



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 01:40 AM UTC

PDB ID : 6J50 / pdb_00006j50
EMDB ID : EMD-0675
Title : RNA polymerase II elongation complex bound with Spt4/5 and foreign DNA, stalled at SHL(-1) of the nucleosome (tilted conformation)
Authors : Ehara, H.; Kujirai, T.; Fujino, Y.; Shirouzu, M.; Kurumizaka, H.; Sekine, S.
Deposited on : 2019-01-10
Resolution : 4.70 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:

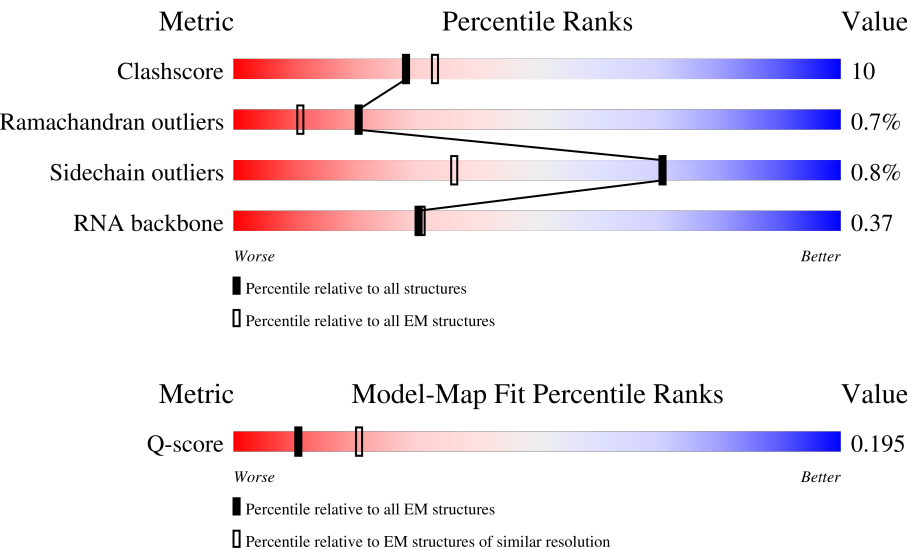
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	1989 (4.20 - 5.20)

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	1743	
2	B	1227	
3	C	304	

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Mol	Chain	Length	Quality of chain
4	D	186	
5	E	214	
6	F	155	
7	G	171	
8	H	145	
9	I	115	
10	J	72	
11	K	118	
12	L	72	
13	P	16	
14	T	198	
15	N	198	
16	V	108	
17	W	911	
18	a	139	
18	e	139	
19	b	106	
19	f	106	
20	c	133	
20	g	133	
21	d	129	
21	h	129	
22	o	41	
23	1	41	

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 47422 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1414	Total	C	N	O	S	0	0
			11139	7025	1941	2103	70		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1157	Total	C	N	O	S	0	0
			9228	5816	1630	1724	58		

- Molecule 3 is a protein called RNA polymerase II third largest subunit B44, part of central core.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	263	Total	C	N	O	S	0	0
			2098	1319	354	413	12		

- Molecule 4 is a protein called RNA polymerase II subunit B32.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	168	Total	C	N	O	S	0	0
			1314	812	237	263	2		

- Molecule 5 is a protein called RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1740	1094	312	324	10		

- Molecule 6 is a protein called RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	84	Total	C	N	O	S	0	0
			677	429	114	131	3		

- Molecule 7 is a protein called RNA polymerase II subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1324	858	214	247	5		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1052	671	169	208	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	111	Total	C	N	O	S	0	0
			917	565	161	180	11		

- Molecule 10 is a protein called RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			545	349	95	95	6		

- Molecule 11 is a protein called RNA polymerase II subunit B12.5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	113	Total	C	N	O	S	0	0
			932	599	160	169	4		

- Molecule 12 is a protein called RNA polymerase subunit ABC10-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			359	221	72	61	5		

- Molecule 13 is a RNA chain called RNA (5'-R(P*GP*CP*CP*UP*GP*GP*UP*GP*UP*C P*UP*UP*GP*GP*GP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	16	Total	C	N	O	P	0	0
			341	151	56	118	16		

- Molecule 14 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	128	Total	C	N	O	P	0	0
			2610	1237	491	755	127		

- Molecule 15 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	123	Total	C	N	O	P	0	0
			2527	1198	458	748	123		

- Molecule 16 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	102	Total	C	N	O	S	0	0
			792	492	143	150	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	7	MET	-	expression tag	UNP C4R0E6

- Molecule 17 is a protein called Protein that forms a complex with Spt4p.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	275	Total	C	N	O	S	0	0
			2226	1425	397	403	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	-2	GLY	-	expression tag	UNP C4R370
W	-1	PRO	-	expression tag	UNP C4R370
W	0	GLY	-	expression tag	UNP C4R370

- Molecule 18 is a protein called Histone H3.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	a	97	Total	C	N	O	S	0	0
			797	503	155	137	2		
18	e	97	Total	C	N	O	S	0	0
			796	501	155	138	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	-3	GLY	-	expression tag	UNP P84243
a	-2	SER	-	expression tag	UNP P84243
a	-1	HIS	-	expression tag	UNP P84243
e	-3	GLY	-	expression tag	UNP P84243
e	-2	SER	-	expression tag	UNP P84243
e	-1	HIS	-	expression tag	UNP P84243

- Molecule 19 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	b	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
19	f	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

There are 6 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
f	-3	GLY	-	expression tag	UNP P62805
f	-2	SER	-	expression tag	UNP P62805
f	-1	HIS	-	expression tag	UNP P62805

- Molecule 20 is a protein called Histone H2A type 1-B/E.

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

There are 6 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
g	-3	GLY	-	expression tag	UNP P04908
g	-2	SER	-	expression tag	UNP P04908
g	-1	HIS	-	expression tag	UNP P04908

- Molecule 21 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	95	Total	C	N	O	S	0	0
			746	468	136	140	2		
21	h	91	Total	C	N	O	S	0	0
			708	447	125	134	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	-6	GLY	-	expression tag	UNP P06899
d	-5	SER	-	expression tag	UNP P06899
d	-4	HIS	-	expression tag	UNP P06899
h	-6	GLY	-	expression tag	UNP P06899
h	-5	SER	-	expression tag	UNP P06899
h	-4	HIS	-	expression tag	UNP P06899

- Molecule 22 is a DNA chain called DNA (41-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	41	Total	C	N	O	P	0	0
			846	399	177	229	41		

- Molecule 23 is a DNA chain called DNA (41-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1	41	Total	C	N	O	P	0	0
			835	401	130	263	41		

- Molecule 24 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
24	A	2	Total	Zn	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
24	B	1	Total 1	Zn 1	0
24	C	1	Total 1	Zn 1	0
24	I	2	Total 2	Zn 2	0
24	J	1	Total 1	Zn 1	0
24	L	1	Total 1	Zn 1	0
24	V	1	Total 1	Zn 1	0

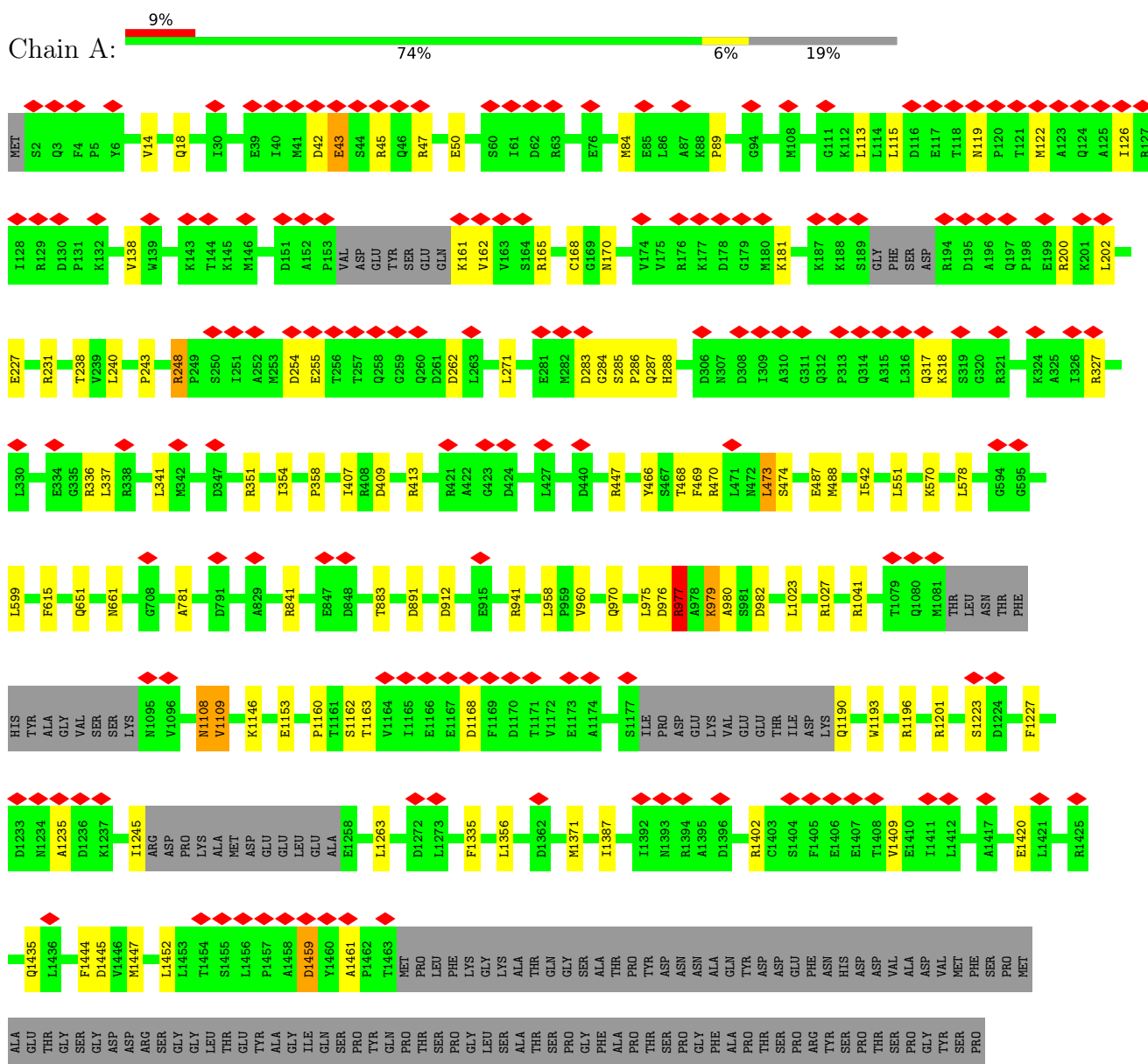
- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
25	A	1	Total 1	Mg 1	0

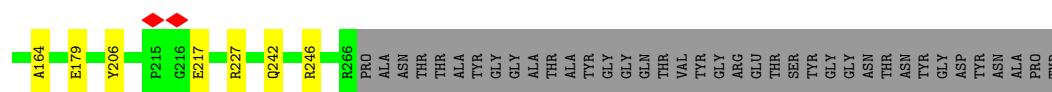
3 Residue-property plots

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.

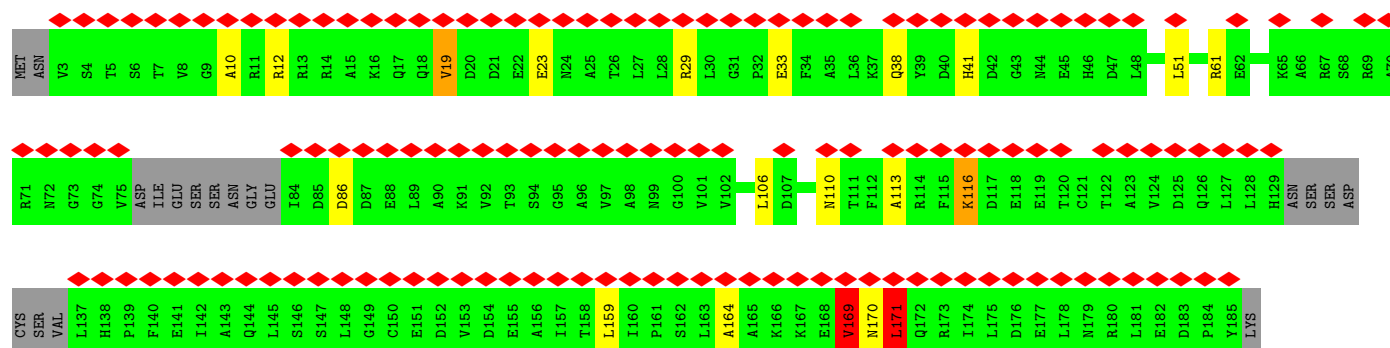
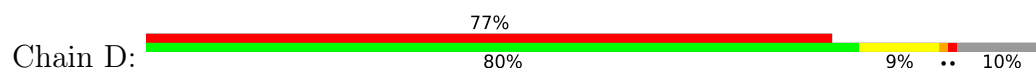
• Molecule 1: DNA-directed RNA polymerase subunit



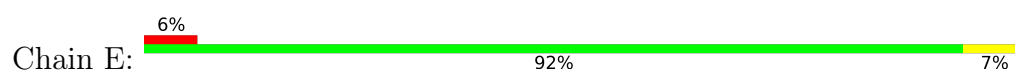




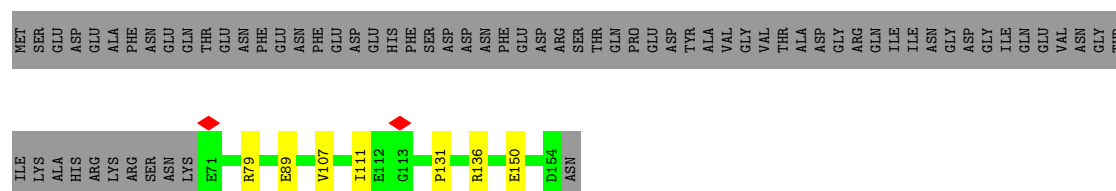
• Molecule 4: RNA polymerase II subunit B32



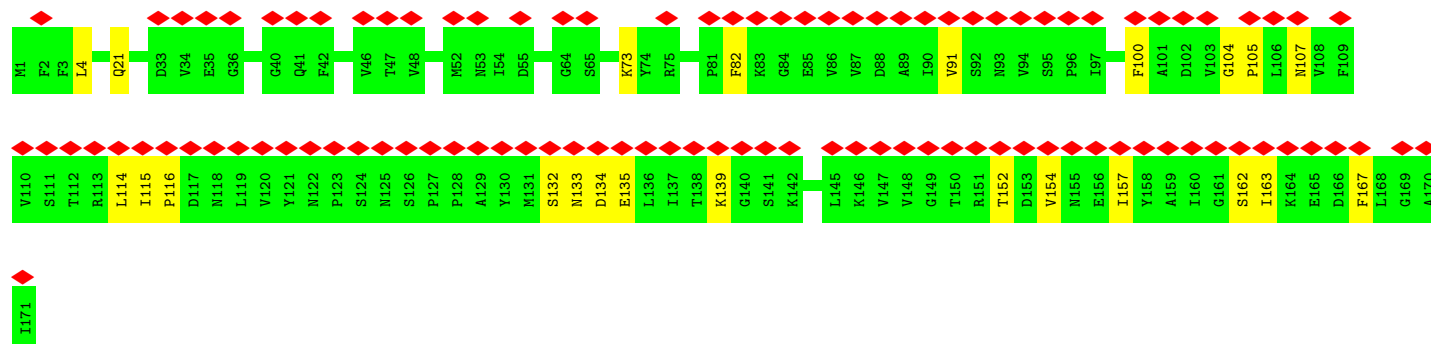
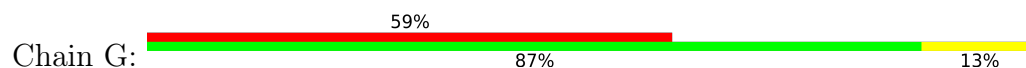
• Molecule 5: RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III



• Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III

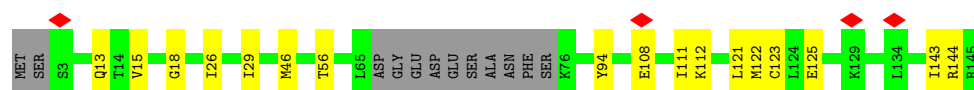


• Molecule 7: RNA polymerase II subunit



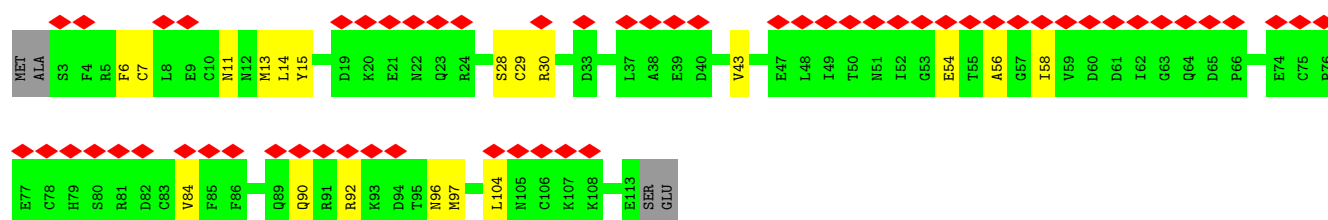
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 



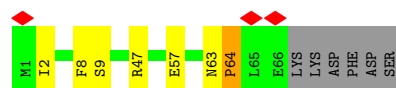
- Molecule 9: DNA-directed RNA polymerase subunit

Chain I: 

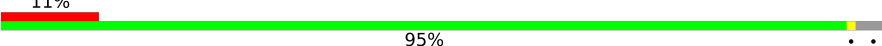


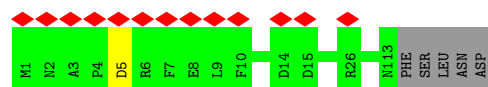
- Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III

Chain J: 



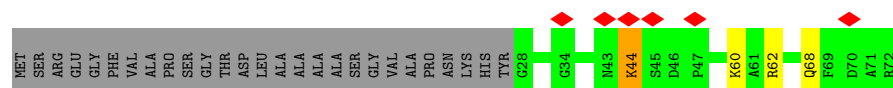
- Molecule 11: RNA polymerase II subunit B12.5

Chain K: 



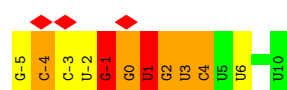
- Molecule 12: RNA polymerase subunit ABC10-alpha

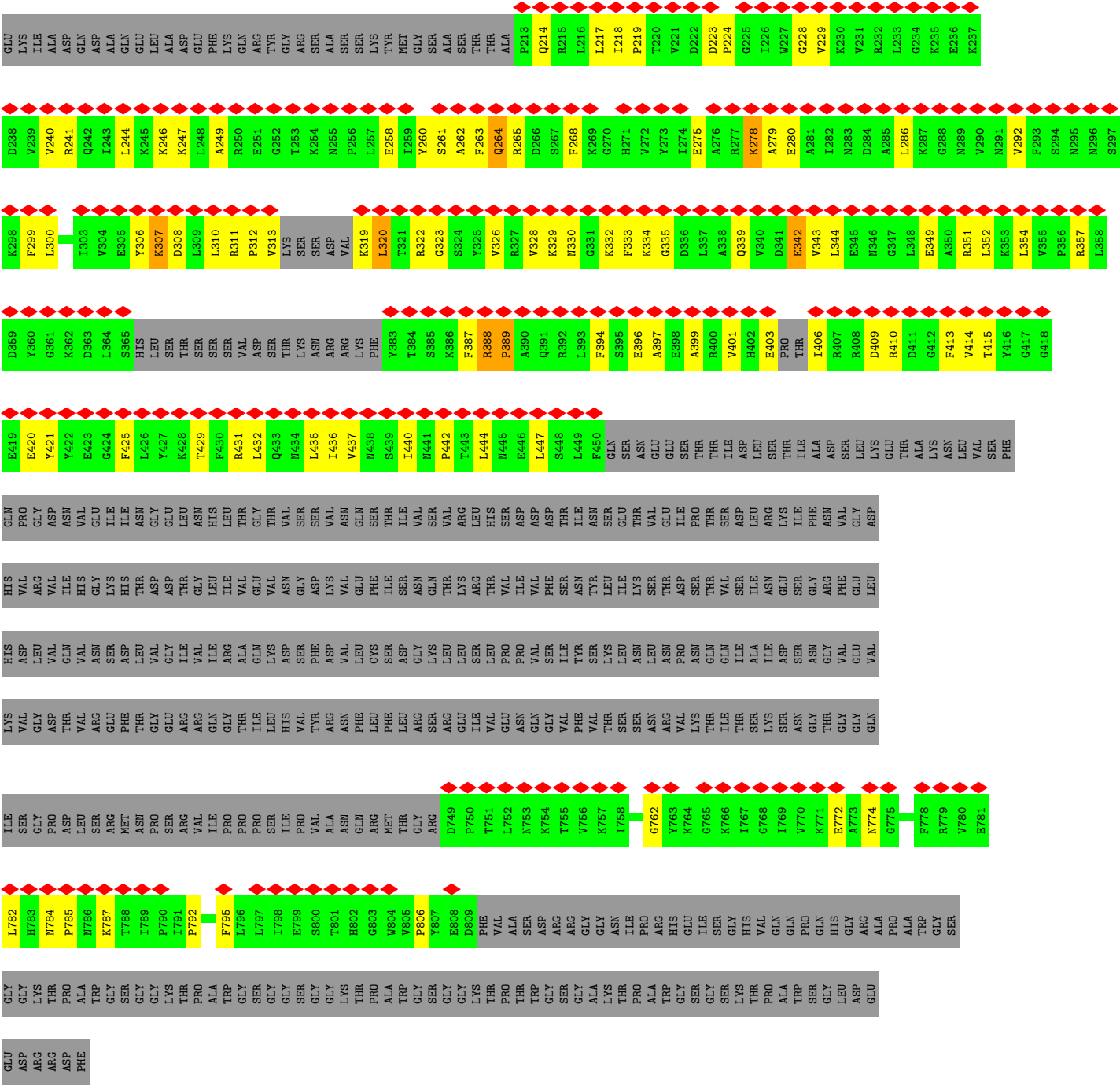
Chain L: 



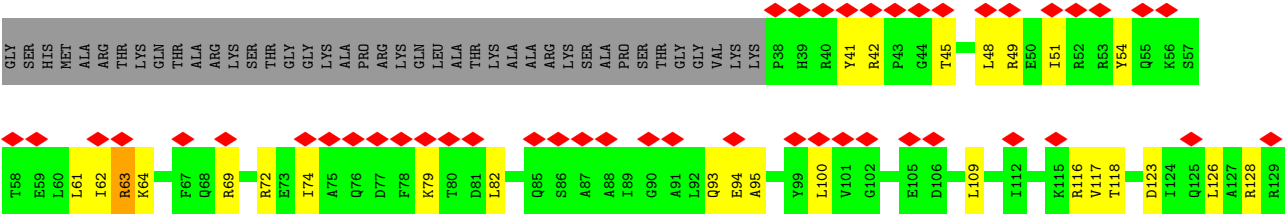
- Molecule 13: RNA (5'-R(P*GP*CP*CP*UP*GP*GP*UP*GP*UP*CP*UP*UP*GP*GP*GP*U)-3')

Chain P: 



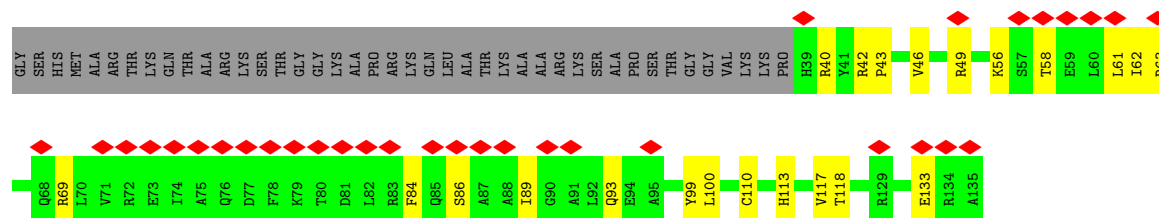


● Molecule 18: Histone H3.3

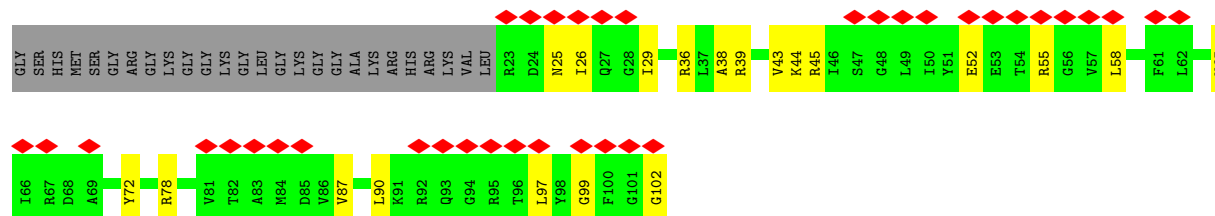




- Molecule 18: Histone H3.3



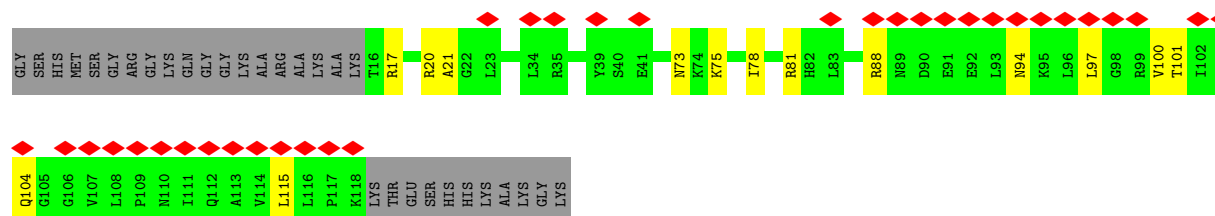
- Molecule 19: Histone H4



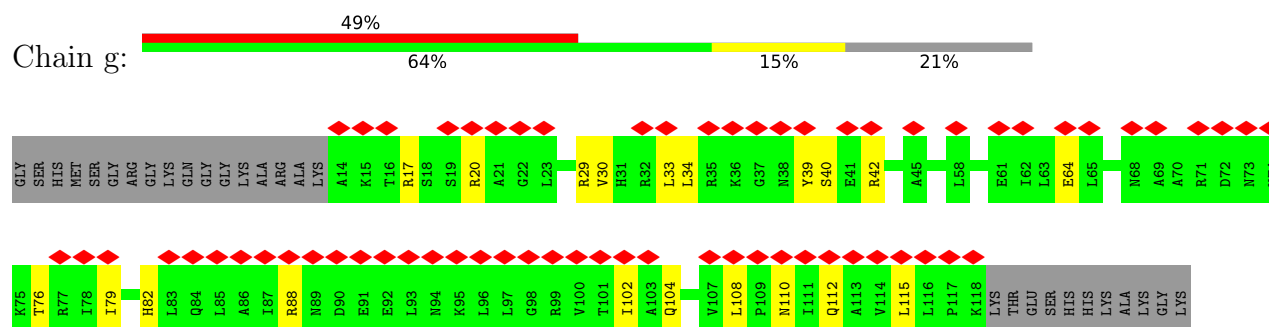
- Molecule 19: Histone H4



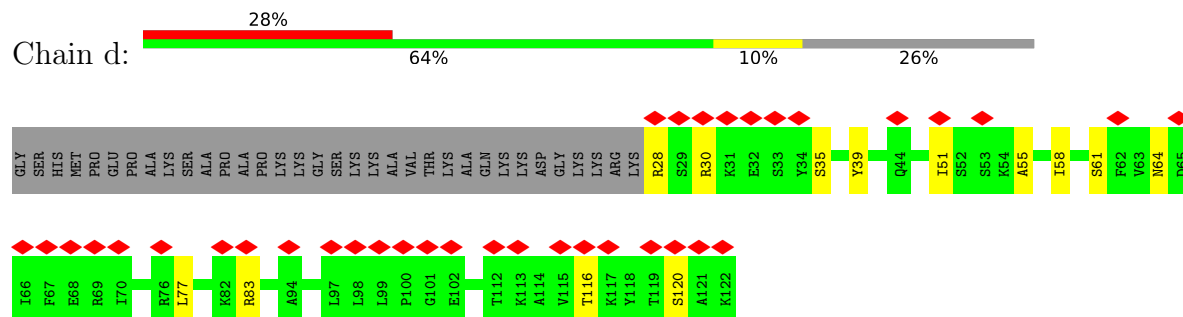
- Molecule 20: Histone H2A type 1-B/E



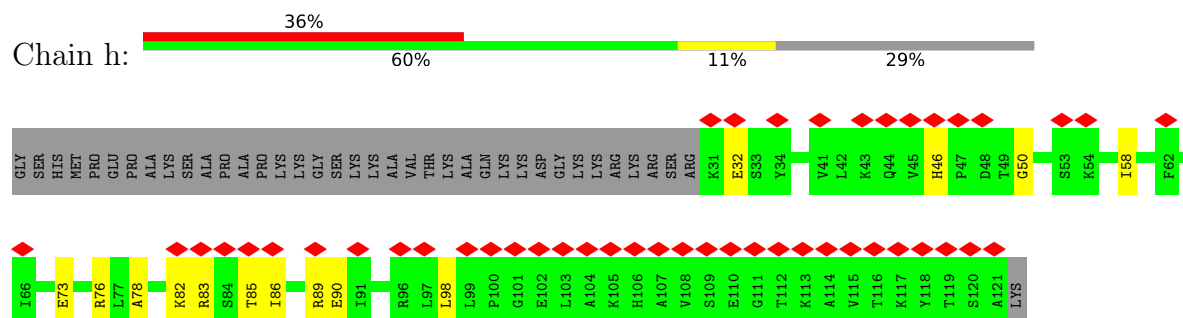
- Molecule 20: Histone H2A type 1-B/E



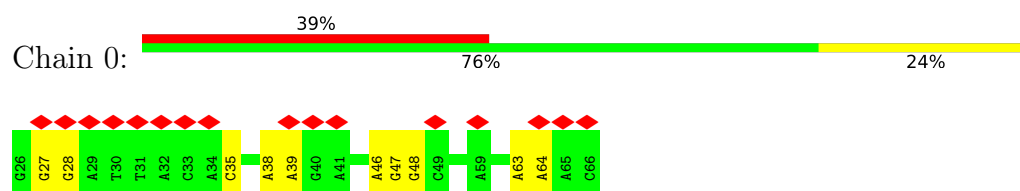
- Molecule 21: Histone H2B type 1-J



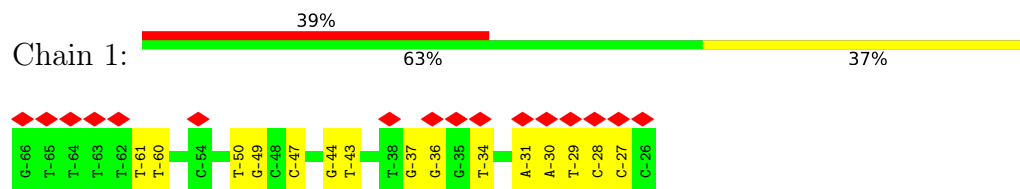
- Molecule 21: Histone H2B type 1-J



- Molecule 22: DNA (41-MER)



- Molecule 23: DNA (41-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	20468	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.056	Depositor
Minimum map value	-0.017	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.016	Depositor
Map size ($\text{\AA}$)	357.6, 357.6, 357.6	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.49, 1.49, 1.49	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.39	0/11345	0.74	3/15331 (0.0%)
2	B	0.43	0/9407	0.79	11/12685 (0.1%)
3	C	0.42	0/2139	0.76	4/2895 (0.1%)
4	D	0.30	0/1326	0.79	4/1788 (0.2%)
5	E	0.37	0/1772	0.73	0/2385
6	F	0.39	0/687	0.68	0/931
7	G	0.32	0/1353	0.79	2/1837 (0.1%)
8	H	0.36	0/1069	0.72	0/1444
9	I	0.32	0/934	0.89	4/1257 (0.3%)
10	J	0.46	0/554	0.80	0/742
11	K	0.40	0/953	0.73	0/1291
12	L	0.38	0/365	0.85	1/484 (0.2%)
13	P	1.01	6/379 (1.6%)	0.66	0/589
14	T	0.52	0/2929	0.65	0/4514
15	N	0.51	0/2831	0.67	0/4368
16	V	0.61	2/808 (0.2%)	0.91	1/1097 (0.1%)
17	W	0.50	2/2267 (0.1%)	0.86	3/3048 (0.1%)
18	a	0.38	0/809	0.74	0/1085
18	e	0.41	0/807	0.67	0/1081
19	b	0.41	0/645	0.76	0/862
19	f	0.40	0/626	0.70	0/837
20	c	0.41	0/806	0.65	0/1089
20	g	0.36	0/820	0.60	0/1107
21	d	0.41	0/757	0.66	0/1015
21	h	0.37	0/719	0.64	0/968
22	o	0.38	0/955	0.59	0/1470
23	l	0.40	0/929	0.61	0/1433
All	All	0.43	10/48991 (0.0%)	0.74	33/67633 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
18	a	0	2
18	e	0	1
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	29	CYS	C-N	8.12	1.43	1.33
13	P	-1	G	C1'-N9	-7.53	1.36	1.48
13	P	4	C	C1'-N1	7.46	1.59	1.48
13	P	2	G	C1'-N9	-7.46	1.36	1.48
17	W	440	ILE	CA-C	-7.43	1.43	1.52
13	P	-5	G	C1'-N9	-6.91	1.36	1.47
16	V	63	ASN	C-N	-6.34	1.24	1.33
13	P	6	U	C1'-N1	5.99	1.57	1.48
13	P	1	U	C1'-N1	5.39	1.56	1.48
17	W	307	LYS	C-N	-5.07	1.27	1.33

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	63	GLN	N-CA-C	-9.61	92.30	108.26
17	W	389	PRO	CA-N-CD	-8.90	99.54	112.00
2	B	63	GLN	N-CA-CB	-8.56	96.81	110.77
16	V	29	CYS	O-C-N	-8.29	114.26	121.31
17	W	388	ARG	CA-C-N	7.11	128.72	119.84
17	W	388	ARG	C-N-CA	7.11	128.72	119.84
2	B	336	ILE	CA-CB-CG2	6.95	122.31	110.50
7	G	133	ASN	CA-C-N	6.58	134.12	121.54
7	G	133	ASN	C-N-CA	6.58	134.12	121.54
4	D	170	ASN	CA-C-N	6.37	133.70	121.54
4	D	170	ASN	C-N-CA	6.37	133.70	121.54
2	B	238	GLY	CA-C-N	6.03	133.06	121.54
2	B	238	GLY	C-N-CA	6.03	133.06	121.54
2	B	60	GLN	CA-C-N	5.88	127.20	119.84
2	B	60	GLN	C-N-CA	5.88	127.20	119.84
1	A	1108	ASN	CA-C-N	5.80	132.41	121.97
1	A	1108	ASN	C-N-CA	5.80	132.41	121.97
1	A	473	LEU	CA-CB-CG	-5.70	96.36	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	932	HIS	N-CA-C	-5.65	98.77	110.80
2	B	330	GLY	N-CA-C	5.62	126.50	113.18
12	L	44	LYS	N-CA-C	5.54	122.61	110.80
3	C	88	GLU	CA-C-N	5.41	131.88	121.54
3	C	88	GLU	C-N-CA	5.41	131.88	121.54
4	D	169	VAL	CA-CB-CG1	5.23	119.30	110.40
3	C	89	ASP	CA-C-N	-5.19	111.59	122.03
3	C	89	ASP	C-N-CA	-5.19	111.59	122.03
4	D	169	VAL	CB-CA-C	5.15	119.73	111.29
2	B	336	ILE	CA-CB-CG1	5.14	119.14	110.40
2	B	499	GLY	N-CA-C	-5.09	101.12	113.18
9	I	58	ILE	CA-C-N	-5.04	115.20	122.45
9	I	58	ILE	C-N-CA	-5.04	115.20	122.45
9	I	54	GLU	CA-C-N	5.03	132.36	121.64
9	I	54	GLU	C-N-CA	5.03	132.36	121.64

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	336	ILE	Mainchain
18	a	42	ARG	Peptide
18	a	63	ARG	Peptide
18	e	63	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11139	0	11169	104	0
2	B	9228	0	9232	96	0
3	C	2098	0	2059	21	0
4	D	1314	0	1314	11	0
5	E	1740	0	1754	15	0
6	F	677	0	693	5	0
7	G	1324	0	1342	13	0
8	H	1052	0	1050	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	917	0	868	10	0
10	J	545	0	561	6	0
11	K	932	0	944	1	0
12	L	359	0	358	3	0
13	P	341	0	170	13	0
14	T	2610	0	1431	117	0
15	N	2527	0	1386	121	0
16	V	792	0	761	170	0
17	W	2226	0	2273	312	0
18	a	797	0	835	24	0
18	e	796	0	832	18	0
19	b	638	0	676	20	0
19	f	619	0	659	18	0
20	c	796	0	848	11	0
20	g	810	0	866	13	0
21	d	746	0	771	10	0
21	h	708	0	727	12	0
22	o	846	0	454	7	0
23	l	835	0	471	26	0
24	A	2	0	0	0	0
24	B	1	0	0	0	0
24	C	1	0	0	0	0
24	I	2	0	0	0	0
24	J	1	0	0	0	0
24	L	1	0	0	0	0
24	V	1	0	0	0	0
25	A	1	0	0	0	0
All	All	47422	0	44504	836	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 10.

All (836) 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)
16:V:81:LEU:HG	17:W:244:LEU:CD2	1.28	1.56
14:T:23:DA:C2	15:N:-22:DG:C2	1.99	1.49
14:T:23:DA:N1	15:N:-22:DG:C2	1.83	1.41
16:V:67:TRP:CE2	17:W:219:PRO:HB3	1.58	1.38
16:V:81:LEU:CG	17:W:244:LEU:HD22	1.57	1.35
16:V:57:LEU:O	17:W:263:PHE:HA	1.16	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:58:VAL:HA	17:W:262:ALA:O	1.26	1.33
16:V:73:ARG:CZ	17:W:217:LEU:HD11	1.59	1.30
16:V:59:ALA:O	17:W:261:SER:CA	1.84	1.24
14:T:23:DA:C2	15:N:-22:DG:N3	2.04	1.23
17:W:409:ASP:HB2	17:W:413:PHE:CD2	1.73	1.22
14:T:23:DA:C4	15:N:-22:DG:N2	2.08	1.22
17:W:333:PHE:CD1	17:W:354:LEU:HD21	1.73	1.21
15:N:-23:DT:H2''	15:N:-22:DG:C8	1.75	1.21
14:T:23:DA:C2	15:N:-22:DG:N2	2.09	1.20
16:V:68:VAL:HB	17:W:275:GLU:OE1	1.40	1.19
16:V:71:TRP:HZ3	17:W:218:ILE:HA	1.03	1.18
16:V:71:TRP:CZ3	17:W:218:ILE:HA	1.77	1.17
17:W:333:PHE:CG	17:W:354:LEU:HD21	1.80	1.16
14:T:23:DA:H2''	14:T:24:DA:C1'	1.76	1.15
16:V:110:GLY:HA2	17:W:312:PRO:CG	1.76	1.15
14:T:28:DG:O6	15:N:-28:DC:N4	1.79	1.15
23:1:-28:DC:C4	23:1:-27:DC:N4	2.16	1.14
16:V:61:GLY:HA3	17:W:247:LYS:HE2	1.24	1.14
16:V:110:GLY:CA	17:W:312:PRO:CG	2.25	1.13
17:W:409:ASP:HB2	17:W:413:PHE:HD2	1.05	1.12
17:W:332:LYS:HD2	17:W:389:PRO:HD3	1.24	1.12
14:T:16:DA:H2''	14:T:17:DA:H5'	1.16	1.11
17:W:399:ALA:HB1	17:W:406:ILE:HD11	1.27	1.11
16:V:67:TRP:HB2	17:W:223:ASP:HB3	1.28	1.10
16:V:85:ARG:HD3	17:W:312:PRO:O	1.49	1.10
16:V:110:GLY:HA2	17:W:312:PRO:HG3	1.23	1.09
14:T:26:DG:H2''	14:T:27:DG:H5'	1.10	1.09
16:V:59:ALA:O	17:W:261:SER:HA	0.92	1.08
14:T:23:DA:C5	15:N:-22:DG:N2	2.22	1.08
16:V:67:TRP:CB	17:W:223:ASP:HB3	1.81	1.08
1:A:976:ASP:O	1:A:977:ARG:HB2	1.51	1.07
16:V:58:VAL:HG22	17:W:263:PHE:HB3	1.37	1.07
16:V:55:GLU:OE2	17:W:265:ARG:HA	1.55	1.06
16:V:57:LEU:O	17:W:263:PHE:CA	2.04	1.04
16:V:73:ARG:CZ	17:W:217:LEU:CD1	2.34	1.04
16:V:110:GLY:CA	17:W:312:PRO:HG2	1.87	1.04
2:B:419:ARG:NH1	15:N:-40:DC:H1'	1.71	1.04
17:W:352:LEU:HD11	17:W:435:LEU:HD11	1.31	1.04
1:A:286:PRO:CG	17:W:268:PHE:CZ	2.41	1.04
2:B:419:ARG:HH11	15:N:-40:DC:H1'	1.14	1.04
14:T:23:DA:C6	15:N:-22:DG:C2	2.45	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:320:LEU:HD22	17:W:432:LEU:CD1	1.88	1.03
17:W:320:LEU:HD22	17:W:432:LEU:HD13	1.37	1.03
16:V:67:TRP:HB2	17:W:223:ASP:CB	1.88	1.02
16:V:110:GLY:HA3	17:W:312:PRO:HG2	1.42	1.02
15:N:24:DC:H2''	15:N:25:DT:C5	1.95	1.02
16:V:81:LEU:HG	17:W:244:LEU:HD23	1.38	1.02
16:V:106:ARG:NH2	17:W:214:GLN:OE1	1.93	1.02
1:A:318:LYS:NZ	14:T:43:DA:C6	2.28	1.01
16:V:67:TRP:CD1	17:W:223:ASP:OD2	2.13	1.01
16:V:106:ARG:CZ	17:W:214:GLN:OE1	2.09	1.01
14:T:16:DA:H2''	14:T:17:DA:C5'	1.90	1.01
17:W:399:ALA:CB	17:W:406:ILE:HD11	1.90	1.00
16:V:67:TRP:CH2	17:W:306:TYR:HB3	1.96	1.00
16:V:81:LEU:CG	17:W:244:LEU:CD2	2.25	1.00
14:T:23:DA:H2'	14:T:24:DA:C8	1.97	0.99
2:B:62:ALA:O	2:B:70:ASN:HA	1.62	0.99
14:T:23:DA:C6	15:N:-22:DG:N2	2.30	0.99
16:V:9:GLU:OE1	17:W:241:ARG:NH2	1.96	0.99
1:A:288:HIS:NE2	17:W:299:PHE:CZ	2.31	0.99
14:T:23:DA:N3	15:N:-22:DG:N2	2.11	0.98
17:W:396:GLU:OE2	17:W:414:VAL:HG23	1.64	0.98
16:V:67:TRP:CZ2	17:W:219:PRO:HB3	1.99	0.97
16:V:73:ARG:HH21	17:W:214:GLN:HA	1.29	0.97
14:T:-25:DA:N1	15:N:25:DT:N3	2.12	0.97
14:T:49:DC:H5''	17:W:330:ASN:HD21	1.26	0.97
16:V:61:GLY:HA3	17:W:247:LYS:CE	1.95	0.96
16:V:55:GLU:CD	17:W:265:ARG:HE	1.74	0.96
16:V:110:GLY:HA3	17:W:312:PRO:CG	1.95	0.96
17:W:399:ALA:HB1	17:W:406:ILE:CD1	1.95	0.96
15:N:-23:DT:C2'	15:N:-22:DG:C8	2.48	0.96
1:A:318:LYS:HD2	14:T:43:DA:C2	2.02	0.95
2:B:62:ALA:HB3	2:B:71:ILE:CG2	1.97	0.95
16:V:66:SER:HB2	17:W:260:TYR:HB3	1.46	0.95
16:V:68:VAL:N	17:W:275:GLU:OE2	1.98	0.95
14:T:23:DA:H2''	14:T:24:DA:N9	1.83	0.94
2:B:62:ALA:CB	2:B:71:ILE:CG2	2.46	0.93
17:W:409:ASP:CB	17:W:413:PHE:CD2	2.50	0.93
14:T:23:DA:N1	15:N:-22:DG:N1	2.15	0.92
16:V:71:TRP:HZ3	17:W:218:ILE:CA	1.81	0.92
16:V:67:TRP:CE2	17:W:219:PRO:CB	2.51	0.91
1:A:286:PRO:CD	17:W:268:PHE:CZ	2.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:278:LYS:HB3	23:1:-30:DA:H4'	1.52	0.91
16:V:67:TRP:CD1	17:W:223:ASP:CG	2.48	0.91
17:W:409:ASP:CB	17:W:413:PHE:HD2	1.81	0.91
17:W:399:ALA:C	17:W:406:ILE:CD1	2.43	0.91
1:A:288:HIS:CD2	17:W:299:PHE:CZ	2.58	0.90
14:T:30:DT:H2''	14:T:31:DT:H71	1.49	0.90
16:V:58:VAL:CA	17:W:262:ALA:O	2.16	0.90
14:T:19:DC:O2	15:N:-19:DG:N2	2.03	0.90
14:T:26:DG:C2'	14:T:27:DG:H5'	1.99	0.90
16:V:73:ARG:NH2	17:W:214:GLN:HA	1.85	0.90
16:V:67:TRP:NE1	17:W:219:PRO:HB3	1.87	0.89
1:A:286:PRO:HD3	17:W:268:PHE:CZ	2.08	0.89
16:V:110:GLY:CA	17:W:312:PRO:HG3	1.99	0.89
2:B:62:ALA:CB	2:B:71:ILE:HG23	2.03	0.88
14:T:23:DA:C6	15:N:-22:DG:N1	2.43	0.87
17:W:258:GLU:OE1	17:W:278:LYS:NZ	2.08	0.87
14:T:29:DA:H61	15:N:-29:DT:H3	1.16	0.87
16:V:85:ARG:NH1	16:V:87:ASP:OD1	2.07	0.87
17:W:394:PHE:HE2	17:W:396:GLU:HG2	1.37	0.87
17:W:409:ASP:O	17:W:410:ARG:HG3	1.75	0.87
17:W:320:LEU:CD2	17:W:432:LEU:HD13	2.05	0.86
14:T:23:DA:H2''	14:T:24:DA:O4'	1.75	0.86
14:T:25:DG:H2''	14:T:26:DG:H5''	1.58	0.86
16:V:67:TRP:HD1	17:W:223:ASP:OD2	1.56	0.86
16:V:68:VAL:HG23	17:W:275:GLU:CD	2.01	0.85
17:W:333:PHE:CG	17:W:354:LEU:CD2	2.59	0.85
17:W:388:ARG:HB2	17:W:389:PRO:HD3	1.58	0.84
14:T:23:DA:C2'	14:T:24:DA:N9	2.41	0.84
17:W:329:LYS:HD2	17:W:436:ILE:HG13	1.59	0.84
14:T:14:DT:H2''	14:T:15:DT:C7	2.08	0.84
17:W:399:ALA:CB	17:W:406:ILE:CD1	2.55	0.84
17:W:352:LEU:HD11	17:W:435:LEU:CD1	2.07	0.83
17:W:357:ARG:C	17:W:389:PRO:HG2	2.02	0.83
17:W:399:ALA:C	17:W:406:ILE:HD11	2.02	0.83
2:B:62:ALA:CB	2:B:71:ILE:HG22	2.09	0.83
14:T:23:DA:N1	15:N:-23:DT:O2	2.12	0.83
5:E:117:PRO:HG2	14:T:22:DC:OP1	1.78	0.83
2:B:62:ALA:HB3	2:B:71:ILE:HG22	1.59	0.82
16:V:71:TRP:CZ2	17:W:307:LYS:HB2	2.14	0.82
14:T:30:DT:C2'	14:T:31:DT:H71	2.08	0.82
1:A:286:PRO:CD	17:W:268:PHE:CE1	2.63	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:500:LYS:H	2:B:500:LYS:HD3	1.42	0.82
16:V:60:VAL:HA	17:W:260:TYR:O	1.79	0.82
17:W:332:LYS:HD2	17:W:388:ARG:HB2	1.59	0.82
16:V:67:TRP:HH2	17:W:306:TYR:HB3	1.42	0.82
16:V:67:TRP:NE1	17:W:219:PRO:HA	1.95	0.82
14:T:16:DA:C2'	14:T:17:DA:H5'	2.06	0.81
16:V:67:TRP:NE1	17:W:219:PRO:CA	2.43	0.81
16:V:68:VAL:CB	17:W:275:GLU:OE1	2.26	0.81
16:V:71:TRP:CZ2	17:W:307:LYS:CB	2.63	0.81
16:V:55:GLU:OE1	17:W:265:ARG:NE	2.13	0.81
15:N:-25:DC:C2	15:N:-24:DT:C5	2.69	0.80
14:T:32:DA:C2	15:N:-31:DA:C2	2.69	0.80
15:N:-41:DT:OP2	15:N:-41:DT:H2'	1.82	0.80
17:W:328:VAL:HA	17:W:435:LEU:HD23	1.64	0.80
17:W:357:ARG:HB3	17:W:389:PRO:HD2	1.64	0.80
14:T:23:DA:C2'	14:T:24:DA:C8	2.65	0.79
16:V:9:GLU:OE2	17:W:241:ARG:NH1	2.13	0.79
16:V:9:GLU:CD	17:W:241:ARG:HH12	1.89	0.79
1:A:318:LYS:NZ	14:T:43:DA:N6	2.29	0.79
2:B:419:ARG:NH1	15:N:-40:DC:C1'	2.45	0.79
1:A:288:HIS:CE1	17:W:299:PHE:CE1	2.70	0.79
16:V:81:LEU:HG	17:W:244:LEU:HD22	0.79	0.78
15:N:-25:DC:C2	15:N:-24:DT:C7	2.66	0.78
16:V:106:ARG:HH21	17:W:214:GLN:HB2	1.49	0.78
14:T:21:DC:H2''	14:T:22:DC:C5	2.19	0.78
14:T:49:DC:H5''	17:W:330:ASN:ND2	1.99	0.78
14:T:25:DG:N2	15:N:-24:DT:C2	2.52	0.77
15:N:-39:DT:H2''	15:N:-38:DT:H72	1.65	0.77
14:T:32:DA:N1	15:N:-31:DA:C2	2.52	0.77
14:T:23:DA:H2	15:N:-22:DG:N3	1.78	0.77
5:E:118:SER:OG	15:N:-18:DG:H5''	1.84	0.77
16:V:73:ARG:NH1	17:W:217:LEU:HD11	1.99	0.77
17:W:394:PHE:CE2	17:W:396:GLU:HG2	2.18	0.77
16:V:66:SER:OG	17:W:275:GLU:OE1	2.03	0.77
16:V:85:ARG:CD	17:W:312:PRO:O	2.30	0.77
16:V:68:VAL:CG2	17:W:275:GLU:CD	2.57	0.77
16:V:67:TRP:NE1	17:W:219:PRO:CB	2.48	0.76
16:V:57:LEU:CG	17:W:240:VAL:HG11	2.15	0.76
1:A:318:LYS:NZ	14:T:43:DA:N1	2.28	0.76
14:T:16:DA:H1'	14:T:17:DA:H5''	1.67	0.76
14:T:23:DA:H61	15:N:-23:DT:H3	1.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:PRO:HG2	17:W:268:PHE:CE2	2.20	0.76
23:1:-28:DC:N4	23:1:-27:DC:N4	2.33	0.76
13:P:1:U:H2'	13:P:2:G:C8	2.21	0.76
16:V:67:TRP:CZ3	17:W:306:TYR:CD2	2.74	0.75
1:A:286:PRO:CG	17:W:268:PHE:CE2	2.68	0.75
16:V:58:VAL:HG12	17:W:261:SER:HB2	1.69	0.75
15:N:-23:DT:H2''	15:N:-22:DG:H8	1.44	0.74
14:T:27:DG:O6	15:N:-27:DC:N4	2.15	0.74
17:W:319:LYS:O	17:W:320:LEU:CB	2.33	0.74
1:A:286:PRO:HG2	17:W:268:PHE:CZ	2.21	0.74
16:V:67:TRP:CB	17:W:224:PRO:HD2	2.18	0.74
1:A:288:HIS:NE2	17:W:299:PHE:CE1	2.55	0.74
16:V:81:LEU:CD2	17:W:244:LEU:HD22	2.17	0.74
14:T:23:DA:C2	15:N:-23:DT:O2	2.41	0.73
14:T:14:DT:H2''	14:T:15:DT:H71	1.70	0.73
16:V:61:GLY:CA	17:W:247:LYS:HE2	2.13	0.73
17:W:328:VAL:HG22	17:W:435:LEU:HD21	1.70	0.73
16:V:57:LEU:HG	17:W:240:VAL:HG11	1.69	0.73
16:V:67:TRP:HB2	17:W:223:ASP:CG	2.13	0.73
16:V:67:TRP:HE1	17:W:219:PRO:CA	1.99	0.73
16:V:67:TRP:HD1	17:W:223:ASP:CG	1.94	0.73
14:T:23:DA:N6	15:N:-23:DT:H3	1.86	0.72
16:V:56:GLY:HA2	17:W:264:GLN:O	1.89	0.72
2:B:868:ILE:HG12	15:N:-47:DC:OP1	1.89	0.72
16:V:58:VAL:CG1	17:W:261:SER:HB2	2.20	0.72
17:W:323:GLY:HA2	17:W:339:GLN:HE21	1.54	0.72
16:V:68:VAL:HB	17:W:275:GLU:CD	2.15	0.72
17:W:388:ARG:HB2	17:W:389:PRO:CD	2.19	0.72
17:W:396:GLU:OE2	17:W:414:VAL:CG2	2.36	0.72
14:T:16:DA:C2'	14:T:17:DA:C5'	2.65	0.72
15:N:-16:DT:H4'	15:N:-15:DA:H5'	1.71	0.72
17:W:326:VAL:HG21	17:W:435:LEU:HD13	1.71	0.72
16:V:57:LEU:HG	17:W:240:VAL:CG1	2.20	0.71
14:T:21:DC:H2''	14:T:22:DC:C6	2.25	0.71
16:V:67:TRP:CZ2	17:W:219:PRO:CB	2.72	0.71
17:W:333:PHE:CD1	17:W:354:LEU:CD2	2.65	0.71
16:V:57:LEU:CB	17:W:240:VAL:HG11	2.20	0.71
14:T:23:DA:N1	15:N:-23:DT:C2	2.59	0.71
1:A:45:ARG:O	1:A:45:ARG:HG2	1.88	0.71
1:A:286:PRO:HG3	17:W:268:PHE:CZ	2.25	0.71
16:V:58:VAL:HG22	17:W:263:PHE:CB	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:PRO:HD3	17:W:268:PHE:CE1	2.26	0.70
14:T:26:DG:H2''	14:T:27:DG:C5'	2.06	0.70
16:V:73:ARG:NE	17:W:217:LEU:CD1	2.54	0.70
15:N:24:DC:H2''	15:N:25:DT:C6	2.27	0.70
2:B:500:LYS:HD3	2:B:500:LYS:N	2.06	0.70
1:A:14:VAL:H	1:A:1435:GLN:HE22	1.40	0.70
16:V:57:LEU:HD23	17:W:240:VAL:HB	1.73	0.70
14:T:14:DT:O4	15:N:-15:DA:N6	2.25	0.70
16:V:71:TRP:CZ2	17:W:307:LYS:HB3	2.26	0.70
14:T:23:DA:C2'	14:T:24:DA:O4'	2.38	0.69
16:V:106:ARG:NH2	17:W:214:GLN:HB2	2.05	0.69
17:W:320:LEU:HD22	17:W:432:LEU:HD11	1.74	0.69
16:V:85:ARG:HD3	17:W:312:PRO:C	2.17	0.69
21:h:83:ARG:HH21	23:1:-34:DT:H5''	1.55	0.69
2:B:71:ILE:HD12	2:B:127:ILE:HG23	1.73	0.69
16:V:71:TRP:HE3	17:W:217:LEU:O	1.75	0.69
17:W:357:ARG:HB3	17:W:389:PRO:CD	2.22	0.69
17:W:332:LYS:HG3	17:W:388:ARG:CB	2.22	0.69
15:N:-25:DC:O2	15:N:-24:DT:C5	2.46	0.69
17:W:399:ALA:CA	17:W:406:ILE:HD11	2.23	0.68
17:W:279:ALA:HB2	23:1:-29:DT:OP1	1.94	0.68
1:A:1160:PRO:HB3	1:A:1190:GLN:HE21	1.56	0.68
16:V:72:LEU:HD21	17:W:310:LEU:HD13	1.74	0.68
16:V:67:TRP:HE1	17:W:219:PRO:HA	1.54	0.68
14:T:32:DA:N1	15:N:-31:DA:N1	2.42	0.67
16:V:61:GLY:N	17:W:260:TYR:O	2.27	0.67
17:W:329:LYS:CD	17:W:436:ILE:HG13	2.24	0.67
17:W:357:ARG:O	17:W:389:PRO:HG2	1.94	0.67
14:T:31:DT:N3	14:T:32:DA:C6	2.63	0.67
17:W:332:LYS:CD	17:W:388:ARG:HB2	2.24	0.67
17:W:357:ARG:HB3	17:W:389:PRO:HG2	1.75	0.67
16:V:73:ARG:NE	17:W:217:LEU:HD11	2.10	0.67
15:N:-25:DC:O2	15:N:-24:DT:C6	2.48	0.66
1:A:243:PRO:O	1:A:248:ARG:NH1	2.28	0.66
16:V:71:TRP:CE3	17:W:217:LEU:O	2.49	0.66
7:G:132:SER:HB2	7:G:135:GLU:HB2	1.78	0.65
12:L:68:GLN:HB3	17:W:784:ASN:HD21	1.61	0.65
17:W:409:ASP:O	17:W:410:ARG:CG	2.43	0.65
17:W:329:LYS:HD2	17:W:436:ILE:CG1	2.25	0.65
16:V:67:TRP:CH2	17:W:306:TYR:CB	2.76	0.65
17:W:351:ARG:HG2	17:W:429:THR:HG22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:HIS:NE2	17:W:299:PHE:HZ	1.92	0.65
16:V:68:VAL:CB	17:W:275:GLU:CD	2.68	0.65
23:1:-31:DA:C6	23:1:-30:DA:N6	2.65	0.65
1:A:466:TYR:HB2	1:A:470:ARG:HH22	1.61	0.64
17:W:409:ASP:CB	17:W:413:PHE:CE2	2.80	0.64
2:B:70:ASN:O	2:B:127:ILE:HA	1.97	0.64
14:T:25:DG:N2	15:N:-24:DT:O2	2.29	0.64
14:T:9:DG:N3	18:e:40:ARG:NH2	2.45	0.64
16:V:66:SER:CB	17:W:260:TYR:HB3	2.24	0.64
2:B:896:ASP:OD2	12:L:60:LYS:NZ	2.30	0.64
16:V:61:GLY:CA	17:W:247:LYS:CE	2.74	0.64
16:V:73:ARG:NH2	17:W:217:LEU:CD1	2.61	0.64
16:V:55:GLU:OE2	17:W:265:ARG:NE	2.31	0.63
16:V:71:TRP:HZ2	17:W:307:LYS:HB2	1.62	0.63
17:W:396:GLU:CD	17:W:414:VAL:CG2	2.70	0.63
16:V:57:LEU:HB3	17:W:240:VAL:HG11	1.79	0.63
14:T:40:DG:H2''	14:T:41:DA:H5''	1.80	0.63
17:W:332:LYS:HG3	17:W:388:ARG:HB3	1.79	0.63
16:V:67:TRP:CZ2	17:W:219:PRO:CG	2.82	0.63
17:W:329:LYS:CG	17:W:436:ILE:HG13	2.28	0.63
16:V:57:LEU:CG	17:W:240:VAL:CG1	2.75	0.63
16:V:67:TRP:H	17:W:224:PRO:HD2	1.62	0.63
14:T:23:DA:C2'	14:T:24:DA:C1'	2.67	0.62
15:N:24:DC:H2''	15:N:25:DT:C7	2.28	0.62
2:B:62:ALA:HB3	2:B:71:ILE:H	1.64	0.62
4:D:159:LEU:HD21	7:G:167:PHE:HB2	1.81	0.62
1:A:161:LYS:CA	14:T:-58:DG:OP1	2.48	0.62
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.32	0.62
18:e:118:THR:OG1	19:f:45:ARG:NH1	2.33	0.62
16:V:68:VAL:HG21	17:W:275:GLU:HB2	1.82	0.62
1:A:982:ASP:O	1:A:1041:ARG:NH2	2.33	0.61
16:V:55:GLU:CD	17:W:265:ARG:NE	2.52	0.61
17:W:352:LEU:CD1	17:W:435:LEU:HD11	2.19	0.61
18:a:116:ARG:NH1	18:a:118:THR:O	2.33	0.61
23:1:-28:DC:C4	23:1:-27:DC:C4	2.88	0.61
17:W:328:VAL:HG22	17:W:435:LEU:CD2	2.30	0.61
17:W:437:VAL:O	17:W:437:VAL:HG22	1.99	0.61
4:D:19:VAL:O	4:D:29:ARG:NH1	2.33	0.61
1:A:318:LYS:HZ1	14:T:43:DA:N6	1.96	0.61
14:T:29:DA:H2'	14:T:30:DT:H72	1.82	0.61
8:H:56:THR:HB	8:H:144:ARG:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:67:TRP:CB	17:W:223:ASP:CB	2.62	0.61
9:I:29:CYS:SG	9:I:30:ARG:N	2.74	0.61
2:B:220:ALA:O	2:B:252:ARG:NH2	2.33	0.61
2:B:233:SER:HG	2:B:356:HIS:HD1	1.47	0.61
16:V:44:ALA:O	16:V:48:GLU:HG2	2.01	0.61
16:V:68:VAL:H	17:W:275:GLU:CD	2.05	0.60
1:A:288:HIS:CE1	17:W:299:PHE:HE1	2.16	0.60
19:f:92:ARG:HH21	21:h:98:LEU:HA	1.65	0.60
19:b:38:ALA:HB1	19:b:43:VAL:HB	1.84	0.60
15:N:-25:DC:H2''	15:N:-24:DT:OP2	1.99	0.60
16:V:84:VAL:HG22	17:W:310:LEU:HD22	1.83	0.60
2:B:969:ARG:NH1	3:C:60:GLU:OE1	2.34	0.60
4:D:41:HIS:HB3	7:G:73:LYS:HD3	1.82	0.60
15:N:-15:DA:H2''	15:N:-14:DA:C8	2.35	0.60
17:W:357:ARG:HB3	17:W:389:PRO:CG	2.31	0.60
16:V:57:LEU:HD23	17:W:240:VAL:CG1	2.32	0.60
3:C:69:ILE:HD11	3:C:144:LEU:HD21	1.84	0.60
16:V:55:GLU:OE2	17:W:265:ARG:HD2	2.01	0.59
14:T:-14:DA:O3'	18:a:63:ARG:NH2	2.35	0.59
1:A:161:LYS:C	14:T:-58:DG:OP1	2.44	0.59
5:E:118:SER:HB3	15:N:-18:DG:H4'	1.83	0.59
14:T:22:DC:H2''	14:T:23:DA:H5''	1.85	0.59
20:g:29:ARG:NH2	21:h:32:GLU:OE1	2.35	0.59
17:W:319:LYS:O	17:W:320:LEU:HB3	2.02	0.59
14:T:-42:DT:OP1	20:c:20:ARG:NH2	2.35	0.59
17:W:413:PHE:CE1	17:W:420:GLU:HB3	2.38	0.59
21:h:73:GLU:OE1	21:h:76:ARG:NH2	2.35	0.59
2:B:995:ARG:NH1	2:B:997:GLU:OE2	2.35	0.59
16:V:62:ASP:HB3	17:W:260:TYR:CD2	2.37	0.59
16:V:67:TRP:CG	17:W:223:ASP:HB3	2.36	0.59
18:a:100:LEU:HD11	19:b:58:LEU:HD13	1.83	0.59
1:A:42:ASP:O	1:A:43:GLU:HG3	2.03	0.59
1:A:318:LYS:HG2	15:N:-42:DG:O6	2.02	0.59
2:B:279:ARG:NH2	2:B:286:ASP:OD1	2.35	0.59
2:B:859:TYR:HD2	2:B:911:ILE:HD11	1.67	0.59
14:T:17:DA:C2	15:N:-16:DT:O2	2.55	0.59
5:E:85:PRO:HA	5:E:112:GLN:HB2	1.85	0.59
17:W:397:ALA:O	17:W:401:VAL:HG23	2.03	0.59
2:B:62:ALA:HB3	2:B:71:ILE:HG23	1.70	0.58
15:N:-40:DC:H6	15:N:-40:DC:O5'	1.86	0.58
8:H:112:LYS:HG2	8:H:125:GLU:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:-25:DA:H2	15:N:25:DT:O2	1.85	0.58
17:W:328:VAL:HA	17:W:435:LEU:CD2	2.33	0.58
18:a:69:ARG:NH1	19:b:25:ASN:OD1	2.37	0.58
20:c:88:ARG:NH1	20:c:94:ASN:OD1	2.35	0.58
17:W:399:ALA:O	17:W:406:ILE:CD1	2.50	0.58
14:T:14:DT:H2''	14:T:15:DT:C5	2.37	0.58
17:W:394:PHE:HE2	17:W:396:GLU:CG	2.14	0.58
17:W:396:GLU:CD	17:W:414:VAL:HG21	2.27	0.58
16:V:73:ARG:NH2	17:W:217:LEU:HD11	2.16	0.58
16:V:106:ARG:NH2	17:W:214:GLN:CD	2.61	0.58
15:N:49:DC:H4'	21:d:30:ARG:HD2	1.85	0.58
17:W:319:LYS:O	17:W:320:LEU:HB2	2.03	0.58
17:W:389:PRO:HD2	17:W:389:PRO:O	2.04	0.58
1:A:570:LYS:HB3	8:H:46:MET:HE1	1.86	0.58
2:B:295:TYR:HD1	2:B:564:PRO:HB3	1.69	0.58
14:T:31:DT:C4	14:T:32:DA:N6	2.72	0.58
18:a:123:ASP:OD1	18:e:113:HIS:NE2	2.37	0.57
1:A:162:VAL:HG23	14:T:-58:DG:P	2.43	0.57
15:N:-3:DA:H5'	19:f:45:ARG:HH12	1.67	0.57
16:V:110:GLY:HA3	17:W:312:PRO:CB	2.32	0.57
1:A:286:PRO:HG3	17:W:268:PHE:CE2	2.38	0.57
1:A:351:ARG:HB2	2:B:1128:LEU:HD11	1.87	0.57
17:W:332:LYS:CG	17:W:388:ARG:HB2	2.35	0.57
17:W:394:PHE:CE2	17:W:396:GLU:CG	2.87	0.57
16:V:55:GLU:OE2	17:W:265:ARG:CD	2.52	0.57
8:H:13:GLN:HE22	8:H:29:ILE:HD12	1.70	0.57
16:V:71:TRP:CZ3	17:W:218:ILE:CA	2.67	0.57
14:T:17:DA:OP1	18:e:69:ARG:NH2	2.36	0.57
17:W:344:LEU:CD1	17:W:349:GLU:HB2	2.35	0.56
2:B:30:LEU:O	2:B:489:ARG:NH1	2.38	0.56
1:A:89:PRO:HB3	1:A:238:THR:HG22	1.87	0.56
16:V:68:VAL:HG23	17:W:275:GLU:OE2	2.05	0.56
2:B:760:ASP:OD1	2:B:760:ASP:N	2.38	0.56
16:V:72:LEU:CD2	17:W:310:LEU:HD13	2.35	0.56
16:V:57:LEU:HD23	17:W:240:VAL:CB	2.36	0.56
14:T:32:DA:C2	15:N:-31:DA:H2	2.23	0.56
19:f:38:ALA:HB1	19:f:43:VAL:HB	1.87	0.56
17:W:279:ALA:N	23:1:-29:DT:OP1	2.39	0.56
21:d:35:SER:O	21:d:39:TYR:HB2	2.05	0.56
1:A:1201:ARG:NH2	1:A:1235:ALA:O	2.38	0.56
14:T:23:DA:C3'	14:T:24:DA:O4'	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:83:ARG:HG2	17:W:762:GLY:HA2	1.88	0.55
16:V:67:TRP:CZ3	17:W:306:TYR:HD2	2.23	0.55
19:f:74:GLU:O	21:h:89:ARG:NH2	2.38	0.55
1:A:50:GLU:CD	17:W:444:LEU:HD11	2.31	0.55
5:E:84:GLU:OE1	5:E:91:THR:OG1	2.20	0.55
16:V:55:GLU:OE2	17:W:265:ARG:CA	2.44	0.55
17:W:396:GLU:CD	17:W:414:VAL:HG23	2.30	0.55
22:0:28:DG:N2	23:1:-27:DC:O2	2.39	0.55
3:C:74:GLU:O	3:C:246:ARG:NH2	2.33	0.55
17:W:409:ASP:HB2	17:W:413:PHE:CE2	2.35	0.55
18:a:62:ILE:O	18:a:93:GLN:NE2	2.40	0.55
1:A:1459:ASP:OD1	1:A:1459:ASP:N	2.34	0.55
13:P:1:U:O2'	13:P:2:G:O4'	2.23	0.55
15:N:29:DG:OP1	19:b:78:ARG:NH1	2.40	0.55
14:T:25:DG:N2	15:N:-24:DT:N3	2.52	0.54
16:V:58:VAL:CG2	17:W:263:PHE:HB3	2.24	0.54
16:V:67:TRP:CG	17:W:223:ASP:CG	2.85	0.54
2:B:822:ASN:O	10:J:47:ARG:NH1	2.39	0.54
16:V:67:TRP:HZ2	17:W:219:PRO:HD3	1.72	0.54
2:B:268:VAL:HA	2:B:330:GLY:HA2	1.88	0.54
14:T:-34:DG:H3'	21:d:83:ARG:HH21	1.73	0.54
17:W:352:LEU:HD11	17:W:435:LEU:HD21	1.90	0.54
15:N:-23:DT:C2	15:N:-22:DG:C5	2.96	0.54
22:0:35:DC:N4	23:1:-36:DG:O6	2.41	0.54
1:A:288:HIS:CD2	17:W:299:PHE:CE1	2.94	0.54
2:B:904:ARG:NH1	17:W:782:LEU:O	2.41	0.54
15:N:-15:DA:C5	15:N:-14:DA:N6	2.76	0.54
16:V:67:TRP:HB3	17:W:224:PRO:HD2	1.89	0.54
1:A:1452:LEU:HD22	6:F:131:PRO:HB3	1.90	0.53
16:V:43:GLN:NE2	16:V:47:ASN:OD1	2.39	0.53
17:W:409:ASP:OD2	17:W:415:THR:OG1	2.21	0.53
15:N:-26:DC:H2''	15:N:-25:DC:C5	2.44	0.53
10:J:8:PHE:HB2	10:J:47:ARG:HH22	1.73	0.53
15:N:-23:DT:N3	15:N:-22:DG:C6	2.77	0.53
3:C:146:LYS:NZ	10:J:57:GLU:OE2	2.34	0.53
17:W:280:GLU:OE2	23:1:-30:DA:H5''	2.09	0.53
18:a:128:ARG:NH2	18:a:134:ARG:O	2.42	0.53
20:c:81:ARG:NH1	18:e:56:LYS:O	2.42	0.53
2:B:270:GLN:HB3	2:B:329:ARG:HD3	1.89	0.53
16:V:67:TRP:H	17:W:224:PRO:CD	2.22	0.53
14:T:14:DT:C4	15:N:-15:DA:N6	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLU:OE1	17:W:444:LEU:HD11	2.09	0.53
3:C:20:MET:SD	3:C:227:ARG:NH2	2.75	0.53
9:I:90:GLN:HE21	9:I:92:ARG:HG3	1.74	0.53
17:W:772:GLU:OE2	17:W:774:ASN:ND2	2.42	0.53
1:A:162:VAL:HG23	14:T:-58:DG:O5'	2.10	0.52
1:A:327:ARG:HG3	1:A:1409:VAL:HG21	1.91	0.52
15:N:-42:DG:H4'	15:N:-41:DT:O5'	2.08	0.52
15:N:28:DA:H3'	19:b:78:ARG:HD2	1.91	0.52
16:V:41:SER:HB2	16:V:45:THR:HB	1.91	0.52
23:1:-28:DC:N3	23:1:-27:DC:N4	2.56	0.52
2:B:944:THR:HG21	2:B:1122:ARG:HE	1.75	0.52
14:T:32:DA:H2	15:N:-31:DA:C2	2.26	0.52
1:A:409:ASP:OD1	1:A:409:ASP:N	2.40	0.52
18:e:62:ILE:O	18:e:93:GLN:NE2	2.41	0.52
23:1:-28:DC:C5	23:1:-27:DC:N4	2.75	0.52
21:d:61:SER:HA	21:d:64:ASN:HD22	1.75	0.52
1:A:336:ARG:HH22	2:B:1114:LEU:HD21	1.74	0.52
17:W:413:PHE:HZ	17:W:420:GLU:CD	2.17	0.52
16:V:67:TRP:CH2	17:W:306:TYR:CD2	2.98	0.52
20:c:115:LEU:HD22	18:e:117:VAL:HG13	1.90	0.52
18:e:100:LEU:HD11	19:f:58:LEU:HD13	1.91	0.52
2:B:333:ALA:HB3	2:B:336:ILE:HD11	1.92	0.52
16:V:67:TRP:CZ2	17:W:219:PRO:HG3	2.45	0.52
16:V:110:GLY:CA	17:W:312:PRO:CB	2.87	0.52
5:E:117:PRO:CG	14:T:22:DC:OP1	2.54	0.51
5:E:118:SER:OG	15:N:-18:DG:C5'	2.57	0.51
23:1:-28:DC:N4	23:1:-27:DC:H42	2.07	0.51
14:T:49:DC:C5'	17:W:330:ASN:HD21	2.11	0.51
18:a:45:THR:O	18:a:49:ARG:HB2	2.10	0.51
20:c:78:ILE:H	21:d:51:ILE:HA	1.76	0.51
16:V:68:VAL:HG11	17:W:261:SER:OG	2.10	0.51
21:d:55:ALA:HA	21:d:58:ILE:HD12	1.91	0.51
1:A:18:GLN:HB3	2:B:1215:ARG:HB2	1.93	0.51
1:A:1402:ARG:NH2	1:A:1420:GLU:OE1	2.43	0.51
2:B:316:ILE:HG23	2:B:321:VAL:HG23	1.92	0.51
23:1:-29:DT:H2''	23:1:-28:DC:C5	2.45	0.51
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.92	0.51
7:G:100:PHE:HB3	7:G:107:ASN:HD21	1.75	0.51
14:T:22:DC:C2	15:N:-21:DG:N2	2.79	0.51
18:a:79:LYS:HB3	18:a:82:LEU:HD11	1.93	0.51
1:A:318:LYS:CD	14:T:43:DA:C2	2.86	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:ILE:HG21	2:B:355:PRO:HG3	1.93	0.51
14:T:16:DA:C1'	14:T:17:DA:H5''	2.37	0.51
17:W:349:GLU:HG2	17:W:431:ARG:HA	1.92	0.51
1:A:227:GLU:OE1	1:A:231:ARG:NH1	2.44	0.51
16:V:57:LEU:O	17:W:263:PHE:CB	2.59	0.51
20:c:101:THR:HG23	19:f:97:LEU:HD13	1.93	0.51
18:e:99:TYR:OH	18:e:133:GLU:OE2	2.29	0.51
16:V:67:TRP:HB2	17:W:224:PRO:HD2	1.93	0.51
17:W:332:LYS:HG3	17:W:388:ARG:HB2	1.93	0.51
1:A:351:ARG:NE	1:A:487:GLU:OE1	2.44	0.50
14:T:19:DC:O2	15:N:-18:DG:N2	2.44	0.50
21:d:58:ILE:HG12	19:f:99:GLY:HA2	1.93	0.50
19:f:29:ILE:HB	19:f:55:ARG:HE	1.77	0.50
2:B:419:ARG:NH1	15:N:-40:DC:C2	2.76	0.50
14:T:30:DT:C2'	14:T:31:DT:C7	2.84	0.50
15:N:51:DG:OP1	21:d:28:ARG:NH1	2.45	0.50
17:W:388:ARG:CB	17:W:389:PRO:CD	2.88	0.50
1:A:354:ILE:HG22	1:A:469:PHE:HB2	1.93	0.50
22:0:63:DA:H2''	22:0:64:DA:H2'	1.93	0.50
2:B:260:THR:HG22	2:B:308:PRO:HB2	1.94	0.50
16:V:73:ARG:CZ	17:W:217:LEU:HD12	2.36	0.50
16:V:57:LEU:CD2	17:W:240:VAL:CG1	2.89	0.50
16:V:67:TRP:CH2	17:W:306:TYR:HD2	2.29	0.50
16:V:67:TRP:N	17:W:224:PRO:HD2	2.26	0.50
17:W:300:LEU:CD1	23:1:-28:DC:OP1	2.59	0.50
2:B:62:ALA:HB2	2:B:71:ILE:HG23	1.89	0.50
2:B:62:ALA:HB3	2:B:71:ILE:N	2.26	0.50
4:D:113:ALA:O	4:D:116:LYS:NZ	2.43	0.50
14:T:30:DT:H2'	14:T:31:DT:H71	1.92	0.50
16:V:67:TRP:CG	17:W:223:ASP:CB	2.94	0.50
17:W:409:ASP:C	17:W:410:ARG:HG3	2.37	0.50
2:B:1187:ASN:HD21	2:B:1190:ASN:HB3	1.77	0.49
2:B:1101:ASP:O	2:B:1122:ARG:NH1	2.45	0.49
9:I:7:CYS:HB2	9:I:14:LEU:HD21	1.94	0.49
4:D:33:GLU:O	4:D:38:GLN:NE2	2.45	0.49
15:N:-25:DC:C2	15:N:-24:DT:H73	2.46	0.49
3:C:74:GLU:HG3	3:C:242:GLN:HE22	1.77	0.49
14:T:-25:DA:C2	15:N:25:DT:O2	2.65	0.49
16:V:28:GLY:HA3	16:V:33:ASP:CG	2.38	0.49
17:W:286:LEU:HD22	17:W:292:VAL:HG21	1.93	0.49
18:a:95:ALA:HB2	19:b:97:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:-26:DC:C2	15:N:-25:DC:C5	3.01	0.49
16:V:73:ARG:NH2	17:W:214:GLN:CA	2.68	0.49
20:g:110:ASN:OD1	20:g:112:GLN:NE2	2.45	0.49
2:B:419:ARG:HH11	15:N:-40:DC:C1'	2.03	0.49
5:E:27:TYR:HA	5:E:63:PRO:HA	1.95	0.49
15:N:-45:DG:OP1	17:W:334:LYS:HE3	2.12	0.49
15:N:4:DG:H4'	15:N:5:DT:H5'	1.95	0.49
16:V:110:GLY:HA3	17:W:312:PRO:HB2	1.93	0.49
1:A:161:LYS:HA	14:T:-58:DG:OP1	2.11	0.49
1:A:841:ARG:NH2	1:A:1108:ASN:OD1	2.46	0.49
18:a:61:LEU:HD22	19:b:36:ARG:HD2	1.95	0.49
19:f:34:ILE:HA	19:f:37:LEU:HD12	1.94	0.49
1:A:43:GLU:OE2	17:W:335:GLY:O	2.31	0.49
1:A:286:PRO:HD2	17:W:268:PHE:CE1	2.44	0.49
2:B:859:TYR:HE2	2:B:941:LEU:HD12	1.77	0.49
8:H:15:VAL:HG22	8:H:26:ILE:HG22	1.94	0.49
16:V:9:GLU:CD	17:W:241:ARG:NH1	2.67	0.49
17:W:409:ASP:OD2	17:W:413:PHE:CE2	2.66	0.49
18:e:46:VAL:HG22	18:e:49:ARG:HH12	1.77	0.49
5:E:19:LYS:NZ	5:E:33:GLU:O	2.38	0.48
16:V:73:ARG:HH21	17:W:214:GLN:CA	2.12	0.48
17:W:357:ARG:CB	17:W:389:PRO:HG2	2.42	0.48
1:A:283:ASP:OD1	1:A:283:ASP:N	2.46	0.48
17:W:403:GLU:O	17:W:403:GLU:HG3	2.12	0.48
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.95	0.48
5:E:118:SER:CB	15:N:-18:DG:H4'	2.42	0.48
17:W:437:VAL:O	17:W:437:VAL:CG2	2.61	0.48
19:f:79:LYS:HD2	22:0:27:DG:H5''	1.94	0.48
18:a:45:THR:O	18:a:49:ARG:CB	2.62	0.48
18:a:126:LEU:HD21	18:e:110:CYS:HA	1.95	0.48
18:e:86:SER:HA	18:e:89:ILE:HD12	1.95	0.48
1:A:122:MET:HE1	1:A:138:VAL:HG13	1.96	0.48
2:B:62:ALA:HB1	2:B:71:ILE:HG22	1.89	0.48
1:A:1193:TRP:HZ3	9:I:43:VAL:HG21	1.79	0.48
2:B:851:PHE:O	2:B:1094:ARG:NH1	2.46	0.48
14:T:30:DT:H2''	14:T:31:DT:C7	2.34	0.48
20:g:30:VAL:HA	20:g:33:LEU:HD12	1.95	0.48
1:A:912:ASP:OD1	1:A:912:ASP:N	2.42	0.48
2:B:63:GLN:OE1	17:W:249:ALA:HB1	2.13	0.48
5:E:142:ASN:HB3	5:E:145:HIS:HD2	1.79	0.48
17:W:399:ALA:O	17:W:406:ILE:HD11	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:d:116:THR:O	21:d:120:SER:OG	2.28	0.48
2:B:401:LEU:HD13	2:B:538:ILE:HG21	1.96	0.47
16:V:67:TRP:CB	17:W:223:ASP:CG	2.84	0.47
16:V:81:LEU:CG	17:W:244:LEU:HD23	2.22	0.47
13:P:-4:C:H4'	13:P:-4:C:OP1	2.14	0.47
2:B:780:VAL:HG22	2:B:795:ILE:HG23	1.96	0.47
3:C:47:LEU:HB2	3:C:158:ILE:HB	1.95	0.47
16:V:60:VAL:CA	17:W:260:TYR:O	2.59	0.47
16:V:84:VAL:CG2	17:W:310:LEU:HD22	2.44	0.47
1:A:14:VAL:H	1:A:1435:GLN:NE2	2.10	0.47
2:B:273:PRO:HD2	2:B:276:ILE:HD12	1.97	0.47
1:A:113:LEU:O	1:A:165:ARG:NH2	2.47	0.47
1:A:115:LEU:HB2	1:A:122:MET:HE2	1.96	0.47
5:E:189:LEU:HD13	5:E:213:CYS:HB2	1.97	0.47
16:V:67:TRP:CD1	17:W:219:PRO:HA	2.49	0.47
19:b:29:ILE:HB	19:b:55:ARG:HE	1.79	0.47
1:A:1227:PHE:HB2	1:A:1245:ILE:HD11	1.97	0.47
2:B:969:ARG:HH22	3:C:59:ASP:HB2	1.80	0.47
10:J:9:SER:OG	10:J:47:ARG:NH2	2.47	0.47
19:b:99:GLY:HA2	21:h:58:ILE:HG12	1.97	0.47
20:g:76:THR:HG22	21:h:50:GLY:H	1.78	0.47
23:1:-37:DG:H2''	23:1:-36:DG:C8	2.50	0.47
1:A:254:ASP:OD1	1:A:254:ASP:N	2.48	0.47
1:A:285:SER:O	1:A:285:SER:OG	2.30	0.47
17:W:278:LYS:HB3	23:1:-30:DA:C4'	2.35	0.47
17:W:413:PHE:HE1	17:W:420:GLU:HB3	1.78	0.47
17:W:399:ALA:O	17:W:406:ILE:HD12	2.13	0.47
2:B:225:ILE:HD13	2:B:248:LYS:HD3	1.97	0.47
11:K:5:ASP:OD1	17:W:787:LYS:NZ	2.48	0.47
17:W:279:ALA:CB	23:1:-29:DT:OP1	2.61	0.47
3:C:13:GLN:HE21	3:C:16:GLU:HG2	1.79	0.46
13:P:-1:G:H2'	13:P:0:G:H5''	1.97	0.46
14:T:16:DA:C2'	14:T:17:DA:H5''	2.46	0.46
16:V:84:VAL:CG2	17:W:310:LEU:CD2	2.93	0.46
20:c:104:GLN:OE1	18:e:58:THR:OG1	2.29	0.46
22:0:46:DA:N6	23:1:-47:DC:N3	2.63	0.46
14:T:28:DG:N2	15:N:-27:DC:O2	2.48	0.46
15:N:-25:DC:C2	15:N:-24:DT:H71	2.49	0.46
16:V:71:TRP:CD1	17:W:310:LEU:HD12	2.50	0.46
17:W:308:ASP:HA	17:W:311:ARG:HG3	1.96	0.46
18:e:61:LEU:HD22	19:f:36:ARG:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1109:VAL:HG13	1:A:1335:PHE:HE2	1.80	0.46
2:B:299:ASP:OD2	2:B:385:ARG:NH1	2.37	0.46
1:A:358:PRO:HD2	2:B:833:TYR:CE1	2.51	0.46
1:A:542:ILE:HD12	1:A:578:LEU:HD13	1.98	0.46
15:N:17:DA:H2''	15:N:18:DG:H8	1.81	0.46
16:V:57:LEU:HG	17:W:240:VAL:HG12	1.96	0.46
2:B:164:MET:HB2	2:B:194:PHE:HE1	1.81	0.46
13:P:-2:U:H6	13:P:-2:U:O5'	1.98	0.46
20:g:79:ILE:HG12	20:g:82:HIS:CG	2.49	0.46
1:A:119:ASN:HB3	1:A:122:MET:HB3	1.98	0.46
13:P:-1:G:H2'	13:P:-1:G:N3	2.30	0.46
14:T:23:DA:N6	15:N:-22:DG:N1	2.63	0.46
14:T:31:DT:H2'	14:T:32:DA:C8	2.51	0.46
1:A:1162:SER:OG	1:A:1163:THR:N	2.49	0.46
16:V:73:ARG:HG2	17:W:217:LEU:HD13	1.96	0.46
13:P:2:G:O5'	13:P:2:G:H8	1.99	0.46
14:T:-14:DA:H2''	14:T:-13:DA:H8	1.80	0.46
14:T:16:DA:H1'	14:T:17:DA:C5'	2.39	0.46
20:c:97:LEU:HD22	20:c:100:VAL:HG21	1.98	0.46
1:A:1168:ASP:OD2	1:A:1196:ARG:NE	2.49	0.46
16:V:57:LEU:CD2	17:W:240:VAL:HG12	2.46	0.46
2:B:557:GLU:HB2	2:B:582:ILE:HD12	1.97	0.45
2:B:984:HIS:NE2	2:B:1028:GLU:OE1	2.36	0.45
4:D:51:LEU:HD11	7:G:4:LEU:HG	1.98	0.45
17:W:352:LEU:CD1	17:W:435:LEU:HD21	2.46	0.45
19:b:39:ARG:NH1	19:b:44:LYS:O	2.45	0.45
2:B:419:ARG:NH1	15:N:-40:DC:N1	2.60	0.45
2:B:1219:GLU:O	4:D:12:ARG:NH2	2.49	0.45
15:N:-15:DA:C4	15:N:-14:DA:C6	3.03	0.45
17:W:322:ARG:HD3	17:W:342:GLU:HA	1.99	0.45
13:P:-2:U:O5'	13:P:-2:U:C6	2.69	0.45
16:V:91:PRO:HB2	16:V:93:ASP:OD1	2.14	0.45
17:W:399:ALA:CB	17:W:406:ILE:HD13	2.44	0.45
18:e:99:TYR:HD1	19:f:95:ARG:HH22	1.64	0.45
14:T:-25:DA:C2	15:N:25:DT:N3	2.77	0.45
2:B:73:LYS:HG2	2:B:125:THR:HG22	1.99	0.45
18:a:48:LEU:HD13	18:a:51:ILE:HD12	1.99	0.45
23:1:-61:DT:H2'	23:1:-60:DT:C6	2.52	0.45
23:1:-44:DG:H2'	23:1:-43:DT:H71	1.99	0.45
18:e:40:ARG:HD2	18:e:40:ARG:HA	1.80	0.45
1:A:979:LYS:O	1:A:980:ALA:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1461:ALA:HB1	7:G:21:GLN:HB2	1.99	0.45
2:B:870:ILE:HG13	17:W:387:PHE:CZ	2.52	0.45
14:T:17:DA:H2''	14:T:18:DC:C6	2.51	0.45
18:a:45:THR:HG22	18:a:49:ARG:HH11	1.81	0.45
22:0:47:DG:H2''	22:0:48:DG:C8	2.51	0.45
23:1:-28:DC:N3	23:1:-27:DC:C4	2.85	0.45
3:C:53:ASN:ND2	3:C:59:ASP:OD1	2.47	0.45
15:N:-23:DT:C4	15:N:-22:DG:O6	2.70	0.45
19:b:38:ALA:O	19:b:43:VAL:N	2.46	0.45
8:H:94:TYR:HD2	8:H:143:ILE:HD12	1.80	0.45
12:L:60:LYS:HE3	12:L:60:LYS:HB3	1.81	0.45
14:T:26:DG:O6	15:N:-26:DC:N3	2.49	0.45
15:N:-19:DG:H2''	15:N:-18:DG:C8	2.51	0.45
20:g:64:GLU:HA	21:h:46:HIS:HE1	1.82	0.45
1:A:1146:LYS:NZ	2:B:254:ASP:OD2	2.38	0.44
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.53	0.44
17:W:409:ASP:OD2	17:W:413:PHE:HE2	2.00	0.44
14:T:31:DT:C2	14:T:32:DA:C5	3.05	0.44
15:N:34:DC:H6	15:N:34:DC:H2'	1.69	0.44
3:C:32:LEU:HD12	3:C:32:LEU:HA	1.83	0.44
15:N:-23:DT:C4	15:N:-22:DG:C6	3.06	0.44
2:B:688:GLU:OE2	2:B:740:HIS:NE2	2.38	0.44
3:C:38:ALA:HA	3:C:164:ALA:HB3	1.99	0.44
3:C:45:ILE:HA	3:C:159:ALA:HA	1.99	0.44
14:T:-18:DC:H1'	14:T:-17:DT:H5'	2.00	0.44
17:W:344:LEU:HD12	17:W:349:GLU:HB2	2.00	0.44
1:A:286:PRO:O	1:A:288:HIS:N	2.50	0.44
2:B:62:ALA:HB1	2:B:71:ILE:CG2	2.41	0.44
15:N:3:DC:H2''	15:N:4:DG:C8	2.52	0.44
16:V:59:ALA:N	17:W:262:ALA:O	2.50	0.44
1:A:599:LEU:HD13	8:H:123:CYS:HB2	1.98	0.44
4:D:23:GLU:HB3	7:G:82:PHE:HD1	1.83	0.44
21:h:78:ALA:O	21:h:82:LYS:N	2.50	0.44
15:N:-38:DT:H6	15:N:-38:DT:H3'	1.82	0.44
15:N:28:DA:H2''	15:N:29:DG:H8	1.82	0.44
17:W:442:PRO:HB2	17:W:447:LEU:CD1	2.48	0.44
2:B:71:ILE:HG12	2:B:73:LYS:HE3	2.00	0.44
18:a:41:TYR:HE2	18:a:45:THR:H	1.64	0.44
20:c:73:ASN:HB3	20:c:75:LYS:HD3	2.00	0.44
3:C:148:ARG:HG2	3:C:149:ASN:H	1.83	0.43
2:B:265:LEU:HD22	2:B:353:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:278:LYS:HB2	17:W:280:GLU:HG2	2.00	0.43
6:F:107:VAL:HG11	6:F:111:ILE:HD11	2.00	0.43
7:G:116:PRO:HD2	7:G:163:ILE:HG13	1.99	0.43
2:B:1073:TYR:HE2	3:C:179:GLU:HA	1.83	0.43
3:C:18:GLU:OE2	3:C:206:TYR:OH	2.34	0.43
15:N:15:DT:H2''	15:N:16:DA:C8	2.53	0.43
1:A:45:ARG:O	1:A:45:ARG:CG	2.59	0.43
2:B:64:HIS:O	2:B:64:HIS:CG	2.70	0.43
15:N:-40:DC:O5'	15:N:-40:DC:C6	2.70	0.43
1:A:1153:GLU:OE1	1:A:1196:ARG:NH1	2.44	0.43
14:T:23:DA:N6	15:N:-22:DG:H1	2.17	0.43
17:W:792:PRO:HG2	17:W:795:PHE:CD2	2.54	0.43
1:A:468:THR:OG1	1:A:470:ARG:NH1	2.52	0.43
15:N:-28:DC:H2''	15:N:-27:DC:C6	2.54	0.43
1:A:407:ILE:HG12	1:A:413:ARG:HG2	2.00	0.43
15:N:52:DC:H1'	15:N:53:DC:H5'	2.01	0.43
17:W:421:TYR:HA	17:W:425:PHE:O	2.19	0.43
22:O:38:DA:H2''	22:O:39:DA:C8	2.53	0.43
14:T:16:DA:C6	14:T:17:DA:C6	3.07	0.43
15:N:-22:DG:H4'	15:N:-22:DG:OP1	2.18	0.43
17:W:332:LYS:HE3	17:W:357:ARG:HB2	2.01	0.43
20:g:88:ARG:HB3	20:g:108:LEU:HD11	2.01	0.43
1:A:891:ASP:HA	1:A:941:ARG:HH12	1.83	0.43
5:E:189:LEU:HD11	5:E:195:VAL:HG13	2.01	0.43
14:T:-37:DG:H2''	14:T:-36:DT:C5	2.54	0.43
15:N:18:DG:OP1	18:a:64:LYS:N	2.52	0.43
7:G:91:VAL:HG23	7:G:139:LYS:HA	2.01	0.42
14:T:-13:DA:P	18:a:63:ARG:HH22	2.42	0.42
16:V:106:ARG:NH1	17:W:214:GLN:OE1	2.48	0.42
19:f:38:ALA:O	19:f:42:GLY:N	2.52	0.42
1:A:286:PRO:O	1:A:288:HIS:ND1	2.53	0.42
1:A:958:LEU:HD13	1:A:1023:LEU:HD22	2.01	0.42
2:B:70:ASN:HB2	2:B:128:ASP:O	2.18	0.42
16:V:59:ALA:O	17:W:261:SER:C	2.58	0.42
16:V:85:ARG:HD3	17:W:312:PRO:CA	2.48	0.42
17:W:258:GLU:OE1	17:W:278:LYS:CE	2.67	0.42
23:1:-31:DA:C5	23:1:-30:DA:N6	2.87	0.42
13:P:3:U:H2'	13:P:4:C:O4'	2.19	0.42
17:W:333:PHE:CD2	17:W:354:LEU:CD2	3.00	0.42
19:b:29:ILE:O	19:b:55:ARG:NH2	2.37	0.42
1:A:341:LEU:HD23	1:A:341:LEU:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1445:ASP:HB3	1:A:1447:MET:HE3	2.01	0.42
2:B:436:ASN:O	2:B:438:ASN:N	2.48	0.42
2:B:756:ILE:HG12	2:B:770:GLN:HG2	2.02	0.42
5:E:116:THR:CG2	15:N:-18:DG:OP1	2.68	0.42
16:V:59:ALA:N	17:W:262:ALA:H	2.18	0.42
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.77	0.42
7:G:115:ILE:HG23	7:G:163:ILE:HD11	2.01	0.42
16:V:67:TRP:CE3	17:W:306:TYR:CD2	3.07	0.42
19:b:87:VAL:HG11	19:b:102:GLY:HA3	2.02	0.42
20:c:17:ARG:O	20:c:21:ALA:N	2.50	0.42
20:g:17:ARG:HA	20:g:20:ARG:HB2	2.00	0.42
2:B:190:MET:SD	2:B:190:MET:N	2.86	0.42
2:B:336:ILE:H	2:B:341:ARG:HH21	1.67	0.42
14:T:23:DA:H2''	14:T:24:DA:H1'	1.83	0.42
18:a:117:VAL:HG11	19:b:44:LYS:HD3	2.01	0.42
1:A:841:ARG:NE	1:A:1387:ILE:O	2.44	0.42
16:V:15:CYS:HB3	16:V:32:CYS:SG	2.59	0.42
17:W:352:LEU:HD11	17:W:435:LEU:CD2	2.49	0.42
18:a:94:GLU:OE2	20:g:104:GLN:N	2.52	0.42
19:b:52:GLU:OE2	19:b:55:ARG:NH1	2.53	0.42
19:b:65:VAL:HG13	19:b:90:LEU:HD21	2.01	0.42
19:b:90:LEU:HD23	19:b:90:LEU:HA	1.78	0.42
1:A:168:CYS:SG	1:A:170:ASN:ND2	2.93	0.42
1:A:615:PHE:HB3	8:H:121:LEU:HD21	2.01	0.42
15:N:-42:DG:H2''	15:N:-41:DT:C6	2.55	0.42
15:N:-25:DC:C2'	15:N:-24:DT:OP2	2.68	0.42
15:N:62:DG:H1'	15:N:63:DG:H5'	2.01	0.42
17:W:344:LEU:HD11	17:W:349:GLU:HB2	2.00	0.42
18:a:54:TYR:HD2	19:b:39:ARG:HB2	1.84	0.42
20:g:102:ILE:HG23	21:h:58:ILE:HG21	2.02	0.42
1:A:781:ALA:N	2:B:696:GLU:OE2	2.45	0.42
2:B:101:PRO:HG2	2:B:172:LEU:HD11	2.01	0.42
4:D:61:ARG:NH1	4:D:86:ASP:OD1	2.52	0.42
15:N:-16:DT:H1'	15:N:-15:DA:C4	2.55	0.42
19:f:32:PRO:HA	19:f:35:ARG:HB2	2.01	0.42
2:B:251:GLY:HA2	2:B:256:GLY:HA3	2.02	0.42
2:B:761:HIS:HB2	2:B:1024:ALA:HB2	2.01	0.42
6:F:89:GLU:OE2	6:F:136:ARG:NE	2.51	0.42
14:T:4:DC:N4	15:N:-5:DG:O6	2.53	0.42
21:h:85:THR:OG1	21:h:86:ILE:N	2.52	0.42
1:A:883:THR:O	1:A:1027:ARG:NH2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1263:LEU:HD12	1:A:1263:LEU:HA	1.93	0.41
2:B:154:ASN:OD1	2:B:155:LYS:N	2.45	0.41
6:F:79:ARG:NH1	6:F:150:GLU:OE2	2.48	0.41
10:J:63:ASN:HA	10:J:64:PRO:HD2	1.89	0.41
15:N:23:DG:H1'	15:N:24:DC:H5'	2.02	0.41
15:N:25:DT:H2''	15:N:26:DA:N7	2.35	0.41
20:g:34:LEU:HA	20:g:39:TYR:CD2	2.55	0.41
2:B:290:LEU:HD22	9:I:6:PHE:HZ	1.85	0.41
3:C:66:LEU:HD11	3:C:155:ILE:HD12	2.02	0.41
9:I:84:VAL:HG22	9:I:104:LEU:HD21	2.01	0.41
13:P:1:U:H5'	13:P:1:U:H6	1.85	0.41
14:T:31:DT:N3	14:T:32:DA:N6	2.67	0.41
17:W:265:ARG:HA	17:W:265:ARG:HD2	1.71	0.41
18:e:118:THR:HG23	19:f:45:ARG:HG2	2.02	0.41
5:E:131:ILE:HA	5:E:131:ILE:HD13	1.77	0.41
13:P:3:U:H3	14:T:41:DA:H61	1.68	0.41
15:N:4:DG:H2''	15:N:5:DT:C5	2.55	0.41
16:V:57:LEU:C	17:W:240:VAL:HG11	2.45	0.41
20:c:78:ILE:HB	21:d:51:ILE:HG13	2.03	0.41
1:A:1444:PHE:CZ	6:F:89:GLU:HA	2.55	0.41
2:B:71:ILE:O	2:B:73:LYS:HG3	2.20	0.41
14:T:-25:DA:C2	15:N:25:DT:C2	3.08	0.41
14:T:-23:DC:OP2	18:a:72:ARG:NH2	2.49	0.41
16:V:84:VAL:HG22	17:W:310:LEU:CD2	2.49	0.41
20:g:40:SER:OG	20:g:42:ARG:O	2.33	0.41
1:A:181:LYS:HB3	1:A:202:LEU:HD11	2.03	0.41
13:P:2:G:H2'	13:P:3:U:C6	2.56	0.41
14:T:-48:DC:H2''	14:T:-47:DT:H5'	2.03	0.41
17:W:228:GLY:HA3	17:W:299:PHE:CZ	2.55	0.41
18:a:48:LEU:HD11	20:g:115:LEU:HB3	2.03	0.41
19:b:26:ILE:HD11	19:b:55:ARG:HB3	2.01	0.41
23:1:-31:DA:C2	23:1:-30:DA:C6	3.08	0.41
1:A:551:LEU:HD23	1:A:551:LEU:HA	1.89	0.41
1:A:1356:LEU:HD13	1:A:1371:MET:HE1	2.03	0.41
4:D:106:LEU:O	4:D:110:ASN:N	2.53	0.41
9:I:15:TYR:N	9:I:28:SER:O	2.37	0.41
15:N:-16:DT:C4'	15:N:-15:DA:H5'	2.46	0.41
18:e:42:ARG:HA	18:e:43:PRO:HD3	1.88	0.41
19:f:47:SER:OG	19:f:48:GLY:N	2.38	0.41
1:A:84:MET:HE2	1:A:271:LEU:HD13	2.03	0.41
2:B:1212:ILE:HD13	2:B:1212:ILE:HA	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:114:LEU:HD13	7:G:162:SER:HB2	2.03	0.41
15:N:21:DG:H2'	15:N:22:DT:H71	2.01	0.41
17:W:332:LYS:NZ	17:W:357:ARG:O	2.30	0.41
17:W:352:LEU:HD21	17:W:435:LEU:CD1	2.50	0.41
1:A:240:LEU:HD12	1:A:240:LEU:HA	1.87	0.41
1:A:447:ARG:HB2	1:A:488:MET:HG2	2.03	0.41
1:A:970:GLN:HA	1:A:975:LEU:HB2	2.03	0.41
2:B:1073:TYR:CE1	2:B:1080:LYS:HG2	2.55	0.41
4:D:169:VAL:C	4:D:171:LEU:H	2.28	0.41
7:G:104:GLY:HA3	7:G:105:PRO:HD3	1.96	0.41
7:G:152:THR:HA	7:G:157:ILE:HG22	2.02	0.41
9:I:13:MET:HE3	9:I:13:MET:HB2	1.89	0.41
9:I:96:ASN:OD1	9:I:97:MET:N	2.48	0.41
13:P:3:U:H3	14:T:41:DA:N6	2.18	0.41
15:N:-42:DG:H2''	15:N:-41:DT:O5'	2.21	0.41
15:N:-7:DG:H2''	15:N:-6:DG:N7	2.35	0.41
15:N:7:DC:H5'	19:b:45:ARG:HH21	1.86	0.41
17:W:229:VAL:HG21	17:W:286:LEU:HD11	2.03	0.41
18:a:109:LEU:HD23	18:a:109:LEU:HA	1.89	0.41
23:1:-50:DT:H2''	23:1:-49:DG:C8	2.55	0.41
1:A:262:ASP:OD1	1:A:317:GLN:NE2	2.54	0.41
2:B:371:LEU:HA	2:B:371:LEU:HD23	1.76	0.41
2:B:839:MET:HE2	2:B:839:MET:HB3	1.91	0.41
2:B:840:ILE:HG12	2:B:992:VAL:HG12	2.03	0.41
3:C:125:GLY:HA2	3:C:126:ASN:HA	1.76	0.41
1:A:474:SER:OG	1:A:651:GLN:NE2	2.54	0.40
3:C:143:LEU:HG	10:J:2:ILE:HD11	2.03	0.40
14:T:-14:DA:H2''	14:T:-13:DA:C8	2.55	0.40
14:T:29:DA:H2'	14:T:30:DT:C7	2.51	0.40
15:N:24:DC:C2'	15:N:25:DT:C7	2.97	0.40
15:N:42:DA:H2''	15:N:43:DA:C8	2.56	0.40
16:V:67:TRP:HZ2	17:W:219:PRO:CD	2.33	0.40
16:V:73:ARG:NH2	17:W:217:LEU:HD12	2.34	0.40
17:W:322:ARG:CD	17:W:342:GLU:HG3	2.51	0.40
17:W:784:ASN:HB2	17:W:785:PRO:HD3	2.02	0.40
2:B:119:MET:O	2:B:153:GLY:N	2.53	0.40
2:B:833:TYR:HD2	2:B:992:VAL:HG11	1.86	0.40
3:C:63:SER:HA	3:C:66:LEU:HD12	2.03	0.40
17:W:322:ARG:CD	17:W:342:GLU:HA	2.51	0.40
17:W:357:ARG:O	17:W:389:PRO:CG	2.67	0.40
2:B:649:LYS:HE2	2:B:649:LYS:HB3	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:-42:DG:C4'	15:N:-41:DT:O5'	2.69	0.40
17:W:409:ASP:HB3	17:W:413:PHE:CD2	2.50	0.40
19:f:75:HIS:NE2	21:h:90:GLU:HG3	2.37	0.40
1:A:122:MET:HE3	1:A:126:ILE:HD11	2.02	0.40
2:B:293:ILE:HG12	2:B:372:GLY:HA2	2.04	0.40
15:N:-15:DA:C5	15:N:-14:DA:C6	3.09	0.40
2:B:262:LYS:HA	2:B:273:PRO:HA	2.03	0.40
2:B:285:PRO:HB2	9:I:11:ASN:HB3	2.04	0.40
15:N:-26:DC:H2''	15:N:-25:DC:C6	2.56	0.40
15:N:-26:DC:C2	15:N:-25:DC:C4	3.09	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	1402/1743 (80%)	1345 (96%)	47 (3%)	10 (1%)	18	55
2	B	1145/1227 (93%)	1081 (94%)	56 (5%)	8 (1%)	18	55
3	C	261/304 (86%)	253 (97%)	6 (2%)	2 (1%)	16	53
4	D	162/186 (87%)	149 (92%)	9 (6%)	4 (2%)	4	26
5	E	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
6	F	82/155 (53%)	80 (98%)	2 (2%)	0	100	100
7	G	169/171 (99%)	160 (95%)	7 (4%)	2 (1%)	10	43
8	H	129/145 (89%)	125 (97%)	2 (2%)	2 (2%)	7	37
9	I	109/115 (95%)	102 (94%)	6 (6%)	1 (1%)	14	49
10	J	64/72 (89%)	61 (95%)	2 (3%)	1 (2%)	7	37
11	K	111/118 (94%)	110 (99%)	1 (1%)	0	100	100
12	L	43/72 (60%)	42 (98%)	0	1 (2%)	5	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	V	100/108 (93%)	97 (97%)	3 (3%)	0	100	100
17	W	265/911 (29%)	246 (93%)	17 (6%)	2 (1%)	16	53
18	a	95/139 (68%)	85 (90%)	10 (10%)	0	100	100
18	e	95/139 (68%)	86 (90%)	9 (10%)	0	100	100
19	b	78/106 (74%)	74 (95%)	4 (5%)	0	100	100
19	f	76/106 (72%)	69 (91%)	7 (9%)	0	100	100
20	c	101/133 (76%)	92 (91%)	9 (9%)	0	100	100
20	g	103/133 (77%)	94 (91%)	9 (9%)	0	100	100
21	d	93/129 (72%)	91 (98%)	2 (2%)	0	100	100
21	h	89/129 (69%)	87 (98%)	2 (2%)	0	100	100
All	All	4983/6555 (76%)	4736 (95%)	214 (4%)	33 (1%)	20	55

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	GLU
1	A	287	GLN
1	A	960	VAL
1	A	1109	VAL
2	B	155	LYS
2	B	239	SER
2	B	337	ARG
3	C	89	ASP
7	G	134	ASP
8	H	108	GLU
12	L	44	LYS
17	W	320	LEU
1	A	284	GLY
1	A	977	ARG
1	A	1223	SER
2	B	62	ALA
2	B	177	GLU
2	B	299	ASP
4	D	169	VAL
4	D	171	LEU
7	G	154	VAL
8	H	18	GLY
1	A	979	LYS

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Mol	Chain	Res	Type
4	D	10	ALA
4	D	164	ALA
9	I	56	ALA
1	A	47	ARG
3	C	217	GLU
1	A	43	GLU
2	B	437	LEU
2	B	238	GLY
10	J	64	PRO
17	W	806	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	1227/1528 (80%)	1221 (100%)	6 (0%)	81	82
2	B	1012/1077 (94%)	1002 (99%)	10 (1%)	68	76
3	C	236/264 (89%)	236 (100%)	0	100	100
4	D	143/160 (89%)	140 (98%)	3 (2%)	47	65
5	E	196/197 (100%)	195 (100%)	1 (0%)	81	82
6	F	75/137 (55%)	75 (100%)	0	100	100
7	G	148/148 (100%)	148 (100%)	0	100	100
8	H	120/130 (92%)	118 (98%)	2 (2%)	53	68
9	I	106/109 (97%)	106 (100%)	0	100	100
10	J	60/66 (91%)	60 (100%)	0	100	100
11	K	104/109 (95%)	104 (100%)	0	100	100
12	L	38/56 (68%)	37 (97%)	1 (3%)	40	61
16	V	86/92 (94%)	85 (99%)	1 (1%)	63	74
17	W	241/796 (30%)	235 (98%)	6 (2%)	42	62
18	a	83/112 (74%)	82 (99%)	1 (1%)	63	74
18	e	82/112 (73%)	81 (99%)	1 (1%)	63	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	b	65/81 (80%)	64 (98%)	1 (2%)	57	71
19	f	63/81 (78%)	63 (100%)	0	100	100
20	c	82/102 (80%)	82 (100%)	0	100	100
20	g	83/102 (81%)	83 (100%)	0	100	100
21	d	81/107 (76%)	80 (99%)	1 (1%)	63	74
21	h	77/107 (72%)	77 (100%)	0	100	100
All	All	4408/5673 (78%)	4374 (99%)	34 (1%)	70	78

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	ARG
1	A	248	ARG
1	A	473	LEU
1	A	661	ASN
1	A	977	ARG
1	A	1459	ASP
2	B	69	ASP
2	B	70	ASN
2	B	71	ILE
2	B	233	SER
2	B	428	CYS
2	B	466	MET
2	B	500	LYS
2	B	578	VAL
2	B	582	ILE
2	B	618	LYS
4	D	19	VAL
4	D	116	LYS
4	D	171	LEU
5	E	131	ILE
8	H	111	ILE
8	H	122	MET
12	L	62	ARG
16	V	33	ASP
17	W	246	LYS
17	W	264	GLN
17	W	278	LYS
17	W	313	VAL
17	W	342	GLU

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Mol	Chain	Res	Type
17	W	343	VAL
18	a	74	ILE
19	b	72	TYR
21	d	77	LEU
18	e	84	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	287	GLN
1	A	340	ASN
1	A	400	HIS
1	A	446	ASN
1	A	452	HIS
1	A	563	GLN
1	A	651	GLN
1	A	661	ASN
1	A	1190	GLN
1	A	1261	GLN
1	A	1435	GLN
2	B	735	HIS
2	B	842	ASN
2	B	887	HIS
2	B	1062	ASN
2	B	1097	HIS
2	B	1174	ASN
3	C	8	ASN
3	C	13	GLN
3	C	126	ASN
3	C	188	HIS
3	C	242	GLN
4	D	179	ASN
5	E	4	ASN
5	E	51	ASN
5	E	94	ASN
5	E	112	GLN
5	E	120	ASN
5	E	145	HIS
5	E	193	GLN
7	G	21	GLN
7	G	125	ASN

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Mol	Chain	Res	Type
8	H	13	GLN
8	H	136	GLN
9	I	90	GLN
9	I	105	ASN
17	W	330	ASN
17	W	339	GLN
17	W	402	HIS
17	W	434	ASN
17	W	784	ASN
18	a	108	ASN
20	c	24	GLN
21	d	60	ASN
21	d	64	ASN
18	e	68	GLN
20	g	31	HIS
20	g	112	GLN
21	h	64	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	P	15/16 (93%)	6 (40%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	P	-4	C
13	P	-3	C
13	P	-1	G
13	P	0	G
13	P	1	U
13	P	3	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 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.

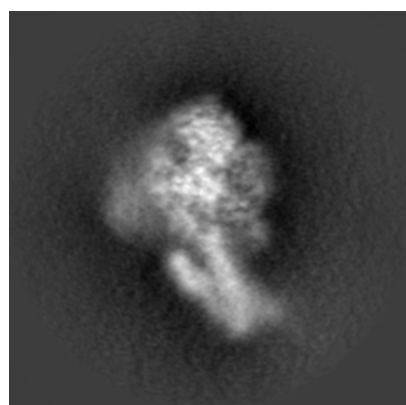
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0675. These allow visual inspection of the internal detail of the map and identification of artifacts.

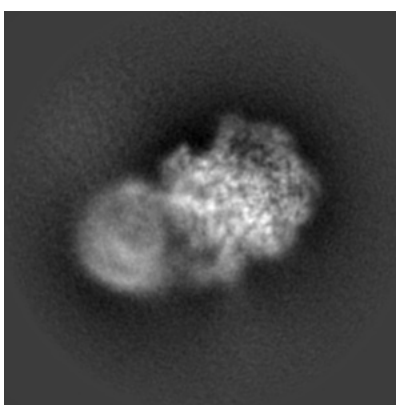
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

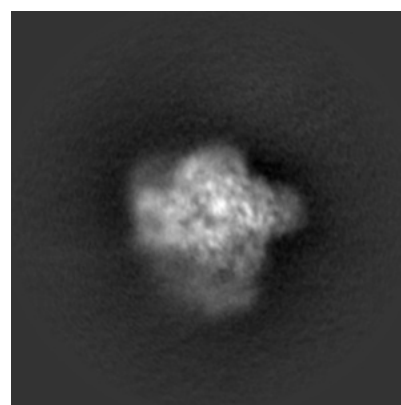
6.1.1 Primary map



X



Y

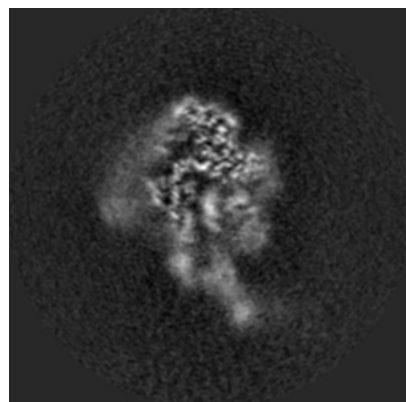


Z

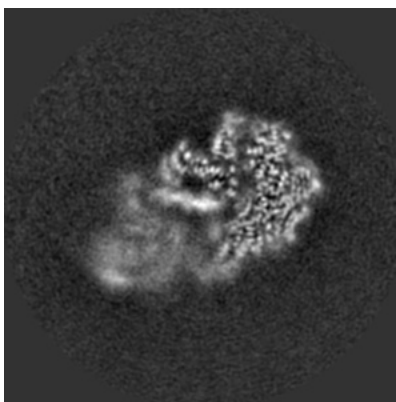
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

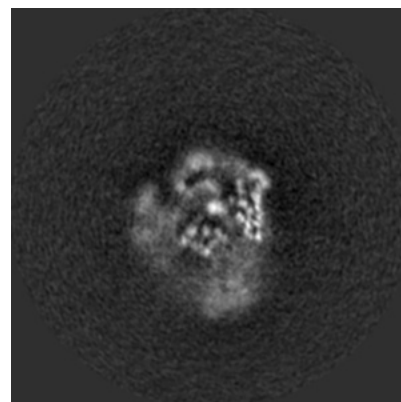
6.2.1 Primary map



X Index: 120



Y Index: 120

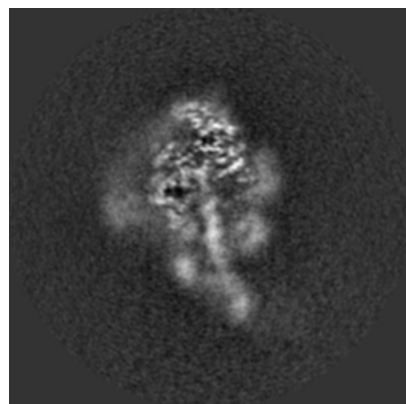


Z Index: 120

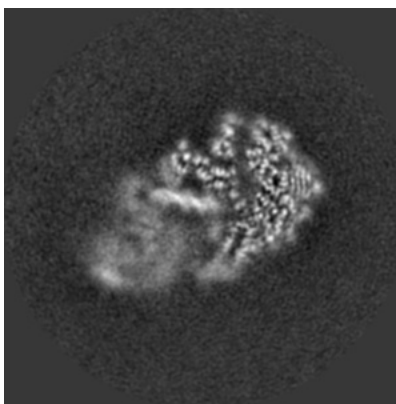
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

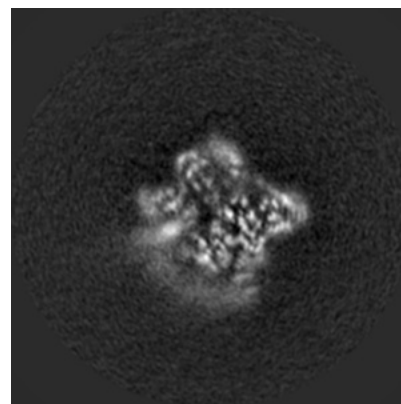
6.3.1 Primary map



X Index: 125



Y Index: 122

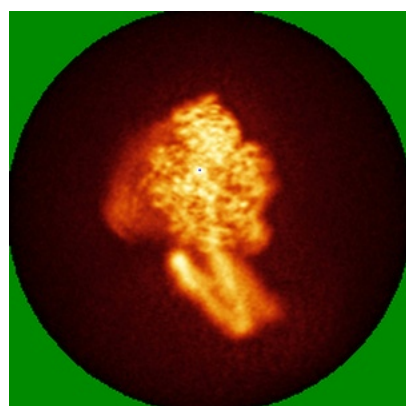


Z Index: 133

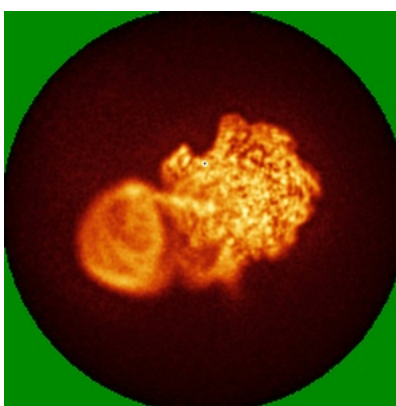
The images above show the largest variance slices of the map in three orthogonal directions.

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

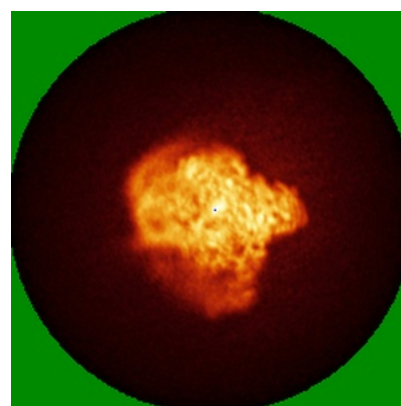
6.4.1 Primary map



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

This section was not generated.

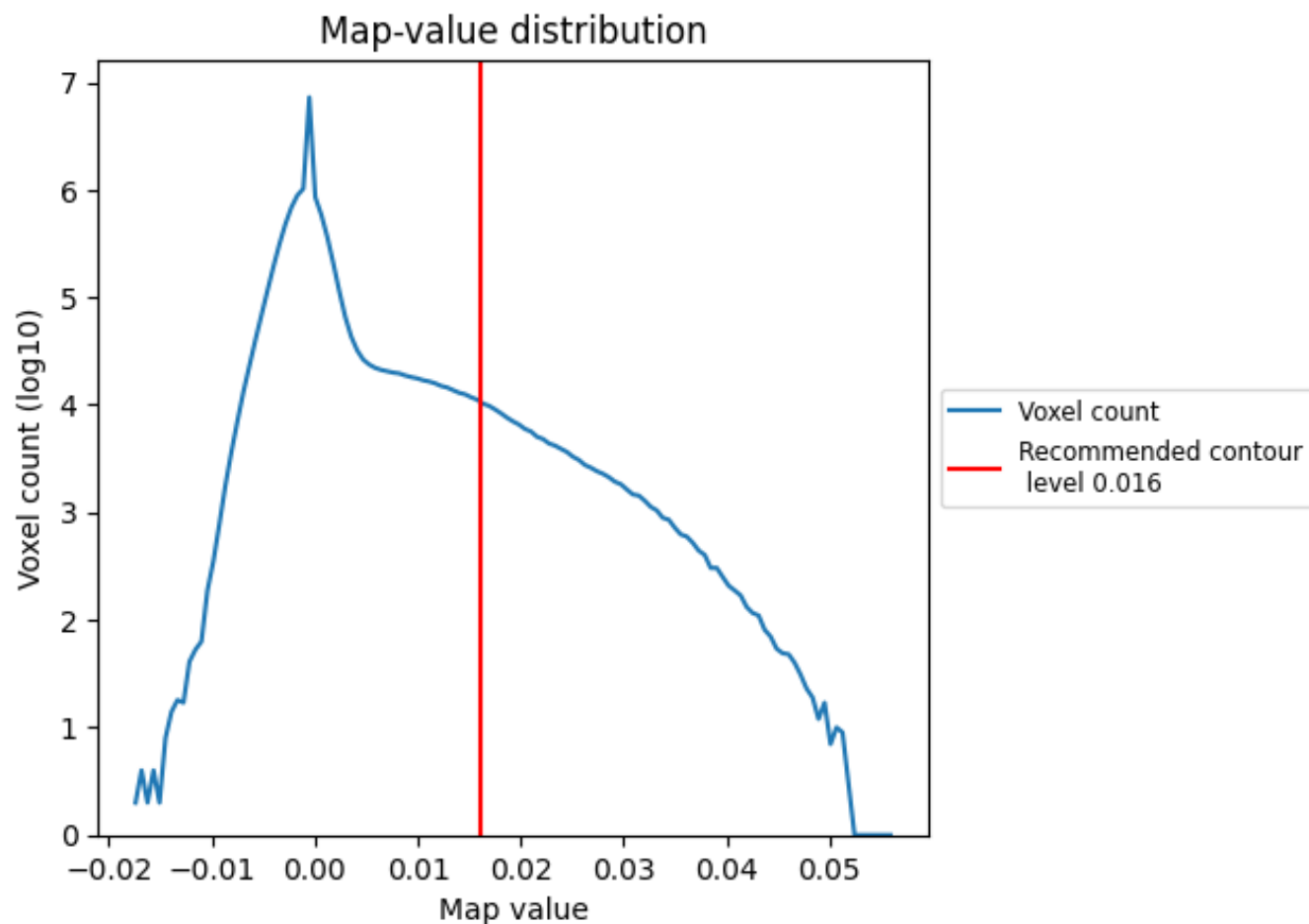
6.6 Mask visualisation

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

7 Map analysis [i](#)

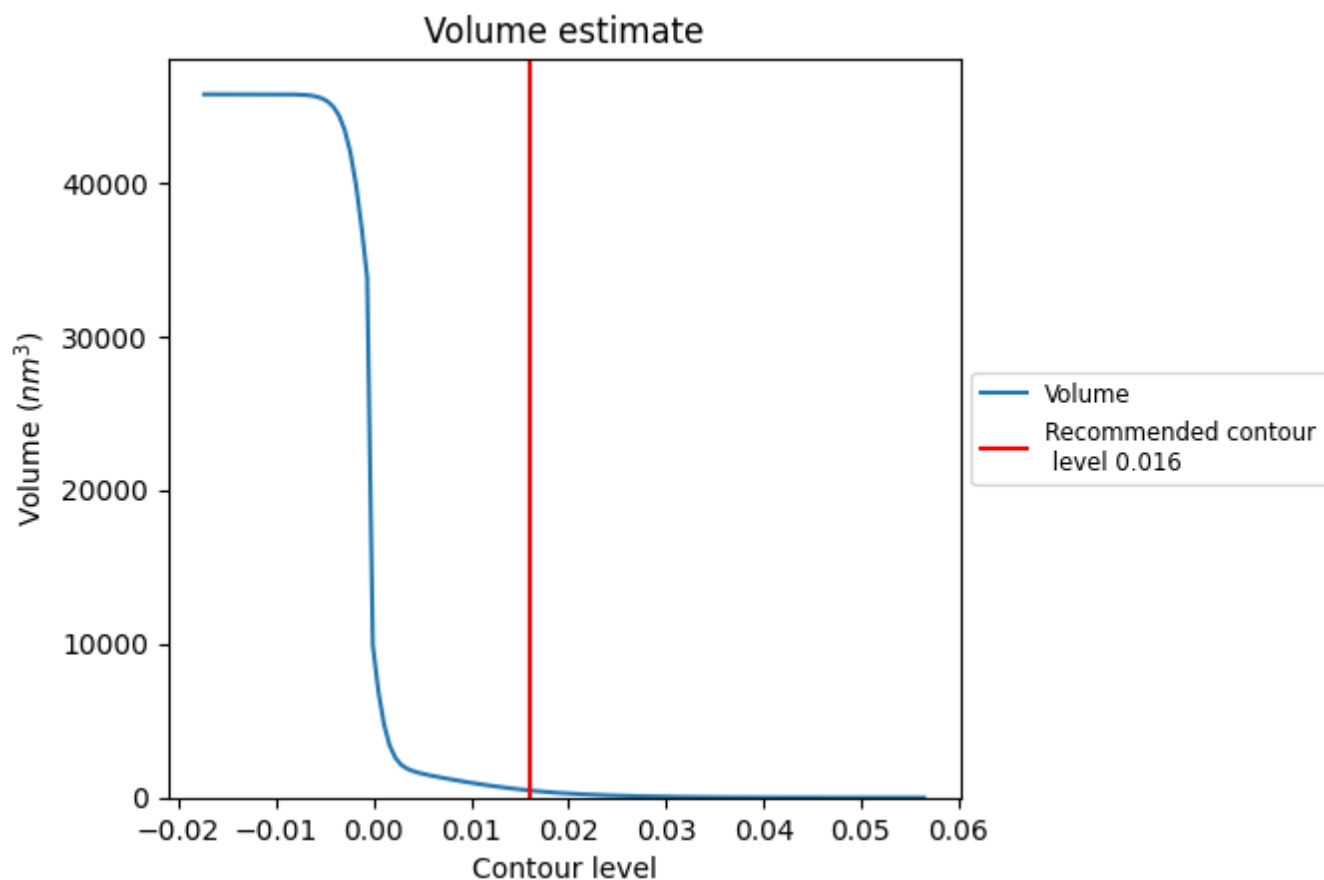
This section contains the results of statistical analysis of the map.

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.

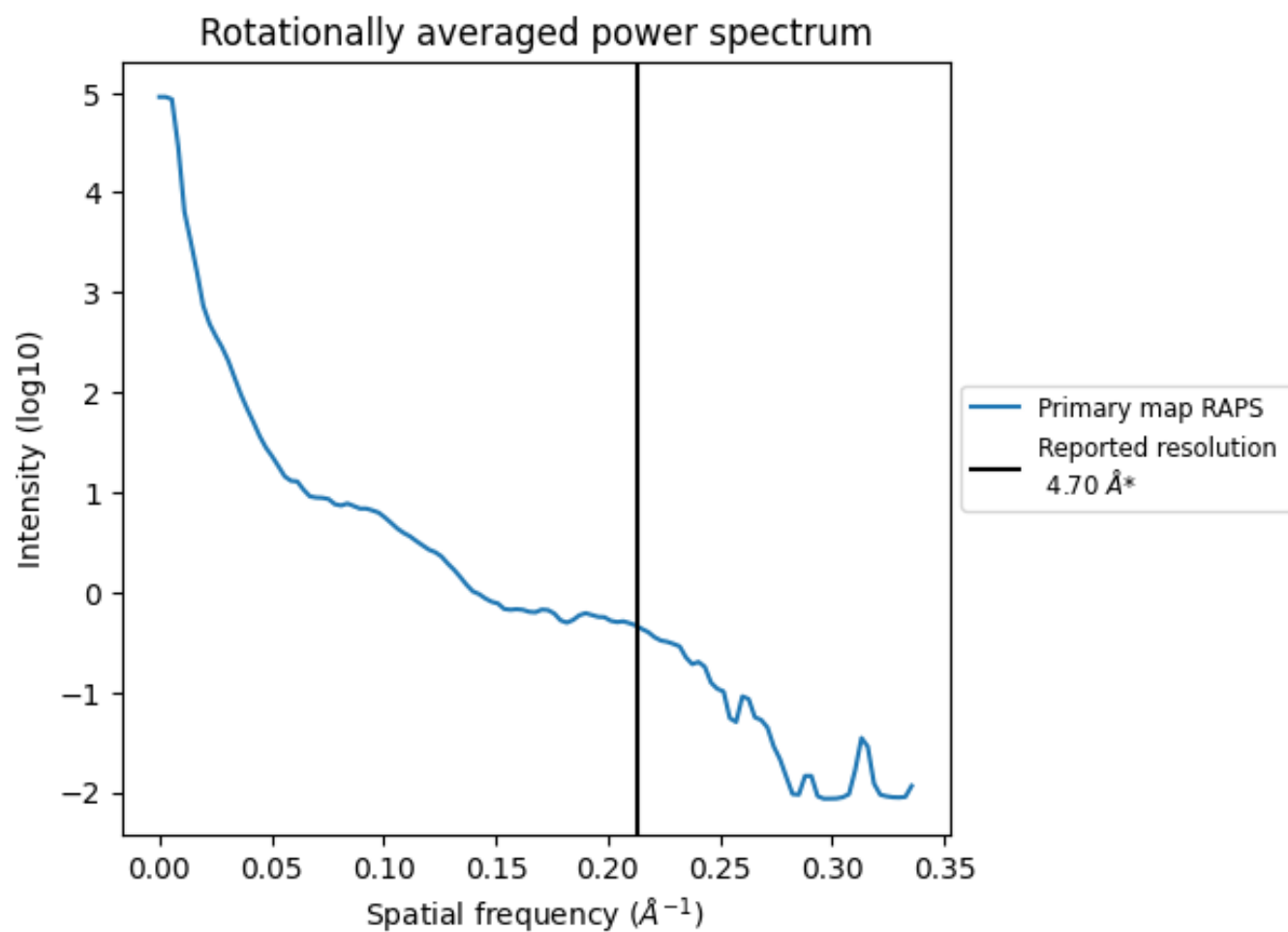
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 464 nm³; this corresponds to an approximate mass of 419 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 ⓘ

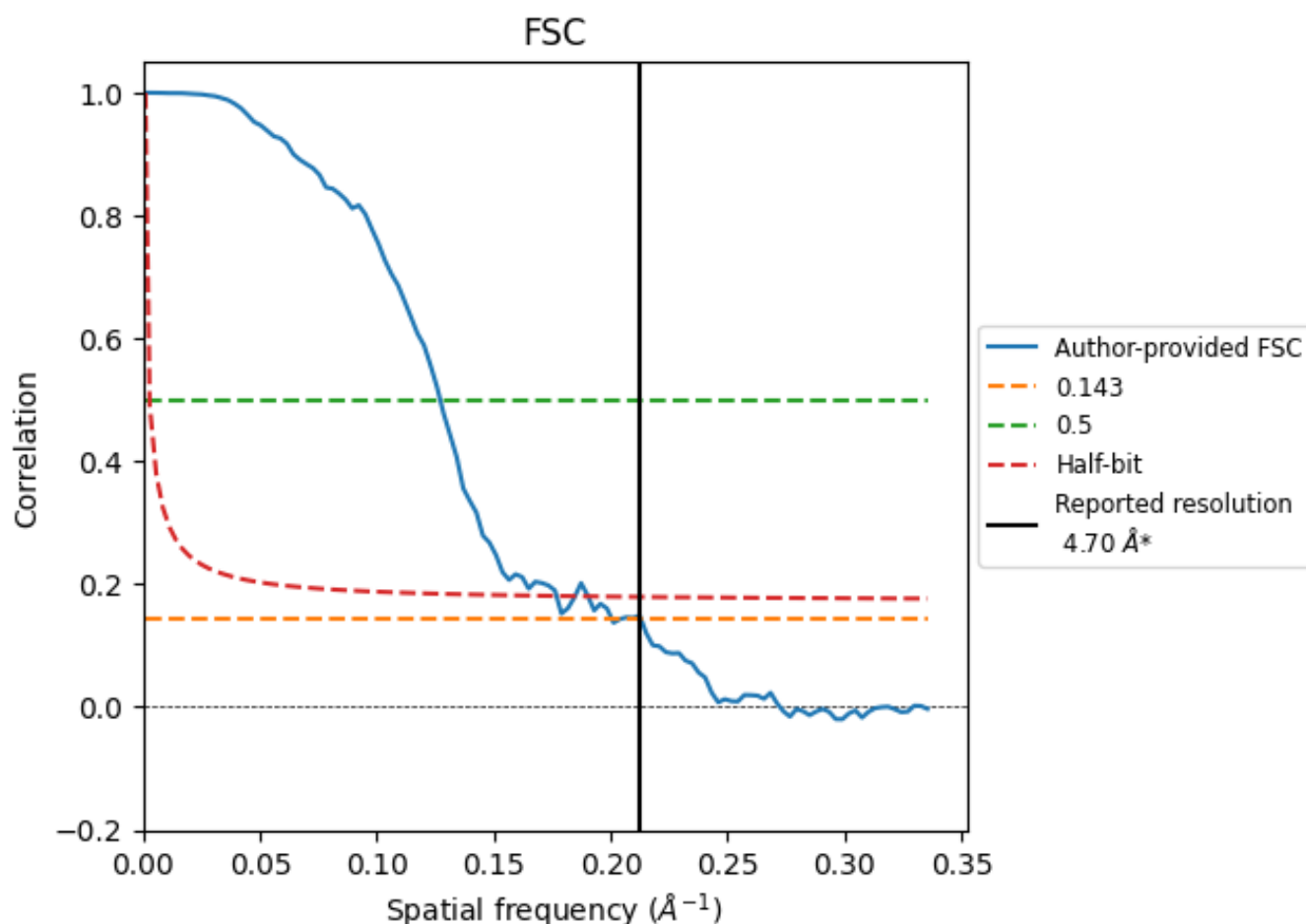


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

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 0.213 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

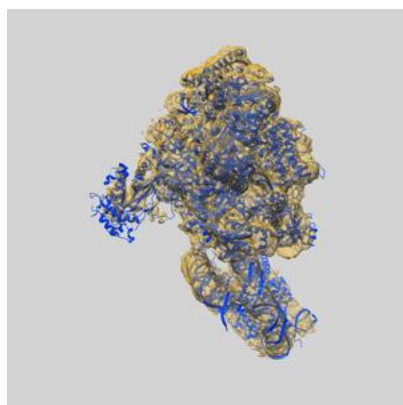
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.99	7.86	5.66
Unmasked-calculated*	-	-	-

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

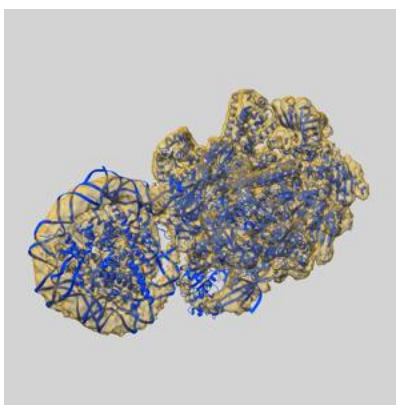
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0675 and PDB model 6J50. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

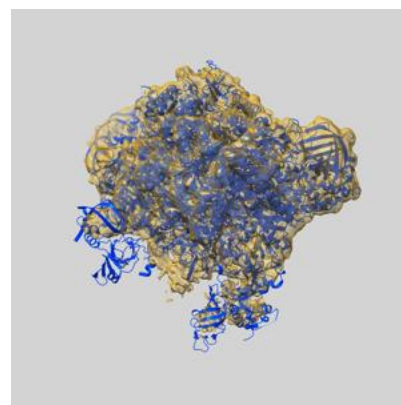
9.1 Map-model overlay [i](#)



X



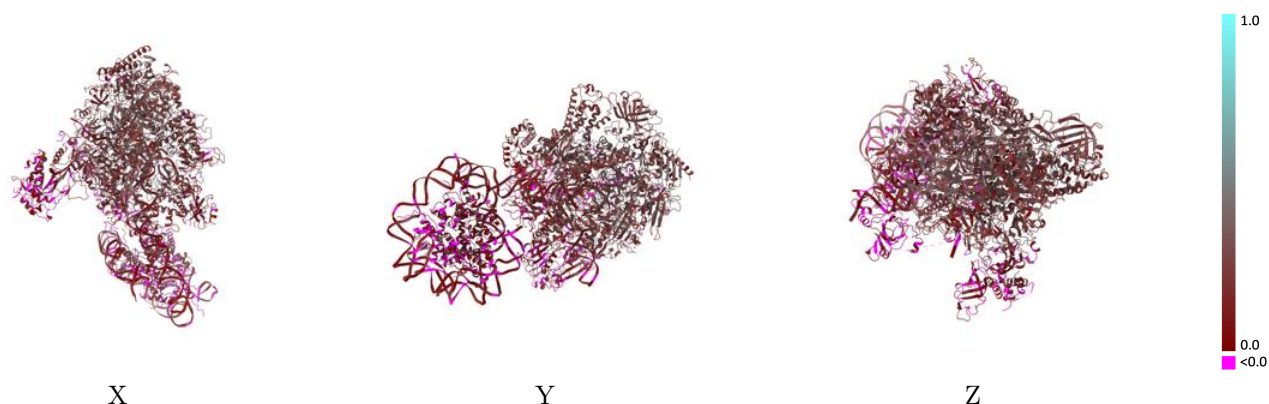
Y



Z

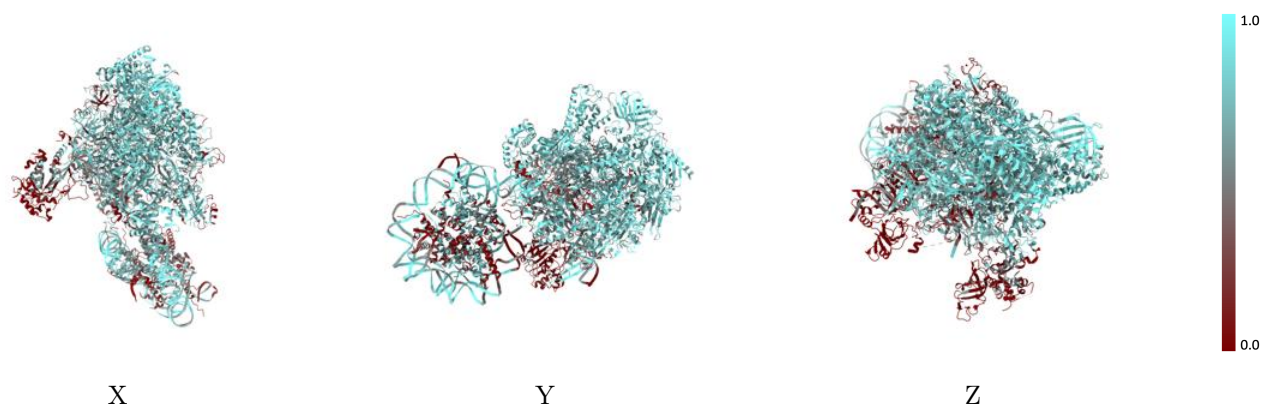
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



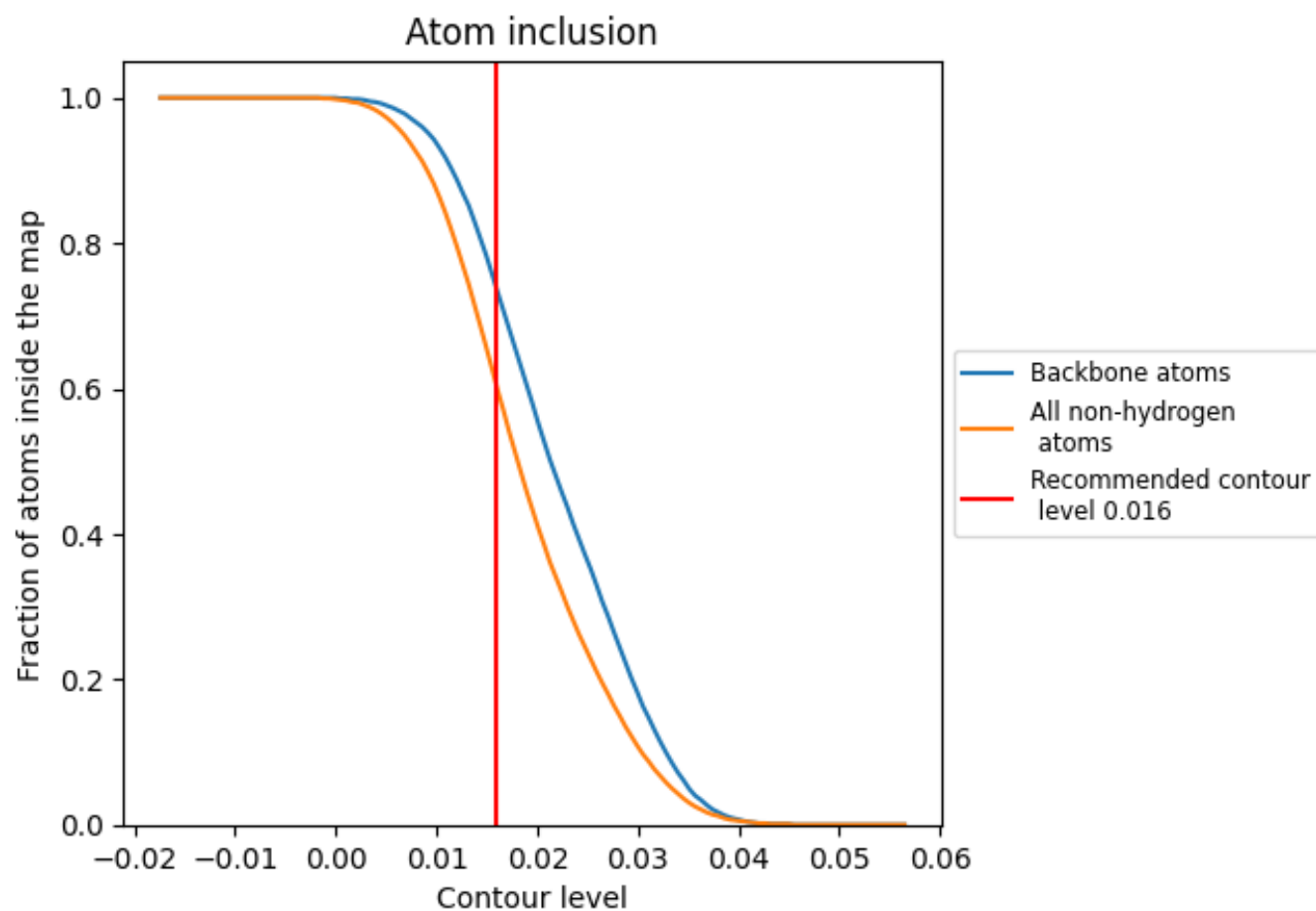
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 60% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6020	 0.1950
0	 0.5140	 0.0670
1	 0.4870	 0.0400
A	 0.6750	 0.2600
B	 0.6900	 0.2670
C	 0.7930	 0.2900
D	 0.1350	 0.0710
E	 0.7630	 0.2550
F	 0.7630	 0.2760
G	 0.3210	 0.1350
H	 0.8380	 0.2910
I	 0.3960	 0.1190
J	 0.7720	 0.2650
K	 0.7220	 0.2690
L	 0.7300	 0.2360
N	 0.7250	 0.1120
P	 0.7510	 0.1950
T	 0.7450	 0.1280
V	 0.1220	 0.0580
W	 0.0840	 0.0770
a	 0.4400	 0.0490
b	 0.4740	 0.0700
c	 0.5550	 0.0940
d	 0.5030	 0.1010
e	 0.5140	 0.1080
f	 0.5360	 0.0940
g	 0.3430	 0.0630
h	 0.4160	 0.0960

