Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 12:59 AM EST

PDB ID	:	3NVK
Title	:	Structural basis for substrate placement by an archaeal box C/D ribonucleo-protein particle
Authors	:	Xue, S.; Wang, R.; Li, H.
Deposited on	:	2010-07-08
Resolution	:	3.21 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.21 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	Percentile Ranks	Value
Rfree		0.276
Clashscore		52
Ramachandran outliers		1.7%
Sidechain outliers		18.8%
RSRZ outliers		2.3%
RNA backbone		0.16

Worse ← → *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
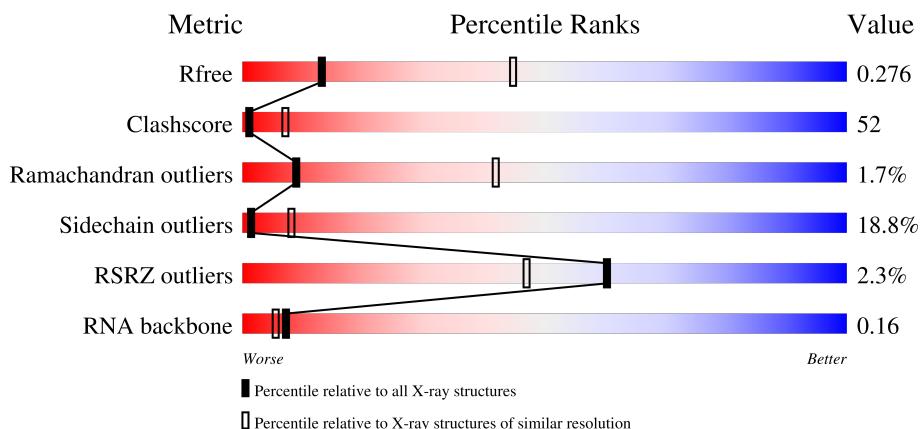
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	376	2% / 35% / 47% / 13% · ·
1	F	376	2% / 35% / 48% / 13% · ·
2	E	129	4% / 22% / 62% / 9% / 6%
2	H	129	5% / 23% / 56% / 15% / 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	I	234	33% 53% 11%
3	J	234	34% 53% 10%
4	K	34	6% 15% 44% 9% 29%
4	L	34	3% 12% 18% 35% 6% 29%
5	G	13	8% 15% 77%
5	S	13	15% 8% 77%
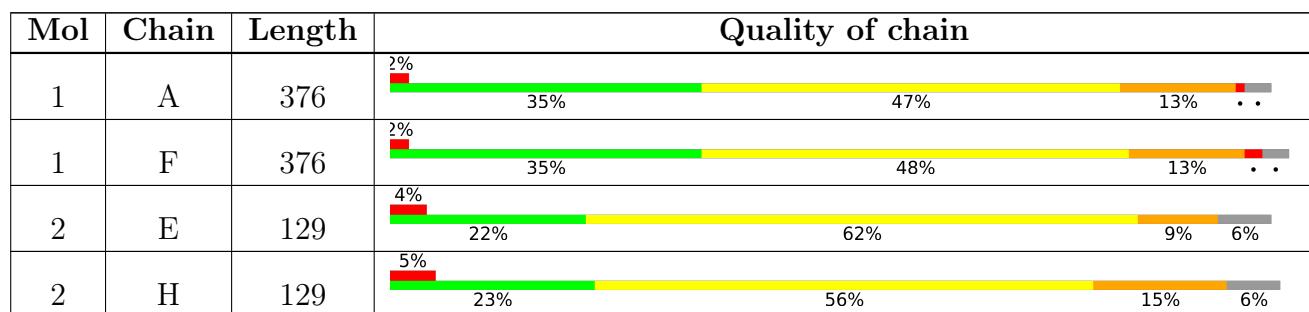
2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 12606 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NOP5/NOP56 related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2948	1883	513	545	7			
1	F	363	Total	C	N	O	S	0	0	0
			2948	1883	513	545	7			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP Q8U4M1
A	-4	HIS	-	expression tag	UNP Q8U4M1
A	-3	HIS	-	expression tag	UNP Q8U4M1
A	-2	HIS	-	expression tag	UNP Q8U4M1
A	-1	HIS	-	expression tag	UNP Q8U4M1
A	0	HIS	-	expression tag	UNP Q8U4M1
A	1	HIS	-	expression tag	UNP Q8U4M1
A	2	VAL	-	expression tag	UNP Q8U4M1
A	3	MET	-	expression tag	UNP Q8U4M1
A	4	ILE	-	expression tag	UNP Q8U4M1
A	368	LEU	-	expression tag	UNP Q8U4M1
A	369	VAL	-	expression tag	UNP Q8U4M1
A	370	LEU	-	expression tag	UNP Q8U4M1
F	-5	MET	-	expression tag	UNP Q8U4M1
F	-4	HIS	-	expression tag	UNP Q8U4M1
F	-3	HIS	-	expression tag	UNP Q8U4M1
F	-2	HIS	-	expression tag	UNP Q8U4M1
F	-1	HIS	-	expression tag	UNP Q8U4M1
F	0	HIS	-	expression tag	UNP Q8U4M1
F	1	HIS	-	expression tag	UNP Q8U4M1
F	2	VAL	-	expression tag	UNP Q8U4M1
F	3	MET	-	expression tag	UNP Q8U4M1
F	4	ILE	-	expression tag	UNP Q8U4M1
F	368	LEU	-	expression tag	UNP Q8U4M1
F	369	VAL	-	expression tag	UNP Q8U4M1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	370	LEU	-	expression tag	UNP Q8U4M1

- Molecule 2 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	121	Total	C	N	O	S	0	0	0
			926	591	153	179	3			
2	H	121	Total	C	N	O	S	0	0	0
			926	591	153	179	3			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	MET	-	expression tag	UNP Q8U160
E	-3	HIS	-	expression tag	UNP Q8U160
E	-2	HIS	-	expression tag	UNP Q8U160
E	-1	HIS	-	expression tag	UNP Q8U160
E	0	HIS	-	expression tag	UNP Q8U160
E	1	HIS	-	expression tag	UNP Q8U160
E	2	HIS	-	expression tag	UNP Q8U160
H	-4	MET	-	expression tag	UNP Q8U160
H	-3	HIS	-	expression tag	UNP Q8U160
H	-2	HIS	-	expression tag	UNP Q8U160
H	-1	HIS	-	expression tag	UNP Q8U160
H	0	HIS	-	expression tag	UNP Q8U160
H	1	HIS	-	expression tag	UNP Q8U160
H	2	HIS	-	expression tag	UNP Q8U160

- Molecule 3 is a protein called Fibrillarin-like rRNA/tRNA 2'-O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	227	Total	C	N	O	S	0	0	0
			1822	1174	312	334	2			
3	J	227	Total	C	N	O	S	0	0	0
			1822	1174	312	334	2			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-6	MET	-	expression tag	UNP Q8U4M2
I	-5	HIS	-	expression tag	UNP Q8U4M2
I	-4	HIS	-	expression tag	UNP Q8U4M2

Continued on next page...

Continued from previous page...

| Chain	Residue	Modelled	Actual	Comment	Reference
I	-3	HIS	-	expression tag	UNP Q8U4M2
I	-2	HIS	-	expression tag	UNP Q8U4M2
I	-1	HIS	-	expression tag	UNP Q8U4M2
I	0	HIS	-	expression tag	UNP Q8U4M2
J	-6	MET	-	expression tag	UNP Q8U4M2
J	-5	HIS	-	expression tag	UNP Q8U4M2
J	-4	HIS	-	expression tag	UNP Q8U4M2
J	-3	HIS	-	expression tag	UNP Q8U4M2
J	-2	HIS	-	expression tag	UNP Q8U4M2
J	-1	HIS	-	expression tag	UNP Q8U4M2
J	0	HIS	-	expression tag	UNP Q8U4M2

- Molecule 4 is a RNA chain called RNA (5'-R(*GP*CP*CP*GP*UP*UP*GP*AP*AP*GP* CP*UP*CP*UP*GP*AP*CP*CP*GP*AP*AP*AP*GP*GP*CP*GP*UP*GP*AP*UP*G P*AP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	24	Total	C	N	O	P	0	0	0
			518	231	98	165	24			
4	L	24	Total	C	N	O	P	0	0	0
			518	231	98	165	24			

- Molecule 5 is a RNA chain called RNA (5'-R(*GP*AP*GP*CP*UP*UP*CP*AP*AP*CP* GP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	3	Total	C	N	O	P	0	0	0
			63	28	10	22	3			
5	S	3	Total	C	N	O	P	0	0	0
			63	28	10	22	3			

- Molecule 6 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).

SAM
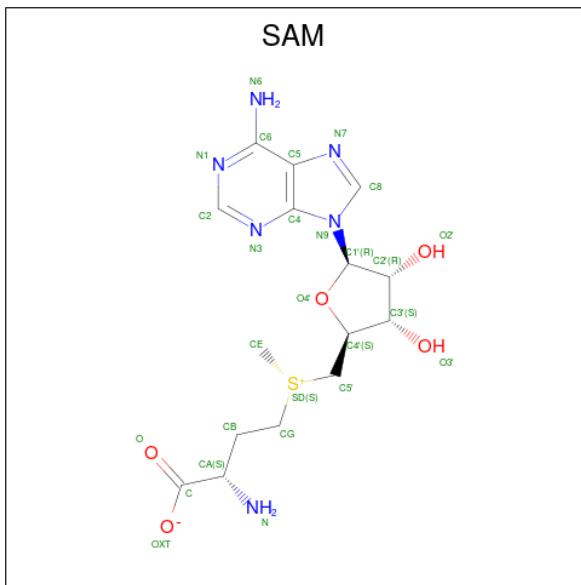
| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	I	1	Total	C	N	O	S	0	0
			26	15	6	4	1		
6	J	1	Total	C	N	O	S	0	0
			26	15	6	4	1		

3 Residue-property plots ⓘ

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

• Molecule 1: NOP5/NOP56 related protein
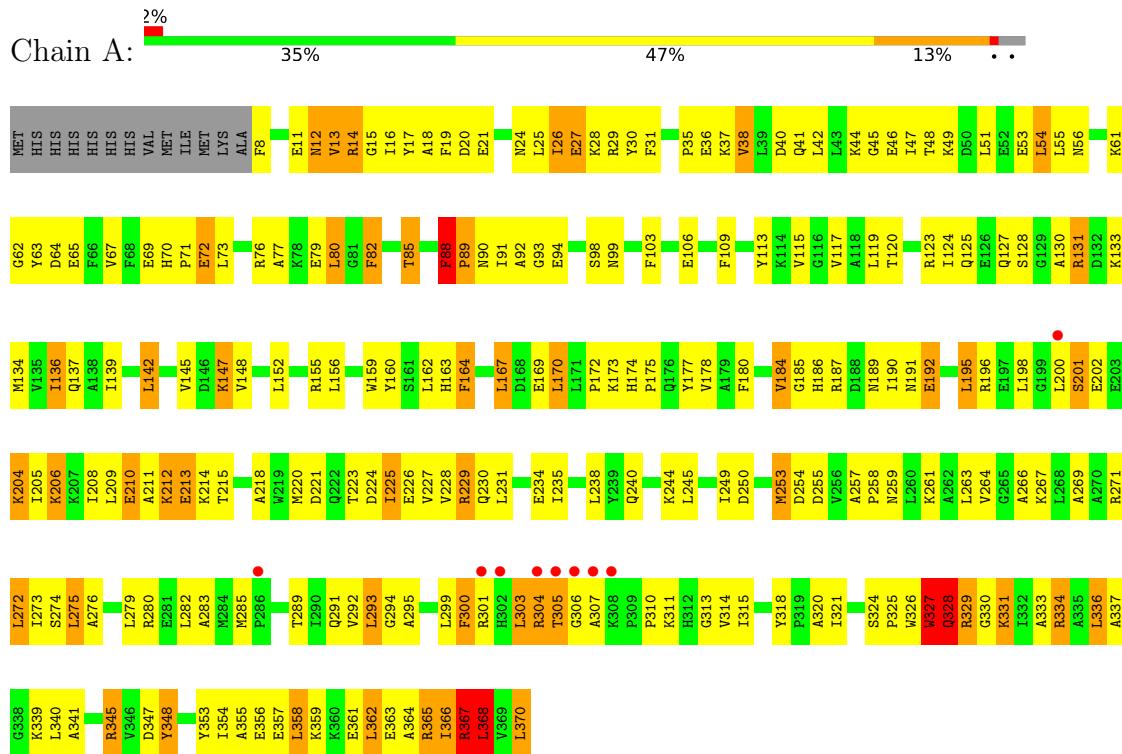
• Molecule 1: NOP5/NOP56 related protein
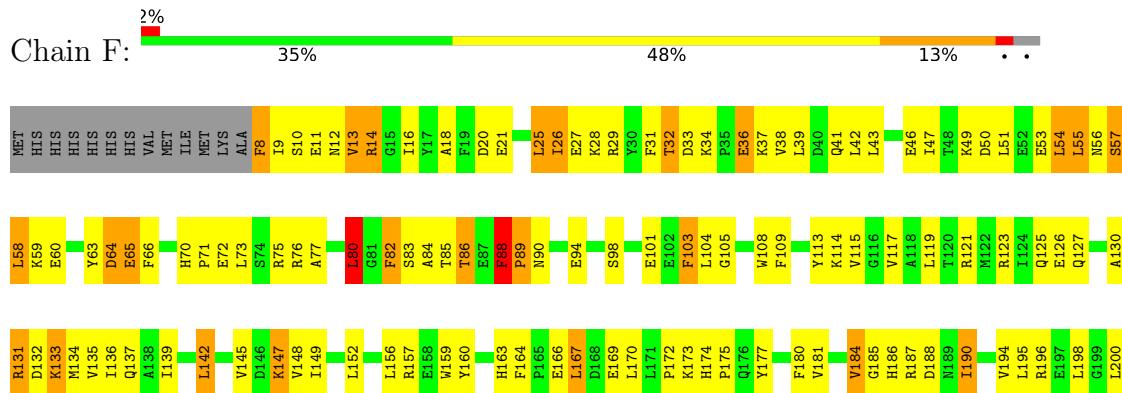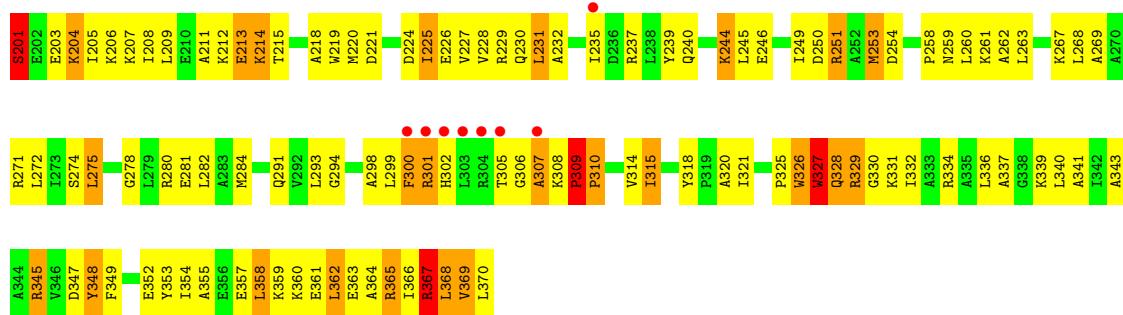
- Molecule 2: 50S ribosomal protein L7Ae
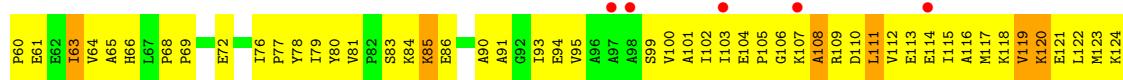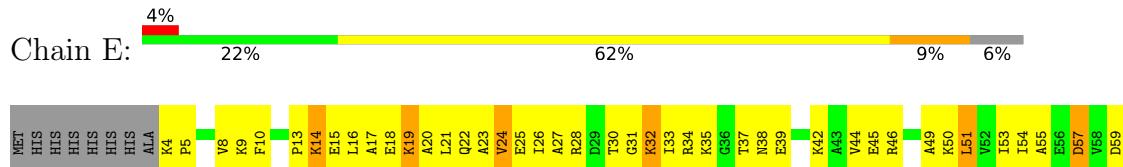
Chain E:

- Molecule 2: 50S ribosomal protein L7Ae
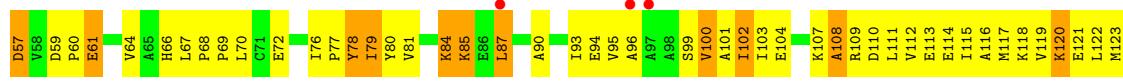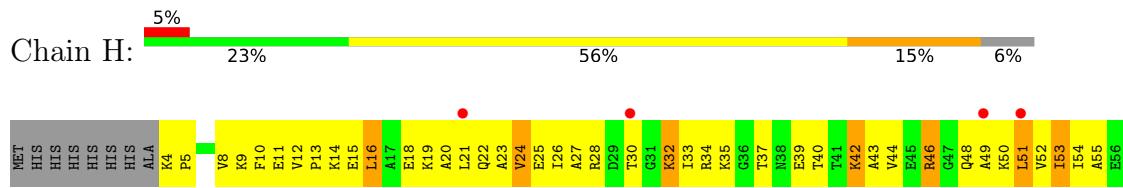
Chain H:

- Molecule 3: Fibrillarin-like rRNA/tRNA 2'-O-methyltransferase

Chain I:

• Molecule 3: Fibrillarin-like rRNA/tRNA 2'-O-methyltransferase

Chain J:

• Molecule 4: RNA (5'-R(*GP*CP*CP*GP*UP*UP*GP*AP*AP*GP*CP*UP*CP*UP*GP*AP
*CP*CP*GP*AP*AP*AP*GP*GP*CP*GP*UP*GP*AP*UP*GP*AP*GP*C)-3')

Chain K:

• Molecule 4: RNA (5'-R(*GP*CP*CP*GP*UP*UP*GP*AP*AP*GP*CP*UP*CP*UP*GP*AP
*CP*CP*GP*AP*AP*AP*GP*GP*CP*GP*UP*GP*AP*UP*GP*AP*GP*C)-3')

Chain L:

• Molecule 5: RNA (5'-R(*GP*AP*GP*CP*UP*UP*CP*AP*AP*CP*GP*GP*C)-3')

Chain G:

• Molecule 5: RNA (5'-R(*GP*AP*GP*CP*UP*UP*CP*AP*AP*CP*GP*GP*C)-3')

Chain S:
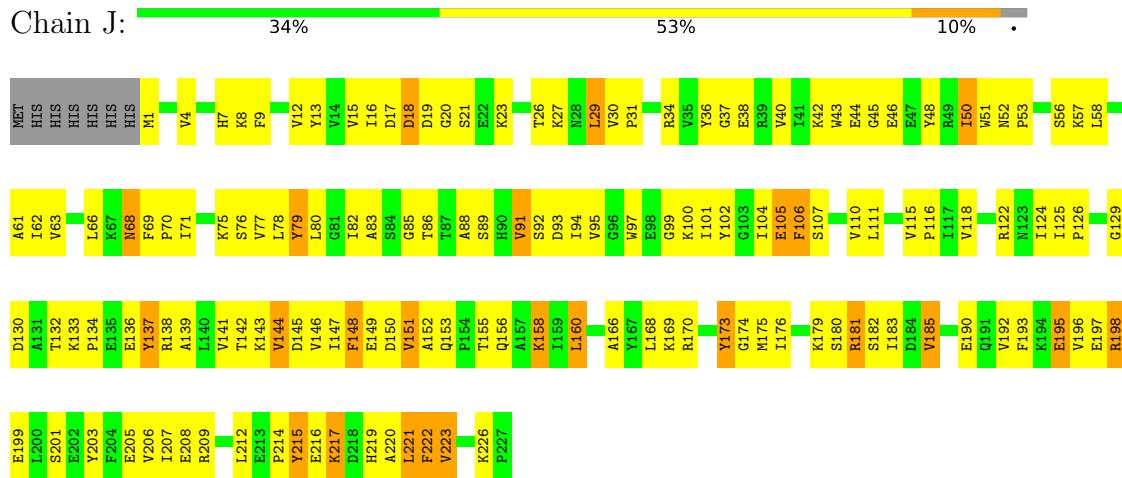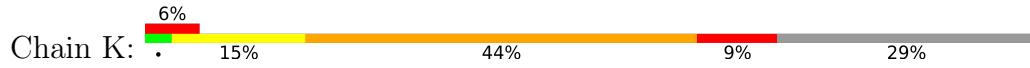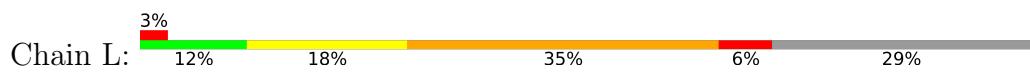
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	330.04Å 94.55Å 97.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.69 – 3.21 39.69 – 3.21	Depositor EDS
% Data completeness (in resolution range)	79.6 (39.69-3.21) 78.7 (39.69-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.230 , 0.288 0.217 , 0.276	Depositor DCC
R_{free} test set	4297 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å^2)	80.2	Xtriage
Anisotropy	0.711	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 64.9	EDS
L-test for twinning[2]	$< |L| > = 0.43, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.064 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12606	wwPDB-VP
Average B, all atoms (Å^2)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality (i)

5.1   Standard geometry (i)

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

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	0.55	1/3002 (0.0%)	0.79	2/4042 (0.0%)
1	F	0.54	1/3002 (0.0%)	0.80	2/4042 (0.0%)
2	E	0.42	0/938	0.70	1/1264 (0.1%)
2	H	0.42	0/938	0.69	0/1264
3	I	0.52	0/1861	0.76	0/2515
3	J	0.57	0/1861	0.82	2/2515 (0.1%)
4	K	0.48	0/580	1.06	3/903 (0.3%)
4	L	0.50	0/580	1.05	3/903 (0.3%)
5	G	0.44	0/69	1.06	0/105
5	S	0.31	0/69	0.84	0/105
All	All	0.52	2/12900 (0.0%)	0.81	13/17658 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	F	0	4
3	J	0	1
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	327	TRP	CB-CG	6.17	1.61	1.50
1	F	327	TRP	CB-CG	5.77	1.60	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	66	LEU	CA-CB-CG	8.31	134.42	115.30
4	L	17	C	C6-N1-C2	-7.36	117.36	120.30
4	L	17	C	C5-C6-N1	6.34	124.17	121.00
1	F	368	LEU	N-CA-C	6.31	128.03	111.00
1	A	368	LEU	N-CA-C	5.71	126.41	111.00
2	E	31	GLY	N-CA-C	-5.68	98.91	113.10
3	J	174	GLY	N-CA-C	-5.45	99.48	113.10
4	K	17	C	C6-N1-C2	-5.34	118.16	120.30
1	F	309	PRO	N-CA-C	5.31	125.89	112.10
1	A	370	LEU	CA-CB-CG	5.23	127.33	115.30
4	L	7	G	C3'-C2'-C1'	5.17	105.64	101.50
4	K	5	C	C2-N1-C1'	-5.16	113.13	118.80
4	K	22	U	C5-C6-N1	5.02	125.21	122.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	LEU	Peptide
1	A	367	ARG	Peptide
1	A	88	PHE	Peptide
1	F	309	PRO	Peptide
1	F	367	ARG	Peptide
1	F	80	LEU	Peptide
1	F	88	PHE	Peptide
3	J	20	GLY	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2948	0	2995	306	0
1	F	2948	0	2995	307	0
2	E	926	0	977	138	0
2	H	926	0	977	142	0
3	I	1822	0	1869	167	0
3	J	1822	0	1869	162	0
4	K	518	0	261	74	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	518	0	261	56	0
5	G	63	0	33	2	0
5	S	63	0	33	4	0
6	I	26	0	21	4	0
6	J	26	0	22	5	0
All	All	12606	0	12313	1295	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 52.

All (1295) 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:170:LEU:HD23	1:A:208:ILE:HG22	1.27	1.14
3:I:95:VAL:HG12	3:I:99:GLY:HA3	1.22	1.11
1:F:301:ARG:HB3	1:F:307:ALA:HB3	1.13	1.08
1:F:190:ILE:HD11	1:F:212:LYS:HD2	1.09	1.06
1:F:47:ILE:HG13	1:F:51:LEU:HD23	1.38	1.06
1:F:184:VAL:HG21	1:F:190:ILE:HG22	1.40	1.03
3:I:144:VAL:O	3:I:169:LYS:HG2	1.61	1.01
1:F:170:LEU:HD23	1:F:208:ILE:HG22	1.40	1.01
3:J:95:VAL:HG12	3:J:99:GLY:HA3	1.38	1.00
1:F:301:ARG:HB3	1:F:307:ALA:CB	1.91	1.00
1:A:190:ILE:HD11	1:A:212:LYS:HB2	1.43	0.98
1:F:16:ILE:HD11	1:F:42:LEU:HD11	1.42	0.98
3:I:91:VAL:O	3:I:95:VAL:HG23	1.60	0.98
1:F:184:VAL:CG2	1:F:190:ILE:HG22	1.94	0.97
3:I:4:VAL:HG22	3:I:15:VAL:HG12	1.44	0.96
2:H:49:ALA:HB3	2:H:76:ILE:HD13	1.47	0.95
2:E:14:LYS:HD2	2:E:14:LYS:N	1.80	0.95
1:A:152:LEU:HD21	1:F:148:VAL:HG21	1.47	0.94
1:F:190:ILE:HD11	1:F:212:LYS:CD	1.97	0.94
1:A:280:ARG:HG3	1:A:348:TYR:HE1	1.31	0.93
1:F:200:LEU:HD12	1:F:204:LYS:HG2	1.51	0.93
1:F:174:HIS:HB2	1:F:175:PRO:HD3	1.49	0.93
2:H:109:ARG:HG2	2:H:109:ARG:HH11	1.34	0.93
3:J:102:TYR:HE1	3:J:142:THR:H	1.17	0.92
3:J:75:LYS:HZ3	3:J:145:ASP:HB3	1.35	0.92
1:F:119:LEU:O	1:F:119:LEU:HD23	1.70	0.92
4:L:10:C:H3'	4:L:11:G:H5"	1.51	0.91
1:F:251:ARG:HG3	1:F:251:ARG:HH11	1.32	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:66:HIS:O	2:E:69:PRO:HD2	1.71	0.91
4:K:22:U:HO2'	4:K:23:G:H8	0.92	0.89
1:F:190:ILE:CD1	1:F:212:LYS:HD2	2.00	0.89
4:L:7:G:H4'	4:L:8:A:OP1	1.73	0.89
1:F:113:TYR:HE2	3:J:122:ARG:HH21	1.14	0.89
1:F:203:GLU:OE1	1:F:207:LYS:HD2	1.72	0.88
2:E:19:LYS:HD3	2:E:20:ALA:N	1.87	0.88
1:F:251:ARG:HH11	1:F:251:ARG:CG	1.86	0.88
1:F:275:LEU:HD23	1:F:275:LEU:H	1.38	0.88
4:K:10:C:H3'	4:K:11:G:H5"	1.51	0.88
1:A:163:HIS:HE1	1:A:187:ARG:H	1.21	0.88
3:I:28:ASN:HB2	3:I:49:ARG:HG3	1.55	0.88
4:K:7:G:H4'	4:K:8:A:OP1	1.73	0.88
2:H:108:ALA:HA	2:H:111:LEU:HD12	1.57	0.86
4:L:22:U:HO2'	4:L:23:G:H8	1.20	0.86
1:A:167:LEU:HA	1:A:170:LEU:HB2	1.57	0.86
1:F:328:GLN:HG2	1:F:329:ARG:H	1.40	0.85
2:H:37:THR:HG21	2:H:64:VAL:HG12	1.58	0.85
1:A:70:HIS:ND1	1:A:71:PRO:HD2	1.92	0.85
4:K:11:G:H22	4:K:15:G:H1'	1.40	0.85
1:A:163:HIS:CE1	1:A:187:ARG:HB2	2.11	0.84
1:A:163:HIS:NE2	1:A:187:ARG:HB2	1.93	0.84
3:J:36:TYR:HB3	3:J:86:THR:HG22	1.59	0.84
3:I:194:LYS:HD2	3:I:209:ARG:HH22	1.42	0.84
3:I:190:GLU:O	3:I:194:LYS:HG2	1.79	0.83
1:F:355:ALA:O	1:F:358:LEU:HD12	1.79	0.83
1:A:258:PRO:HD2	1:A:347:ASP:OD1	1.78	0.82
1:F:55:LEU:HD12	1:F:56:ASN:N	1.93	0.82
2:H:118:LYS:O	2:H:122:LEU:HG	1.79	0.82
3:J:105:GLU:OE2	6:J:228:SAM:H1'	1.80	0.82
3:J:79:TYR:CE1	3:J:88:ALA:HB2	2.13	0.82
3:J:111:LEU:HD11	3:J:126:PRO:HB3	1.60	0.82
4:K:15:G:O2'	4:K:16:G:H8	1.63	0.81
1:A:364:ALA:HA	1:A:367:ARG:HH22	1.45	0.81
2:E:57:ASP:HB2	2:E:84:LYS:HD3	1.63	0.81
2:H:54:ILE:HG22	2:H:55:ALA:H	1.45	0.81
4:L:7:G:H1'	4:L:21:A:H61	1.45	0.81
1:A:289:THR:HG22	4:K:5:C:OP1	1.81	0.81
1:A:195:LEU:HD11	1:A:208:ILE:HD11	1.63	0.81
2:E:117:MET:O	2:E:120:LYS:HG3	1.80	0.80
1:F:180:PHE:O	1:F:184:VAL:HG12	1.81	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:211:ASN:HD21	3:I:213:GLU:HG2	1.45	0.80
4:K:21:A:O2'	4:K:22:U:H5'	1.82	0.80
4:K:15:G:HO2'	4:K:16:G:H8	0.81	0.80
1:F:326:TRP:HD1	1:F:327:TRP:H	1.29	0.80
2:E:14:LYS:HD2	2:E:14:LYS:H	1.43	0.80
2:E:51:LEU:HD11	2:E:79:ILE:HD13	1.62	0.80
1:A:365:ARG:O	1:A:367:ARG:NH1	2.14	0.80
3:J:151:VAL:HG23	3:J:151:VAL:O	1.79	0.80
4:K:8:A:H4'	4:K:9:C:OP1	1.79	0.79
1:F:82:PHE:CD1	1:F:82:PHE:N	2.47	0.79
1:A:240:GLN:O	1:A:244:LYS:HG2	1.83	0.79
1:A:280:ARG:HG3	1:A:348:TYR:CE1	2.16	0.79
2:H:28:ARG:HD2	2:H:28:ARG:O	1.81	0.79
1:A:190:ILE:HD11	1:A:212:LYS:CB	2.11	0.79
3:I:28:ASN:ND2	3:I:49:ARG:HD2	1.97	0.79
3:J:75:LYS:NZ	3:J:145:ASP:HB3	1.97	0.79
3:I:95:VAL:CG1	3:I:99:GLY:HA3	2.07	0.79
3:I:211:ASN:HD22	3:I:213:GLU:H	1.30	0.79
3:J:75:LYS:NZ	3:J:146:VAL:HG23	1.97	0.79
1:A:299:LEU:HG	1:A:310:PRO:HB3	1.65	0.79
1:A:253:MET:HB3	1:A:261:LYS:HD2	1.63	0.78
1:F:55:LEU:HD13	1:F:82:PHE:CE2	2.18	0.78
4:K:22:U:O2'	4:K:23:G:H8	1.66	0.78
3:J:193:PHE:CE2	3:J:220:ALA:HB3	2.18	0.78
3:I:102:TYR:HE1	3:I:142:THR:H	1.32	0.78
3:J:43:TRP:HB3	3:J:48:TYR:HE1	1.47	0.78
1:A:184:VAL:CG2	1:A:190:ILE:HG22	2.13	0.78
1:F:156:LEU:O	1:F:156:LEU:HD23	1.84	0.78
2:E:15:GLU:HA	2:E:18:GLU:OE1	1.83	0.78
1:A:366:ILE:HD11	4:K:21:A:OP1	1.84	0.77
4:L:7:G:H1'	4:L:21:A:N6	1.99	0.77
2:H:108:ALA:HA	2:H:111:LEU:CD1	2.14	0.77
2:E:108:ALA:HA	2:E:111:LEU:HD12	1.65	0.77
1:A:301:ARG:HB3	1:A:307:ALA:HB3	1.66	0.77
1:F:301:ARG:CB	1:F:307:ALA:HB3	2.06	0.77
2:E:115:ILE:HD12	2:E:116:ALA:N	2.00	0.77
2:H:49:ALA:HB3	2:H:76:ILE:CD1	2.14	0.77
2:H:108:ALA:HA	2:H:111:LEU:HB2	1.65	0.77
3:J:83:ALA:H	3:J:105:GLU:HG2	1.50	0.77
2:E:16:LEU:O	2:E:19:LYS:HG3	1.85	0.77
4:L:10:C:N4	4:L:16:G:O6	2.17	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LEU:HD23	1:A:275:LEU:H	1.48	0.76
3:I:205:GLU:HG2	3:I:207:ILE:HG22	1.67	0.76
3:I:34:ARG:HH11	3:I:40:VAL:HG11	1.50	0.76
2:H:48:GLN:HB3	2:H:103:ILE:HD13	1.66	0.76
1:A:163:HIS:CE1	1:A:187:ARG:H	2.03	0.75
1:F:326:TRP:HD1	1:F:327:TRP:N	1.84	0.75
1:F:359:LYS:O	1:F:363:GLU:HG3	1.86	0.75
2:E:108:ALA:HA	2:E:111:LEU:CD1	2.17	0.75
1:A:301:ARG:O	1:A:306:GLY:HA2	1.86	0.75
4:K:15:G:O2'	4:K:16:G:C8	2.37	0.75
1:A:180:PHE:CE2	1:A:184:VAL:HG21	2.22	0.75
4:L:11:G:H22	4:L:15:G:H1'	1.49	0.75
3:I:36:TYR:HB3	3:I:86:THR:HG22	1.67	0.75
1:A:170:LEU:CD2	1:A:208:ILE:HG22	2.13	0.74
2:E:118:LYS:NZ	2:E:122:LEU:HD11	2.01	0.74
1:F:326:TRP:CD1	1:F:327:TRP:N	2.54	0.74
1:A:225:ILE:HG22	1:A:226:GLU:N	2.02	0.74
1:A:362:LEU:HD12	1:A:362:LEU:O	1.85	0.74
2:E:59:ASP:HA	2:E:60:PRO:C	2.08	0.74
3:I:211:ASN:ND2	3:I:213:GLU:HG2	2.01	0.74
1:F:163:HIS:NE2	1:F:187:ARG:HB2	2.01	0.74
1:F:88:PHE:HB3	1:F:89:PRO:HD3	1.69	0.74
1:A:198:LEU:HB2	1:A:200:LEU:HD23	1.67	0.74
4:L:16:G:O2'	4:L:17:C:H6	1.70	0.74
1:F:360:LYS:HE3	3:J:183:ILE:O	1.88	0.74
1:A:26:ILE:HG22	1:A:27:GLU:N	2.03	0.73
2:E:22:GLN:HB2	2:E:25:GLU:OE2	1.88	0.73
2:H:109:ARG:CG	2:H:110:ASP:H	1.99	0.73
4:K:8:A:C8	4:K:18:G:C6	2.75	0.73
1:A:69:GLU:OE2	1:A:93:GLY:HA3	1.88	0.73
3:J:57:LYS:HE2	6:J:228:SAM:O	1.88	0.73
4:L:8:A:H4'	4:L:9:C:OP1	1.88	0.73
2:H:39:GLU:HA	2:H:42:LYS:HB2	1.71	0.73
4:L:16:G:O2'	4:L:17:C:C6	2.41	0.73
3:J:58:LEU:CD1	3:J:148:PHE:HE1	2.01	0.73
4:L:15:G:O2'	4:L:16:G:H8	1.70	0.73
4:L:21:A:O2'	4:L:22:U:C6	2.40	0.73
1:F:11:GLU:OE2	3:J:138:ARG:HD2	1.87	0.73
1:F:308:LYS:HD2	1:F:308:LYS:N	2.02	0.73
1:A:291:GLN:HB3	1:A:337:ALA:HB2	1.70	0.73
2:E:63:ILE:HD12	4:K:19:U:O2	1.89	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:PHE:HE2	3:J:102:TYR:HE2	1.35	0.72
2:H:66:HIS:O	2:H:69:PRO:HD2	1.88	0.72
2:E:38:ASN:HB2	4:K:20:G:O6	1.89	0.72
1:A:119:LEU:O	1:A:119:LEU:HD23	1.89	0.72
2:E:119:VAL:O	2:E:123:MET:HG2	1.90	0.72
2:E:16:LEU:CD2	2:E:118:LYS:HG2	2.20	0.72
4:L:15:G:O2'	4:L:16:G:C8	2.42	0.72
4:L:16:G:C4	4:L:17:C:C5	2.77	0.72
1:A:180:PHE:O	1:A:184:VAL:HG12	1.88	0.71
2:H:112:VAL:O	2:H:115:ILE:HG13	1.90	0.71
3:J:150:ASP:CG	6:J:228:SAM:HE3	2.11	0.71
4:L:8:A:C6	4:L:21:A:C8	2.78	0.71
2:H:115:ILE:HD12	2:H:116:ALA:H	1.55	0.71
3:J:4:VAL:HG22	3:J:15:VAL:HG12	1.71	0.71
1:A:200:LEU:HD12	1:A:204:LYS:HG2	1.72	0.71
2:H:108:ALA:CA	2:H:111:LEU:HB2	2.20	0.71
3:J:75:LYS:HZ3	3:J:145:ASP:CB	2.04	0.71
2:E:49:ALA:HB3	2:E:76:ILE:HD13	1.71	0.71
3:I:79:TYR:CE1	3:I:88:ALA:HB2	2.25	0.71
4:L:22:U:O2'	4:L:23:G:H8	1.74	0.71
1:A:20:ASP:HB3	1:A:24:ASN:HB2	1.73	0.71
1:A:125:GLN:HB3	1:A:131:ARG:HH12	1.56	0.71
2:H:50:LYS:HZ3	2:H:103:ILE:HD12	1.56	0.71
3:J:198:ARG:HG3	3:J:199:GLU:N	2.05	0.71
3:I:83:ALA:HB2	6:I:228:SAM:H5'2	1.71	0.70
1:A:362:LEU:HD12	1:A:362:LEU:C	2.11	0.70
1:F:14:ARG:O	1:F:31:PHE:HD2	1.73	0.70
2:H:50:LYS:NZ	2:H:104:GLU:H	1.88	0.70
2:H:94:GLU:HG2	2:H:95:VAL:N	2.06	0.70
2:H:109:ARG:CG	2:H:110:ASP:N	2.54	0.70
3:I:118:VAL:HG12	3:I:124:ILE:HB	1.72	0.70
2:E:37:THR:HG21	2:E:64:VAL:HG12	1.73	0.70
2:H:115:ILE:HD12	2:H:116:ALA:N	2.06	0.70
4:K:7:G:H1'	4:K:21:A:H61	1.56	0.70
1:F:364:ALA:HA	1:F:367:ARG:NH2	2.07	0.70
1:A:329:ARG:HG2	1:A:330:GLY:H	1.56	0.70
2:E:54:ILE:HG22	2:E:55:ALA:H	1.57	0.70
3:I:105:GLU:OE2	6:I:228:SAM:H1'	1.91	0.70
2:E:32:LYS:HG3	2:E:33:ILE:H	1.57	0.70
3:I:193:PHE:CE2	3:I:220:ALA:HB3	2.25	0.70
3:J:75:LYS:HZ1	3:J:146:VAL:HG23	1.54	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:258:PRO:HD2	1:F:347:ASP:OD1	1.92	0.70
1:A:213:GLU:OE1	1:A:213:GLU:HA	1.90	0.70
1:F:59:LYS:NZ	1:F:64:ASP:HA	2.06	0.69
1:F:200:LEU:CD1	1:F:204:LYS:HG2	2.20	0.69
1:F:341:ALA:O	1:F:345:ARG:HG2	1.91	0.69
2:E:115:ILE:HD12	2:E:116:ALA:H	1.58	0.69
1:A:11:GLU:OE2	3:I:138:ARG:NH2	2.25	0.69
2:E:108:ALA:O	2:E:112:VAL:HG23	1.93	0.69
3:I:70:PRO:HD2	3:I:175:MET:CE	2.22	0.69
4:L:10:C:N4	4:L:16:G:C6	2.60	0.69
1:A:18:ALA:O	1:A:26:ILE:HB	1.92	0.69
1:A:301:ARG:HD3	1:A:307:ALA:HB3	1.74	0.69
1:F:16:ILE:HD11	1:F:42:LEU:CD1	2.21	0.69
2:E:42:LYS:HE2	4:K:6:U:OP2	1.93	0.69
2:H:122:LEU:HD12	2:H:123:MET:N	2.08	0.69
1:A:88:PHE:HB3	1:A:89:PRO:HD3	1.74	0.68
1:A:361:GLU:O	1:A:365:ARG:HG2	1.93	0.68
1:A:190:ILE:CD1	1:A:212:LYS:HB2	2.21	0.68
1:F:12:ASN:OD1	1:F:13:VAL:N	2.25	0.68
2:H:112:VAL:HG23	2:H:115:ILE:HD11	1.75	0.68
4:L:21:A:O2'	4:L:22:U:H5'	1.94	0.68
2:H:32:LYS:NZ	2:H:34:ARG:H	1.90	0.68
3:J:145:ASP:O	3:J:168:LEU:HD11	1.93	0.68
1:F:33:ASP:OD1	1:F:38:VAL:HG22	1.93	0.68
1:A:191:ASN:O	1:A:195:LEU:HB2	1.94	0.68
1:A:299:LEU:HA	1:A:310:PRO:HB3	1.76	0.68
1:F:284:MET:HE3	2:H:66:HIS:HB2	1.76	0.68
1:F:291:GLN:HB3	1:F:337:ALA:HB2	1.75	0.68
2:H:23:ALA:O	2:H:27:ALA:HB2	1.93	0.68
1:A:354:ILE:HD12	1:A:354:ILE:O	1.93	0.68
1:F:88:PHE:O	1:F:90:ASN:N	2.27	0.68
3:I:79:TYR:CD1	3:I:88:ALA:HB2	2.29	0.68
1:F:254:ASP:OD1	1:F:261:LYS:HE3	1.94	0.67
3:J:58:LEU:HD12	3:J:148:PHE:HE1	1.58	0.67
3:J:102:TYR:HE1	3:J:142:THR:N	1.91	0.67
1:A:283:ALA:O	1:A:345:ARG:HD3	1.94	0.67
1:F:209:LEU:O	1:F:212:LYS:HG2	1.95	0.67
1:F:198:LEU:HB2	1:F:200:LEU:HD23	1.76	0.67
3:I:151:VAL:HG23	3:I:151:VAL:O	1.94	0.67
4:K:10:C:N4	4:K:16:G:O6	2.28	0.67
2:H:109:ARG:HG3	2:H:110:ASP:N	2.10	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:58:LEU:HD12	3:J:148:PHE:CE1	2.29	0.67
3:J:70:PRO:HD2	3:J:175:MET:HE1	1.76	0.67
3:J:173:TYR:N	3:J:173:TYR:CD2	2.62	0.67
1:A:271:ARG:O	1:A:275:LEU:HD23	1.95	0.67
1:A:136:ILE:HD11	1:A:274:SER:HA	1.77	0.67
2:H:24:VAL:HA	2:H:27:ALA:HB3	1.77	0.67
1:A:184:VAL:HG21	1:A:190:ILE:HG22	1.76	0.67
1:F:280:ARG:O	1:F:284:MET:HB2	1.95	0.67
1:F:328:GLN:CG	1:F:329:ARG:H	2.07	0.67
4:K:11:G:N2	4:K:15:G:H1'	2.08	0.67
1:A:55:LEU:HB3	1:A:82:PHE:CE2	2.30	0.67
1:A:294:GLY:H	1:A:314:VAL:HG23	1.60	0.67
2:E:16:LEU:HD11	2:E:115:ILE:HG22	1.75	0.67
1:A:20:ASP:CB	1:A:24:ASN:HB2	2.25	0.66
1:F:364:ALA:HA	1:F:367:ARG:CZ	2.25	0.66
1:F:14:ARG:O	1:F:31:PHE:CD2	2.49	0.66
3:I:149:GLU:OE1	3:I:156:GLN:HB2	1.96	0.66
1:F:300:PHE:O	1:F:301:ARG:HB2	1.94	0.66
1:A:94:GLU:O	1:A:98:SER:HB3	1.94	0.66
1:A:275:LEU:HG	1:A:293:LEU:HD13	1.75	0.66
2:E:20:ALA:O	2:E:24:VAL:HG12	1.96	0.66
3:J:85:GLY:O	3:J:89:SER:HB3	1.94	0.66
1:A:299:LEU:HG	1:A:310:PRO:CB	2.25	0.66
4:L:11:G:N2	4:L:15:G:H1'	2.11	0.66
1:A:125:GLN:OE1	1:A:131:ARG:NH1	2.29	0.66
1:F:237:ARG:NH2	1:F:237:ARG:HB2	2.11	0.66
3:J:43:TRP:HB3	3:J:48:TYR:CE1	2.31	0.66
1:A:280:ARG:CG	1:A:348:TYR:HE1	2.08	0.66
2:E:21:LEU:HD23	2:E:81:VAL:HG21	1.77	0.66
3:J:83:ALA:N	3:J:105:GLU:HG2	2.11	0.66
1:A:259:ASN:HB2	1:A:347:ASP:OD2	1.94	0.66
1:A:152:LEU:HB2	1:A:235:ILE:CD1	2.26	0.65
1:F:357:GLU:OE1	3:J:182:SER:HA	1.95	0.65
1:A:113:TYR:O	1:A:117:VAL:HG12	1.96	0.65
3:J:29:LEU:HD22	3:J:97:TRP:CZ2	2.31	0.65
3:J:148:PHE:HD2	3:J:149:GLU:N	1.93	0.65
3:J:106:PHE:HD1	3:J:107:SER:N	1.94	0.65
3:I:158:LYS:O	3:I:158:LYS:HD3	1.96	0.65
3:I:53:PRO:HB2	3:I:215:TYR:CE1	2.31	0.65
3:I:26:THR:HG21	3:I:93:ASP:HB2	1.79	0.65
3:J:115:VAL:N	3:J:116:PRO:HD2	2.12	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ASN:HB3	1:A:15:GLY:H	1.62	0.65
1:A:137:GLN:HE21	1:F:159:TRP:HB2	1.62	0.65
1:F:358:LEU:HA	1:F:361:GLU:HB2	1.79	0.65
2:E:50:LYS:HZ3	2:E:103:ILE:HD12	1.58	0.65
2:E:25:GLU:HG3	2:E:26:ILE:HD12	1.77	0.65
2:H:84:LYS:HD3	2:H:96:ALA:HB1	1.79	0.65
3:I:148:PHE:HD2	3:I:149:GLU:N	1.95	0.65
4:K:21:A:O2'	4:K:22:U:C6	2.45	0.65
2:E:21:LEU:HD13	2:E:21:LEU:O	1.97	0.65
1:A:41:GLN:O	1:A:46:GLU:HB2	1.97	0.64
1:A:70:HIS:CE1	1:A:71:PRO:HD2	2.32	0.64
1:A:355:ALA:HA	1:A:358:LEU:HD11	1.79	0.64
3:I:68:ASN:OD1	3:I:68:ASN:N	2.30	0.64
4:K:16:G:C4	4:K:17:C:C5	2.86	0.64
1:A:152:LEU:HB2	1:A:235:ILE:HD11	1.80	0.64
1:F:136:ILE:HD11	1:F:278:GLY:HA2	1.79	0.64
2:E:4:LYS:N	2:E:5:PRO:HD3	2.11	0.64
3:I:70:PRO:HD2	3:I:175:MET:HE2	1.78	0.64
4:L:8:A:C8	4:L:18:G:C6	2.85	0.64
4:L:8:A:H1'	4:L:9:C:H5'	1.79	0.64
1:A:128:SER:HB3	1:A:131:ARG:HH21	1.63	0.64
3:I:115:VAL:N	3:I:116:PRO:HD2	2.13	0.64
1:A:184:VAL:HG22	1:A:190:ILE:HG22	1.79	0.64
1:F:361:GLU:O	1:F:365:ARG:HG2	1.97	0.64
2:E:4:LYS:N	2:E:5:PRO:CD	2.61	0.64
3:I:102:TYR:HD1	3:I:141:VAL:HB	1.61	0.64
4:K:15:G:O2'	4:K:16:G:O5'	2.15	0.64
1:F:101:GLU:HB3	1:F:108:TRP:CD1	2.32	0.64
2:H:109:ARG:O	2:H:112:VAL:HG12	1.98	0.64
4:K:7:G:H1'	4:K:21:A:N6	2.13	0.64
3:I:198:ARG:HG3	3:I:199:GLU:N	2.13	0.64
2:E:106:GLY:O	2:E:109:ARG:HG2	1.98	0.63
3:J:147:ILE:HG21	3:J:160:LEU:HD23	1.80	0.63
2:E:44:VAL:HG13	2:E:76:ILE:HD12	1.80	0.63
1:F:212:LYS:HG3	1:F:213:GLU:N	2.12	0.63
1:A:300:PHE:HE2	1:A:304:ARG:NE	1.96	0.63
1:F:142:LEU:HD23	1:F:142:LEU:C	2.19	0.63
3:I:51:TRP:HE1	3:I:56:SER:HB3	1.64	0.63
1:A:364:ALA:C	1:A:367:ARG:HH12	2.02	0.63
1:F:125:GLN:NE2	1:F:131:ARG:NH1	2.46	0.63
2:H:109:ARG:HG2	2:H:109:ARG:NH1	2.08	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:300:PHE:CD2	1:F:301:ARG:N	2.65	0.63
2:E:107:LYS:O	2:E:108:ALA:HB3	1.98	0.63
2:H:109:ARG:HG2	2:H:110:ASP:H	1.62	0.63
4:L:21:A:O2'	4:L:22:U:C5'	2.46	0.63
1:F:163:HIS:CE1	1:F:186:HIS:CD2	2.86	0.63
2:E:10:PHE:HZ	2:E:78:TYR:O	1.82	0.63
3:I:193:PHE:HE2	3:I:220:ALA:HB3	1.64	0.63
1:A:200:LEU:CD1	1:A:204:LYS:HG2	2.29	0.63
1:F:54:LEU:HD12	1:F:58:LEU:HD13	1.81	0.63
1:A:167:LEU:CD1	1:A:180:PHE:CE1	2.82	0.62
1:F:353:TYR:CE2	1:F:355:ALA:HB3	2.33	0.62
3:I:168:LEU:HD12	3:I:169:LYS:H	1.64	0.62
1:A:336:LEU:CD2	1:A:340:LEU:HG	2.29	0.62
2:H:42:LYS:HE2	4:L:6:U:OP2	1.98	0.62
3:I:71:ILE:HD12	3:I:175:MET:HE3	1.81	0.62
4:L:16:G:N3	4:L:17:C:C6	2.67	0.62
1:A:167:LEU:HD11	1:A:180:PHE:CE1	2.34	0.62
1:A:198:LEU:HB2	1:A:200:LEU:CD2	2.28	0.62
2:E:50:LYS:HZ3	2:E:104:GLU:H	1.47	0.62
3:I:102:TYR:CD1	3:I:141:VAL:HB	2.35	0.62
4:L:16:G:C4	4:L:17:C:C6	2.87	0.62
1:A:133:LYS:O	1:A:136:ILE:HG22	1.99	0.62
1:F:156:LEU:HD11	1:F:232:ALA:HB2	1.81	0.62
2:H:32:LYS:HG3	2:H:33:ILE:H	1.65	0.62
3:J:106:PHE:CD1	3:J:107:SER:N	2.68	0.62
1:F:73:LEU:O	1:F:77:ALA:HB2	1.98	0.62
1:F:301:ARG:HD3	1:F:307:ALA:HB1	1.82	0.62
3:I:179:LYS:HG3	3:I:219:HIS:CE1	2.34	0.62
3:J:1:MET:SD	3:J:18:ASP:O	2.58	0.62
2:H:107:LYS:O	2:H:108:ALA:HB3	1.99	0.62
4:K:21:A:HO2'	4:K:22:U:H6	1.41	0.62
3:J:208:GLU:HB3	3:J:223:VAL:HG13	1.80	0.62
1:F:281:GLU:CD	1:F:281:GLU:H	2.04	0.61
2:E:118:LYS:O	2:E:122:LEU:HD13	1.99	0.61
4:K:10:C:C3'	4:K:11:G:H5"	2.26	0.61
3:J:102:TYR:CE1	3:J:141:VAL:HA	2.35	0.61
1:F:94:GLU:OE1	3:J:143:LYS:HD2	1.99	0.61
3:J:7:HIS:HB3	3:J:12:VAL:O	2.00	0.61
1:A:325:PRO:HD2	1:A:328:GLN:HG3	1.81	0.61
1:F:89:PRO:HG3	3:J:166:ALA:HA	1.82	0.61
1:F:113:TYR:HE2	3:J:122:ARG:NH2	1.92	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ARG:N	1:A:367:ARG:HH12	1.98	0.61
3:I:148:PHE:C	3:I:148:PHE:CD2	2.74	0.61
1:A:195:LEU:HD21	1:A:208:ILE:HD11	1.82	0.61
1:F:291:GLN:NE2	4:L:5:C:H41	1.99	0.61
2:H:50:LYS:HZ3	2:H:104:GLU:H	1.48	0.61
4:K:21:A:O2'	4:K:22:U:C5'	2.49	0.61
2:E:100:VAL:HG12	2:E:101:ALA:H	1.65	0.61
3:I:34:ARG:NH1	3:I:40:VAL:HG11	2.15	0.61
3:J:50:ILE:HG23	3:J:51:TRP:N	2.15	0.61
1:A:354:ILE:HD11	1:A:358:LEU:HD21	1.81	0.61
1:F:190:ILE:O	1:F:190:ILE:HG13	1.99	0.61
1:F:348:TYR:C	1:F:348:TYR:CD2	2.74	0.61
4:L:8:A:C1'	4:L:9:C:H5'	2.31	0.61
3:I:135:GLU:O	3:I:138:ARG:HB3	2.01	0.61
3:I:204:PHE:CB	3:I:224:VAL:HB	2.31	0.61
1:F:177:TYR:O	1:F:180:PHE:HB3	2.00	0.60
1:F:209:LEU:HD23	1:F:212:LYS:HD2	1.83	0.60
4:K:15:G:O5'	4:K:15:G:H8	1.84	0.60
4:L:6:U:H1'	4:L:23:G:N2	2.14	0.60
1:A:49:LYS:HG2	1:A:53:GLU:HG3	1.83	0.60
1:A:227:VAL:O	1:A:230:GLN:HB2	2.00	0.60
3:I:221:LEU:HD23	3:I:222:PHE:N	2.16	0.60
3:J:118:VAL:HG12	3:J:124:ILE:HB	1.83	0.60
1:F:11:GLU:OE2	3:J:138:ARG:NH2	2.28	0.60
1:F:275:LEU:H	1:F:275:LEU:CD2	2.11	0.60
1:F:224:ASP:O	1:F:227:VAL:HG12	2.01	0.60
1:A:26:ILE:HG22	1:A:27:GLU:H	1.66	0.60
1:F:225:ILE:HG22	1:F:226:GLU:N	2.17	0.60
1:F:227:VAL:HG13	1:F:228:VAL:N	2.17	0.60
1:A:249:ILE:O	1:A:253:MET:HB2	2.01	0.60
1:F:88:PHE:HE2	3:J:134:PRO:HB2	1.63	0.60
4:L:13:A:N7	4:L:14:A:N7	2.50	0.60
2:E:18:GLU:HA	2:E:21:LEU:HB3	1.82	0.60
2:E:38:ASN:CB	4:K:20:G:O6	2.49	0.60
2:H:10:PHE:CG	2:H:122:LEU:HD13	2.37	0.60
2:H:51:LEU:HB3	2:H:102:ILE:HD11	1.83	0.60
3:J:190:GLU:OE2	3:J:209:ARG:NH1	2.35	0.60
1:F:253:MET:HB3	1:F:261:LYS:HD2	1.84	0.60
2:H:104:GLU:O	2:H:104:GLU:HG3	2.01	0.60
3:I:173:TYR:CZ	3:I:225:ARG:HD2	2.37	0.60
2:E:23:ALA:O	2:E:27:ALA:HB2	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:83:ALA:HA	3:J:105:GLU:CG	2.32	0.60
1:A:348:TYR:HD2	1:A:348:TYR:C	2.05	0.59
1:F:184:VAL:HG22	1:F:190:ILE:HG22	1.80	0.59
1:A:301:ARG:CD	1:A:307:ALA:HB3	2.31	0.59
3:I:204:PHE:HB3	3:I:224:VAL:HB	1.83	0.59
1:A:359:LYS:O	1:A:363:GLU:HG3	2.01	0.59
1:F:329:ARG:O	1:F:331:LYS:N	2.35	0.59
4:K:6:U:H1'	4:K:23:G:N2	2.17	0.59
4:L:15:G:H4'	4:L:16:G:OP1	2.03	0.59
2:E:50:LYS:HB2	2:E:102:ILE:O	2.03	0.59
2:H:51:LEU:H	2:H:102:ILE:HD12	1.67	0.59
1:F:167:LEU:HA	1:F:170:LEU:HB2	1.82	0.59
1:F:331:LYS:HG2	1:F:334:ARG:NH2	2.17	0.59
3:I:148:PHE:HD2	3:I:148:PHE:C	2.05	0.59
1:A:170:LEU:C	1:A:172:PRO:HD3	2.23	0.59
1:F:82:PHE:H	1:F:82:PHE:HD1	1.46	0.59
3:J:43:TRP:CB	3:J:48:TYR:HE1	2.15	0.59
2:E:10:PHE:CZ	2:E:78:TYR:O	2.56	0.59
2:E:51:LEU:HD12	2:E:115:ILE:HD13	1.83	0.59
3:I:158:LYS:HD2	3:I:162:ASP:CG	2.23	0.59
1:F:200:LEU:HD12	1:F:204:LYS:CG	2.27	0.59
3:J:78:LEU:N	3:J:144:VAL:HG11	2.18	0.59
3:J:130:ASP:OD1	3:J:132:THR:HB	2.03	0.59
1:A:156:LEU:HD12	1:A:231:LEU:HB3	1.85	0.59
1:F:174:HIS:HB2	1:F:175:PRO:CD	2.30	0.59
3:I:7:HIS:HE1	3:I:9:PHE:CD1	2.21	0.59
1:F:49:LYS:HG3	1:F:50:ASP:N	2.17	0.58
1:F:58:LEU:HD23	1:F:66:PHE:HE2	1.68	0.58
2:H:59:ASP:HA	2:H:60:PRO:C	2.22	0.58
3:I:118:VAL:CG1	3:I:124:ILE:HB	2.33	0.58
3:I:152:ALA:O	3:I:153:GLN:HG2	2.02	0.58
4:K:3:C:O2'	4:K:4:U:P	2.61	0.58
5:S:3:C:H2'	5:S:3:C:O2	2.04	0.58
1:A:160:TYR:O	1:A:160:TYR:CD2	2.56	0.58
1:A:211:ALA:O	1:A:214:LYS:O	2.22	0.58
2:E:66:HIS:C	2:E:69:PRO:HD2	2.24	0.58
2:E:118:LYS:HZ2	2:E:122:LEU:HD21	1.67	0.58
1:A:125:GLN:HB3	1:A:131:ARG:NH1	2.18	0.58
1:A:163:HIS:CE1	1:A:186:HIS:CD2	2.92	0.58
2:E:59:ASP:OD1	3:I:181:ARG:NH1	2.36	0.58
2:H:15:GLU:O	2:H:18:GLU:N	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PHE:CD1	1:A:92:ALA:HA	2.38	0.58
1:A:365:ARG:NH2	4:K:17:C:OP1	2.37	0.58
1:F:163:HIS:CE1	1:F:187:ARG:HB2	2.37	0.58
2:E:13:PRO:HB2	2:E:16:LEU:H	1.68	0.58
3:J:91:VAL:O	3:J:95:VAL:HG23	2.04	0.58
4:K:7:G:C4'	4:K:8:A:OP1	2.49	0.58
1:F:190:ILE:HB	1:F:195:LEU:HD11	1.85	0.58
1:A:156:LEU:HB2	1:A:231:LEU:HD23	1.86	0.58
1:A:348:TYR:C	1:A:348:TYR:CD2	2.77	0.58
1:F:58:LEU:O	1:F:63:TYR:HD2	1.86	0.58
3:J:70:PRO:HD2	3:J:175:MET:CE	2.34	0.58
3:J:144:VAL:O	3:J:169:LYS:HG2	2.02	0.58
1:F:42:LEU:HD23	1:F:46:GLU:O	2.03	0.58
1:F:220:MET:HB3	1:F:224:ASP:HB2	1.85	0.58
1:A:366:ILE:CD1	4:K:21:A:OP1	2.51	0.57
1:F:12:ASN:HD21	1:F:104:LEU:HD11	1.69	0.57
1:F:365:ARG:HD2	1:F:366:ILE:HD12	1.85	0.57
1:F:94:GLU:O	1:F:98:SER:HB3	2.03	0.57
2:H:57:ASP:N	2:H:57:ASP:OD1	2.37	0.57
2:H:61:GLU:O	2:H:61:GLU:HG3	2.05	0.57
3:J:106:PHE:CD1	3:J:106:PHE:C	2.77	0.57
3:J:148:PHE:HD2	3:J:148:PHE:C	2.07	0.57
4:K:8:A:H1'	4:K:9:C:H5'	1.87	0.57
1:A:301:ARG:CB	1:A:307:ALA:HB3	2.35	0.57
2:H:109:ARG:HH11	2:H:109:ARG:CG	2.14	0.57
3:J:83:ALA:HA	3:J:105:GLU:HG2	1.85	0.57
4:K:19:U:H4'	4:K:20:G:OP2	2.04	0.57
1:F:366:ILE:O	1:F:366:ILE:HG22	2.04	0.57
1:F:166:GLU:H	1:F:166:GLU:CD	2.07	0.57
1:F:302:HIS:HD2	1:F:307:ALA:O	1.87	0.57
2:E:50:LYS:NZ	2:E:104:GLU:H	2.02	0.57
3:I:29:LEU:HD22	3:I:97:TRP:CZ2	2.39	0.57
3:J:75:LYS:NZ	3:J:145:ASP:CB	2.66	0.57
3:J:195:GLU:OE1	3:J:195:GLU:O	2.22	0.57
4:K:1:A:O2'	4:K:2:G:P	2.62	0.57
1:A:201:SER:OG	1:A:204:LYS:HB2	2.05	0.57
1:F:160:TYR:O	1:F:160:TYR:CD2	2.57	0.57
2:H:54:ILE:HG23	2:H:99:SER:HB3	1.85	0.57
2:E:18:GLU:O	2:E:22:GLN:HG2	2.04	0.57
3:J:214:PRO:HD2	3:J:215:TYR:CD2	2.40	0.57
1:F:8:PHE:HB3	1:F:9:ILE:HG13	1.86	0.57

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:GLN:NE2	3:I:112:ARG:NH2	2.52	0.56
1:F:14:ARG:C	1:F:31:PHE:CD2	2.78	0.56
1:A:295:ALA:HB2	1:A:313:GLY:H	1.70	0.56
3:I:88:ALA:HA	3:I:91:VAL:HG13	1.85	0.56
4:K:1:A:O2'	4:K:2:G:OP1	2.23	0.56
1:F:149:ILE:HG21	1:F:239:TYR:HE2	1.71	0.56
1:F:205:ILE:O	1:F:209:LEU:HD12	2.05	0.56
2:E:42:LYS:HE2	4:K:6:U:P	2.46	0.56
3:J:102:TYR:CD1	3:J:141:VAL:HG12	2.40	0.56
1:A:362:LEU:O	1:A:365:ARG:HB2	2.05	0.56
2:E:33:ILE:O	2:E:34:ARG:HB2	2.03	0.56
2:E:118:LYS:HZ3	2:E:122:LEU:HD11	1.70	0.56
3:J:51:TRP:HE1	3:J:56:SER:HB3	1.70	0.56
4:L:8:A:N1	4:L:21:A:C8	2.73	0.56
1:A:167:LEU:HD11	1:A:180:PHE:CD1	2.40	0.56
1:A:339:LYS:HG3	1:A:362:LEU:HB2	1.87	0.56
1:A:367:ARG:NE	1:A:367:ARG:CA	2.67	0.56
1:F:298:ALA:O	1:F:299:LEU:HB2	2.05	0.56
2:H:112:VAL:CG2	2:H:115:ILE:HD11	2.36	0.56
1:A:353:TYR:CE2	1:A:355:ALA:HB3	2.40	0.56
1:F:32:THR:HG21	1:F:49:LYS:HZ1	1.68	0.56
2:E:51:LEU:CD1	2:E:79:ILE:HD13	2.31	0.56
3:I:123:ASN:OD1	3:I:124:ILE:HG13	2.05	0.56
3:I:217:LYS:O	3:I:219:HIS:ND1	2.35	0.56
3:J:79:TYR:HD2	3:J:79:TYR:C	2.09	0.56
4:K:16:G:C4	4:K:17:C:C6	2.94	0.56
2:E:15:GLU:O	2:E:16:LEU:C	2.44	0.56
2:E:28:ARG:HD2	2:E:91:ALA:O	2.06	0.56
3:J:94:ILE:HG22	3:J:95:VAL:N	2.21	0.56
4:K:16:G:N3	4:K:17:C:C6	2.74	0.56
1:F:300:PHE:O	1:F:301:ARG:CB	2.53	0.56
2:E:15:GLU:O	2:E:17:ALA:N	2.39	0.56
3:J:61:ALA:CB	3:J:221:LEU:HD12	2.36	0.56
3:J:148:PHE:C	3:J:148:PHE:CD2	2.79	0.56
1:A:204:LYS:HE3	1:A:204:LYS:HA	1.87	0.56
1:A:318:TYR:HB3	1:A:321:ILE:HG13	1.87	0.56
1:F:18:ALA:O	1:F:25:LEU:O	2.24	0.56
3:J:17:ASP:O	3:J:18:ASP:C	2.43	0.56
4:K:17:C:O2'	4:K:18:G:H5"	2.05	0.56
1:A:364:ALA:CA	1:A:367:ARG:HH22	2.18	0.55
1:F:156:LEU:HD21	1:F:181:VAL:HG21	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:280:ARG:CB	1:F:348:TYR:HE1	2.19	0.55
2:H:50:LYS:NZ	2:H:103:ILE:HD12	2.21	0.55
2:H:79:ILE:HD12	2:H:80:TYR:H	1.71	0.55
4:K:3:C:O2'	4:K:4:U:OP2	2.23	0.55
1:A:8:PHE:O	1:A:92:ALA:HB2	2.06	0.55
1:F:49:LYS:O	1:F:53:GLU:HG3	2.05	0.55
2:E:78:TYR:C	2:E:79:ILE:HD12	2.26	0.55
1:F:341:ALA:HB1	1:F:345:ARG:HH12	1.71	0.55
2:E:78:TYR:OH	2:E:123:MET:HE3	2.07	0.55
2:H:12:VAL:HG22	2:H:13:PRO:O	2.06	0.55
2:H:68:PRO:HB2	2:H:69:PRO:HD3	1.89	0.55
3:I:85:GLY:O	3:I:89:SER:HB3	2.06	0.55
2:E:24:VAL:O	2:E:27:ALA:N	2.39	0.55
2:H:22:GLN:HA	2:H:25:GLU:HB2	1.89	0.55
2:H:102:ILE:HD12	2:H:102:ILE:H	1.71	0.55
3:I:108:PRO:HB3	3:I:128:LEU:HD11	1.88	0.55
3:J:147:ILE:HG21	3:J:160:LEU:CD2	2.36	0.55
1:F:157:ARG:HH11	1:F:174:HIS:CD2	2.25	0.55
2:E:20:ALA:HA	2:E:23:ALA:HB3	1.88	0.55
3:J:75:LYS:HZ2	3:J:146:VAL:HG23	1.71	0.55
1:F:348:TYR:C	1:F:348:TYR:HD2	2.10	0.55
2:H:15:GLU:HA	2:H:18:GLU:HB3	1.89	0.55
2:H:113:GLU:OE1	2:H:113:GLU:N	2.28	0.55
3:J:181:ARG:HB2	3:J:185:VAL:HG13	1.89	0.55
1:A:328:GLN:CD	1:A:328:GLN:H	2.10	0.55
1:F:33:ASP:OD2	1:F:37:LYS:HD3	2.07	0.55
1:F:88:PHE:HB3	1:F:89:PRO:CD	2.37	0.55
1:F:190:ILE:CD1	1:F:209:LEU:HD23	2.37	0.55
1:F:212:LYS:CG	1:F:213:GLU:N	2.70	0.55
1:F:119:LEU:O	1:F:119:LEU:CD2	2.52	0.55
1:A:367:ARG:NE	1:A:367:ARG:HA	2.22	0.54
1:F:306:GLY:O	1:F:307:ALA:HB2	2.07	0.54
1:F:114:LYS:HG2	1:F:115:VAL:N	2.21	0.54
3:I:39:ARG:O	3:I:50:ILE:HB	2.06	0.54
3:I:79:TYR:C	3:I:79:TYR:CD2	2.80	0.54
1:F:163:HIS:CD2	1:F:163:HIS:O	2.60	0.54
2:E:37:THR:CG2	2:E:64:VAL:HG12	2.37	0.54
2:E:107:LYS:O	2:E:108:ALA:CB	2.55	0.54
3:I:83:ALA:H	3:I:105:GLU:HG2	1.72	0.54
3:I:155:THR:O	3:I:158:LYS:N	2.38	0.54
3:J:95:VAL:CG1	3:J:99:GLY:HA3	2.24	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:TYR:N	1:A:63:TYR:CD2	2.75	0.54
3:I:147:ILE:CD1	3:I:168:LEU:HB2	2.38	0.54
1:F:109:PHE:HE2	3:J:102:TYR:CE2	2.21	0.54
1:A:109:PHE:HE2	3:I:102:TYR:HE2	1.55	0.54
2:E:50:LYS:NZ	2:E:103:ILE:HD12	2.22	0.54
2:H:51:LEU:H	2:H:102:ILE:CD1	2.20	0.54
3:I:1:MET:SD	3:I:17:ASP:O	2.66	0.54
3:J:193:PHE:CE2	3:J:220:ALA:CB	2.89	0.54
1:F:268:LEU:HD12	1:F:268:LEU:O	2.08	0.54
1:A:130:ALA:HB2	1:F:218:ALA:HB1	1.90	0.54
1:A:292:VAL:HG23	1:A:292:VAL:O	2.07	0.54
3:I:211:ASN:ND2	3:I:213:GLU:H	2.01	0.54
4:K:16:G:O2'	4:K:17:C:O5'	2.25	0.54
1:F:169:GLU:O	1:F:169:GLU:HG3	2.08	0.54
2:H:77:PRO:HB3	2:H:119:VAL:HG21	1.89	0.54
2:H:94:GLU:HG2	2:H:95:VAL:H	1.73	0.54
4:L:15:G:O2'	4:L:16:G:O5'	2.19	0.54
1:F:163:HIS:CE1	1:F:187:ARG:H	2.26	0.53
2:H:14:LYS:HD2	2:H:14:LYS:N	2.23	0.53
2:H:30:THR:HG22	2:H:30:THR:O	2.08	0.53
2:H:54:ILE:HG22	2:H:55:ALA:N	2.20	0.53
4:L:7:G:C4'	4:L:8:A:OP1	2.52	0.53
1:A:295:ALA:O	1:A:299:LEU:HB2	2.07	0.53
3:J:137:TYR:N	3:J:137:TYR:CD2	2.76	0.53
1:A:148:VAL:O	1:A:152:LEU:HG	2.08	0.53
1:A:255:ASP:O	1:A:255:ASP:OD2	2.26	0.53
1:F:133:LYS:HA	1:F:136:ILE:HD12	1.90	0.53
1:F:259:ASN:O	1:F:262:ALA:N	2.41	0.53
4:L:8:A:C6	4:L:21:A:N7	2.77	0.53
1:A:16:ILE:HD11	1:A:42:LEU:HD11	1.88	0.53
1:F:55:LEU:HD13	1:F:82:PHE:CZ	2.43	0.53
1:A:62:GLY:C	1:A:63:TYR:HD2	2.12	0.53
1:A:331:LYS:HG2	1:A:334:ARG:NH2	2.23	0.53
1:A:365:ARG:C	1:A:367:ARG:NH1	2.62	0.53
1:F:126:GLU:O	1:F:131:ARG:NH2	2.41	0.53
1:F:280:ARG:HA	1:F:348:TYR:CD1	2.43	0.53
1:F:343:ALA:O	1:F:347:ASP:HB2	2.09	0.53
1:A:136:ILE:CD1	1:A:274:SER:HA	2.39	0.53
1:F:284:MET:HE1	2:H:66:HIS:O	2.09	0.53
2:H:50:LYS:CE	2:H:104:GLU:H	2.22	0.53
1:A:220:MET:HB3	1:A:224:ASP:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:59:LYS:HZ2	1:F:64:ASP:HA	1.73	0.53
1:F:70:HIS:ND1	1:F:71:PRO:HD2	2.24	0.53
1:F:240:GLN:O	1:F:244:LYS:HG2	2.08	0.53
1:A:98:SER:HA	3:I:143:LYS:HD3	1.89	0.53
1:A:295:ALA:O	1:A:299:LEU:HD13	2.08	0.53
1:F:170:LEU:C	1:F:172:PRO:HD3	2.30	0.53
2:H:55:ALA:CB	2:H:84:LYS:HB3	2.38	0.53
2:H:55:ALA:HB1	2:H:84:LYS:HB3	1.91	0.53
3:I:158:LYS:HD3	3:I:158:LYS:C	2.29	0.53
2:H:21:LEU:HD13	2:H:21:LEU:O	2.09	0.53
1:F:318:TYR:CD1	1:F:320:ALA:HB3	2.44	0.52
1:F:251:ARG:CG	1:F:251:ARG:NH1	2.55	0.52
3:I:118:VAL:HG21	3:I:126:PRO:HG3	1.90	0.52
4:K:12:A:H2'	4:K:13:A:O4'	2.08	0.52
1:F:43:LEU:HD21	3:J:139:ALA:HB3	1.90	0.52
1:F:145:VAL:O	1:F:149:ILE:HG13	2.10	0.52
2:E:32:LYS:HE2	2:E:33:ILE:H	1.74	0.52
2:H:24:VAL:HG23	2:H:33:ILE:HD13	1.91	0.52
1:A:109:PHE:HE2	3:I:102:TYR:CE2	2.28	0.52
1:A:186:HIS:O	1:A:189:ASN:HB2	2.10	0.52
3:I:53:PRO:HB2	3:I:215:TYR:CD1	2.45	0.52
2:H:49:ALA:CB	2:H:76:ILE:HD13	2.30	0.52
3:J:195:GLU:OE1	3:J:195:GLU:C	2.48	0.52
4:K:10:C:N4	4:K:16:G:C6	2.78	0.52
1:F:203:GLU:OE2	1:F:204:LYS:N	2.42	0.52
2:H:122:LEU:HD12	2:H:123:MET:H	1.73	0.52
3:I:58:LEU:HD23	3:I:58:LEU:O	2.10	0.52
3:I:79:TYR:C	3:I:79:TYR:HD2	2.12	0.52
3:J:27:LYS:O	3:J:93:ASP:HB3	2.09	0.52
1:A:63:TYR:N	1:A:63:TYR:HD2	2.07	0.52
4:K:8:A:C1'	4:K:9:C:H5'	2.39	0.52
1:F:57:SER:O	1:F:60:GLU:HB3	2.10	0.52
2:E:19:LYS:HD2	2:E:115:ILE:HG23	1.92	0.52
2:H:37:THR:CG2	2:H:64:VAL:HG12	2.36	0.52
1:A:205:ILE:C	1:A:205:ILE:HD12	2.31	0.52
1:A:264:VAL:CG1	1:A:340:LEU:HD21	2.39	0.52
1:A:325:PRO:O	1:A:329:ARG:HB2	2.09	0.52
1:F:55:LEU:CD1	1:F:82:PHE:CZ	2.93	0.52
3:J:61:ALA:HB1	3:J:221:LEU:HD12	1.92	0.52
1:A:13:VAL:HG22	1:A:115:VAL:HB	1.91	0.52
1:A:55:LEU:HB3	1:A:82:PHE:CZ	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:GLU:O	1:F:76:ARG:HG2	2.10	0.52
1:F:149:ILE:HD13	1:F:239:TYR:CD2	2.45	0.52
2:E:22:GLN:O	2:E:25:GLU:HG2	2.10	0.52
3:I:95:VAL:HG12	3:I:99:GLY:CA	2.15	0.52
1:A:269:ALA:O	1:A:273:ILE:HG13	2.09	0.51
2:H:40:THR:O	2:H:44:VAL:HG23	2.10	0.51
1:A:195:LEU:CD1	1:A:208:ILE:HD11	2.37	0.51
1:A:205:ILE:O	1:A:209:LEU:HB2	2.11	0.51
1:F:229:ARG:O	1:F:229:ARG:HG2	2.10	0.51
2:E:32:LYS:HE2	2:E:33:ILE:N	2.25	0.51
1:A:70:HIS:ND1	1:A:71:PRO:CD	2.70	0.51
1:A:318:TYR:CD2	1:A:336:LEU:HD11	2.45	0.51
2:H:81:VAL:HG23	2:H:81:VAL:O	2.10	0.51
2:H:107:LYS:O	2:H:108:ALA:CB	2.58	0.51
3:I:28:ASN:HB2	3:I:49:ARG:CG	2.36	0.51
3:J:79:TYR:C	3:J:79:TYR:CD2	2.83	0.51
1:A:11:GLU:CD	3:I:138:ARG:HH21	2.13	0.51
1:A:14:ARG:HD2	1:A:30:TYR:CZ	2.45	0.51
1:F:253:MET:HE2	1:F:269:ALA:CB	2.40	0.51
1:F:329:ARG:O	1:F:332:ILE:HG13	2.11	0.51
1:F:341:ALA:HB1	1:F:345:ARG:NH1	2.26	0.51
2:E:34:ARG:O	2:E:100:VAL:HG13	2.10	0.51
2:H:66:HIS:CD2	2:H:67:LEU:HD23	2.45	0.51
4:K:16:G:O2'	4:K:17:C:C6	2.63	0.51
1:F:66:PHE:O	1:F:84:ALA:HA	2.11	0.51
1:F:163:HIS:HE1	1:F:186:HIS:CD2	2.28	0.51
2:E:19:LYS:HD2	2:E:115:ILE:CG2	2.40	0.51
2:H:19:LYS:O	2:H:23:ALA:HB2	2.11	0.51
3:J:149:GLU:OE1	3:J:156:GLN:HB2	2.11	0.51
1:F:284:MET:CE	2:H:66:HIS:HB2	2.40	0.51
3:I:147:ILE:HD11	3:I:168:LEU:HB2	1.92	0.51
3:J:92:SER:HA	3:J:101:ILE:HD11	1.93	0.51
1:A:301:ARG:HB3	1:A:307:ALA:CB	2.40	0.51
1:F:208:ILE:HG13	1:F:209:LEU:N	2.25	0.51
3:I:17:ASP:OD2	3:I:23:LYS:HE2	2.11	0.51
2:E:57:ASP:N	2:E:57:ASP:OD1	2.44	0.51
3:I:24:ILE:HD13	3:I:62:ILE:HG22	1.93	0.51
3:J:222:PHE:CD1	3:J:222:PHE:N	2.79	0.51
1:A:91:ILE:HD12	1:A:91:ILE:H	1.77	0.50
1:A:174:HIS:HB2	1:A:175:PRO:HD3	1.94	0.50
1:F:11:GLU:CD	3:J:138:ARG:HH21	2.14	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:8:VAL:HG23	2:H:8:VAL:O	2.11	0.50
2:H:121:GLU:HG2	2:H:122:LEU:N	2.25	0.50
3:J:13:TYR:N	3:J:13:TYR:CD2	2.79	0.50
1:F:13:VAL:HG22	1:F:115:VAL:HB	1.93	0.50
1:F:267:LYS:NZ	1:F:271:ARG:HH22	2.09	0.50
1:F:300:PHE:CG	1:F:301:ARG:N	2.78	0.50
3:I:114:LEU:C	3:I:116:PRO:HD2	2.30	0.50
1:A:73:LEU:O	1:A:77:ALA:HB2	2.11	0.50
1:A:128:SER:HB3	1:A:131:ARG:NH2	2.24	0.50
2:E:26:ILE:O	2:E:26:ILE:HG22	2.11	0.50
2:H:32:LYS:HZ1	2:H:34:ARG:H	1.57	0.50
2:H:110:ASP:OD1	2:H:113:GLU:OE2	2.28	0.50
3:J:57:LYS:HZ3	3:J:216:GLU:HG3	1.75	0.50
3:J:83:ALA:CA	3:J:105:GLU:HG2	2.41	0.50
1:A:305:THR:HG22	1:A:306:GLY:N	2.26	0.50
1:F:166:GLU:HG2	1:F:211:ALA:HB1	1.93	0.50
2:E:21:LEU:HD11	2:E:86:GLU:HG3	1.93	0.50
2:H:115:ILE:O	2:H:119:VAL:HG22	2.11	0.50
1:A:220:MET:SD	1:A:225:ILE:HD12	2.51	0.50
1:A:291:GLN:HB3	1:A:337:ALA:CB	2.40	0.50
3:I:168:LEU:HD12	3:I:169:LYS:N	2.26	0.50
1:F:227:VAL:CG1	1:F:228:VAL:N	2.74	0.50
1:F:308:LYS:HB3	1:F:309:PRO:HD2	1.94	0.50
3:I:145:ASP:OD1	3:I:169:LYS:HD2	2.12	0.50
3:J:179:LYS:O	3:J:179:LYS:HG2	2.11	0.50
1:A:169:GLU:O	1:A:169:GLU:HG3	2.12	0.50
2:H:4:LYS:N	2:H:5:PRO:HD3	2.27	0.50
2:H:53:ILE:HB	2:H:79:ILE:HG23	1.93	0.50
3:J:50:ILE:CG2	3:J:51:TRP:N	2.73	0.50
1:F:214:LYS:O	1:F:214:LYS:HG2	2.07	0.50
3:I:176:ILE:HD11	3:I:178:VAL:HG22	1.94	0.50
3:J:75:LYS:HG2	3:J:145:ASP:HB2	1.94	0.50
1:F:8:PHE:CZ	1:F:65:GLU:OE1	2.65	0.50
1:F:8:PHE:HZ	1:F:65:GLU:OE1	1.94	0.50
1:F:170:LEU:HD23	1:F:208:ILE:CG2	2.29	0.50
3:I:71:ILE:HG22	3:I:71:ILE:O	2.11	0.50
3:I:158:LYS:O	3:I:159:ILE:C	2.49	0.50
4:K:11:G:C8	4:K:13:A:OP2	2.65	0.50
4:L:10:C:C3'	4:L:11:G:H5"	2.34	0.50
1:F:246:GLU:HA	1:F:249:ILE:HD12	1.94	0.49
1:F:253:MET:HE2	1:F:269:ALA:HB3	1.92	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:27:ALA:HA	2:E:107:LYS:O	2.11	0.49
2:E:113:GLU:O	2:E:116:ALA:HB3	2.12	0.49
1:A:285:MET:CE	1:A:289:THR:O	2.60	0.49
1:F:132:ASP:OD1	1:F:133:LYS:HG2	2.12	0.49
1:F:294:GLY:HA3	1:F:314:VAL:HG22	1.93	0.49
3:J:70:PRO:HB2	3:J:146:VAL:CG2	2.41	0.49
4:L:15:G:O5'	4:L:15:G:H8	1.94	0.49
1:A:294:GLY:H	1:A:314:VAL:CG2	2.23	0.49
1:F:237:ARG:HB2	1:F:237:ARG:HH21	1.76	0.49
1:F:345:ARG:O	1:F:349:PHE:HD1	1.95	0.49
1:F:366:ILE:HD12	1:F:366:ILE:N	2.27	0.49
2:H:39:GLU:O	2:H:42:LYS:HB3	2.11	0.49
2:H:50:LYS:HB2	2:H:102:ILE:O	2.12	0.49
3:I:7:HIS:CE1	3:I:9:PHE:CD1	3.00	0.49
3:I:34:ARG:CZ	3:I:40:VAL:HG21	2.42	0.49
3:J:78:LEU:HB2	3:J:144:VAL:HG21	1.94	0.49
4:L:13:A:C8	4:L:14:A:C8	3.00	0.49
1:A:214:LYS:O	1:A:215:THR:HB	2.11	0.49
2:E:15:GLU:OE1	2:E:18:GLU:OE2	2.29	0.49
2:H:112:VAL:O	2:H:115:ILE:CD1	2.60	0.49
3:I:70:PRO:HD2	3:I:175:MET:HE1	1.94	0.49
3:J:42:LYS:HZ1	3:J:45:GLY:C	2.15	0.49
4:K:13:A:N7	4:K:14:A:N7	2.60	0.49
1:A:221:ASP:C	1:A:223:THR:H	2.16	0.49
1:F:101:GLU:HB2	1:F:105:GLY:O	2.12	0.49
1:F:280:ARG:HB2	1:F:348:TYR:HE1	1.77	0.49
1:F:328:GLN:HG2	1:F:329:ARG:N	2.20	0.49
2:E:8:VAL:HA	2:E:80:TYR:CZ	2.48	0.49
2:H:32:LYS:HZ3	2:H:34:ARG:H	1.57	0.49
3:I:102:TYR:HE1	3:I:142:THR:N	2.04	0.49
3:I:104:ILE:HG22	3:I:104:ILE:O	2.11	0.49
3:J:217:LYS:HB2	3:J:217:LYS:NZ	2.27	0.49
1:A:220:MET:HG2	1:F:134:MET:CE	2.43	0.49
1:F:196:ARG:HG3	1:F:205:ILE:HG21	1.94	0.49
2:E:19:LYS:O	2:E:23:ALA:N	2.46	0.49
3:I:36:TYR:CE2	3:I:38:GLU:HB3	2.47	0.49
3:J:149:GLU:HG3	3:J:151:VAL:HG22	1.95	0.49
1:A:152:LEU:CB	1:A:235:ILE:HD11	2.42	0.49
1:F:157:ARG:HH11	1:F:174:HIS:HD2	1.60	0.49
1:F:291:GLN:HE22	4:L:5:C:H41	1.60	0.49
3:I:193:PHE:CE2	3:I:220:ALA:CB	2.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:21:A:O2'	4:L:22:U:H6	1.92	0.49
1:A:29:ARG:NH2	1:A:53:GLU:HB3	2.28	0.49
1:A:51:LEU:O	1:A:55:LEU:HD13	2.13	0.49
2:E:45:GLU:HG3	2:E:46:ARG:HG3	1.95	0.49
1:A:109:PHE:CE2	3:I:100:LYS:HB3	2.47	0.49
1:A:159:TRP:HA	1:F:137:GLN:HG3	1.95	0.49
3:I:102:TYR:N	3:I:102:TYR:CD2	2.80	0.49
1:A:275:LEU:H	1:A:275:LEU:CD2	2.20	0.49
2:H:112:VAL:O	2:H:115:ILE:CG1	2.60	0.49
1:A:200:LEU:HD12	1:A:204:LYS:CG	2.43	0.48
1:F:190:ILE:O	1:F:212:LYS:NZ	2.46	0.48
1:F:271:ARG:O	1:F:275:LEU:HD23	2.13	0.48
1:F:327:TRP:O	1:F:328:GLN:O	2.31	0.48
2:E:18:GLU:HA	2:E:21:LEU:CB	2.43	0.48
2:H:52:VAL:O	2:H:78:TYR:HA	2.13	0.48
3:I:149:GLU:HG3	3:I:151:VAL:HG22	1.95	0.48
1:A:206:LYS:O	1:A:210:GLU:HG2	2.12	0.48
1:F:32:THR:HG21	1:F:49:LYS:NZ	2.28	0.48
2:E:32:LYS:HG3	2:E:33:ILE:N	2.25	0.48
2:E:94:GLU:HG2	2:E:95:VAL:N	2.28	0.48
3:J:152:ALA:O	3:J:153:GLN:HG2	2.14	0.48
4:K:2:G:O2'	4:K:3:C:OP2	2.26	0.48
1:A:355:ALA:O	1:A:359:LYS:HB2	2.13	0.48
1:F:59:LYS:HZ3	1:F:64:ASP:HA	1.78	0.48
1:F:211:ALA:O	1:F:214:LYS:O	2.31	0.48
1:F:362:LEU:HA	1:F:365:ARG:HB2	1.94	0.48
1:A:88:PHE:HE2	3:I:134:PRO:HB2	1.78	0.48
1:A:341:ALA:HB1	1:A:345:ARG:HH12	1.79	0.48
3:I:53:PRO:HB3	3:I:60:ALA:HA	1.95	0.48
3:I:71:ILE:HD12	3:I:175:MET:CE	2.41	0.48
3:I:78:LEU:CD2	3:I:80:LEU:HD21	2.44	0.48
1:F:362:LEU:HD12	1:F:362:LEU:O	2.14	0.48
2:H:39:GLU:OE2	4:L:7:G:H2'	2.14	0.48
3:J:58:LEU:HD23	3:J:58:LEU:O	2.13	0.48
1:F:280:ARG:HA	1:F:348:TYR:CE1	2.48	0.48
2:H:10:PHE:HE2	2:H:123:MET:HE2	1.78	0.48
3:I:207:ILE:O	3:I:208:GLU:HB2	2.14	0.48
4:K:16:G:O2'	4:K:17:C:H6	1.96	0.48
1:A:12:ASN:HB3	1:A:14:ARG:H	1.79	0.48
1:A:19:PHE:HD2	1:A:24:ASN:O	1.97	0.48
1:F:26:ILE:HG22	1:F:27:GLU:N	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:284:MET:HE3	1:F:284:MET:HA	1.96	0.48
3:J:151:VAL:O	3:J:151:VAL:CG2	2.51	0.48
1:A:225:ILE:O	1:A:228:VAL:N	2.47	0.48
1:F:13:VAL:HG22	1:F:115:VAL:CB	2.44	0.48
4:K:10:C:H3'	4:K:11:G:C5'	2.34	0.48
1:A:329:ARG:HG2	1:A:330:GLY:N	2.28	0.48
1:F:345:ARG:O	1:F:349:PHE:CD1	2.67	0.48
3:J:76:SER:O	3:J:144:VAL:HG12	2.14	0.48
4:K:15:G:H1'	4:K:16:G:C8	2.49	0.48
1:A:177:TYR:O	1:A:180:PHE:HB3	2.14	0.47
1:A:299:LEU:CG	1:A:310:PRO:HB3	2.41	0.47
1:A:300:PHE:HE2	1:A:304:ARG:CZ	2.27	0.47
1:A:355:ALA:O	1:A:358:LEU:HD12	2.14	0.47
1:F:26:ILE:HG22	1:F:27:GLU:H	1.78	0.47
2:E:61:GLU:O	2:E:65:ALA:HB2	2.13	0.47
2:H:51:LEU:HD23	2:H:51:LEU:O	2.14	0.47
3:I:7:HIS:CE1	3:I:8:LYS:HG2	2.49	0.47
1:A:88:PHE:O	1:A:90:ASN:N	2.46	0.47
1:A:261:LYS:HE2	1:A:266:ALA:HB2	1.95	0.47
1:F:29:ARG:HH22	1:F:53:GLU:HB3	1.79	0.47
3:I:78:LEU:HD21	3:I:80:LEU:HD21	1.95	0.47
3:J:183:ILE:HD12	3:J:196:VAL:CG2	2.44	0.47
1:F:103:PHE:C	1:F:104:LEU:HD12	2.35	0.47
1:F:147:LYS:HD3	1:F:147:LYS:HA	1.68	0.47
2:H:48:GLN:CB	2:H:103:ILE:HD13	2.42	0.47
1:F:70:HIS:O	1:F:86:THR:HG23	2.13	0.47
1:F:114:LYS:CG	1:F:115:VAL:N	2.77	0.47
2:H:28:ARG:O	2:H:28:ARG:CD	2.57	0.47
2:H:50:LYS:NZ	2:H:104:GLU:N	2.61	0.47
3:J:36:TYR:CB	3:J:86:THR:HG22	2.39	0.47
1:A:254:ASP:OD1	1:A:261:LYS:HE3	2.13	0.47
2:H:53:ILE:HG12	2:H:87:LEU:HD11	1.96	0.47
3:I:80:LEU:HD11	3:I:163:ASN:ND2	2.29	0.47
3:J:58:LEU:HD13	3:J:148:PHE:HE1	1.75	0.47
1:A:320:ALA:O	1:A:324:SER:OG	2.32	0.47
1:F:149:ILE:HG21	1:F:239:TYR:CE2	2.49	0.47
2:H:5:PRO:O	2:H:8:VAL:HG22	2.15	0.47
1:A:180:PHE:CE1	1:A:184:VAL:HG11	2.50	0.47
1:A:221:ASP:O	1:A:223:THR:N	2.47	0.47
1:F:301:ARG:HD3	1:F:307:ALA:CB	2.44	0.47
1:F:325:PRO:O	1:F:329:ARG:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:85:LYS:HE3	2:E:94:GLU:O	2.13	0.47
3:I:143:LYS:HG2	3:I:167:TYR:O	2.14	0.47
3:I:210:LEU:HD12	3:I:210:LEU:C	2.35	0.47
3:J:79:TYR:CD1	3:J:88:ALA:HB2	2.48	0.47
4:L:10:C:H3'	4:L:11:G:C5'	2.34	0.47
1:A:231:LEU:HD12	1:A:231:LEU:HA	1.61	0.47
3:J:214:PRO:HD2	3:J:215:TYR:CE2	2.50	0.47
1:A:272:LEU:HD12	1:A:272:LEU:HA	1.71	0.47
1:F:71:PRO:HB2	1:F:72:GLU:OE2	2.14	0.47
2:E:100:VAL:HG12	2:E:101:ALA:N	2.30	0.47
2:H:79:ILE:HD12	2:H:80:TYR:N	2.29	0.47
3:I:52:ASN:HA	3:I:53:PRO:HD3	1.79	0.47
3:J:57:LYS:NZ	3:J:216:GLU:HG3	2.30	0.47
4:L:17:C:O2'	4:L:18:G:H5"	2.15	0.47
3:I:152:ALA:HB1	3:I:182:SER:OG	2.15	0.47
3:J:71:ILE:O	3:J:71:ILE:HG22	2.15	0.47
3:J:142:THR:O	3:J:143:LYS:C	2.53	0.47
1:A:47:ILE:HG13	1:A:51:LEU:HD23	1.96	0.46
1:A:51:LEU:O	1:A:51:LEU:HD12	2.14	0.46
1:A:271:ARG:O	1:A:274:SER:HB3	2.15	0.46
1:F:152:LEU:O	1:F:235:ILE:HD11	2.15	0.46
1:F:275:LEU:HG	1:F:293:LEU:HD13	1.97	0.46
2:E:32:LYS:CG	2:E:33:ILE:H	2.24	0.46
2:E:118:LYS:CE	2:E:122:LEU:HD11	2.44	0.46
2:H:20:ALA:O	2:H:24:VAL:HG12	2.15	0.46
3:J:38:GLU:OE1	3:J:38:GLU:N	2.48	0.46
1:A:20:ASP:HB3	1:A:24:ASN:CB	2.44	0.46
1:A:99:ASN:HD22	1:A:99:ASN:HA	1.62	0.46
1:A:212:LYS:HG3	1:A:213:GLU:N	2.26	0.46
1:A:334:ARG:NH1	4:K:22:U:C5	2.83	0.46
1:A:362:LEU:C	1:A:362:LEU:CD1	2.81	0.46
1:F:135:VAL:O	1:F:139:ILE:HG22	2.15	0.46
1:F:221:ASP:OD1	1:F:221:ASP:N	2.49	0.46
2:E:19:LYS:CD	2:E:20:ALA:N	2.70	0.46
2:E:39:GLU:OE2	4:K:7:G:H2'	2.16	0.46
1:A:18:ALA:O	1:A:25:LEU:O	2.31	0.46
1:A:35:PRO:HA	1:A:38:VAL:HG23	1.98	0.46
1:A:80:LEU:O	1:A:80:LEU:HG	2.15	0.46
1:F:328:GLN:CG	1:F:329:ARG:N	2.77	0.46
4:L:4:U:C4	5:S:2:G:O6	2.69	0.46
1:A:180:PHE:CZ	1:A:184:VAL:HG11	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ARG:HA	1:A:365:ARG:HD3	1.60	0.46
1:F:201:SER:O	1:F:205:ILE:HG23	2.15	0.46
3:I:64:ASN:ND2	3:I:213:GLU:O	2.39	0.46
3:I:83:ALA:N	3:I:105:GLU:HG2	2.31	0.46
3:J:148:PHE:CD2	3:J:149:GLU:N	2.80	0.46
1:A:19:PHE:HD1	1:A:92:ALA:HA	1.79	0.46
1:A:218:ALA:CB	1:F:130:ALA:HB2	2.46	0.46
2:H:68:PRO:O	2:H:72:GLU:HG3	2.15	0.46
3:J:197:GLU:HG3	3:J:206:VAL:HG11	1.98	0.46
1:A:180:PHE:O	1:A:184:VAL:N	2.49	0.46
2:E:78:TYR:O	2:E:119:VAL:HG21	2.15	0.46
2:E:104:GLU:HG3	2:E:104:GLU:O	2.16	0.46
2:H:24:VAL:HG22	2:H:90:ALA:O	2.16	0.46
3:I:133:LYS:HA	3:I:134:PRO:HD3	1.76	0.46
1:A:45:GLY:HA2	1:A:73:LEU:HD13	1.97	0.46
4:K:1:A:HO2'	4:K:2:G:P	2.37	0.46
4:K:15:G:H4'	4:K:16:G:OP1	2.16	0.46
1:A:27:GLU:HG3	1:A:28:LYS:N	2.31	0.46
1:A:119:LEU:HD21	1:A:123:ARG:NH1	2.30	0.46
1:F:13:VAL:HG22	1:F:115:VAL:HG11	1.97	0.46
1:F:41:GLN:O	1:F:46:GLU:HB2	2.16	0.46
1:F:245:LEU:O	1:F:249:ILE:HG13	2.16	0.46
1:F:365:ARG:HA	1:F:365:ARG:HD3	1.47	0.46
2:H:117:MET:O	2:H:120:LYS:HG3	2.16	0.46
3:I:28:ASN:HD22	3:I:49:ARG:HD2	1.79	0.46
4:K:11:G:H22	4:K:15:G:C1'	2.19	0.46
1:A:40:ASP:O	1:A:44:LYS:HE2	2.15	0.46
1:A:119:LEU:HD23	1:A:119:LEU:C	2.36	0.46
1:A:147:LYS:HA	1:A:147:LYS:HD3	1.57	0.46
1:A:291:GLN:OE1	4:K:5:C:H5	1.99	0.46
1:F:12:ASN:HD21	1:F:104:LEU:CD1	2.29	0.46
1:F:33:ASP:OD1	1:F:38:VAL:CG2	2.62	0.46
1:F:163:HIS:HE1	1:F:187:ARG:H	1.63	0.46
2:E:81:VAL:O	2:E:81:VAL:HG23	2.16	0.46
2:H:66:HIS:C	2:H:69:PRO:HD2	2.37	0.46
4:L:16:G:C5	4:L:17:C:C5	3.03	0.46
1:F:70:HIS:C	1:F:86:THR:HG23	2.37	0.46
1:F:80:LEU:HA	1:F:80:LEU:HD22	1.67	0.46
2:E:32:LYS:CE	2:E:33:ILE:H	2.29	0.46
2:H:109:ARG:CG	2:H:109:ARG:NH1	2.73	0.46
3:J:70:PRO:HB2	3:J:146:VAL:HG21	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:203:TYR:OH	3:J:226:LYS:HE3	2.16	0.46
1:A:56:ASN:OD1	1:A:82:PHE:HZ	1.98	0.45
1:A:155:ARG:NE	1:A:155:ARG:HA	2.30	0.45
1:A:264:VAL:HG11	1:A:340:LEU:HD21	1.97	0.45
1:A:362:LEU:O	1:A:365:ARG:N	2.43	0.45
1:F:14:ARG:C	1:F:31:PHE:HD2	2.13	0.45
2:E:78:TYR:CE2	2:E:123:MET:HE1	2.51	0.45
2:H:53:ILE:HA	2:H:79:ILE:HG23	1.98	0.45
2:H:103:ILE:O	2:H:104:GLU:HG2	2.16	0.45
3:I:104:ILE:HD12	3:I:137:TYR:CZ	2.51	0.45
3:J:57:LYS:NZ	3:J:219:HIS:CE1	2.84	0.45
3:J:173:TYR:N	3:J:173:TYR:HD2	2.12	0.45
1:A:279:LEU:HD12	1:A:279:LEU:O	2.17	0.45
1:F:220:MET:HB2	1:F:225:ILE:HD13	1.98	0.45
1:F:294:GLY:H	1:F:314:VAL:HG23	1.81	0.45
1:F:300:PHE:HD2	1:F:301:ARG:H	1.58	0.45
2:E:15:GLU:O	2:E:18:GLU:OE1	2.34	0.45
2:H:20:ALA:HA	2:H:23:ALA:HB3	1.98	0.45
4:L:11:G:N2	4:L:16:G:N7	2.64	0.45
1:A:67:VAL:HG22	1:A:85:THR:HG23	1.98	0.45
1:F:54:LEU:CD1	1:F:58:LEU:HD13	2.46	0.45
1:F:203:GLU:C	1:F:203:GLU:CD	2.75	0.45
2:E:77:PRO:HB3	2:E:119:VAL:HG11	1.97	0.45
3:I:91:VAL:O	3:I:95:VAL:CG2	2.47	0.45
3:J:68:ASN:OD1	3:J:68:ASN:N	2.49	0.45
1:A:180:PHE:C	1:A:184:VAL:HG12	2.37	0.45
2:E:68:PRO:HB2	2:E:69:PRO:HD3	1.98	0.45
3:I:160:LEU:HD23	3:I:160:LEU:HA	1.73	0.45
1:F:125:GLN:NE2	1:F:131:ARG:HH11	2.13	0.45
1:F:336:LEU:O	1:F:336:LEU:HD23	2.17	0.45
2:H:33:ILE:O	2:H:101:ALA:O	2.34	0.45
3:I:66:LEU:CD1	3:I:69:PHE:HB2	2.46	0.45
3:I:101:ILE:HD12	3:I:124:ILE:HG12	1.98	0.45
3:I:102:TYR:CE1	3:I:141:VAL:HA	2.52	0.45
1:A:220:MET:HG2	1:F:134:MET:HE1	1.99	0.45
1:A:333:ALA:O	1:A:337:ALA:HB2	2.16	0.45
1:A:336:LEU:HD23	1:A:340:LEU:HG	1.98	0.45
1:A:348:TYR:HD2	1:A:348:TYR:O	1.98	0.45
1:A:366:ILE:CG2	1:A:366:ILE:O	2.64	0.45
2:H:32:LYS:HE2	2:H:33:ILE:H	1.81	0.45
3:I:29:LEU:HD21	3:I:97:TRP:CE2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:168:LEU:HD12	3:I:168:LEU:HA	1.63	0.45
1:F:12:ASN:ND2	1:F:104:LEU:HD11	2.32	0.45
2:E:32:LYS:H	2:E:104:GLU:HG3	1.81	0.45
1:F:75:ARG:NH1	1:F:76:ARG:HH21	2.15	0.45
3:I:2:VAL:HG23	3:I:2:VAL:O	2.17	0.45
3:I:40:VAL:HG12	3:I:49:ARG:HA	1.98	0.45
3:I:63:VAL:HG11	3:I:215:TYR:OH	2.17	0.45
3:I:118:VAL:HG21	3:I:126:PRO:CG	2.46	0.45
1:A:163:HIS:HB2	1:A:220:MET:HG3	1.98	0.45
1:A:200:LEU:N	1:A:200:LEU:HD22	2.32	0.45
2:E:19:LYS:HA	2:E:22:GLN:HG2	1.99	0.45
2:H:32:LYS:CG	2:H:33:ILE:H	2.30	0.45
3:J:105:GLU:OE2	3:J:105:GLU:HA	2.17	0.45
3:J:115:VAL:N	3:J:116:PRO:CD	2.79	0.45
1:A:152:LEU:HD21	1:F:148:VAL:CG2	2.34	0.45
1:F:251:ARG:HG3	1:F:251:ARG:NH1	2.13	0.45
3:J:7:HIS:HB3	3:J:12:VAL:C	2.37	0.45
4:K:8:A:N7	4:K:18:G:C5	2.85	0.45
1:A:358:LEU:HA	1:A:361:GLU:HB2	1.98	0.44
1:F:366:ILE:HD12	1:F:366:ILE:H	1.81	0.44
2:E:16:LEU:CD1	2:E:115:ILE:HG22	2.44	0.44
2:E:35:LYS:HD2	4:K:18:G:N7	2.32	0.44
2:E:85:LYS:HD2	2:E:85:LYS:HA	1.51	0.44
2:E:120:LYS:HE3	2:E:121:GLU:N	2.32	0.44
2:H:32:LYS:O	2:H:103:ILE:O	2.34	0.44
3:J:70:PRO:O	3:J:75:LYS:HD3	2.17	0.44
1:F:119:LEU:HD21	1:F:123:ARG:CZ	2.47	0.44
3:J:152:ALA:C	3:J:153:GLN:HG2	2.37	0.44
3:J:222:PHE:N	3:J:222:PHE:HD1	2.15	0.44
1:F:34:LYS:O	1:F:37:LYS:HB3	2.17	0.44
1:F:369:VAL:O	1:F:369:VAL:CG2	2.65	0.44
2:H:32:LYS:HE2	2:H:33:ILE:N	2.32	0.44
2:H:33:ILE:HG23	2:H:102:ILE:HG23	1.99	0.44
3:I:12:VAL:C	3:I:13:TYR:CD2	2.90	0.44
3:J:7:HIS:ND1	3:J:8:LYS:N	2.65	0.44
3:J:75:LYS:CE	3:J:145:ASP:HB3	2.46	0.44
1:A:13:VAL:HG22	1:A:115:VAL:CB	2.48	0.44
1:F:27:GLU:HG3	1:F:28:LYS:N	2.32	0.44
2:H:35:LYS:HE3	4:L:18:G:O6	2.17	0.44
3:I:155:THR:O	3:I:157:ALA:N	2.51	0.44
4:L:10:C:O2	4:L:10:C:H2'	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LEU:HD23	1:A:293:LEU:HA	1.70	0.44
1:F:55:LEU:HD12	1:F:56:ASN:H	1.75	0.44
1:F:291:GLN:CD	4:L:5:C:H5	2.21	0.44
2:E:24:VAL:HA	2:E:27:ALA:HB3	1.99	0.44
3:J:183:ILE:HB	3:J:192:VAL:HG21	2.00	0.44
1:A:62:GLY:C	1:A:63:TYR:CD2	2.91	0.44
1:F:354:ILE:O	1:F:357:GLU:HB3	2.17	0.44
2:E:54:ILE:HG23	2:E:99:SER:HB3	1.98	0.44
2:E:78:TYR:OH	2:E:123:MET:CE	2.66	0.44
2:H:85:LYS:HA	2:H:85:LYS:HD2	1.51	0.44
1:A:29:ARG:HH22	1:A:53:GLU:HB3	1.82	0.44
1:A:326:TRP:CD1	1:A:326:TRP:N	2.85	0.44
1:A:354:ILE:HD12	1:A:354:ILE:C	2.38	0.44
1:F:175:PRO:HG3	1:F:239:TYR:CE1	2.53	0.44
1:F:315:ILE:O	1:F:315:ILE:HG12	2.18	0.44
2:E:54:ILE:HG22	2:E:55:ALA:N	2.30	0.44
2:E:63:ILE:HD12	4:K:19:U:O4'	2.17	0.44
2:H:24:VAL:HG23	2:H:33:ILE:CD1	2.47	0.44
3:J:79:TYR:HD2	3:J:80:LEU:N	2.16	0.44
5:S:3:C:H2'	5:S:4:U:O5'	2.18	0.44
1:A:76:ARG:HA	1:A:79:GLU:HB3	2.00	0.44
2:E:14:LYS:N	2:E:14:LYS:CD	2.63	0.44
3:I:33:GLN:HE22	3:I:120:GLU:HB2	1.83	0.44
3:J:124:ILE:HG22	3:J:125:ILE:N	2.32	0.44
3:J:179:LYS:HG3	3:J:219:HIS:CE1	2.53	0.44
3:J:150:ASP:CG	6:J:228:SAM:CE	2.84	0.44
1:A:192:GLU:HG2	1:A:205:ILE:HD13	1.98	0.43
1:F:318:TYR:O	1:F:321:ILE:N	2.51	0.43
2:E:112:VAL:O	2:E:115:ILE:HG13	2.18	0.43
3:J:102:TYR:HD1	3:J:141:VAL:HG12	1.82	0.43
1:A:295:ALA:CA	1:A:313:GLY:H	2.31	0.43
1:F:253:MET:CB	1:F:261:LYS:HD2	2.48	0.43
1:F:259:ASN:O	1:F:260:LEU:C	2.57	0.43
2:E:108:ALA:HA	2:E:111:LEU:HD13	1.99	0.43
4:K:13:A:C8	4:K:14:A:C8	3.06	0.43
1:A:267:LYS:HD3	1:A:271:ARG:NH1	2.33	0.43
1:F:109:PHE:CE2	3:J:100:LYS:HB3	2.53	0.43
1:F:114:LYS:HG2	1:F:115:VAL:H	1.83	0.43
2:E:15:GLU:C	2:E:17:ALA:N	2.71	0.43
3:I:82:ILE:HG21	3:I:103:GLY:HA3	2.00	0.43
1:A:11:GLU:CD	1:A:11:GLU:N	2.72	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ALA:HB3	1:A:134:MET:HE3	1.99	0.43
1:A:280:ARG:HA	1:A:348:TYR:CD1	2.54	0.43
1:F:117:VAL:HG22	1:F:121:ARG:NH1	2.33	0.43
1:F:190:ILE:HD12	1:F:209:LEU:HD23	2.00	0.43
1:F:361:GLU:HG2	3:J:185:VAL:HG21	1.99	0.43
3:I:2:VAL:HG21	3:I:41:ILE:HG12	2.00	0.43
3:I:43:TRP:CG	3:I:44:GLU:N	2.86	0.43
3:J:89:SER:O	3:J:92:SER:HB3	2.17	0.43
1:A:253:MET:HE1	1:A:273:ILE:HD12	1.99	0.43
1:A:327:TRP:HB3	1:A:328:GLN:CD	2.38	0.43
1:F:334:ARG:NH1	4:L:22:U:C5	2.87	0.43
2:E:63:ILE:HG22	2:E:64:VAL:HG13	2.00	0.43
3:I:160:LEU:O	3:I:160:LEU:HD22	2.18	0.43
3:I:161:ILE:O	3:I:165:LYS:HG3	2.18	0.43
3:I:181:ARG:HB2	3:I:185:VAL:HG13	1.99	0.43
3:J:30:VAL:O	3:J:31:PRO:C	2.57	0.43
4:K:16:G:C5	4:K:17:C:C5	3.07	0.43
1:A:14:ARG:O	1:A:14:ARG:HG3	2.18	0.43
1:A:163:HIS:O	1:A:187:ARG:HD3	2.18	0.43
1:A:185:GLY:HA3	1:A:229:ARG:HH12	1.82	0.43
1:A:196:ARG:HD3	1:A:202:GLU:OE1	2.18	0.43
1:F:196:ARG:CG	1:F:205:ILE:HG21	2.49	0.43
1:F:198:LEU:HB2	1:F:200:LEU:CD2	2.45	0.43
3:I:29:LEU:CD2	3:I:97:TRP:CZ2	3.02	0.43
3:I:52:ASN:OD1	3:I:54:HIS:HB2	2.19	0.43
3:I:195:GLU:O	3:I:198:ARG:HG3	2.19	0.43
3:J:82:ILE:HG22	3:J:104:ILE:N	2.33	0.43
1:A:300:PHE:CE2	1:A:304:ARG:CZ	3.02	0.43
1:F:175:PRO:HA	1:F:239:TYR:HE1	1.82	0.43
3:I:43:TRP:HB3	3:I:48:TYR:CE1	2.54	0.43
3:J:9:PHE:CE2	3:J:69:PHE:HB3	2.53	0.43
3:J:75:LYS:HZ3	3:J:145:ASP:C	2.21	0.43
4:L:8:A:C5	4:L:21:A:N7	2.87	0.43
2:H:9:LYS:NZ	2:H:124:LYS:O	2.51	0.43
2:H:15:GLU:HG3	2:H:16:LEU:N	2.34	0.43
3:I:26:THR:HG22	3:I:27:LYS:H	1.83	0.43
3:I:82:ILE:HD13	3:I:103:GLY:HA3	2.01	0.43
4:L:6:U:C2	4:L:23:G:N1	2.87	0.43
1:A:14:ARG:O	1:A:31:PHE:CD2	2.71	0.43
1:A:326:TRP:O	1:A:327:TRP:CB	2.66	0.43
2:E:26:ILE:O	2:E:107:LYS:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:106:PHE:HB2	3:J:129:GLY:O	2.18	0.43
1:A:120:THR:O	1:A:124:ILE:HG13	2.19	0.43
1:F:101:GLU:CB	1:F:105:GLY:O	2.66	0.43
2:E:16:LEU:HD21	2:E:118:LYS:HG2	1.99	0.43
2:H:78:TYR:N	2:H:78:TYR:CD2	2.87	0.43
4:L:6:U:H1'	4:L:23:G:C2	2.53	0.43
4:L:6:U:C1'	4:L:23:G:N2	2.81	0.43
1:F:34:LYS:HB3	1:F:36:GLU:HG3	2.01	0.42
2:E:68:PRO:O	2:E:72:GLU:HG3	2.18	0.42
3:I:71:ILE:CD1	3:I:175:MET:HE3	2.46	0.42
3:J:16:ILE:HA	3:J:21:SER:O	2.19	0.42
3:J:99:GLY:C	3:J:100:LYS:HG3	2.38	0.42
5:G:4:U:O2	5:G:4:U:H2'	2.19	0.42
1:A:214:LYS:HD2	1:A:214:LYS:HA	1.74	0.42
1:A:301:ARG:CZ	1:A:307:ALA:HB2	2.49	0.42
2:H:50:LYS:HZ3	2:H:104:GLU:N	2.14	0.42
3:I:58:LEU:HD11	3:I:69:PHE:HE2	1.84	0.42
4:K:22:U:O2'	4:K:23:G:P	2.77	0.42
4:L:8:A:C4'	4:L:9:C:OP1	2.63	0.42
1:A:14:ARG:C	1:A:31:PHE:CD2	2.93	0.42
1:A:45:GLY:O	1:A:73:LEU:HD12	2.20	0.42
1:A:221:ASP:C	1:A:223:THR:N	2.72	0.42
1:A:327:TRP:HA	1:A:327:TRP:CE3	2.55	0.42
2:E:21:LEU:HG	2:E:86:GLU:HG2	2.00	0.42
2:H:11:GLU:O	2:H:11:GLU:HG2	2.19	0.42
3:I:61:ALA:O	3:I:66:LEU:HB2	2.19	0.42
3:I:104:ILE:HG22	6:I:228:SAM:H2	2.01	0.42
3:J:12:VAL:C	3:J:13:TYR:CD2	2.93	0.42
3:J:42:LYS:HZ3	3:J:46:GLU:N	2.18	0.42
3:J:43:TRP:CG	3:J:44:GLU:N	2.87	0.42
3:J:75:LYS:HZ1	3:J:146:VAL:CG2	2.28	0.42
1:A:220:MET:CB	1:A:225:ILE:HD13	2.50	0.42
1:A:240:GLN:O	1:A:244:LYS:CG	2.63	0.42
1:F:196:ARG:C	1:F:198:LEU:H	2.23	0.42
1:F:309:PRO:N	1:F:310:PRO:HD3	2.35	0.42
2:E:4:LYS:O	2:E:4:LYS:HG2	2.19	0.42
3:J:52:ASN:ND2	3:J:53:PRO:HD2	2.35	0.42
4:K:10:C:O2	4:K:10:C:H2'	2.19	0.42
1:A:103:PHE:CD1	1:A:103:PHE:N	2.87	0.42
1:A:136:ILE:O	1:A:139:ILE:HG22	2.19	0.42
1:F:13:VAL:HG22	1:F:115:VAL:CG1	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:ILE:HA	1:F:139:ILE:HG22	2.00	0.42
1:F:362:LEU:O	1:F:365:ARG:HB2	2.20	0.42
2:E:9:LYS:NZ	2:E:124:LYS:O	2.50	0.42
2:E:18:GLU:O	2:E:22:GLN:N	2.45	0.42
2:H:119:VAL:HA	2:H:122:LEU:HG	2.02	0.42
3:J:42:LYS:NZ	3:J:46:GLU:N	2.67	0.42
3:J:58:LEU:HD21	3:J:69:PHE:HE2	1.85	0.42
5:S:3:C:O2	5:S:3:C:C2'	2.67	0.42
1:A:49:LYS:HB3	1:A:49:LYS:HE3	1.87	0.42
1:A:329:ARG:O	1:A:331:LYS:N	2.52	0.42
1:F:231:LEU:HA	1:F:231:LEU:HD23	1.79	0.42
1:F:293:LEU:HD23	1:F:293:LEU:HA	1.66	0.42
2:E:51:LEU:CD1	2:E:115:ILE:HD13	2.50	0.42
2:E:116:ALA:O	2:E:119:VAL:HG12	2.19	0.42
2:H:44:VAL:HG11	2:H:70:LEU:HG	2.01	0.42
3:I:13:TYR:CD1	3:I:48:TYR:HE2	2.38	0.42
3:I:17:ASP:O	3:I:18:ASP:C	2.58	0.42
5:G:3:C:H2'	5:G:4:U:H6	1.85	0.42
1:F:227:VAL:O	1:F:230:GLN:HB2	2.20	0.42
2:H:43:ALA:HA	2:H:46:ARG:HD2	2.00	0.42
2:H:54:ILE:N	2:H:79:ILE:O	2.35	0.42
1:A:8:PHE:CE1	1:A:63:TYR:HD1	2.37	0.42
1:A:160:TYR:HE2	1:A:164:PHE:HB3	1.84	0.42
1:A:301:ARG:CZ	1:A:307:ALA:CB	2.97	0.42
1:A:324:SER:HA	1:A:325:PRO:HD3	1.73	0.42
1:F:160:TYR:O	1:F:160:TYR:CG	2.73	0.42
2:H:37:THR:HG22	2:H:37:THR:O	2.20	0.42
3:I:158:LYS:C	3:I:158:LYS:CD	2.87	0.42
3:J:43:TRP:CB	3:J:48:TYR:CE1	2.97	0.42
3:J:179:LYS:HB3	3:J:182:SER:OG	2.20	0.42
1:A:37:LYS:O	1:A:41:GLN:NE2	2.53	0.42
1:A:72:GLU:OE2	1:A:72:GLU:HA	2.18	0.42
1:A:136:ILE:HA	1:A:139:ILE:HG22	2.02	0.42
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.91	0.42
1:A:280:ARG:HA	1:A:348:TYR:CE1	2.55	0.42
1:F:70:HIS:CG	1:F:71:PRO:HD2	2.55	0.42
1:F:163:HIS:NE2	1:F:187:ARG:CB	2.80	0.42
1:F:196:ARG:C	1:F:198:LEU:N	2.73	0.42
1:F:352:GLU:HG2	6:J:228:SAM:H3'	2.01	0.42
2:H:66:HIS:NE2	2:H:67:LEU:HD23	2.35	0.42
2:H:117:MET:O	2:H:121:GLU:OE1	2.38	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LEU:HD21	1:A:123:ARG:CZ	2.50	0.42
1:A:345:ARG:H	1:A:345:ARG:HG2	1.57	0.42
3:I:28:ASN:ND2	3:I:49:ARG:CD	2.78	0.42
3:I:43:TRP:HB3	3:I:48:TYR:HE1	1.84	0.42
3:J:205:GLU:HG2	3:J:207:ILE:HG22	2.02	0.42
4:K:8:A:C8	4:K:18:G:C5	3.08	0.42
1:A:195:LEU:HD11	1:A:208:ILE:CD1	2.44	0.41
2:E:104:GLU:O	2:E:105:PRO:C	2.58	0.41
2:H:20:ALA:HA	2:H:23:ALA:CB	2.49	0.41
2:H:35:LYS:HA	2:H:100:VAL:CG2	2.50	0.41
2:H:46:ARG:HD3	2:H:48:GLN:HG3	2.02	0.41
3:I:57:LYS:HB2	3:I:57:LYS:NZ	2.34	0.41
3:J:53:PRO:HG3	3:J:63:VAL:HG21	2.02	0.41
4:K:22:U:O2'	4:K:23:G:O5'	2.38	0.41
1:A:42:LEU:HD23	1:A:42:LEU:HA	1.91	0.41
3:J:37:GLY:N	3:J:38:GLU:OE1	2.53	0.41
4:K:9:C:O2'	4:K:10:C:P	2.78	0.41
1:A:42:LEU:HD23	1:A:46:GLU:O	2.19	0.41
1:F:39:LEU:HA	1:F:39:LEU:HD23	1.82	0.41
1:F:299:LEU:HD12	1:F:300:PHE:H	1.85	0.41
2:E:5:PRO:O	2:E:8:VAL:HG23	2.20	0.41
2:H:81:VAL:HG21	2:H:87:LEU:HG	2.03	0.41
3:J:106:PHE:HD1	3:J:107:SER:H	1.65	0.41
4:L:11:G:C8	4:L:13:A:OP2	2.73	0.41
1:A:94:GLU:O	1:A:98:SER:CB	2.66	0.41
1:A:301:ARG:C	1:A:306:GLY:HA2	2.40	0.41
1:A:341:ALA:HB1	1:A:345:ARG:NH1	2.35	0.41
1:F:20:ASP:HA	1:F:26:ILE:HD11	2.01	0.41
1:F:345:ARG:NH2	2:H:66:HIS:CE1	2.89	0.41
2:E:59:ASP:O	4:K:19:U:N3	2.53	0.41
1:A:113:TYR:HA	3:I:125:ILE:CD1	2.50	0.41
1:A:162:LEU:HA	1:A:162:LEU:HD23	1.87	0.41
1:A:229:ARG:O	1:A:229:ARG:HG2	2.20	0.41
2:H:23:ALA:O	2:H:27:ALA:CB	2.66	0.41
2:H:112:VAL:HG22	2:H:113:GLU:N	2.35	0.41
3:I:117:ILE:H	3:I:117:ILE:HG12	1.70	0.41
1:F:47:ILE:CG1	1:F:51:LEU:HD23	2.28	0.41
1:F:49:LYS:HG3	1:F:50:ASP:H	1.84	0.41
2:E:78:TYR:CD2	2:E:78:TYR:N	2.88	0.41
3:I:81:GLY:O	6:I:228:SAM:H5'1	2.20	0.41
3:J:133:LYS:O	3:J:137:TYR:CE2	2.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:6:U:H1'	4:K:23:G:C2	2.55	0.41
4:L:8:A:C5	4:L:18:G:C2	3.09	0.41
1:A:227:VAL:CG1	1:A:228:VAL:N	2.84	0.41
1:A:366:ILE:O	1:A:368:LEU:HG	2.20	0.41
1:F:339:LYS:HG3	1:F:362:LEU:HB2	2.03	0.41
2:E:68:PRO:N	2:E:69:PRO:CD	2.84	0.41
3:I:28:ASN:CB	3:I:49:ARG:HG3	2.40	0.41
1:A:12:ASN:ND2	1:A:13:VAL:H	2.19	0.41
1:A:142:LEU:HB3	1:A:245:LEU:HD12	2.02	0.41
1:A:160:TYR:CE2	1:A:164:PHE:HB3	2.56	0.41
1:A:295:ALA:CB	1:A:313:GLY:H	2.32	0.41
1:A:356:GLU:OE2	1:A:359:LYS:HE2	2.20	0.41
1:F:70:HIS:HB3	1:F:73:LEU:HG	2.02	0.41
1:F:214:LYS:HE2	1:F:214:LYS:HB3	1.28	0.41
2:E:64:VAL:C	2:E:66:HIS:N	2.74	0.41
2:E:110:ASP:C	2:E:112:VAL:H	2.24	0.41
3:I:212:LEU:HD13	3:I:212:LEU:HA	1.78	0.41
4:K:9:C:HO2'	4:K:10:C:P	2.44	0.41
1:A:12:ASN:HB2	1:A:17:TYR:HE1	1.85	0.41
1:A:16:ILE:CG2	1:A:54:LEU:HD23	2.51	0.41
1:A:109:PHE:CZ	3:I:100:LYS:HB3	2.56	0.41
1:A:134:MET:CE	1:F:220:MET:HG2	2.51	0.41
1:A:210:GLU:HG2	1:A:210:GLU:H	1.55	0.41
1:A:291:GLN:CD	4:K:5:C:H5	2.24	0.41
1:F:42:LEU:HD23	1:F:42:LEU:HA	1.89	0.41
1:F:88:PHE:O	1:F:89:PRO:C	2.60	0.41
1:F:174:HIS:CB	1:F:175:PRO:HD3	2.32	0.41
1:F:244:LYS:HG2	1:F:244:LYS:H	1.65	0.41
1:F:284:MET:CE	1:F:284:MET:HA	2.51	0.41
1:F:340:LEU:HD23	1:F:340:LEU:HA	1.88	0.41
3:I:173:TYR:N	3:I:173:TYR:CD2	2.88	0.41
3:J:102:TYR:HD1	3:J:141:VAL:CG1	2.33	0.41
3:J:158:LYS:HE3	3:J:158:LYS:HB2	1.96	0.41
1:A:90:ASN:O	1:A:91:ILE:C	2.59	0.41
1:A:167:LEU:HA	1:A:170:LEU:CB	2.41	0.41
1:A:336:LEU:HD23	1:A:336:LEU:O	2.20	0.41
1:F:321:ILE:HG22	1:F:321:ILE:O	2.19	0.41
2:E:25:GLU:HA	2:E:90:ALA:O	2.20	0.41
2:H:121:GLU:CG	2:H:122:LEU:N	2.84	0.41
3:I:51:TRP:CZ2	3:I:58:LEU:HD23	2.56	0.41
3:I:52:ASN:ND2	3:I:53:PRO:HD2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:78:LEU:N	3:I:144:VAL:HG11	2.36	0.41
1:F:8:PHE:O	1:F:18:ALA:HA	2.20	0.40
1:F:267:LYS:NZ	1:F:271:ARG:NH2	2.69	0.40
2:E:21:LEU:O	2:E:24:VAL:HG13	2.21	0.40
2:E:118:LYS:CD	2:E:122:LEU:HD11	2.51	0.40
3:I:13:TYR:CD2	3:I:13:TYR:N	2.89	0.40
3:I:90:HIS:O	3:I:93:ASP:N	2.52	0.40
3:J:168:LEU:HD12	3:J:168:LEU:HA	1.70	0.40
1:A:145:VAL:O	1:A:145:VAL:HG12	2.20	0.40
1:A:184:VAL:CG1	1:A:185:GLY:N	2.84	0.40
2:E:64:VAL:O	2:E:66:HIS:N	2.54	0.40
3:I:102:TYR:N	3:I:102:TYR:HD2	2.18	0.40
4:K:14:A:H2'	4:K:15:G:H5'	2.03	0.40
1:F:219:TRP:CD1	1:F:219:TRP:C	2.94	0.40
2:H:54:ILE:O	2:H:81:VAL:HG22	2.21	0.40
2:H:113:GLU:O	2:H:116:ALA:HB3	2.21	0.40
3:I:35:VAL:HG12	3:I:36:TYR:N	2.36	0.40
3:I:51:TRP:CZ2	3:I:58:LEU:CD2	3.04	0.40
3:J:53:PRO:HB2	3:J:215:TYR:CE1	2.56	0.40
1:A:328:GLN:O	1:A:329:ARG:HB3	2.21	0.40
1:F:80:LEU:O	1:F:82:PHE:CE1	2.75	0.40
1:F:301:ARG:O	1:F:306:GLY:C	2.60	0.40
2:E:16:LEU:HD22	2:E:118:LYS:HG2	2.03	0.40
2:E:57:ASP:OD1	2:E:83:SER:HA	2.21	0.40
2:H:32:LYS:CE	2:H:33:ILE:H	2.34	0.40
2:H:33:ILE:HG12	2:H:102:ILE:HG22	2.04	0.40
2:H:112:VAL:O	2:H:114:GLU:N	2.55	0.40
3:I:29:LEU:CD2	3:I:97:TRP:CE2	3.05	0.40
3:J:62:ILE:O	3:J:62:ILE:HG22	2.20	0.40
1:A:155:ARG:HA	1:A:155:ARG:HE	1.86	0.40
1:A:257:ALA:HA	1:A:347:ASP:CG	2.42	0.40
1:A:273:ILE:O	1:A:276:ALA:HB3	2.22	0.40
1:A:354:ILE:O	1:A:357:GLU:HB2	2.22	0.40
1:F:31:PHE:HD1	1:F:38:VAL:HG11	1.86	0.40
1:F:55:LEU:CD1	1:F:56:ASN:N	2.76	0.40
1:F:184:VAL:CG1	1:F:185:GLY:N	2.84	0.40
1:F:194:VAL:O	1:F:198:LEU:HG	2.20	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	361/376 (96%)	309 (86%)	45 (12%)	7 (2%)	8	39
1	F	361/376 (96%)	310 (86%)	40 (11%)	11 (3%)	4	28
2	E	119/129 (92%)	99 (83%)	19 (16%)	1 (1%)	19	58
2	H	119/129 (92%)	104 (87%)	13 (11%)	2 (2%)	9	42
3	I	225/234 (96%)	199 (88%)	25 (11%)	1 (0%)	34	69
3	J	225/234 (96%)	202 (90%)	21 (9%)	2 (1%)	17	56
All	All	1410/1478 (95%)	1223 (87%)	163 (12%)	24 (2%)	9	42

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	PHE
1	F	88	PHE
1	F	328	GLN
1	A	89	PRO
1	A	328	GLN
1	F	89	PRO
1	F	301	ARG
1	F	307	ALA
1	F	330	GLY
1	A	26	ILE
1	F	329	ARG
2	E	108	ALA
1	F	26	ILE
1	F	201	SER
1	F	300	PHE
2	H	42	LYS
1	A	329	ARG
1	A	331	LYS
2	H	108	ALA
3	J	215	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	J	151	VAL
3	I	151	VAL
1	F	310	PRO
1	A	178	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	309/321 (96%)	245 (79%)	64 (21%)	1	6
1	F	309/321 (96%)	247 (80%)	62 (20%)	1	6
2	E	98/105 (93%)	83 (85%)	15 (15%)	2	13
2	H	98/105 (93%)	79 (81%)	19 (19%)	1	7
3	I	197/204 (97%)	166 (84%)	31 (16%)	2	12
3	J	197/204 (97%)	161 (82%)	36 (18%)	1	8
All	All	1208/1260 (96%)	981 (81%)	227 (19%)	1	8

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	13	VAL
1	A	14	ARG
1	A	21	GLU
1	A	27	GLU
1	A	36	GLU
1	A	38	VAL
1	A	48	THR
1	A	54	LEU
1	A	61	LYS
1	A	64	ASP
1	A	65	GLU
1	A	72	GLU
1	A	80	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	82	PHE
1	A	85	THR
1	A	88	PHE
1	A	106	GLU
1	A	131	ARG
1	A	136	ILE
1	A	142	LEU
1	A	147	LYS
1	A	164	PHE
1	A	167	LEU
1	A	170	LEU
1	A	173	LYS
1	A	184	VAL
1	A	192	GLU
1	A	195	LEU
1	A	201	SER
1	A	204	LYS
1	A	206	LYS
1	A	210	GLU
1	A	212	LYS
1	A	213	GLU
1	A	225	ILE
1	A	229	ARG
1	A	234	GLU
1	A	250	ASP
1	A	253	MET
1	A	263	LEU
1	A	272	LEU
1	A	275	LEU
1	A	282	LEU
1	A	293	LEU
1	A	300	PHE
1	A	303	LEU
1	A	304	ARG
1	A	305	THR
1	A	311	LYS
1	A	315	ILE
1	A	327	TRP
1	A	328	GLN
1	A	334	ARG
1	A	336	LEU
1	A	345	ARG

Continued from previous page...

Mol	Chain	Res	Type
1	A	348	TYR
1	A	358	LEU
1	A	362	LEU
1	A	365	ARG
1	A	366	ILE
1	A	367	ARG
1	A	368	LEU
1	A	370	LEU
1	F	8	PHE
1	F	10	SER
1	F	13	VAL
1	F	14	ARG
1	F	21	GLU
1	F	25	LEU
1	F	32	THR
1	F	36	GLU
1	F	54	LEU
1	F	55	LEU
1	F	57	SER
1	F	58	LEU
1	F	64	ASP
1	F	65	GLU
1	F	80	LEU
1	F	82	PHE
1	F	83	SER
1	F	85	THR
1	F	86	THR
1	F	88	PHE
1	F	103	PHE
1	F	127	GLN
1	F	131	ARG
1	F	133	LYS
1	F	142	LEU
1	F	147	LYS
1	F	164	PHE
1	F	167	LEU
1	F	173	LYS
1	F	184	VAL
1	F	188	ASP
1	F	190	ILE
1	F	201	SER
1	F	204	LYS

Continued from previous page...

Mol	Chain	Res	Type
1	F	206	LYS
1	F	213	GLU
1	F	214	LYS
1	F	215	THR
1	F	225	ILE
1	F	231	LEU
1	F	244	LYS
1	F	250	ASP
1	F	251	ARG
1	F	253	MET
1	F	263	LEU
1	F	272	LEU
1	F	274	SER
1	F	275	LEU
1	F	282	LEU
1	F	305	THR
1	F	315	ILE
1	F	326	TRP
1	F	327	TRP
1	F	345	ARG
1	F	348	TYR
1	F	358	LEU
1	F	362	LEU
1	F	365	ARG
1	F	367	ARG
1	F	368	LEU
1	F	369	VAL
1	F	370	LEU
2	E	14	LYS
2	E	19	LYS
2	E	24	VAL
2	E	30	THR
2	E	32	LYS
2	E	51	LEU
2	E	53	ILE
2	E	57	ASP
2	E	63	ILE
2	E	85	LYS
2	E	93	ILE
2	E	111	LEU
2	E	114	GLU
2	E	119	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	120	LYS
2	H	16	LEU
2	H	24	VAL
2	H	26	ILE
2	H	32	LYS
2	H	46	ARG
2	H	51	LEU
2	H	53	ILE
2	H	57	ASP
2	H	61	GLU
2	H	78	TYR
2	H	79	ILE
2	H	84	LYS
2	H	85	LYS
2	H	87	LEU
2	H	93	ILE
2	H	100	VAL
2	H	102	ILE
2	H	120	LYS
2	H	124	LYS
3	I	1	MET
3	I	5	LYS
3	I	23	LYS
3	I	26	THR
3	I	29	LEU
3	I	34	ARG
3	I	47	GLU
3	I	57	LYS
3	I	66	LEU
3	I	68	ASN
3	I	72	LYS
3	I	77	VAL
3	I	79	TYR
3	I	104	ILE
3	I	118	VAL
3	I	136	GLU
3	I	138	ARG
3	I	144	VAL
3	I	148	PHE
3	I	158	LYS
3	I	160	LEU
3	I	175	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	176	ILE
3	I	180	SER
3	I	181	ARG
3	I	198	ARG
3	I	202	GLU
3	I	207	ILE
3	I	210	LEU
3	I	211	ASN
3	I	212	LEU
3	J	18	ASP
3	J	19	ASP
3	J	23	LYS
3	J	26	THR
3	J	29	LEU
3	J	34	ARG
3	J	40	VAL
3	J	50	ILE
3	J	68	ASN
3	J	77	VAL
3	J	79	TYR
3	J	91	VAL
3	J	105	GLU
3	J	106	PHE
3	J	110	VAL
3	J	136	GLU
3	J	137	TYR
3	J	144	VAL
3	J	148	PHE
3	J	155	THR
3	J	158	LYS
3	J	160	LEU
3	J	170	ARG
3	J	173	TYR
3	J	176	ILE
3	J	180	SER
3	J	181	ARG
3	J	185	VAL
3	J	195	GLU
3	J	198	ARG
3	J	201	SER
3	J	212	LEU
3	J	217	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	J	221	LEU
3	J	222	PHE
3	J	223	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	41	GLN
1	A	99	ASN
1	A	127	GLN
1	A	137	GLN
1	A	163	HIS
1	A	186	HIS
1	A	302	HIS
1	F	125	GLN
1	F	150	ASN
1	F	163	HIS
1	F	174	HIS
1	F	176	GLN
1	F	186	HIS
1	F	291	GLN
1	F	302	HIS
3	I	28	ASN
3	I	163	ASN
3	I	211	ASN
3	J	219	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	K	24/34 (70%)	17 (70%)	4 (16%)
4	L	23/34 (67%)	17 (73%)	3 (13%)
5	G	2/13 (15%)	0	0
5	S	2/13 (15%)	1 (50%)	0
All	All	51/94 (54%)	35 (68%)	7 (13%)

All (35) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	K	2	G
4	K	3	C
4	K	4	U
4	K	5	C
4	K	7	G
4	K	8	A
4	K	9	C
4	K	10	C
4	K	11	G
4	K	15	G
4	K	16	G
4	K	17	C
4	K	19	U
4	K	20	G
4	K	21	A
4	K	22	U
4	K	23	G
4	L	2	G
4	L	4	U
4	L	5	C
4	L	7	G
4	L	8	A
4	L	9	C
4	L	10	C
4	L	11	G
4	L	12	A
4	L	13	A
4	L	15	G
4	L	16	G
4	L	17	C
4	L	20	G
4	L	21	A
4	L	22	U
4	L	23	G
5	S	4	U

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	K	1	A
4	K	7	G
4	K	8	A
4	K	15	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L	7	G
4	L	8	A
4	L	15	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
6	SAM	I	228	-	23,28,29	1.29	2 (8%)	18,40,42	2.17	6 (33%)
6	SAM	J	228	-	23,28,29	1.15	1 (4%)	18,40,42	1.80	4 (22%)

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
6	SAM	I	228	-	-	5/9/31/33	0/3/3/3
6	SAM	J	228	-	-	3/9/31/33	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	228	SAM	C2-N3	3.93	1.38	1.32
6	J	228	SAM	C2-N3	3.86	1.38	1.32
6	I	228	SAM	C2-N1	2.39	1.38	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	228	SAM	N3-C2-N1	-5.52	120.05	128.68
6	I	228	SAM	O4'-C4'-C5'	5.41	122.56	108.88
6	I	228	SAM	N3-C2-N1	-5.10	120.71	128.68
6	J	228	SAM	O4'-C4'-C5'	3.35	117.35	108.88
6	I	228	SAM	O4'-C1'-C2'	-2.93	102.64	106.93
6	I	228	SAM	CG-SD-C5'	2.58	109.98	103.40
6	I	228	SAM	O3'-C3'-C4'	-2.34	104.28	111.05
6	J	228	SAM	C4-C5-N7	-2.34	106.97	109.40
6	I	228	SAM	C4-C5-N7	-2.19	107.11	109.40
6	J	228	SAM	O4'-C1'-C2'	-2.19	103.73	106.93

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	228	SAM	O-C-CA-CB
6	I	228	SAM	N-CA-CB-CG
6	I	228	SAM	CB-CG-SD-CE
6	I	228	SAM	CB-CG-SD-C5'
6	J	228	SAM	CA-CB-CG-SD
6	J	228	SAM	CB-CG-SD-CE
6	J	228	SAM	CB-CG-SD-C5'
6	I	228	SAM	CA-CB-CG-SD

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	228	SAM	4	0
6	J	228	SAM	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 then 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.

Ligand SAM I 228

Bond lengths
Bond angles
Torsions
Rings

Ligand SAM J 228

Bond lengths
Bond angles
Torsions
Rings
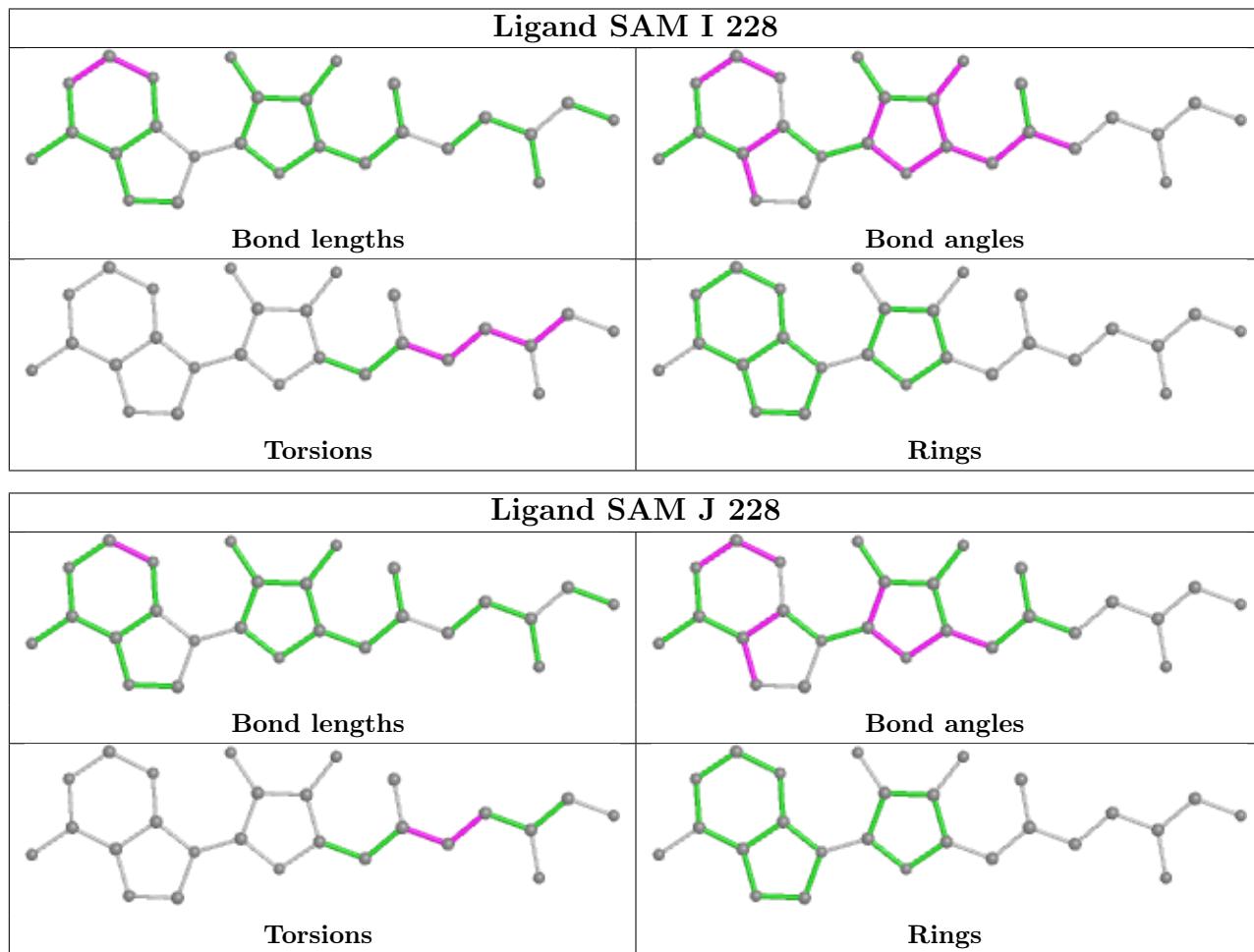
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	363/376 (96%)	0.25	9 (2%)	57	43	62, 87, 136, 227	0
1	F	363/376 (96%)	0.23	8 (2%)	62	48	66, 93, 125, 232	0
2	E	121/129 (93%)	0.43	5 (4%)	37	24	107, 146, 174, 186	0
2	H	121/129 (93%)	0.39	7 (5%)	23	13	104, 142, 171, 181	0
3	I	227/234 (97%)	0.23	2 (0%)	84	75	56, 79, 114, 143	0
3	J	227/234 (97%)	0.21	0	100	100	60, 77, 102, 130	0
4	K	24/34 (70%)	0.14	2 (8%)	11	6	120, 135, 253, 271	0
4	L	24/34 (70%)	0.12	1 (4%)	36	23	113, 133, 230, 267	0
5	G	3/13 (23%)	-0.43	0	100	100	232, 232, 239, 240	0
5	S	3/13 (23%)	0.12	0	100	100	235, 235, 255, 264	0
All	All	1476/1572 (93%)	0.26	34 (2%)	60	47	56, 91, 169, 271	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	303	LEU	8.6
1	F	305	THR	6.0
1	F	300	PHE	5.7
1	F	304	ARG	5.7
1	F	302	HIS	5.3
1	A	305	THR	5.3
1	A	302	HIS	5.1
1	A	307	ALA	4.2
4	K	1	A	4.1
4	L	1	A	3.9
1	A	306	GLY	3.7
2	H	30	THR	3.6
1	F	301	ARG	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	97	ALA	3.2
2	H	96	ALA	3.0
4	K	2	G	3.0
2	E	98	ALA	2.7
2	H	49	ALA	2.5
1	A	301	ARG	2.4
1	A	304	ARG	2.4
2	E	107	LYS	2.4
2	H	21	LEU	2.3
2	E	114	GLU	2.1
3	I	22	GLU	2.1
1	F	307	ALA	2.1
2	H	87	LEU	2.1
2	E	103	ILE	2.1
2	H	51	LEU	2.1
1	F	235	ILE	2.1
2	H	97	ALA	2.1
1	A	286	PRO	2.1
3	I	18	ASP	2.0
1	A	308	LYS	2.0
1	A	200	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
6	SAM	J	228	26/27	0.92	0.31	65,81,117,128	0
6	SAM	I	228	26/27	0.95	0.38	69,82,122,128	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SAM J 228:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around SAM I 228:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.