



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Sep 18, 2017 – 12:00 PM EDT

PDB ID : 5WFE
EMDB ID: : EMD-8827
Title : Cas1-Cas2-IHF-DNA holo-complex
Authors : Wright, A.V.; Liu, J.J.; Nogales, E.; Doudna, J.A.
Deposited on : unknown
Resolution : 3.64 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

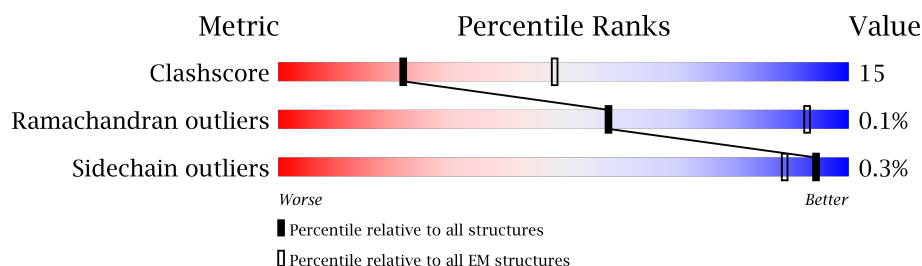
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.64 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	305	59% 27% 14%
1	B	305	68% 24% 9%
1	C	305	62% 22% 16%
1	D	305	68% 21% 11%
2	E	103	53% 38% 9%
2	F	103	52% 39% 9%
3	G	28	21% 79%
4	H	61	33% 41% 26%
5	I	95	27% 54% 19%

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Mol	Chain	Length	Quality of chain
6	J	62	<div><div></div><div>45%</div><div></div><div>52%</div><div></div></div>
7	K	99	<div><div></div><div>70%</div><div></div><div>27%</div><div></div></div>
8	L	94	<div><div></div><div>71%</div><div></div><div>28%</div><div></div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15523 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CRISPR-associated endonuclease Cas1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	262	Total	C	N	O	S	0	0
			2018	1290	358	363	7		
1	B	279	Total	C	N	O	S	0	0
			2157	1382	382	386	7		
1	C	256	Total	C	N	O	S	0	0
			1964	1254	349	354	7		
1	D	272	Total	C	N	O	S	0	0
			2096	1341	373	375	7		

- Molecule 2 is a protein called CRISPR-associated endoribonuclease Cas2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	94	Total	C	N	O	S	0	0
			739	475	128	132	4		
2	F	94	Total	C	N	O	S	0	0
			739	475	128	132	4		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	95	GLY	-	expression tag	UNP P45956
E	96	SER	-	expression tag	UNP P45956
E	97	SER	-	expression tag	UNP P45956
E	98	GLU	-	expression tag	UNP P45956
E	99	ASN	-	expression tag	UNP P45956
E	100	LEU	-	expression tag	UNP P45956
E	101	TYR	-	expression tag	UNP P45956
E	102	PHE	-	expression tag	UNP P45956
E	103	GLN	-	expression tag	UNP P45956
F	95	GLY	-	expression tag	UNP P45956
F	96	SER	-	expression tag	UNP P45956
F	97	SER	-	expression tag	UNP P45956
F	98	GLU	-	expression tag	UNP P45956

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Chain	Residue	Modelled	Actual	Comment	Reference
F	99	ASN	-	expression tag	UNP P45956
F	100	LEU	-	expression tag	UNP P45956
F	101	TYR	-	expression tag	UNP P45956
F	102	PHE	-	expression tag	UNP P45956
F	103	GLN	-	expression tag	UNP P45956

- Molecule 3 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	28	Total	C	N	O	P	0	0
			578	275	118	158	27		

- Molecule 4 is a DNA chain called DNA (45-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	45	Total	C	N	O	P	0	0
			907	436	146	281	44		

- Molecule 5 is a DNA chain called DNA (76-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	77	Total	C	N	O	P	0	0
			1570	753	279	461	77		

- Molecule 6 is a DNA chain called DNA (61-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	60	Total	C	N	O	P	0	0
			1244	597	228	359	60		

- Molecule 7 is a protein called Integration host factor subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	96	Total	C	N	O	S	0	0
			769	481	143	144	1		

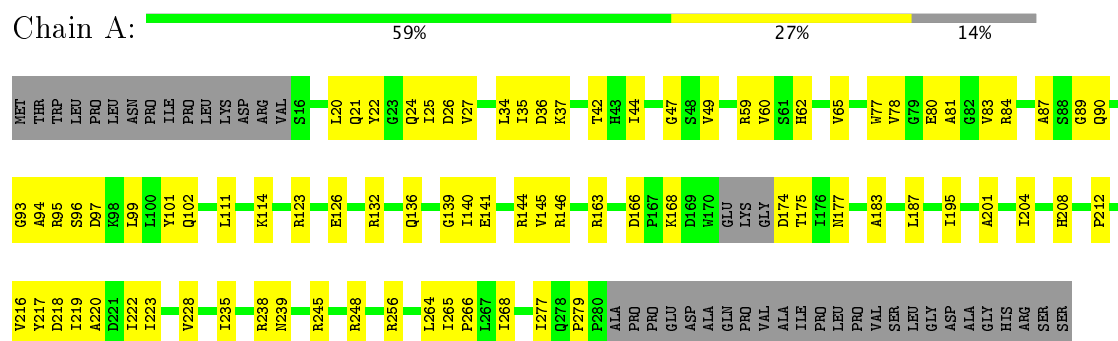
- Molecule 8 is a protein called Integration host factor subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	94	Total	C	N	O	S	0	0
			742	461	139	139	3		

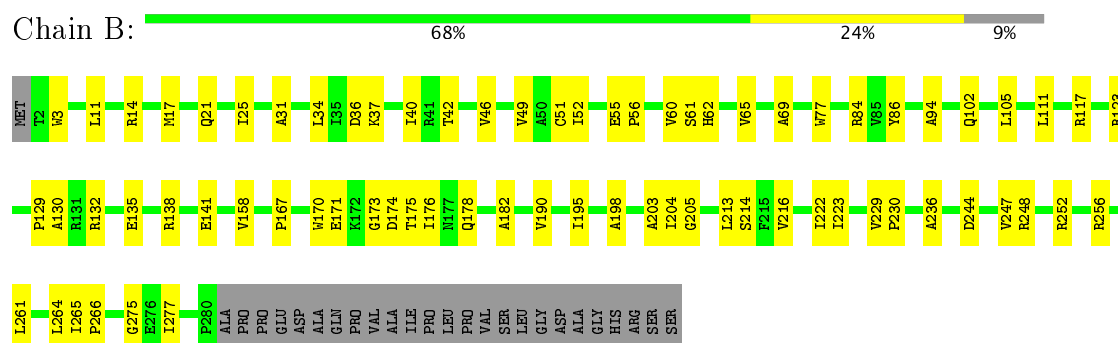
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

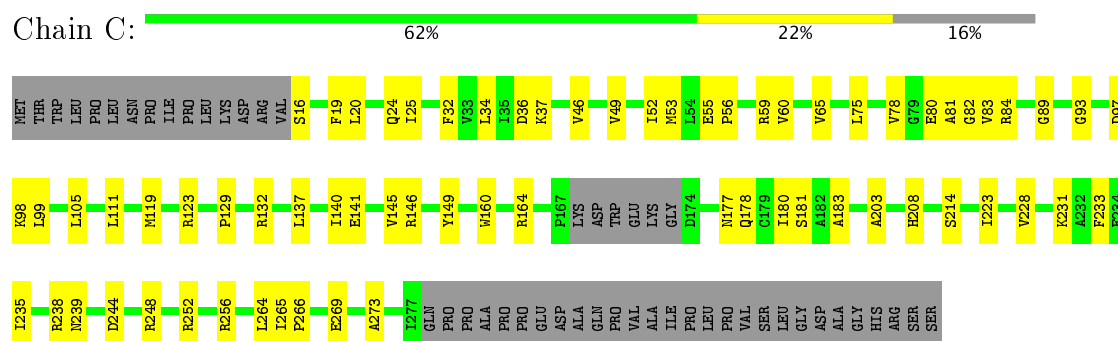
- Molecule 1: CRISPR-associated endonuclease Cas1



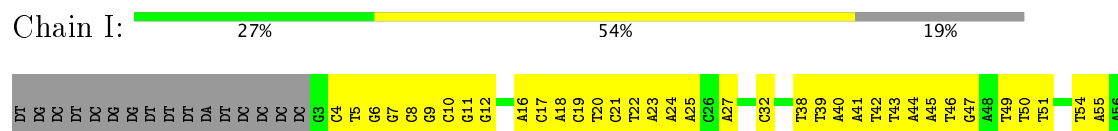
- Molecule 1: CRISPR-associated endonuclease Cas1

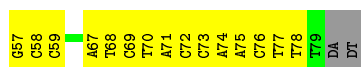


- Molecule 1: CRISPR-associated endonuclease Cas1



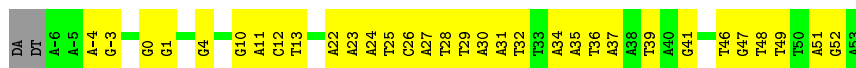
- Molecule 1: CRISPR-associated endonuclease Cas1





- Molecule 6: DNA (61-MER)

Chain J: 45% 52% .



- Molecule 7: Integration host factor subunit alpha

Chain K: 70% 27% .



- Molecule 8: Integration host factor subunit beta

Chain L: 71% 28% .



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	86000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.5	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 >2	RMSZ	# Z >2
1	A	0.27	0/2057	0.43	0/2789
1	B	0.27	0/2202	0.43	0/2990
1	C	0.26	0/1999	0.41	0/2708
1	D	0.25	0/2137	0.40	0/2898
2	E	0.29	0/753	0.46	0/1024
2	F	0.31	0/753	0.47	0/1024
3	G	0.60	0/652	0.89	0/1005
4	H	0.59	0/1010	1.08	0/1556
5	I	0.61	0/1759	1.05	0/2710
6	J	0.53	0/1398	1.03	0/2159
7	K	0.25	0/780	0.38	0/1043
8	L	0.26	0/755	0.40	0/1010
All	All	0.39	0/16255	0.68	0/22916

There are no bond length outliers.

There are no bond angle outliers.

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	2018	0	2069	58	0
1	B	2157	0	2219	59	0
1	C	1964	0	2020	51	0
1	D	2096	0	2163	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	739	0	756	34	0
2	F	739	0	756	45	0
3	G	578	0	314	32	0
4	H	907	0	514	29	0
5	I	1570	0	872	75	0
6	J	1244	0	683	45	0
7	K	769	0	781	23	0
8	L	742	0	749	35	0
All	All	15523	0	13896	430	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (430) 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)
6:J:29:DT:N3	8:L:64:PRO:HB3	1.22	1.46
6:J:29:DT:C2	8:L:64:PRO:CB	2.09	1.35
6:J:29:DT:N3	8:L:64:PRO:CB	1.89	1.33
6:J:29:DT:C4	8:L:64:PRO:HB3	1.66	1.30
6:J:29:DT:C2	8:L:64:PRO:HB2	1.66	1.27
5:I:57:DG:H2'	5:I:58:DC:C6	1.79	1.16
6:J:29:DT:C2	8:L:64:PRO:HB3	1.79	1.13
2:F:38:LYS:HG3	2:F:39:ILE:N	1.42	1.13
2:F:38:LYS:CG	2:F:39:ILE:N	2.20	1.00
5:I:57:DG:N7	5:I:58:DC:N4	2.12	0.97
6:J:27:DA:H2''	6:J:28:DT:H73	1.42	0.96
5:I:57:DG:C8	5:I:58:DC:N4	2.34	0.96
4:H:38:DG:N2	5:I:10:DC:O2	2.02	0.92
5:I:32:DC:O2	6:J:41:DG:N2	2.02	0.91
6:J:29:DT:O2	8:L:64:PRO:HB2	1.71	0.90
5:I:57:DG:C8	5:I:58:DC:C4	2.61	0.89
5:I:57:DG:H2''	5:I:58:DC:H5'	1.54	0.88
2:F:38:LYS:HG3	2:F:39:ILE:H	1.38	0.86
5:I:57:DG:C2'	5:I:58:DC:C6	2.60	0.84
2:F:38:LYS:CG	2:F:39:ILE:H	1.87	0.82
1:B:135:GLU:HG3	1:B:138:ARG:HH11	1.46	0.80
5:I:32:DC:OP1	8:L:42:ARG:NH2	2.13	0.80
1:A:59:ARG:NH1	3:G:2:DA:OP1	2.16	0.78
1:C:80:GLU:OE2	1:C:252:ARG:NH1	2.20	0.74
1:B:190:VAL:HB	1:B:261:LEU:HD21	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:39:DT:H4'	7:K:60:ARG:HB2	1.70	0.74
1:B:25:ILE:HB	1:B:60:VAL:HA	1.70	0.73
1:A:123:ARG:NH1	1:A:141:GLU:OE2	2.20	0.73
5:I:44:DA:C4	6:J:29:DT:O4	2.41	0.73
1:B:132:ARG:NH1	5:I:73:DC:O2	2.22	0.73
5:I:44:DA:C5	6:J:29:DT:O4	2.43	0.72
1:D:55:GLU:OE2	1:D:248:ARG:NH1	2.22	0.72
8:L:82:PRO:O	8:L:87:ARG:NH1	2.23	0.72
3:G:21:DA:H2'	3:G:22:DA:C8	2.25	0.72
1:C:119:MET:O	1:C:123:ARG:HB2	1.91	0.71
2:E:2:SER:HB2	2:E:61:ALA:HB3	1.72	0.71
4:H:38:DG:N1	5:I:10:DC:N3	2.29	0.70
2:E:18:ARG:HD3	2:E:21:ILE:HD12	1.74	0.70
5:I:57:DG:C2'	5:I:58:DC:H5'	2.20	0.70
1:D:163:ARG:NH1	1:D:164:ARG:O	2.25	0.69
1:C:59:ARG:NH1	4:H:2:DT:OP1	2.24	0.69
2:E:77:ARG:HH22	2:E:94:VAL:HA	1.57	0.69
2:E:5:VAL:HG21	2:F:5:VAL:HG21	1.75	0.69
7:K:91:VAL:HG21	8:L:78:PRO:HG3	1.73	0.69
6:J:29:DT:H3	8:L:64:PRO:CB	2.04	0.68
1:A:59:ARG:HA	1:B:61:SER:HA	1.74	0.68
5:I:32:DC:N3	6:J:41:DG:N1	2.30	0.68
2:F:38:LYS:HD2	2:F:39:ILE:HD13	1.76	0.67
4:H:19:DT:H2'	4:H:20:DG:C8	2.29	0.67
5:I:72:DC:H2''	5:I:73:DC:C6	2.29	0.67
1:A:163:ARG:HA	1:A:177:ASN:HD21	1.60	0.67
3:G:7:DC:H2'	3:G:8:DA:C8	2.30	0.67
2:F:38:LYS:O	2:F:41:GLU:N	2.28	0.67
6:J:27:DA:C2'	6:J:28:DT:H73	2.21	0.66
1:B:11:LEU:HD12	1:B:14:ARG:HD2	1.77	0.66
1:C:129:PRO:HG2	1:C:132:ARG:HG3	1.76	0.65
1:C:123:ARG:NH1	1:C:141:GLU:OE2	2.28	0.65
3:G:19:DT:H2'	3:G:20:DA:C8	2.33	0.64
6:J:34:DA:OP1	8:L:56:ARG:NH2	2.30	0.64
2:F:4:LEU:HD23	2:F:23:LEU:HD21	1.79	0.64
5:I:57:DG:H2'	5:I:58:DC:N1	2.10	0.64
6:J:27:DA:H2''	6:J:28:DT:C7	2.24	0.64
2:F:38:LYS:HD2	2:F:39:ILE:CD1	2.29	0.63
7:K:77:ARG:HB3	8:L:91:ASN:HA	1.80	0.62
1:A:111:LEU:HD13	1:A:277:ILE:HD11	1.81	0.62
2:E:55:ASN:ND2	2:E:75:LEU:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:LEU:HD13	1:C:25:ILE:HD11	1.81	0.62
2:E:6:VAL:HB	2:E:31:TYR:HB2	1.81	0.62
2:F:83:LEU:HD22	2:F:88:LEU:HD12	1.82	0.62
1:C:32:PHE:HE2	1:C:46:VAL:HG23	1.65	0.61
2:E:18:ARG:NH1	2:E:46:GLN:OE1	2.33	0.61
1:A:126:GLU:OE2	1:A:144:ARG:NH1	2.33	0.61
1:C:183:ALA:HB1	1:C:228:VAL:HG12	1.82	0.61
3:G:11:DA:H2''	3:G:12:DC:H2'	1.81	0.61
2:F:38:LYS:HG3	2:F:39:ILE:CA	2.26	0.61
5:I:76:DC:H2''	5:I:77:DT:H72	1.81	0.61
1:C:248:ARG:NH2	3:G:23:DT:OP1	2.34	0.60
6:J:35:DA:N3	7:K:60:ARG:NH2	2.49	0.60
1:A:96:SER:OG	1:B:203:ALA:O	2.17	0.60
3:G:20:DA:H2'	3:G:21:DA:C8	2.36	0.60
1:A:24:GLN:HB2	1:A:35:ILE:HB	1.84	0.59
3:G:22:DA:H2'	3:G:23:DT:C6	2.38	0.59
1:A:183:ALA:HB1	1:A:228:VAL:HG12	1.84	0.59
4:H:3:DT:H2'	4:H:4:DT:H71	1.84	0.59
7:K:3:LEU:HB2	8:L:36:THR:HG21	1.84	0.59
1:A:245:ARG:HH21	4:H:22:DT:H3'	1.67	0.59
5:I:41:DA:H2''	5:I:42:DT:C7	2.32	0.59
5:I:41:DA:H2''	5:I:42:DT:H71	1.83	0.59
4:H:37:DC:H4'	4:H:38:DG:OP1	2.03	0.59
1:B:36:ASP:OD1	1:B:37:LYS:N	2.36	0.58
5:I:45:DA:N6	8:L:64:PRO:HG2	2.17	0.58
1:D:187:LEU:HD22	1:D:228:VAL:HG21	1.85	0.58
1:D:252:ARG:NH2	2:F:84:ASP:O	2.37	0.58
5:I:57:DG:C8	5:I:58:DC:C5	2.92	0.57
1:B:198:ALA:HB2	1:B:265:ILE:HD12	1.86	0.57
1:D:4:LEU:HD21	2:E:49:GLY:HA3	1.87	0.57
6:J:29:DT:C5	8:L:64:PRO:HB3	2.36	0.57
3:G:16:DT:H2''	3:G:17:DA:C8	2.40	0.56
1:A:87:ALA:HB2	1:B:69:ALA:HB2	1.87	0.56
5:I:57:DG:C5	5:I:58:DC:C4	2.93	0.56
1:A:102:GLN:NE2	1:A:204:ILE:O	2.39	0.56
5:I:57:DG:N7	5:I:58:DC:C4	2.72	0.56
5:I:5:DT:H2''	5:I:6:DG:C8	2.39	0.56
5:I:58:DC:OP2	5:I:58:DC:H2'	2.05	0.56
1:C:25:ILE:HB	1:C:60:VAL:HG22	1.87	0.56
1:A:146:ARG:HD3	6:J:51:DA:H1'	1.88	0.56
1:C:81:ALA:HB3	1:C:252:ARG:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:GLU:N	3:G:24:DT:OP2	2.39	0.56
1:B:117:ARG:NH2	6:J:4:DG:OP1	2.38	0.55
1:D:180:ILE:HD11	1:D:233:PHE:HE1	1.71	0.55
1:C:78:VAL:O	1:D:62:HIS:NE2	2.37	0.55
2:F:14:ARG:NH1	3:G:5:DA:OP1	2.34	0.55
1:B:31:ALA:HB2	2:F:17:GLY:HA2	1.89	0.55
3:G:17:DA:H2'	3:G:18:DG:C8	2.41	0.55
1:D:66:ARG:NH2	3:G:25:DG:OP2	2.39	0.55
1:B:244:ASP:O	1:B:248:ARG:HD3	2.06	0.55
1:B:129:PRO:HA	5:I:73:DC:H5"	1.89	0.55
1:B:129:PRO:HB2	1:B:132:ARG:HD3	1.89	0.55
3:G:20:DA:H2'	3:G:21:DA:H8	1.72	0.55
1:A:223:ILE:HD13	1:A:264:LEU:HD21	1.89	0.55
1:D:224:LYS:O	1:D:228:VAL:HB	2.07	0.55
7:K:59:GLN:HE21	7:K:72:PRO:HB2	1.72	0.55
1:C:36:ASP:OD1	1:C:37:LYS:N	2.40	0.54
2:E:70:PHE:O	2:E:87:ARG:NH1	2.40	0.54
1:D:112:ARG:NH2	1:D:206:PHE:O	2.39	0.54
1:C:24:GLN:NE2	4:H:2:DT:OP1	2.41	0.54
2:F:70:PHE:HE2	2:F:80:PRO:HB3	1.72	0.54
1:A:208:HIS:ND1	1:A:218:ASP:OD1	2.36	0.54
1:D:146:ARG:HA	1:D:149:TYR:HD2	1.71	0.54
2:F:6:VAL:HB	2:F:31:TYR:HB2	1.90	0.54
1:D:36:ASP:OD1	1:D:37:LYS:N	2.40	0.54
5:I:58:DC:H1'	5:I:59:DC:C6	2.43	0.53
1:A:60:VAL:N	1:B:60:VAL:O	2.40	0.53
1:A:93:GLY:HA3	1:A:99:LEU:HD11	1.90	0.53
1:A:78:VAL:O	1:B:62:HIS:NE2	2.38	0.53
2:E:25:GLU:HG3	2:E:31:TYR:HE1	1.72	0.53
1:B:102:GLN:NE2	1:B:204:ILE:O	2.42	0.53
3:G:18:DG:H3'	3:G:19:DT:H71	1.89	0.53
2:F:38:LYS:O	2:F:39:ILE:C	2.48	0.53
2:F:38:LYS:O	2:F:40:ARG:N	2.42	0.53
5:I:19:DC:H2'	5:I:20:DT:H71	1.91	0.53
5:I:54:DT:H2"	5:I:55:DA:N7	2.24	0.53
8:L:43:ILE:HB	8:L:51:PHE:HB2	1.90	0.53
1:B:123:ARG:HG2	1:B:222:ILE:HA	1.91	0.52
2:E:5:VAL:HG22	2:E:32:VAL:HG22	1.91	0.52
2:E:70:PHE:HE2	2:E:80:PRO:HB3	1.74	0.52
5:I:22:DT:H2"	5:I:23:DA:C8	2.45	0.52
6:J:29:DT:C4	8:L:64:PRO:CB	2.61	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ILE:HG22	2:E:92:LEU:HA	1.91	0.52
1:D:118:LYS:HE3	1:D:122:LEU:HD11	1.90	0.52
7:K:30:PHE:HE1	8:L:26:VAL:HG13	1.75	0.52
1:B:84:ARG:NH1	1:B:213:LEU:HD11	2.24	0.51
1:A:187:LEU:HD21	1:A:220:ALA:O	2.11	0.51
5:I:74:DA:H2"	5:I:75:DA:H8	1.75	0.51
1:C:59:ARG:HA	1:D:61:SER:HA	1.91	0.51
7:K:63:ARG:HD3	7:K:68:GLY:HA2	1.92	0.51
1:A:132:ARG:NH2	1:A:140:ILE:HD11	2.26	0.51
5:I:44:DA:C8	8:L:64:PRO:HG3	2.45	0.51
1:A:166:ASP:HB3	1:A:168:LYS:HG2	1.91	0.51
1:A:248:ARG:HH12	4:H:23:DT:H5"	1.76	0.51
1:A:34:LEU:HB3	1:A:42:THR:HB	1.92	0.51
4:H:33:DT:H2"	4:H:34:DC:C5	2.45	0.51
1:B:175:THR:HG22	1:B:236:ALA:HA	1.91	0.51
1:B:49:VAL:HG12	1:B:51:CYS:H	1.76	0.51
1:D:256:ARG:HD3	2:F:65:GLU:HB2	1.93	0.51
1:C:65:VAL:HG11	1:D:77:TRP:CD2	2.45	0.51
3:G:24:DT:H2'	3:G:25:DG:C8	2.46	0.51
1:B:21:GLN:HB3	1:B:55:GLU:HB2	1.92	0.50
3:G:4:DC:H2"	3:G:5:DA:H8	1.76	0.50
1:B:105:LEU:HD23	1:B:111:LEU:HD13	1.94	0.50
1:B:167:PRO:HA	1:B:170:TRP:CE2	2.47	0.50
1:A:25:ILE:HB	1:A:60:VAL:HA	1.92	0.50
1:B:55:GLU:OE2	1:B:248:ARG:NH2	2.44	0.50
1:D:54:LEU:HB2	1:D:77:TRP:HA	1.94	0.50
1:B:174:ASP:O	1:B:176:ILE:N	2.45	0.50
4:H:15:DC:C6	4:H:16:DT:H72	2.47	0.50
1:C:141:GLU:O	1:C:145:VAL:HB	2.11	0.50
1:A:62:HIS:CG	1:B:56:PRO:HA	2.47	0.50
1:A:77:TRP:CD2	1:B:65:VAL:HG11	2.47	0.50
1:C:19:PHE:HE1	1:C:53:MET:HG3	1.77	0.49
1:B:261:LEU:HD23	1:B:264:LEU:HD12	1.94	0.49
5:I:46:DT:H2"	5:I:47:DG:C8	2.46	0.49
1:C:235:ILE:HG12	1:C:238:ARG:NH2	2.27	0.49
6:J:31:DA:H2"	6:J:32:DT:OP2	2.11	0.49
1:D:34:LEU:HB3	1:D:42:THR:HB	1.94	0.49
3:G:15:DG:H2'	3:G:16:DT:H71	1.94	0.49
1:C:93:GLY:HA3	1:C:99:LEU:HD11	1.95	0.49
2:E:76:ASN:OD1	2:E:77:ARG:N	2.45	0.49
6:J:30:DA:H2"	6:J:31:DA:OP2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:ILE:HB	1:C:266:PRO:HD3	1.95	0.49
2:E:23:LEU:HD22	2:E:33:GLY:HA3	1.95	0.49
4:H:32:DT:H2"	4:H:33:DT:H72	1.94	0.49
5:I:11:DG:H1'	5:I:12:DG:C8	2.48	0.49
8:L:54:HIS:HB3	8:L:56:ARG:NH1	2.28	0.49
1:A:24:GLN:NE2	3:G:2:DA:OP1	2.38	0.49
5:I:73:DC:H1'	5:I:74:DA:C8	2.48	0.49
6:J:46:DT:OP2	7:K:4:THR:HB	2.13	0.49
1:B:252:ARG:NH1	2:E:84:ASP:O	2.45	0.49
5:I:74:DA:H2"	5:I:75:DA:C8	2.48	0.49
7:K:3:LEU:HB3	8:L:43:ILE:HG12	1.93	0.49
2:E:61:ALA:HB2	2:F:3:MET:HG3	1.94	0.48
1:A:219:ILE:HA	1:A:222:ILE:HD12	1.95	0.48
1:D:17:MET:HA	1:D:51:CYS:O	2.13	0.48
2:F:18:ARG:NH1	2:F:46:GLN:OE1	2.44	0.48
1:A:36:ASP:OD1	1:A:37:LYS:N	2.45	0.48
1:B:248:ARG:O	1:B:252:ARG:HB2	2.13	0.48
2:F:38:LYS:CD	2:F:39:ILE:HD13	2.42	0.48
5:I:57:DG:N9	5:I:58:DC:C4	2.82	0.48
5:I:4:DC:H4'	5:I:5:DT:OP1	2.14	0.48
7:K:43:GLN:NE2	7:K:53:ASP:OD1	2.46	0.48
1:A:60:VAL:O	1:B:60:VAL:N	2.47	0.48
1:B:123:ARG:NH1	1:B:141:GLU:OE2	2.38	0.48
1:A:89:GLY:HA3	1:B:86:TYR:OH	2.13	0.48
1:D:9:ILE:HD11	1:D:14:ARG:HG2	1.95	0.48
4:H:17:DG:H2"	4:H:18:DG:H5"	1.96	0.48
1:C:78:VAL:HB	1:C:82:GLY:HA2	1.94	0.48
4:H:18:DG:H2'	4:H:19:DT:C6	2.49	0.48
1:C:231:LYS:HE3	1:C:235:ILE:HD11	1.95	0.48
5:I:24:DA:H2"	5:I:25:DA:H8	1.79	0.48
1:A:195:ILE:HD12	1:A:216:VAL:HG22	1.96	0.48
1:B:195:ILE:HD12	1:B:216:VAL:HG22	1.96	0.48
2:E:7:VAL:HG11	2:F:27:ARG:HG3	1.96	0.47
1:A:265:ILE:HB	1:A:266:PRO:HD3	1.96	0.47
6:J:36:DT:H2'	6:J:37:DA:C5	2.48	0.47
1:C:178:GLN:NE2	1:C:244:ASP:OD2	2.46	0.47
3:G:16:DT:H2"	3:G:17:DA:H8	1.79	0.47
1:A:84:ARG:NH1	4:H:25:DT:OP1	2.36	0.47
5:I:57:DG:C4	5:I:58:DC:C4	3.03	0.47
3:G:12:DC:H2"	3:G:13:DG:C8	2.50	0.47
6:J:10:DG:H2"	6:J:11:DA:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:5:VAL:N	2:E:59:ALA:O	2.47	0.47
5:I:9:DG:H2'	5:I:10:DC:C6	2.50	0.47
5:I:74:DA:OP2	5:I:74:DA:H8	1.97	0.47
6:J:22:DA:H2''	6:J:23:DA:H8	1.79	0.47
6:J:27:DA:C2'	6:J:28:DT:C7	2.90	0.47
1:D:40:ILE:HG22	2:F:92:LEU:HA	1.96	0.47
3:G:11:DA:H1'	3:G:12:DC:H5'	1.96	0.47
1:B:178:GLN:NE2	1:B:244:ASP:OD1	2.48	0.47
1:B:265:ILE:HB	1:B:266:PRO:HD3	1.97	0.47
1:B:174:ASP:C	1:B:176:ILE:H	2.18	0.47
2:E:25:GLU:O	2:F:89:VAL:HG11	2.14	0.47
2:E:6:VAL:HG11	2:E:19:LEU:HD13	1.96	0.47
5:I:45:DA:C2	8:L:65:LYS:HB2	2.49	0.46
5:I:45:DA:H1'	5:I:46:DT:C6	2.50	0.46
1:B:222:ILE:HG22	1:B:223:ILE:HG23	1.98	0.46
4:H:29:DG:H2'	4:H:30:DT:C6	2.50	0.46
8:L:54:HIS:HB3	8:L:56:ARG:HH12	1.79	0.46
1:B:34:LEU:O	1:B:42:THR:N	2.43	0.46
1:C:119:MET:O	1:C:123:ARG:CB	2.62	0.46
1:C:20:LEU:HD22	1:C:34:LEU:HD22	1.98	0.46
1:D:68:ALA:HB1	1:D:75:LEU:HD13	1.97	0.46
2:F:72:THR:HG21	2:F:80:PRO:HD3	1.97	0.46
8:L:58:PRO:HB3	8:L:74:GLY:N	2.29	0.46
1:A:141:GLU:O	1:A:145:VAL:HG23	2.16	0.46
1:A:219:ILE:HG12	1:A:268:ILE:HG12	1.98	0.46
1:C:252:ARG:HD2	1:C:256:ARG:NH2	2.31	0.46
1:D:31:ALA:HB2	2:E:17:GLY:HA2	1.97	0.46
2:E:76:ASN:HD22	2:F:27:ARG:CZ	2.28	0.46
1:A:21:GLN:HG2	1:A:22:TYR:CD1	2.51	0.46
5:I:24:DA:H2''	5:I:25:DA:C8	2.51	0.46
5:I:51:DT:C6	5:I:51:DT:H5'	2.50	0.46
8:L:63:ASN:O	8:L:67:GLY:N	2.35	0.46
1:A:80:GLU:OE2	4:H:23:DT:H2'	2.16	0.46
1:A:163:ARG:HA	1:A:177:ASN:ND2	2.29	0.46
1:C:55:GLU:HB3	1:C:56:PRO:HD2	1.98	0.46
2:E:68:PHE:HB3	2:F:3:MET:SD	2.55	0.46
2:F:38:LYS:HG2	2:F:39:ILE:HG12	1.98	0.46
2:F:16:ARG:NH1	4:H:15:DC:OP2	2.39	0.46
7:K:92:GLU:HA	8:L:76:TYR:H	1.81	0.46
1:A:136:GLN:HG2	5:I:21:DC:O3'	2.15	0.46
1:A:235:ILE:HG12	1:A:238:ARG:NH2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:VAL:HG12	1:D:149:TYR:CE2	2.50	0.46
2:F:51:ALA:HB3	2:F:73:PHE:HE2	1.80	0.46
6:J:25:DT:OP1	7:K:45:LYS:HD2	2.16	0.46
1:B:77:TRP:N	1:B:86:TYR:O	2.47	0.45
3:G:26:DG:H2''	3:G:27:DG:H5''	1.98	0.45
5:I:67:DA:C8	5:I:68:DT:H72	2.51	0.45
1:A:101:TYR:HE1	1:A:277:ILE:HB	1.82	0.45
1:A:217:TYR:OH	4:H:28:DT:N3	2.47	0.45
1:C:146:ARG:HA	1:C:149:TYR:HD2	1.80	0.45
3:G:24:DT:H2''	3:G:25:DG:H5'	1.99	0.45
4:H:2:DT:H2'	4:H:3:DT:H71	1.99	0.45
5:I:57:DG:N9	5:I:58:DC:C5	2.85	0.45
1:C:248:ARG:NH2	3:G:23:DT:H5''	2.32	0.45
5:I:27:DA:C8	5:I:27:DA:H5'	2.52	0.45
7:K:29:LEU:HA	7:K:32:GLU:HB3	1.99	0.45
1:B:205:GLY:HA3	1:B:214:SER:HB2	1.99	0.45
5:I:58:DC:H1'	5:I:59:DC:C5	2.50	0.45
6:J:36:DT:H2'	6:J:37:DA:C4	2.52	0.45
1:C:55:GLU:OE2	1:C:81:ALA:HA	2.17	0.45
1:D:265:ILE:HB	1:D:266:PRO:HD3	1.97	0.45
6:J:27:DA:H1'	6:J:28:DT:C7	2.47	0.45
7:K:48:GLY:HA2	7:K:86:LYS:HD3	1.99	0.45
1:D:9:ILE:HG22	2:E:39:ILE:HD12	1.99	0.45
7:K:92:GLU:HB2	8:L:75:LYS:HB2	1.99	0.45
1:A:65:VAL:HG11	1:B:77:TRP:CG	2.52	0.45
1:C:180:ILE:HD11	1:C:233:PHE:HE1	1.82	0.45
1:C:59:ARG:NH2	1:D:26:ASP:OD1	2.44	0.45
1:D:19:PHE:HB2	2:F:84:ASP:OD2	2.17	0.45
5:I:54:DT:OP1	8:L:27:LYS:NZ	2.45	0.45
7:K:11:TYR:OH	7:K:15:LYS:NZ	2.42	0.45
2:F:18:ARG:HD3	2:F:21:ILE:HD12	1.98	0.44
6:J:25:DT:H1'	6:J:26:DC:H5'	1.99	0.44
5:I:38:DT:H1'	5:I:39:DT:H5'	1.98	0.44
1:C:52:ILE:HB	1:C:75:LEU:HD23	1.98	0.44
2:F:51:ALA:HB3	2:F:73:PHE:CE2	2.52	0.44
1:A:81:ALA:HB2	1:A:256:ARG:HE	1.82	0.44
5:I:11:DG:H2''	5:I:12:DG:OP2	2.17	0.44
1:A:101:TYR:CE2	1:A:279:PRO:HB3	2.52	0.44
2:F:4:LEU:N	2:F:33:GLY:O	2.48	0.44
4:H:36:DC:H2''	4:H:37:DC:C5	2.52	0.44
1:B:34:LEU:HB3	1:B:42:THR:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:4:DC:H2''	3:G:5:DA:C8	2.53	0.44
5:I:39:DT:H2''	5:I:40:DA:C8	2.53	0.44
2:F:76:ASN:OD1	2:F:77:ARG:N	2.51	0.44
2:F:10:ASN:HD21	4:H:13:DT:P	2.40	0.44
1:C:149:TYR:HB3	1:C:160:TRP:CZ2	2.53	0.44
1:D:105:LEU:HD22	1:D:275:GLY:HA3	1.99	0.44
1:D:132:ARG:HD2	1:D:136:GLN:OE1	2.18	0.44
1:D:167:PRO:HA	1:D:170:TRP:CD2	2.52	0.44
2:F:66:THR:OG1	2:F:68:PHE:O	2.36	0.44
5:I:17:DC:H2''	5:I:18:DA:H8	1.83	0.44
1:D:99:LEU:HD22	1:D:201:ALA:HB2	2.00	0.43
4:H:1:DA:H2'	4:H:2:DT:H71	1.99	0.43
2:E:4:LEU:N	2:E:33:GLY:O	2.39	0.43
5:I:16:DA:H1'	5:I:17:DC:H5'	2.00	0.43
5:I:23:DA:H2''	5:I:24:DA:H8	1.83	0.43
1:D:174:ASP:O	1:D:176:ILE:N	2.50	0.43
8:L:63:ASN:N	8:L:68:ASP:O	2.34	0.43
1:A:146:ARG:NH1	6:J:51:DA:N3	2.66	0.43
1:B:158:VAL:HG11	1:B:176:ILE:HD13	2.01	0.43
2:F:37:ALA:O	2:F:38:LYS:C	2.55	0.43
3:G:21:DA:H2'	3:G:22:DA:H8	1.78	0.43
6:J:12:DC:H2''	6:J:13:DT:H72	2.00	0.43
1:C:164:ARG:O	1:C:177:ASN:ND2	2.50	0.43
2:E:8:THR:HA	2:E:56:VAL:HG22	2.00	0.43
6:J:48:DT:C6	6:J:49:DT:H72	2.53	0.43
1:A:99:LEU:HD22	1:A:201:ALA:HB2	2.00	0.43
2:F:70:PHE:CE2	2:F:80:PRO:HB3	2.54	0.43
1:B:229:VAL:N	1:B:230:PRO:HD2	2.34	0.43
1:C:265:ILE:O	1:C:269:GLU:HG3	2.19	0.43
1:D:25:ILE:HD13	1:D:34:LEU:HA	2.01	0.43
2:E:8:THR:HB	2:E:11:VAL:HG21	2.00	0.43
8:L:14:GLN:OE1	8:L:16:HIS:NE2	2.51	0.43
1:A:95:ARG:HB3	1:A:97:ASP:OD1	2.18	0.43
2:F:8:THR:HB	2:F:11:VAL:HG21	2.01	0.43
6:J:47:DG:H2'	6:J:48:DT:H71	2.00	0.43
1:A:212:PRO:HB3	1:B:94:ALA:O	2.19	0.42
1:B:130:ALA:O	1:B:132:ARG:HD2	2.19	0.42
1:B:182:ALA:HB3	1:B:247:VAL:HG11	2.00	0.42
3:G:14:DA:H2''	3:G:15:DG:H8	1.84	0.42
5:I:70:DT:H1'	5:I:71:DA:H5'	2.01	0.42
4:H:12:DG:C2	4:H:13:DT:C2	3.06	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:58:DC:OP2	5:I:58:DC:H3'	2.19	0.42
7:K:46:LEU:HB2	7:K:49:PHE:HB3	2.01	0.42
2:F:5:VAL:HG22	2:F:32:VAL:HG22	2.01	0.42
5:I:49:DT:C6	5:I:50:DT:H72	2.54	0.42
8:L:4:SER:HA	8:L:7:ILE:HD12	2.01	0.42
2:F:38:LYS:HG2	2:F:39:ILE:H	1.80	0.42
6:J:-4:DA:H2''	6:J:-3:DG:C8	2.55	0.42
1:C:203:ALA:HB1	1:D:96:SER:HB2	2.02	0.42
1:B:256:ARG:HD3	2:E:65:GLU:HA	2.02	0.42
3:G:11:DA:C2	3:G:12:DC:C2	3.06	0.42
2:E:10:ASN:HD21	3:G:13:DG:P	2.43	0.42
6:J:24:DA:C2'	6:J:25:DT:H71	2.48	0.42
1:C:83:VAL:HG13	1:C:84:ARG:HG2	2.02	0.42
1:D:195:ILE:HD12	1:D:216:VAL:HG22	2.00	0.42
5:I:57:DG:H2'	5:I:58:DC:C5	2.45	0.42
5:I:77:DT:C6	5:I:78:DT:H72	2.54	0.42
6:J:26:DC:H2''	6:J:27:DA:C8	2.55	0.42
1:A:174:ASP:OD1	1:A:175:THR:N	2.53	0.42
4:H:16:DT:H2''	4:H:17:DG:C8	2.55	0.42
5:I:11:DG:C8	5:I:11:DG:H5'	2.55	0.42
1:A:20:LEU:HD21	1:A:44:ILE:HD11	2.02	0.42
1:B:171:GLU:C	1:B:173:GLY:H	2.23	0.42
1:C:105:LEU:HD23	1:C:111:LEU:HD13	2.02	0.42
4:H:17:DG:H2''	4:H:18:DG:H8	1.85	0.42
1:A:26:ASP:OD1	1:A:27:VAL:N	2.47	0.42
1:B:17:MET:HA	1:B:51:CYS:O	2.19	0.42
2:E:4:LEU:HD11	2:E:58:MET:SD	2.59	0.42
1:C:181:SER:OG	3:G:27:DG:N3	2.32	0.42
5:I:45:DA:H2''	5:I:46:DT:H72	2.01	0.42
1:A:90:GLN:HB3	1:A:94:ALA:HB2	2.01	0.41
1:D:35:ILE:HG13	1:D:41:ARG:HG2	2.02	0.41
6:J:46:DT:OP1	7:K:5:LYS:HG3	2.20	0.41
1:B:167:PRO:HA	1:B:170:TRP:CD2	2.55	0.41
1:C:269:GLU:O	1:C:273:ALA:HB2	2.20	0.41
1:C:83:VAL:HG21	1:C:248:ARG:HG3	2.01	0.41
2:E:12:PRO:HG3	2:E:52:GLU:HG3	2.01	0.41
5:I:43:DT:H1'	5:I:44:DA:C2	2.56	0.41
1:B:77:TRP:HB2	1:B:86:TYR:HB3	2.01	0.41
2:E:6:VAL:O	2:E:31:TYR:N	2.35	0.41
2:F:37:ALA:O	2:F:38:LYS:O	2.38	0.41
4:H:30:DT:H2''	4:H:31:DG:H5''	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:39:DT:H2''	5:I:40:DA:OP2	2.19	0.41
1:C:208:HIS:O	1:C:214:SER:HB3	2.20	0.41
1:D:117:ARG:NH2	1:D:128:ALA:O	2.52	0.41
6:J:0:DG:H2''	6:J:1:DG:N7	2.35	0.41
6:J:22:DA:H2''	6:J:23:DA:C8	2.55	0.41
5:I:44:DA:H4'	8:L:72:LEU:HD11	2.02	0.41
1:D:16:SER:HB3	1:D:252:ARG:HG3	2.02	0.41
7:K:63:ARG:HA	7:K:71:ILE:H	1.85	0.41
1:D:21:GLN:HB3	1:D:55:GLU:OE1	2.21	0.41
5:I:69:DC:C2'	5:I:70:DT:H72	2.51	0.41
7:K:83:PRO:O	7:K:88:LYS:HE3	2.21	0.41
1:D:6:LEU:HD23	1:D:70:GLN:HB3	2.03	0.41
1:B:3:TRP:CG	4:H:25:DT:H1'	2.55	0.41
2:F:9:GLU:HB3	2:F:55:ASN:OD1	2.21	0.41
5:I:17:DC:H4'	5:I:18:DA:OP1	2.20	0.41
1:B:275:GLY:C	1:B:277:ILE:H	2.23	0.41
1:D:47:GLY:HA3	2:E:22:TRP:CD1	2.56	0.41
5:I:57:DG:C3'	5:I:58:DC:C6	3.03	0.41
1:C:16:SER:N	1:C:49:VAL:HA	2.36	0.41
1:C:56:PRO:HG3	3:G:24:DT:OP2	2.21	0.41
1:A:80:GLU:N	1:A:83:VAL:HG12	2.36	0.41
1:C:97:ASP:OD1	1:C:98:LYS:N	2.54	0.41
5:I:7:DG:H2''	5:I:8:DC:OP2	2.22	0.41
1:A:111:LEU:HD23	1:A:114:LYS:HD2	2.03	0.40
1:C:223:ILE:HD13	1:C:264:LEU:HD21	2.03	0.40
1:A:139:GLY:HA2	6:J:52:DG:N2	2.36	0.40
1:B:46:VAL:HG23	1:B:52:ILE:HD12	2.02	0.40
5:I:8:DC:C2	5:I:9:DG:C8	3.10	0.40
8:L:7:ILE:HG23	8:L:22:VAL:HG12	2.03	0.40
6:J:39:DT:H2'	6:J:39:DT:H6	1.68	0.40
1:C:89:GLY:HA3	1:D:86:TYR:OH	2.22	0.40
4:H:16:DT:H2''	4:H:17:DG:H8	1.86	0.40
7:K:77:ARG:H	8:L:91:ASN:CG	2.25	0.40
1:A:47:GLY:C	1:A:49:VAL:H	2.24	0.40
1:C:137:LEU:HD23	1:C:140:ILE:HD12	2.03	0.40
6:J:25:DT:P	7:K:51:ASN:HD21	2.43	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	258/305 (85%)	245 (95%)	13 (5%)	0	100	100
1	B	277/305 (91%)	260 (94%)	17 (6%)	0	100	100
1	C	252/305 (83%)	241 (96%)	11 (4%)	0	100	100
1	D	270/305 (88%)	258 (96%)	11 (4%)	1 (0%)	38	76
2	E	92/103 (89%)	88 (96%)	4 (4%)	0	100	100
2	F	92/103 (89%)	86 (94%)	6 (6%)	0	100	100
7	K	94/99 (95%)	92 (98%)	2 (2%)	0	100	100
8	L	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
All	All	1427/1619 (88%)	1360 (95%)	66 (5%)	1 (0%)	58	87

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	175	THR

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/245 (85%)	208 (100%)	1 (0%)	91	97
1	B	225/245 (92%)	225 (100%)	0	100	100
1	C	203/245 (83%)	202 (100%)	1 (0%)	91	97
1	D	218/245 (89%)	218 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	79/87 (91%)	79 (100%)	0	100	100
2	F	79/87 (91%)	79 (100%)	0	100	100
7	K	82/86 (95%)	82 (100%)	0	100	100
8	L	78/79 (99%)	77 (99%)	1 (1%)	73	89
All	All	1173/1319 (89%)	1170 (100%)	3 (0%)	94	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	ASN
1	C	239	ASN
8	L	42	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
1	A	239	ASN
1	B	177	ASN
1	C	90	GLN
1	C	239	ASN
2	F	10	ASN
7	K	59	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.