



Full wwPDB EM Validation Report ⓘ

Oct 22, 2024 – 12:20 AM JST

PDB ID : 8IHT
EMDB ID : EMD-35455
Title : Rpd3S bound to the nucleosome
Authors : Zhang, Y.; Gang, C.
Deposited on : 2023-02-23
Resolution : 3.72 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
Mogul	: 1.8.5 (274361), CSD as541be (2020)
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)	: 2.39

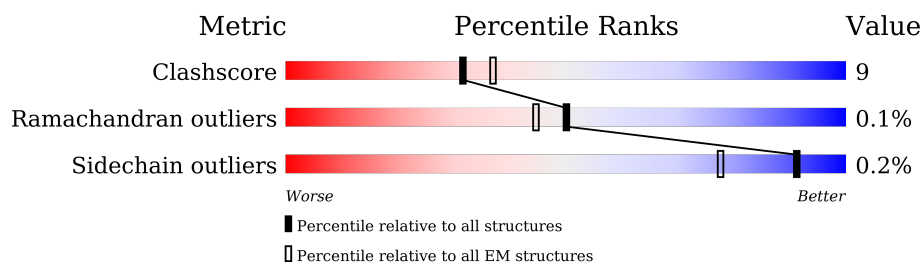
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.72 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	135	
1	E	135	
2	B	102	
2	F	102	
3	C	129	
3	G	129	
4	D	122	
4	H	122	
5	I	164	

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Mol	Chain	Length	Quality of chain
6	J	165	<div><div></div><div>36%</div><div>61%</div><div></div></div>
7	M	684	<div><div></div><div>46%</div><div>8%</div><div>45%</div><div></div></div>
7	O	684	<div><div></div><div>19%</div><div></div><div>78%</div><div></div></div>
8	N	401	<div><div></div><div>61%</div><div>13%</div><div>26%</div><div></div></div>
8	P	401	<div><div></div><div>37%</div><div>9%</div><div>54%</div><div></div></div>
9	K	1536	<div><div></div><div>33%</div><div>6%</div><div>61%</div><div></div></div>
10	L	433	<div><div></div><div>79%</div><div>15%</div><div>5%</div><div></div></div>

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 27545 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 H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	121	Total	C	N	O	S	0	0
			925	581	184	159	1		
1	E	100	Total	C	N	O	S	0	0
			779	490	151	136	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ALA	CYS	engineered mutation	UNP A0A310TTQ1
E	110	ALA	CYS	engineered mutation	UNP A0A310TTQ1

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	80	Total	C	N	O	S	0	0
			607	381	119	106	1		
2	F	82	Total	C	N	O	S	0	0
			609	385	117	106	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	107	Total	C	N	O	0	0
			801	499	161	141		
3	G	106	Total	C	N	O	0	0
			760	473	151	136		

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	94	Total	C	N	O	S	0	0
			711	452	126	131	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	89	Total	C	N	O	S	0	0
			639	398	120	120	1		

- Molecule 5 is a DNA chain called DNA (164-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	158	Total	C	N	O	P	0	0
			3216	1527	581	950	158		

- Molecule 6 is a DNA chain called DNA (165-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	159	Total	C	N	O	P	0	0
			3280	1551	621	949	159		

- Molecule 7 is a protein called RCO1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	375	Total	C	N	O	S	0	0
			2844	1789	500	544	11		
7	O	153	Total	C	N	O	S	0	0
			1125	718	193	209	5		

- Molecule 8 is a protein called Chromatin modification-related protein EAF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	295	Total	C	N	O	S	0	0
			2212	1412	373	416	11		
8	P	184	Total	C	N	O	S	0	0
			1320	847	213	254	6		

- Molecule 9 is a protein called Transcriptional regulatory protein SIN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	598	Total	C	N	O	S	0	0
			4668	2982	810	861	15		

- Molecule 10 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	410	Total	C	N	O	S	0	0
			3047	1924	524	578	21		

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

Mol	Chain	Residues	Atoms		AltConf
11	L	1	Total	Zn	0
			1	1	

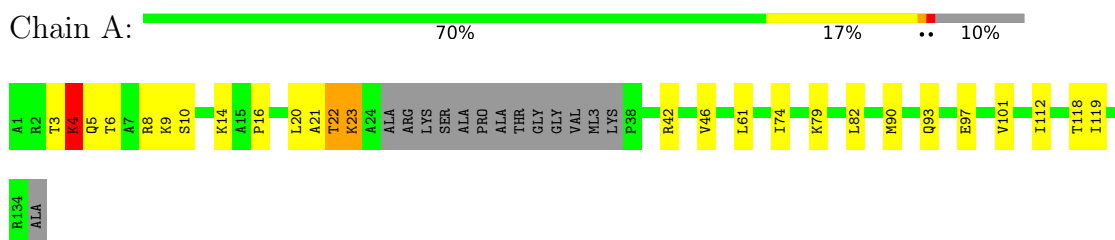
- Molecule 12 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
12	L	1	Total	Ca	0
			1	1	

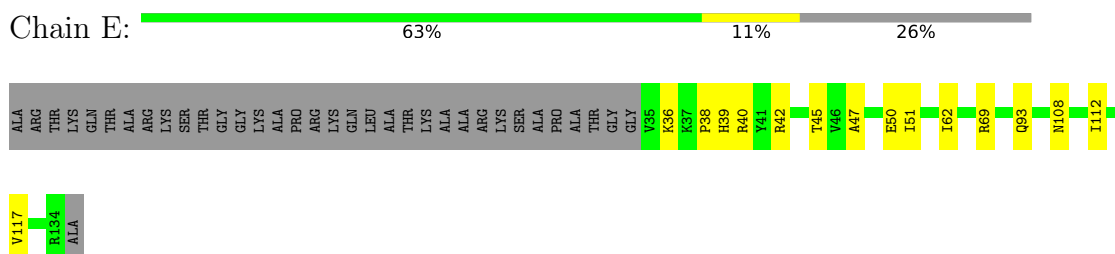
3 Residue-property plots [i](#)

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. 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.

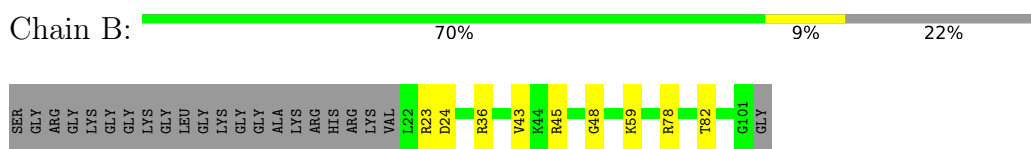
- Molecule 1: Histone H3



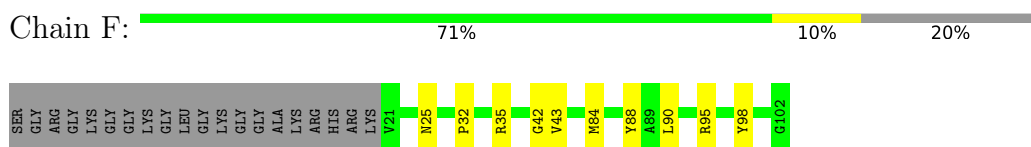
- Molecule 1: Histone H3



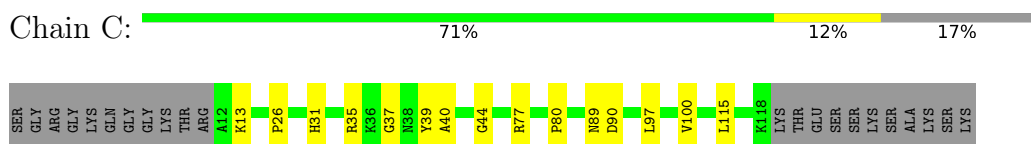
- Molecule 2: Histone H4



- Molecule 2: Histone H4

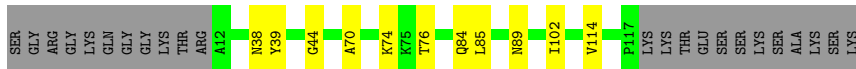


- Molecule 3: Histone H2A



- Molecule 3: Histone H2A

Chain G: 



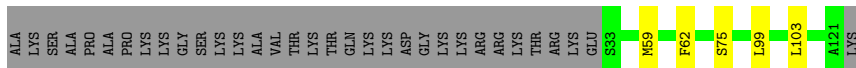
- Molecule 4: Histone H2B

Chain D: 



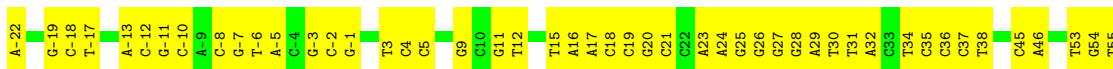
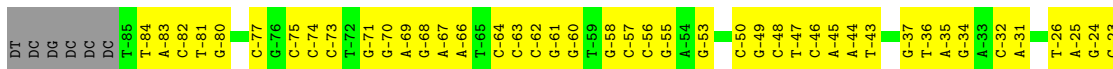
- Molecule 4: Histone H2B

Chain H: 



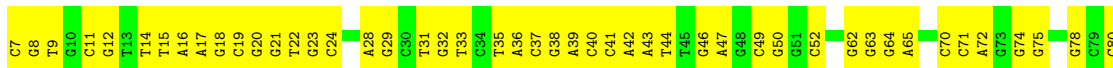
- Molecule 5: DNA (164-MER)

Chain I: 



- Molecule 6: DNA (165-MER)

Chain J: 



- Molecule 7: RCO1 isoform 1

Chain M: 

L401	G402	D403	E406	D407	S408	A409	E410	A411	A421	R422	ASP	LEU	HIS	VAL	GLU	HIS	ASP	ASN	GLU	PHE	TYR
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	107252	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 ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA, ML3

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	0.42	0/937	0.55	0/1256
1	E	0.42	0/777	0.51	0/1045
2	B	0.50	0/613	0.54	0/824
2	F	0.47	0/616	0.51	0/827
3	C	0.42	0/811	0.47	0/1093
3	G	0.29	0/769	0.44	0/1043
4	D	0.48	0/721	0.47	0/969
4	H	0.31	0/647	0.42	0/877
5	I	0.75	0/3601	0.96	0/5548
6	J	0.73	0/3685	0.90	0/5688
7	M	0.34	0/2904	0.53	1/3928 (0.0%)
7	O	0.28	0/1147	0.46	1/1547 (0.1%)
8	N	0.31	0/2256	0.46	0/3057
8	P	0.27	0/1344	0.44	0/1836
9	K	0.30	0/4762	0.43	1/6444 (0.0%)
10	L	0.35	0/3116	0.50	0/4226
All	All	0.48	0/28706	0.64	3/40208 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	452	VAL	N-CA-C	-7.71	90.18	111.00
9	K	1081	ASN	CB-CA-C	5.32	121.04	110.40
7	O	289	PRO	N-CA-C	-5.27	98.40	112.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	925	0	936	27	0
1	E	779	0	771	15	0
2	B	607	0	606	8	0
2	F	609	0	597	7	0
3	C	801	0	815	14	0
3	G	760	0	754	8	0
4	D	711	0	718	11	0
4	H	639	0	610	3	0
5	I	3216	0	1770	97	0
6	J	3280	0	1782	87	0
7	M	2844	0	2569	39	0
7	O	1125	0	1008	18	0
8	N	2212	0	2068	32	0
8	P	1320	0	1180	27	0
9	K	4668	0	4404	65	0
10	L	3047	0	2781	41	0
11	L	1	0	0	0	0
12	L	1	0	0	0	0
All	All	27545	0	23369	431	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 9.

All (431) 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)
5:I:11:DG:H2''	5:I:12:DT:H5''	1.70	0.73
5:I:-73:DC:N3	6:J:74:DG:N2	2.37	0.72
5:I:-68:DG:H2'	5:I:-67:DA:C8	2.25	0.71
5:I:-7:DG:H2''	5:I:-6:DT:H71	1.74	0.69
1:A:20:LEU:CB	1:A:23:LYS:H	2.05	0.69
5:I:30:DT:H2'	5:I:31:DT:H71	1.75	0.68
1:E:38:PRO:HG2	1:E:40:ARG:HG3	1.76	0.67
6:J:49:DC:H2'	6:J:50:DG:C8	2.28	0.67
6:J:31:DT:H2'	6:J:32:DG:C8	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LYS:O	1:A:5:GLN:HG2	1.97	0.63
5:I:69:DC:H2''	5:I:70:DC:H5''	1.81	0.62
7:M:315:SER:O	7:M:316:MET:C	2.38	0.62
5:I:-70:DG:H2''	5:I:-69:DA:C8	2.34	0.62
1:A:8:ARG:HD3	1:A:14:LYS:NZ	2.15	0.61
1:A:16:PRO:HG2	9:K:787:VAL:HG12	1.82	0.61
6:J:-8:DG:C8	6:J:-8:DG:H5'	2.36	0.61
1:A:8:ARG:CZ	1:A:22:THR:HG21	2.32	0.60
6:J:64:DG:H2''	6:J:65:DA:H5'	1.82	0.60
6:J:14:DT:H2''	6:J:15:DT:H71	1.83	0.59
1:E:40:ARG:HH21	5:I:9:DG:H1'	1.68	0.58
5:I:12:DT:OP1	8:N:83:GLY:N	2.36	0.58
5:I:62:DT:H2''	5:I:63:DA:H8	1.68	0.58
10:L:142:ALA:HB3	10:L:306:MET:HG3	1.86	0.58
7:O:351:PHE:CE1	8:P:333:ARG:HB3	2.39	0.57
9:K:1196:LEU:HD11	9:K:1219:LEU:HD11	1.86	0.57
7:O:564:ARG:HH22	7:O:565:LYS:HG3	1.70	0.57
1:A:14:LYS:HE2	1:A:22:THR:HG23	1.87	0.56
9:K:962:LYS:O	9:K:966:TRP:N	2.37	0.56
8:N:269:LEU:HD11	8:N:275:GLN:HG3	1.87	0.56
3:G:44:GLY:HA2	5:I:38:DT:H5''	1.86	0.56
8:N:124:GLU:HA	8:N:127:LYS:HD3	1.87	0.56
1:A:14:LYS:HG2	1:A:21:ALA:H	1.70	0.56
7:O:336:PHE:HE1	8:P:355:LEU:HD21	1.71	0.56
5:I:-6:DT:H1'	5:I:-5:DA:C5	2.42	0.55
8:N:111:LEU:O	8:N:115:ALA:N	2.39	0.55
9:K:853:PRO:HA	9:K:884:HIS:CE1	2.41	0.55
5:I:53:DT:H2''	5:I:54:DG:C8	2.41	0.55
9:K:1186:LEU:HD23	10:L:351:TYR:CZ	2.42	0.55
8:P:222:LEU:HD11	8:P:359:THR:HG21	1.88	0.55
7:O:357:ILE:HD11	8:P:229:LYS:HA	1.88	0.55
5:I:54:DG:H2''	5:I:55:DT:C7	2.37	0.55
5:I:-71:DG:H2''	5:I:-70:DG:C8	2.42	0.55
8:P:376:ASP:HB3	8:P:379:PRO:HB3	1.88	0.55
6:J:22:DT:H1'	6:J:23:DG:H5'	1.89	0.54
6:J:35:DT:H2''	6:J:36:DA:C8	2.42	0.54
10:L:402:GLY:O	10:L:403:ASP:C	2.46	0.54
5:I:-44:DA:H1'	5:I:-43:DT:H5'	1.88	0.54
4:D:112:THR:HA	4:D:115:VAL:HG12	1.89	0.54
9:K:960:THR:O	9:K:963:LYS:HB3	2.06	0.54
3:C:115:LEU:HD21	1:E:112:ILE:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:45:DC:H2''	5:I:46:DA:N7	2.22	0.54
9:K:906:ARG:HB3	9:K:910:ARG:HH21	1.73	0.54
6:J:81:DA:H2''	6:J:82:DG:OP2	2.06	0.54
1:A:8:ARG:HD3	1:A:14:LYS:HZ1	1.73	0.53
8:P:226:ILE:HA	8:P:229:LYS:HD3	1.90	0.53
6:J:31:DT:H2'	6:J:32:DG:H8	1.72	0.53
6:J:62:DG:C2	6:J:63:DG:C2	2.97	0.53
7:M:99:PRO:HB2	7:M:101:THR:HG23	1.89	0.53
8:N:256:MET:HA	8:N:259:ASN:HB2	1.90	0.53
5:I:16:DA:H1'	5:I:17:DA:N7	2.24	0.53
6:J:-48:DC:H2''	6:J:-47:DC:C5	2.44	0.53
6:J:37:DC:H2''	6:J:38:DG:C8	2.44	0.53
8:N:99:ALA:O	8:N:101:ASN:ND2	2.42	0.53
10:L:89:VAL:HG22	10:L:112:VAL:HG11	1.90	0.53
3:G:85:LEU:O	3:G:89:ASN:ND2	2.41	0.52
3:C:89:ASN:ND2	7:M:54:ILE:HG21	2.25	0.52
6:J:42:DA:H5'	6:J:42:DA:C8	2.44	0.52
7:M:396:THR:CB	9:K:796:ILE:HD13	2.38	0.52
1:E:42:ARG:O	1:E:45:THR:HG22	2.10	0.52
5:I:-46:DC:H1'	5:I:-45:DA:C8	2.45	0.52
5:I:-8:DC:H2''	5:I:-7:DG:C8	2.45	0.52
6:J:-4:DG:H2''	6:J:-3:DA:C8	2.45	0.52
6:J:23:DG:H1'	6:J:24:DC:H5'	1.91	0.52
10:L:335:ASP:OD2	10:L:336:LYS:N	2.42	0.52
7:O:262:PHE:HA	7:O:269:SER:HA	1.91	0.52
7:O:344:ASP:OD1	7:O:345:SER:N	2.42	0.52
4:D:86:ILE:HA	4:D:90:GLU:OE1	2.10	0.52
5:I:-13:DA:C8	5:I:-13:DA:H5'	2.45	0.52
5:I:-35:DA:H1'	5:I:-34:DG:O4'	2.11	0.51
9:K:810:ILE:HD11	9:K:919:LEU:HD23	1.92	0.51
2:B:48:GLY:H	6:J:7:DC:P	2.33	0.51
9:K:748:CYS:SG	9:K:749:GLU:N	2.83	0.51
9:K:962:LYS:O	9:K:965:HIS:N	2.44	0.51
6:J:-5:DG:H2''	6:J:-4:DG:C8	2.45	0.51
1:E:69:ARG:HB3	2:F:25:ASN:ND2	2.26	0.51
5:I:-50:DC:H2''	5:I:-49:DG:C8	2.46	0.51
8:N:60:LYS:NZ	8:N:61:LEU:O	2.43	0.51
9:K:1013:LEU:HD22	9:K:1257:MET:SD	2.51	0.51
5:I:63:DA:H1'	5:I:64:DT:OP2	2.10	0.51
6:J:15:DT:H2''	6:J:16:DA:O4'	2.11	0.51
3:C:31:HIS:CE1	3:C:35:ARG:HH22	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:66:DC:H2''	5:I:67:DA:C8	2.45	0.51
8:N:117:GLU:O	8:N:121:SER:N	2.33	0.51
6:J:82:DG:H2''	6:J:83:DT:OP2	2.11	0.51
3:C:40:ALA:HA	3:G:38:ASN:HD22	1.76	0.51
5:I:-80:DG:H5'	5:I:-80:DG:C8	2.46	0.51
6:J:3:DC:H4'	6:J:4:DG:OP1	2.10	0.51
6:J:32:DG:H2'	6:J:33:DT:H71	1.92	0.51
6:J:83:DT:H2''	6:J:84:DA:C8	2.46	0.51
6:J:62:DG:N2	6:J:63:DG:C2	2.79	0.51
10:L:184:ASP:HB3	10:L:207:SER:HA	1.92	0.51
9:K:1219:LEU:HD23	9:K:1224:PHE:HB2	1.93	0.50
10:L:279:ASP:HA	10:L:314:THR:OG1	2.12	0.50
8:P:299:TYR:H	8:P:302:GLU:HB2	1.75	0.50
10:L:406:GLU:O	10:L:407:ASP:HB2	2.11	0.50
7:M:553:ASP:HA	8:P:272:PRO:HD2	1.92	0.50
9:K:1075:GLN:O	9:K:1079:ARG:N	2.37	0.50
7:M:85:LEU:O	7:M:86:GLU:C	2.49	0.50
9:K:853:PRO:HA	9:K:884:HIS:HE1	1.76	0.50
5:I:15:DT:H2''	5:I:16:DA:C8	2.46	0.50
7:M:441:ASP:HB3	7:M:463:LYS:HD3	1.94	0.50
10:L:401:LEU:O	10:L:402:GLY:C	2.46	0.50
5:I:55:DT:H2''	5:I:56:DC:H5'	1.94	0.50
6:J:-14:DA:H2''	6:J:-13:DA:C8	2.46	0.49
7:M:522:ILE:HG13	9:K:683:THR:HG23	1.92	0.49
8:P:366:LEU:HD12	8:P:374:PHE:CE1	2.47	0.49
5:I:-56:DC:H2''	5:I:-55:DG:N7	2.27	0.49
7:M:410:ASN:OD1	7:M:411:SER:N	2.45	0.49
8:N:238:TYR:HA	8:N:242:ASP:HB2	1.95	0.49
5:I:67:DA:C8	5:I:67:DA:H5'	2.47	0.49
7:M:424:ARG:O	7:M:434:SER:HA	2.12	0.49
8:N:254:VAL:HG13	8:N:331:LEU:HD22	1.94	0.49
1:A:119:ILE:HD13	2:B:43:VAL:HG11	1.94	0.49
6:J:-72:DC:H2''	6:J:-71:DA:C8	2.48	0.49
7:O:351:PHE:HD1	8:P:297:LEU:HA	1.75	0.49
5:I:-26:DT:H2''	5:I:-25:DA:C8	2.48	0.49
8:P:246:CYS:HB2	8:P:387:TYR:CE1	2.48	0.49
5:I:-82:DC:H1'	5:I:-81:DT:C5	2.47	0.49
5:I:26:DG:H2''	5:I:27:DG:C8	2.48	0.49
5:I:67:DA:H2''	5:I:68:DT:H5''	1.95	0.49
8:N:33:PRO:HG3	8:N:74:GLY:O	2.12	0.49
9:K:1303:ILE:HG13	9:K:1314:ILE:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:26:PRO:HG3	4:D:37:TYR:CE2	2.47	0.49
8:N:246:CYS:HA	8:N:387:TYR:HA	1.94	0.49
1:A:3:THR:O	1:A:4:LYS:O	2.30	0.49
3:C:77:ARG:HA	4:D:50:GLY:O	2.13	0.49
3:C:100:VAL:HG11	2:F:98:TYR:CE2	2.48	0.49
1:E:47:ALA:HA	1:E:50:GLU:HG2	1.93	0.49
5:I:64:DT:H2''	5:I:65:DA:H8	1.78	0.49
6:J:39:DA:C4	6:J:40:DC:C5	3.01	0.49
6:J:63:DG:H2''	6:J:64:DG:C8	2.48	0.49
5:I:-13:DA:H5'	5:I:-13:DA:H8	1.78	0.49
5:I:67:DA:C2	6:J:-66:DG:C2	3.01	0.49
9:K:778:LEU:HD21	10:L:171:ILE:HD11	1.95	0.49
10:L:163:LEU:HD11	10:L:168:LEU:HD11	1.95	0.49
8:P:223:GLN:NE2	8:P:224:ILE:O	2.46	0.49
5:I:67:DA:N6	6:J:-67:DT:O4	2.46	0.48
6:J:-44:DG:H2''	6:J:-43:DA:C8	2.48	0.48
5:I:-83:DA:H2'	5:I:-83:DA:N3	2.27	0.48
6:J:-54:DC:H2''	6:J:-53:DA:C8	2.48	0.48
8:P:264:GLU:HA	8:P:267:GLN:NE2	2.28	0.48
4:H:99:LEU:HD23	4:H:103:LEU:HB3	1.95	0.48
5:I:-63:DC:H1'	5:I:-62:DC:O4'	2.13	0.48
6:J:-22:DG:H2''	6:J:-21:DG:H8	1.78	0.48
7:M:264:SER:HB2	7:M:282:PHE:CE1	2.48	0.48
9:K:771:ASP:OD1	9:K:772:ASP:N	2.46	0.48
2:F:90:LEU:HB3	2:F:95:ARG:O	2.12	0.48
6:J:47:DA:H5'	6:J:47:DA:C8	2.48	0.48
8:P:269:LEU:HD22	8:P:274:SER:HB3	1.95	0.48
3:C:97:LEU:HD21	4:D:62:PHE:HE1	1.79	0.48
9:K:798:HIS:CG	10:L:283:CYS:HB3	2.49	0.48
1:A:9:LYS:O	1:A:10:SER:OG	2.30	0.48
1:A:20:LEU:CB	1:A:23:LYS:HB3	2.43	0.48
8:P:333:ARG:NH2	8:P:387:TYR:OH	2.46	0.48
8:P:358:GLN:O	8:P:362:PHE:N	2.41	0.48
3:G:39:TYR:HB3	4:H:75:SER:HB2	1.94	0.48
5:I:-71:DG:H2''	5:I:-70:DG:H8	1.77	0.48
9:K:666:VAL:HG11	7:O:552:PHE:HD1	1.78	0.48
6:J:-37:DG:H2''	6:J:-36:DG:C8	2.48	0.48
7:M:54:ILE:O	7:M:55:THR:OG1	2.30	0.48
7:M:404:ASP:O	7:M:407:ILE:HG22	2.14	0.47
9:K:961:ASN:O	9:K:964:ILE:HB	2.14	0.47
5:I:56:DC:H2''	5:I:57:DA:N7	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:37:GLY:HA3	3:C:39:TYR:HE2	1.79	0.47
3:C:115:LEU:HD22	1:E:117:VAL:HG13	1.97	0.47
5:I:59:DA:H2'	5:I:60:DT:H71	1.96	0.47
7:M:120:SER:O	9:K:918:GLU:HB2	2.15	0.47
7:M:416:ILE:O	7:M:446:PRO:HG2	2.14	0.47
9:K:672:ALA:O	9:K:676:ILE:HG12	2.14	0.47
8:P:360:GLU:O	8:P:364:VAL:HG23	2.15	0.47
5:I:-3:DG:H1'	5:I:-2:DC:H5'	1.97	0.47
7:M:88:ASP:O	7:M:91:GLY:N	2.48	0.47
9:K:1209:ARG:O	9:K:1213:ARG:HG3	2.15	0.47
10:L:377:PHE:O	10:L:381:GLU:HG3	2.14	0.47
1:A:4:LYS:HB2	1:A:5:GLN:H	1.48	0.47
1:A:6:THR:OG1	7:M:271:SER:N	2.48	0.47
1:E:62:ILE:O	1:E:93:GLN:NE2	2.48	0.47
7:M:478:ILE:HG13	7:M:480:HIS:H	1.79	0.47
9:K:834:ILE:O	9:K:838:ILE:HD12	2.14	0.47
10:L:212:GLY:O	10:L:213:GLU:HG2	2.15	0.47
6:J:-11:DC:H2''	6:J:-10:DG:H8	1.80	0.47
7:M:287:LEU:HA	7:M:348:PRO:HG2	1.96	0.47
7:M:382:THR:HG22	7:M:384:ARG:H	1.80	0.47
8:N:15:LEU:O	8:N:97:ILE:HA	2.14	0.47
7:O:323:GLU:O	7:O:327:ILE:HD12	2.15	0.47
2:B:23:ARG:HG3	2:B:24:ASP:N	2.29	0.47
8:N:106:ALA:O	8:N:110:ARG:HG2	2.15	0.47
1:A:61:LEU:O	2:B:36:ARG:NH2	2.40	0.46
5:I:-84:DT:H3'	5:I:-83:DA:H8	1.80	0.46
5:I:-18:DC:H2'	5:I:-17:DT:H72	1.96	0.46
5:I:4:DC:H2''	5:I:5:DC:C5	2.49	0.46
6:J:-27:DC:H2''	6:J:-26:DC:C5	2.51	0.46
9:K:962:LYS:O	9:K:963:LYS:C	2.51	0.46
5:I:28:DG:H2''	5:I:29:DA:H8	1.81	0.46
5:I:35:DC:OP2	5:I:35:DC:H2'	2.15	0.46
6:J:-43:DA:H2''	6:J:-42:DG:H8	1.81	0.46
9:K:963:LYS:HE3	9:K:970:LYS:HB3	1.97	0.46
9:K:1234:ASN:O	10:L:359:ASN:ND2	2.48	0.46
6:J:-56:DG:H4'	6:J:-55:DA:OP1	2.14	0.46
10:L:65:ARG:HB2	10:L:409:ALA:HB2	1.98	0.46
7:O:355:ASN:O	7:O:359:GLU:N	2.39	0.46
3:C:80:PRO:HD3	4:D:55:ALA:HB2	1.96	0.46
9:K:993:ASP:OD1	9:K:1011:LYS:HE3	2.15	0.46
7:M:452:VAL:O	7:M:453:PRO:C	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:69:ARG:HB3	4:D:98:LEU:HD13	1.97	0.46
6:J:-31:DA:C6	6:J:-30:DA:C6	3.04	0.46
7:O:327:ILE:HG13	7:O:337:ALA:HB1	1.97	0.46
7:M:103:SER:O	7:M:104:GLU:C	2.50	0.46
7:M:567:PHE:HB3	7:O:569:PHE:CE2	2.51	0.46
5:I:-19:DG:H5'	9:K:937:GLN:HE21	1.81	0.46
5:I:35:DC:H2''	5:I:36:DC:C5	2.51	0.46
6:J:80:DC:H2''	6:J:81:DA:C8	2.51	0.46
5:I:19:DC:H2''	5:I:20:DG:C8	2.50	0.46
8:N:276:SER:O	8:N:280:GLU:HG2	2.16	0.46
8:P:290:ASP:OD1	8:P:323:ILE:HG23	2.16	0.46
8:P:366:LEU:O	8:P:370:VAL:N	2.49	0.46
5:I:20:DG:H4'	5:I:21:DC:OP1	2.15	0.45
5:I:63:DA:H2''	5:I:64:DT:OP1	2.16	0.45
3:G:84:GLN:NE2	3:G:102:ILE:HB	2.31	0.45
10:L:60:LYS:HE2	10:L:332:VAL:HG21	1.97	0.45
10:L:149:LEU:HB3	10:L:161:CYS:HB3	1.99	0.45
10:L:104:PHE:O	10:L:106:VAL:N	2.50	0.45
1:A:90:MET:O	1:A:93:GLN:N	2.48	0.45
1:A:112:ILE:HD12	3:G:114:VAL:HB	1.97	0.45
1:A:42:ARG:NH2	5:I:-5:DA:OP1	2.48	0.45
1:A:79:LYS:HD3	1:A:82:LEU:HD21	1.99	0.45
6:J:-42:DG:H8	6:J:-42:DG:H5'	1.81	0.45
6:J:32:DG:C2'	6:J:33:DT:H71	2.47	0.45
7:M:120:SER:OG	9:K:919:LEU:HD22	2.17	0.45
9:K:1013:LEU:HD23	9:K:1253:ALA:HB1	1.98	0.45
4:D:78:ALA:HB2	4:D:90:GLU:OE1	2.16	0.45
5:I:-67:DA:H2''	5:I:-66:DA:C8	2.51	0.45
5:I:20:DG:H2''	5:I:21:DC:O5'	2.17	0.45
6:J:-59:DT:H2''	6:J:-58:DC:C6	2.52	0.45
10:L:19:ARG:NH2	10:L:299:LYS:O	2.50	0.45
9:K:714:LYS:HB2	9:K:714:LYS:NZ	2.32	0.45
9:K:1131:GLN:O	9:K:1277:THR:HG22	2.17	0.45
3:C:90:ASP:OD1	7:M:59:ILE:HD11	2.17	0.45
5:I:-61:DG:C6	5:I:-60:DG:C6	3.05	0.45
5:I:-37:DG:H2'	5:I:-36:DT:H71	1.98	0.45
7:M:503:GLN:HE21	7:M:539:ILE:HG12	1.82	0.45
8:N:227:LYS:O	8:N:231:VAL:HG23	2.17	0.45
10:L:242:ILE:HG12	10:L:247:TYR:HD1	1.82	0.45
10:L:316:ARG:O	10:L:320:ARG:HG3	2.17	0.45
7:M:300:ASP:OD1	7:M:300:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:186:ASP:OD1	10:L:187:VAL:N	2.50	0.44
10:L:410:GLU:O	10:L:411:ALA:C	2.55	0.44
1:A:14:LYS:HE3	1:A:21:ALA:HB3	1.99	0.44
5:I:62:DT:H2''	5:I:63:DA:C8	2.51	0.44
5:I:29:DA:H2'	5:I:30:DT:H71	2.00	0.44
5:I:58:DG:H2''	5:I:59:DA:C8	2.53	0.44
6:J:41:DC:N3	6:J:42:DA:N6	2.66	0.44
8:N:85:LYS:NZ	8:N:86:SER:OG	2.50	0.44
9:K:1194:MET:HB3	9:K:1194:MET:HE2	1.86	0.44
10:L:81:GLU:HG3	10:L:104:PHE:HZ	1.82	0.44
5:I:-74:DC:C5	6:J:75:DG:C6	3.06	0.44
10:L:198:TYR:CE2	10:L:225:GLY:HA2	2.52	0.44
1:E:36:ML3:HM1A	8:N:88:TRP:CZ3	2.53	0.44
6:J:-25:DC:H1'	6:J:-24:DT:C5	2.52	0.44
6:J:2:DG:C5	6:J:3:DC:C4	3.06	0.44
9:K:785:HIS:ND1	9:K:787:VAL:HG22	2.33	0.44
9:K:1027:GLU:O	9:K:1031:GLU:HG2	2.17	0.44
5:I:-13:DA:H1'	5:I:-12:DC:H5'	2.00	0.44
5:I:-11:DG:C4	5:I:-10:DC:C5	3.05	0.44
9:K:809:LYS:O	9:K:813:GLU:HG3	2.18	0.44
6:J:40:DC:C2	6:J:41:DC:C5	3.06	0.44
7:M:113:LEU:HD22	9:K:911:GLU:HG3	2.00	0.44
10:L:236:VAL:HG22	10:L:376:ILE:HD13	2.00	0.44
1:A:97:GLU:O	1:A:101:VAL:HG23	2.18	0.44
6:J:-21:DG:C2	6:J:-20:DC:C4	3.06	0.44
7:M:477:LYS:NZ	7:M:489:TYR:HB3	2.33	0.44
8:N:125:GLN:O	8:N:129:LYS:N	2.49	0.44
2:F:32:PRO:HA	2:F:35:ARG:HG2	2.00	0.43
5:I:-58:DG:H2''	5:I:-57:DC:C6	2.52	0.43
5:I:28:DG:H2''	5:I:29:DA:C8	2.54	0.43
7:M:93:ILE:HD13	9:K:890:THR:HA	1.99	0.43
8:N:123:LEU:HD23	8:N:127:LYS:HG3	1.99	0.43
5:I:26:DG:N2	6:J:-25:DC:O2	2.51	0.43
9:K:1117:THR:HB	9:K:1120:LEU:HG	1.99	0.43
10:L:45:ILE:HG12	10:L:146:ALA:HA	2.00	0.43
8:P:248:LEU:HD13	8:P:326:TYR:CE2	2.52	0.43
8:P:262:GLU:O	8:P:266:SER:HB3	2.18	0.43
1:A:74:ILE:HD11	2:B:59:LYS:HE2	2.00	0.43
1:E:39:HIS:O	1:E:39:HIS:ND1	2.51	0.43
5:I:-75:DC:H1'	6:J:75:DG:H1	1.83	0.43
5:I:-25:DA:H2''	5:I:-24:DG:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:568:GLN:O	7:M:572:SER:N	2.50	0.43
9:K:898:LEU:HD23	9:K:898:LEU:HA	1.89	0.43
9:K:1137:ASN:HA	9:K:1304:GLU:HA	2.00	0.43
10:L:198:TYR:CZ	10:L:225:GLY:HA2	2.53	0.43
1:E:45:THR:HG21	6:J:70:DC:OP1	2.18	0.43
6:J:17:DA:C6	6:J:18:DG:C6	3.06	0.43
6:J:43:DA:H1'	6:J:44:DT:H5'	2.00	0.43
9:K:1134:SER:HB3	9:K:1307:LYS:HB3	2.00	0.43
10:L:84:ASP:OD2	10:L:88:ARG:NH2	2.52	0.43
7:O:265:ALA:O	7:O:350:GLN:HB2	2.18	0.43
8:P:257:VAL:HG21	8:P:328:ALA:HB2	2.01	0.43
1:A:118:THR:HA	2:B:45:ARG:O	2.18	0.43
3:G:76:THR:N	5:I:58:DG:OP1	2.51	0.43
6:J:71:DC:H2''	6:J:72:DA:N7	2.33	0.43
7:M:290:PRO:HG2	8:N:307:ASP:HB2	2.01	0.43
7:M:499:ASN:OD1	7:M:500:LYS:N	2.52	0.43
2:B:23:ARG:HG3	2:B:24:ASP:H	1.83	0.43
2:B:78:ARG:NH2	2:B:82:THR:HG22	2.34	0.43
6:J:-9:DC:H6	6:J:-9:DC:H5'	1.84	0.43
7:O:293:PRO:O	7:O:296:LEU:HG	2.18	0.43
8:P:246:CYS:HB2	8:P:387:TYR:CD1	2.54	0.43
1:A:46:VAL:HB	6:J:9:DT:OP1	2.19	0.43
5:I:-7:DG:C2	6:J:8:DG:N2	2.87	0.43
6:J:-20:DC:C2	6:J:-19:DG:C5	3.07	0.43
6:J:84:DA:H2''	6:J:85:DA:C8	2.53	0.43
9:K:676:ILE:HD12	9:K:709:TYR:HD1	1.82	0.43
5:I:-32:DC:H2''	5:I:-31:DA:H8	1.83	0.43
6:J:37:DC:H2''	6:J:38:DG:H8	1.84	0.43
8:N:117:GLU:HA	8:N:120:LYS:HB2	2.01	0.43
9:K:949:ILE:HD11	9:K:1142:THR:HG23	1.99	0.43
9:K:1036:HIS:CB	9:K:1212:ARG:HH22	2.32	0.43
10:L:220:GLU:OE1	10:L:221:LEU:N	2.51	0.43
5:I:23:DA:H2''	5:I:24:DA:C8	2.54	0.42
6:J:52:DC:H5'	6:J:52:DC:C6	2.54	0.42
9:K:1290:VAL:HG12	9:K:1294:MET:HE1	2.02	0.42
2:F:84:MET:HG3	2:F:88:TYR:CE2	2.54	0.42
5:I:-48:DC:H2''	5:I:-47:DT:C7	2.49	0.42
6:J:17:DA:H2''	6:J:18:DG:H8	1.83	0.42
7:M:396:THR:O	7:M:459:ASN:ND2	2.51	0.42
8:N:88:TRP:O	8:N:90:GLU:HG2	2.19	0.42
9:K:1309:THR:O	9:K:1310:LEU:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:332:LEU:HD22	8:P:374:PHE:CE1	2.55	0.42
3:C:13:LYS:NZ	6:J:46:DG:OP1	2.51	0.42
1:E:108:ASN:ND2	2:F:42:GLY:O	2.52	0.42
6:J:-22:DG:C2	6:J:-21:DG:C5	3.08	0.42
6:J:3:DC:H2''	6:J:4:DG:N7	2.34	0.42
1:E:51:ILE:HD11	2:F:43:VAL:O	2.19	0.42
6:J:14:DT:H2''	6:J:15:DT:C7	2.49	0.42
9:K:926:LYS:NZ	9:K:1226:GLU:OE2	2.52	0.42
9:K:1013:LEU:HD12	9:K:1065:LEU:HD11	2.00	0.42
5:I:34:DT:H2''	5:I:35:DC:OP2	2.18	0.42
6:J:21:DG:C8	6:J:21:DG:H5'	2.55	0.42
10:L:280:ARG:HG3	10:L:281:LEU:HG	2.00	0.42
1:E:40:ARG:NH2	5:I:9:DG:H1'	2.34	0.42
5:I:70:DC:H2''	5:I:71:DT:H5'	2.02	0.42
9:K:824:ASN:O	9:K:828:ILE:HG12	2.20	0.42
5:I:-49:DG:H2''	5:I:-48:DC:C6	2.55	0.42
6:J:-37:DG:H2''	6:J:-36:DG:N7	2.35	0.42
6:J:-70:DG:C2	6:J:-69:DG:C6	3.07	0.42
9:K:909:GLN:O	9:K:913:ASN:N	2.53	0.42
1:A:4:LYS:H	1:A:4:LYS:HG2	1.54	0.42
5:I:-47:DT:H2''	5:I:-46:DC:C5	2.54	0.42
5:I:37:DC:H6	5:I:37:DC:H2'	1.69	0.42
9:K:757:ARG:HG3	9:K:781:GLU:HG2	2.01	0.42
5:I:-77:DC:O2	6:J:78:DG:N2	2.53	0.41
5:I:-23:DC:H2''	5:I:-22:DA:H5'	2.01	0.41
6:J:0:DG:C4	6:J:1:DC:C5	3.08	0.41
6:J:71:DC:C2	6:J:72:DA:C6	3.08	0.41
9:K:860:MET:O	9:K:864:LYS:HE2	2.20	0.41
9:K:879:ILE:O	9:K:883:LEU:N	2.46	0.41
4:D:50:GLY:HA3	5:I:-53:DG:OP1	2.19	0.41
6:J:19:DC:H2''	6:J:20:DG:C8	2.55	0.41
7:M:565:LYS:HA	7:M:565:LYS:HD3	1.96	0.41
8:N:258:LEU:HD21	8:N:285:LEU:HD23	2.02	0.41
6:J:-41:DA:H1'	6:J:-40:DC:H5'	2.02	0.41
8:N:253:THR:H	8:N:256:MET:CE	2.33	0.41
7:O:288:ASP:CB	7:O:289:PRO:HD3	2.51	0.41
3:C:44:GLY:HA2	6:J:38:DG:H5''	2.02	0.41
5:I:64:DT:H2''	5:I:65:DA:C8	2.56	0.41
6:J:-43:DA:C4	6:J:-42:DG:N7	2.88	0.41
5:I:19:DC:H2''	5:I:20:DG:H8	1.86	0.41
5:I:24:DA:H2''	5:I:25:DG:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:52:LYS:HE3	7:M:52:LYS:HB3	1.90	0.41
7:M:378:LYS:HB2	7:M:378:LYS:HE2	1.90	0.41
7:O:336:PHE:CE1	8:P:355:LEU:HD21	2.53	0.41
8:P:248:LEU:HD22	8:P:326:TYR:CD2	2.55	0.41
5:I:-64:DC:H3'	7:M:51:ARG:HD2	2.03	0.41
6:J:-2:DC:H2''	6:J:-1:DA:H8	1.85	0.41
7:M:340:LEU:O	7:M:343:ILE:HG22	2.20	0.41
8:N:16:ALA:HB1	8:N:92:VAL:HG11	2.03	0.41
8:N:27:ILE:HG13	8:N:27:ILE:O	2.21	0.41
4:D:107:ALA:O	4:D:111:GLY:N	2.50	0.41
3:G:70:ALA:O	3:G:74:LYS:N	2.54	0.41
9:K:782:TRP:CE2	10:L:226:VAL:HG21	2.55	0.41
5:I:18:DC:H2''	5:I:19:DC:C6	2.55	0.41
6:J:38:DG:C2	6:J:39:DA:C5	3.08	0.41
9:K:1081:ASN:N	9:K:1081:ASN:OD1	2.53	0.41
10:L:39:PRO:HB3	10:L:280:ARG:HD3	2.03	0.41
10:L:186:ASP:OD1	10:L:274:ASP:HB2	2.20	0.41
1:A:8:ARG:HD3	1:A:14:LYS:HZ3	1.86	0.41
5:I:-7:DG:C4	5:I:-6:DT:C4	3.09	0.41
5:I:27:DG:H2''	5:I:28:DG:N7	2.36	0.41
6:J:11:DC:C2	6:J:12:DG:C5	3.09	0.41
6:J:81:DA:H2''	6:J:82:DG:C8	2.56	0.41
8:N:251:ASP:O	8:N:256:MET:HE3	2.20	0.41
10:L:131:ALA:HB1	10:L:173:LEU:HG	2.02	0.41
7:O:305:GLU:HG2	7:O:309:LYS:NZ	2.35	0.41
8:P:325:ILE:HG13	8:P:326:TYR:N	2.36	0.41
5:I:67:DA:N1	6:J:-67:DT:C4	2.89	0.41
8:N:38:TYR:N	8:N:59:GLN:O	2.54	0.41
9:K:1018:ILE:HD13	9:K:1018:ILE:HA	1.92	0.41
10:L:340:TYR:HE2	10:L:421:ALA:HB3	1.86	0.41
4:D:87:THR:HG22	4:D:90:GLU:HG3	2.04	0.40
5:I:31:DT:H2''	5:I:32:DA:C8	2.56	0.40
6:J:42:DA:H1'	6:J:43:DA:H5'	2.03	0.40
5:I:-58:DG:H2''	5:I:-57:DC:H5'	2.02	0.40
8:N:354:LEU:HD12	8:N:354:LEU:HA	1.88	0.40
8:N:386:LEU:H	8:N:386:LEU:HG	1.66	0.40
9:K:666:VAL:HG11	7:O:552:PHE:CD1	2.56	0.40
10:L:19:ARG:HH21	10:L:302:GLY:CA	2.35	0.40
5:I:-2:DC:H2''	5:I:-1:DG:C8	2.56	0.40
5:I:56:DC:H6	5:I:56:DC:H2'	1.76	0.40
9:K:835:VAL:HA	9:K:838:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:1148:PHE:CZ	9:K:1312:VAL:HG11	2.57	0.40
9:K:1180:PHE:CD2	10:L:340:TYR:HB2	2.56	0.40
1:A:23:LYS:HB3	1:A:23:LYS:HE2	1.61	0.40
1:E:36:ML3:HM2A	8:N:18:HIS:CD2	2.57	0.40
4:H:59:MET:HA	4:H:62:PHE:HB3	2.04	0.40
6:J:-69:DG:C2	6:J:-68:DA:C2	3.09	0.40
6:J:28:DA:C6	6:J:29:DG:C6	3.09	0.40
5:I:3:DT:H2''	5:I:4:DC:C6	2.56	0.40
6:J:20:DG:H1'	6:J:21:DG:H5''	2.03	0.40
9:K:1196:LEU:HB3	9:K:1227:SER:HB2	2.04	0.40
10:L:94:LEU:HD23	10:L:94:LEU:HA	1.80	0.40
10:L:150:HIS:NE2	10:L:186:ASP:OD2	2.50	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	117/135 (87%)	109 (93%)	7 (6%)	1 (1%)	14	46
1	E	97/135 (72%)	91 (94%)	6 (6%)	0	100	100
2	B	78/102 (76%)	73 (94%)	5 (6%)	0	100	100
2	F	80/102 (78%)	76 (95%)	4 (5%)	0	100	100
3	C	105/129 (81%)	104 (99%)	1 (1%)	0	100	100
3	G	104/129 (81%)	104 (100%)	0	0	100	100
4	D	92/122 (75%)	88 (96%)	4 (4%)	0	100	100
4	H	87/122 (71%)	85 (98%)	2 (2%)	0	100	100
7	M	363/684 (53%)	339 (93%)	24 (7%)	0	100	100
7	O	149/684 (22%)	143 (96%)	5 (3%)	1 (1%)	19	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	N	289/401 (72%)	279 (96%)	10 (4%)	0	100	100
8	P	182/401 (45%)	178 (98%)	4 (2%)	0	100	100
9	K	590/1536 (38%)	568 (96%)	22 (4%)	0	100	100
10	L	406/433 (94%)	392 (97%)	14 (3%)	0	100	100
All	All	2739/5115 (54%)	2629 (96%)	108 (4%)	2 (0%)	50	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
7	O	289	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	87/108 (81%)	84 (97%)	3 (3%)	32	56
1	E	72/108 (67%)	72 (100%)	0	100	100
2	B	56/78 (72%)	56 (100%)	0	100	100
2	F	54/78 (69%)	54 (100%)	0	100	100
3	C	75/101 (74%)	75 (100%)	0	100	100
3	G	69/101 (68%)	69 (100%)	0	100	100
4	D	72/102 (71%)	72 (100%)	0	100	100
4	H	60/102 (59%)	60 (100%)	0	100	100
7	M	286/653 (44%)	286 (100%)	0	100	100
7	O	108/653 (16%)	108 (100%)	0	100	100
8	N	216/359 (60%)	216 (100%)	0	100	100
8	P	123/359 (34%)	123 (100%)	0	100	100
9	K	468/1391 (34%)	467 (100%)	1 (0%)	92	95
10	L	291/367 (79%)	291 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2037/4560 (45%)	2033 (100%)	4 (0%)	91	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	22	THR
1	A	23	LYS
9	K	951	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	25	ASN
3	G	38	ASN
3	G	73	ASN
3	G	82	HIS
4	H	60	ASN
8	N	18	HIS
9	K	937	GLN
8	P	263	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	ML3	E	36	1	10,11,12	0.72	0	10,14,16	0.74	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ML3	E	36	1	-	1/8/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	36	ML3	SG-CD-CE-NZ

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	36	ML3	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.