



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 05:38 PM UTC

PDB ID : 7C0M / pdb_00007c0m
EMDB ID : EMD-30267
Title : Human cGAS-nucleosome complex
Authors : Kujirai, T.; Zierhut, C.; Takizawa, Y.; Kim, R.; Negishi, L.; Uruma, N.; Hirai, S.; Funabiki, H.; Kurumizaka, H.
Deposited on : 2020-05-01
Resolution : 3.90 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 : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

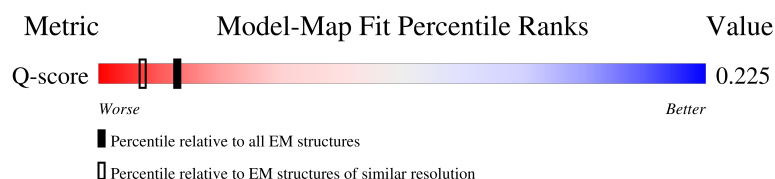
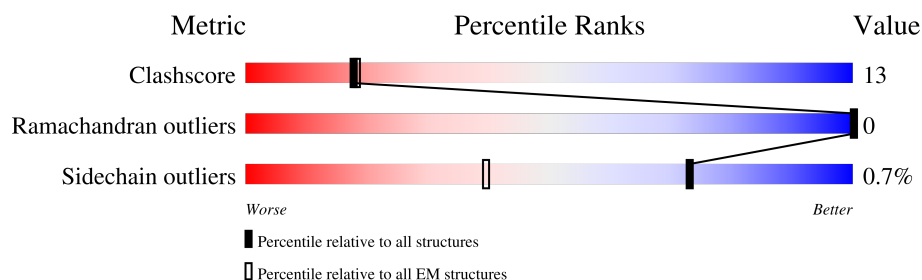
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	139	 55% 14% 30%
1	E	139	 55% 14% 30%
1	a	139	 51% 19% 30%
1	e	139	 55% 15% 30%

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Mol	Chain	Length	Quality of chain
2	B	106	
2	F	106	
2	b	106	
2	f	106	
3	C	133	
3	G	133	
3	c	133	
3	g	133	
4	D	129	
4	H	129	
4	d	129	
4	h	129	
5	I	145	
5	i	145	
6	J	145	
6	j	145	
7	K	380	
7	k	380	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 29816 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 H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	97	Total	C	N	O	S	0	0
			801	505	155	137	4		
1	E	97	Total	C	N	O	S	0	0
			799	503	155	137	4		
1	a	97	Total	C	N	O	S	0	0
			801	505	155	137	4		
1	e	97	Total	C	N	O	S	0	0
			799	503	155	137	4		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P68431
A	-2	SER	-	expression tag	UNP P68431
A	-1	HIS	-	expression tag	UNP P68431
A	0	MET	-	expression tag	UNP P68431
E	-3	GLY	-	expression tag	UNP P68431
E	-2	SER	-	expression tag	UNP P68431
E	-1	HIS	-	expression tag	UNP P68431
E	0	MET	-	expression tag	UNP P68431
a	-3	GLY	-	expression tag	UNP P68431
a	-2	SER	-	expression tag	UNP P68431
a	-1	HIS	-	expression tag	UNP P68431
a	0	MET	-	expression tag	UNP P68431
e	-3	GLY	-	expression tag	UNP P68431
e	-2	SER	-	expression tag	UNP P68431
e	-1	HIS	-	expression tag	UNP P68431
e	0	MET	-	expression tag	UNP P68431

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	83	Total	C	N	O	S	0	0
			661	418	129	113	1		
2	F	78	Total	C	N	O	S	0	0
			618	391	120	106	1		
2	b	83	Total	C	N	O	S	0	0
			661	418	129	113	1		
2	f	78	Total	C	N	O	S	0	0
			618	391	120	106	1		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P62805
B	-2	SER	-	expression tag	UNP P62805
B	-1	HIS	-	expression tag	UNP P62805
B	0	MET	-	expression tag	UNP P62805
F	-3	GLY	-	expression tag	UNP P62805
F	-2	SER	-	expression tag	UNP P62805
F	-1	HIS	-	expression tag	UNP P62805
F	0	MET	-	expression tag	UNP P62805
b	-3	GLY	-	expression tag	UNP P62805
b	-2	SER	-	expression tag	UNP P62805
b	-1	HIS	-	expression tag	UNP P62805
b	0	MET	-	expression tag	UNP P62805
f	-3	GLY	-	expression tag	UNP P62805
f	-2	SER	-	expression tag	UNP P62805
f	-1	HIS	-	expression tag	UNP P62805
f	0	MET	-	expression tag	UNP P62805

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	103	Total	C	N	O	0	0
			796	502	155	139		
3	G	105	Total	C	N	O	0	0
			810	511	158	141		
3	c	103	Total	C	N	O	0	0
			796	502	155	139		
3	g	105	Total	C	N	O	0	0
			810	511	158	141		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP P04908
C	-2	SER	-	expression tag	UNP P04908
C	-1	HIS	-	expression tag	UNP P04908
C	0	MET	-	expression tag	UNP P04908
G	-3	GLY	-	expression tag	UNP P04908
G	-2	SER	-	expression tag	UNP P04908
G	-1	HIS	-	expression tag	UNP P04908
G	0	MET	-	expression tag	UNP P04908
c	-3	GLY	-	expression tag	UNP P04908
c	-2	SER	-	expression tag	UNP P04908
c	-1	HIS	-	expression tag	UNP P04908
c	0	MET	-	expression tag	UNP P04908
g	-3	GLY	-	expression tag	UNP P04908
g	-2	SER	-	expression tag	UNP P04908
g	-1	HIS	-	expression tag	UNP P04908
g	0	MET	-	expression tag	UNP P04908

- Molecule 4 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	95	Total	C	N	O	S	0	0
			745	468	136	139	2		
4	H	93	Total	C	N	O	S	0	0
			725	456	130	137	2		
4	d	95	Total	C	N	O	S	0	0
			745	468	136	139	2		
4	h	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP P06899
D	-2	SER	-	expression tag	UNP P06899
D	-1	HIS	-	expression tag	UNP P06899
D	0	MET	-	expression tag	UNP P06899
H	-3	GLY	-	expression tag	UNP P06899
H	-2	SER	-	expression tag	UNP P06899
H	-1	HIS	-	expression tag	UNP P06899
H	0	MET	-	expression tag	UNP P06899
d	-3	GLY	-	expression tag	UNP P06899
d	-2	SER	-	expression tag	UNP P06899
d	-1	HIS	-	expression tag	UNP P06899

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Chain	Residue	Modelled	Actual	Comment	Reference
d	0	MET	-	expression tag	UNP P06899
h	-3	GLY	-	expression tag	UNP P06899
h	-2	SER	-	expression tag	UNP P06899
h	-1	HIS	-	expression tag	UNP P06899
h	0	MET	-	expression tag	UNP P06899

- Molecule 5 is a DNA chain called DNA (145-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	145	Total	C	N	O	P	0	0
			2952	1404	537	867	144		
5	i	145	Total	C	N	O	P	0	0
			2952	1404	537	867	144		

- Molecule 6 is a DNA chain called DNA (145-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	145	Total	C	N	O	P	0	0
			2987	1416	558	869	144		
6	j	145	Total	C	N	O	P	0	0
			2987	1416	558	869	144		

- Molecule 7 is a protein called Cyclic GMP-AMP synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	366	Total	C	N	O	S	3	0
			3013	1924	520	554	15		
7	k	366	Total	C	N	O	S	3	0
			3013	1924	520	554	15		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	149	GLY	-	expression tag	UNP Q8N884
K	150	SER	-	expression tag	UNP Q8N884
K	523	GLU	-	expression tag	UNP Q8N884
K	524	ASN	-	expression tag	UNP Q8N884
K	525	LEU	-	expression tag	UNP Q8N884
K	526	TYR	-	expression tag	UNP Q8N884
K	527	PHE	-	expression tag	UNP Q8N884
K	528	GLN	-	expression tag	UNP Q8N884
k	149	GLY	-	expression tag	UNP Q8N884

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Chain	Residue	Modelled	Actual	Comment	Reference
k	150	SER	-	expression tag	UNP Q8N884
k	523	GLU	-	expression tag	UNP Q8N884
k	524	ASN	-	expression tag	UNP Q8N884
k	525	LEU	-	expression tag	UNP Q8N884
k	526	TYR	-	expression tag	UNP Q8N884
k	527	PHE	-	expression tag	UNP Q8N884
k	528	GLN	-	expression tag	UNP Q8N884

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

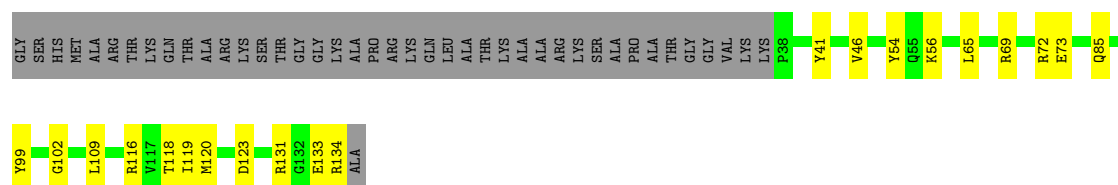
Mol	Chain	Residues	Atoms		AltConf
8	K	1	Total 1	Zn 1	0
8	k	1	Total 1	Zn 1	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

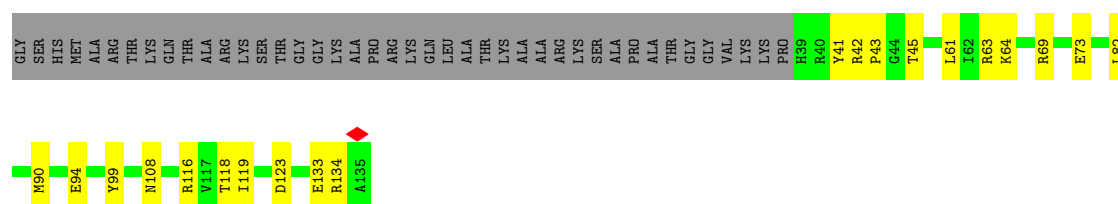
• Molecule 1: Histone H3.1

Chain A: 



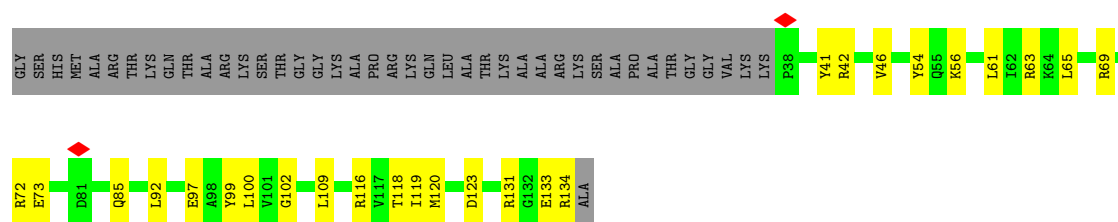
• Molecule 1: Histone H3.1

Chain E: 



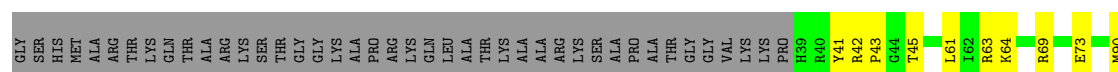
• Molecule 1: Histone H3.1

Chain a: 



• Molecule 1: Histone H3.1

Chain e: 





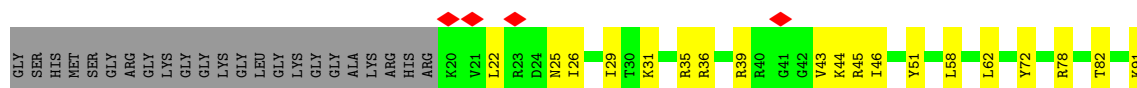
• Molecule 2: Histone H4



• Molecule 2: Histone H4



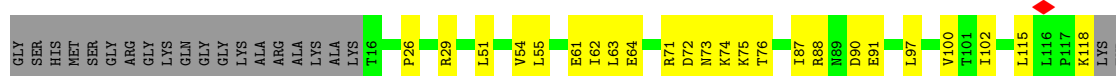
• Molecule 2: Histone H4



• Molecule 2: Histone H4



• Molecule 3: Histone H2A type 1-B/E



GLU
SER
HIS
HIS
LYS
ALA
LYS
LYS

• Molecule 3: Histone H2A type 1-B/E



GLY
SER
HIS
MET
SER
GLY
ARG
GLY
LYS
GLN
GLY
LYS
LYS
ALA
ALA
ALA
LYS
A14
K15
T16
R17
Q24
R29
V30
H31
R32
K36
R42
P48
V49
Y50
V54
L55
T59
L63
R81
L85
A86
I87
R88
N89
E92
L97
T102
L108

L115
K118
LYS
THR
GLU
SER
HIS
HIS
LYS
ALA
LYS
GLY
LYS

• Molecule 3: Histone H2A type 1-B/E



GLY
SER
MET
SER
GLY
ARG
GLY
LYS
GLN
GLY
LYS
LYS
ALA
ALA
ALA
LYS
LYS
T16
P26
R29
L51
V54
L55
E61
I62
L63
E64
R71
D72
N73
K74
K75
T76
I87
R88
N89
D90
E91
E92
L93
L97
V100
T101
I102
Q112
A113
V114
L115

L116
P117
K118
LYS
THR
GLU
SER
HIS
HIS
LYS
ALA
GLY
LYS

• Molecule 3: Histone H2A type 1-B/E



GLY
SER
HIS
MET
SER
GLY
ARG
GLY
LYS
GLN
GLY
LYS
LYS
ALA
ALA
ALA
LYS
LYS
A14
K15
T16
R17
Q24
R29
V30
H31
R32
K36
R42
P48
V49
Y50
V54
L55
T59
L63
R81
L85
A86
I87
R88
N89
E92
L97
T102
L108

Q112
A113
V114
L115
P117
K118
LYS
THR
GLU
SER
HIS
HIS
LYS
ALA
GLY
LYS

• Molecule 4: Histone H2B type 1-J

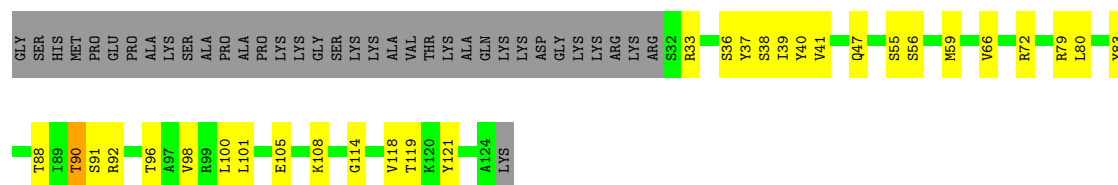


GLY
SER
HIS
MET
PRO
GLU
PRO
ALA
LYS
SER
PRO
ALA
ALA
PRO
LYS
LYS
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SER
LYS
LYS
LYS
VAL
THR
LYS
LYS
ALA
GLN
LYS
LYS
ASP
GLY
LYS
LYS
ARG
R31
S32
R33
K34
E35
S36
Y37
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P50
D51
M59
N63
D68
I69
F70
E71

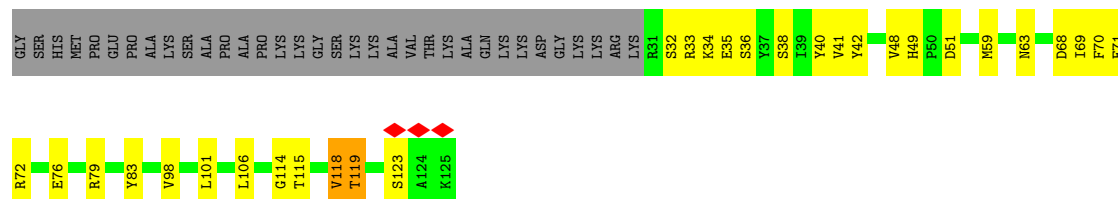
R72
R79
Y83
V98
L101
G114
T115
V118
T119
K125

• Molecule 4: Histone H2B type 1-J

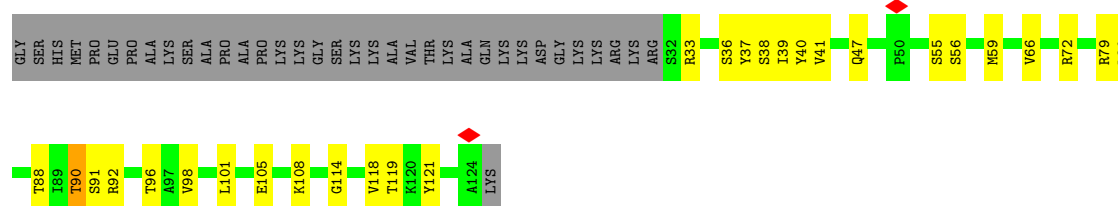




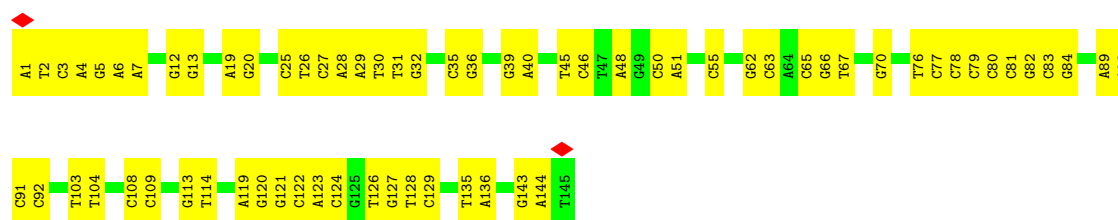
• Molecule 4: Histone H2B type 1-J



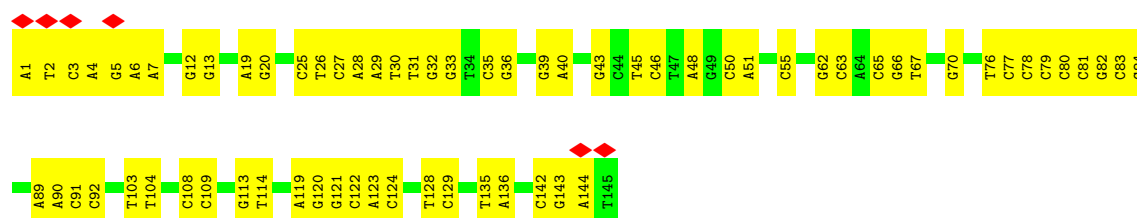
• Molecule 4: Histone H2B type 1-J



• Molecule 5: DNA (145-MER)

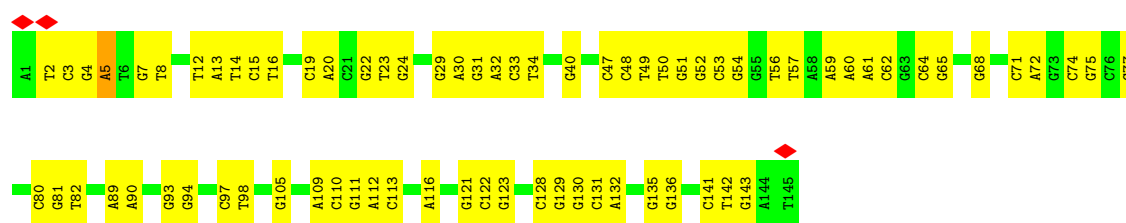


• Molecule 5: DNA (145-MER)



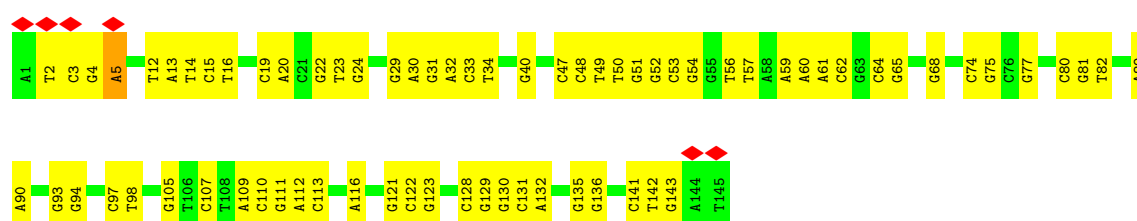
- Molecule 6: DNA (145-MER)

Chain J:  49% 50%



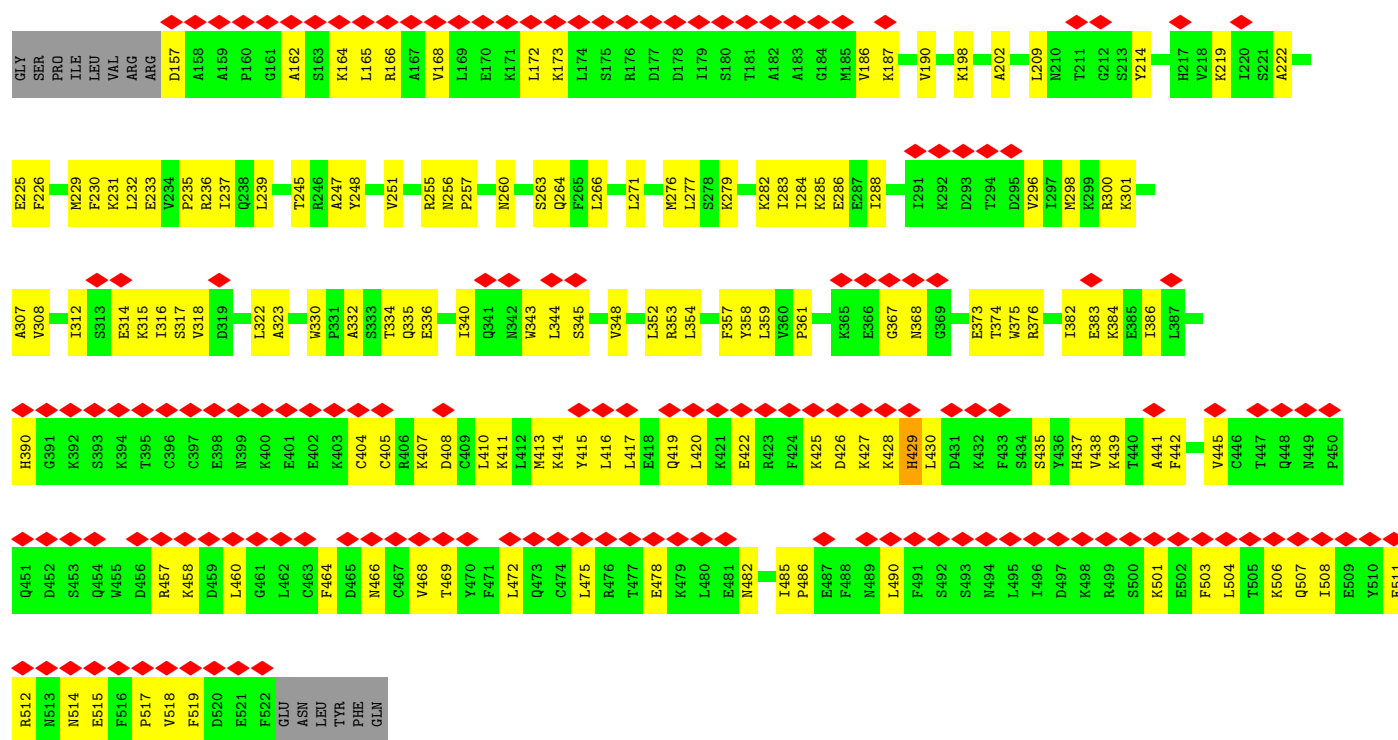
- Molecule 6: DNA (145-MER)

Chain j:  51% 48%

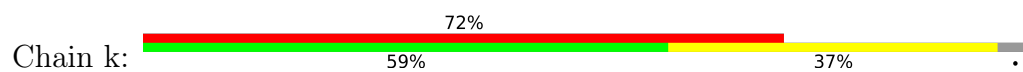


- Molecule 7: Cyclic GMP-AMP synthase

Chain K:  41% 58% 38%



- Molecule 7: Cyclic GMP-AMP synthase



L475	R476	T477	E478	K479	L480	E481	N482	Y483	F484	I485	P486	E487	F488	N489	L490	F491	S492	S493	N494	L495	I496	D497	K498	R499	S500	K501	E502	F503	L504	T505	K506	Q507	I508	E509	Y510	E511	R512	N513	N514	E515	F516	P517	V518	F519	D520	E521	F522	GLU	ASN	LEU	TYR	PHE	GLN						
Y415	L416	L417	E418	Q419	L420	K421	E422	R423	F424	K425	D426	K427	K428	H429	L430	D431	K432	F433	N434	S435	Y436	H437	V438	K439	T440	A441	F442	F443	H444	V445	C446	T447	Q448	N449	P450	Q451	D452	S453	Q454	W455	D456	R457	K458	D459	L460	G461	L462	C463	F464	D465	N466	C467	V468	T469	Y470	F471	L472	Q473	C474
L352	R353	L354	K355	P356	F357	Y358	P361	K362	H363	A364	K365	E366	G367	N368	G369	F370	Q371	E372	E373	T374	W375	R376	H381	I382	E383	K384	E385	I386	L387	N388	N389	H390	G391	K392	S393	K394	T395	C396	C397	E398	N399	K400	E401	E402	K403	C404	C405	R406	K407	D408	C409	L410	K411	L412	M413	K414			
I284	K285	E286	E287	I288	N289	D290	I291	K292	D293	T294	D295	V296	I297	M298	K299	R300	K301	R302	G303	G304	S305	P306	A307	V308	T309	L310	L311	I312	S313	E314	K315	I316	S317	V318	D319	I320	T321	L322	W330	P331	A332	S333	T334	Q335	E336	G337	L338	R339	I340	Q341	N342	W343	L344	S345	A346	K347	V348	R349	
H217	V218	K219	I220	S221	A222	P223	N224	E225	F226	D227	V228	M229	F230	K231	L232	E233	V234	P235	R236	I237	Q238	L239	E240	E241	Y242	S243	N244	T245	R246	A247	Y248	Y249	F250	V251	R255	E256	P257	N260	S263	Q264	F265	L266	E267	L271	S274	K275	M276	L277	S278	K279	F280	R281	K282	I283					
GLY	SER	PRO	ILE	LEU	VAL	ARG	D157	A158	A159	P160	G161	A162	S163	K164	L165	R166	A167	V168	L169	E170	K171	L172	K173	L174	S175	R176	D177	D178	I179	S180	T181	A182	A183	G184	M185	V186	K187	G188	V189	V190	D191	L195	R196	A202	F203	R204	L208	L209	W210	T211	G212	S213	Y214	Y215	E216				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	160075	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.058	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0119	Depositor
Map size (Å)	262.5, 262.5, 262.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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	A	0.63	0/813	0.53	0/1090
1	E	0.62	0/810	0.53	0/1086
1	a	0.63	0/813	0.53	0/1090
1	e	0.62	0/810	0.53	0/1086
2	B	0.67	0/668	0.57	0/894
2	F	0.68	0/625	0.55	0/837
2	b	0.66	0/668	0.57	0/894
2	f	0.68	0/625	0.55	0/837
3	C	0.64	0/806	0.59	0/1089
3	G	0.57	0/820	0.48	0/1107
3	c	0.64	0/806	0.59	0/1089
3	g	0.57	0/820	0.48	0/1107
4	D	0.62	0/756	0.53	0/1015
4	H	0.61	0/736	0.55	0/990
4	d	0.62	0/756	0.53	0/1015
4	h	0.61	0/736	0.55	0/990
5	I	0.44	0/3308	0.49	1/5099 (0.0%)
5	i	0.44	0/3308	0.49	1/5099 (0.0%)
6	J	0.45	0/3354	0.47	1/5180 (0.0%)
6	j	0.44	0/3354	0.47	1/5180 (0.0%)
7	K	0.22	0/3074	0.50	1/4124 (0.0%)
7	k	0.21	0/3074	0.50	0/4124
All	All	0.49	0/31540	0.51	5/45022 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	j	5	DA	C2'-C3'-O3'	-5.91	102.64	111.50
6	J	5	DA	C2'-C3'-O3'	-5.90	102.65	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	48	DA	C2'-C3'-O3'	-5.54	103.19	111.50
5	i	48	DA	C2'-C3'-O3'	-5.52	103.22	111.50
7	K	233	GLU	N-CA-C	5.25	117.41	111.11

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	801	0	839	19	0
1	E	799	0	836	23	0
1	a	801	0	839	23	0
1	e	799	0	836	24	0
2	B	661	0	709	20	0
2	F	618	0	659	22	0
2	b	661	0	709	23	0
2	f	618	0	659	25	0
3	C	796	0	848	30	0
3	G	810	0	866	23	0
3	c	796	0	848	29	0
3	g	810	0	866	22	0
4	D	745	0	771	31	0
4	H	725	0	745	32	0
4	d	745	0	771	37	0
4	h	725	0	745	30	0
5	I	2952	0	1629	58	0
5	i	2952	0	1629	64	0
6	J	2987	0	1630	60	0
6	j	2987	0	1630	60	0
7	K	3013	0	3042	134	0
7	k	3013	0	3042	120	0
8	K	1	0	0	0	0
8	k	1	0	0	0	0
All	All	29816	0	25148	736	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 13.

All (736) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:114:GLY:O	4:d:118:VAL:HG12	1.64	0.97
4:D:114:GLY:O	4:D:118:VAL:HG12	1.64	0.96
2:b:91:LYS:HZ1	4:d:79:ARG:HE	1.23	0.87
4:d:33:ARG:HH22	6:j:121:DG:H21	1.23	0.86
2:B:91:LYS:HZ3	4:D:79:ARG:HE	1.26	0.83
4:D:33:ARG:HH22	6:J:121:DG:H21	1.23	0.81
7:K:368:ASN:O	4:d:119:THR:HG21	1.81	0.81
7:K:285:LYS:HZ3	5:i:43:DG:C5'	1.94	0.80
7:k:514:ASN:HD22	7:k:517:PRO:HG3	1.46	0.80
4:H:38:SER:HA	4:H:59:MET:HE2	1.64	0.80
7:K:514:ASN:HD22	7:K:517:PRO:HG3	1.46	0.80
4:d:36:SER:HB2	4:d:63:ASN:HD21	1.47	0.79
7:K:285:LYS:NZ	5:i:43:DG:H5''	1.96	0.79
4:h:38:SER:HA	4:h:59:MET:HE2	1.64	0.79
4:D:36:SER:HB2	4:D:63:ASN:HD21	1.47	0.78
7:K:427:LYS:HD2	5:i:33:DG:OP2	1.82	0.78
7:k:312:ILE:HB	7:k:316:ILE:HB	1.67	0.77
7:K:368:ASN:O	4:d:119:THR:CG2	2.34	0.76
7:K:503:PHE:HA	7:K:506:LYS:HE3	1.67	0.76
7:k:503:PHE:HA	7:k:506:LYS:HE3	1.67	0.75
1:A:41:TYR:HA	5:I:143:DG:H5''	1.68	0.75
1:E:133:GLU:O	1:E:134:ARG:NE	2.19	0.74
7:K:312:ILE:HB	7:K:316:ILE:HB	1.67	0.74
1:a:41:TYR:HA	5:i:143:DG:H5''	1.68	0.74
1:e:63:ARG:NH2	6:j:59:DA:O3'	2.21	0.74
1:e:133:GLU:O	1:e:134:ARG:NE	2.19	0.74
1:E:63:ARG:NH2	6:J:59:DA:O3'	2.20	0.73
7:K:285:LYS:NZ	5:i:43:DG:C5'	2.51	0.73
2:f:92:ARG:HH21	4:h:101:LEU:HA	1.54	0.73
7:K:414:LYS:HZ1	7:K:439:LYS:HB2	1.55	0.71
2:F:92:ARG:HH21	4:H:101:LEU:HA	1.54	0.71
7:K:300:ARG:HD2	6:j:107:DC:H4'	1.71	0.71
7:K:482:ASN:HD22	7:K:485:ILE:HD12	1.57	0.70
6:J:129:DG:N2	6:J:130:DG:C2	2.60	0.70
7:k:482:ASN:HD22	7:k:485:ILE:HD12	1.56	0.70
6:j:129:DG:N2	6:j:130:DG:C2	2.60	0.69
1:E:41:TYR:HA	6:J:143:DG:H5''	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:41:TYR:HA	6:j:143:DG:H5''	1.73	0.69
4:H:72:ARG:HB3	4:H:101:LEU:HD21	1.74	0.69
4:h:72:ARG:HB3	4:h:101:LEU:HD21	1.74	0.69
7:K:428:LYS:O	7:K:428:LYS:HG3	1.94	0.68
1:E:42:ARG:N	6:J:143:DG:OP1	2.27	0.67
7:k:428:LYS:HG3	7:k:428:LYS:O	1.94	0.67
3:G:29:ARG:NH1	4:H:36:SER:O	2.27	0.67
1:e:42:ARG:N	6:j:143:DG:OP1	2.27	0.67
7:K:285:LYS:HZ1	5:i:43:DG:H5''	1.58	0.67
3:g:29:ARG:NH1	4:h:36:SER:O	2.27	0.67
4:h:33:ARG:HH12	5:i:121:DG:H21	1.43	0.66
7:k:226:PHE:HB2	7:k:318:VAL:HG12	1.78	0.66
5:I:4:DA:H2''	5:I:5:DG:C8	2.31	0.66
5:i:4:DA:H2''	5:i:5:DG:C8	2.31	0.66
7:K:314:GLU:HA	7:K:314:GLU:OE1	1.95	0.66
4:H:33:ARG:HH12	5:I:121:DG:H21	1.43	0.66
7:K:226:PHE:HB2	7:K:318:VAL:HG12	1.78	0.66
3:c:26:PRO:HG3	4:d:40:TYR:CZ	2.31	0.66
3:C:26:PRO:HG3	4:D:40:TYR:CZ	2.31	0.65
1:A:73:GLU:OE1	2:B:25:ASN:ND2	2.29	0.65
7:k:314:GLU:HA	7:k:314:GLU:OE1	1.95	0.65
3:C:64:GLU:HB2	4:D:48:VAL:HG11	1.78	0.65
6:J:49:DT:H2'	6:J:50:DT:H71	1.80	0.64
1:a:73:GLU:OE1	2:b:25:ASN:ND2	2.29	0.64
3:c:64:GLU:HB2	4:d:48:VAL:HG11	1.78	0.64
1:E:61:LEU:HD12	2:F:37:LEU:HD23	1.80	0.63
3:c:73:ASN:O	3:c:75:LYS:HG3	1.99	0.63
7:k:414:LYS:HZ2	7:k:435:SER:HB3	1.62	0.63
3:c:90:ASP:OD2	7:k:255:ARG:NH1	2.30	0.63
7:K:284:ILE:HD12	7:K:308:VAL:HG21	1.81	0.63
6:j:49:DT:H2'	6:j:50:DT:H71	1.80	0.63
1:A:69:ARG:NH2	6:J:90:DA:OP2	2.30	0.63
3:C:90:ASP:OD2	7:K:255:ARG:NH1	2.30	0.63
1:a:69:ARG:NH2	6:j:90:DA:OP2	2.30	0.63
7:k:284:ILE:HD12	7:k:308:VAL:HG21	1.81	0.62
7:k:405:CYS:HB2	7:k:460:LEU:HD13	1.82	0.62
3:C:64:GLU:OE1	7:K:236:ARG:NH2	2.29	0.61
1:e:61:LEU:HD12	2:f:37:LEU:HD23	1.80	0.61
3:C:73:ASN:O	3:C:75:LYS:HG3	1.99	0.61
7:K:405:CYS:HB2	7:K:460:LEU:HD13	1.82	0.61
7:k:251:VAL:HG13	7:k:271:LEU:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:33:DC:H1'	6:J:34:DT:H5'	1.82	0.61
7:k:414:LYS:HZ1	7:k:439:LYS:HB2	1.65	0.61
6:j:33:DC:H1'	6:j:34:DT:H5'	1.82	0.61
7:k:352:LEU:HD12	7:k:382:ILE:HG23	1.83	0.60
7:K:251:VAL:HG13	7:K:271:LEU:HB3	1.83	0.60
3:g:32:ARG:NH1	6:j:29:DG:OP1	2.34	0.60
3:g:17:ARG:HD3	4:h:121:TYR:OH	2.02	0.60
7:k:414:LYS:NZ	7:k:439:LYS:HB2	2.17	0.60
3:G:32:ARG:NH1	6:J:29:DG:OP1	2.34	0.60
3:C:88:ARG:NH2	3:C:100:VAL:O	2.35	0.59
3:c:88:ARG:NH2	3:c:100:VAL:O	2.35	0.59
3:G:42:ARG:HB2	4:H:88:THR:HG22	1.84	0.59
7:K:352:LEU:HD12	7:K:382:ILE:HD12	1.83	0.59
7:k:352:LEU:HD12	7:k:382:ILE:HD12	1.83	0.59
7:K:168:VAL:HG21	7:K:519:PHE:HD2	1.68	0.59
3:c:64:GLU:OE1	7:k:236:ARG:NH2	2.29	0.59
2:F:47:SER:OG	2:F:48:GLY:N	2.35	0.59
7:k:168:VAL:HG21	7:k:519:PHE:HD2	1.68	0.59
3:G:17:ARG:HD3	4:H:121:TYR:OH	2.02	0.59
7:K:414:LYS:NZ	7:K:439:LYS:HB2	2.17	0.59
1:a:116:ARG:NH1	1:a:120:MET:SD	2.76	0.59
1:A:116:ARG:NH1	1:A:120:MET:SD	2.76	0.58
2:f:47:SER:OG	2:f:48:GLY:N	2.35	0.58
7:K:352:LEU:HD12	7:K:382:ILE:HG23	1.84	0.58
6:j:53:DC:H2''	6:j:54:DG:C8	2.39	0.58
6:J:53:DC:H2''	6:J:54:DG:C8	2.39	0.58
6:j:2:DT:H1'	6:j:3:DC:H5'	1.84	0.58
3:g:42:ARG:HB2	4:h:88:THR:HG22	1.84	0.58
2:b:92:ARG:HH21	4:d:101:LEU:HA	1.68	0.58
2:B:91:LYS:HZ1	4:D:79:ARG:HH21	1.52	0.58
6:J:2:DT:H1'	6:J:3:DC:H5'	1.84	0.58
7:K:464:PHE:O	7:K:468:VAL:HG23	2.04	0.58
6:J:60:DA:H2''	6:J:61:DA:H8	1.69	0.57
2:f:75:HIS:HB2	4:h:96:THR:HG21	1.86	0.57
7:K:413[A]:MET:HB3	7:K:438:VAL:HG11	1.86	0.57
6:j:60:DA:H2''	6:j:61:DA:H8	1.70	0.57
2:B:92:ARG:HH21	4:D:101:LEU:HA	1.68	0.57
6:j:4:DG:H4'	6:j:5:DA:H5'	1.87	0.57
7:k:279:LYS:O	7:k:283:ILE:HG13	2.05	0.57
7:k:413[A]:MET:HB3	7:k:438:VAL:HG11	1.86	0.57
3:G:24:GLN:NE2	4:H:47:GLN:OE1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:164:LYS:O	7:K:168:VAL:HG23	2.04	0.57
7:k:464:PHE:O	7:k:468:VAL:HG23	2.04	0.57
6:J:47:DC:H2''	6:J:48:DC:C6	2.39	0.57
4:d:33:ARG:HH22	6:j:121:DG:N2	2.00	0.57
7:k:237:ILE:HB	7:k:251:VAL:HG23	1.86	0.57
3:C:72:ASP:C	3:C:74:LYS:H	2.12	0.57
4:D:33:ARG:HH22	6:J:121:DG:N2	2.00	0.57
5:I:128:DT:H2''	5:I:129:DC:C5	2.40	0.57
6:J:93:DG:H2''	6:J:94:DG:O5'	2.05	0.57
3:g:24:GLN:NE2	4:h:47:GLN:OE1	2.37	0.57
5:i:103:DT:H2'	5:i:104:DT:H71	1.87	0.57
7:K:237:ILE:HB	7:K:251:VAL:HG23	1.86	0.57
7:k:336:GLU:HB2	7:k:486:PRO:HG3	1.87	0.57
2:F:75:HIS:HB2	4:H:96:THR:HG21	1.86	0.56
7:K:367:GLY:O	4:d:123:SER:HB2	2.05	0.56
4:H:33:ARG:HH22	5:I:121:DG:N2	2.04	0.56
7:K:279:LYS:O	7:K:283:ILE:HG13	2.05	0.56
6:j:47:DC:H2''	6:j:48:DC:C6	2.39	0.56
7:k:164:LYS:O	7:k:168:VAL:HG23	2.04	0.56
7:k:437:HIS:HD2	7:k:490:LEU:HD23	1.70	0.56
7:K:245:THR:HG23	7:K:248:TYR:H	1.70	0.56
4:h:33:ARG:HH22	5:i:121:DG:N2	2.04	0.56
5:i:77:DC:H2''	5:i:78:DC:C5	2.41	0.56
6:j:93:DG:H2''	6:j:94:DG:O5'	2.05	0.56
5:I:77:DC:H2''	5:I:78:DC:C5	2.41	0.56
5:I:83:DC:H2''	5:I:84:DG:C8	2.41	0.56
5:i:128:DT:H2''	5:i:129:DC:C5	2.40	0.56
6:J:4:DG:H4'	6:J:5:DA:H5'	1.87	0.56
7:K:336:GLU:HB2	7:K:486:PRO:HG3	1.87	0.56
7:K:427:LYS:O	7:K:427:LYS:HG3	2.06	0.56
3:g:88:ARG:NH2	3:g:97:LEU:O	2.39	0.56
7:k:245:THR:HG23	7:k:248:TYR:H	1.70	0.56
5:I:89:DA:H1'	5:I:90:DA:C8	2.42	0.55
7:K:245:THR:HG21	7:K:248:TYR:HB2	1.88	0.55
7:K:263:SER:HA	7:K:266:LEU:HD23	1.88	0.55
7:k:507:GLN:O	7:k:511:GLU:HG2	2.07	0.55
7:k:427:LYS:O	7:k:427:LYS:HG3	2.06	0.55
1:E:116:ARG:HH22	1:E:123:ASP:CG	2.14	0.55
3:c:72:ASP:C	3:c:74:LYS:H	2.12	0.55
1:e:116:ARG:HH22	1:e:123:ASP:CG	2.14	0.55
7:K:414:LYS:HZ2	7:K:435:SER:HB3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:437:HIS:HD2	7:K:490:LEU:HD23	1.70	0.55
5:i:83:DC:H2''	5:i:84:DG:C8	2.41	0.55
3:G:88:ARG:NH2	3:G:97:LEU:O	2.39	0.55
5:I:103:DT:H2'	5:I:104:DT:H71	1.87	0.55
7:k:263:SER:HA	7:k:266:LEU:HD23	1.88	0.55
1:A:119:ILE:HD13	2:B:43:VAL:HG21	1.89	0.55
5:i:89:DA:H1'	5:i:90:DA:C8	2.41	0.55
6:j:64:DC:H2''	6:j:65:DG:C8	2.42	0.55
6:J:64:DC:H2''	6:J:65:DG:C8	2.42	0.55
1:e:99:TYR:OH	1:e:133:GLU:OE1	2.26	0.54
4:h:55:SER:OG	4:h:56:SER:N	2.40	0.54
7:k:237:ILE:HD12	7:k:239:LEU:HD21	1.90	0.54
6:j:141:DC:H2'	6:j:142:DT:C6	2.42	0.54
7:K:410:LEU:HD12	7:K:442:PHE:CD1	2.43	0.54
4:h:36:SER:OG	4:h:37:TYR:N	2.40	0.54
3:c:87:ILE:HD13	3:c:97:LEU:HD12	1.89	0.54
3:C:87:ILE:HD13	3:C:97:LEU:HD12	1.89	0.54
1:E:99:TYR:OH	1:E:133:GLU:OE1	2.26	0.54
7:K:507:GLN:O	7:K:511:GLU:HG2	2.07	0.54
3:c:71:ARG:HH21	7:k:354:LEU:HA	1.72	0.54
7:k:245:THR:HG21	7:k:248:TYR:HB2	1.88	0.54
3:C:71:ARG:HH21	7:K:354:LEU:HA	1.72	0.54
1:a:119:ILE:HD13	2:b:43:VAL:HG21	1.89	0.54
3:C:90:ASP:CG	7:K:255:ARG:HH12	2.16	0.54
6:J:141:DC:H2'	6:J:142:DT:C6	2.42	0.54
3:c:76:THR:HG22	7:k:354:LEU:HD11	1.90	0.54
3:c:90:ASP:CG	7:k:255:ARG:HH12	2.16	0.54
5:i:35:DC:H2''	5:i:36:DG:C8	2.43	0.54
4:H:114:GLY:O	4:H:118:VAL:HG23	2.08	0.53
7:k:504:LEU:HA	7:k:507:GLN:HG2	1.90	0.53
3:G:31:HIS:CD2	3:G:48:PRO:HG2	2.43	0.53
7:K:237:ILE:HD12	7:K:239:LEU:HD21	1.90	0.53
7:K:277:LEU:HD11	7:K:361:PRO:HG2	1.90	0.53
7:K:416:LEU:O	7:K:420:LEU:HG	2.08	0.53
1:E:69:ARG:HB3	2:F:25:ASN:HD21	1.74	0.53
5:I:2:DT:H2''	5:I:3:DC:C6	2.43	0.53
5:I:35:DC:H2''	5:I:36:DG:C8	2.44	0.53
3:g:31:HIS:CD2	3:g:48:PRO:HG2	2.43	0.53
7:k:410:LEU:HD12	7:k:442:PHE:CD1	2.43	0.53
7:k:408:ASP:OD1	7:k:457:ARG:NH1	2.42	0.53
6:j:129:DG:H2''	6:j:130:DG:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:63:LEU:HD11	4:H:41:VAL:HG13	1.91	0.53
1:e:69:ARG:HB3	2:f:25:ASN:HD21	1.74	0.53
5:I:108:DC:H2''	5:I:109:DC:C5	2.43	0.52
5:i:108:DC:H2''	5:i:109:DC:C5	2.44	0.52
7:k:416:LEU:O	7:k:420:LEU:HG	2.08	0.52
5:i:2:DT:H2''	5:i:3:DC:C6	2.44	0.52
5:i:89:DA:H1'	5:i:90:DA:N7	2.24	0.52
3:C:61:GLU:HG2	7:K:255:ARG:HH21	1.75	0.52
3:C:76:THR:HG22	7:K:354:LEU:HD11	1.90	0.52
1:a:99:TYR:OH	1:a:133:GLU:OE1	2.26	0.52
7:k:277:LEU:HD11	7:k:361:PRO:HG2	1.90	0.52
1:A:99:TYR:OH	1:A:133:GLU:OE1	2.26	0.52
5:I:89:DA:H1'	5:I:90:DA:N7	2.24	0.52
6:J:129:DG:H2''	6:J:130:DG:C8	2.44	0.52
7:K:408:ASP:OD1	7:K:457:ARG:NH1	2.42	0.52
7:K:437:HIS:CD2	7:K:490:LEU:HD23	2.44	0.52
3:g:63:LEU:HD11	4:h:41:VAL:HG13	1.91	0.52
7:K:504:LEU:HA	7:K:507:GLN:HG2	1.90	0.52
3:g:54:VAL:HG21	4:h:98:VAL:HG21	1.91	0.52
2:f:39:ARG:NH1	2:f:44:LYS:O	2.41	0.52
2:f:84:MET:HE1	2:f:102:GLY:HA2	1.91	0.52
2:F:84:MET:HE1	2:F:102:GLY:HA2	1.91	0.52
4:h:114:GLY:O	4:h:118:VAL:HG23	2.08	0.52
7:k:437:HIS:CD2	7:k:490:LEU:HD23	2.44	0.52
4:H:55:SER:OG	4:H:56:SER:N	2.40	0.52
7:k:164:LYS:HE3	7:k:515:GLU:HB3	1.92	0.52
3:C:54:VAL:HG21	4:D:98:VAL:HG21	1.92	0.52
4:H:36:SER:OG	4:H:37:TYR:N	2.40	0.52
7:K:478:GLU:HA	7:K:501:LYS:HZ2	1.75	0.52
3:C:61:GLU:CG	7:K:255:ARG:HH21	2.23	0.51
5:I:25:DC:H2''	5:I:26:DT:C5	2.45	0.51
6:J:112:DA:C4	6:J:113:DC:C5	2.98	0.51
1:e:119:ILE:HG13	2:f:50:ILE:HG13	1.92	0.51
3:g:16:THR:HA	6:j:30:DA:H5''	1.92	0.51
3:G:16:THR:HA	6:J:30:DA:H5''	1.92	0.51
7:K:422:GLU:HG3	7:K:425:LYS:HZ2	1.76	0.51
7:K:478:GLU:HA	7:K:501:LYS:NZ	2.25	0.51
3:c:87:ILE:HD12	3:c:102:ILE:HD11	1.93	0.51
5:i:25:DC:H2''	5:i:26:DT:C5	2.45	0.51
6:j:112:DA:C4	6:j:113:DC:C5	2.99	0.51
3:C:100:VAL:HG22	2:F:96:THR:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:68:ASP:OD2	2:F:98:TYR:OH	2.23	0.51
3:c:61:GLU:CG	7:k:255:ARG:HH21	2.24	0.51
3:c:91:GLU:HB3	7:k:257:PRO:HB3	1.93	0.51
3:c:100:VAL:HG22	2:f:96:THR:HB	1.93	0.51
4:d:68:ASP:OD2	2:f:98:TYR:OH	2.23	0.51
5:i:1:DA:C8	5:i:2:DT:H72	2.46	0.51
5:i:19:DA:H2''	5:i:20:DG:C8	2.46	0.51
6:j:19:DC:H2''	6:j:20:DA:C8	2.46	0.51
6:J:19:DC:H2''	6:J:20:DA:C8	2.46	0.51
2:b:91:LYS:NZ	4:d:79:ARG:HH21	2.09	0.51
1:e:118:THR:HG21	2:f:45:ARG:HH11	1.75	0.51
5:i:79:DC:H1'	5:i:80:DC:C5	2.46	0.51
2:B:91:LYS:NZ	4:D:79:ARG:HH21	2.09	0.51
2:F:39:ARG:NH1	2:F:44:LYS:O	2.41	0.51
3:G:54:VAL:HG21	4:H:98:VAL:HG21	1.90	0.51
1:A:120:MET:N	1:A:123:ASP:OD2	2.43	0.51
3:c:61:GLU:HG2	7:k:255:ARG:HH21	1.75	0.51
7:k:503:PHE:O	7:k:506:LYS:HG2	2.11	0.51
5:I:19:DA:H2''	5:I:20:DG:C8	2.45	0.51
5:I:79:DC:H1'	5:I:80:DC:C5	2.46	0.51
5:i:31:DT:H2''	5:i:32:DG:H5''	1.93	0.51
7:k:478:GLU:HA	7:k:501:LYS:NZ	2.25	0.51
2:B:92:ARG:HH21	4:D:101:LEU:HD23	1.75	0.51
5:I:1:DA:C8	5:I:2:DT:H72	2.46	0.51
7:K:164:LYS:HE3	7:K:515:GLU:HB3	1.92	0.51
3:c:55:LEU:HD11	4:d:70:PHE:HB2	1.93	0.51
6:j:23:DT:H2''	6:j:24:DG:C8	2.46	0.51
1:E:118:THR:HG21	2:F:45:ARG:HH11	1.75	0.50
6:J:23:DT:H2''	6:J:24:DG:C8	2.46	0.50
7:K:332:ALA:O	7:K:335:GLN:HG3	2.10	0.50
2:b:92:ARG:HH21	4:d:101:LEU:HD23	1.75	0.50
7:k:301:LYS:NZ	7:k:307:ALA:O	2.42	0.50
7:k:332:ALA:O	7:k:335:GLN:HG3	2.11	0.50
7:k:410:LEU:HD12	7:k:442:PHE:HD1	1.77	0.50
6:J:56:DT:H4'	6:J:57:DT:OP1	2.11	0.50
3:c:54:VAL:HG21	4:d:98:VAL:HG21	1.92	0.50
5:i:62:DG:H1'	5:i:63:DC:H5'	1.94	0.50
5:i:70:DG:C2	6:j:77:DG:N2	2.79	0.50
7:k:407:LYS:O	7:k:411:LYS:HG2	2.12	0.50
5:I:31:DT:H2''	5:I:32:DG:H5''	1.93	0.50
5:I:70:DG:C2	6:J:77:DG:N2	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:91:GLU:HB3	7:K:257:PRO:HB3	1.93	0.50
2:b:78:ARG:NH2	4:d:83:TYR:OH	2.44	0.50
3:g:50:TYR:HD2	4:h:118:VAL:HG21	1.77	0.50
3:C:87:ILE:HD12	3:C:102:ILE:HD11	1.93	0.50
7:K:368:ASN:O	4:d:119:THR:HG23	2.09	0.50
7:K:407:LYS:O	7:K:411:LYS:HG2	2.12	0.50
7:K:301:LYS:NZ	7:K:307:ALA:O	2.43	0.50
5:i:5:DG:H2''	5:i:6:DA:H5''	1.94	0.50
2:B:78:ARG:NH2	4:D:83:TYR:OH	2.44	0.49
1:E:119:ILE:HG13	2:F:50:ILE:HG13	1.92	0.49
7:k:478:GLU:HA	7:k:501:LYS:HZ2	1.77	0.49
3:G:50:TYR:HD2	4:H:118:VAL:HG21	1.77	0.49
7:K:503:PHE:O	7:K:506:LYS:HG2	2.11	0.49
3:C:55:LEU:HD11	4:D:70:PHE:HB2	1.93	0.49
5:I:62:DG:H1'	5:I:63:DC:H5'	1.94	0.49
5:I:123:DA:H1'	5:I:124:DC:H5'	1.94	0.49
7:K:427:LYS:HG3	7:K:429:HIS:HD2	1.78	0.49
7:k:344:LEU:HG	7:k:348:VAL:HG11	1.93	0.49
3:C:63:LEU:HD11	4:D:41:VAL:HG13	1.95	0.49
7:K:315:LYS:HG3	7:K:316:ILE:HG13	1.95	0.49
3:g:85:LEU:O	3:g:89:ASN:HB2	2.13	0.49
3:G:85:LEU:O	3:G:89:ASN:HB2	2.13	0.49
7:k:383:GLU:OE1	7:k:439:LYS:HE3	2.13	0.49
5:I:5:DG:H2''	5:I:6:DA:H5''	1.95	0.49
7:K:173:LYS:HA	7:K:173:LYS:HE3	1.95	0.49
7:K:344:LEU:HG	7:K:348:VAL:HG11	1.93	0.49
7:k:315:LYS:HG3	7:k:316:ILE:HG13	1.95	0.49
1:e:118:THR:HG22	2:f:45:ARG:HD3	1.95	0.49
6:j:4:DG:H2''	6:j:5:DA:C8	2.48	0.49
6:J:4:DG:H2''	6:J:5:DA:C8	2.48	0.49
7:K:282:LYS:O	7:K:286:GLU:HG2	2.13	0.49
7:k:166:ARG:HG3	7:k:166:ARG:HH11	1.78	0.49
7:k:427:LYS:HG3	7:k:429:HIS:HD2	1.78	0.49
1:A:56:LYS:O	3:G:81:ARG:NH1	2.46	0.49
1:E:43:PRO:HG2	6:J:68:DG:H5''	1.95	0.49
6:j:56:DT:H4'	6:j:57:DT:OP1	2.11	0.49
7:k:173:LYS:HA	7:k:173:LYS:HE3	1.95	0.49
7:K:410:LEU:HD12	7:K:442:PHE:HD1	1.77	0.49
6:j:59:DA:H2''	6:j:60:DA:H8	1.78	0.49
7:k:345:SER:HG	7:k:348:VAL:H	1.56	0.49
7:K:373:GLU:OE2	7:K:373:GLU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:420:LEU:HD23	7:K:518:VAL:HG21	1.95	0.48
2:B:62:LEU:HD23	2:B:62:LEU:HA	1.66	0.48
4:H:90:THR:HG22	4:H:91:SER:H	1.78	0.48
7:K:166:ARG:HG3	7:K:166:ARG:HH11	1.78	0.48
3:g:92:GLU:OE2	4:h:105:GLU:N	2.32	0.48
7:k:219:LYS:HB2	7:k:222:ALA:HB3	1.96	0.48
3:G:55:LEU:O	3:G:59:THR:HG22	2.13	0.48
1:a:56:LYS:O	3:g:81:ARG:NH1	2.46	0.48
1:e:43:PRO:HG2	6:j:68:DG:H5''	1.95	0.48
7:k:382:ILE:O	7:k:386:ILE:HG12	2.13	0.48
3:C:26:PRO:HG3	4:D:40:TYR:CE1	2.48	0.48
7:K:382:ILE:O	7:K:386:ILE:HG12	2.13	0.48
7:K:383:GLU:OE1	7:K:439:LYS:HE3	2.13	0.48
1:e:63:ARG:HG3	1:e:64:LYS:H	1.78	0.48
7:k:373:GLU:OE2	7:k:373:GLU:N	2.46	0.48
3:G:92:GLU:OE2	4:H:105:GLU:N	2.32	0.48
4:h:90:THR:HG22	4:h:91:SER:H	1.78	0.48
7:k:330:TRP:CZ3	7:k:353:ARG:HG2	2.49	0.48
7:K:225:GLU:HG2	7:K:317:SER:OG	2.14	0.48
5:i:83:DC:H2''	5:i:84:DG:H8	1.79	0.48
2:B:44:LYS:HD2	3:G:115:LEU:HB3	1.95	0.48
5:I:83:DC:H2''	5:I:84:DG:H8	1.79	0.48
3:c:26:PRO:HG3	4:d:40:TYR:CE1	2.48	0.48
1:E:63:ARG:HG3	1:E:64:LYS:H	1.78	0.48
1:E:118:THR:HG22	2:F:45:ARG:HD3	1.95	0.48
7:K:422:GLU:HG3	7:K:425:LYS:NZ	2.29	0.48
3:c:63:LEU:HD11	4:d:41:VAL:HG13	1.94	0.48
6:j:129:DG:N2	6:j:130:DG:N2	2.62	0.48
3:C:26:PRO:HG2	3:C:29:ARG:HB3	1.96	0.47
3:G:81:ARG:HH21	3:G:85:LEU:HD21	1.79	0.47
1:e:73:GLU:OE1	2:f:25:ASN:HB3	2.14	0.47
3:g:81:ARG:HH21	3:g:85:LEU:HD21	1.79	0.47
7:k:225:GLU:HG2	7:k:317:SER:OG	2.14	0.47
7:k:282:LYS:O	7:k:286:GLU:HG2	2.13	0.47
4:H:33:ARG:HH22	5:I:121:DG:H21	1.62	0.47
5:i:123:DA:H1'	5:i:124:DC:H5'	1.94	0.47
7:k:420:LEU:HD23	7:k:518:VAL:HG21	1.95	0.47
6:j:80:DC:H2''	6:j:81:DG:C8	2.50	0.47
1:A:102:GLY:O	1:A:131:ARG:NH2	2.48	0.47
2:f:38:ALA:HB3	2:f:46:ILE:HD11	1.97	0.47
6:j:129:DG:C2	6:j:130:DG:C2	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:38:SER:HA	4:D:59:MET:HE2	1.96	0.47
3:G:36:LYS:HD2	3:G:36:LYS:O	2.15	0.47
4:H:108:LYS:HA	4:H:108:LYS:HD3	1.56	0.47
1:a:102:GLY:O	1:a:131:ARG:NH2	2.47	0.47
6:j:3:DC:H2''	6:j:4:DG:H2'	1.97	0.47
5:I:29:DA:H1'	5:I:30:DT:H5'	1.97	0.47
5:I:80:DC:H5''	5:I:80:DC:C6	2.50	0.47
6:J:59:DA:H2''	6:J:60:DA:H8	1.78	0.47
6:J:80:DC:H2''	6:J:81:DG:C8	2.50	0.47
7:K:219:LYS:HB2	7:K:222:ALA:HB3	1.96	0.47
2:b:91:LYS:HZ2	4:d:79:ARG:HH21	1.61	0.47
3:g:55:LEU:O	3:g:59:THR:HG22	2.13	0.47
1:A:118:THR:HA	2:B:45:ARG:O	2.15	0.47
1:E:73:GLU:OE1	2:F:25:ASN:HB3	2.14	0.47
6:J:129:DG:C2	6:J:130:DG:C2	3.02	0.47
7:K:202:ALA:HB2	7:K:264:GLN:NE2	2.30	0.47
7:K:285:LYS:HZ3	5:i:43:DG:P	2.37	0.47
7:K:345:SER:HG	7:K:348:VAL:H	1.56	0.47
2:b:44:LYS:HD2	3:g:115:LEU:HB3	1.95	0.47
3:g:36:LYS:HD2	3:g:36:LYS:O	2.15	0.47
5:i:80:DC:H5''	5:i:80:DC:C6	2.50	0.47
6:j:97:DC:H2'	6:j:98:DT:H71	1.95	0.47
7:k:504:LEU:HG	7:k:508:ILE:HD11	1.97	0.47
2:F:38:ALA:HB3	2:F:46:ILE:HD11	1.97	0.47
6:J:105:DG:C8	6:J:105:DG:H5'	2.50	0.47
7:K:330:TRP:CZ3	7:K:353:ARG:HG2	2.49	0.47
5:i:29:DA:H1'	5:i:30:DT:H5'	1.97	0.47
1:A:116:ARG:NH2	1:A:123:ASP:OD1	2.48	0.47
4:h:108:LYS:HA	4:h:108:LYS:HD3	1.56	0.47
7:k:414:LYS:NZ	7:k:435:SER:HB3	2.30	0.47
7:k:422:GLU:HG3	7:k:425:LYS:NZ	2.29	0.47
1:a:116:ARG:NH2	1:a:123:ASP:OD1	2.48	0.47
2:b:31:LYS:HE3	2:b:35:ARG:HH21	1.80	0.47
2:b:62:LEU:HD23	2:b:62:LEU:HA	1.66	0.47
2:f:62:LEU:HD23	2:f:62:LEU:HA	1.65	0.47
7:k:202:ALA:HB2	7:k:264:GLN:NE2	2.30	0.47
7:k:248:TYR:HB3	7:k:374:THR:HG21	1.97	0.47
6:J:61:DA:C4	6:J:62:DC:C5	3.04	0.46
7:K:390:HIS:NE2	7:K:404:CYS:SG	2.89	0.46
7:K:466:ASN:O	7:K:469:THR:OG1	2.28	0.46
7:K:504:LEU:HG	7:K:508:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:118:THR:HA	2:b:45:ARG:O	2.15	0.46
5:i:143:DG:H2''	5:i:144:DA:C8	2.50	0.46
6:j:105:DG:C8	6:j:105:DG:H5'	2.50	0.46
6:J:129:DG:N2	6:J:130:DG:N2	2.62	0.46
7:K:430:LEU:HD11	7:K:507:GLN:OE1	2.15	0.46
4:h:41:VAL:HB	4:h:59:MET:HE1	1.98	0.46
5:I:81:DC:H2''	5:I:82:DG:C8	2.50	0.46
6:J:97:DC:H2'	6:J:98:DT:H71	1.95	0.46
3:c:26:PRO:HG2	3:c:29:ARG:HB3	1.96	0.46
1:e:63:ARG:NH1	5:i:90:DA:H4'	2.31	0.46
5:i:81:DC:H2''	5:i:82:DG:C8	2.50	0.46
2:B:31:LYS:HE3	2:B:35:ARG:HH21	1.80	0.46
5:I:2:DT:H2''	5:I:3:DC:C5	2.51	0.46
6:J:3:DC:H2''	6:J:4:DG:H2'	1.97	0.46
6:J:29:DG:H2''	6:J:30:DA:H8	1.81	0.46
4:d:38:SER:HA	4:d:59:MET:HE2	1.96	0.46
6:j:29:DG:H2''	6:j:30:DA:H8	1.81	0.46
6:j:89:DA:H1'	6:j:90:DA:C8	2.51	0.46
6:j:128:DC:H2''	6:j:129:DG:C8	2.51	0.46
5:I:143:DG:H2''	5:I:144:DA:C8	2.51	0.46
6:J:59:DA:H2''	6:J:60:DA:C8	2.51	0.46
5:I:27:DC:H1'	5:I:28:DA:C8	2.51	0.46
1:e:118:THR:HA	2:f:45:ARG:O	2.15	0.46
6:j:61:DA:C4	6:j:62:DC:C5	3.04	0.46
7:k:468:VAL:O	7:k:472:LEU:HG	2.16	0.46
3:C:115:LEU:HD11	1:E:108:ASN:HD21	1.81	0.46
4:D:34:LYS:HD2	4:D:35:GLU:N	2.31	0.46
4:d:34:LYS:HD2	4:d:35:GLU:N	2.31	0.46
7:k:390:HIS:NE2	7:k:404:CYS:SG	2.89	0.46
2:B:35:ARG:O	2:B:39:ARG:HG2	2.16	0.46
5:I:80:DC:H5''	5:I:80:DC:H6	1.81	0.46
7:K:468:VAL:O	7:K:472:LEU:HG	2.16	0.46
4:d:41:VAL:HB	4:d:59:MET:HE1	1.97	0.46
4:h:33:ARG:NH1	5:i:121:DG:H21	2.12	0.46
7:k:430:LEU:HD11	7:k:507:GLN:OE1	2.15	0.46
2:B:22:LEU:HB3	2:B:25:ASN:HD21	1.80	0.46
2:F:77:LYS:HE3	4:H:92:ARG:CZ	2.46	0.46
2:b:91:LYS:HZ1	4:d:79:ARG:NE	2.03	0.46
4:H:41:VAL:HB	4:H:59:MET:HE1	1.97	0.45
6:J:128:DC:H2''	6:J:129:DG:C8	2.51	0.45
2:f:77:LYS:HE3	4:h:92:ARG:CZ	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:j:13:DA:H1'	6:j:14:DT:H5'	1.99	0.45
5:I:55:DC:C6	5:I:55:DC:H5'	2.51	0.45
7:K:322:LEU:HD21	7:K:361:PRO:HG2	1.97	0.45
5:i:80:DC:H5''	5:i:80:DC:H6	1.81	0.45
6:j:59:DA:H2''	6:j:60:DA:C8	2.51	0.45
7:k:162:ALA:O	7:k:166:ARG:HG2	2.17	0.45
4:H:59:MET:HE3	4:H:59:MET:O	2.16	0.45
7:K:414:LYS:NZ	7:K:435:SER:HB3	2.30	0.45
2:b:35:ARG:O	2:b:39:ARG:HG2	2.16	0.45
4:h:33:ARG:HH22	5:i:121:DG:H21	1.62	0.45
7:k:165:LEU:HD21	7:k:464:PHE:CD2	2.51	0.45
7:k:475:LEU:HD21	7:k:504:LEU:HD23	1.97	0.45
4:D:41:VAL:HB	4:D:59:MET:HE1	1.97	0.45
4:D:69:ILE:HD13	4:D:69:ILE:HA	1.82	0.45
1:a:120:MET:N	1:a:123:ASP:OD2	2.44	0.45
2:b:26:ILE:HD12	2:b:26:ILE:HA	1.83	0.45
5:I:76:DT:H2''	5:I:77:DC:C6	2.51	0.45
7:K:165:LEU:HD21	7:K:464:PHE:CD2	2.51	0.45
7:K:475:LEU:HD21	7:K:504:LEU:HD23	1.97	0.45
7:K:478:GLU:OE2	7:K:501:LYS:HD3	2.16	0.45
5:i:27:DC:H1'	5:i:28:DA:C8	2.51	0.45
5:i:76:DT:H2''	5:i:77:DC:C6	2.51	0.45
7:k:322:LEU:HD21	7:k:361:PRO:HG2	1.97	0.45
1:E:119:ILE:HD13	2:F:43:VAL:HG21	1.97	0.45
6:J:89:DA:H1'	6:J:90:DA:C8	2.51	0.45
1:E:118:THR:HA	2:F:45:ARG:O	2.16	0.45
3:c:51:LEU:HD21	4:d:70:PHE:CD1	2.52	0.45
4:D:32:SER:OG	4:D:33:ARG:N	2.49	0.45
1:e:119:ILE:HD13	2:f:43:VAL:HG21	1.97	0.45
4:h:59:MET:HE3	4:h:59:MET:O	2.16	0.45
7:k:209:LEU:HD11	7:k:358:TYR:OH	2.17	0.45
1:A:65:LEU:HD12	1:A:65:LEU:HA	1.74	0.45
2:B:35:ARG:NH2	2:B:51:TYR:OH	2.50	0.45
5:I:12:DG:H2''	5:I:13:DG:C8	2.52	0.45
7:K:162:ALA:O	7:K:166:ARG:HG2	2.17	0.45
4:d:32:SER:OG	4:d:33:ARG:N	2.49	0.45
5:i:2:DT:H2''	5:i:3:DC:C5	2.51	0.45
7:k:478:GLU:OE2	7:k:501:LYS:HD3	2.16	0.45
6:J:110:DC:H2''	6:J:111:DG:C8	2.52	0.45
7:K:384:LYS:HB3	7:K:384:LYS:HE3	1.83	0.45
2:b:22:LEU:HB3	2:b:25:ASN:HD21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:115:LEU:HD11	1:e:108:ASN:HD21	1.81	0.45
6:j:15:DC:H2''	6:j:16:DT:OP2	2.17	0.45
3:C:51:LEU:HD21	4:D:70:PHE:CD1	2.52	0.44
3:G:17:ARG:CD	4:H:121:TYR:OH	2.65	0.44
3:g:17:ARG:CD	4:h:121:TYR:OH	2.65	0.44
5:i:55:DC:H5'	5:i:55:DC:C6	2.51	0.44
6:j:110:DC:H2''	6:j:111:DG:C8	2.52	0.44
7:k:422:GLU:HG3	7:k:425:LYS:HZ2	1.82	0.44
6:J:51:DG:H2''	6:J:52:DG:H8	1.82	0.44
7:K:209:LEU:HD11	7:K:358:TYR:OH	2.17	0.44
7:K:248:TYR:HB3	7:K:374:THR:HG21	1.97	0.44
1:a:54:TYR:CE1	2:b:36:ARG:HD2	2.52	0.44
3:G:55:LEU:HD13	4:H:66:VAL:HG13	2.00	0.44
1:a:61:LEU:N	1:a:97:GLU:OE2	2.49	0.44
1:a:100:LEU:HD23	1:a:100:LEU:HA	1.77	0.44
5:i:12:DG:H2''	5:i:13:DG:C8	2.52	0.44
7:k:330:TRP:CD1	7:k:357:PHE:HB3	2.53	0.44
1:E:63:ARG:NH1	5:I:90:DA:H4'	2.31	0.44
7:K:187:LYS:HB2	7:K:214:TYR:CD1	2.53	0.44
7:K:330:TRP:CD1	7:K:357:PHE:HB3	2.52	0.44
7:K:469:THR:HG23	7:K:512:ARG:HH12	1.83	0.44
4:D:115:THR:O	4:D:118:VAL:HG13	2.17	0.44
1:a:118:THR:OG1	2:b:45:ARG:HG2	2.18	0.44
6:j:122:DC:H2''	6:j:123:DG:C8	2.53	0.44
6:j:131:DC:H2''	6:j:132:DA:C8	2.52	0.44
3:G:87:ILE:HD12	3:G:102:ILE:HD11	1.99	0.44
3:g:87:ILE:HD12	3:g:102:ILE:HD11	2.00	0.44
7:k:187:LYS:HB2	7:k:214:TYR:CD1	2.53	0.44
5:I:50:DC:H2''	5:I:51:DA:H8	1.83	0.44
6:J:13:DA:H1'	6:J:14:DT:H5'	1.99	0.44
6:J:122:DC:H2''	6:J:123:DG:C8	2.53	0.44
4:d:115:THR:O	4:d:118:VAL:HG13	2.17	0.44
2:f:73:THR:OG1	2:f:85:ASP:OD2	2.35	0.44
6:j:51:DG:H2''	6:j:52:DG:H8	1.82	0.44
1:A:54:TYR:CE1	2:B:36:ARG:HD2	2.53	0.44
1:A:118:THR:OG1	2:B:45:ARG:HG2	2.18	0.44
3:c:62:ILE:HD13	3:c:62:ILE:HA	1.83	0.44
3:C:29:ARG:HE	3:C:29:ARG:HB2	1.65	0.43
3:C:64:GLU:CD	7:K:236:ARG:HH21	2.23	0.43
1:E:41:TYR:HB3	1:E:45:THR:CG2	2.48	0.43
2:F:62:LEU:HD23	2:F:62:LEU:HA	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:100:LEU:HA	4:H:100:LEU:HD23	1.68	0.43
6:J:12:DT:H2''	6:J:13:DA:C8	2.53	0.43
6:J:15:DC:H2''	6:J:16:DT:OP2	2.17	0.43
7:k:248:TYR:HB3	7:k:374:THR:CG2	2.48	0.43
7:k:334:THR:HG22	7:k:485:ILE:HG12	2.00	0.43
5:I:91:DC:H1'	5:I:92:DC:H5'	2.00	0.43
7:K:410:LEU:HD21	7:K:414:LYS:HE3	2.01	0.43
5:i:122:DC:H2''	5:i:123:DA:C8	2.53	0.43
7:k:469:THR:HG23	7:k:512:ARG:HH12	1.82	0.43
4:H:72:ARG:HB3	4:H:101:LEU:CD2	2.47	0.43
2:b:35:ARG:NH2	2:b:51:TYR:OH	2.50	0.43
3:g:55:LEU:HD13	4:h:66:VAL:HG13	2.00	0.43
6:j:12:DT:H2''	6:j:13:DA:C8	2.53	0.43
7:k:157:ASP:O	7:k:458:LYS:HD2	2.18	0.43
7:k:288:ILE:HD12	7:k:296:VAL:O	2.18	0.43
4:D:115:THR:HA	4:D:118:VAL:CG1	2.48	0.43
5:I:122:DC:H2''	5:I:123:DA:C8	2.53	0.43
6:J:122:DC:H2''	6:J:123:DG:H8	1.82	0.43
7:K:248:TYR:HB3	7:K:374:THR:CG2	2.48	0.43
1:a:109:LEU:HD23	1:a:109:LEU:HA	1.77	0.43
7:k:368:ASN:OD1	7:k:368:ASN:N	2.52	0.43
5:I:4:DA:H2''	5:I:5:DG:H8	1.83	0.43
6:J:131:DC:H2''	6:J:132:DA:C8	2.52	0.43
1:a:92:LEU:HD23	1:a:92:LEU:HA	1.79	0.43
7:k:186:VAL:O	7:k:190:VAL:HG23	2.19	0.43
7:K:288:ILE:HD12	7:K:296:VAL:O	2.18	0.43
1:a:72:ARG:NH1	5:i:50:DC:OP1	2.51	0.43
4:d:42:TYR:OH	5:i:20:DG:H3'	2.18	0.43
4:d:106:LEU:HD12	4:d:106:LEU:HA	1.80	0.43
4:d:115:THR:HA	4:d:118:VAL:CG1	2.48	0.43
5:i:91:DC:H1'	5:i:92:DC:H5'	2.00	0.43
6:j:122:DC:H2''	6:j:123:DG:H8	1.82	0.43
7:K:157:ASP:O	7:K:458:LYS:HD2	2.18	0.43
7:K:186:VAL:O	7:K:190:VAL:HG23	2.18	0.43
7:K:334:THR:HG22	7:K:485:ILE:HG12	1.99	0.43
1:e:90:MET:O	1:e:94:GLU:HG2	2.19	0.43
1:e:100:LEU:HA	1:e:100:LEU:HD23	1.75	0.43
5:i:142:DC:H6	5:i:142:DC:H2'	1.65	0.43
7:k:340:ILE:HG22	7:k:343:TRP:CE3	2.54	0.43
7:K:420:LEU:HD21	7:K:518:VAL:HG11	2.00	0.43
7:k:416:LEU:HD21	7:k:508:ILE:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:MET:O	1:E:94:GLU:HG2	2.19	0.43
5:I:91:DC:H5'	5:I:91:DC:C6	2.54	0.43
7:K:198:LYS:HE3	7:K:198:LYS:HB2	1.78	0.43
7:K:368:ASN:OD1	7:K:368:ASN:N	2.52	0.43
7:K:416:LEU:HD21	7:K:508:ILE:HG12	1.99	0.43
1:A:99:TYR:HH	1:A:133:GLU:CD	2.26	0.43
4:D:42:TYR:OH	5:I:20:DG:H3'	2.18	0.43
6:J:31:DG:H2''	6:J:32:DA:C8	2.54	0.43
5:i:91:DC:C6	5:i:91:DC:H5'	2.54	0.43
6:j:31:DG:H2''	6:j:32:DA:C8	2.54	0.43
2:F:73:THR:OG1	2:F:85:ASP:OD2	2.35	0.42
4:H:80:LEU:HD13	4:H:96:THR:OG1	2.19	0.42
7:K:300:ARG:HD2	6:j:107:DC:C4'	2.45	0.42
1:e:41:TYR:HB3	1:e:45:THR:CG2	2.48	0.42
5:i:66:DG:H2''	5:i:67:DT:C6	2.54	0.42
5:i:50:DC:H2''	5:i:51:DA:H8	1.83	0.42
3:G:81:ARG:HA	3:G:81:ARG:HD2	1.79	0.42
1:a:63:ARG:HD3	1:a:63:ARG:HA	1.87	0.42
5:i:39:DG:H1'	5:i:40:DA:C8	2.55	0.42
5:i:119:DA:H2''	5:i:120:DG:N7	2.35	0.42
5:I:66:DG:H2''	5:I:67:DT:C6	2.55	0.42
5:I:119:DA:H2''	5:I:120:DG:N7	2.35	0.42
7:K:209:LEU:HD13	7:K:231:LYS:HD3	2.02	0.42
7:k:247:ALA:O	7:k:376:ARG:HA	2.19	0.42
1:A:109:LEU:HD23	1:A:109:LEU:HA	1.77	0.42
4:H:79:ARG:NE	4:H:83:TYR:OH	2.53	0.42
6:J:40:DG:C8	6:J:40:DG:H5'	2.55	0.42
4:d:49:HIS:O	4:d:51:ASP:N	2.52	0.42
5:i:3:DC:H2''	5:i:4:DA:H8	1.84	0.42
6:j:15:DC:H5'	6:j:15:DC:C6	2.55	0.42
7:k:248:TYR:HA	7:k:375:TRP:O	2.19	0.42
7:k:420:LEU:HD21	7:k:518:VAL:HG11	2.00	0.42
1:A:72:ARG:NH1	5:I:50:DC:OP1	2.51	0.42
4:D:71:GLU:OE1	4:H:79:ARG:NH2	2.53	0.42
5:I:6:DA:H2''	5:I:7:DA:H8	1.85	0.42
7:K:190:VAL:HG13	7:K:230:PHE:HZ	1.85	0.42
7:K:348:VAL:O	7:K:352:LEU:HD23	2.20	0.42
7:k:190:VAL:HG13	7:k:230:PHE:CZ	2.54	0.42
7:k:190:VAL:HG13	7:k:230:PHE:HZ	1.85	0.42
7:k:237:ILE:O	7:k:237:ILE:HG13	2.20	0.42
3:C:91:GLU:H	7:K:257:PRO:HG2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:3:DC:H2''	5:I:4:DA:H8	1.84	0.42
7:K:340:ILE:HG22	7:K:343:TRP:CE3	2.54	0.42
7:K:441:ALA:O	7:K:445:VAL:HG23	2.20	0.42
1:e:42:ARG:HG3	6:j:143:DG:P	2.59	0.42
1:e:116:ARG:NH2	1:e:123:ASP:OD1	2.53	0.42
7:k:172:LEU:HD21	7:k:415:TYR:CG	2.55	0.42
7:k:410:LEU:HD21	7:k:414:LYS:HE3	2.01	0.42
4:D:49:HIS:O	4:D:51:ASP:N	2.52	0.42
1:E:82:LEU:HD23	1:E:82:LEU:HA	1.86	0.42
5:I:39:DG:H1'	5:I:40:DA:C8	2.54	0.42
6:J:135:DG:H2''	6:J:136:DG:C8	2.55	0.42
4:d:72:ARG:HB3	4:d:101:LEU:HD13	2.02	0.42
7:K:190:VAL:HG13	7:K:230:PHE:CZ	2.54	0.42
7:K:248:TYR:HA	7:K:375:TRP:O	2.19	0.42
6:j:111:DG:C2	6:j:112:DA:C5	3.08	0.42
7:k:441:ALA:O	7:k:445:VAL:HG23	2.20	0.42
3:C:62:ILE:HD12	3:C:62:ILE:HG23	1.80	0.42
3:C:87:ILE:HD13	3:C:97:LEU:CD1	2.49	0.42
2:F:35:ARG:HD3	2:F:46:ILE:HD12	2.02	0.42
3:G:108:LEU:HD23	3:G:108:LEU:HA	1.75	0.42
6:J:15:DC:H5'	6:J:15:DC:C6	2.55	0.42
7:K:172:LEU:HD21	7:K:415:TYR:CG	2.55	0.42
7:K:426:ASP:N	7:K:426:ASP:OD1	2.48	0.42
4:h:80:LEU:HD13	4:h:96:THR:OG1	2.19	0.42
7:k:348:VAL:O	7:k:352:LEU:HD23	2.20	0.42
7:k:384:LYS:HE3	7:k:384:LYS:HB3	1.82	0.42
7:k:475:LEU:HA	7:k:501:LYS:HE2	2.02	0.42
1:A:85:GLN:NE2	2:B:82:THR:HG23	2.34	0.41
5:I:66:DG:H2''	5:I:67:DT:C5	2.55	0.41
6:J:22:DG:C8	6:J:22:DG:H5'	2.55	0.41
7:K:413[A]:MET:HB3	7:K:438:VAL:CG1	2.50	0.41
7:K:475:LEU:HA	7:K:501:LYS:HE2	2.02	0.41
2:b:72:TYR:OH	4:d:76:GLU:OE2	2.36	0.41
3:c:87:ILE:HD13	3:c:97:LEU:CD1	2.49	0.41
5:i:6:DA:H2''	5:i:7:DA:C8	2.55	0.41
5:i:66:DG:H2''	5:i:67:DT:C5	2.55	0.41
5:i:90:DA:H1'	5:i:91:DC:H5'	2.00	0.41
4:D:72:ARG:HB3	4:D:101:LEU:HD13	2.02	0.41
4:H:33:ARG:NH1	5:I:121:DG:H21	2.12	0.41
4:H:39:ILE:HG13	4:H:40:TYR:N	2.35	0.41
5:I:26:DT:H2''	5:I:27:DC:C5	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:359:LEU:HD23	7:K:359:LEU:HA	1.79	0.41
1:a:85:GLN:NE2	2:b:82:THR:HG23	2.34	0.41
4:d:71:GLU:OE1	4:h:79:ARG:NH2	2.53	0.41
6:j:74:DC:H1'	6:j:75:DG:H5'	2.02	0.41
7:k:187:LYS:HB2	7:k:214:TYR:CE1	2.55	0.41
7:k:415:TYR:O	7:k:419:GLN:HG2	2.20	0.41
7:k:466:ASN:O	7:k:469:THR:OG1	2.28	0.41
5:I:90:DA:H1'	5:I:91:DC:H5'	2.00	0.41
6:J:74:DC:H1'	6:J:75:DG:H5'	2.02	0.41
6:J:111:DG:C2	6:J:112:DA:C5	3.08	0.41
6:j:22:DG:H5'	6:j:22:DG:C8	2.55	0.41
6:j:135:DG:H2''	6:j:136:DG:C8	2.55	0.41
7:k:209:LEU:HD23	7:k:229:MET:HE2	2.01	0.41
7:k:271:LEU:HD11	7:k:276:MET:HE2	2.03	0.41
1:E:42:ARG:HG3	6:J:143:DG:P	2.59	0.41
7:K:209:LEU:HD23	7:K:229:MET:HE2	2.01	0.41
1:a:65:LEU:HD12	1:a:65:LEU:HA	1.74	0.41
5:i:26:DT:H2''	5:i:27:DC:C5	2.56	0.41
5:I:6:DA:H2''	5:I:7:DA:C8	2.55	0.41
5:I:113:DG:H1'	5:I:114:DT:H5'	2.02	0.41
7:K:187:LYS:HB2	7:K:214:TYR:CE1	2.55	0.41
7:K:235:PRO:HD2	7:K:260:ASN:ND2	2.36	0.41
7:K:247:ALA:O	7:K:376:ARG:HA	2.19	0.41
2:f:35:ARG:CD	2:f:46:ILE:HD12	2.51	0.41
7:k:209:LEU:HD13	7:k:231:LYS:HD3	2.02	0.41
5:I:45:DT:H2''	5:I:46:DC:C6	2.55	0.41
7:K:285:LYS:HD2	7:K:298:MET:SD	2.60	0.41
7:k:235:PRO:HD2	7:k:260:ASN:ND2	2.36	0.41
7:K:417:LEU:HD22	7:K:438:VAL:CG2	2.51	0.41
4:d:69:ILE:HD13	4:d:69:ILE:HA	1.82	0.41
1:e:92:LEU:HA	1:e:92:LEU:HD23	1.91	0.41
2:f:80:THR:O	2:f:80:THR:OG1	2.38	0.41
5:i:6:DA:H2''	5:i:7:DA:H8	1.85	0.41
5:i:45:DT:H2''	5:i:46:DC:C6	2.55	0.41
7:k:285:LYS:HD2	7:k:298:MET:SD	2.60	0.41
2:F:35:ARG:CD	2:F:46:ILE:HD12	2.51	0.41
5:I:135:DT:C2	5:I:136:DA:C8	3.09	0.41
7:K:271:LEU:HD11	7:K:276:MET:HE2	2.03	0.41
1:a:42:ARG:N	5:i:143:DG:OP1	2.53	0.41
3:C:62:ILE:HD13	3:C:62:ILE:HA	1.83	0.41
1:E:42:ARG:O	1:E:45:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:36:DG:O6	6:J:109:DA:N6	2.54	0.41
7:K:232:LEU:N	7:K:323:ALA:O	2.54	0.41
7:K:415:TYR:O	7:K:419:GLN:HG2	2.20	0.41
1:a:46:VAL:HB	6:j:82:DT:OP1	2.21	0.41
3:c:90:ASP:OD1	3:c:93:LEU:N	2.50	0.41
3:c:91:GLU:H	7:k:257:PRO:HG2	1.85	0.41
2:f:31:LYS:NZ	2:f:35:ARG:HH21	2.19	0.41
2:f:50:ILE:HD13	2:f:50:ILE:HA	1.88	0.41
3:g:108:LEU:HA	3:g:108:LEU:HD23	1.75	0.41
5:i:113:DG:H1'	5:i:114:DT:H5'	2.02	0.41
5:i:135:DT:C2	5:i:136:DA:C8	3.09	0.41
6:j:40:DG:C8	6:j:40:DG:H5'	2.55	0.41
6:j:116:DA:H5'	6:j:116:DA:C8	2.56	0.41
7:k:417:LEU:HD22	7:k:438:VAL:CG2	2.51	0.41
5:l:65:DC:H2''	5:l:66:DG:C8	2.56	0.41
6:J:116:DA:C8	6:J:116:DA:H5'	2.56	0.41
7:K:344:LEU:CG	7:K:348:VAL:HG11	2.51	0.41
2:b:29:ILE:HG13	2:b:58:LEU:HD23	2.03	0.41
2:b:43:VAL:HG11	2:b:46:ILE:HG12	2.03	0.41
4:h:39:ILE:HG13	4:h:40:TYR:N	2.35	0.41
5:i:36:DG:O6	6:j:109:DA:N6	2.54	0.41
5:i:65:DC:H2''	5:i:66:DG:C8	2.56	0.41
7:k:362:LYS:HD2	7:k:376:ARG:HD3	2.03	0.41
7:k:381:HIS:CE1	7:k:382:ILE:HG12	2.56	0.41
2:F:31:LYS:NZ	2:F:35:ARG:HH21	2.19	0.40
7:K:237:ILE:HG13	7:K:237:ILE:O	2.20	0.40
7:K:413[A]:MET:HE1	7:K:442:PHE:CD2	2.56	0.40
3:c:64:GLU:CD	7:k:236:ARG:HH21	2.23	0.40
2:f:35:ARG:O	2:f:39:ARG:HG2	2.22	0.40
7:k:233:GLU:OE1	7:k:235:PRO:HD3	2.21	0.40
7:k:348:VAL:HG22	7:k:352:LEU:HD23	2.03	0.40
1:A:46:VAL:HB	6:J:82:DT:OP1	2.21	0.40
2:f:92:ARG:NH2	4:h:101:LEU:HA	2.29	0.40
2:B:92:ARG:NH2	4:D:101:LEU:HA	2.35	0.40
6:J:71:DC:C2	6:J:72:DA:N7	2.90	0.40
7:k:392:LYS:HE2	7:k:392:LYS:HB3	1.93	0.40
3:C:26:PRO:HB3	4:D:40:TYR:CE1	2.56	0.40
6:J:7:DG:C2	6:J:8:DT:C2	3.10	0.40
3:c:26:PRO:HB3	4:d:40:TYR:CE1	2.56	0.40
7:k:420:LEU:HB3	7:k:507:GLN:OE1	2.22	0.40
2:B:43:VAL:HG11	2:B:46:ILE:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:126:DT:H2''	5:I:127:DG:C8	2.56	0.40
7:K:256:ASN:HA	7:K:257:PRO:HD3	1.91	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	A	95/139 (68%)	92 (97%)	3 (3%)	0	100	100
1	E	95/139 (68%)	95 (100%)	0	0	100	100
1	a	95/139 (68%)	92 (97%)	3 (3%)	0	100	100
1	e	95/139 (68%)	94 (99%)	1 (1%)	0	100	100
2	B	81/106 (76%)	74 (91%)	7 (9%)	0	100	100
2	F	76/106 (72%)	72 (95%)	4 (5%)	0	100	100
2	b	81/106 (76%)	74 (91%)	7 (9%)	0	100	100
2	f	76/106 (72%)	72 (95%)	4 (5%)	0	100	100
3	C	101/133 (76%)	93 (92%)	8 (8%)	0	100	100
3	G	103/133 (77%)	93 (90%)	10 (10%)	0	100	100
3	c	101/133 (76%)	93 (92%)	8 (8%)	0	100	100
3	g	103/133 (77%)	93 (90%)	10 (10%)	0	100	100
4	D	93/129 (72%)	87 (94%)	6 (6%)	0	100	100
4	H	91/129 (70%)	83 (91%)	8 (9%)	0	100	100
4	d	93/129 (72%)	87 (94%)	6 (6%)	0	100	100
4	h	91/129 (70%)	83 (91%)	8 (9%)	0	100	100
7	K	365/380 (96%)	351 (96%)	14 (4%)	0	100	100
7	k	365/380 (96%)	351 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2200/2788 (79%)	2079 (94%)	121 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	85/113 (75%)	84 (99%)	1 (1%)	63	72
1	E	84/113 (74%)	84 (100%)	0	100	100
1	a	85/113 (75%)	84 (99%)	1 (1%)	63	72
1	e	84/113 (74%)	84 (100%)	0	100	100
2	B	68/81 (84%)	68 (100%)	0	100	100
2	F	63/81 (78%)	63 (100%)	0	100	100
2	b	68/81 (84%)	68 (100%)	0	100	100
2	f	63/81 (78%)	63 (100%)	0	100	100
3	C	82/102 (80%)	81 (99%)	1 (1%)	63	72
3	G	83/102 (81%)	83 (100%)	0	100	100
3	c	82/102 (80%)	81 (99%)	1 (1%)	63	72
3	g	83/102 (81%)	83 (100%)	0	100	100
4	D	81/107 (76%)	79 (98%)	2 (2%)	42	62
4	H	79/107 (74%)	77 (98%)	2 (2%)	42	62
4	d	81/107 (76%)	79 (98%)	2 (2%)	42	62
4	h	79/107 (74%)	77 (98%)	2 (2%)	42	62
7	K	337/349 (97%)	336 (100%)	1 (0%)	86	85
7	k	337/349 (97%)	336 (100%)	1 (0%)	86	85
All	All	1924/2310 (83%)	1910 (99%)	14 (1%)	73	78

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	ARG
3	C	118	LYS
4	D	118	VAL
4	D	119	THR
4	H	90	THR
4	H	119	THR
7	K	429	HIS
1	a	134	ARG
3	c	118	LYS
4	d	118	VAL
4	d	119	THR
4	h	90	THR
4	h	119	THR
7	k	429	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
2	B	25	ASN
3	C	24	GLN
3	C	73	ASN
3	C	84	GLN
4	D	63	ASN
4	D	82	HIS
4	D	95	GLN
4	D	109	HIS
1	E	108	ASN
3	G	38	ASN
3	G	73	ASN
4	H	109	HIS
7	K	192	HIS
7	K	210	ASN
7	K	264	GLN
7	K	289	ASN
7	K	335	GLN
7	K	429	HIS
7	K	466	ASN
7	K	482	ASN
7	K	514	ASN
3	c	24	GLN
3	c	73	ASN
3	c	84	GLN

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Mol	Chain	Res	Type
4	d	63	ASN
4	d	82	HIS
4	d	95	GLN
4	d	109	HIS
1	e	108	ASN
3	g	38	ASN
3	g	73	ASN
7	k	192	HIS
7	k	210	ASN
7	k	264	GLN
7	k	289	ASN
7	k	335	GLN
7	k	429	HIS
7	k	466	ASN
7	k	482	ASN
7	k	514	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

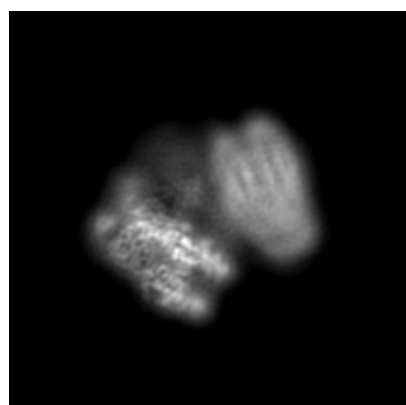
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30267. These allow visual inspection of the internal detail of the map and identification of artifacts.

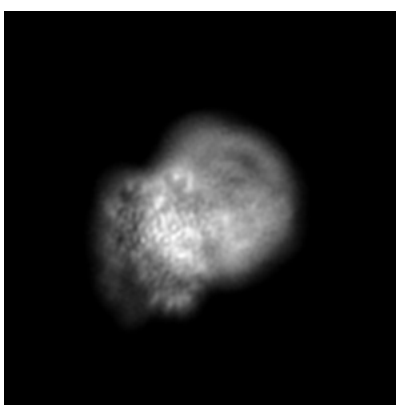
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

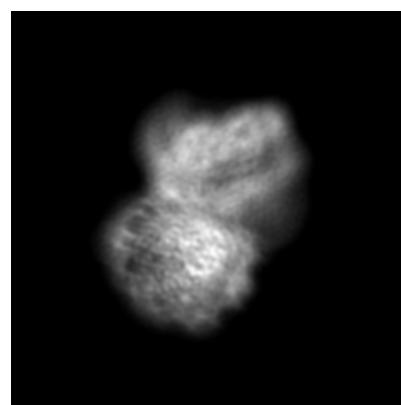
6.1.1 Primary map



X



Y

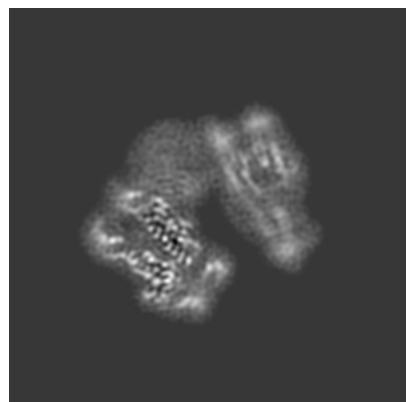


Z

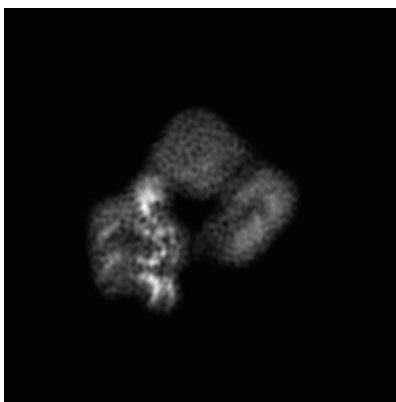
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

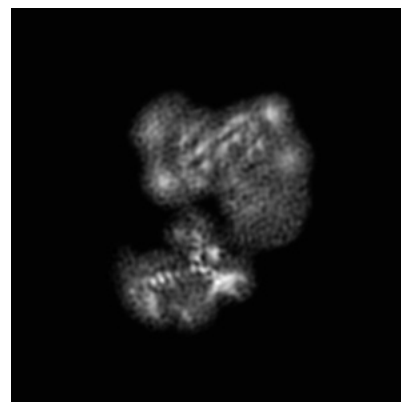
6.2.1 Primary map



X Index: 125



Y Index: 125

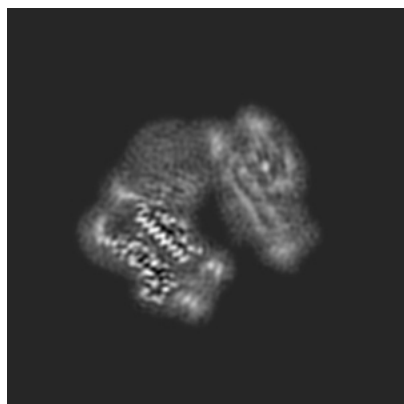


Z Index: 125

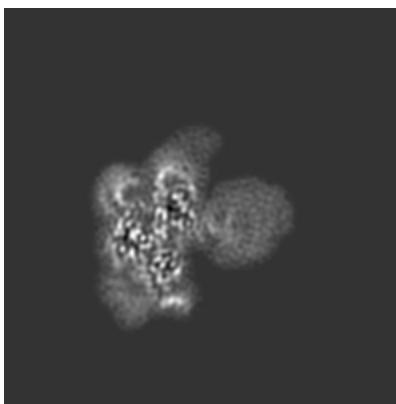
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

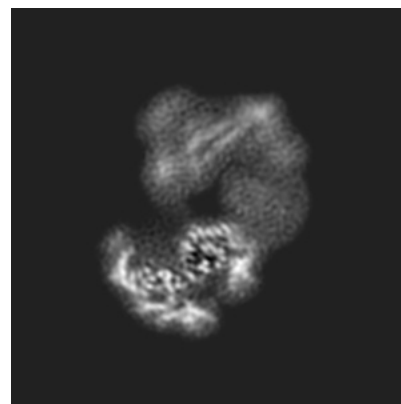
6.3.1 Primary map



X Index: 121



Y Index: 104

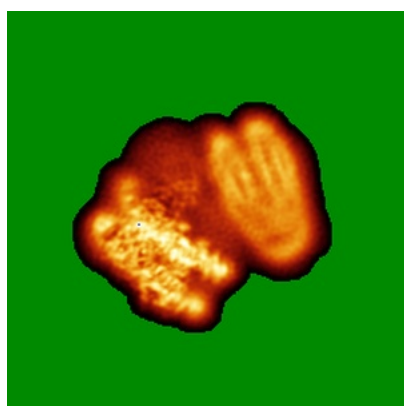


Z Index: 115

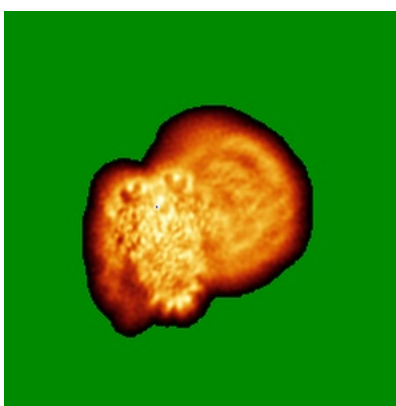
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

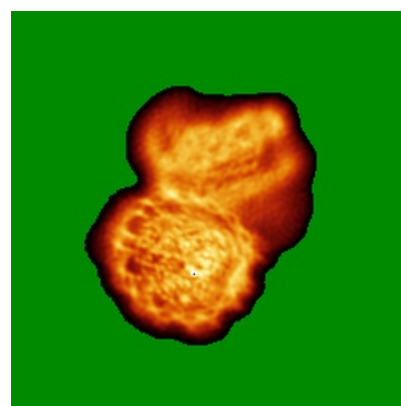
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0119. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

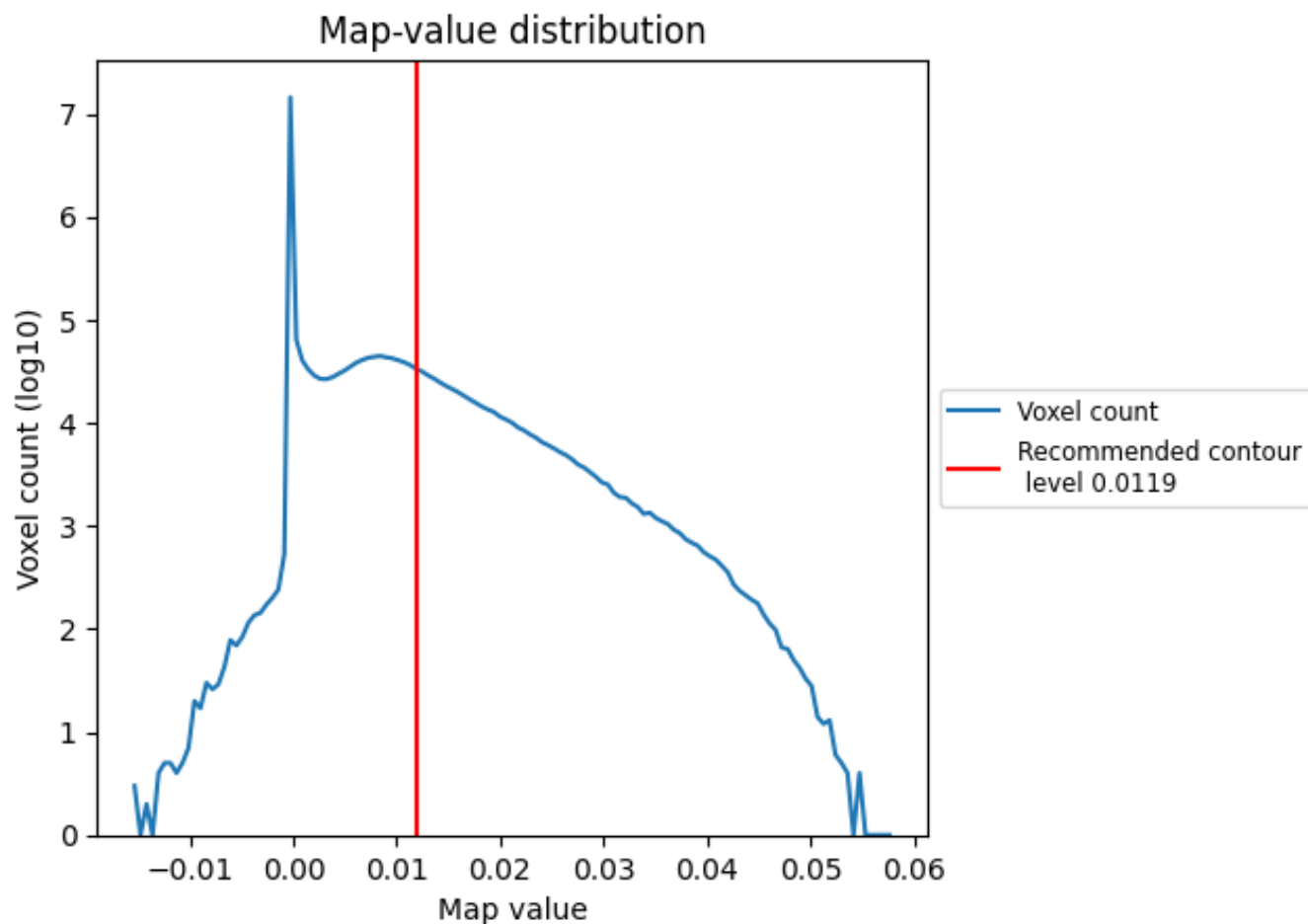
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

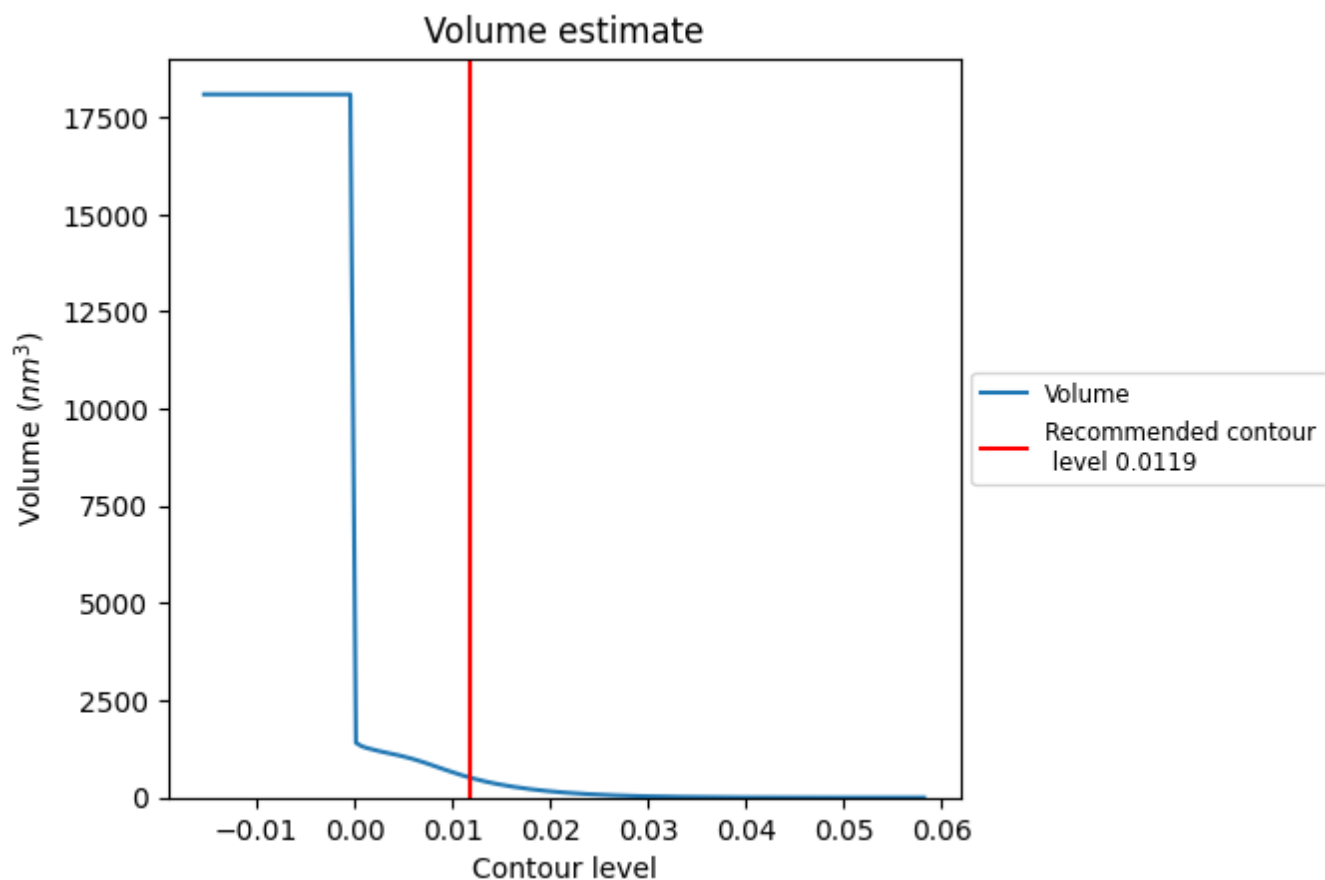
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

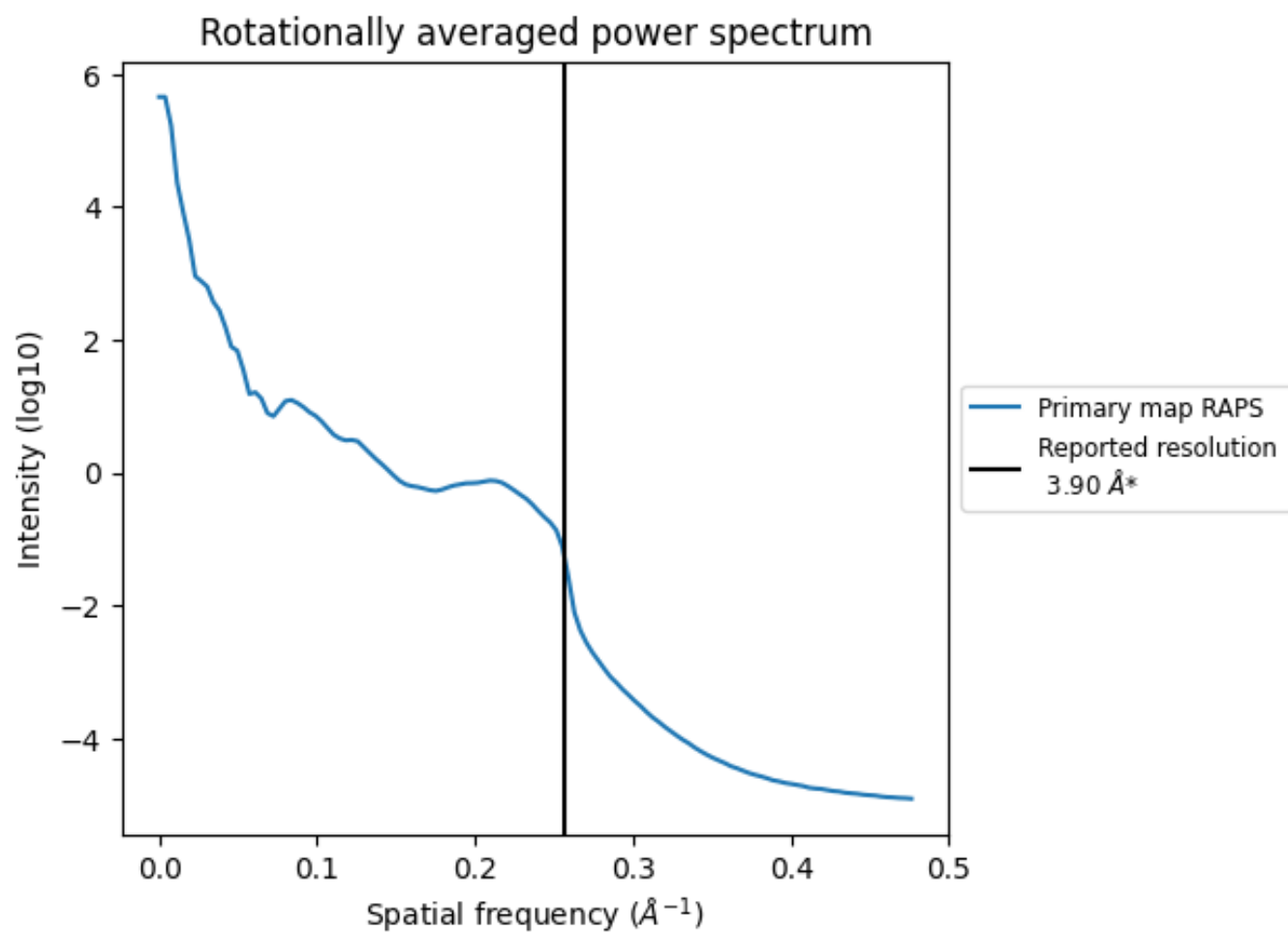
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 509 nm^3 ; this corresponds to an approximate mass of 460 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

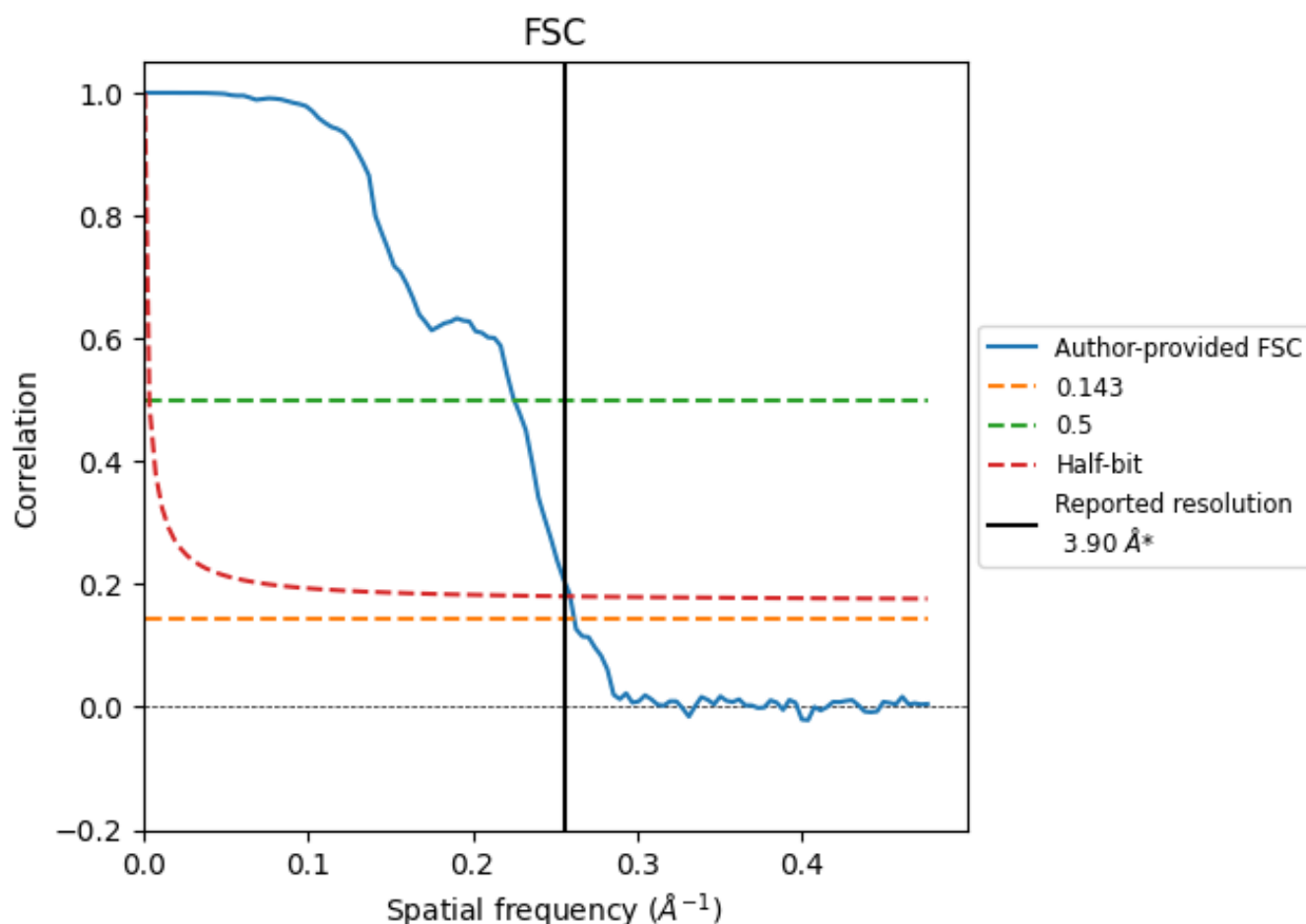


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

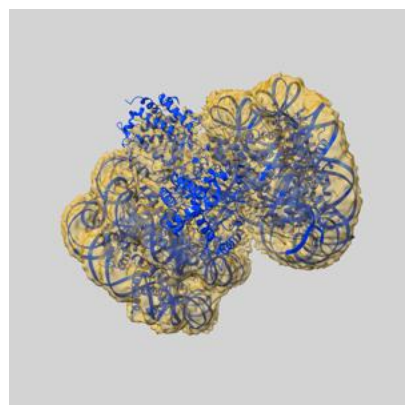
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.82	4.44	3.86
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

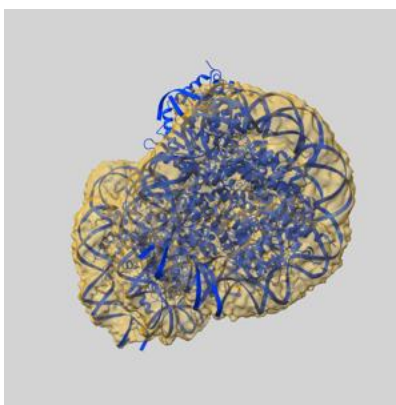
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30267 and PDB model 7C0M. Per-residue inclusion information can be found in section 3 on page 9.

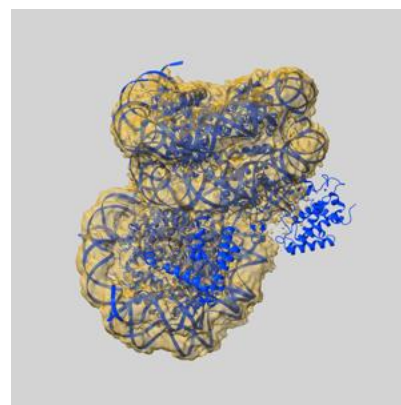
9.1 Map-model overlay [i](#)



X



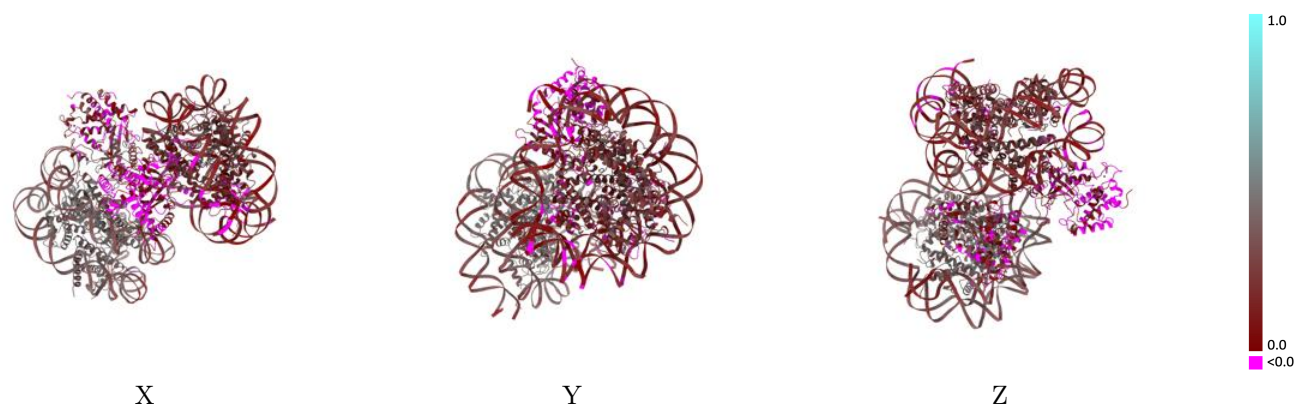
Y



Z

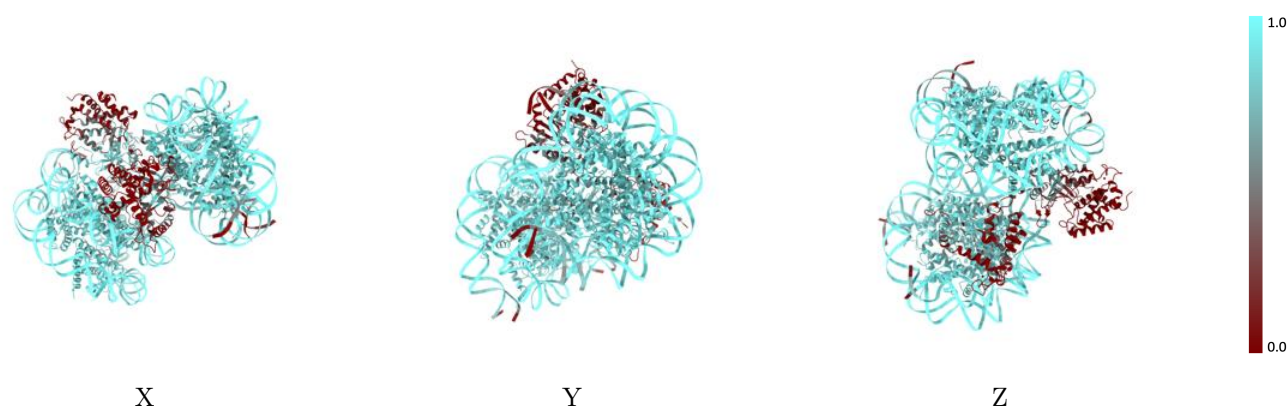
The images above show the 3D surface view of the map at the recommended contour level 0.0119 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



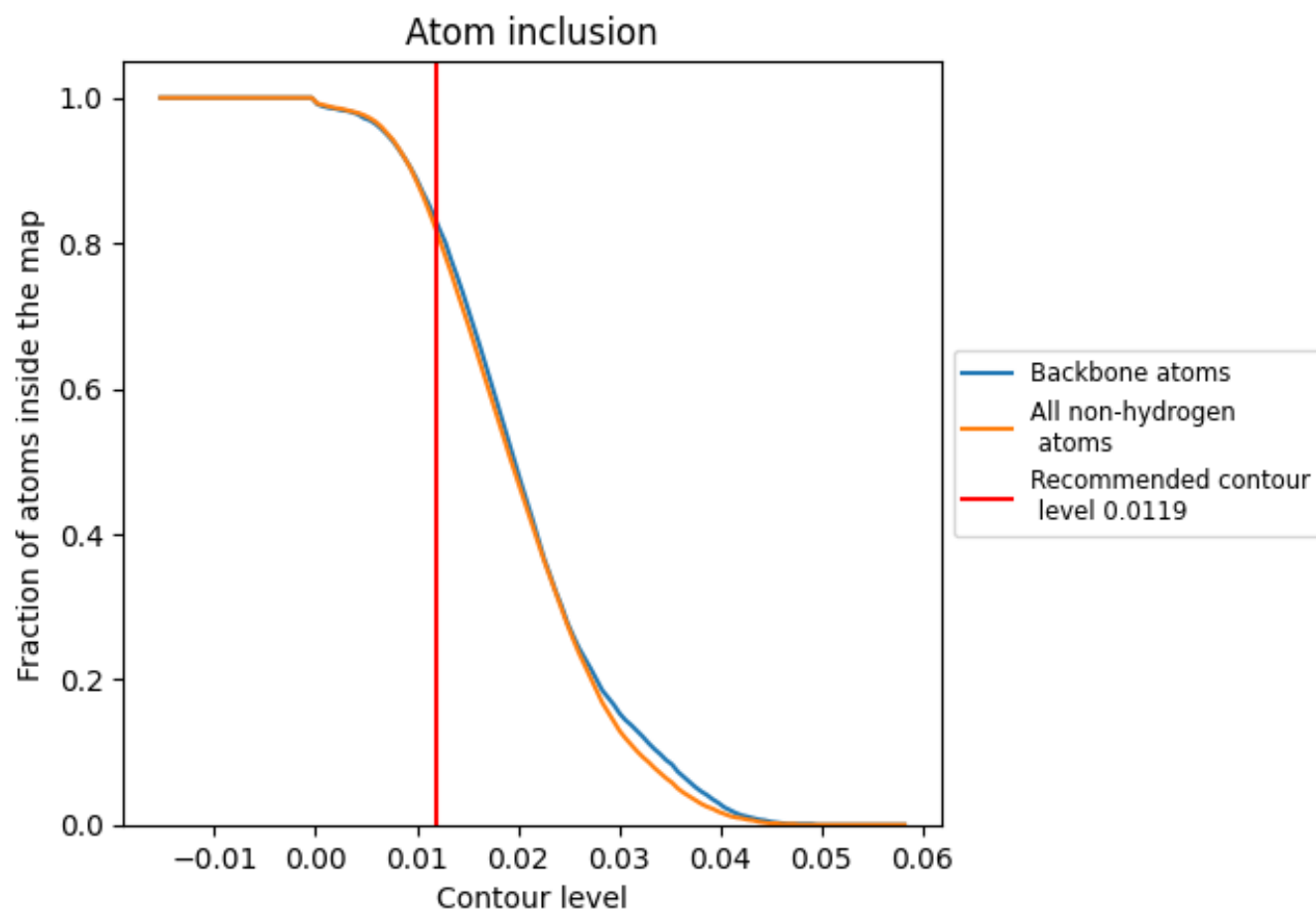
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0119).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0119) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8190	 0.2250
A	 0.9520	 0.3820
B	 0.9340	 0.3980
C	 0.9470	 0.4110
D	 0.9630	 0.3930
E	 0.9560	 0.4010
F	 0.9820	 0.4290
G	 0.9440	 0.3940
H	 0.9690	 0.3920
I	 0.9640	 0.3010
J	 0.9610	 0.3050
K	 0.4990	 0.1440
a	 0.9340	 0.1330
b	 0.9040	 0.1540
c	 0.9100	 0.2140
d	 0.9280	 0.2120
e	 0.9350	 0.1980
f	 0.9530	 0.2350
g	 0.9010	 0.1850
h	 0.9410	 0.2230
i	 0.9000	 0.1440
j	 0.8970	 0.1380
k	 0.2170	 0.0310

