Full wwPDB EM Validation Report ⓘ

Apr 9, 2025 – 03:17 PM JST

PDB ID	:	9IPU / pdb_00009ipu
EMDB ID	:	EMD-60781
Title	:	cryo-EM structure of the RNF168(1-193)/UbcH5c-Ub ubiquitylation module bound to H1.0-K63-Ub3 modified chromatosome
Authors	:	Ai, H.S.; Deng, Z.H.; Liu, L.
Deposited on	:	2024-07-11
Resolution	:	4.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

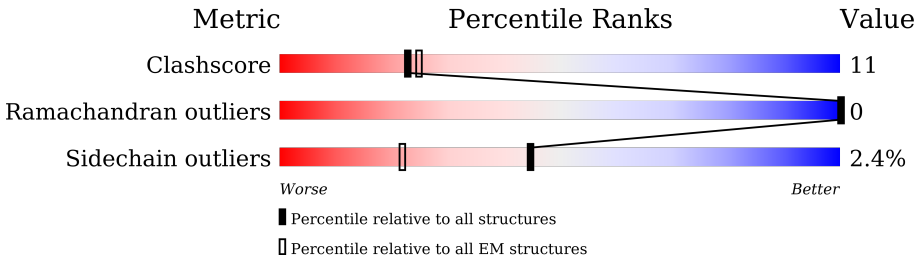
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 4.30 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	I	194	35% · 63%
2	A	135	51% 21% 27%
2	E	135	50% 21% 28%
3	B	102	60% 19% · 19%
3	F	102	61% 21% 19%
4	C	129	72% 12% · 16%
4	G	129	71% 12% · 16%
5	D	125	60% 15% 25%
5	H	125	62% 12% · 25%

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Mol	Chain	Length	Quality of chain
6	K	147	
7	L	193	
8	M	75	
9	J	171	
10	N	171	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 15750 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 Histone H1.0.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	72	Total	C	N	O	S	0	0
			526	327	97	100	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	82	CYS	LYS	conflict	UNP P07305

- Molecule 2 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	98	Total	C	N	O	S	0	0
			810	511	157	140	2		
2	E	97	Total	C	N	O	S	0	0
			801	505	155	139	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	SER	CYS	conflict	UNP Q71DI3
E	110	SER	CYS	conflict	UNP Q71DI3

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	83	Total	C	N	O	S	0	0
			668	422	132	113	1		
3	F	83	Total	C	N	O	S	0	0
			662	419	129	113	1		

- Molecule 4 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	109	Total	C	N	O	S	0	0
			833	523	164	145	1		
4	G	109	Total	C	N	O	S	0	0
			833	523	164	145	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	15	CYS	LYS	conflict	UNP P04908
G	15	CYS	LYS	conflict	UNP P04908

- Molecule 5 is a protein called Histone H2B type 1-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	94	Total	C	N	O	S	0	0
			735	461	134	138	2		
5	H	94	Total	C	N	O	S	0	0
			735	461	134	138	2		

- Molecule 6 is a protein called Ubiquitin-conjugating enzyme E2 D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	147	Total	C	N	O	S	0	0
			1125	726	187	207	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	21	SER	CYS	conflict	UNP P61077
K	107	SER	CYS	conflict	UNP P61077
K	111	SER	CYS	conflict	UNP P61077

- Molecule 7 is a protein called E3 ubiquitin-protein ligase RNF168.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	83	Total	C	N	O	S	0	0
			641	404	115	112	10		

- Molecule 8 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	61	Total	C	N	O	S	0	0
			407	251	68	87	1		

- Molecule 9 is a DNA chain called DNA (171-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	170	Total	C	N	O	P	0	0
			3488	1653	645	1020	170		

- Molecule 10 is a DNA chain called DNA (171-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	170	Total	C	N	O	P	0	0
			3484	1652	643	1019	170		

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

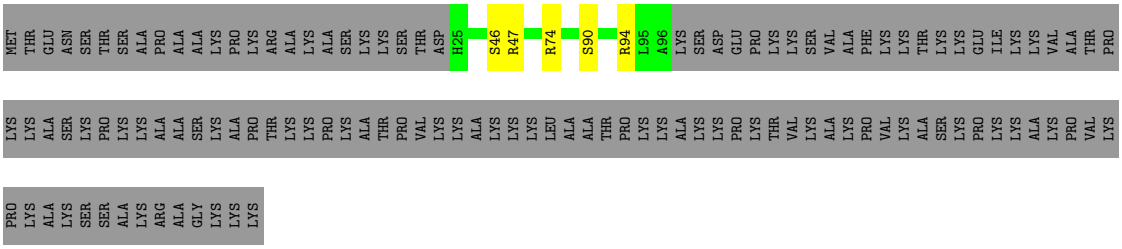
Mol	Chain	Residues	Atoms		AltConf
11	L	2	Total	Zn	0
			2	2	

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. 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.

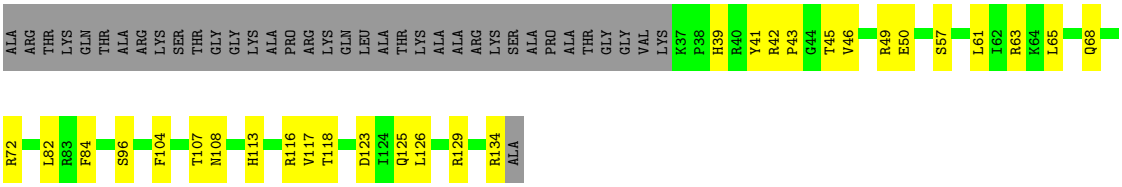
- Molecule 1: Histone H1.0

Chain I:



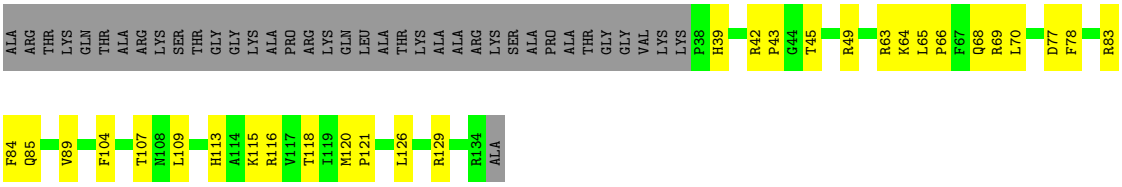
- Molecule 2: Histone H3.2

Chain A:



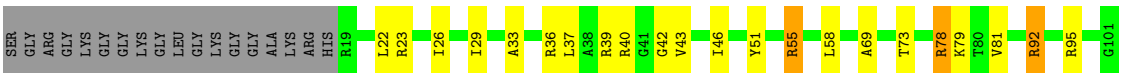
- Molecule 2: Histone H3.2

Chain E:



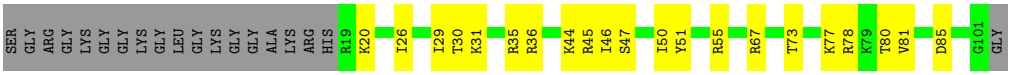
- Molecule 3: Histone H4

Chain B:



• Molecule 3: Histone H4

Chain F:

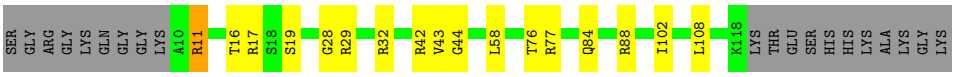


• Molecule 4: Histone H2A type 1-B/E

Chain C:

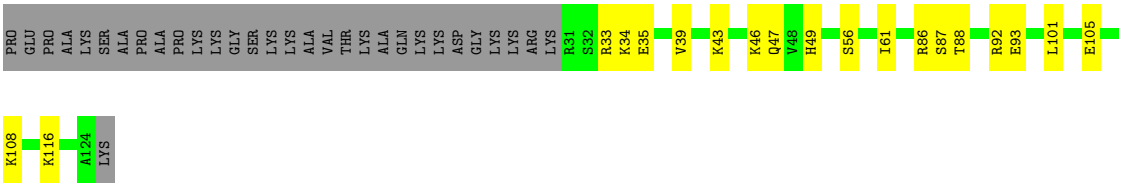
• Molecule 4: Histone H2A type 1-B/E

Chain G:



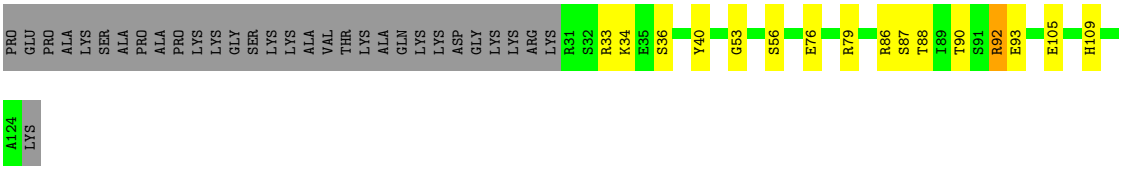
• Molecule 5: Histone H2B type 1-K

Chain D:



• Molecule 5: Histone H2B type 1-K

Chain H:

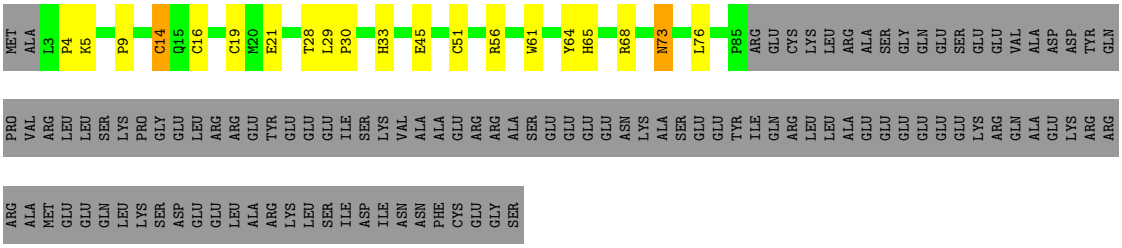


• Molecule 6: Ubiquitin-conjugating enzyme E2 D3

Chain K:

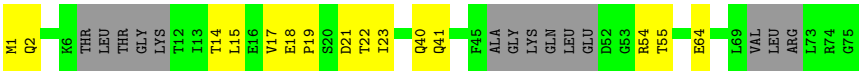
• Molecule 7: E3 ubiquitin-protein ligase RNF168

Chain L:



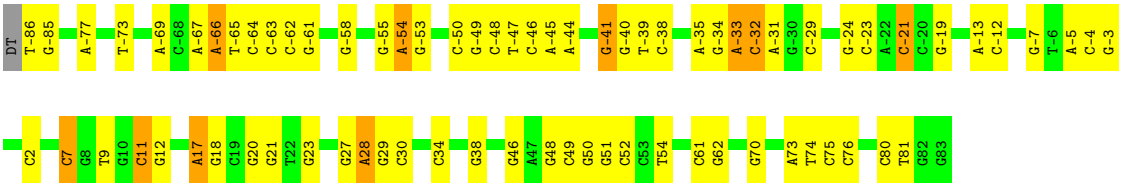
• Molecule 8: Ubiquitin

Chain M:



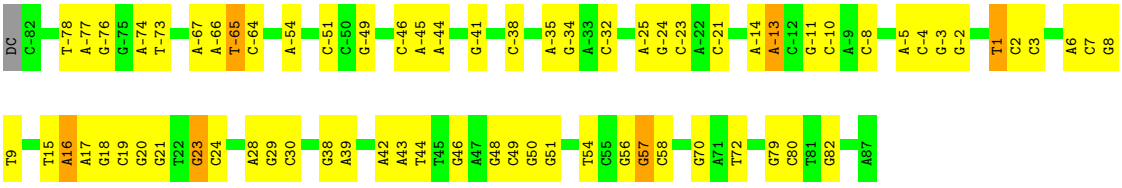
• Molecule 9: DNA (171-MER)

Chain J:



• Molecule 10: DNA (171-MER)

Chain N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36240	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	I	0.59	0/532	0.79	1/716 (0.1%)
2	A	0.34	0/822	0.55	0/1102
2	E	0.33	0/813	0.55	0/1090
3	B	0.35	0/675	0.58	0/903
3	F	0.35	0/669	0.58	0/896
4	C	0.32	0/843	0.53	0/1139
4	G	0.30	0/843	0.52	0/1139
5	D	0.34	0/746	0.48	0/1003
5	H	0.32	0/746	0.48	0/1003
6	K	0.27	0/1160	0.43	0/1589
7	L	0.25	0/658	0.53	0/902
8	M	0.25	0/409	0.42	0/556
9	J	0.82	6/3913 (0.2%)	1.32	28/6038 (0.5%)
10	N	0.81	6/3908 (0.2%)	1.30	28/6029 (0.5%)
All	All	0.61	12/16737 (0.1%)	1.00	57/24105 (0.2%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	N	79	DG	C3'-O3'	-7.20	1.34	1.44
10	N	-78	DT	C1'-N1	6.26	1.57	1.49
10	N	-77	DA	C3'-O3'	5.98	1.51	1.44
10	N	82	DG	C3'-O3'	-5.94	1.36	1.44
9	J	-69	DA	C3'-O3'	-5.92	1.36	1.44
10	N	-78	DT	C3'-O3'	5.88	1.51	1.44
9	J	-85	DG	C3'-O3'	-5.67	1.36	1.44
9	J	75	DC	C1'-N1	-5.50	1.39	1.47
9	J	-77	DA	C3'-O3'	-5.34	1.37	1.44
9	J	-86	DT	C1'-N1	5.34	1.56	1.49
9	J	-73	DT	C1'-N1	5.17	1.55	1.49
10	N	72	DT	C1'-N1	5.05	1.55	1.49

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J	21	DG	O4'-C1'-N9	9.69	114.78	108.00
10	N	54	DT	P-O3'-C3'	8.00	129.30	119.70
9	J	54	DT	P-O3'-C3'	7.60	128.82	119.70
9	J	-58	DG	P-O3'-C3'	7.58	128.79	119.70
10	N	-2	DG	O4'-C1'-N9	7.39	113.17	108.00
9	J	75	DC	O4'-C1'-N1	7.32	113.12	108.00
10	N	-10	DC	O4'-C1'-N1	7.30	113.11	108.00
9	J	20	DG	P-O3'-C3'	7.21	128.35	119.70
10	N	-77	DA	O5'-P-OP2	-7.20	99.22	105.70
9	J	-32	DC	O4'-C1'-N1	7.03	112.92	108.00
9	J	34	DC	P-O3'-C3'	6.92	128.00	119.70
9	J	29	DG	C3'-C2'-C1'	-6.79	94.35	102.50
10	N	43	DA	P-O3'-C3'	6.78	127.84	119.70
9	J	-33	DA	P-O3'-C3'	6.76	127.81	119.70
10	N	42	DA	P-O3'-C3'	6.69	127.73	119.70
10	N	57	DG	P-O3'-C3'	6.50	127.50	119.70
9	J	30	DC	O4'-C1'-N1	6.44	112.51	108.00
10	N	23	DG	P-O3'-C3'	6.41	127.39	119.70
9	J	-38	DC	P-O3'-C3'	6.40	127.38	119.70
10	N	-32	DC	O4'-C1'-N1	6.34	112.44	108.00
10	N	-38	DC	P-O3'-C3'	6.26	127.21	119.70
10	N	-14	DA	P-O3'-C3'	6.19	127.13	119.70
10	N	16	DA	O4'-C1'-N9	6.19	112.33	108.00
9	J	-41	DG	P-O3'-C3'	6.19	127.12	119.70
10	N	30	DC	O4'-C1'-N1	6.06	112.24	108.00
9	J	11	DC	O4'-C1'-N1	6.03	112.22	108.00
9	J	75	DC	C6-N1-C2	6.00	122.70	120.30
9	J	-29	DC	P-O3'-C3'	5.99	126.89	119.70
9	J	17	DA	O4'-C1'-N9	-5.99	103.81	108.00
10	N	-76	DG	O4'-C1'-N9	5.97	112.18	108.00
10	N	-13	DA	P-O3'-C3'	5.97	126.86	119.70
9	J	-21	DC	P-O3'-C3'	5.83	126.69	119.70
9	J	7	DC	O4'-C1'-N1	5.82	112.08	108.00
10	N	-65	DT	N3-C4-O4	5.72	123.33	119.90
9	J	18	DG	P-O3'-C3'	5.69	126.53	119.70
10	N	-51	DC	P-O3'-C3'	5.62	126.44	119.70
10	N	-21	DC	O4'-C1'-N1	5.62	111.93	108.00
9	J	23	DG	P-O3'-C3'	5.61	126.43	119.70
10	N	-11	DG	O4'-C1'-N9	5.51	111.86	108.00
9	J	75	DC	C3'-C2'-C1'	-5.37	96.06	102.50
9	J	-66	DA	OP1-P-O3'	5.34	116.96	105.20
10	N	-8	DC	O4'-C1'-N1	5.33	111.73	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	N	-65	DT	C5-C4-O4	-5.33	121.17	124.90
10	N	-49	DG	O4'-C1'-N9	5.30	111.71	108.00
9	J	-65	DT	P-O3'-C3'	5.26	126.01	119.70
9	J	-21	DC	O4'-C1'-N1	5.26	111.68	108.00
9	J	28	DA	P-O3'-C3'	5.20	125.93	119.70
10	N	-13	DA	O5'-P-OP2	-5.16	101.05	105.70
9	J	76	DC	O4'-C1'-N1	5.14	111.60	108.00
10	N	44	DT	O4'-C1'-N1	5.13	111.59	108.00
9	J	-53	DG	C1'-O4'-C4'	-5.13	104.97	110.10
10	N	1	DT	P-O3'-C3'	5.11	125.83	119.70
1	I	47	ARG	NE-CZ-NH1	5.11	122.86	120.30
9	J	-54	DA	P-O3'-C3'	5.08	125.80	119.70
10	N	-23	DC	C1'-O4'-C4'	-5.05	105.05	110.10
10	N	-49	DG	O4'-C1'-C2'	-5.02	101.88	105.90
10	N	29	DG	O4'-C1'-N9	5.01	111.51	108.00

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	I	526	0	524	4	0
2	A	810	0	851	45	0
2	E	801	0	839	48	0
3	B	668	0	719	21	0
3	F	662	0	708	20	0
4	C	833	0	883	23	0
4	G	833	0	883	21	0
5	D	735	0	756	31	0
5	H	735	0	756	36	0
6	K	1125	0	1079	31	0
7	L	641	0	613	15	0
8	M	407	0	325	9	0
9	J	3488	0	1908	96	0
10	N	3484	0	1908	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	L	2	0	0	0	0
All	All	15750	0	12752	314	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 11.

All (314) 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)
2:E:49:ARG:HH12	10:N:-66:DA:C5’	1.11	1.59
2:E:49:ARG:NH1	10:N:-66:DA:H5”	1.12	1.42
2:A:49:ARG:NH1	9:J:-66:DA:H5”	1.08	1.39
2:A:45:THR:HG21	10:N:70:DG:OP1	1.30	1.27
2:A:49:ARG:CZ	9:J:-66:DA:H5”	1.64	1.27
2:A:49:ARG:NH1	9:J:-66:DA:C5’	2.02	1.22
2:E:49:ARG:NH1	10:N:-66:DA:C5’	1.81	1.17
2:A:45:THR:CG2	10:N:70:DG:OP1	1.93	1.17
3:B:78:ARG:HB2	9:J:28:DA:OP2	1.42	1.16
2:E:42:ARG:HG2	9:J:70:DG:P	1.89	1.12
2:E:49:ARG:HD3	10:N:-65:DT:OP1	1.50	1.12
2:E:49:ARG:NH1	10:N:-66:DA:C4’	2.23	1.02
2:E:49:ARG:CZ	10:N:-66:DA:H4’	1.91	1.00
4:C:32:ARG:HE	10:N:-44:DA:P	1.86	0.97
4:C:32:ARG:HD3	10:N:-44:DA:OP2	1.65	0.95
2:E:49:ARG:CZ	10:N:-66:DA:H5”	1.94	0.94
2:A:49:ARG:HH12	9:J:-66:DA:H5”	1.12	0.93
3:F:47:SER:HB2	10:N:7:DC:OP1	1.70	0.90
5:D:56:SER:HB3	10:N:-54:DA:OP2	1.71	0.89
4:C:77:ARG:CZ	10:N:-54:DA:H4’	2.04	0.87
1:I:74:ARG:NH1	10:N:80:DC:OP1	2.07	0.86
2:A:43:PRO:HG2	10:N:-5:DA:H5’	1.55	0.86
4:C:32:ARG:NE	10:N:-44:DA:OP1	2.09	0.84
5:H:33:ARG:HD3	9:J:-46:DC:H5”	1.58	0.84
5:H:33:ARG:HD3	9:J:-46:DC:C5’	2.09	0.83
4:G:32:ARG:HD3	9:J:-44:DA:OP2	1.79	0.83
2:E:45:THR:HG21	9:J:70:DG:OP1	1.79	0.82
2:E:63:ARG:HD3	10:N:17:DA:H4’	1.62	0.81
5:H:56:SER:HB3	9:J:-54:DA:P	2.20	0.81
2:A:49:ARG:CZ	9:J:-66:DA:C5’	2.50	0.81
3:B:78:ARG:CB	9:J:28:DA:OP2	2.27	0.80
3:B:78:ARG:HB2	9:J:28:DA:P	2.22	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:11:ARG:HB3	9:J:-41:DG:OP1	1.83	0.79
4:C:32:ARG:NE	10:N:-44:DA:P	2.57	0.77
2:E:42:ARG:CG	9:J:70:DG:P	2.70	0.77
3:B:46:ILE:O	9:J:7:DC:H3'	1.85	0.76
2:A:118:THR:N	10:N:-3:DG:OP1	2.20	0.74
2:E:49:ARG:CZ	10:N:-66:DA:C4'	2.63	0.74
2:E:68:GLN:HG2	2:E:89:VAL:HG11	1.69	0.74
7:L:64:TYR:O	7:L:68:ARG:NH1	2.21	0.73
5:D:87:SER:OG	10:N:-35:DA:H3'	1.88	0.72
2:A:41:TYR:OH	9:J:-67:DA:H4'	1.88	0.71
5:H:40:TYR:OH	10:N:48:DG:OP1	2.07	0.71
5:D:86:ARG:NH1	10:N:-34:DG:C2'	2.53	0.70
4:C:32:ARG:CD	10:N:-44:DA:OP2	2.39	0.70
5:H:86:ARG:NH1	9:J:-34:DG:C2'	2.54	0.70
5:D:34:LYS:O	9:J:49:DC:H5"	1.92	0.70
5:H:56:SER:CB	9:J:-54:DA:OP1	2.40	0.70
2:A:61:LEU:O	3:B:36:ARG:NH1	2.25	0.69
2:E:42:ARG:HD2	9:J:70:DG:OP2	1.93	0.68
2:E:42:ARG:HG2	9:J:70:DG:OP1	1.93	0.68
2:E:42:ARG:HG2	9:J:70:DG:O5'	1.94	0.68
6:K:4:LYS:NZ	7:L:21:GLU:OE2	2.27	0.68
8:M:22:THR:HG22	8:M:55:THR:HG22	1.75	0.67
2:A:45:THR:HG22	10:N:70:DG:OP1	1.94	0.67
5:D:33:ARG:HH22	9:J:48:DG:H21	1.39	0.67
5:D:33:ARG:NH2	9:J:48:DG:H21	1.93	0.67
4:G:77:ARG:CZ	10:N:57:DG:H4'	2.25	0.67
5:H:56:SER:HB3	9:J:-54:DA:OP1	1.94	0.67
2:E:70:LEU:HD22	3:F:29:ILE:HD11	1.77	0.67
6:K:35:ALA:HB3	6:K:52:LEU:HB2	1.75	0.67
5:D:33:ARG:HD3	10:N:-46:DC:C5'	2.25	0.67
9:J:11:DC:H2"	9:J:12:DG:C8	2.30	0.67
2:E:65:LEU:HD12	10:N:17:DA:H2'	1.75	0.66
3:F:36:ARG:NH2	9:J:-13:DA:OP2	2.28	0.66
5:H:86:ARG:NH2	9:J:-33:DA:OP2	2.29	0.66
10:N:-65:DT:H1'	10:N:-64:DC:H5'	1.78	0.66
6:K:22:SER:OG	6:K:36:THR:OG1	2.14	0.65
10:N:49:DC:H2'	10:N:50:DG:C8	2.32	0.65
5:D:86:ARG:HH12	10:N:-34:DG:C2'	2.11	0.64
10:N:50:DG:H2"	10:N:51:DG:OP2	1.97	0.64
2:A:61:LEU:HD12	3:B:37:LEU:HD23	1.78	0.64
2:A:63:ARG:HD3	9:J:17:DA:H4'	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:86:ARG:NH1	10:N:-34:DG:H3'	2.11	0.64
5:H:86:ARG:NH1	9:J:-34:DG:H3'	2.13	0.63
4:G:77:ARG:HB2	10:N:58:DC:OP1	1.97	0.63
2:A:39:HIS:CD2	9:J:-67:DA:H5"	2.33	0.63
5:H:86:ARG:HH12	9:J:-34:DG:C2'	2.10	0.63
4:G:44:GLY:HA2	10:N:38:DG:OP1	1.99	0.63
5:H:76:GLU:OE1	5:H:79:ARG:NH2	2.32	0.63
3:B:29:ILE:HD13	3:B:58:LEU:HD23	1.81	0.62
2:A:50:GLU:OE2	3:B:39:ARG:NE	2.32	0.62
1:I:94:ARG:NH1	9:J:80:DC:OP1	2.33	0.62
2:E:84:PHE:O	9:J:-24:DG:H3'	2.00	0.62
4:C:115:LEU:HD13	3:F:44:LYS:HB2	1.82	0.62
2:E:42:ARG:NH1	9:J:70:DG:OP2	2.24	0.62
2:A:49:ARG:HH12	9:J:-66:DA:C5'	1.87	0.61
9:J:61:DC:H2"	9:J:62:DG:C8	2.36	0.61
2:E:42:ARG:CG	9:J:70:DG:OP1	2.48	0.60
3:B:36:ARG:HH21	10:N:-13:DA:P	2.23	0.60
5:H:33:ARG:CD	9:J:-46:DC:C5'	2.79	0.60
6:K:38:MET:HG2	6:K:49:VAL:HG22	1.82	0.60
5:D:86:ARG:NH1	10:N:-34:DG:C3'	2.64	0.60
5:D:87:SER:OG	10:N:-35:DA:C3'	2.50	0.59
4:C:32:ARG:NH2	5:D:35:GLU:OE1	2.34	0.59
4:C:77:ARG:NE	10:N:-54:DA:H4'	2.17	0.59
5:D:35:GLU:OE2	10:N:-45:DA:H5"	2.02	0.59
2:E:45:THR:CG2	9:J:70:DG:OP1	2.50	0.59
3:F:80:THR:CG2	10:N:28:DA:H5"	2.33	0.58
7:L:29:LEU:HD12	7:L:33:HIS:HB2	1.84	0.58
2:A:43:PRO:HG2	10:N:-5:DA:C5'	2.29	0.58
2:E:64:LYS:HB2	10:N:18:DG:OP2	2.03	0.58
4:G:76:THR:O	5:H:53:GLY:N	2.32	0.58
2:A:43:PRO:CG	10:N:-5:DA:H5'	2.32	0.58
3:B:36:ARG:NH2	10:N:-13:DA:P	2.77	0.58
2:E:118:THR:N	9:J:-3:DG:OP1	2.37	0.58
6:K:87:ASP:O	6:K:92:GLN:N	2.37	0.58
2:A:41:TYR:HH	9:J:-67:DA:H4'	1.68	0.57
1:I:46:SER:OG	10:N:3:DC:OP1	2.22	0.57
3:F:80:THR:HG22	10:N:28:DA:H5"	1.86	0.57
2:A:41:TYR:OH	9:J:-67:DA:C4'	2.52	0.57
3:F:77:LYS:HE3	5:H:92:ARG:HH12	1.69	0.56
4:C:42:ARG:HG3	5:D:88:THR:HG23	1.86	0.56
2:A:104:PHE:HA	2:A:107:THR:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:77:ARG:NE	10:N:57:DG:H4'	2.19	0.56
9:J:51:DG:H1'	9:J:52:DC:H5'	1.88	0.56
3:F:36:ARG:HH22	9:J:-13:DA:P	2.28	0.56
5:D:33:ARG:HD3	10:N:-46:DC:H5'	1.86	0.56
5:D:86:ARG:HH12	10:N:-34:DG:H2"	1.70	0.55
2:A:42:ARG:HD2	10:N:70:DG:P	2.47	0.55
5:H:86:ARG:NH1	9:J:-34:DG:H2'	2.20	0.55
7:L:4:PRO:HG3	7:L:76:LEU:HD13	1.87	0.55
5:H:86:ARG:NH1	9:J:-34:DG:C3'	2.70	0.55
3:B:92:ARG:HH22	5:D:101:LEU:HD23	1.71	0.55
6:K:77:ASN:HD21	6:K:114:ASN:HB2	1.71	0.55
2:A:117:VAL:N	10:N:-3:DG:OP1	2.40	0.55
8:M:17:VAL:HG21	8:M:21:ASP:HB2	1.87	0.55
2:A:68:GLN:HE21	2:A:72:ARG:HE	1.53	0.54
3:F:46:ILE:HG23	3:F:50:ILE:HD12	1.88	0.54
5:H:33:ARG:NH2	10:N:49:DC:H1'	2.21	0.54
6:K:108:SER:O	6:K:112:ASP:N	2.40	0.54
6:K:30:MET:O	6:K:33:TRP:NE1	2.41	0.54
5:H:56:SER:HB3	9:J:-54:DA:OP2	2.07	0.54
4:G:32:ARG:CD	9:J:-44:DA:OP2	2.55	0.54
6:K:60:TYR:CG	6:K:61:PRO:HA	2.44	0.53
4:C:13:LYS:H	4:C:13:LYS:HD3	1.73	0.53
2:E:49:ARG:NH2	10:N:-66:DA:H4'	2.20	0.53
6:K:34:GLN:HE21	6:K:51:PHE:HB3	1.74	0.53
7:L:16:CYS:HB3	7:L:19:CYS:SG	2.48	0.53
10:N:-66:DA:H2"	10:N:-65:DT:H72	1.91	0.53
9:J:-50:DC:H2"	9:J:-49:DG:C8	2.44	0.52
9:J:-64:DC:H2"	9:J:-63:DC:C6	2.45	0.52
2:E:49:ARG:HH12	10:N:-66:DA:H5"	0.37	0.52
3:B:36:ARG:NH2	10:N:-13:DA:OP1	2.43	0.52
5:D:33:ARG:HH22	9:J:48:DG:N2	2.07	0.52
5:H:87:SER:H	9:J:-34:DG:P	2.33	0.52
2:A:49:ARG:CZ	9:J:-66:DA:H4'	2.40	0.51
7:L:4:PRO:HB3	7:L:76:LEU:HD22	1.93	0.51
6:K:86:LEU:HG	6:K:88:ILE:HG12	1.92	0.51
6:K:76:PRO:HD2	6:K:113:PRO:HB3	1.92	0.51
4:G:32:ARG:HE	9:J:-44:DA:P	2.33	0.51
2:A:49:ARG:NH2	9:J:-66:DA:H5"	2.22	0.50
9:J:-7:DG:C6	10:N:6:DA:N6	2.79	0.50
4:C:43:VAL:O	9:J:38:DG:H3'	2.11	0.50
3:F:26:ILE:HD11	3:F:55:ARG:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:33:ARG:HD3	10:N:-46:DC:H5”	1.93	0.50
2:A:57:SER:O	3:B:40:ARG:NH2	2.44	0.50
7:L:4:PRO:N	7:L:5:LYS:HA	2.27	0.49
9:J:-47:DT:H2”	9:J:-46:DC:C6	2.48	0.49
10:N:-66:DA:H2”	10:N:-65:DT:C7	2.42	0.49
5:H:56:SER:OG	9:J:-54:DA:OP1	2.31	0.49
7:L:30:PRO:HD3	7:L:61:TRP:CD2	2.47	0.49
2:A:125:GLN:O	2:A:134:ARG:NH2	2.45	0.49
7:L:51:CYS:HB3	7:L:56:ARG:N	2.28	0.49
5:H:87:SER:OG	9:J:-35:DA:H3’	2.13	0.49
4:G:42:ARG:HG3	5:H:88:THR:HG23	1.95	0.48
9:J:-40:DG:H2”	9:J:-39:DT:OP2	2.12	0.48
2:E:69:ARG:HH22	10:N:17:DA:P	2.36	0.48
5:H:33:ARG:HH22	10:N:49:DC:H1’	1.79	0.48
7:L:9:PRO:O	7:L:14:CYS:HB2	2.13	0.48
4:G:29:ARG:NH1	5:H:36:SER:O	2.46	0.48
7:L:64:TYR:HD2	7:L:65:HIS:CD2	2.32	0.48
4:G:42:ARG:HB2	10:N:38:DG:H4’	1.96	0.48
5:H:33:ARG:CD	9:J:-46:DC:H5’	2.44	0.48
10:N:15:DT:H2”	10:N:16:DA:C8	2.48	0.48
3:F:45:ARG:HD3	9:J:-4:DC:H5”	1.95	0.48
5:H:87:SER:OG	9:J:-35:DA:C3’	2.62	0.48
9:J:-32:DC:H2”	9:J:-31:DA:OP2	2.14	0.48
4:C:102:ILE:HG23	5:D:61:ILE:HD13	1.95	0.48
2:E:49:ARG:NH2	10:N:-66:DA:H5”	2.27	0.48
2:A:117:VAL:H	10:N:-3:DG:P	2.37	0.48
3:F:31:LYS:HG2	3:F:35:ARG:HH12	1.79	0.48
3:F:73:THR:HG21	3:F:81:VAL:HG22	1.95	0.47
6:K:35:ALA:O	6:K:52:LEU:N	2.39	0.47
2:E:77:ASP:OD1	2:E:78:PHE:N	2.47	0.47
5:H:33:ARG:CD	9:J:-46:DC:H5”	2.39	0.47
6:K:33:TRP:HB2	6:K:54:ILE:HB	1.95	0.47
4:G:42:ARG:HB2	10:N:38:DG:O3’	2.14	0.47
4:C:80:PRO:HB3	5:D:61:ILE:HD12	1.97	0.47
5:D:46:LYS:HA	5:D:46:LYS:HD3	1.71	0.47
6:K:79:ASN:OD1	6:K:83:SER:N	2.48	0.47
3:F:46:ILE:O	10:N:7:DC:H5’	2.15	0.47
2:E:49:ARG:NH1	10:N:-66:DA:H4’	2.00	0.47
2:E:66:PRO:HD3	10:N:17:DA:O5’	2.15	0.47
7:L:45:GLU:OE1	7:L:45:GLU:N	2.38	0.47
9:J:-19:DG:H1	10:N:19:DC:H42	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:105:GLU:HG3	5:H:109:HIS:HD2	1.80	0.46
2:A:42:ARG:HD2	10:N:70:DG:O5'	2.16	0.46
2:E:42:ARG:CD	9:J:70:DG:OP2	2.63	0.46
7:L:51:CYS:HB3	7:L:56:ARG:H	1.80	0.46
2:A:116:ARG:HB2	10:N:-3:DG:P	2.56	0.46
2:E:49:ARG:CZ	10:N:-66:DA:C5'	2.63	0.46
2:A:84:PHE:O	10:N:-24:DG:H3'	2.16	0.46
3:B:33:ALA:HA	3:B:36:ARG:NH1	2.31	0.46
9:J:-55:DG:N2	10:N:56:DG:N2	2.63	0.46
10:N:19:DC:H2"	10:N:20:DG:C8	2.51	0.45
1:I:90:SER:HB2	9:J:2:DC:C5'	2.46	0.45
4:C:87:ILE:HD12	4:C:102:ILE:HD11	1.97	0.45
2:A:41:TYR:HH	9:J:-67:DA:C4'	2.27	0.45
2:A:123:ASP:OD1	2:E:113:HIS:NE2	2.45	0.45
2:A:108:ASN:ND2	3:B:42:GLY:O	2.50	0.45
4:G:16:THR:O	4:G:19:SER:OG	2.29	0.45
9:J:-21:DC:H42	10:N:21:DG:H1	1.63	0.44
2:A:46:VAL:HG22	9:J:9:DT:P	2.58	0.44
3:F:31:LYS:HG3	3:F:51:TYR:CE1	2.51	0.44
8:M:14:THR:HA	8:M:15:LEU:HA	1.70	0.44
10:N:-74:DA:H2"	10:N:-73:DT:H72	1.99	0.44
2:E:104:PHE:HA	2:E:107:THR:HG22	2.00	0.44
5:H:86:ARG:HH12	9:J:-34:DG:H2"	1.82	0.44
9:J:80:DC:H2"	9:J:81:DT:C5	2.52	0.44
4:C:16:THR:O	4:C:19:SER:OG	2.28	0.44
2:E:116:ARG:NH1	2:E:118:THR:O	2.50	0.44
6:K:87:ASP:O	6:K:91:SER:N	2.51	0.44
2:E:39:HIS:CD2	10:N:-67:DA:H5"	2.53	0.44
4:G:17:ARG:HH21	4:G:28:GLY:HA2	1.82	0.44
6:K:30:MET:HA	6:K:33:TRP:HE1	1.82	0.44
2:A:49:ARG:CZ	9:J:-66:DA:C4'	2.96	0.44
6:K:75:HIS:NE2	6:K:109:LEU:O	2.33	0.44
10:N:-66:DA:C2'	10:N:-65:DT:H72	2.48	0.44
5:H:34:LYS:O	10:N:49:DC:H5"	2.18	0.43
6:K:45:TYR:HB3	6:K:50:PHE:HZ	1.82	0.43
6:K:77:ASN:ND2	6:K:114:ASN:O	2.50	0.43
8:M:22:THR:HA	8:M:55:THR:HA	2.00	0.43
4:C:67:GLY:HA3	5:D:49:HIS:CD2	2.53	0.43
3:F:47:SER:HA	10:N:7:DC:H5'	2.00	0.43
9:J:-45:DA:C2	10:N:46:DG:N2	2.87	0.43
2:A:46:VAL:HA	2:A:49:ARG:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:30:PRO:HB2	7:L:56:ARG:NH2	2.34	0.43
2:A:113:HIS:CG	2:E:126:LEU:HD22	2.54	0.43
4:C:42:ARG:HD3	9:J:38:DG:H4'	2.00	0.43
6:K:75:HIS:CE1	6:K:109:LEU:HG	2.54	0.43
4:G:43:VAL:O	10:N:38:DG:H3'	2.18	0.43
8:M:1:MET:N	8:M:18:GLU:OE1	2.50	0.43
8:M:23:ILE:HG12	8:M:54:ARG:O	2.19	0.43
9:J:27:DG:N2	9:J:28:DA:C2	2.87	0.43
5:D:86:ARG:NH1	10:N:-34:DG:H2'	2.34	0.42
6:K:44:PRO:HA	6:K:139:ARG:CZ	2.49	0.42
3:B:73:THR:HG21	3:B:81:VAL:HA	2.01	0.42
5:D:34:LYS:HG2	9:J:50:DG:OP1	2.20	0.42
2:E:49:ARG:NH2	10:N:-66:DA:C5'	2.82	0.42
3:F:30:THR:HB	9:J:-12:DC:OP2	2.19	0.42
6:K:87:ASP:OD1	6:K:88:ILE:N	2.51	0.42
10:N:7:DC:H2'	10:N:8:DG:C8	2.54	0.42
2:E:85:GLN:HA	9:J:-24:DG:O5'	2.20	0.42
2:E:120:MET:HB2	2:E:121:PRO:HD2	2.01	0.42
4:G:84:GLN:NE2	4:G:102:ILE:HB	2.35	0.42
10:N:-25:DA:H1'	10:N:-24:DG:C8	2.53	0.42
5:D:56:SER:HB3	10:N:-54:DA:P	2.59	0.42
6:K:109:LEU:HD12	6:K:112:ASP:O	2.20	0.42
6:K:17:PRO:HA	6:K:18:PRO:HD3	1.91	0.42
6:K:60:TYR:CD1	6:K:61:PRO:HA	2.54	0.42
8:M:1:MET:HG2	8:M:19:PRO:HD3	2.01	0.42
2:A:42:ARG:HG3	10:N:70:DG:H3'	2.01	0.42
2:A:126:LEU:HD22	2:E:113:HIS:CG	2.54	0.42
4:C:11:ARG:HD3	10:N:-41:DG:H5'	2.02	0.42
5:H:86:ARG:CZ	9:J:-34:DG:H3'	2.50	0.42
8:M:2:GLN:O	8:M:64:GLU:N	2.34	0.42
9:J:46:DG:N2	10:N:-45:DA:C2	2.88	0.42
10:N:-4:DC:H2"	10:N:-3:DG:C8	2.55	0.42
4:G:42:ARG:HA	10:N:39:DA:OP1	2.19	0.42
3:B:26:ILE:HG13	3:B:55:ARG:HG3	2.01	0.42
8:M:40:GLN:HA	8:M:41:GLN:HA	1.48	0.41
9:J:-48:DC:C6	9:J:-47:DT:H72	2.55	0.41
4:G:17:ARG:NH2	4:G:28:GLY:HA2	2.35	0.41
5:H:33:ARG:HD2	9:J:-46:DC:H5'	2.02	0.41
6:K:56:PHE:CD1	6:K:65:PRO:HB3	2.56	0.41
3:B:51:TYR:O	3:B:55:ARG:HD3	2.20	0.41
5:D:105:GLU:OE2	5:D:108:LYS:NZ	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:43:PRO:HA	10:N:9:DT:H5'	2.02	0.41
4:C:32:ARG:NE	10:N:-44:DA:OP2	2.52	0.41
3:B:69:ALA:O	3:B:73:THR:HG23	2.21	0.41
2:E:42:ARG:HG3	9:J:70:DG:OP1	2.20	0.41
5:H:90:THR:OG1	5:H:93:GLU:OE1	2.32	0.41
4:C:11:ARG:CD	10:N:-41:DG:H5"	2.50	0.41
4:C:24:GLN:OE1	5:D:47:GLN:NE2	2.54	0.41
5:D:39:VAL:HG12	5:D:43:LYS:HE3	2.02	0.41
4:G:88:ARG:HB2	4:G:108:LEU:HD13	2.03	0.41
5:D:33:ARG:CD	10:N:-46:DC:H5'	2.50	0.41
5:D:93:GLU:OE1	5:D:93:GLU:N	2.51	0.41
2:E:65:LEU:HD23	2:E:65:LEU:HA	1.94	0.41
2:A:108:ASN:HB2	3:B:43:VAL:HG22	2.03	0.41
5:H:33:ARG:NH2	10:N:49:DC:C1'	2.83	0.41
6:K:22:SER:N	6:K:36:THR:O	2.46	0.41
6:K:77:ASN:OD1	6:K:114:ASN:N	2.48	0.41
9:J:-62:DC:H2'	9:J:-61:DG:C8	2.56	0.41
9:J:49:DC:H2'	9:J:50:DG:C8	2.56	0.41
2:E:83:ARG:CZ	9:J:-23:DC:H5"	2.51	0.41
3:F:78:ARG:NH2	3:F:85:ASP:OD2	2.54	0.41
9:J:73:DA:H2"	9:J:74:DT:H72	2.02	0.41
3:B:79:LYS:HE2	3:B:79:LYS:HB2	1.86	0.40
7:L:28:THR:OG1	7:L:73:ASN:OD1	2.23	0.40
10:N:1:DT:H1'	10:N:2:DC:H5'	2.03	0.40
4:C:44:GLY:HA2	9:J:38:DG:OP1	2.21	0.40
3:F:80:THR:HG21	10:N:28:DA:H5"	2.04	0.40
2:E:43:PRO:HG2	9:J:-5:DA:H5'	2.04	0.40
2:E:109:LEU:HD23	2:E:109:LEU:HA	1.88	0.40
6:K:106:ILE:O	6:K:110:LEU:HG	2.20	0.40
2:A:82:LEU:HD23	2:A:82:LEU:HA	1.91	0.40
4:G:58:LEU:HD23	4:G:58:LEU:HA	1.84	0.40
5:H:33:ARG:HH22	10:N:48:DG:H21	1.69	0.40
6:K:44:PRO:HB2	6:K:138:SER:HB2	2.02	0.40
2:A:41:TYR:HB3	2:A:45:THR:OG1	2.21	0.40
3:F:77:LYS:HE3	5:H:92:ARG:NH1	2.34	0.40
10:N:23:DG:H2"	10:N:24:DC:OP2	2.22	0.40

There are no symmetry-related clashes.

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 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	I	70/194 (36%)	69 (99%)	1 (1%)	0	100	100
2	A	96/135 (71%)	95 (99%)	1 (1%)	0	100	100
2	E	95/135 (70%)	93 (98%)	2 (2%)	0	100	100
3	B	81/102 (79%)	75 (93%)	6 (7%)	0	100	100
3	F	81/102 (79%)	79 (98%)	2 (2%)	0	100	100
4	C	107/129 (83%)	104 (97%)	3 (3%)	0	100	100
4	G	107/129 (83%)	107 (100%)	0	0	100	100
5	D	92/125 (74%)	91 (99%)	1 (1%)	0	100	100
5	H	92/125 (74%)	89 (97%)	3 (3%)	0	100	100
6	K	145/147 (99%)	140 (97%)	5 (3%)	0	100	100
7	L	81/193 (42%)	71 (88%)	10 (12%)	0	100	100
8	M	53/75 (71%)	47 (89%)	6 (11%)	0	100	100
All	All	1100/1591 (69%)	1060 (96%)	40 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 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	I	54/158 (34%)	54 (100%)	0	100	100
2	A	86/110 (78%)	83 (96%)	3 (4%)	31	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	85/110 (77%)	83 (98%)	2 (2%)	44 64
3	B	69/78 (88%)	63 (91%)	6 (9%)	8 26
3	F	68/78 (87%)	66 (97%)	2 (3%)	37 58
4	C	84/99 (85%)	82 (98%)	2 (2%)	44 64
4	G	84/99 (85%)	83 (99%)	1 (1%)	67 79
5	D	80/104 (77%)	78 (98%)	2 (2%)	42 63
5	H	80/104 (77%)	79 (99%)	1 (1%)	65 77
6	K	120/132 (91%)	119 (99%)	1 (1%)	79 85
7	L	74/176 (42%)	72 (97%)	2 (3%)	40 60
8	M	35/68 (52%)	35 (100%)	0	100 100
All	All	919/1316 (70%)	897 (98%)	22 (2%)	45 64

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	65	LEU
2	A	96	SER
2	A	129	ARG
3	B	22	LEU
3	B	23	ARG
3	B	55	ARG
3	B	78	ARG
3	B	92	ARG
3	B	95	ARG
4	C	13	LYS
4	C	108	LEU
5	D	92	ARG
5	D	116	LYS
2	E	115	LYS
2	E	129	ARG
3	F	20	LYS
3	F	67	ARG
4	G	11	ARG
5	H	92	ARG
6	K	97	LEU
7	L	14	CYS
7	L	73	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
2	A	68	GLN
8	M	25	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.