



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:19 AM UTC

PDB ID : 9L12 / pdb_00009l12
Title : Crystal structure of Cas12h ternary complex
Authors : Xiang, W.; Chen, J.; Liu, L.
Deposited on : 2024-12-13
Resolution : 3.81 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

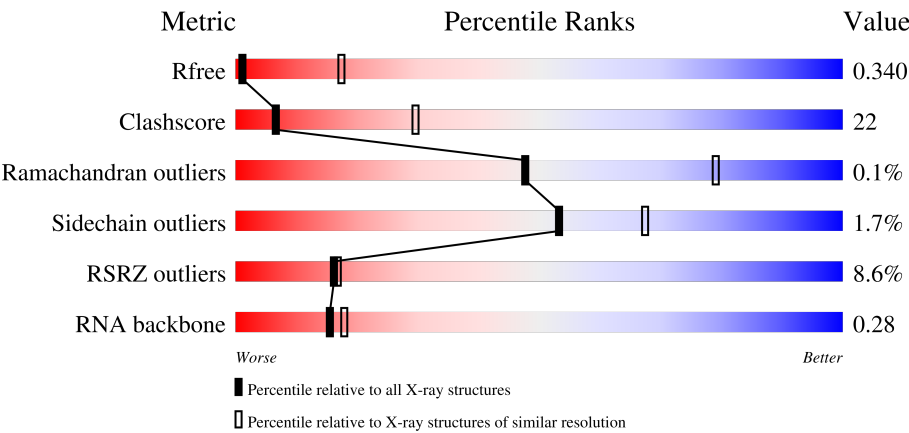
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.81 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1043 (3.98-3.66)
Clashscore	190562	1075 (3.98-3.66)
Ramachandran outliers	187476	1029 (3.98-3.66)
Sidechain outliers	187428	1024 (3.98-3.66)
RSRZ outliers	180081	1042 (3.98-3.66)
RNA backbone	3983	1009 (4.52-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	870	9% 63% 34% ..
1	E	870	8% 63% 34% .
1	I	870	9% 60% 37% ..
2	B	28	50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	28	4% 29% 71%
2	J	28	4% 43% 57%
3	C	15	7% 40% 40% 20%
3	G	15	60% 40%
3	K	15	40% 33% 27%
4	D	56	14% 20% 61% 20%
4	H	56	12% 18% 54% 29%
4	L	56	7% 16% 54% 30%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 26996 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 Cas12h.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	861	Total	C	N	O	S	0	0	0
			6961	4431	1227	1276	27			
1	E	870	Total	C	N	O	S	0	0	0
			6923	4391	1224	1282	26			
1	I	864	Total	C	N	O	S	0	0	0
			6995	4452	1234	1282	27			

- Molecule 2 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	28	Total	C	N	O	P	0	0	0
			574	273	99	174	28			
2	F	28	Total	C	N	O	P	0	0	0
			574	273	99	174	28			
2	J	28	Total	C	N	O	P	0	0	0
			574	273	99	174	28			

- Molecule 3 is a DNA chain called DNA (5'-D(P*AP*GP*TP*CP*GP*AP*TP*GP*TP*TP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	P	0	0	0
			247	118	41	76	12			
3	G	15	Total	C	N	O	P	0	0	0
			306	147	48	96	15			
3	K	11	Total	C	N	O	P	0	0	0
			227	108	39	69	11			

- Molecule 4 is a RNA chain called RNA (56-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	56	Total 1204	C 536	N 225	O 387	P 56	0	0	0
4	H	56	Total 1204	C 536	N 225	O 387	P 56	0	0	0
4	L	56	Total 1204	C 536	N 225	O 387	P 56	0	0	0

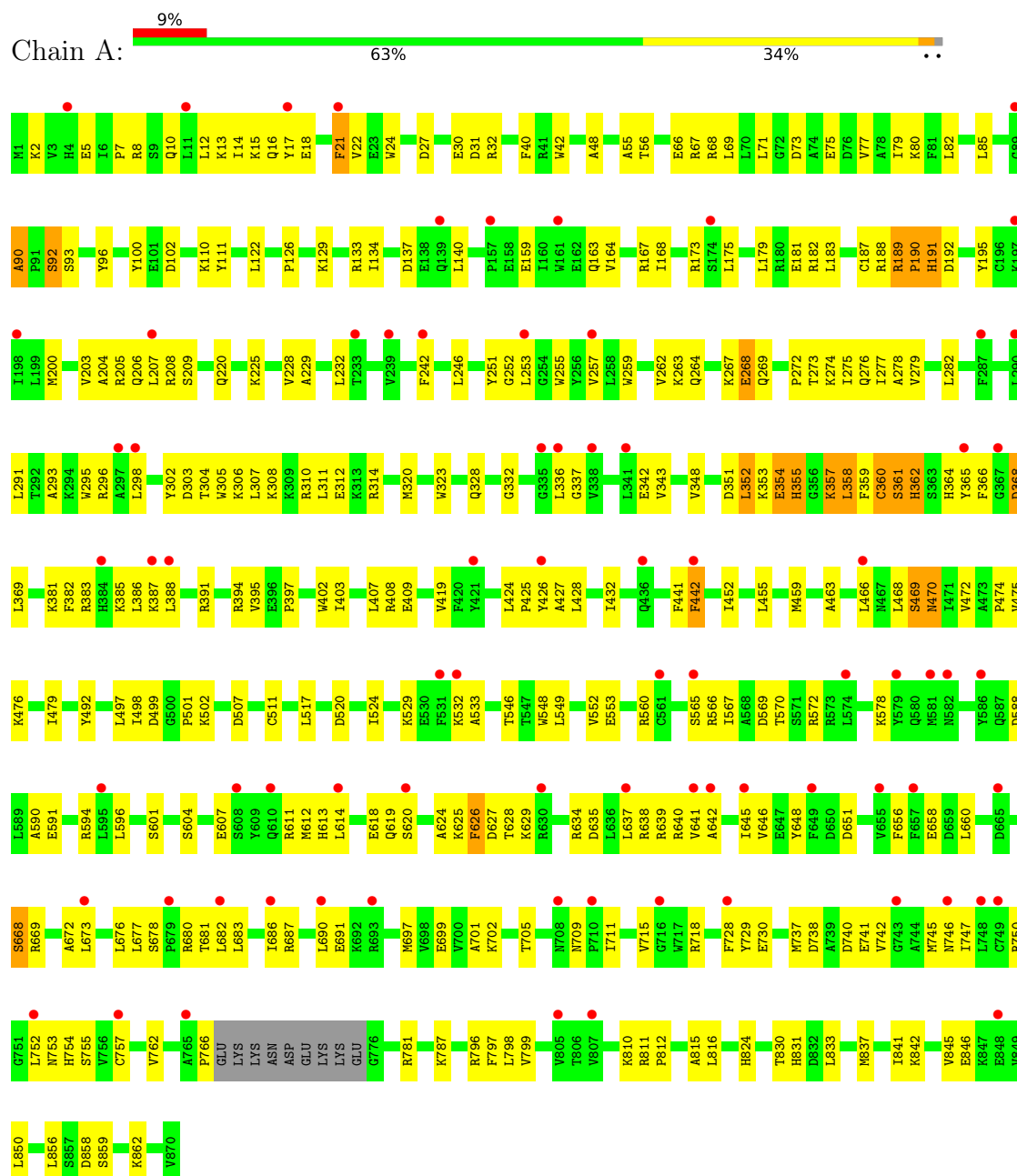
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mg 1	0	0
5	E	1	Total 1	Mg 1	0	0
5	I	1	Total 1	Mg 1	0	0

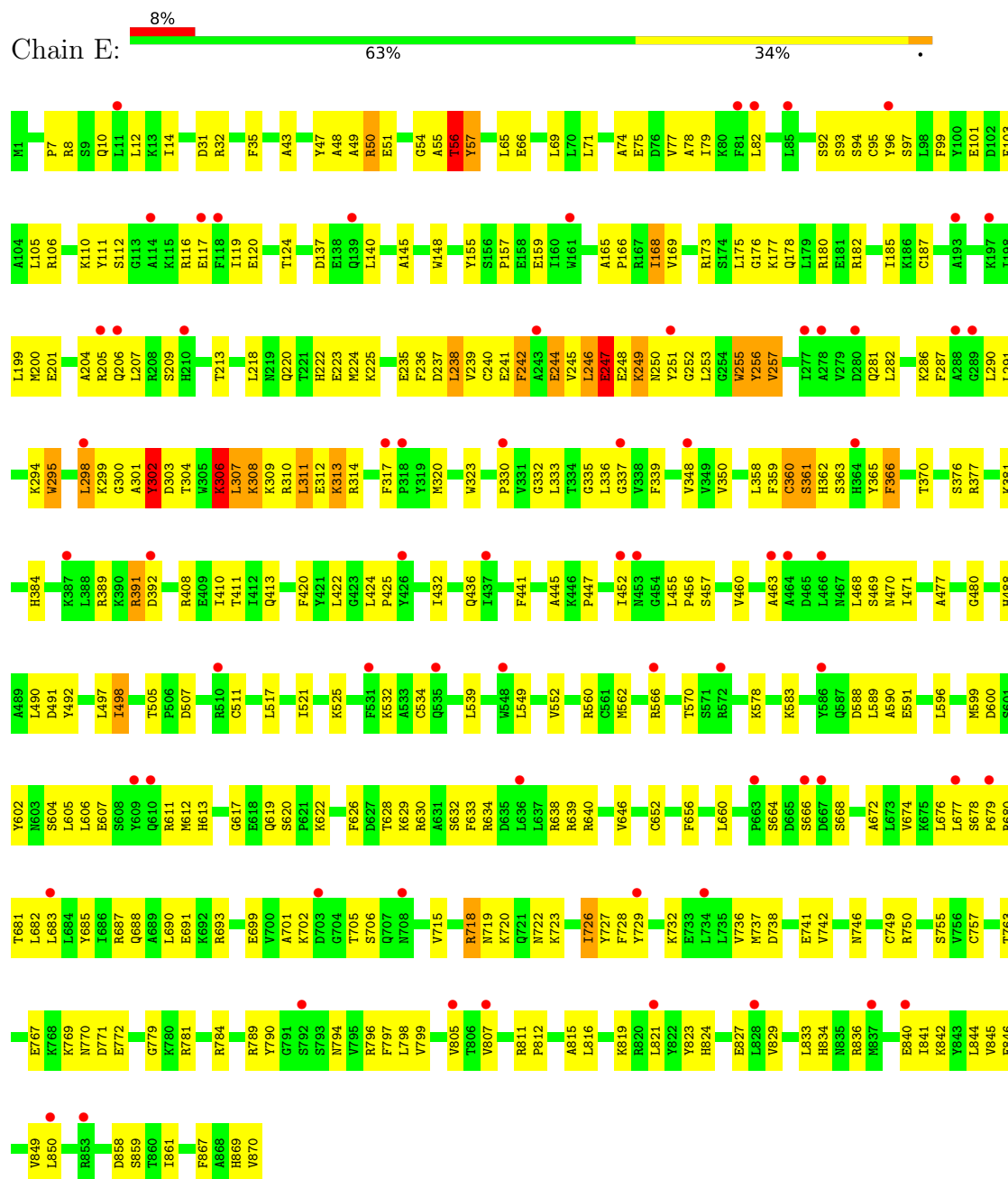
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

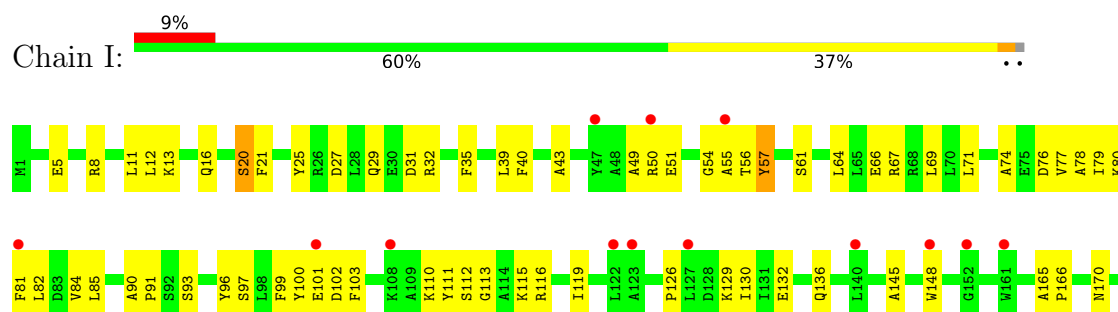
• Molecule 1: Cas12h

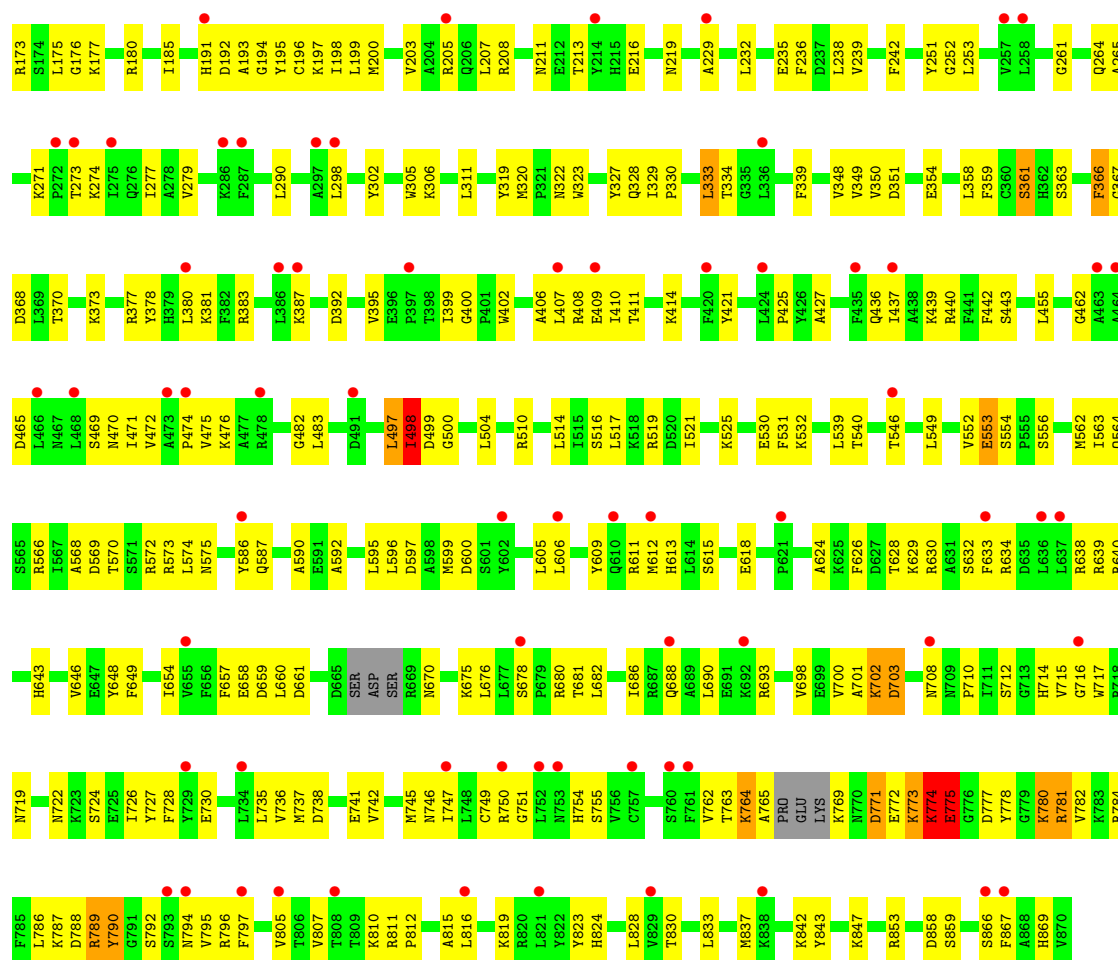


● Molecule 1: Cas12h



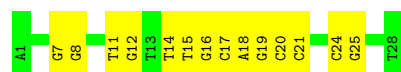
● Molecule 1: Cas12h





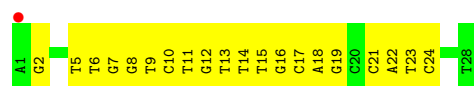
• Molecule 2: DNA (28-MER)

Chain B: 50% 50%



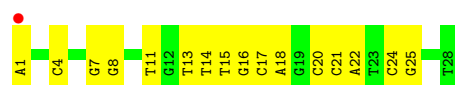
• Molecule 2: DNA (28-MER)

Chain F: 4% 29% 71%

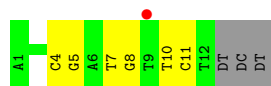


• Molecule 2: DNA (28-MER)

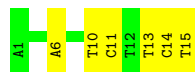
Chain J: 4% 43% 57%



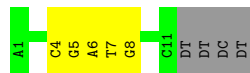
- Molecule 3: DNA (5'-D(P*AP*GP*TP*CP*GP*AP*TP*GP*TP*TP*CP*T)-3')



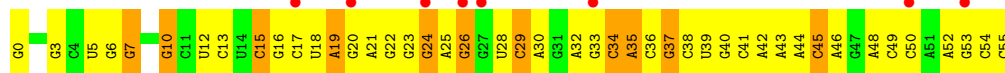
- Molecule 3: DNA (5'-D(P*AP*GP*TP*CP*GP*AP*TP*GP*TP*TP*CP*T)-3')



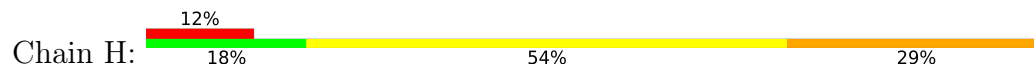
- Molecule 3: DNA (5'-D(P*AP*GP*TP*CP*GP*AP*TP*GP*TP*TP*CP*T)-3')



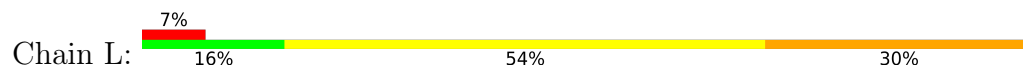
- Molecule 4: RNA (56-MER)



- Molecule 4: RNA (56-MER)



- Molecule 4: RNA (56-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	155.53Å 155.53Å 479.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.42 – 3.81 28.42 – 3.81	Depositor EDS
% Data completeness (in resolution range)	62.5 (28.42-3.81) 41.6 (28.42-3.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.85 (at 3.86Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.334 , 0.339 0.336 , 0.340	Depositor DCC
R_{free} test set	28879 reflections (43.09%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	1.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.089 for -h,-k,l	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	26996	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.30	2/7110 (0.0%)	0.87	38/9577 (0.4%)
1	E	0.33	7/7067 (0.1%)	0.86	44/9526 (0.5%)
1	I	0.24	0/7142	0.76	32/9614 (0.3%)
2	B	0.31	0/641	0.52	0/986
2	F	0.30	0/641	0.53	0/986
2	J	0.28	0/641	0.57	0/986
3	C	0.26	0/275	0.52	0/421
3	G	0.26	0/340	0.52	0/521
3	K	0.23	0/253	0.58	0/387
4	D	0.19	0/1347	0.42	0/2098
4	H	0.21	0/1347	0.44	0/2098
4	L	0.17	0/1347	0.40	0/2098
All	All	0.28	9/28151 (0.0%)	0.75	114/39298 (0.3%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	93	SER	CA-C	7.15	1.62	1.52
1	E	92	SER	CA-C	6.96	1.62	1.52
1	E	470	ASN	N-CA	6.51	1.54	1.46
1	E	92	SER	N-CA	-6.46	1.37	1.46
1	E	469	SER	CA-C	-5.97	1.45	1.52
1	E	469	SER	CA-CB	5.66	1.62	1.53
1	A	190	PRO	N-CD	5.43	1.55	1.47
1	A	122	LEU	CA-C	-5.20	1.45	1.52
1	E	93	SER	N-CA	-5.18	1.40	1.46

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	LEU	N-CA-C	23.32	139.85	111.40
1	A	469	SER	N-CA-C	22.25	135.73	111.03
1	E	361	SER	N-CA-C	20.21	138.65	110.35
1	E	498	ILE	N-CA-C	16.47	125.91	110.42
1	E	469	SER	N-CA-C	15.72	128.12	111.14
1	E	256	TYR	N-CA-C	-14.41	88.49	109.96
1	A	470	ASN	N-CA-C	-14.03	83.21	107.61
1	I	702	LYS	CB-CA-C	-13.98	89.52	111.74
1	I	482	GLY	N-CA-C	13.96	139.90	115.61
1	I	789	ARG	N-CA-C	13.67	128.51	111.69
1	A	92	SER	N-CA-C	-13.60	89.60	109.59
1	A	190	PRO	CB-CA-C	-13.37	89.49	111.56
1	E	257	VAL	N-CA-C	-12.78	101.00	113.53
1	E	362	HIS	N-CA-C	-12.76	90.83	109.59
1	A	497	LEU	CB-CA-C	-12.59	89.20	110.22
1	I	469	SER	N-CA-C	12.50	127.06	111.69
1	A	337	GLY	N-CA-C	-12.10	87.71	110.83
1	E	169	VAL	N-CA-C	-11.57	93.08	108.35
1	A	395	VAL	N-CA-CB	-11.26	99.74	111.90
1	E	360	CYS	CB-CA-C	-11.22	88.33	112.78
1	E	361	SER	N-CA-CB	-11.01	91.39	109.56
1	E	497	LEU	CB-CA-C	-10.57	92.57	110.22
1	A	668	SER	N-CA-C	10.53	124.13	112.97
1	A	336	LEU	CB-CA-C	-10.41	93.30	110.79
1	E	626	PHE	N-CA-C	-10.36	94.37	109.59
1	A	497	LEU	N-CA-C	10.09	125.00	108.96
1	A	395	VAL	N-CA-C	9.99	121.55	107.37
1	I	498	ILE	N-CA-C	9.97	120.72	111.45
1	A	627	ASP	N-CA-C	-9.93	94.99	109.59
1	A	93	SER	N-CA-C	-9.89	101.08	113.55
1	I	553	GLU	N-CA-C	-9.89	95.05	109.59
1	A	268	GLU	N-CA-C	-9.84	95.13	109.59
1	E	256	TYR	CB-CA-C	9.71	124.14	110.16
1	E	666	SER	N-CA-C	9.49	124.68	112.34
1	I	469	SER	CB-CA-C	-9.45	93.40	110.70
1	E	772	GLU	N-CA-C	9.37	122.42	110.33
1	I	774	LYS	CB-CA-C	9.37	129.06	110.42
1	E	169	VAL	N-CA-CB	9.26	126.55	111.36
1	A	191	HIS	N-CA-C	-9.26	101.50	113.17
1	E	168	ILE	N-CA-C	-9.25	93.73	107.51
1	I	781	ARG	N-CA-C	9.04	124.12	113.18
1	A	469	SER	CB-CA-C	-9.00	97.00	110.95
1	E	470	ASN	N-CA-C	-8.98	93.87	108.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	470	ASN	N-CA-C	-8.57	92.76	108.02
1	A	470	ASN	N-CA-CB	8.41	123.58	110.71
1	I	703	ASP	N-CA-CB	8.39	126.89	111.11
1	I	483	LEU	N-CA-C	-8.33	95.32	108.90
1	E	469	SER	CB-CA-C	-8.31	97.77	110.90
1	E	497	LEU	N-CA-C	8.26	122.09	108.96
1	A	391	ARG	N-CA-C	8.13	123.55	112.90
1	A	269	GLN	N-CA-C	-8.02	95.34	108.41
1	A	668	SER	N-CA-CB	-7.92	99.41	110.65
1	I	780	LYS	CB-CA-C	7.85	126.04	110.42
1	E	391	ARG	CB-CA-C	-7.70	96.15	110.01
1	E	723	LYS	N-CA-C	7.65	119.70	111.36
1	E	363	SER	N-CA-CB	7.58	123.38	110.57
1	A	268	GLU	CB-CA-C	7.27	121.17	110.26
1	E	392	ASP	N-CA-C	-7.19	101.74	111.87
1	I	497	LEU	CB-CA-C	-7.16	98.06	109.80
1	I	483	LEU	N-CA-CB	7.03	122.49	110.68
1	E	769	LYS	CB-CA-C	-7.00	97.25	109.02
1	I	553	GLU	CB-CA-C	6.99	120.74	110.26
1	I	703	ASP	N-CA-C	-6.94	93.01	107.37
1	I	392	ASP	N-CA-C	-6.93	103.11	112.26
1	A	553	GLU	N-CA-C	-6.91	97.57	108.63
1	I	20	SER	CB-CA-C	-6.88	101.59	112.05
1	A	498	ILE	N-CA-C	6.78	116.87	110.30
1	I	554	SER	N-CA-C	-6.76	96.14	108.85
1	I	21	PHE	N-CA-C	6.66	121.45	113.12
1	E	770	ASN	N-CA-C	-6.64	97.34	109.56
1	E	335	GLY	N-CA-C	6.61	122.06	113.27
1	A	394	ARG	CB-CA-C	6.56	123.00	110.27
1	A	391	ARG	CB-CA-C	-6.54	96.52	109.67
1	E	337	GLY	N-CA-C	-6.42	104.70	112.48
1	A	366	PHE	N-CA-C	-6.35	95.93	107.75
1	A	361	SER	CB-CA-C	6.29	121.04	109.71
1	A	628	THR	N-CA-C	-6.29	105.64	113.38
1	E	769	LYS	N-CA-C	6.18	122.28	114.31
1	A	190	PRO	N-CA-C	6.04	124.91	112.47
1	E	626	PHE	CB-CA-C	5.99	119.24	110.26
1	A	442	PHE	N-CA-C	-5.98	105.64	113.12
1	A	93	SER	N-CA-CB	5.95	119.03	110.40
1	A	353	LYS	N-CA-C	5.88	117.36	111.07
1	I	788	ASP	N-CA-C	-5.86	104.53	111.03
1	A	626	PHE	N-CA-C	-5.84	103.18	111.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	302	TYR	N-CA-C	-5.81	104.95	111.28
1	E	498	ILE	N-CA-CB	-5.77	104.13	110.65
1	A	269	GLN	N-CA-CB	5.76	119.64	110.65
1	I	366	PHE	N-CA-C	-5.75	95.80	107.41
1	I	20	SER	N-CA-C	5.71	118.57	108.24
1	E	56	THR	N-CA-C	-5.70	103.00	110.53
1	E	771	ASP	CB-CA-C	-5.70	100.17	111.91
1	E	366	PHE	N-CA-C	-5.64	97.27	107.75
1	E	552	VAL	CB-CA-C	5.64	119.25	111.19
1	E	498	ILE	CB-CA-C	-5.62	104.62	111.87
1	E	362	HIS	CB-CA-C	5.61	118.67	110.26
1	I	361	SER	CB-CA-C	5.60	120.14	110.45
1	I	367	GLY	N-CA-C	-5.60	99.92	113.18
1	E	332	GLY	N-CA-C	5.55	119.73	111.18
1	E	247	GLU	N-CA-C	-5.55	105.23	111.28
1	I	790	TYR	N-CA-C	-5.41	102.19	110.14
1	I	775	GLU	N-CA-CB	-5.36	101.43	110.49
1	A	368	ASP	N-CA-C	-5.34	96.51	107.67
1	A	189	ARG	CB-CA-C	5.33	116.61	109.42
1	E	359	PHE	CA-C-N	-5.27	113.05	122.32
1	E	359	PHE	C-N-CA	-5.27	113.05	122.32
1	E	306	LYS	N-CA-C	-5.27	105.54	111.28
1	E	295	TRP	N-CA-C	5.20	116.64	111.07
1	I	774	LYS	N-CA-C	-5.20	99.73	110.80
1	I	788	ASP	CB-CA-C	5.19	118.99	110.95
1	I	333	LEU	CB-CA-C	-5.17	100.29	110.11
1	I	57	TYR	N-CA-CB	-5.09	102.57	110.87
1	A	360	CYS	N-CA-C	5.04	116.47	108.96
1	E	718	ARG	N-CA-C	-5.03	102.94	110.23

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	6961	0	7009	259	2
1	E	6923	0	6872	343	0
1	I	6995	0	7048	342	2
2	B	574	0	318	19	0
2	F	574	0	318	30	0
2	J	574	0	318	18	0
3	C	247	0	138	5	0
3	G	306	0	173	4	0
3	K	227	0	126	9	0
4	D	1204	0	610	50	0
4	H	1204	0	610	85	0
4	L	1204	0	610	56	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
5	I	1	0	0	0	0
All	All	26996	0	24150	1085	3

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 22.

All (1085) 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)
4:H:27:G:N2	4:H:28:U:H1'	1.19	1.48
1:E:241:GLU:OE1	1:E:287:PHE:CZ	1.80	1.35
4:H:6:G:H1	4:H:29:C:N4	1.26	1.33
4:H:27:G:N2	4:H:28:U:C1'	1.95	1.28
1:I:790:TYR:CE2	1:I:828:LEU:HD11	1.70	1.26
1:E:241:GLU:OE1	1:E:287:PHE:HZ	1.08	1.23
1:E:237:ASP:C	1:E:238:LEU:HD23	1.61	1.23
1:I:763:THR:C	1:I:778:TYR:OH	1.81	1.23
1:I:764:LYS:HB2	1:I:778:TYR:CE2	1.72	1.22
1:E:255:TRP:CE3	1:E:302:TYR:OH	1.96	1.17
1:A:15:LYS:HE3	1:A:361:SER:OG	1.41	1.17
1:E:236:PHE:CD2	1:E:240:CYS:SG	2.38	1.17
1:I:762:VAL:O	1:I:778:TYR:CE1	1.98	1.15
1:A:79:ILE:HD12	1:A:80:LYS:N	1.61	1.13
1:E:245:VAL:HG12	1:E:249:LYS:HD3	1.17	1.12
1:I:789:ARG:HG3	1:I:790:TYR:CD1	1.85	1.11
1:I:769:LYS:HE3	1:I:769:LYS:HA	1.32	1.11
4:H:26:G:C2	4:H:27:G:N7	2.20	1.10
4:H:27:G:C2	4:H:28:U:N1	2.21	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:309:LYS:HA	1:E:309:LYS:HE2	1.32	1.07
1:I:764:LYS:HB2	1:I:778:TYR:HE2	0.91	1.07
1:I:702:LYS:CG	1:I:702:LYS:O	1.88	1.05
1:I:702:LYS:O	1:I:702:LYS:HG3	1.26	1.04
1:E:246:LEU:HA	1:E:249:LYS:HB2	1.04	1.04
1:A:79:ILE:HD12	1:A:80:LYS:H	1.14	1.02
1:E:246:LEU:CA	1:E:249:LYS:HB2	1.89	1.01
1:I:790:TYR:CD2	1:I:807:VAL:HG21	1.95	1.01
1:E:246:LEU:HD12	1:E:253:LEU:CB	1.91	1.00
1:I:51:GLU:N	1:I:51:GLU:OE2	1.95	1.00
1:I:790:TYR:HE2	1:I:828:LEU:HD11	1.17	0.99
4:H:27:G:C2	4:H:28:U:C6	2.50	0.99
1:A:469:SER:O	1:A:507:ASP:OD1	1.79	0.99
1:A:15:LYS:CE	1:A:361:SER:OG	2.12	0.97
1:I:497:LEU:HD12	1:I:497:LEU:O	1.61	0.97
1:E:245:VAL:HG12	1:E:249:LYS:CD	1.93	0.97
1:E:727:TYR:CE2	1:E:845:VAL:HG11	2.00	0.96
1:I:769:LYS:HE2	1:I:774:LYS:HB2	1.46	0.96
1:E:245:VAL:O	1:E:249:LYS:N	1.98	0.95
1:I:634:ARG:HE	1:I:638:ARG:HH12	1.15	0.95
1:E:237:ASP:O	1:E:238:LEU:HD23	1.67	0.94
1:E:246:LEU:HA	1:E:249:LYS:CB	1.97	0.94
1:E:51:GLU:OE1	1:E:56:THR:OG1	1.85	0.93
1:I:789:ARG:HG3	1:I:790:TYR:CE1	2.04	0.92
1:E:706:SER:HB2	1:E:718:ARG:HH11	1.34	0.91
1:I:790:TYR:CE2	1:I:828:LEU:CD1	2.54	0.90
2:F:2:DG:H1	4:H:55:C:H42	1.19	0.90
1:A:351:ASP:C	1:A:352:LEU:HD23	1.97	0.89
1:I:750:ARG:HG2	1:I:755:SER:HA	1.54	0.89
1:A:24:TRP:CD1	1:A:355:HIS:HD2	1.90	0.89
1:I:762:VAL:O	1:I:778:TYR:CZ	2.25	0.89
4:L:4:C:N3	4:L:32:A:N6	2.21	0.89
1:I:764:LYS:CB	1:I:778:TYR:HE2	1.85	0.88
1:E:66:GLU:HA	1:E:69:LEU:HB2	1.53	0.88
1:I:16:GLN:HB3	1:I:359:PHE:HB2	1.54	0.88
1:E:634:ARG:HH22	2:F:13:DT:H3'	1.39	0.88
1:I:771:ASP:CB	1:I:774:LYS:HE3	2.03	0.88
1:E:239:VAL:HG22	1:E:290:LEU:HD13	1.56	0.87
1:I:763:THR:O	1:I:778:TYR:OH	1.91	0.87
4:H:27:G:N2	4:H:28:U:N1	2.19	0.86
1:E:246:LEU:O	1:E:250:ASN:N	2.09	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:26:G:C6	4:H:27:G:O6	2.30	0.85
1:I:762:VAL:O	1:I:778:TYR:HE1	1.54	0.85
1:I:765:ALA:O	1:I:795:VAL:O	1.93	0.85
1:E:706:SER:CB	1:E:718:ARG:HH11	1.90	0.84
1:E:252:GLY:HA3	2:F:6:DT:H5'	1.60	0.84
1:E:307:LEU:HD12	1:E:307:LEU:O	1.77	0.84
1:E:241:GLU:OE1	1:E:287:PHE:CE1	2.30	0.84
1:E:308:LYS:HD3	1:E:308:LYS:C	2.02	0.84
1:I:771:ASP:HB2	1:I:774:LYS:HE3	1.57	0.84
1:E:245:VAL:CG1	1:E:249:LYS:HD3	2.04	0.83
1:E:313:LYS:HB2	1:E:313:LYS:NZ	1.93	0.83
1:A:388:LEU:HD21	1:A:397:PRO:HB3	1.59	0.83
1:E:391:ARG:O	1:E:391:ARG:HG2	1.77	0.83
1:I:790:TYR:OH	1:I:828:LEU:HG	1.79	0.82
1:E:613:HIS:HB3	4:H:15:C:H4'	1.60	0.82
1:I:771:ASP:O	1:I:774:LYS:HD3	1.80	0.82
3:G:13:DT:H2''	3:G:14:DC:H5''	1.62	0.82
1:E:308:LYS:HD3	1:E:308:LYS:O	1.79	0.81
1:I:792:SER:HB3	1:I:794:ASN:OD1	1.79	0.81
1:I:778:TYR:HB3	1:I:782:VAL:CB	2.10	0.81
1:I:789:ARG:CG	1:I:790:TYR:CE1	2.64	0.81
1:E:246:LEU:HD23	1:E:249:LYS:HG2	1.61	0.81
1:E:246:LEU:HD12	1:E:253:LEU:CA	2.11	0.80
4:H:27:G:C2'	4:H:28:U:OP1	2.28	0.80
1:I:790:TYR:HE2	1:I:828:LEU:CD1	1.90	0.80
1:E:244:GLU:O	1:E:247:GLU:HG3	1.80	0.80
1:E:816:LEU:HD22	1:E:819:LYS:HG3	1.64	0.80
1:I:634:ARG:NH1	1:I:675:LYS:O	2.15	0.80
1:E:750:ARG:HG2	1:E:755:SER:HA	1.61	0.80
4:H:27:G:H21	4:H:28:U:H1'	0.90	0.80
1:E:706:SER:CB	1:E:718:ARG:NH1	2.45	0.79
1:I:587:GLN:HA	1:I:640:ARG:HH22	1.48	0.79
1:A:15:LYS:HE3	1:A:361:SER:CB	2.11	0.79
4:H:27:G:N1	4:H:28:U:C2	2.51	0.79
1:E:678:SER:HB3	2:F:14:DT:H5''	1.65	0.79
1:A:669:ARG:NH2	4:D:46:A:OP1	2.15	0.78
1:E:246:LEU:HD13	1:E:251:TYR:O	1.83	0.78
1:E:255:TRP:HE3	1:E:302:TYR:OH	1.66	0.78
1:I:777:ASP:OD1	1:I:778:TYR:O	1.99	0.78
1:E:145:ALA:HA	1:E:148:TRP:HD1	1.50	0.77
1:I:596:LEU:HD21	1:I:634:ARG:HG3	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:764:LYS:HD3	1:I:765:ALA:H	1.46	0.77
1:E:797:PHE:HB2	1:E:816:LEU:HB2	1.66	0.76
4:H:27:G:C2	4:H:28:U:C2	2.73	0.76
1:I:778:TYR:CB	1:I:782:VAL:HG11	2.16	0.76
1:E:302:TYR:HE2	1:E:306:LYS:NZ	1.84	0.76
1:E:619:GLN:NE2	2:F:9:DT:O2	2.17	0.76
4:H:27:G:C6	4:H:28:U:C4	2.72	0.76
1:I:786:LEU:O	1:I:790:TYR:O	2.02	0.76
1:A:678:SER:HB3	1:A:681:THR:HB	1.68	0.76
1:E:302:TYR:HE2	1:E:306:LYS:HZ2	1.34	0.76
1:I:85:LEU:O	1:I:208:ARG:NH1	2.17	0.76
1:A:110:LYS:NZ	3:C:7:DT:O2	2.17	0.76
1:I:126:PRO:HG2	1:I:129:LYS:HB2	1.68	0.76
1:A:16:GLN:HE21	1:A:359:PHE:HD2	1.33	0.76
4:H:27:G:C2	4:H:28:U:C1'	2.65	0.76
1:E:50:ARG:HD2	1:E:320:MET:HB3	1.66	0.75
1:A:796:ARG:HE	1:A:811:ARG:HB3	1.50	0.75
1:E:639:ARG:NH2	1:E:688:GLN:OE1	2.20	0.75
1:E:660:LEU:HA	1:E:702:LYS:HE2	1.68	0.75
4:H:27:G:H2'	4:H:28:U:OP1	1.87	0.75
1:E:236:PHE:CE2	1:E:240:CYS:SG	2.79	0.75
1:E:664:SER:HB3	1:E:702:LYS:HE3	1.66	0.75
1:I:334:THR:O	2:J:22:DA:N6	2.19	0.75
1:E:239:VAL:O	1:E:242:PHE:HB3	1.87	0.75
1:I:789:ARG:HG3	1:I:790:TYR:HD1	1.52	0.75
1:E:51:GLU:OE2	1:E:56:THR:HG23	1.87	0.74
1:A:15:LYS:CD	1:A:361:SER:OG	2.34	0.74
1:A:24:TRP:CD1	1:A:355:HIS:CD2	2.74	0.74
1:E:252:GLY:CA	2:F:6:DT:H5'	2.17	0.74
1:E:309:LYS:HA	1:E:309:LYS:CE	2.14	0.74
1:E:238:LEU:HD23	1:E:238:LEU:N	2.02	0.74
1:E:238:LEU:CD1	1:E:286:LYS:O	2.36	0.74
2:F:16:DG:H2''	2:F:17:DC:H5''	1.68	0.74
1:E:237:ASP:O	1:E:238:LEU:CD2	2.36	0.74
1:E:812:PRO:HG2	1:E:815:ALA:HB2	1.69	0.74
1:I:368:ASP:OD2	1:I:383:ARG:NH2	2.18	0.74
4:L:36:C:O2'	4:L:38:C:OP1	2.04	0.74
1:E:255:TRP:O	1:E:256:TYR:C	2.31	0.73
1:I:778:TYR:HB3	1:I:782:VAL:HB	1.68	0.73
1:E:32:ARG:NH2	1:E:323:TRP:O	2.21	0.73
4:H:6:G:N1	4:H:29:C:N4	2.06	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:4:DC:H42	4:L:53:G:H1	1.34	0.73
1:A:253:LEU:HB3	1:A:305:TRP:HH2	1.53	0.73
1:I:442:PHE:HE1	1:I:654:ILE:HG21	1.53	0.73
1:A:79:ILE:CD1	1:A:80:LYS:N	2.49	0.73
4:H:26:G:N3	4:H:27:G:N7	2.38	0.72
1:I:11:LEU:HD22	1:I:421:TYR:HB3	1.69	0.72
1:A:14:ILE:HG21	1:A:358:LEU:HD23	1.70	0.72
1:E:307:LEU:HA	1:E:310:ARG:HD3	1.70	0.72
1:I:32:ARG:NH2	1:I:323:TRP:O	2.23	0.72
1:I:778:TYR:CG	1:I:782:VAL:HG11	2.24	0.72
1:A:102:ASP:OD2	1:A:191:HIS:ND1	2.21	0.72
1:I:497:LEU:O	1:I:497:LEU:CD1	2.38	0.72
1:I:639:ARG:HD3	4:L:36:C:H4'	1.72	0.72
1:I:774:LYS:HD2	1:I:774:LYS:N	2.04	0.72
1:A:619:GLN:NE2	4:D:50:C:O2	2.23	0.71
1:I:778:TYR:CB	1:I:782:VAL:CG1	2.68	0.71
2:J:16:DG:H2''	2:J:17:DC:H5''	1.72	0.71
1:E:101:GLU:HG2	1:E:180:ARG:HD2	1.72	0.71
1:E:348:VAL:HB	1:E:360:CYS:HB2	1.72	0.71
1:E:241:GLU:CD	1:E:287:PHE:CE1	2.68	0.71
4:H:26:G:N1	4:H:27:G:O6	2.24	0.71
1:A:352:LEU:HD23	1:A:352:LEU:N	2.03	0.71
4:H:27:G:N3	4:H:28:U:C6	2.59	0.71
1:A:277:ILE:HD11	4:D:54:C:H4'	1.73	0.70
1:E:237:ASP:C	1:E:238:LEU:CD2	2.55	0.70
1:I:546:THR:HG23	1:I:562:MET:HE1	1.74	0.70
1:A:73:ASP:HB3	1:A:182:ARG:HH21	1.56	0.70
1:A:797:PHE:O	1:A:815:ALA:HB1	1.90	0.70
1:E:687:ARG:NH2	1:E:699:GLU:OE1	2.22	0.70
1:E:726:ILE:HD11	1:E:728:PHE:CZ	2.26	0.70
1:A:14:ILE:HG23	1:A:359:PHE:O	1.91	0.70
1:E:727:TYR:HE2	1:E:845:VAL:HG11	1.55	0.70
1:A:68:ARG:NE	1:A:75:GLU:OE2	2.25	0.70
1:E:307:LEU:HD12	1:E:307:LEU:C	2.16	0.70
1:A:499:ASP:OD2	1:A:648:TYR:OH	2.10	0.69
1:I:380:LEU:HD21	1:I:407:LEU:HD22	1.72	0.69
1:E:49:ALA:HB3	1:E:56:THR:OG1	1.92	0.69
1:A:24:TRP:NE1	1:A:355:HIS:HD2	1.90	0.69
1:E:124:THR:HG21	1:I:192:ASP:HA	1.73	0.69
1:E:789:ARG:HB2	1:E:869:HIS:HB2	1.75	0.69
1:I:778:TYR:HB3	1:I:782:VAL:CG1	2.23	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:43:A:H2'	4:L:44:A:H8	1.56	0.69
1:A:308:LYS:NZ	1:A:312:GLU:OE1	2.25	0.69
1:I:472:VAL:HG12	1:I:474:PRO:HD3	1.73	0.69
1:I:261:GLY:HA2	1:I:279:VAL:HG22	1.75	0.69
1:I:51:GLU:HG2	1:I:54:GLY:CA	2.23	0.68
4:D:10:G:H22	4:D:26:G:H1	1.39	0.68
1:E:668:SER:O	1:E:674:VAL:HG11	1.93	0.68
1:I:778:TYR:HB3	1:I:782:VAL:HG11	1.75	0.68
1:A:7:PRO:O	1:A:8:ARG:NH1	2.27	0.68
1:E:74:ALA:O	1:E:78:ALA:N	2.22	0.68
1:A:492:TYR:HD2	1:A:492:TYR:O	1.77	0.68
1:E:65:LEU:O	1:E:69:LEU:N	2.26	0.68
1:E:705:THR:O	1:E:746:ASN:ND2	2.26	0.68
4:L:10:G:H1	4:L:25:A:H61	1.41	0.68
1:A:672:ALA:O	1:A:676:LEU:N	2.23	0.68
1:E:560:ARG:NH2	4:H:15:C:O2'	2.26	0.68
1:E:300:GLY:O	1:E:303:ASP:HB2	1.94	0.68
1:A:133:ARG:NH2	1:A:137:ASP:OD2	2.27	0.67
1:A:32:ARG:NH2	1:A:323:TRP:O	2.28	0.67
1:I:778:TYR:CB	1:I:782:VAL:HB	2.24	0.67
1:I:812:PRO:HG2	1:I:815:ALA:HB2	1.75	0.67
1:E:236:PHE:HD2	1:E:240:CYS:SG	2.16	0.67
1:I:66:GLU:HA	1:I:69:LEU:HB2	1.75	0.67
1:E:255:TRP:O	1:E:257:VAL:N	2.27	0.67
1:I:769:LYS:HE3	1:I:769:LYS:CA	2.16	0.67
1:I:790:TYR:CD2	1:I:807:VAL:CG2	2.76	0.67
1:E:767:GLU:O	1:E:794:ASN:ND2	2.28	0.67
1:I:790:TYR:HD2	1:I:807:VAL:HG21	1.52	0.67
1:I:794:ASN:O	1:I:795:VAL:HG13	1.95	0.67
1:A:705:THR:HG21	1:A:747:ILE:HG13	1.76	0.67
1:I:762:VAL:O	1:I:778:TYR:OH	2.13	0.67
1:I:805:VAL:HG23	1:I:830:THR:HG22	1.77	0.67
1:A:368:ASP:OD2	1:A:383:ARG:NE	2.26	0.66
1:E:391:ARG:O	1:E:391:ARG:CG	2.43	0.66
1:E:255:TRP:O	1:E:257:VAL:HG23	1.95	0.66
4:L:16:G:O2'	4:L:19:A:N6	2.28	0.66
1:I:25:TYR:HE2	1:I:329:ILE:HD11	1.59	0.66
1:A:387:LYS:HB3	4:D:34:C:H42	1.58	0.66
4:H:26:G:C2	4:H:27:G:C5	2.83	0.66
1:I:790:TYR:CE2	1:I:828:LEU:HD21	2.30	0.66
1:E:309:LYS:HE2	1:E:309:LYS:CA	2.18	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:ILE:HG13	1:E:168:ILE:O	1.95	0.66
1:E:861:ILE:HD12	1:E:861:ILE:O	1.95	0.65
4:H:27:G:N2	4:H:28:U:C2	2.64	0.65
1:E:456:PRO:O	1:E:492:TYR:OH	2.13	0.65
4:H:27:G:H2'	4:H:27:G:N3	2.11	0.65
1:I:504:LEU:HD13	1:I:504:LEU:O	1.96	0.65
1:A:469:SER:O	1:A:507:ASP:CG	2.39	0.65
4:L:39:U:H2'	4:L:40:G:H8	1.62	0.65
1:A:209:SER:HB2	2:B:18:DA:H1'	1.79	0.65
1:E:589:LEU:HD21	1:E:640:ARG:HG2	1.78	0.65
1:A:745:MET:HG3	1:A:856:LEU:HD13	1.79	0.65
4:L:24:G:H2'	4:L:25:A:C8	2.32	0.65
1:E:525:LYS:NZ	1:E:604:SER:OG	2.30	0.65
1:I:796:ARG:HD2	1:I:811:ARG:HA	1.79	0.65
2:B:17:DC:H42	4:D:40:G:H1	1.45	0.64
1:E:245:VAL:O	1:E:248:GLU:HB3	1.97	0.64
1:E:727:TYR:CE2	1:E:845:VAL:CG1	2.78	0.64
1:I:700:VAL:HG11	1:I:751:GLY:HA2	1.78	0.64
1:I:769:LYS:HA	1:I:769:LYS:CE	2.16	0.64
1:E:241:GLU:CD	1:E:287:PHE:CZ	2.74	0.64
1:A:229:ALA:HA	1:A:232:LEU:HG	1.79	0.64
1:A:251:TYR:HD1	1:A:252:GLY:H	1.46	0.64
1:A:660:LEU:HA	1:A:702:LYS:HG2	1.78	0.64
1:E:247:GLU:OE1	1:E:248:GLU:N	2.30	0.64
4:H:26:G:N1	4:H:27:G:C6	2.66	0.64
1:I:556:SER:HB2	4:L:19:A:H1'	1.79	0.64
1:A:272:PRO:HB3	1:A:276:GLN:HB2	1.77	0.64
1:E:408:ARG:HB2	2:F:21:DC:OP2	1.98	0.64
1:A:17:TYR:CE2	1:A:22:VAL:HG21	2.33	0.64
1:E:632:SER:HB3	4:H:3:G:O2'	1.97	0.64
1:I:49:ALA:O	1:I:319:TYR:CE1	2.50	0.64
4:H:27:G:H21	4:H:28:U:C1'	1.81	0.64
1:I:81:PHE:HE2	1:I:176:GLY:HA2	1.63	0.64
1:A:566:ARG:O	1:A:570:THR:OG1	2.12	0.63
4:H:10:G:H1	4:H:25:A:H61	1.45	0.63
1:I:738:ASP:HB3	1:I:741:GLU:HB2	1.79	0.63
1:E:596:LEU:HD22	1:E:634:ARG:HG3	1.80	0.63
1:E:238:LEU:HD13	1:E:286:LYS:O	1.97	0.63
4:H:21:A:H2'	4:H:22:G:H8	1.63	0.63
2:B:7:DG:H2'	2:B:8:DG:C8	2.34	0.63
1:E:239:VAL:CG2	1:E:290:LEU:HD13	2.28	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:TRP:NE1	1:A:355:HIS:CD2	2.67	0.63
1:A:175:LEU:O	1:A:179:LEU:HD23	1.98	0.63
1:A:368:ASP:O	1:A:382:PHE:HA	1.99	0.63
1:I:629:LYS:O	1:I:633:PHE:N	2.32	0.63
1:E:726:ILE:O	1:E:736:VAL:HG23	1.98	0.63
4:H:36:C:O2'	4:H:38:C:OP1	2.17	0.63
1:I:49:ALA:O	1:I:319:TYR:HE1	1.82	0.63
1:I:208:ARG:HA	1:I:211:ASN:HB3	1.81	0.63
1:I:597:ASP:HB2	1:I:676:LEU:HD21	1.81	0.63
1:I:613:HIS:CD2	4:L:15:C:H4'	2.34	0.62
1:I:235:GLU:HB3	1:I:298:LEU:HD21	1.81	0.62
1:E:246:LEU:HD23	1:E:249:LYS:CG	2.29	0.62
1:A:441:PHE:CD1	1:A:441:PHE:C	2.78	0.62
1:I:437:ILE:HD11	1:I:455:LEU:HD22	1.80	0.62
1:E:688:GLN:NE2	4:H:37:G:N7	2.48	0.62
1:E:858:ASP:OD2	1:E:859:SER:N	2.31	0.62
4:L:39:U:H2'	4:L:40:G:C8	2.35	0.62
1:I:101:GLU:HG2	1:I:180:ARG:HD2	1.81	0.62
1:A:364:HIS:CD2	4:D:0:G:H8	2.17	0.62
1:I:833:LEU:O	1:I:837:MET:N	2.30	0.62
1:A:159:GLU:O	1:A:163:GLN:NE2	2.31	0.62
1:E:32:ARG:NH1	1:E:206:GLN:OE1	2.29	0.61
1:E:611:ARG:NH2	1:E:620:SER:O	2.33	0.61
1:I:499:ASP:OD2	1:I:648:TYR:OH	2.17	0.61
1:I:646:VAL:HG12	1:I:693:ARG:HH11	1.64	0.61
1:I:771:ASP:HB3	1:I:774:LYS:HE3	1.78	0.61
2:B:16:DG:H2''	2:B:17:DC:H5''	1.83	0.61
1:E:239:VAL:N	1:E:290:LEU:HD11	2.14	0.61
1:E:313:LYS:HB2	1:E:313:LYS:HZ3	1.66	0.61
1:E:336:LEU:HD12	1:E:336:LEU:O	2.01	0.61
1:I:737:MET:HE3	1:I:742:VAL:HG22	1.81	0.61
1:I:784:ARG:HA	1:I:787:LYS:HB3	1.82	0.61
4:D:43:A:H2'	4:D:44:A:H8	1.64	0.61
1:E:209:SER:HB2	2:F:18:DA:H1'	1.83	0.61
1:E:680:ARG:HA	1:E:683:LEU:HB2	1.81	0.61
1:E:706:SER:HB2	1:E:718:ARG:NH1	2.07	0.61
1:I:790:TYR:HH	1:I:823:TYR:HE2	1.47	0.61
4:H:26:G:O6	4:H:27:G:O6	2.17	0.61
1:A:354:GLU:HB3	1:A:355:HIS:ND1	2.15	0.61
1:A:472:VAL:HG12	1:A:474:PRO:HD3	1.82	0.61
1:A:524:ILE:HD13	1:A:567:ILE:HG12	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:GLU:HB3	1:A:427:ALA:HB1	1.83	0.61
1:A:683:LEU:HB3	1:A:697:MET:HE1	1.83	0.60
1:A:766:PRO:HG2	1:A:796:ARG:HG2	1.84	0.60
1:E:299:LYS:HD2	1:E:300:GLY:N	2.16	0.60
1:A:264:GLN:OE1	1:A:273:THR:OG1	2.13	0.60
1:E:145:ALA:HA	1:E:148:TRP:CD1	2.34	0.60
4:H:34:C:H2'	4:H:35:A:C8	2.36	0.60
1:A:328:GLN:OE1	2:B:19:DG:N2	2.34	0.60
1:A:658:GLU:HG2	1:A:702:LYS:HD3	1.83	0.60
1:E:299:LYS:HD2	1:E:299:LYS:C	2.27	0.60
1:I:773:LYS:C	1:I:774:LYS:O	2.40	0.60
1:A:278:ALA:O	1:A:282:LEU:N	2.35	0.60
4:D:39:U:H2'	4:D:40:G:C8	2.37	0.60
2:J:7:DG:H1	4:L:50:C:H42	1.48	0.60
1:A:678:SER:HB2	2:B:14:DT:OP2	2.00	0.60
1:E:96:TYR:OH	3:G:6:DA:OP2	2.18	0.60
1:E:333:LEU:CD1	1:E:377:ARG:HA	2.32	0.60
1:A:441:PHE:O	1:A:754:HIS:CD2	2.55	0.59
1:I:539:LEU:HD23	1:I:540:THR:H	1.65	0.59
1:A:364:HIS:CE1	1:A:387:LYS:HA	2.37	0.59
1:I:25:TYR:CE2	1:I:329:ILE:HD11	2.36	0.59
1:I:51:GLU:HG2	1:I:54:GLY:C	2.27	0.59
1:I:51:GLU:HG2	1:I:54:GLY:O	2.02	0.59
1:I:572:ARG:HA	1:I:575:ASN:HB2	1.84	0.59
1:I:769:LYS:HD3	1:I:769:LYS:O	2.01	0.59
1:A:687:ARG:NH2	1:A:699:GLU:OE1	2.36	0.59
1:I:322:ASN:OD1	1:I:323:TRP:N	2.36	0.59
1:A:17:TYR:CE2	1:A:22:VAL:CG2	2.85	0.59
1:A:85:LEU:O	1:A:208:ARG:NH1	2.35	0.59
1:A:409:GLU:CD	2:B:20:DC:H4'	2.28	0.59
1:A:14:ILE:HD13	1:A:358:LEU:CD2	2.33	0.59
1:A:728:PHE:HB3	1:A:730:GLU:OE2	2.03	0.58
1:E:560:ARG:NH2	1:E:612:MET:HE3	2.18	0.58
1:I:504:LEU:HD13	1:I:504:LEU:C	2.27	0.58
1:I:569:ASP:O	1:I:573:ARG:HB2	2.02	0.58
1:E:706:SER:HB3	1:E:718:ARG:NH1	2.16	0.58
4:H:27:G:O2'	4:H:28:U:OP1	2.21	0.58
1:A:687:ARG:HE	1:A:697:MET:HE2	1.68	0.58
4:D:21:A:H2'	4:D:22:G:C8	2.38	0.58
1:E:7:PRO:O	1:E:8:ARG:NH1	2.35	0.58
4:H:27:G:C6	4:H:28:U:C5	2.91	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:216:GLU:HA	1:I:219:ASN:OD1	2.03	0.58
1:I:634:ARG:NE	1:I:638:ARG:HH12	1.94	0.58
1:E:117:GLU:OE2	1:I:191:HIS:NE2	2.37	0.58
1:E:241:GLU:OE2	1:E:287:PHE:HE1	1.86	0.58
1:A:718:ARG:NH2	1:A:740:ASP:OD1	2.36	0.58
1:E:50:ARG:CG	1:E:50:ARG:HH11	2.15	0.58
1:E:239:VAL:HG23	1:E:290:LEU:CD2	2.34	0.58
1:I:115:LYS:O	1:I:119:ILE:HG13	2.02	0.58
1:A:858:ASP:OD1	1:A:859:SER:N	2.37	0.58
1:A:15:LYS:HG3	1:A:361:SER:OG	2.03	0.58
1:A:640:ARG:NH2	4:D:35:A:OP1	2.37	0.58
1:I:410:ILE:HA	1:I:425:PRO:HD2	1.86	0.58
1:A:220:GLN:OE1	1:A:310:ARG:NH2	2.37	0.58
1:A:364:HIS:CD2	1:A:385:LYS:HD2	2.39	0.58
1:A:111:TYR:HB2	2:B:25:DG:OP1	2.04	0.58
1:A:332:GLY:HA2	1:A:409:GLU:HB3	1.86	0.58
1:A:408:ARG:HB2	2:B:21:DC:OP2	2.03	0.58
1:E:488:HIS:CD2	1:E:870:VAL:HG21	2.39	0.58
1:I:765:ALA:C	1:I:795:VAL:O	2.47	0.58
4:D:34:C:H2'	4:D:35:A:C8	2.39	0.57
1:E:298:LEU:O	1:E:301:ALA:HB3	2.04	0.57
1:A:468:LEU:HD11	1:A:676:LEU:HD12	1.86	0.57
1:E:252:GLY:H	2:F:5:DT:H2''	1.69	0.57
1:I:5:GLU:HB3	1:I:427:ALA:HB1	1.87	0.57
1:E:239:VAL:CG2	1:E:290:LEU:CD1	2.81	0.57
1:E:365:TYR:HB2	4:H:1:G:C6	2.40	0.57
1:I:71:LEU:HB3	1:I:74:ALA:HB3	1.87	0.57
1:I:858:ASP:OD1	1:I:859:SER:N	2.38	0.57
1:A:715:VAL:HB	1:A:824:HIS:HE2	1.70	0.57
1:E:201:GLU:O	1:E:205:ARG:HG3	2.02	0.57
1:E:241:GLU:CD	1:E:287:PHE:HE1	2.11	0.57
4:H:46:A:H2'	4:H:47:G:H8	1.70	0.57
1:I:746:ASN:HA	1:I:749:CYS:HB2	1.87	0.57
1:A:179:LEU:O	1:A:183:LEU:HB2	2.04	0.57
1:I:442:PHE:CE1	1:I:654:ILE:HG21	2.37	0.57
1:I:789:ARG:HG2	1:I:790:TYR:CE1	2.40	0.57
1:A:354:GLU:HB3	1:A:355:HIS:CE1	2.40	0.57
1:E:432:ILE:HG12	1:E:436:GLN:HG3	1.86	0.57
4:H:39:U:H2'	4:H:40:G:H8	1.70	0.57
1:I:77:VAL:HG13	1:I:175:LEU:HD22	1.86	0.57
1:I:596:LEU:CD2	1:I:634:ARG:HG3	2.33	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:763:THR:CA	1:I:778:TYR:OH	2.53	0.57
4:D:43:A:H2'	4:D:44:A:C8	2.39	0.56
1:I:790:TYR:CE2	1:I:828:LEU:CG	2.87	0.56
1:A:511:CYS:SG	1:A:594:ARG:HG3	2.44	0.56
1:A:634:ARG:HD2	1:A:676:LEU:O	2.05	0.56
1:E:248:GLU:HA	1:E:248:GLU:OE1	2.05	0.56
1:E:255:TRP:N	1:E:255:TRP:CD1	2.73	0.56
1:E:726:ILE:HG12	1:E:727:TYR:N	2.19	0.56
1:E:727:TYR:CD2	1:E:845:VAL:HG11	2.41	0.56
1:I:97:SER:HB2	1:I:103:PHE:CG	2.40	0.56
1:I:764:LYS:HD3	1:I:765:ALA:N	2.19	0.56
1:A:126:PRO:HG2	1:A:129:LYS:HB2	1.88	0.56
1:A:192:ASP:OD2	1:A:355:HIS:CE1	2.57	0.56
1:E:204:ALA:HA	1:E:207:LEU:HD12	1.88	0.56
1:E:719:ASN:OD1	1:E:722:ASN:HB3	2.04	0.56
1:I:790:TYR:HE2	1:I:828:LEU:HD21	1.68	0.56
1:I:790:TYR:OH	1:I:828:LEU:CG	2.52	0.56
4:D:10:G:N2	4:D:26:G:H1	2.04	0.56
1:I:99:PHE:HE2	1:I:199:LEU:HD23	1.70	0.56
1:E:445:ALA:O	1:E:784:ARG:NH1	2.38	0.56
1:I:792:SER:O	1:I:795:VAL:HG13	2.05	0.56
1:A:611:ARG:NH2	1:A:620:SER:O	2.39	0.56
1:E:246:LEU:HD12	1:E:253:LEU:N	2.21	0.56
1:E:468:LEU:O	1:E:471:ILE:HD13	2.05	0.56
4:H:27:G:C4	4:H:28:U:C6	2.94	0.56
1:A:560:ARG:NH2	4:D:15:C:O2	2.39	0.56
4:D:16:G:H1'	4:D:19:A:H61	1.70	0.56
1:I:350:VAL:O	1:I:358:LEU:N	2.35	0.56
4:L:17:C:H5'	4:L:18:U:C5	2.40	0.56
1:A:569:ASP:OD1	1:A:572:ARG:NH2	2.38	0.56
1:E:105:LEU:HD11	1:E:177:LYS:HD2	1.88	0.56
1:E:306:LYS:O	1:E:310:ARG:HG3	2.06	0.56
4:H:28:U:O2	4:H:28:U:H2'	2.06	0.56
1:A:66:GLU:HA	1:A:69:LEU:HB2	1.88	0.55
1:E:660:LEU:HB2	1:E:679:PRO:HG3	1.88	0.55
1:E:48:ALA:HB1	1:E:55:ALA:HB1	1.88	0.55
1:E:106:ARG:O	1:E:173:ARG:NH2	2.38	0.55
1:E:779:GLY:HA3	3:G:15:DT:O3'	2.06	0.55
4:H:41:C:H2'	4:H:42:A:O4'	2.05	0.55
1:I:112:SER:O	1:I:116:ARG:HG3	2.06	0.55
1:E:71:LEU:HB3	1:E:74:ALA:HB3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:27:G:C5	4:H:28:U:C5	2.95	0.55
1:E:56:THR:C	1:E:57:TYR:HD1	2.14	0.55
4:H:39:U:H2'	4:H:40:G:C8	2.42	0.55
1:A:225:LYS:HE3	1:A:311:LEU:HD21	1.87	0.55
1:A:709:ASN:OD1	1:A:711:ILE:N	2.36	0.55
1:E:94:SER:OG	1:E:173:ARG:O	2.25	0.55
1:E:313:LYS:HB2	1:E:313:LYS:HZ2	1.70	0.55
1:E:796:ARG:HD2	1:E:811:ARG:HB3	1.89	0.55
1:I:229:ALA:HA	1:I:232:LEU:HG	1.88	0.55
1:E:471:ILE:HB	1:E:505:THR:OG1	2.07	0.55
1:E:646:VAL:HG22	1:E:690:LEU:HD23	1.88	0.55
2:F:9:DT:H2'	2:F:10:DC:C6	2.42	0.55
1:I:78:ALA:O	1:I:82:LEU:N	2.33	0.55
1:A:21:PHE:CD1	1:A:21:PHE:C	2.85	0.55
4:D:52:A:H2'	4:D:53:G:C8	2.42	0.55
1:A:295:TRP:CE3	1:A:296:ARG:HB2	2.42	0.55
1:A:737:MET:HE1	1:A:856:LEU:HD21	1.87	0.55
4:D:5:U:H2'	4:D:6:G:C8	2.41	0.55
2:F:5:DT:H3	4:H:52:A:H2	1.54	0.55
1:A:611:ARG:NH1	4:D:49:C:O2'	2.40	0.54
1:E:57:TYR:CD1	1:E:57:TYR:N	2.73	0.54
1:E:97:SER:HB2	1:E:103:PHE:CD1	2.42	0.54
2:F:7:DG:H2'	2:F:8:DG:C8	2.42	0.54
1:I:277:ILE:HD11	4:L:54:C:H4'	1.90	0.54
1:I:701:ALA:HB3	1:I:750:ARG:HD3	1.88	0.54
1:I:772:GLU:O	1:I:774:LYS:HD2	2.06	0.54
1:A:173:ARG:NH1	3:C:8:DG:OP2	2.41	0.54
1:A:348:VAL:O	1:A:360:CYS:HB2	2.07	0.54
1:A:441:PHE:HE2	1:A:455:LEU:HD11	1.72	0.54
1:E:628:THR:O	1:E:632:SER:HB2	2.06	0.54
4:H:27:G:H22	4:H:28:U:H1'	1.54	0.54
1:I:8:ARG:NH2	1:I:688:GLN:OE1	2.40	0.54
1:I:771:ASP:C	1:I:774:LYS:HD3	2.31	0.54
1:A:310:ARG:HH21	1:A:314:ARG:HD2	1.72	0.54
4:H:6:G:C6	4:H:29:C:N4	2.74	0.54
4:L:45:C:H2'	4:L:46:A:O4'	2.08	0.54
1:A:242:PHE:O	1:A:246:LEU:HG	2.07	0.54
1:I:381:LYS:HE2	1:I:402:TRP:CZ3	2.43	0.54
1:I:471:ILE:HD11	1:I:590:ALA:HB2	1.89	0.54
1:A:441:PHE:CE2	1:A:455:LEU:HD11	2.42	0.54
1:A:799:VAL:HG23	1:A:816:LEU:HD22	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:SER:OG	1:E:94:SER:O	2.26	0.54
1:E:224:MET:SD	1:E:314:ARG:NH1	2.81	0.54
1:E:339:PHE:C	1:E:339:PHE:CD2	2.85	0.54
1:I:51:GLU:CG	1:I:54:GLY:CA	2.86	0.54
1:A:17:TYR:C	1:A:17:TYR:CD2	2.85	0.54
1:A:293:ALA:HB3	1:A:298:LEU:HD11	1.88	0.54
4:D:16:G:O2'	4:D:19:A:N1	2.41	0.54
1:E:302:TYR:C	1:E:302:TYR:CD2	2.85	0.54
4:D:36:C:O2'	4:D:38:C:OP1	2.26	0.54
4:H:13:C:H2'	4:H:14:U:C6	2.43	0.54
1:A:635:ASP:OD1	1:A:638:ARG:NH1	2.41	0.54
1:E:298:LEU:O	1:E:301:ALA:N	2.41	0.54
1:E:532:LYS:NZ	4:H:50:C:H5''	2.23	0.54
1:E:816:LEU:HD13	1:E:821:LEU:HD21	1.90	0.54
1:I:373:LYS:HD2	1:I:378:TYR:HE1	1.72	0.54
4:D:41:C:H2'	4:D:42:A:O4'	2.09	0.53
1:E:51:GLU:HB2	1:E:54:GLY:O	2.08	0.53
1:E:239:VAL:HG22	1:E:290:LEU:CD1	2.32	0.53
1:E:295:TRP:C	1:E:295:TRP:CD1	2.85	0.53
1:I:790:TYR:HB3	1:I:807:VAL:HG11	1.90	0.53
1:E:549:LEU:HB3	1:E:562:MET:HB3	1.90	0.53
4:H:46:A:H2'	4:H:47:G:C8	2.43	0.53
1:I:715:VAL:HB	1:I:824:HIS:CE1	2.43	0.53
1:E:155:TYR:HB3	1:E:159:GLU:HB2	1.91	0.53
4:H:21:A:H2'	4:H:22:G:C8	2.41	0.53
1:I:745:MET:O	1:I:749:CYS:N	2.37	0.53
1:A:187:CYS:SG	1:A:189:ARG:O	2.63	0.53
1:E:306:LYS:N	1:E:306:LYS:HD2	2.22	0.53
1:E:600:ASP:OD1	1:E:630:ARG:NE	2.37	0.53
1:I:27:ASP:HB3	1:I:195:TYR:OH	2.09	0.53
1:I:564:GLN:OE1	4:L:20:G:N2	2.41	0.53
1:I:574:LEU:HD21	1:I:599:MET:HG2	1.91	0.53
1:I:592:ALA:HA	1:I:595:LEU:HB3	1.90	0.53
4:L:52:A:H2'	4:L:53:G:C8	2.44	0.53
1:E:678:SER:CB	2:F:14:DT:H5''	2.36	0.53
1:I:613:HIS:CG	4:L:15:C:H4'	2.42	0.53
1:A:842:LYS:O	1:A:846:GLU:HG3	2.09	0.53
1:I:387:LYS:HB3	4:L:34:C:H42	1.73	0.53
1:I:789:ARG:CG	1:I:790:TYR:CD1	2.75	0.53
1:A:295:TRP:HE3	1:A:296:ARG:HB2	1.73	0.53
1:E:517:LEU:HD11	1:E:570:THR:HG23	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:829:VAL:HB	1:E:833:LEU:HD23	1.90	0.53
1:E:578:LYS:HE2	4:H:5:U:H5''	1.90	0.53
1:I:797:PHE:HD2	1:I:816:LEU:HB2	1.73	0.53
1:A:364:HIS:ND1	1:A:387:LYS:HG3	2.24	0.52
1:I:51:GLU:HG2	1:I:54:GLY:N	2.24	0.52
1:A:529:LYS:O	1:A:533:ALA:N	2.42	0.52
1:A:753:ASN:OD1	1:A:757:CYS:N	2.34	0.52
4:H:37:G:O2'	4:H:38:C:OP2	2.27	0.52
1:A:21:PHE:O	1:A:24:TRP:N	2.43	0.52
1:A:387:LYS:HB3	4:D:34:C:N4	2.24	0.52
1:I:132:GLU:HG3	1:I:136:GLN:HE22	1.74	0.52
1:I:566:ARG:O	1:I:570:THR:OG1	2.21	0.52
1:E:7:PRO:HB2	4:H:37:G:H1	1.74	0.52
1:E:111:TYR:HD1	1:E:116:ARG:HH21	1.57	0.52
1:E:246:LEU:CD1	1:E:253:LEU:N	2.73	0.52
3:G:10:DT:H2''	3:G:11:DC:OP2	2.08	0.52
4:H:52:A:H2'	4:H:53:G:C8	2.44	0.52
1:I:145:ALA:HA	1:I:148:TRP:HD1	1.75	0.52
1:A:13:LYS:HE3	1:A:419:VAL:HG11	1.90	0.52
1:A:71:LEU:HD22	1:A:183:LEU:HD11	1.90	0.52
1:E:178:GLN:O	1:E:182:ARG:HB2	2.09	0.52
1:E:525:LYS:HG2	1:E:605:LEU:HD13	1.92	0.52
1:I:678:SER:OG	1:I:681:THR:HB	2.09	0.52
1:E:119:ILE:HG22	1:E:157:PRO:HB3	1.91	0.52
1:E:622:LYS:HE2	1:E:622:LYS:HA	1.91	0.52
1:I:552:VAL:HG12	1:I:553:GLU:O	2.10	0.52
1:E:246:LEU:HD23	1:E:249:LYS:CB	2.39	0.52
1:E:246:LEU:C	1:E:249:LYS:HB2	2.35	0.52
1:A:8:ARG:HD2	4:D:37:G:H5''	1.92	0.52
1:A:15:LYS:CG	1:A:361:SER:OG	2.58	0.52
1:E:246:LEU:CD1	1:E:253:LEU:CA	2.85	0.52
1:E:246:LEU:CD2	1:E:249:LYS:CB	2.87	0.52
1:I:20:SER:O	1:I:20:SER:OG	2.15	0.52
2:B:7:DG:H1	4:D:50:C:H42	1.58	0.51
1:E:566:ARG:O	1:E:570:THR:OG1	2.19	0.51
4:H:27:G:N1	4:H:28:U:N3	2.58	0.51
1:E:43:ALA:HA	1:E:82:LEU:HD11	1.92	0.51
1:E:306:LYS:N	1:E:306:LYS:CD	2.74	0.51
1:E:511:CYS:SG	1:E:591:GLU:HA	2.51	0.51
1:I:8:ARG:HD3	4:L:37:G:H5''	1.92	0.51
1:I:643:HIS:CD2	4:L:35:A:H5'	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:TYR:HE1	1:A:102:ASP:HB2	1.75	0.51
1:A:279:VAL:HA	1:A:282:LEU:HB2	1.92	0.51
4:D:24:G:H2'	4:D:25:A:C8	2.44	0.51
1:E:311:LEU:HD23	1:E:311:LEU:O	2.11	0.51
1:I:549:LEU:HB3	1:I:562:MET:HB3	1.91	0.51
1:I:722:ASN:OD1	1:I:724:SER:OG	2.19	0.51
1:A:302:TYR:CE1	1:A:306:LYS:HD2	2.45	0.51
1:A:639:ARG:O	4:D:35:A:O2'	2.27	0.51
2:F:21:DC:H2''	2:F:22:DA:C8	2.46	0.51
1:A:192:ASP:OD2	1:A:355:HIS:NE2	2.44	0.51
1:E:242:PHE:C	1:E:242:PHE:CD2	2.86	0.51
1:E:619:GLN:HE21	2:F:8:DG:H21	1.58	0.51
4:H:49:C:H2'	4:H:50:C:C6	2.45	0.51
1:I:634:ARG:HE	1:I:638:ARG:NH1	1.95	0.51
1:A:259:TRP:CE2	1:A:263:LYS:HD2	2.45	0.51
1:I:51:GLU:HG2	1:I:54:GLY:H	1.76	0.51
1:I:790:TYR:CZ	1:I:828:LEU:HG	2.46	0.51
1:A:476:LYS:NZ	1:A:651:ASP:OD2	2.41	0.51
1:I:96:TYR:OH	3:K:6:DA:OP2	2.29	0.51
1:I:568:ALA:HB2	4:L:21:A:H5''	1.91	0.51
1:A:614:LEU:HD22	1:A:618:GLU:HG3	1.93	0.51
1:E:727:TYR:CD2	1:E:845:VAL:HG21	2.46	0.51
1:I:370:THR:OG1	1:I:381:LYS:HB3	2.10	0.51
1:A:850:LEU:CD1	1:E:420:PHE:HB2	2.40	0.50
1:E:588:ASP:OD1	1:E:591:GLU:N	2.41	0.50
1:E:50:ARG:NH1	1:E:50:ARG:HG3	2.26	0.50
1:I:750:ARG:HG3	1:I:867:PHE:CD1	2.47	0.50
1:A:611:ARG:HD3	4:D:49:C:O2'	2.11	0.50
1:E:10:GLN:HG2	1:E:365:TYR:CD1	2.46	0.50
1:A:48:ALA:HB1	1:A:55:ALA:HB1	1.93	0.50
1:I:611:ARG:NH1	4:L:50:C:O4'	2.45	0.50
1:A:715:VAL:HB	1:A:824:HIS:NE2	2.27	0.50
1:I:253:LEU:HD23	1:I:305:TRP:CE3	2.47	0.50
1:I:476:LYS:O	1:I:498:ILE:HG22	2.11	0.50
1:E:790:TYR:CD1	1:E:807:VAL:HB	2.47	0.50
4:H:45:C:H2'	4:H:46:A:O4'	2.11	0.50
1:I:110:LYS:HB3	3:K:8:DG:H5'	1.94	0.50
1:I:823:TYR:HD2	1:I:828:LEU:HD23	1.77	0.50
1:E:239:VAL:CA	1:E:290:LEU:HD11	2.42	0.50
1:E:365:TYR:HD1	1:E:366:PHE:CD2	2.30	0.50
1:E:611:ARG:HH22	1:E:619:GLN:CD	2.19	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:100:TYR:HD2	1:I:196:CYS:SG	2.34	0.50
1:I:363:SER:O	1:I:366:PHE:O	2.29	0.50
1:I:442:PHE:HA	1:I:754:HIS:CE1	2.47	0.50
1:I:517:LEU:HD13	1:I:573:ARG:HD3	1.93	0.50
1:E:680:ARG:HB3	2:F:15:DT:OP2	2.12	0.50
2:F:2:DG:H1	4:H:55:C:N4	1.98	0.50
1:I:634:ARG:NH2	2:J:13:DT:O5'	2.45	0.50
1:A:830:THR:OG1	1:A:831:HIS:N	2.44	0.50
1:A:546:THR:HA	1:A:549:LEU:HD12	1.94	0.49
1:E:50:ARG:CG	1:E:50:ARG:NH1	2.73	0.49
1:E:738:ASP:HB3	1:E:741:GLU:HB2	1.94	0.49
1:E:750:ARG:O	1:E:755:SER:N	2.39	0.49
1:I:789:ARG:HB2	1:I:869:HIS:HB2	1.94	0.49
1:E:607:GLU:O	1:E:611:ARG:HD2	2.11	0.49
1:E:796:ARG:HD3	1:E:812:PRO:O	2.13	0.49
4:H:22:G:H2'	4:H:23:G:O4'	2.12	0.49
4:H:26:G:N1	4:H:27:G:C5	2.80	0.49
1:I:51:GLU:HG3	1:I:54:GLY:HA3	1.93	0.49
1:I:264:GLN:OE1	1:I:273:THR:OG1	2.30	0.49
1:E:302:TYR:CE2	1:E:306:LYS:NZ	2.73	0.49
4:L:6:G:H22	4:L:30:A:H1'	1.76	0.49
4:D:7:G:N2	4:D:29:C:H1'	2.28	0.49
4:D:21:A:H2'	4:D:22:G:H8	1.78	0.49
1:I:442:PHE:HB3	1:I:698:VAL:HG11	1.94	0.49
1:A:209:SER:OG	2:B:17:DC:O2	2.24	0.49
1:I:265:ALA:HB2	1:I:279:VAL:HG13	1.95	0.49
1:I:775:GLU:OE1	1:I:775:GLU:HA	2.12	0.49
1:A:687:ARG:O	1:A:691:GLU:HG3	2.12	0.49
1:E:333:LEU:HD13	1:E:376:SER:O	2.11	0.49
1:E:521:ILE:O	1:E:525:LYS:HG3	2.13	0.49
1:I:436:GLN:O	1:I:440:ARG:HB2	2.12	0.49
1:I:476:LYS:HG3	1:I:498:ILE:HG22	1.95	0.49
1:A:204:ALA:O	1:A:208:ARG:HG3	2.13	0.49
1:A:642:ALA:O	1:A:646:VAL:HG23	2.12	0.49
1:I:764:LYS:N	1:I:778:TYR:OH	2.40	0.49
1:I:790:TYR:HE2	1:I:828:LEU:CD2	2.26	0.49
1:A:205:ARG:CZ	2:B:19:DG:H4'	2.42	0.49
1:A:381:LYS:HG2	1:A:402:TRP:CE3	2.48	0.49
1:A:596:LEU:HD22	1:A:637:LEU:HD12	1.95	0.49
1:E:57:TYR:HD1	1:E:57:TYR:N	2.10	0.49
1:I:67:ARG:CZ	1:I:79:ILE:HD11	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:719:ASN:OD1	1:I:722:ASN:N	2.43	0.49
1:A:21:PHE:O	1:A:24:TRP:HB3	2.13	0.49
1:A:850:LEU:HD21	1:E:14:ILE:O	2.13	0.49
4:H:6:G:H1	4:H:29:C:H42	0.58	0.49
1:I:29:GLN:HE22	1:I:327:TYR:N	2.11	0.49
1:I:327:TYR:HD2	4:L:40:G:H1'	1.78	0.49
1:A:578:LYS:HE2	4:D:5:U:H5''	1.95	0.49
1:A:737:MET:HE2	1:A:742:VAL:HG22	1.93	0.49
1:E:411:THR:HG23	1:E:425:PRO:HD3	1.94	0.48
1:I:16:GLN:O	1:I:359:PHE:N	2.45	0.48
1:I:177:LYS:HG3	1:I:180:ARG:NH2	2.28	0.48
1:I:408:ARG:HB2	2:J:21:DC:OP2	2.13	0.48
1:I:586:TYR:C	1:I:640:ARG:HH12	2.21	0.48
1:A:517:LEU:HD11	1:A:570:THR:HG23	1.95	0.48
1:E:532:LYS:HZ3	4:H:50:C:H5''	1.77	0.48
1:E:749:CYS:SG	1:E:750:ARG:N	2.86	0.48
1:E:110:LYS:HG3	2:F:24:DC:H4'	1.94	0.48
1:E:220:GLN:HA	1:E:223:GLU:HB2	1.96	0.48
1:I:61:SER:HA	1:I:64:LEU:HB2	1.96	0.48
1:I:778:TYR:CB	1:I:782:VAL:CB	2.81	0.48
1:A:705:THR:HG21	1:A:747:ILE:CG1	2.41	0.48
1:E:97:SER:HB2	1:E:103:PHE:CG	2.48	0.48
1:E:137:ASP:HB3	1:E:140:LEU:HB2	1.95	0.48
1:I:475:VAL:HG12	1:I:500:GLY:HA3	1.94	0.48
4:L:7:G:N2	4:L:29:C:H1'	2.28	0.48
1:A:552:VAL:HG11	1:A:565:SER:HB3	1.94	0.48
1:E:534:CYS:SG	1:E:539:LEU:HB2	2.53	0.48
1:I:110:LYS:NZ	3:K:8:DG:N3	2.60	0.48
1:A:30:GLU:OE2	1:A:188:ARG:NH2	2.47	0.48
4:D:45:C:H2'	4:D:46:A:O4'	2.12	0.48
1:I:173:ARG:NE	3:K:7:DT:H5'	2.29	0.48
1:A:369:LEU:HA	1:A:382:PHE:HB3	1.96	0.48
1:E:249:LYS:O	1:E:250:ASN:HB2	2.14	0.48
1:E:701:ALA:HB2	1:E:781:ARG:HH12	1.78	0.48
1:I:12:LEU:HD11	1:I:348:VAL:HG21	1.96	0.48
1:I:80:LYS:O	1:I:84:VAL:HG23	2.13	0.48
1:I:251:TYR:HD1	1:I:252:GLY:H	1.60	0.48
1:A:442:PHE:HE1	1:A:752:LEU:HD23	1.79	0.48
1:A:452:ILE:O	1:A:455:LEU:HG	2.13	0.48
3:C:10:DT:H2''	3:C:11:DC:OP2	2.14	0.48
1:E:841:ILE:O	1:E:845:VAL:HG23	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:849:VAL:HG12	1:E:850:LEU:H	1.79	0.48
1:I:639:ARG:NH1	4:L:37:G:OP1	2.47	0.48
1:I:680:ARG:HB3	2:J:15:DT:OP2	2.12	0.48
4:L:37:G:O2'	4:L:38:C:OP2	2.29	0.48
1:E:225:LYS:HG3	1:E:311:LEU:HD11	1.96	0.48
1:E:611:ARG:HH22	1:E:619:GLN:NE2	2.12	0.48
1:E:619:GLN:HE21	2:F:8:DG:N2	2.12	0.48
1:E:726:ILE:O	1:E:736:VAL:HA	2.13	0.48
1:I:443:SER:O	1:I:781:ARG:NH2	2.36	0.48
1:I:670:ASN:O	1:I:675:LYS:NZ	2.34	0.48
1:I:762:VAL:HA	1:I:819:LYS:O	2.14	0.48
1:A:67:ARG:HG2	1:A:75:GLU:OE1	2.14	0.47
1:I:516:SER:HA	1:I:519:ARG:HB3	1.95	0.47
1:A:100:TYR:CE1	1:A:102:ASP:HB2	2.49	0.47
1:I:327:TYR:CD2	4:L:40:G:H1'	2.49	0.47
1:I:531:PHE:HE2	4:L:17:C:H41	1.62	0.47
1:A:77:VAL:HG13	1:A:175:LEU:HD22	1.95	0.47
1:E:12:LEU:N	1:E:422:LEU:O	2.48	0.47
1:A:17:TYR:CZ	1:A:22:VAL:HG21	2.49	0.47
1:E:224:MET:HE1	1:E:310:ARG:HH21	1.79	0.47
1:E:456:PRO:HB3	1:I:76:ASP:OD2	2.14	0.47
1:I:165:ALA:HB3	1:I:166:PRO:HD3	1.97	0.47
1:I:235:GLU:O	1:I:239:VAL:HG23	2.14	0.47
1:I:328:GLN:HE21	1:I:411:THR:HG21	1.79	0.47
1:I:510:ARG:O	1:I:514:LEU:N	2.48	0.47
1:I:659:ASP:OD1	1:I:661:ASP:HB2	2.15	0.47
1:A:386:LEU:HG	1:A:387:LYS:H	1.79	0.47
1:A:660:LEU:HD22	1:A:673:LEU:HD23	1.97	0.47
4:D:34:C:P	4:D:34:C:H6	2.37	0.47
1:I:90:ALA:N	1:I:91:PRO:HD2	2.29	0.47
1:I:605:LEU:O	1:I:609:TYR:N	2.47	0.47
1:E:309:LYS:CE	1:E:309:LYS:CA	2.86	0.47
1:I:771:ASP:HB2	1:I:774:LYS:CE	2.36	0.47
1:A:32:ARG:HD2	1:A:206:GLN:OE1	2.15	0.47
1:A:507:ASP:HA	1:A:590:ALA:HB1	1.95	0.47
1:E:137:ASP:CG	1:E:140:LEU:HD23	2.40	0.47
1:E:441:PHE:HD2	1:E:447:PRO:HB3	1.79	0.47
1:E:463:ALA:HB2	1:E:656:PHE:HB2	1.95	0.47
1:E:507:ASP:OD1	1:E:590:ALA:HB1	2.13	0.47
1:E:619:GLN:NE2	2:F:9:DT:H1'	2.29	0.47
4:L:43:A:H2'	4:L:44:A:C8	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:LYS:HA	1:A:403:ILE:O	2.15	0.47
1:A:624:ALA:HB2	2:B:11:DT:OP1	2.15	0.47
2:F:6:DT:H2'	2:F:7:DG:C8	2.49	0.47
1:I:387:LYS:NZ	4:L:1:G:OP2	2.45	0.47
1:A:27:ASP:HB3	1:A:195:TYR:OH	2.15	0.47
1:E:238:LEU:HB2	1:E:290:LEU:HG	1.95	0.47
4:L:18:U:H5'	4:L:19:A:C2	2.49	0.47
1:A:738:ASP:OD1	1:A:741:GLU:N	2.44	0.47
1:E:299:LYS:C	1:E:299:LYS:CD	2.86	0.47
1:I:112:SER:O	1:I:116:ARG:N	2.48	0.47
1:I:126:PRO:O	1:I:130:ILE:HG13	2.14	0.47
1:I:624:ALA:HB3	2:J:11:DT:H5'	1.97	0.47
1:A:257:VAL:HG13	1:A:275:ILE:HG21	1.96	0.46
1:I:116:ARG:NH1	2:J:24:DC:OP1	2.45	0.46
1:A:680:ARG:HB3	2:B:15:DT:OP2	2.16	0.46
1:E:255:TRP:N	1:E:255:TRP:HD1	2.12	0.46
1:E:629:LYS:HA	4:H:4:C:H5''	1.97	0.46
1:E:646:VAL:HG12	1:E:693:ARG:HH11	1.81	0.46
1:E:679:PRO:O	1:E:683:LEU:N	2.36	0.46
1:I:173:ARG:CZ	3:K:7:DT:H5'	2.45	0.46
1:I:339:PHE:HA	1:I:351:ASP:O	2.16	0.46
1:A:441:PHE:CD1	1:A:441:PHE:O	2.69	0.46
1:E:117:GLU:HB3	1:I:191:HIS:CD2	2.50	0.46
1:E:757:CYS:SG	1:E:867:PHE:HA	2.56	0.46
1:I:51:GLU:CG	1:I:54:GLY:C	2.88	0.46
1:I:660:LEU:HA	1:I:702:LYS:HD3	1.97	0.46
1:I:789:ARG:HD3	1:I:869:HIS:HB2	1.96	0.46
1:A:10:GLN:HG2	1:A:365:TYR:CD1	2.50	0.46
1:E:117:GLU:HB3	1:I:191:HIS:NE2	2.31	0.46
1:E:490:LEU:O	1:E:491:ASP:HB2	2.14	0.46
1:I:51:GLU:CG	1:I:54:GLY:HA3	2.45	0.46
1:I:606:LEU:HA	1:I:609:TYR:HB3	1.97	0.46
1:I:736:VAL:HG13	1:I:853:ARG:HA	1.97	0.46
1:I:790:TYR:HE2	1:I:828:LEU:CG	2.26	0.46
1:E:116:ARG:O	1:E:120:GLU:HG3	2.16	0.46
1:I:50:ARG:NH2	4:L:42:A:OP1	2.49	0.46
1:I:51:GLU:H	1:I:51:GLU:CD	2.22	0.46
1:I:96:TYR:HA	1:I:200:MET:HG2	1.96	0.46
1:I:688:GLN:NE2	4:L:37:G:N7	2.64	0.46
1:I:805:VAL:HG23	1:I:830:THR:CG2	2.43	0.46
1:A:705:THR:HG22	1:A:746:ASN:HB2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:LEU:O	1:A:837:MET:N	2.43	0.46
1:E:105:LEU:HD11	1:E:177:LYS:CD	2.45	0.46
1:E:302:TYR:O	1:E:306:LYS:HD3	2.15	0.46
1:E:664:SER:HB3	1:E:702:LYS:CE	2.42	0.46
1:I:50:ARG:O	1:I:50:ARG:HG2	2.16	0.46
1:I:773:LYS:O	1:I:774:LYS:C	2.57	0.46
1:I:333:LEU:HG	1:I:339:PHE:CE1	2.51	0.46
1:I:703:ASP:HB2	1:I:750:ARG:HH12	1.81	0.46
1:A:18:GLU:HB3	1:A:357:LYS:O	2.16	0.46
1:A:164:VAL:O	1:A:168:ILE:HG12	2.16	0.46
1:A:601:SER:HA	1:A:604:SER:HB3	1.97	0.46
1:E:460:VAL:HB	1:E:652:CYS:HA	1.97	0.46
1:A:42:TRP:CD1	1:A:42:TRP:N	2.84	0.46
1:I:611:ARG:HD3	4:L:49:C:O2'	2.15	0.46
1:I:790:TYR:CE2	1:I:828:LEU:CD2	2.98	0.46
1:A:21:PHE:CD1	1:A:22:VAL:N	2.84	0.46
1:I:29:GLN:HE22	1:I:327:TYR:H	1.63	0.46
1:I:111:TYR:CE2	1:I:119:ILE:HD12	2.51	0.46
1:I:113:GLY:N	1:I:116:ARG:HE	2.14	0.46
1:E:726:ILE:HD13	1:E:742:VAL:HG21	1.98	0.45
1:I:716:GLY:HA3	1:I:727:TYR:O	2.16	0.45
1:A:810:LYS:HE3	1:A:810:LYS:HB2	1.74	0.45
1:I:239:VAL:O	1:I:242:PHE:HB3	2.15	0.45
1:I:632:SER:HB3	4:L:3:G:O2'	2.16	0.45
1:I:712:SER:OG	1:I:730:GLU:OE1	2.28	0.45
1:A:303:ASP:O	1:A:307:LEU:N	2.49	0.45
1:E:370:THR:OG1	1:E:381:LYS:HB3	2.16	0.45
1:E:638:ARG:CG	1:E:677:LEU:HD22	2.46	0.45
1:E:687:ARG:O	1:E:691:GLU:HG3	2.16	0.45
1:A:167:ARG:HE	1:A:167:ARG:HB3	1.57	0.45
1:A:310:ARG:NH1	4:D:44:A:H4'	2.31	0.45
4:D:53:G:O5'	4:D:53:G:H8	1.99	0.45
1:E:333:LEU:CD1	1:E:408:ARG:HA	2.46	0.45
1:I:810:LYS:H	1:I:810:LYS:HG2	1.63	0.45
2:J:25:DG:H22	3:K:4:DC:H42	1.63	0.45
1:A:463:ALA:O	1:A:474:PRO:HA	2.15	0.45
1:E:441:PHE:CE2	1:E:447:PRO:HG3	2.51	0.45
1:E:672:ALA:O	1:E:676:LEU:N	2.44	0.45
1:I:40:PHE:CE2	1:I:320:MET:HG3	2.52	0.45
1:I:213:THR:OG1	2:J:16:DG:N2	2.49	0.45
1:I:773:LYS:O	1:I:774:LYS:O	2.33	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ASP:O	1:A:524:ILE:HG13	2.17	0.45
1:I:626:PHE:CD1	1:I:628:THR:HG22	2.51	0.45
1:E:389:ARG:NH2	4:H:3:G:O6	2.43	0.45
1:I:39:LEU:HD23	1:I:39:LEU:HA	1.85	0.45
1:I:790:TYR:OH	1:I:828:LEU:CD2	2.65	0.45
1:A:362:HIS:NE2	4:D:0:G:OP3	2.46	0.45
1:A:459:MET:HG3	1:A:479:ILE:HD11	1.99	0.45
1:E:245:VAL:O	1:E:249:LYS:HD2	2.16	0.45
1:E:477:ALA:HA	1:E:498:ILE:HG13	1.99	0.45
1:E:602:TYR:CZ	1:E:606:LEU:HD21	2.51	0.45
1:A:14:ILE:HD13	1:A:358:LEU:HD22	1.99	0.45
1:A:282:LEU:HB3	1:A:291:LEU:HD21	1.97	0.45
1:E:55:ALA:O	1:E:57:TYR:CE1	2.70	0.45
1:A:257:VAL:HG13	1:A:275:ILE:CG2	2.47	0.45
1:A:686:ILE:O	1:A:690:LEU:HD23	2.17	0.45
1:E:583:LYS:HG3	4:H:31:G:O2'	2.17	0.45
2:F:19:DG:H1	4:H:38:C:H42	1.63	0.45
1:I:194:GLY:O	1:I:198:ILE:HG13	2.17	0.45
1:A:441:PHE:O	1:A:754:HIS:HD2	1.98	0.44
1:A:683:LEU:HD23	1:A:697:MET:HE3	1.98	0.44
4:H:26:G:N1	4:H:27:G:N7	2.63	0.44
1:I:49:ALA:HB2	1:I:56:THR:OG1	2.17	0.44
1:I:678:SER:HB3	2:J:14:DT:OP2	2.17	0.44
1:A:267:LYS:O	1:A:268:GLU:C	2.61	0.44
1:A:474:PRO:HD2	1:A:502:LYS:O	2.17	0.44
1:E:330:PRO:HA	1:E:411:THR:HA	1.99	0.44
1:I:377:ARG:HD2	1:I:406:ALA:HB1	1.98	0.44
1:E:578:LYS:HE3	1:E:599:MET:SD	2.57	0.44
4:H:26:G:C4	4:H:27:G:N7	2.84	0.44
1:I:349:VAL:HG22	1:I:359:PHE:HD1	1.82	0.44
1:I:549:LEU:HD22	1:I:563:ILE:HA	1.99	0.44
1:A:17:TYR:CD2	1:A:17:TYR:O	2.70	0.44
1:A:251:TYR:HE2	4:D:54:C:H1'	1.82	0.44
1:A:492:TYR:O	1:A:492:TYR:CD2	2.65	0.44
1:E:31:ASP:HB3	1:E:199:LEU:HD21	1.99	0.44
1:E:47:TYR:HA	1:E:317:PHE:HB3	1.99	0.44
4:H:29:C:H2'	4:H:30:A:O5'	2.17	0.44
1:I:13:LYS:O	1:I:361:SER:OG	2.16	0.44
1:I:363:SER:HA	4:L:1:G:C8	2.52	0.44
1:I:611:ARG:NH1	4:L:49:C:O2'	2.50	0.44
1:I:717:TRP:CE2	1:I:842:LYS:HG3	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ARG:HB2	1:A:426:TYR:CZ	2.52	0.44
1:A:12:LEU:HD23	1:A:12:LEU:HA	1.74	0.44
1:A:262:VAL:HG13	1:A:291:LEU:HB3	1.99	0.44
1:A:466:LEU:HD12	1:A:466:LEU:O	2.18	0.44
1:A:613:HIS:CB	4:D:15:C:H4'	2.47	0.44
1:E:242:PHE:CD2	1:E:242:PHE:O	2.70	0.44
1:E:763:THR:HG1	1:E:819:LYS:H	1.62	0.44
1:E:823:TYR:C	1:E:824:HIS:HD1	2.26	0.44
1:I:55:ALA:C	1:I:56:THR:CG2	2.91	0.44
1:I:728:PHE:HB2	1:I:735:LEU:HB2	1.99	0.44
1:E:31:ASP:OD2	1:E:187:CYS:HB2	2.18	0.44
1:E:95:CYS:C	1:E:200:MET:HG2	2.43	0.44
1:E:366:PHE:HE1	1:E:424:LEU:HD12	1.82	0.44
1:E:588:ASP:HB3	1:E:591:GLU:HB2	1.99	0.44
1:I:100:TYR:O	1:I:180:ARG:NH1	2.51	0.44
1:I:790:TYR:OH	1:I:823:TYR:HE2	2.00	0.44
3:C:4:DC:H2''	3:C:5:DG:H8	1.82	0.44
1:E:333:LEU:CD1	1:E:376:SER:O	2.66	0.44
1:A:501:PRO:HG3	1:A:745:MET:SD	2.58	0.44
1:A:532:LYS:HD2	1:A:612:MET:HA	2.00	0.44
1:A:678:SER:HA	2:B:14:DT:OP1	2.17	0.44
1:A:737:MET:CE	1:A:856:LEU:HD11	2.47	0.44
1:E:165:ALA:HB3	1:E:166:PRO:HD3	2.00	0.44
1:E:180:ARG:HA	1:E:185:ILE:HD12	2.00	0.44
1:E:589:LEU:HD21	1:E:640:ARG:CG	2.46	0.44
4:L:5:U:H2'	4:L:6:G:C8	2.52	0.44
1:A:358:LEU:O	1:A:359:PHE:CD1	2.70	0.44
4:D:6:G:H22	4:D:30:A:H1'	1.82	0.44
1:E:457:SER:O	1:E:480:GLY:HA2	2.17	0.44
1:I:462:GLY:HA3	1:I:649:PHE:CE1	2.53	0.44
1:A:296:ARG:HH22	1:A:762:VAL:CG2	2.31	0.43
1:A:619:GLN:HG2	4:D:50:C:H1'	2.00	0.43
4:D:35:A:H2'	4:D:36:C:O4'	2.18	0.43
1:A:79:ILE:HD12	1:A:79:ILE:C	2.35	0.43
1:A:588:ASP:OD1	1:A:591:GLU:N	2.47	0.43
1:E:78:ALA:O	1:E:82:LEU:HG	2.18	0.43
1:E:350:VAL:HB	1:E:358:LEU:HB2	1.99	0.43
1:E:842:LYS:O	1:E:846:GLU:HG3	2.18	0.43
1:I:93:SER:O	1:I:96:TYR:HD1	2.02	0.43
1:I:387:LYS:HB3	4:L:34:C:N4	2.33	0.43
1:I:658:GLU:HB2	1:I:747:ILE:HD13	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:TRP:HB2	1:A:302:TYR:CZ	2.54	0.43
1:A:475:VAL:HB	1:A:501:PRO:HB3	2.00	0.43
2:B:11:DT:H2''	2:B:12:DG:O5'	2.18	0.43
1:E:209:SER:O	1:E:213:THR:OG1	2.29	0.43
1:E:282:LEU:O	1:E:291:LEU:HD21	2.18	0.43
1:I:236:PHE:HA	1:I:239:VAL:HB	2.01	0.43
4:L:25:A:H2'	4:L:26:G:O4'	2.18	0.43
4:L:49:C:H2'	4:L:50:C:C6	2.52	0.43
1:A:304:THR:O	1:A:308:LYS:N	2.42	0.43
1:A:524:ILE:HG12	1:A:548:TRP:HH2	1.83	0.43
4:D:40:G:O5'	4:D:40:G:H8	2.02	0.43
1:E:95:CYS:O	1:E:200:MET:HE3	2.18	0.43
1:E:239:VAL:HG23	1:E:290:LEU:HD21	2.01	0.43
1:E:304:THR:O	1:E:307:LEU:HB3	2.17	0.43
1:A:407:LEU:HD21	1:A:424:LEU:HD22	2.01	0.43
4:H:26:G:C2	4:H:27:G:C8	3.02	0.43
1:I:170:ASN:O	1:I:173:ARG:HG3	2.18	0.43
1:I:530:GLU:HA	2:J:1:DA:OP1	2.18	0.43
4:L:21:A:H2'	4:L:22:G:H8	1.83	0.43
1:A:441:PHE:C	1:A:441:PHE:HD1	2.23	0.43
1:E:295:TRP:CD1	1:E:295:TRP:O	2.71	0.43
1:I:354:GLU:OE2	1:I:354:GLU:N	2.51	0.43
1:I:462:GLY:HA3	1:I:649:PHE:HE1	1.84	0.43
1:E:235:GLU:HG2	1:E:298:LEU:HD11	2.00	0.43
1:E:413:GLN:OE1	4:H:39:U:H4'	2.18	0.43
1:I:600:ASP:OD2	1:I:630:ARG:NH2	2.51	0.43
1:A:16:GLN:NE2	1:A:359:PHE:HD2	2.10	0.43
1:A:90:ALA:O	1:A:92:SER:O	2.36	0.43
1:E:246:LEU:HD22	1:E:249:LYS:HB3	2.01	0.43
1:I:100:TYR:CE2	1:I:193:ALA:HA	2.53	0.43
1:A:220:GLN:HB3	1:A:314:ARG:HH12	1.83	0.43
1:A:637:LEU:O	1:A:641:VAL:HG23	2.19	0.43
2:B:14:DT:H2''	2:B:15:DT:O5'	2.17	0.43
1:E:366:PHE:CE1	1:E:424:LEU:HD12	2.54	0.43
1:I:823:TYR:CD2	1:I:828:LEU:HD23	2.53	0.43
1:A:14:ILE:HG21	1:A:358:LEU:CD2	2.44	0.43
1:A:228:VAL:HA	1:A:304:THR:HG23	2.01	0.43
1:A:833:LEU:O	1:A:837:MET:HG3	2.18	0.43
1:E:282:LEU:O	1:E:291:LEU:HD11	2.19	0.43
1:E:410:ILE:HA	1:E:425:PRO:HD2	2.01	0.43
1:E:578:LYS:HD3	4:H:5:U:O3'	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:798:LEU:O	1:E:805:VAL:HA	2.19	0.43
1:E:827:GLU:OE1	1:E:827:GLU:N	2.52	0.43
2:F:11:DT:H3	4:H:47:G:H1	1.67	0.43
1:I:8:ARG:O	1:I:425:PRO:HA	2.19	0.43
1:I:586:TYR:O	1:I:640:ARG:NH1	2.52	0.43
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.88	0.42
1:A:841:ILE:O	1:A:845:VAL:HG23	2.19	0.42
1:I:43:ALA:HB2	1:I:82:LEU:HD13	2.00	0.42
1:I:302:TYR:OH	1:I:306:LYS:NZ	2.52	0.42
1:I:409:GLU:OE2	2:J:20:DC:H4'	2.18	0.42
1:E:678:SER:OG	1:E:681:THR:OG1	2.13	0.42
1:I:31:ASP:HB3	1:I:199:LEU:HD21	1.99	0.42
1:I:115:LYS:HE3	1:I:115:LYS:HB2	1.74	0.42
1:I:710:PRO:HA	1:I:866:SER:HB3	2.01	0.42
4:L:13:C:H2'	4:L:14:U:C6	2.54	0.42
4:L:13:C:H2'	4:L:14:U:H6	1.84	0.42
1:A:40:PHE:HE1	1:A:320:MET:HG3	1.84	0.42
1:A:203:VAL:O	1:A:207:LEU:HG	2.19	0.42
1:A:355:HIS:ND1	1:A:355:HIS:N	2.67	0.42
1:E:249:LYS:NZ	1:E:281:GLN:CD	2.78	0.42
2:F:12:DG:H1	4:H:45:C:H42	1.68	0.42
2:F:18:DA:N6	4:H:40:G:O6	2.52	0.42
1:I:465:ASP:HB2	1:I:747:ILE:HD12	2.00	0.42
1:A:173:ARG:CZ	3:C:7:DT:H3'	2.49	0.42
1:A:358:LEU:O	1:A:359:PHE:HD1	2.03	0.42
1:A:629:LYS:HD3	4:D:5:U:OP1	2.19	0.42
1:E:797:PHE:O	1:E:815:ALA:HB1	2.19	0.42
1:E:840:GLU:O	1:E:844:LEU:HG	2.20	0.42
1:I:11:LEU:HD21	4:L:38:C:O2'	2.20	0.42
1:I:102:ASP:OD2	1:I:191:HIS:ND1	2.45	0.42
1:I:203:VAL:O	1:I:207:LEU:HG	2.19	0.42
1:I:643:HIS:NE2	4:L:35:A:H5'	2.34	0.42
4:L:3:G:H2'	4:L:4:C:C6	2.54	0.42
1:A:798:LEU:HD23	1:A:815:ALA:HB2	2.02	0.42
1:E:408:ARG:HD3	2:F:22:DA:OP1	2.20	0.42
1:E:629:LYS:O	1:E:633:PHE:N	2.52	0.42
1:E:715:VAL:HB	1:E:824:HIS:NE2	2.34	0.42
1:A:40:PHE:CD1	1:A:323:TRP:HH2	2.38	0.42
1:E:97:SER:OG	1:E:176:GLY:HA3	2.20	0.42
1:I:790:TYR:CG	1:I:807:VAL:HG21	2.48	0.42
2:J:7:DG:H2'	2:J:8:DG:C8	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ILE:HG22	1:A:140:LEU:HD13	2.02	0.42
1:E:246:LEU:HD22	1:E:249:LYS:CB	2.49	0.42
1:I:383:ARG:HD2	1:I:399:ILE:HG21	2.01	0.42
1:I:726:ILE:O	1:I:736:VAL:HA	2.20	0.42
1:A:96:TYR:HA	1:A:200:MET:HG2	2.01	0.42
1:A:463:ALA:HB2	1:A:656:PHE:HB2	2.01	0.42
1:E:706:SER:HB3	1:E:718:ARG:HH12	1.84	0.42
4:H:27:G:N1	4:H:28:U:C4	2.87	0.42
1:I:145:ALA:HA	1:I:148:TRP:CD1	2.54	0.42
1:I:274:LYS:HA	4:L:55:C:H1'	2.01	0.42
1:A:8:ARG:O	1:A:425:PRO:HA	2.20	0.42
1:A:274:LYS:HA	4:D:55:C:H1'	2.02	0.42
1:A:729:TYR:HB2	1:A:841:ILE:HG12	2.02	0.42
1:E:249:LYS:N	1:E:249:LYS:HD2	2.34	0.42
1:E:360:CYS:HB3	1:E:361:SER:H	1.62	0.42
1:I:25:TYR:CZ	1:I:29:GLN:HG3	2.55	0.42
1:I:25:TYR:OH	1:I:414:LYS:HB3	2.20	0.42
1:A:645:ILE:HD12	1:A:686:ILE:HD11	2.02	0.42
1:A:701:ALA:HB3	1:A:750:ARG:NH1	2.34	0.42
1:A:796:ARG:HD2	1:A:812:PRO:O	2.20	0.42
4:H:17:C:H5'	4:H:18:U:C5	2.54	0.42
1:I:682:LEU:HA	1:I:682:LEU:HD12	1.79	0.42
1:I:690:LEU:HD23	1:I:690:LEU:HA	1.84	0.42
1:I:843:TYR:OH	1:I:847:LYS:NZ	2.45	0.42
1:E:333:LEU:HD11	1:E:377:ARG:HA	2.02	0.41
1:E:715:VAL:HG21	1:E:834:HIS:CE1	2.55	0.41
2:F:19:DG:H1	4:H:38:C:N4	2.18	0.41
1:I:40:PHE:HE2	1:I:320:MET:HG3	1.85	0.41
1:I:177:LYS:HG3	1:I:180:ARG:HH22	1.84	0.41
1:E:816:LEU:HD23	1:E:816:LEU:HA	1.90	0.41
1:A:40:PHE:CE1	1:A:320:MET:HG3	2.55	0.41
1:A:787:LYS:HD3	1:A:787:LYS:C	2.45	0.41
1:E:99:PHE:N	1:E:99:PHE:CD1	2.88	0.41
1:E:617:GLY:H	4:H:51:A:C5'	2.33	0.41
1:E:736:VAL:C	1:E:737:MET:HG2	2.46	0.41
1:I:238:LEU:HB2	1:I:290:LEU:HD21	2.01	0.41
1:A:342:GLU:HG2	1:A:343:VAL:H	1.83	0.41
4:D:12:U:H2'	4:D:13:C:C6	2.55	0.41
1:E:457:SER:O	1:E:492:TYR:OH	2.38	0.41
1:E:619:GLN:HE22	2:F:9:DT:H1'	1.85	0.41
1:I:476:LYS:HG3	1:I:498:ILE:CG2	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:657:PHE:CZ	1:I:686:ILE:HG21	2.56	0.41
3:K:5:DG:C2	3:K:6:DA:C4	3.09	0.41
4:D:6:G:N2	4:D:30:A:H1'	2.35	0.41
1:E:55:ALA:O	1:E:57:TYR:HE1	2.04	0.41
1:E:218:LEU:O	1:E:222:HIS:N	2.48	0.41
1:E:701:ALA:HB2	1:E:781:ARG:NH1	2.35	0.41
1:E:833:LEU:HA	1:E:836:ARG:HB2	2.02	0.41
1:I:205:ARG:HA	2:J:18:DA:H2''	2.02	0.41
1:I:708:ASN:O	1:I:746:ASN:ND2	2.48	0.41
1:E:112:SER:O	1:E:116:ARG:N	2.54	0.41
4:H:13:C:H2'	4:H:14:U:H6	1.83	0.41
1:I:56:THR:C	1:I:57:TYR:CG	2.97	0.41
4:L:21:A:H2'	4:L:22:G:C8	2.55	0.41
1:A:48:ALA:HA	1:A:56:THR:O	2.20	0.41
1:A:441:PHE:CD2	1:A:455:LEU:HD21	2.54	0.41
1:I:51:GLU:N	1:I:51:GLU:CD	2.73	0.41
1:I:329:ILE:H	1:I:329:ILE:HD12	1.86	0.41
1:I:532:LYS:HD2	1:I:612:MET:HA	2.02	0.41
4:L:10:G:H2'	4:L:11:C:C6	2.56	0.41
1:A:253:LEU:HB3	1:A:305:TRP:CH2	2.44	0.41
1:E:313:LYS:NZ	1:E:313:LYS:CB	2.73	0.41
1:I:112:SER:HB2	3:K:8:DG:H4'	2.03	0.41
1:I:193:ALA:HB1	1:I:197:LYS:HE3	2.03	0.41
1:I:712:SER:C	1:I:714:HIS:H	2.29	0.41
1:A:31:ASP:OD1	1:A:188:ARG:HG3	2.21	0.41
2:B:24:DC:C4	2:B:25:DG:C6	3.09	0.41
1:E:699:GLU:H	1:E:699:GLU:HG3	1.71	0.41
1:E:729:TYR:CE2	1:E:732:LYS:HA	2.56	0.41
1:E:799:VAL:HG23	1:E:816:LEU:HD21	2.03	0.41
4:H:28:U:O2	4:H:28:U:C2'	2.63	0.41
1:I:271:LYS:HD3	1:I:271:LYS:HA	1.89	0.41
1:I:778:TYR:HB3	1:I:782:VAL:CG2	2.50	0.41
1:I:790:TYR:CD1	1:I:790:TYR:N	2.86	0.41
1:I:790:TYR:CZ	1:I:828:LEU:CG	3.04	0.41
1:I:794:ASN:OD1	1:I:794:ASN:N	2.54	0.41
2:J:21:DC:H2''	2:J:22:DA:C8	2.56	0.41
4:L:27:G:C2	4:L:28:U:H1'	2.56	0.41
1:A:607:GLU:OE2	4:D:48:A:O2'	2.28	0.41
1:E:77:VAL:HG13	1:E:175:LEU:HD22	2.04	0.41
1:E:201:GLU:HG2	1:E:205:ARG:HH21	1.84	0.41
1:E:237:ASP:HB3	1:E:238:LEU:HD23	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:VAL:HA	1:E:290:LEU:HD11	2.03	0.41
1:E:613:HIS:CB	4:H:15:C:H4'	2.41	0.41
1:E:799:VAL:CG2	1:E:816:LEU:HD21	2.51	0.41
2:J:14:DT:H2''	2:J:15:DT:O5'	2.21	0.41
1:A:750:ARG:HG2	1:A:755:SER:HA	2.02	0.40
1:E:246:LEU:HD13	1:E:252:GLY:C	2.46	0.40
1:E:638:ARG:HB3	1:E:685:TYR:HD2	1.86	0.40
1:I:85:LEU:HD12	1:I:85:LEU:HA	1.81	0.40
1:I:99:PHE:CE2	1:I:199:LEU:HD23	2.52	0.40
1:I:789:ARG:C	1:I:790:TYR:HD1	2.29	0.40
1:A:5:GLU:HA	1:A:428:LEU:O	2.21	0.40
2:B:17:DC:N4	4:D:40:G:H1	2.15	0.40
1:E:35:PHE:HD2	1:E:99:PHE:CZ	2.40	0.40
1:E:75:GLU:O	1:E:79:ILE:HG13	2.20	0.40
1:E:209:SER:OG	4:H:40:G:N2	2.54	0.40
1:E:682:LEU:HD12	1:E:682:LEU:HA	1.91	0.40
1:E:742:VAL:HG12	1:E:746:ASN:HD21	1.85	0.40
1:I:399:ILE:HG22	1:I:400:GLY:O	2.21	0.40
1:I:521:ILE:O	1:I:525:LYS:HG3	2.21	0.40
4:L:41:C:H2'	4:L:42:A:O4'	2.22	0.40
1:A:745:MET:HE3	1:A:745:MET:HB3	1.89	0.40
1:E:452:ILE:O	1:E:455:LEU:HG	2.21	0.40
1:I:772:GLU:O	1:I:774:LYS:HE2	2.22	0.40
3:K:4:DC:H2''	3:K:5:DG:H8	1.85	0.40
1:A:2:LYS:O	1:A:432:ILE:HG22	2.22	0.40
1:A:79:ILE:CD1	1:A:79:ILE:C	2.93	0.40
1:A:625:LYS:O	1:A:626:PHE:C	2.65	0.40
1:A:629:LYS:H	1:A:629:LYS:HG3	1.67	0.40
4:D:5:U:H2'	4:D:6:G:H8	1.86	0.40
4:D:16:G:C1'	4:D:19:A:H61	2.31	0.40
1:E:365:TYR:CE1	1:E:384:HIS:CE1	3.10	0.40
1:E:678:SER:HB2	1:E:679:PRO:HD2	2.02	0.40
1:I:328:GLN:O	1:I:330:PRO:HD3	2.22	0.40
1:I:395:VAL:CG1	4:L:33:G:H5'	2.51	0.40
1:A:255:TRP:HB2	1:A:302:TYR:OH	2.22	0.40
1:A:677:LEU:HD12	1:A:682:LEU:HD22	2.04	0.40
2:F:22:DA:C8	2:F:23:DT:H72	2.57	0.40
4:H:43:A:H2'	4:H:44:A:H8	1.86	0.40
1:I:35:PHE:HE1	1:I:185:ILE:HG23	1.87	0.40
1:I:311:LEU:HD23	1:I:311:LEU:HA	1.93	0.40
1:I:439:LYS:HB3	1:I:439:LYS:HE2	1.94	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLU:OE2	1:A:862:LYS:NZ[4_565]	1.84	0.36
1:I:615:SER:OG	1:I:618:GLU:OE2[6_555]	2.04	0.16
1:A:18:GLU:OE1	1:I:853:ARG:O[6_555]	2.12	0.08

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	857/870 (98%)	826 (96%)	29 (3%)	2 (0%)	43	73
1	E	868/870 (100%)	832 (96%)	36 (4%)	0	100	100
1	I	858/870 (99%)	825 (96%)	33 (4%)	0	100	100
All	All	2583/2610 (99%)	2483 (96%)	98 (4%)	2 (0%)	48	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	ALA
1	A	190	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 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	748/757 (99%)	738 (99%)	10 (1%)	61	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	730/757 (96%)	709 (97%)	21 (3%)	37	57
1	I	751/757 (99%)	744 (99%)	7 (1%)	70	74
All	All	2229/2271 (98%)	2191 (98%)	38 (2%)	53	67

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	PHE
1	A	352	LEU
1	A	354	GLU
1	A	355	HIS
1	A	357	LYS
1	A	358	LEU
1	A	362	HIS
1	A	470	ASN
1	A	668	SER
1	A	781	ARG
1	E	50	ARG
1	E	56	THR
1	E	57	TYR
1	E	238	LEU
1	E	242	PHE
1	E	244	GLU
1	E	246	LEU
1	E	247	GLU
1	E	249	LYS
1	E	255	TRP
1	E	294	LYS
1	E	298	LEU
1	E	302	TYR
1	E	306	LYS
1	E	307	LEU
1	E	308	LYS
1	E	311	LEU
1	E	312	GLU
1	E	313	LYS
1	E	720	LYS
1	E	726	ILE
1	I	498	ILE
1	I	764	LYS
1	I	771	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	773	LYS
1	I	774	LYS
1	I	775	GLU
1	I	780	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	215	HIS
1	A	355	HIS
1	A	364	HIS
1	A	430	HIS
1	A	470	ASN
1	A	688	GLN
1	A	834	HIS
1	E	231	ASN
1	E	281	GLN
1	E	322	ASN
1	E	619	GLN
1	E	754	HIS
1	I	136	GLN
1	I	284	GLN
1	I	831	HIS
1	I	835	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	55/56 (98%)	18 (32%)	1 (1%)
4	H	55/56 (98%)	20 (36%)	2 (3%)
4	L	55/56 (98%)	17 (30%)	1 (1%)
All	All	165/168 (98%)	55 (33%)	4 (2%)

All (55) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	3	G
4	D	7	G
4	D	10	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	15	C
4	D	17	C
4	D	18	U
4	D	19	A
4	D	20	G
4	D	23	G
4	D	24	G
4	D	26	G
4	D	28	U
4	D	29	C
4	D	33	G
4	D	34	C
4	D	35	A
4	D	37	G
4	D	45	C
4	H	1	G
4	H	10	G
4	H	15	C
4	H	17	C
4	H	18	U
4	H	19	A
4	H	20	G
4	H	23	G
4	H	24	G
4	H	26	G
4	H	27	G
4	H	28	U
4	H	29	C
4	H	30	A
4	H	33	G
4	H	34	C
4	H	35	A
4	H	37	G
4	H	45	C
4	H	55	C
4	L	3	G
4	L	10	G
4	L	15	C
4	L	17	C
4	L	18	U
4	L	19	A
4	L	20	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L	23	G
4	L	24	G
4	L	26	G
4	L	29	C
4	L	33	G
4	L	34	C
4	L	35	A
4	L	37	G
4	L	45	C
4	L	55	C

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	D	32	A
4	H	27	G
4	H	32	A
4	L	32	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	861/870 (98%)	0.57	78 (9%) 15 16	7, 28, 133, 197	0
1	E	870/870 (100%)	0.46	67 (7%) 19 18	7, 53, 171, 255	0
1	I	864/870 (99%)	0.57	81 (9%) 14 16	7, 40, 130, 217	0
2	B	28/28 (100%)	0.19	0 100 100	10, 45, 186, 198	0
2	F	28/28 (100%)	0.47	1 (3%) 46 32	13, 92, 194, 218	0
2	J	28/28 (100%)	0.21	1 (3%) 46 32	18, 50, 166, 175	0
3	C	12/15 (80%)	0.68	1 (8%) 17 17	23, 51, 195, 220	0
3	G	15/15 (100%)	0.63	0 100 100	40, 84, 186, 228	0
3	K	11/15 (73%)	0.73	0 100 100	58, 91, 145, 176	0
4	D	56/56 (100%)	0.73	8 (14%) 6 9	11, 116, 192, 223	0
4	H	56/56 (100%)	0.83	7 (12%) 8 12	14, 116, 199, 237	0
4	L	56/56 (100%)	0.57	4 (7%) 22 19	12, 89, 136, 217	0
All	All	2885/2907 (99%)	0.54	248 (8%) 16 17	7, 41, 154, 255	0

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	335	GLY	8.3
1	A	531	PHE	7.8
1	I	797	PHE	7.8
1	A	610	GLN	6.8
1	A	297	ALA	6.8
1	I	214	TYR	6.4
1	A	708	ASN	6.2
1	A	388	LEU	6.0
1	A	620	SER	5.9
1	I	397	PRO	5.9
4	H	33	G	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	387	LYS	5.5
1	I	463	ALA	5.5
4	D	33	G	5.3
1	A	11	LEU	5.3
1	I	122	LEU	5.3
1	E	161	TRP	5.1
1	I	407	LEU	5.1
1	E	679	PRO	5.0
1	I	692	LYS	5.0
1	E	821	LEU	5.0
1	I	123	ALA	5.0
1	I	298	LEU	4.9
1	E	850	LEU	4.9
1	E	280	ASP	4.9
1	I	637	LEU	4.8
1	I	273	THR	4.8
1	E	828	LEU	4.8
1	E	734	LEU	4.7
1	A	682	LEU	4.5
1	E	85	LEU	4.4
1	A	686	ILE	4.4
1	A	298	LEU	4.3
1	I	275	ILE	4.3
1	I	747	ILE	4.3
4	L	33	G	4.3
1	A	161	TRP	4.3
4	D	24	G	4.2
1	A	426	TYR	4.2
1	E	118	PHE	4.2
1	A	748	LEU	4.1
1	I	464	ALA	4.1
1	A	673	LEU	4.1
1	A	765	ALA	4.1
1	E	210	HIS	4.1
1	A	586	TYR	4.0
1	A	848	GLU	4.0
1	I	478	ARG	4.0
1	E	586	TYR	3.9
1	E	205	ARG	3.9
1	A	384	HIS	3.9
1	E	251	TYR	3.9
1	I	127	LEU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	197	LYS	3.8
1	I	602	TYR	3.7
1	A	645	ILE	3.7
1	A	338	VAL	3.7
1	I	152	GLY	3.7
1	I	229	ALA	3.7
1	I	688	GLN	3.7
1	I	474	PRO	3.6
1	A	89	GLY	3.6
1	I	636	LEU	3.6
1	I	258	LEU	3.6
1	A	387	LYS	3.5
1	E	11	LEU	3.5
1	A	174	SER	3.5
1	E	609	TYR	3.4
1	A	287	PHE	3.4
1	A	728	PHE	3.4
4	D	27	G	3.4
1	A	614	LEU	3.3
1	E	636	LEU	3.3
1	A	716	GLY	3.3
1	I	409	GLU	3.3
1	E	452	ILE	3.3
1	I	793	SER	3.3
1	A	595	LEU	3.2
1	I	161	TRP	3.2
1	I	829	VAL	3.2
1	A	581	MET	3.2
1	E	81	PHE	3.1
1	A	582	ASN	3.1
1	I	50	ARG	3.1
1	I	734	LEU	3.1
1	E	426	TYR	3.1
1	E	666	SER	3.1
1	E	807	VAL	3.0
1	I	272	PRO	3.0
1	E	206	GLN	3.0
1	I	473	ALA	3.0
1	A	139	GLN	3.0
1	I	466	LEU	3.0
1	A	805	VAL	3.0
1	A	807	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	708	ASN	3.0
1	A	21	PHE	3.0
1	A	749	CYS	2.9
1	A	649	PHE	2.9
1	I	633	PHE	2.9
1	E	289	GLY	2.9
1	I	805	VAL	2.9
1	A	365	TYR	2.9
1	I	380	LEU	2.9
1	A	743	GLY	2.9
1	I	821	LEU	2.9
1	I	757	CYS	2.9
1	A	242	PHE	2.9
1	I	435	PHE	2.9
1	I	586	TYR	2.9
1	I	867	PHE	2.9
1	I	612	MET	2.9
1	E	667	ASP	2.8
4	D	26	G	2.8
1	E	193	ALA	2.8
1	I	108	LYS	2.8
1	A	579	TYR	2.8
1	A	565	SER	2.8
1	A	574	LEU	2.8
1	A	757	CYS	2.8
1	E	277	ILE	2.8
1	I	468	LEU	2.8
1	I	621	PRO	2.8
4	H	17	C	2.8
1	E	535	GLN	2.8
1	I	336	LEU	2.8
1	E	729	TYR	2.8
1	I	655	VAL	2.7
1	I	761	PHE	2.7
1	A	466	LEU	2.7
1	A	642	ALA	2.7
1	A	207	LEU	2.7
1	A	290	LEU	2.7
1	A	197	LYS	2.7
4	H	22	G	2.7
1	I	55	ALA	2.7
1	E	840	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	424	LEU	2.7
1	E	139	GLN	2.6
2	F	1	DA	2.6
1	I	437	ILE	2.6
1	A	710	PRO	2.6
1	E	572	ARG	2.6
1	A	561	CYS	2.6
4	H	21	A	2.6
1	A	257	VAL	2.6
1	A	253	LEU	2.6
1	A	442	PHE	2.6
1	E	531	PHE	2.6
1	I	606	LEU	2.6
1	E	663	PRO	2.6
1	I	546	THR	2.5
1	A	17	TYR	2.5
1	E	96	TYR	2.5
1	A	641	VAL	2.5
4	H	16	G	2.5
1	A	746	ASN	2.5
1	E	114	ALA	2.5
1	E	464	ALA	2.5
1	A	341	LEU	2.5
1	I	816	LEU	2.5
1	A	157	PRO	2.4
1	E	566	ARG	2.4
1	A	239	VAL	2.4
1	I	257	VAL	2.4
1	A	4	HIS	2.4
1	A	637	LEU	2.4
1	I	140	LEU	2.4
1	A	665	ASP	2.4
4	D	17	C	2.4
1	I	387	LYS	2.4
1	E	837	MET	2.4
1	E	330	PRO	2.4
4	L	44	A	2.4
1	I	287	PHE	2.3
1	E	437	ILE	2.3
1	E	853	ARG	2.3
1	I	297	ALA	2.3
1	E	298	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	53	G	2.3
1	I	760	SER	2.3
1	E	337	GLY	2.3
1	A	421	TYR	2.3
1	E	243	ALA	2.3
1	E	805	VAL	2.3
1	A	532	LYS	2.3
1	I	708	ASN	2.3
1	I	794	ASN	2.3
1	E	548	TRP	2.3
1	I	752	LEU	2.3
4	D	50	C	2.3
4	L	36	C	2.3
1	E	453	ASN	2.2
1	I	191	HIS	2.2
1	A	752	LEU	2.2
1	A	198	ILE	2.2
1	A	608	SER	2.2
1	A	655	VAL	2.2
1	E	82	LEU	2.2
1	E	703	ASP	2.2
3	C	9	DT	2.2
1	E	278	ALA	2.2
1	I	47	TYR	2.2
4	H	32	A	2.2
1	A	233	THR	2.2
1	I	838	LYS	2.2
1	I	148	TRP	2.2
1	E	510	ARG	2.2
1	I	808	THR	2.2
1	E	288	ALA	2.2
1	E	610	GLN	2.2
1	E	466	LEU	2.2
1	A	693	ARG	2.1
1	E	392	ASP	2.1
1	E	348	VAL	2.1
1	I	729	TYR	2.1
1	A	367	GLY	2.1
1	A	657	PHE	2.1
1	I	286	LYS	2.1
1	E	792	SER	2.1
1	I	678	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	610	GLN	2.1
1	E	364	HIS	2.1
4	L	24	G	2.1
1	A	436	GLN	2.1
1	I	101	GLU	2.1
1	I	750	ARG	2.1
1	I	866	SER	2.1
1	E	317	PHE	2.1
1	I	81	PHE	2.1
1	A	690	LEU	2.1
2	J	1	DA	2.1
4	D	20	G	2.1
4	H	3	G	2.1
1	A	630	ARG	2.1
1	I	753	ASN	2.1
1	E	677	LEU	2.1
1	E	683	LEU	2.1
1	I	386	LEU	2.1
1	I	716	GLY	2.0
1	A	679	PRO	2.0
1	I	491	ASP	2.0
1	A	336	LEU	2.0
1	E	318	PRO	2.0
1	I	205	ARG	2.0
1	I	420	PHE	2.0
1	E	117	GLU	2.0
1	E	463	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
5	MG	I	901	1/1	0.70	0.36	15,15,15,15	0
5	MG	E	901	1/1	0.95	0.04	19,19,19,19	0
5	MG	A	901	1/1	0.95	0.15	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.