Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2025 – 06:38 PM JST

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:

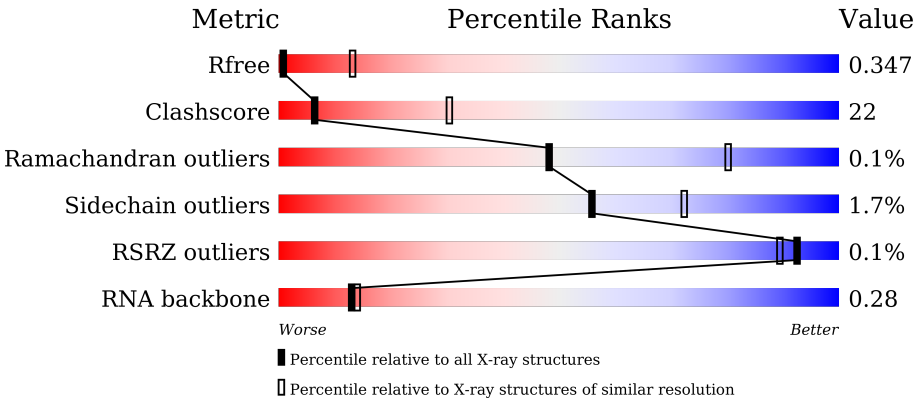
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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}	164625	1155 (4.00-3.64)
Clashscore	180529	1222 (4.00-3.64)
Ramachandran outliers	177936	1182 (4.00-3.64)
Sidechain outliers	177891	1174 (4.00-3.64)
RSRZ outliers	164620	1156 (4.00-3.64)
RNA backbone	3690	1132 (4.62-3.00)

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	870	63% 34% ••
1	E	870	63% 34% •
1	I	870	60% 37% ••
2	B	28	50% 50%

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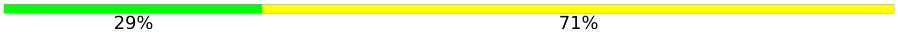
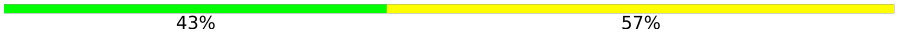
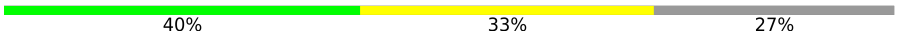
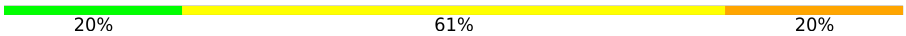
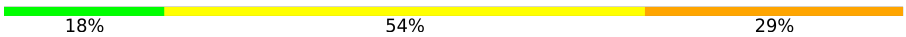
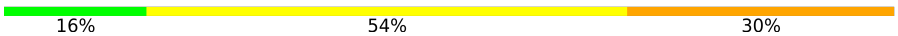
Mol	Chain	Length	Quality of chain
2	F	28	
2	J	28	
3	C	15	
3	G	15	
3	K	15	
4	D	56	
4	H	56	
4	L	56	

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	C	N	O	P	0	0	0
			1204	536	225	387	56			
4	H	56	Total	C	N	O	P	0	0	0
			1204	536	225	387	56			
4	L	56	Total	C	N	O	P	0	0	0
			1204	536	225	387	56			

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

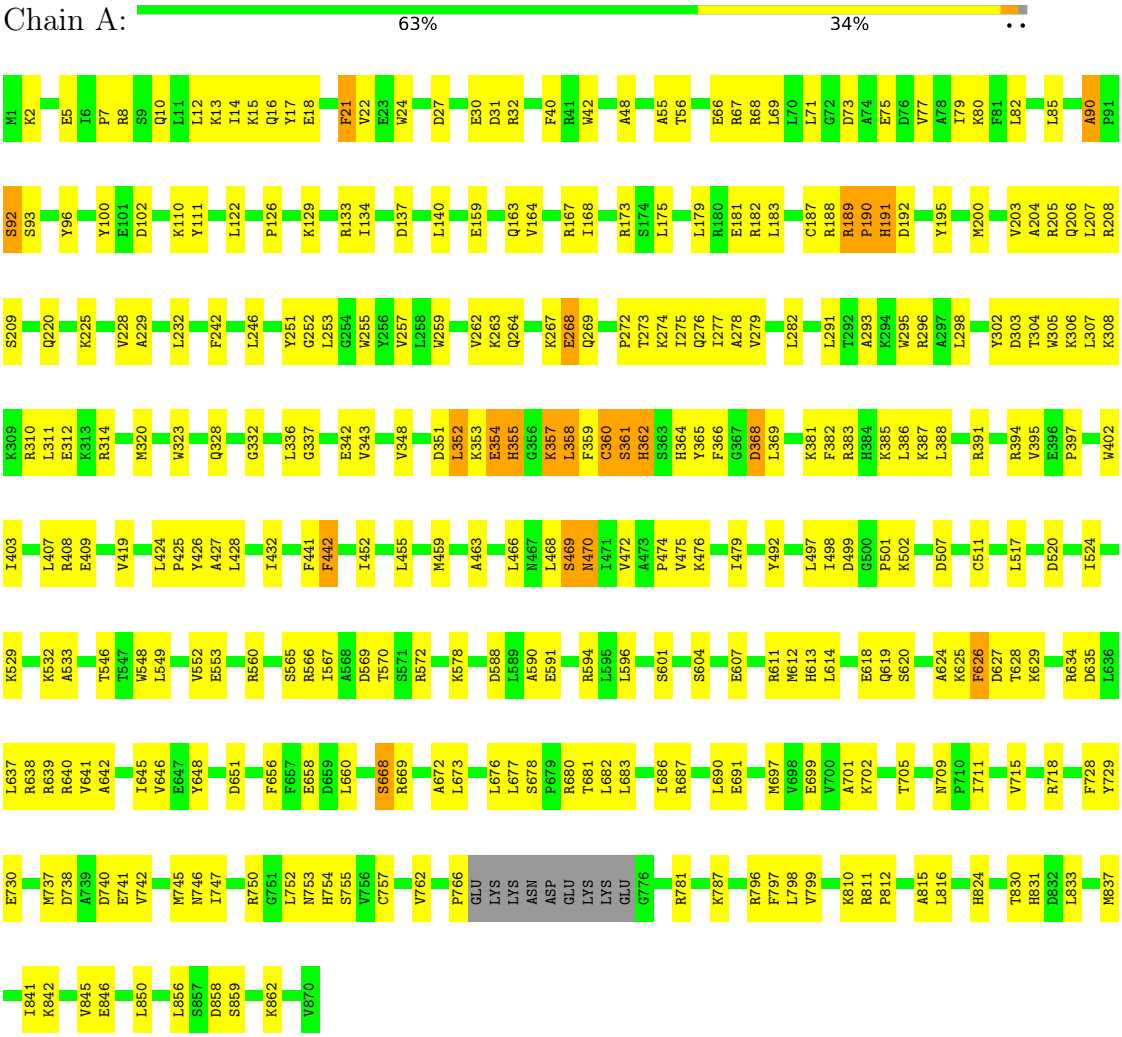
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		
5	I	1	Total	Mg	0	0
			1	1		

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.

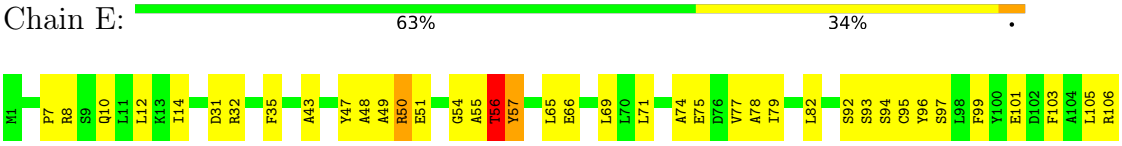
- Molecule 1: Cas12h

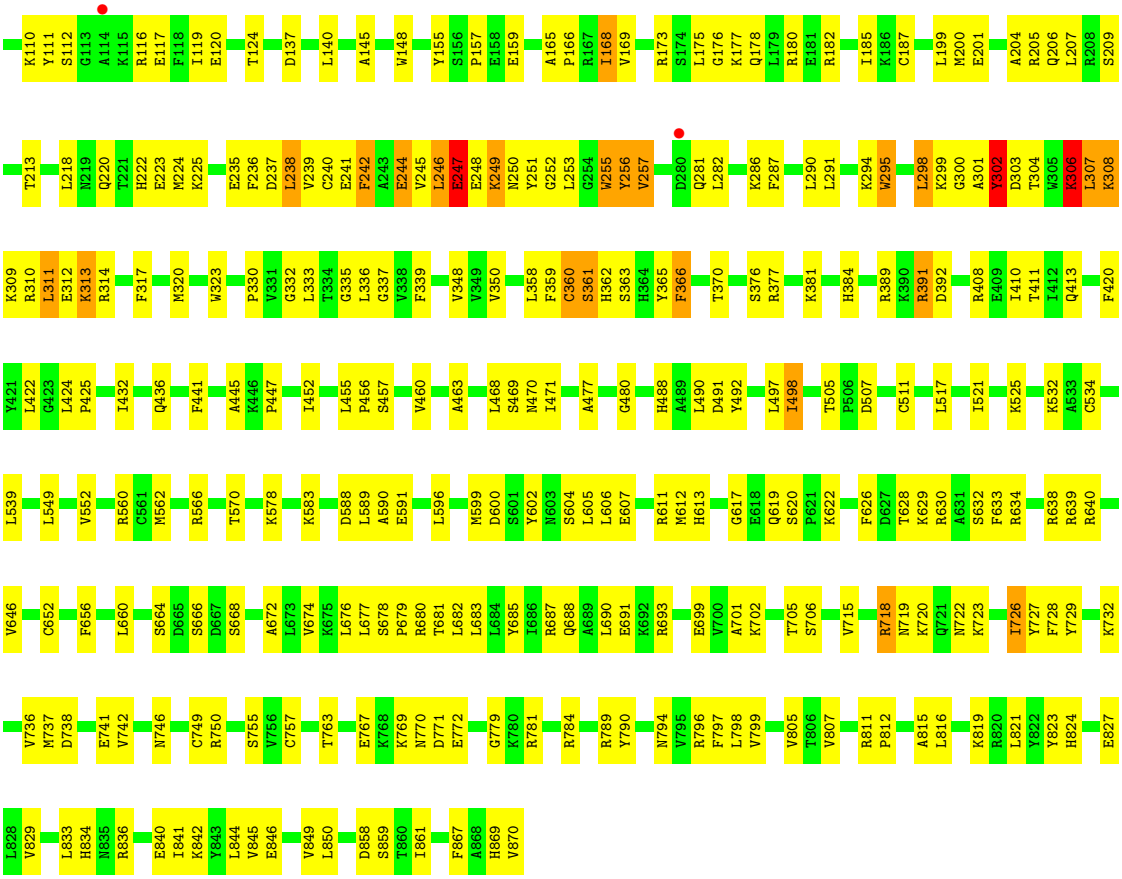
Chain A:



- Molecule 1: Cas12h

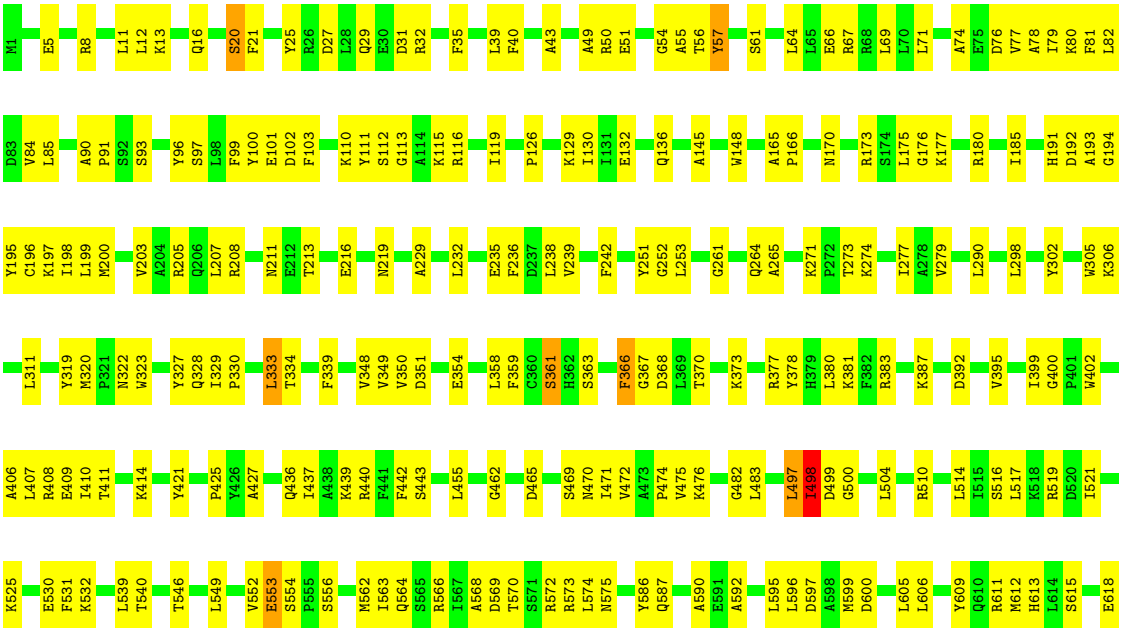
Chain E:





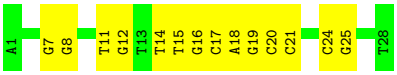
• Molecule 1: Cas12h

Chain I:



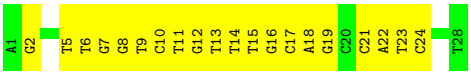
• Molecule 2: DNA (28-MER)

Chain B:



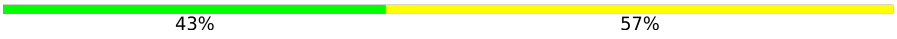
• Molecule 2: DNA (28-MER)

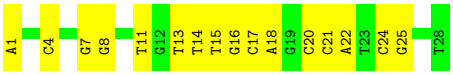
Chain F:



• Molecule 2: DNA (28-MER)

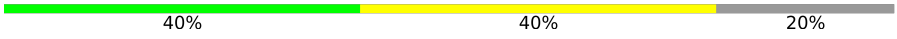
Chain J:





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

Chain C:

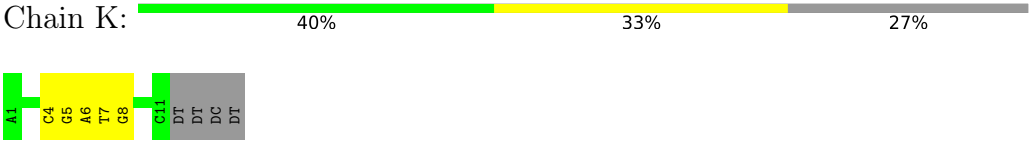


• Molecule 3: DNA (5'-D(P*AP*GP*TP*CP*GP*AP*TP*GP*TP*TP*CP*T)-3')

Chain G:

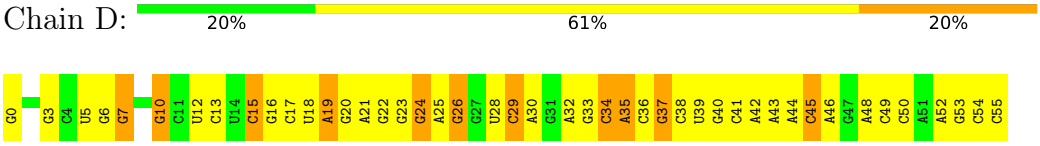
• Molecule 3: DNA (5'-D(P*AP*GP*TP*CP*GP*AP*TP*GP*TP*TP*CP*T)-3')

Chain K:



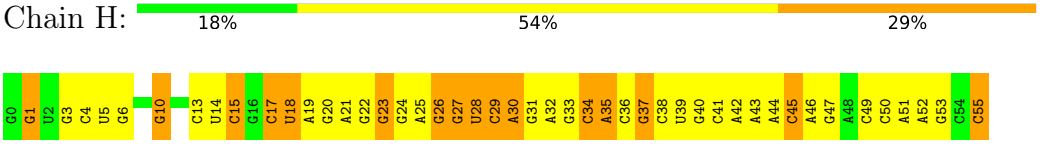
• Molecule 4: RNA (56-MER)

Chain D:



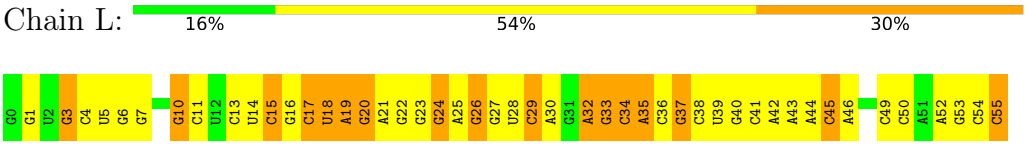
• Molecule 4: RNA (56-MER)

Chain H:



• Molecule 4: RNA (56-MER)

Chain L:



4 Data and refinement statistics (i)

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) 46.7 (28.42-3.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.85 (at 3.86Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.334 , 0.339 0.336 , 0.347	Depositor DCC
R_{free} test set	28744 reflections (3.61%)	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)	0.13 , 110.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.089 for -h,-k,l	Xtriage
F_o,F_c correlation	0.90	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.*

[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

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(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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 (i)

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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	857/870 (98%)	826 (96%)	29 (3%)	2 (0%)	44 74
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 80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	ALA
1	A	190	PRO

5.3.2 Protein sidechains (i)

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%)	65 76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	730/757 (96%)	709 (97%)	21 (3%)	37 59
1	I	751/757 (99%)	744 (99%)	7 (1%)	75 83
All	All	2229/2271 (98%)	2191 (98%)	38 (2%)	56 72

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

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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

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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

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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, 95^{th} 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%)	-1.49	0 100 100	7, 28, 133, 197	0
1	E	870/870 (100%)	-1.45	2 (0%) 92 85	7, 53, 171, 255	0
1	I	864/870 (99%)	-1.50	0 100 100	7, 40, 130, 217	0
2	B	28/28 (100%)	-1.56	0 100 100	10, 45, 186, 198	0
2	F	28/28 (100%)	-1.28	0 100 100	13, 92, 194, 218	0
2	J	28/28 (100%)	-1.59	0 100 100	18, 50, 166, 175	0
3	C	12/15 (80%)	-1.51	0 100 100	23, 51, 195, 220	0
3	G	15/15 (100%)	-1.43	0 100 100	40, 84, 186, 228	0
3	K	11/15 (73%)	-1.61	0 100 100	58, 91, 145, 176	0
4	D	56/56 (100%)	-1.59	0 100 100	11, 116, 192, 223	0
4	H	56/56 (100%)	-1.48	0 100 100	14, 116, 199, 237	0
4	L	56/56 (100%)	-1.89	0 100 100	12, 89, 136, 217	0
All	All	2885/2907 (99%)	-1.49	2 (0%) 92 89	7, 41, 154, 255	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	114	ALA	3.6
1	E	280	ASP	2.1

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 (i)

There are no monosaccharides 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, 95^{th} 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
5	MG	A	901	1/1	1.00	0.03	12,12,12,12	0
5	MG	E	901	1/1	1.00	0.01	19,19,19,19	0
5	MG	I	901	1/1	1.00	0.07	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.