227	ILE
11	c	504	PRO
11	c	505	PRO
11	c	506	THR
11	c	517	VAL
11	c	532	PRO
11	c	550	PRO
12	d	62	ARG
12	d	155	LEU
12	d	263	SER
12	d	271	ILE
12	d	284	LEU
12	d	285	LEU
20	v	385	PHE
20	v	386	GLU
20	v	397	ASN
20	v	398	ASP
20	v	438	ARG
20	v	529	HIS
20	v	530	ARG
20	v	538	LEU
20	v	544	ILE
20	v	576	THR
20	v	582	LEU
20	v	593	LEU
20	v	612	ILE
20	v	652	LEU
20	v	665	ILE
20	v	719	THR
23	t	13	PRO
23	t	76	THR
23	t	77	PRO
23	t	85	THR
23	t	96	PRO
23	t	100	THR
23	t	105	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	t	108	SER
23	t	109	SER
23	t	111	VAL
23	t	133	PRO
23	t	136	VAL
23	t	150	THR
24	u	35	ILE
25	m	33	SER
25	m	35	GLN
25	m	37	ASN
25	m	39	ILE
25	m	45	LEU
25	m	46	THR
25	m	47	LEU
25	m	52	LEU
25	m	60	ILE
25	m	85	ILE
25	m	86	ASN
25	m	92	ILE
25	m	93	ARG
26	j	18	ASN
26	j	19	ILE
26	j	20	ASN
26	j	22	SER
26	j	23	ARG
26	j	29	LEU
26	j	39	VAL
26	j	64	ARG
26	j	74	LEU
28	g	33	LEU
28	g	35	ASN
28	g	41	ARG
28	g	42	THR
28	g	57	ARG
28	g	84	VAL
28	g	85	ILE
29	k	14	ASN
29	k	15	LEU
29	k	39	LYS
29	k	41	MET
29	k	43	LEU
29	k	49	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	k	50	GLU
29	k	82	LEU
29	k	104	SER
29	k	105	LYS
29	k	106	LYS
29	k	109	LEU
28	e	41	ARG
28	e	70	GLU
28	e	88	GLU
28	e	91	ILE
28	e	92	SER
28	e	94	LEU
29	s	15	LEU
29	s	56	THR
29	s	82	LEU
30	l	11	LEU
30	l	15	GLN
30	l	23	LEU
30	l	32	LYS
30	l	36	SER
30	l	37	GLU
30	l	38	ASP
30	l	45	ARG
30	l	47	VAL
30	l	64	VAL
30	l	65	ARG
30	l	70	LYS
30	l	73	VAL
30	l	77	LEU
30	l	79	LYS
30	l	83	LEU
30	l	84	PHE
30	l	85	LYS
24	i	18	PHE
24	i	22	GLN
24	i	40	LYS
26	x	74	LEU
25	z	45	LEU
25	z	54	LYS
25	z	55	LEU
31	r	17	PRO
31	r	44	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	r	63	THR
31	p	17	PRO
31	p	44	PRO
31	p	63	THR
31	p	98	LEU
31	q	17	PRO
31	q	44	PRO
31	q	55	PRO
31	o	17	PRO
31	o	44	PRO
31	o	63	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	HIS
1	A	185	GLN
1	A	254	HIS
1	A	310	ASN
1	A	429	ASN
1	A	532	ASN
1	A	580	ASN
1	A	592	HIS
1	A	658	ASN
1	A	659	HIS
1	A	830	ASN
1	A	864	GLN
1	A	948	HIS
1	A	952	ASN
1	A	1005	GLN
1	A	1067	ASN
1	A	1190	ASN
1	A	1449	ASN
1	A	1466	GLN
1	A	1522	ASN
1	A	1540	ASN
1	A	1618	ASN
1	A	1626	GLN
1	A	1687	HIS
1	A	1730	ASN
1	A	1737	GLN
1	A	1863	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1990	ASN
1	A	2068	ASN
2	C	84	GLN
2	C	103	HIS
2	C	108	GLN
2	C	220	ASN
2	C	251	GLN
2	C	289	ASN
2	C	294	ASN
2	C	403	ASN
2	C	410	GLN
2	C	444	GLN
2	C	511	GLN
2	C	514	GLN
2	C	560	GLN
2	C	588	GLN
2	C	647	ASN
2	C	683	ASN
2	C	726	ASN
2	C	733	ASN
2	C	764	ASN
2	C	797	GLN
2	C	869	HIS
2	C	1004	ASN
3	J	19	HIS
4	O	99	ASN
4	O	121	GLN
4	O	136	ASN
4	O	271	GLN
4	O	273	GLN
4	O	344	ASN
5	P	33	GLN
5	P	79	ASN
5	P	84	ASN
5	P	87	ASN
6	Q	6	ASN
6	Q	85	GLN
6	Q	106	ASN
7	R	35	ASN
7	R	91	HIS
7	R	92	HIS
7	R	227	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	R	255	ASN
7	R	257	ASN
8	S	34	HIS
8	S	173	HIS
9	T	56	HIS
10	Z	84	ASN
10	Z	310	HIS
10	Z	354	HIS
10	Z	441	ASN
11	c	31	HIS
11	c	161	ASN
12	d	79	HIS
12	d	123	ASN
12	d	147	ASN
12	d	248	ASN
12	d	315	ASN
12	d	316	ASN
13	I	99	GLN
13	I	115	GLN
20	v	397	ASN
20	v	596	GLN
20	v	643	HIS
23	t	143	ASN
24	u	24	GLN
24	u	86	ASN
25	m	5	ASN
25	m	12	ASN
25	m	14	GLN
25	m	21	ASN
25	m	30	GLN
25	m	83	GLN
25	m	86	ASN
25	m	94	GLN
26	j	20	ASN
26	j	54	ASN
27	h	50	ASN
28	g	50	ASN
28	g	52	HIS
28	g	86	ASN
29	k	14	ASN
28	e	50	ASN
28	e	64	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	e	66	ASN
28	e	71	ASN
28	e	86	ASN
29	s	8	HIS
30	l	15	GLN
30	l	41	ASN
30	l	43	GLN
30	l	68	GLN
24	i	22	GLN
24	i	24	GLN
26	x	20	ASN
30	y	53	GLN
25	z	12	ASN
25	z	14	GLN
25	z	21	ASN
31	r	85	GLN
31	q	85	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	B	58/679 (8%)	32 (55%)	7 (12%)
17	D	177/214 (82%)	53 (29%)	8 (4%)
18	E	102/112 (91%)	40 (39%)	5 (4%)
19	L	199/1175 (16%)	74 (37%)	9 (4%)
All	All	536/2180 (24%)	199 (37%)	29 (5%)

All (199) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	B	-11	C
16	B	-10	A
16	B	-9	A
16	B	-5	A
16	B	-3	U
16	B	0	G
16	B	1	G
16	B	2	U
16	B	3	A
16	B	9	U
16	B	10	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	B	11	G
16	B	12	C
16	B	16	U
16	B	17	G
16	B	248	A
16	B	249	C
16	B	250	U
16	B	251	A
16	B	252	A
16	B	253	G
16	B	259	U
16	B	260	G
16	B	264	U
16	B	265	A
16	B	266	A
16	B	269	U
16	B	270	C
16	B	271	G
16	B	273	U
16	B	275	G
16	B	276	C
17	D	12	C
17	D	13	A
17	D	14	G
17	D	18	A
17	D	20	U
17	D	27	G
17	D	28	G
17	D	29	G
17	D	33	U
17	D	42	A
17	D	43	G
17	D	44	A
17	D	45	A
17	D	46	C
17	D	71	A
17	D	75	A
17	D	76	U
17	D	77	A
17	D	79	C
17	D	80	G
17	D	82	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	D	95	C
17	D	96	U
17	D	97	U
17	D	100	A
17	D	101	C
17	D	104	G
17	D	109	A
17	D	113	G
17	D	126	A
17	D	127	U
17	D	128	A
17	D	129	G
17	D	130	A
17	D	131	A
17	D	132	A
17	D	139	A
17	D	141	G
17	D	142	C
17	D	151	A
17	D	160	U
17	D	161	U
17	D	162	G
17	D	163	C
17	D	164	C
17	D	165	A
17	D	166	U
17	D	168	U
17	D	170	U
17	D	171	U
17	D	174	G
17	D	175	G
17	D	178	C
18	E	5	G
18	E	12	A
18	E	13	A
18	E	14	C
18	E	15	C
18	E	16	C
18	E	23	G
18	E	24	A
18	E	27	U
18	E	34	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	E	36	U
18	E	42	A
18	E	50	G
18	E	51	A
18	E	52	G
18	E	53	A
18	E	54	U
18	E	56	A
18	E	59	A
18	E	60	G
18	E	62	A
18	E	63	G
18	E	64	U
18	E	65	U
18	E	66	C
18	E	67	C
18	E	68	C
18	E	74	U
18	E	80	U
18	E	85	C
18	E	86	G
18	E	87	U
18	E	88	U
18	E	92	C
18	E	95	A
18	E	98	G
18	E	99	A
18	E	101	U
18	E	102	U
18	E	103	A
19	L	2	C
19	L	3	G
19	L	4	A
19	L	6	U
19	L	12	U
19	L	16	U
19	L	17	U
19	L	18	U
19	L	19	U
19	L	21	G
19	L	23	U
19	L	25	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	L	26	G
19	L	30	A
19	L	31	A
19	L	32	G
19	L	35	U
19	L	36	A
19	L	37	G
19	L	49	U
19	L	50	U
19	L	52	A
19	L	53	G
19	L	54	U
19	L	108	A
19	L	110	A
19	L	111	C
19	L	115	U
19	L	119	G
19	L	120	G
19	L	121	C
19	L	124	C
19	L	129	A
19	L	141	A
19	L	153	U
19	L	1084	A
19	L	1085	G
19	L	1086	U
19	L	1091	G
19	L	1092	A
19	L	1093	C
19	L	1094	G
19	L	1096	C
19	L	1098	C
19	L	1099	G
19	L	1100	A
19	L	1101	C
19	L	1102	C
19	L	1103	C
19	L	1104	U
19	L	1105	C
19	L	1106	G
19	L	1107	C
19	L	1108	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	L	1115	G
19	L	1120	G
19	L	1122	U
19	L	1123	C
19	L	1124	U
19	L	1125	U
19	L	1126	G
19	L	1128	C
19	L	1130	U
19	L	1137	U
19	L	1138	G
19	L	1139	G
19	L	1140	U
19	L	1144	U
19	L	1145	U
19	L	1146	G
19	L	1147	A
19	L	1149	G
19	L	1152	U
19	L	1166	G

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	B	2	U
16	B	9	U
16	B	249	C
16	B	264	U
16	B	265	A
16	B	268	A
16	B	269	U
17	D	17	C
17	D	27	G
17	D	28	G
17	D	81	A
17	D	95	C
17	D	130	A
17	D	131	A
17	D	150	U
18	E	14	C
18	E	23	G
18	E	49	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	E	51	A
18	E	64	U
19	L	3	G
19	L	53	G
19	L	120	G
19	L	1085	G
19	L	1092	A
19	L	1093	C
19	L	1106	G
19	L	1107	C
19	L	1146	G

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	SEP	n	73	14	8,9,10	0.66	0	7,12,14	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	SEP	n	73	14	-	5/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	n	73	SEP	N-CA-CB-OG
14	n	73	SEP	C-CA-CB-OG
14	n	73	SEP	CB-OG-P-O1P
14	n	73	SEP	CB-OG-P-O2P
14	n	73	SEP	CB-OG-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
33	GTP	C	1500	34	33,34,34	0.58	0	50,54,54	0.49	0
32	IHP	A	3000	-	36,36,36	0.77	0	60,60,60	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	GTP	C	1500	34	-	0/22/38/38	0/3/3/3
32	IHP	A	3000	-	-	10/30/54/54	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

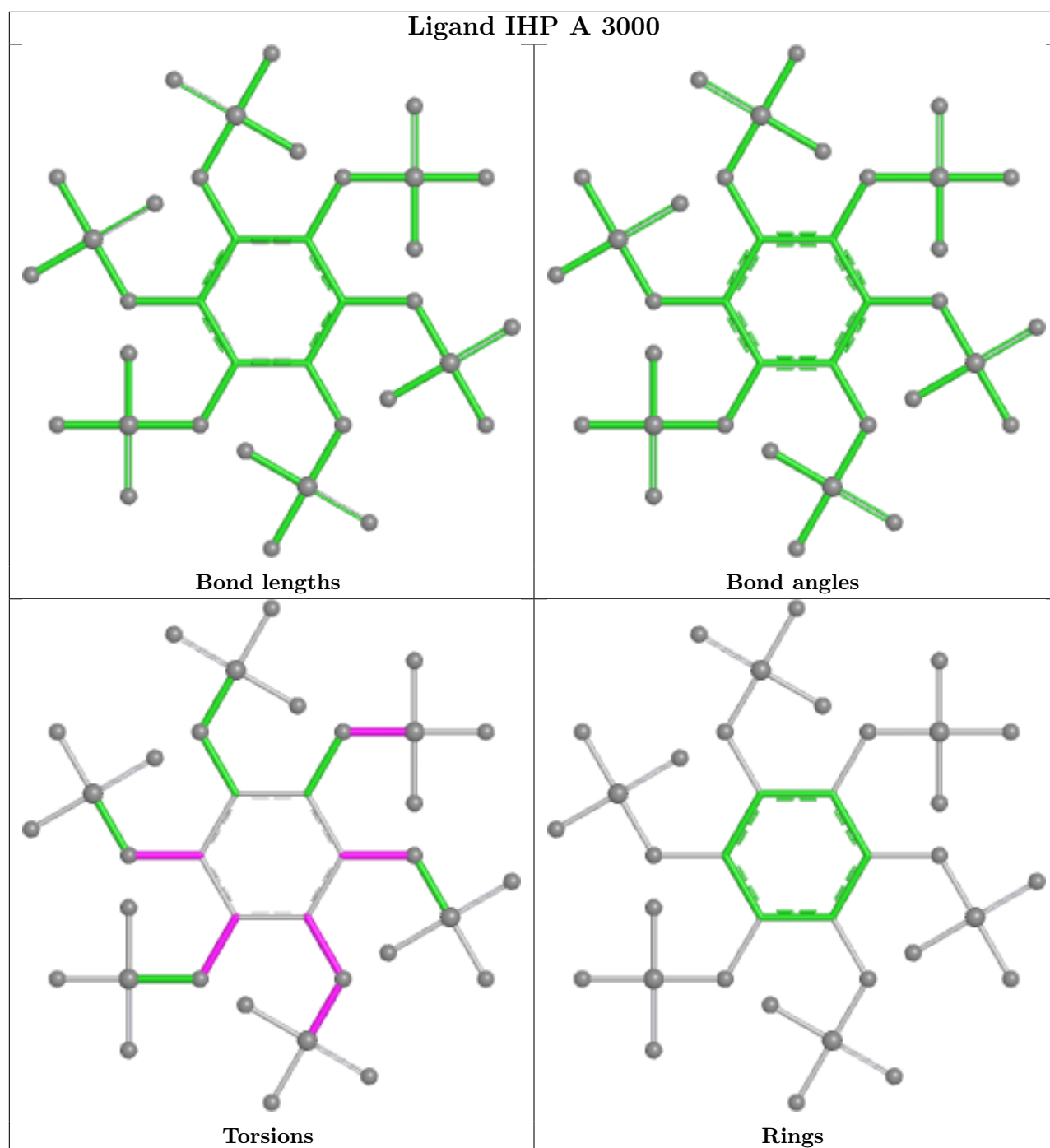
Mol	Chain	Res	Type	Atoms
32	A	3000	IHP	C2-C1-O11-P1
32	A	3000	IHP	C6-C1-O11-P1
32	A	3000	IHP	C3-C2-O12-P2
32	A	3000	IHP	C6-C5-O15-P5
32	A	3000	IHP	C1-C6-O16-P6
32	A	3000	IHP	C1-C2-O12-P2
32	A	3000	IHP	C5-C6-O16-P6
32	A	3000	IHP	C4-O14-P4-O24
32	A	3000	IHP	C6-O16-P6-O26
32	A	3000	IHP	C4-C5-O15-P5

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	C	1500	GTP	1	0
32	A	3000	IHP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

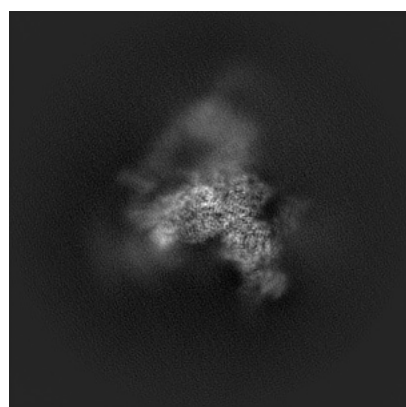
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0687. These allow visual inspection of the internal detail of the map and identification of artifacts.

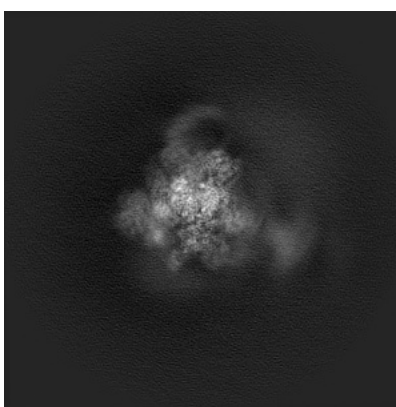
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

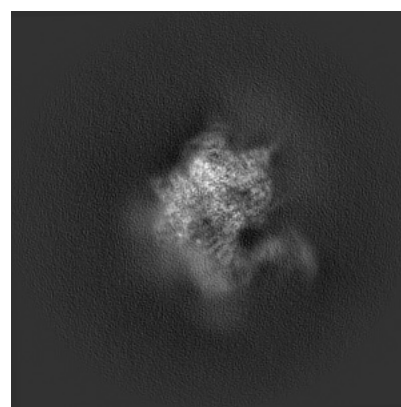
6.1.1 Primary map



X



Y

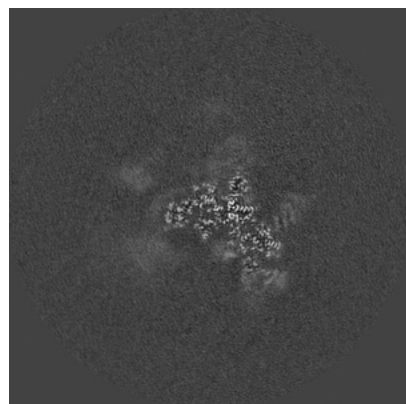


Z

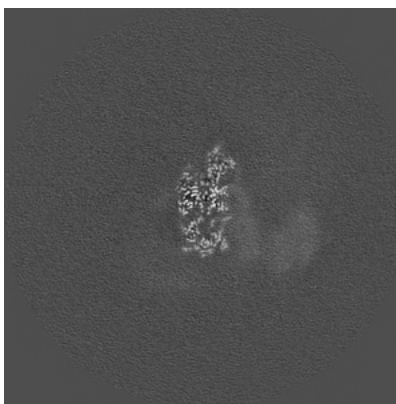
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

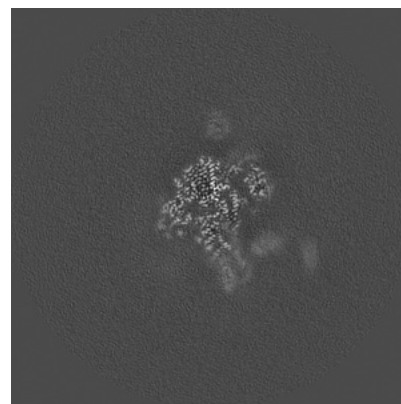
6.2.1 Primary map



X Index: 200



Y Index: 200

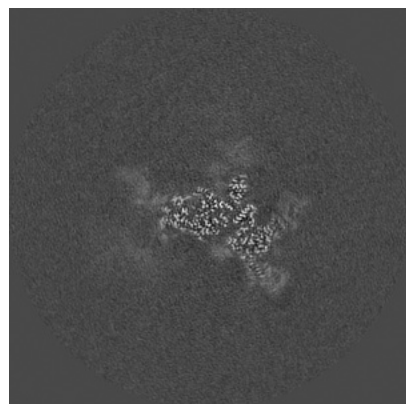


Z Index: 200

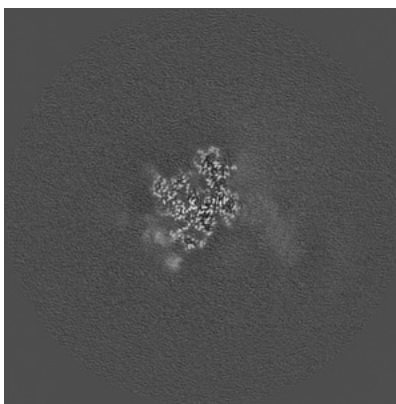
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

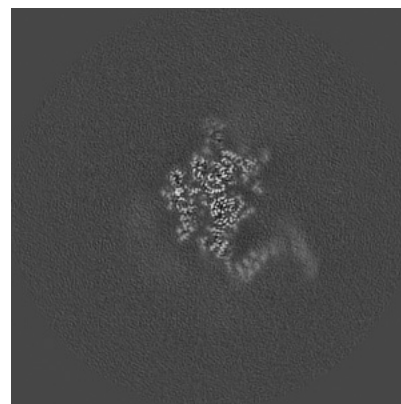
6.3.1 Primary map



X Index: 207



Y Index: 228

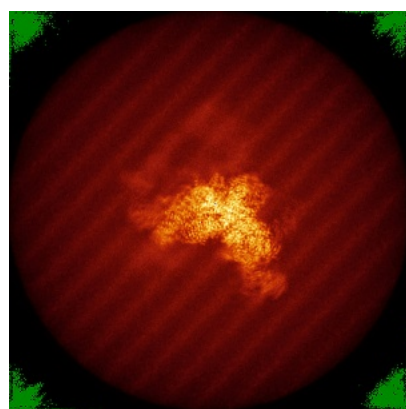


Z Index: 186

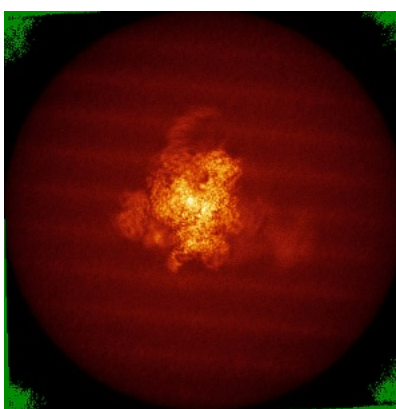
The images above show the largest variance slices of the map in three orthogonal directions.

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

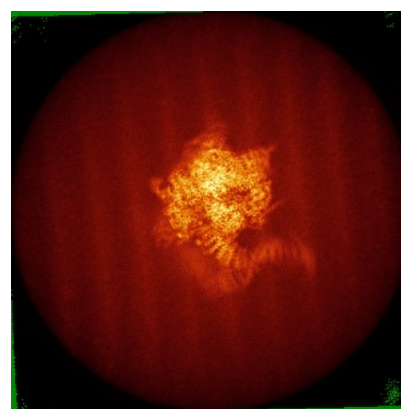
6.4.1 Primary map



X



Y

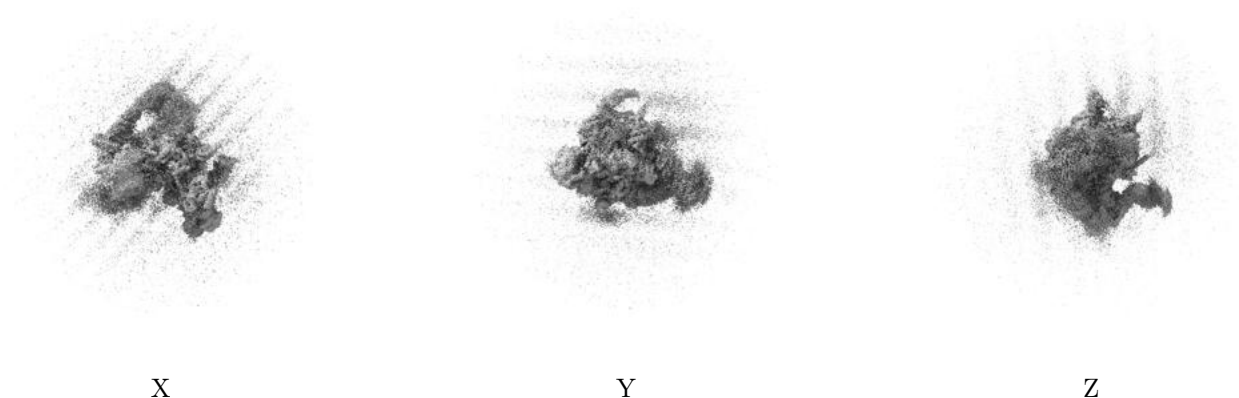


Z

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 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

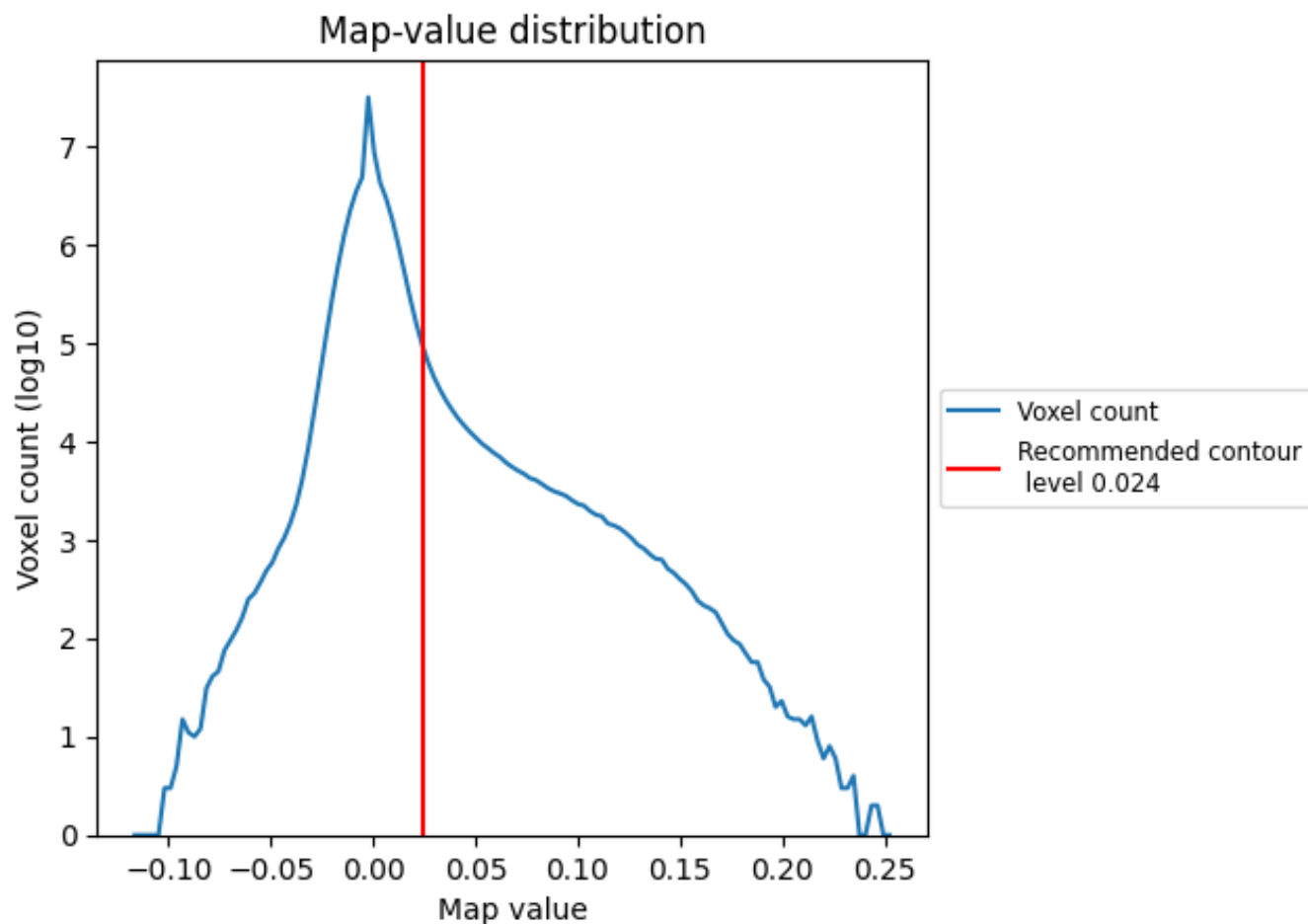
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

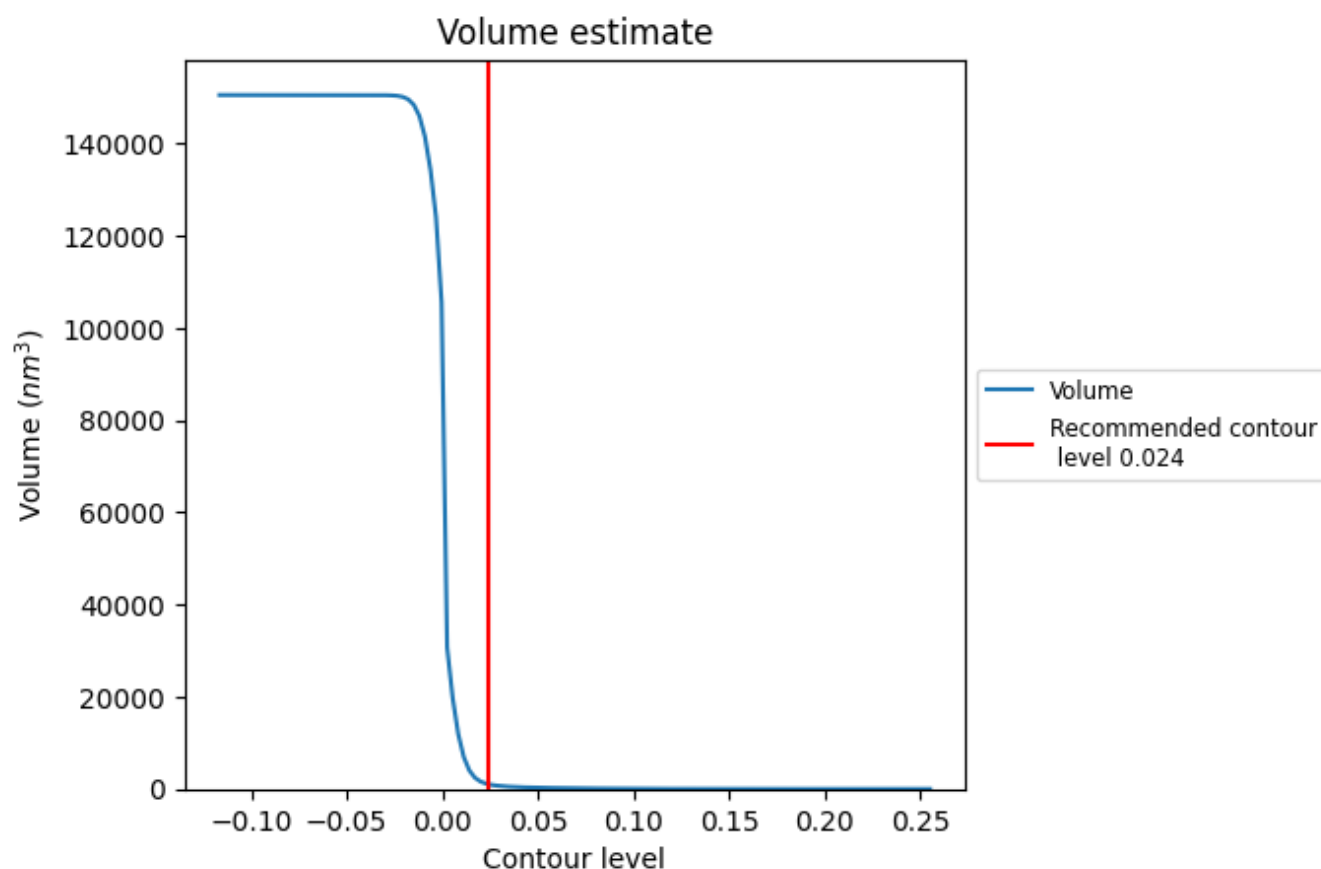
This section contains the results of statistical analysis of the map.

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.

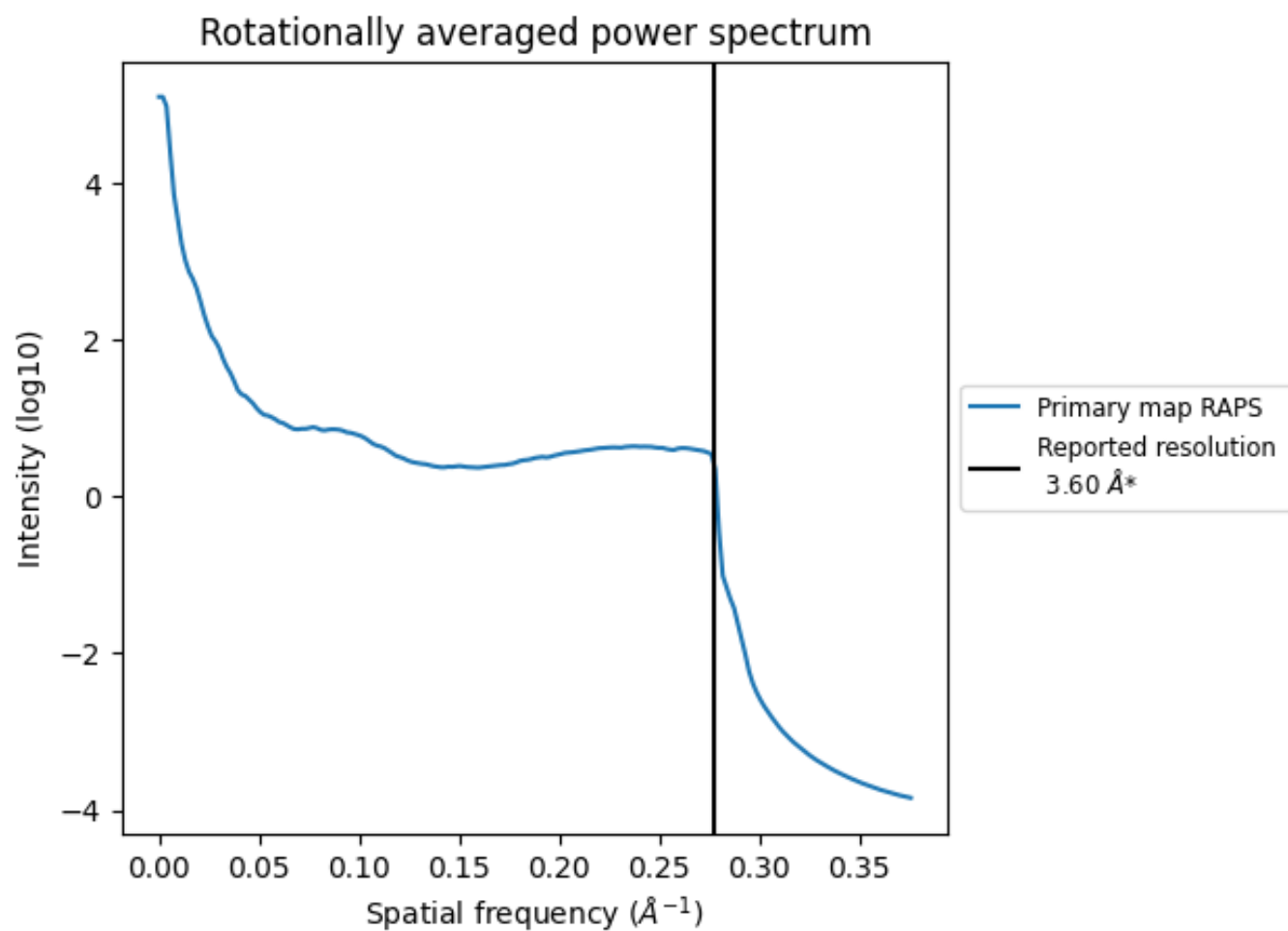
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1055 nm³; this corresponds to an approximate mass of 953 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 0.278 $\text{\AA}^{-1}$

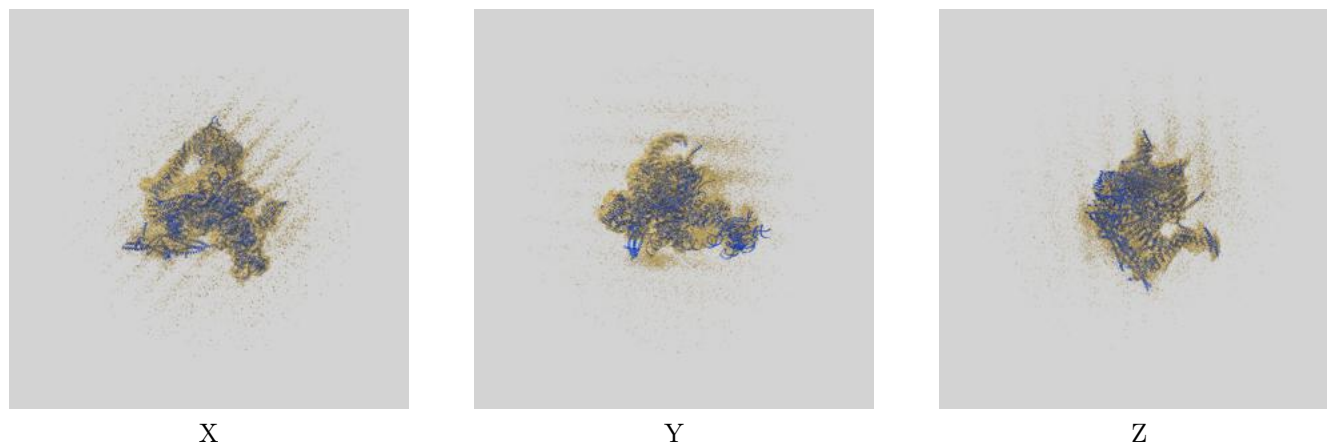
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

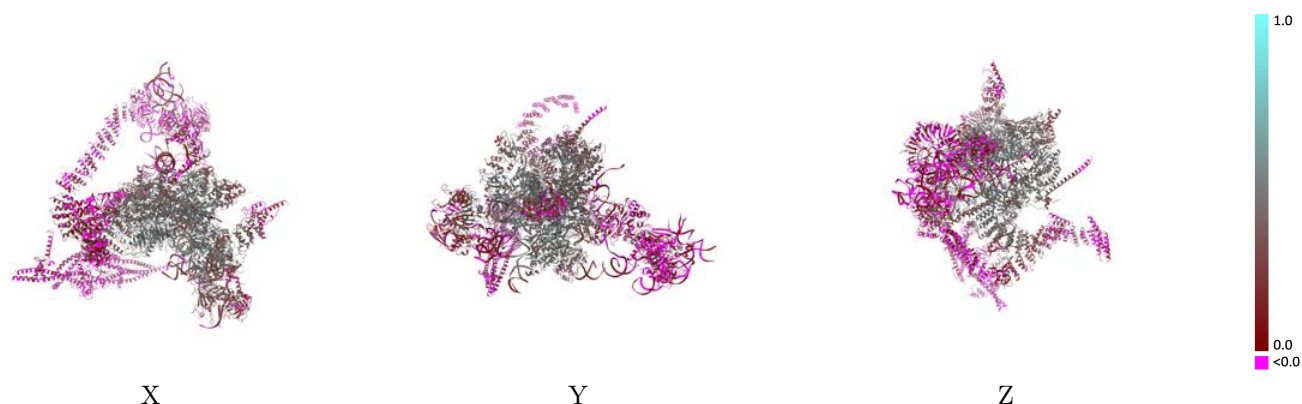
This section contains information regarding the fit between EMDB map EMD-0687 and PDB model 6J6H. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



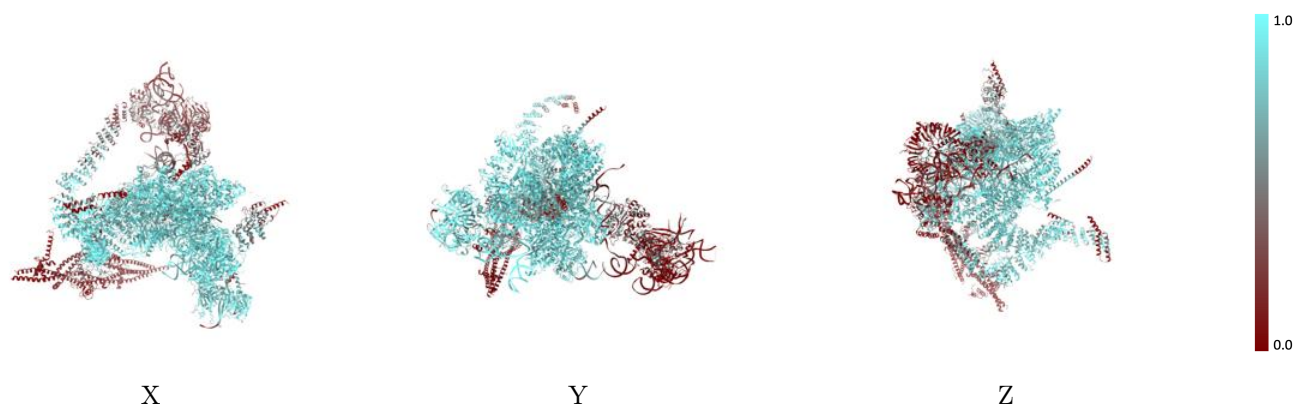
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



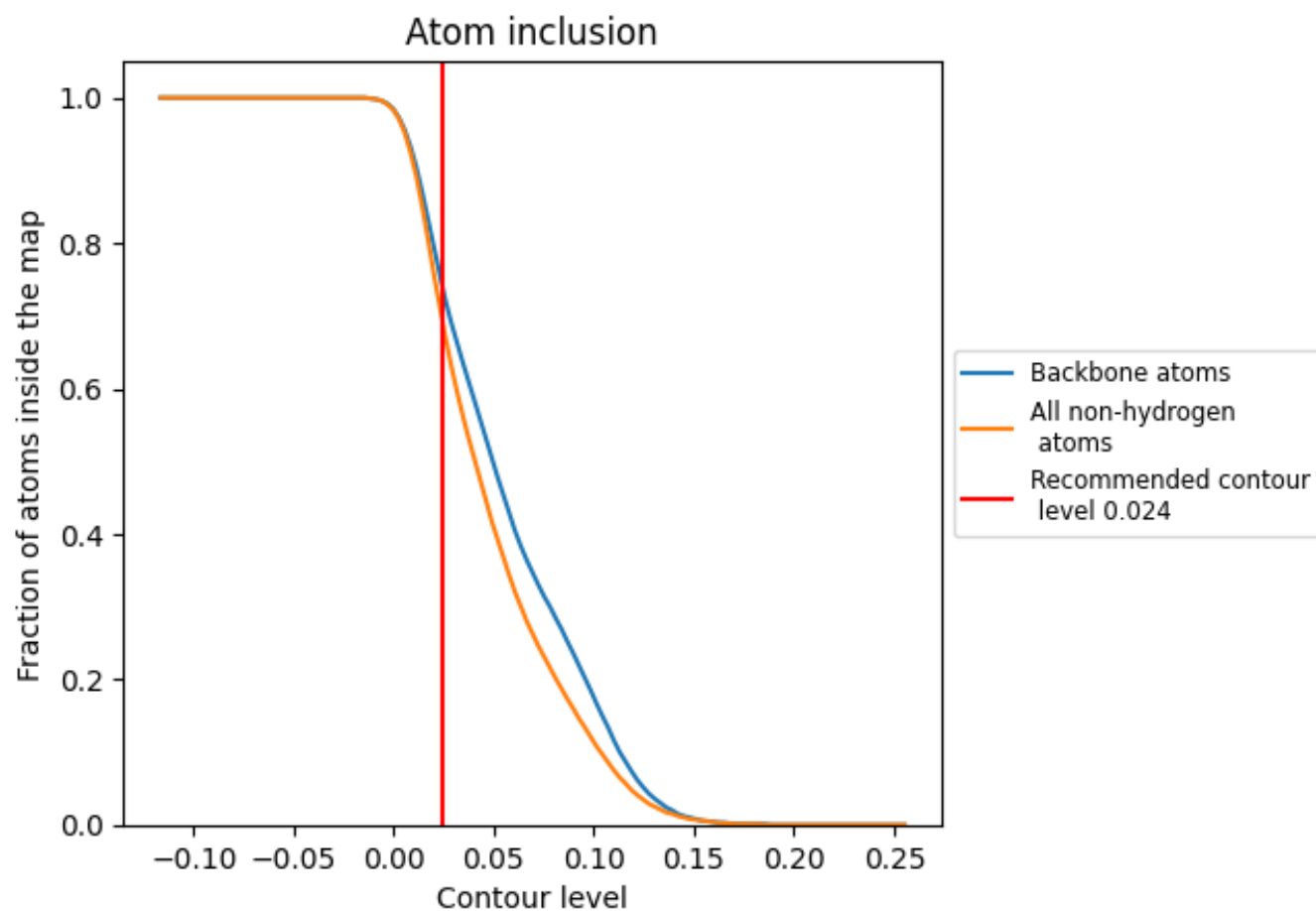
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.024).

9.4 Atom inclusion ⓘ



At the recommended contour level, 74% of all backbone atoms, 70% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6970	 0.2830
A	 0.8380	 0.4070
B	 0.5970	 0.1860
C	 0.9100	 0.4340
D	 0.9260	 0.2930
E	 0.9800	 0.4190
H	 0.4890	 0.0520
I	 0.8190	 0.3750
J	 0.8240	 0.4640
L	 0.3180	 0.0850
O	 0.9340	 0.4800
P	 0.7830	 0.3760
Q	 0.8450	 0.3440
R	 0.9050	 0.4250
S	 0.7250	 0.4160
T	 0.9300	 0.4620
Z	 0.6190	 0.2660
a	 0.1610	 -0.0220
b	 0.2680	 0.0140
c	 0.5120	 0.2380
d	 0.8190	 0.2660
e	 0.1510	 0.0360
g	 0.7730	 0.1370
h	 0.8720	 0.1560
i	 0.8270	 0.1680
j	 0.8250	 0.2710
k	 0.7540	 0.2690
l	 0.8500	 0.3730
m	 0.7120	 0.1760
n	 0.9680	 0.4070
o	 0.1320	 0.0040
p	 0.1420	 0.0180
q	 0.0170	 0.0040
r	 0.1110	 -0.0050
s	 0.2800	 0.0030



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
t	 0.0770	 0.0120
u	 0.0910	 0.0470
v	 0.7020	 0.1310
w	 0.1540	 0.0330
x	 0.0510	 0.0520
y	 0.1120	 0.0000
z	 0.2420	 0.0270