



Full wwPDB EM Validation Report ⓘ

Jul 25, 2026 – 08:10 am BST

PDB ID : 30FH / pdb_000030fh
EMDB ID : EMD-57693
Title : RNA polymerase II initially transcribing complex with a 6-nt RNA and the +1 nucleosome
Authors : Zhan, Y.; Abril-Garrido, J.; Grabbe, F.; Seweryn, P.; Neef, U.; Dienemann, C.; Cramer, P.
Deposited on : 2026-04-22
Resolution : 7.60 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.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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) : 2.50

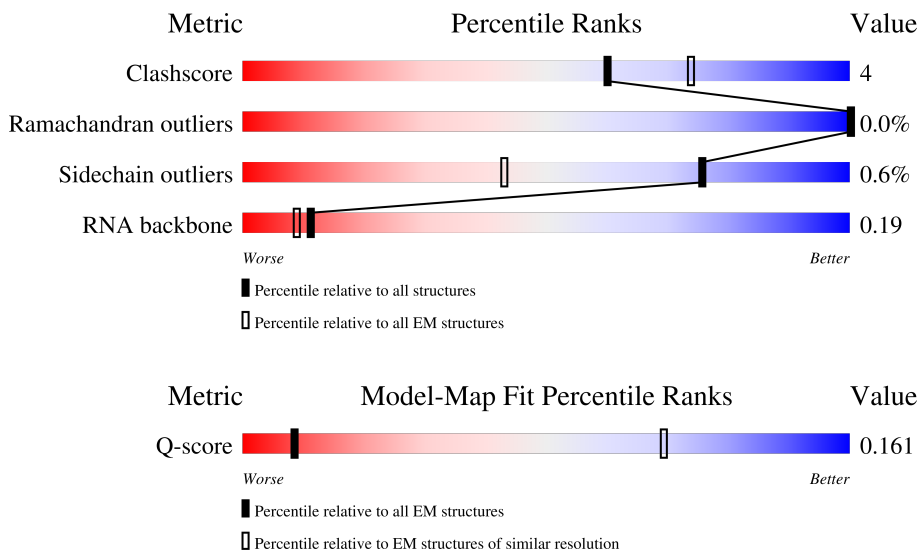
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.60 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	389 (7.10 - 8.10)

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	0	782	
2	1	760	
3	2	548	

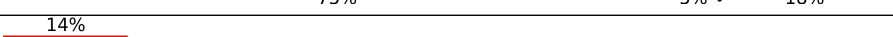
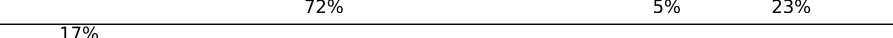
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Mol	Chain	Length	Quality of chain
4	3	462	
5	4	395	
6	5	308	
7	6	71	
8	7	309	
9	A	1984	
10	B	1300	
11	C	275	
12	D	184	
13	E	210	
14	F	127	
15	G	172	
16	H	150	
17	I	125	
18	J	67	
19	K	117	
20	L	58	
21	M	316	
22	N	236	
23	O	339	
24	P	6	
25	Q	517	
26	R	249	
27	T	236	
28	U	376	

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Mol	Chain	Length	Quality of chain
29	V	109	
30	W	439	
31	X	291	
32	a	136	
32	e	136	
33	b	103	
33	f	103	
34	c	130	
34	g	130	
35	d	126	
35	h	126	

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 80807 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 General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	605	Total	C	N	O	S	0	0
			4890	3127	848	885	30		

- Molecule 2 is a protein called TFIIH basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	714	Total	C	N	O	S	0	0
			5751	3683	999	1040	29		

- Molecule 3 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	371	Total	C	N	O	S	0	0
			3016	1922	529	549	16		

- Molecule 4 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	421	Total	C	N	O	S	0	0
			3338	2154	584	587	13		

- Molecule 5 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	347	Total	C	N	O	S	0	0
			2732	1726	471	508	27		

- Molecule 6 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	263	Total	C	N	O	S	0	0
			2066	1323	344	380	19		

- Molecule 7 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	69	Total	C	N	O	S	0	0
			549	352	88	106	3		

- Molecule 8 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	149	Total	C	N	O	S	0	0
			1225	763	212	240	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	1421	Total	C	N	O	S	0	0
			11257	7083	2013	2089	72		

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	1121	Total	C	N	O	S	0	0
			8971	5675	1574	1658	64		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 12 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	128	Total	C	N	O	S	0	0
			1050	656	178	212	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	79	Total	C	N	O	S	0	0
			636	406	108	117	5		

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	114	Total	C	N	O	S	0	0
			928	571	166	180	11		

- Molecule 18 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 19 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 20 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	44	Total	C	N	O	S	0	0
			373	231	72	64	6		

- Molecule 21 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	292	Total	C	N	O	S	0	0
			2253	1403	402	430	18		

- Molecule 22 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	209	Total	C	N	O	P	0	0
			4293	2031	807	1246	209		

- Molecule 23 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	179	Total	C	N	O	S	0	0
			1422	923	251	241	7		

- Molecule 24 is a RNA chain called RNA (5'-R(P*AP*CP*AP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	6	Total	C	N	O	P	0	0
			124	56	22	40	6		

- Molecule 25 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	138	Total	C	N	O	S	0	0
			1138	719	208	208	3		

- Molecule 26 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 27 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	219	Total	C	N	O	P	0	0
			4487	2128	821	1320	218		

- Molecule 28 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	113	Total	C	N	O	S	0	0
			931	585	152	190	4		

- Molecule 29 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 30 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	187	Total	C	N	O	S	0	0
			1535	964	275	285	11		

- Molecule 31 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X	171	Total	C	N	O	S	0	0
			1403	895	243	261	4		

- Molecule 32 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	97	Total	C	N	O	S	0	0
			802	506	155	138	3		
32	e	98	Total	C	N	O	S	0	0
			811	512	157	139	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	103	ALA	GLY	engineered mutation	UNP P84233
e	103	ALA	GLY	engineered mutation	UNP P84233

- Molecule 33 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	82	Total	C	N	O	S	0	0
			653	412	127	113	1		
33	f	80	Total	C	N	O	S	0	0
			638	401	125	111	1		

- Molecule 34 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	c	109	Total	C	N	O	0	0
			843	531	167	145		
34	g	106	Total	C	N	O	0	0
			818	516	160	142		

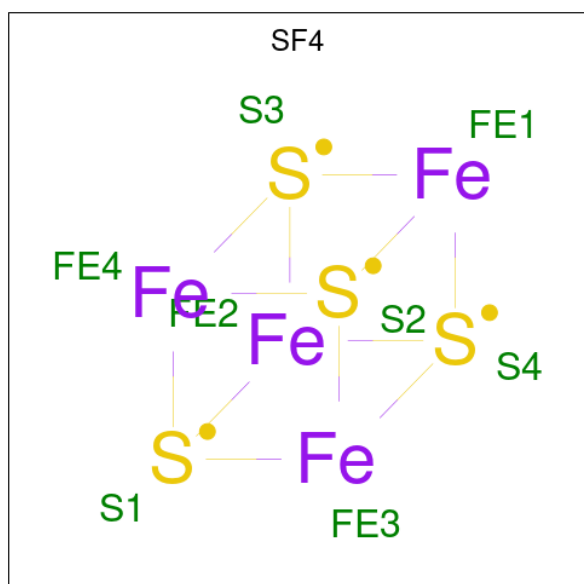
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	100	ARG	GLY	engineered mutation	UNP P06897
g	100	ARG	GLY	engineered mutation	UNP P06897

- Molecule 35 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	97	Total	C	N	O	S	0	0
			766	480	142	142	2		
35	h	95	Total	C	N	O	S	0	0
			744	468	134	140	2		

- Molecule 36 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
36	1	1	Total	Fe	S	0
			8	4	4	

- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
37	4	4	Total 4	Zn 4	0
37	5	1	Total 1	Zn 1	0
37	7	2	Total 2	Zn 2	0
37	A	2	Total 2	Zn 2	0
37	B	1	Total 1	Zn 1	0
37	C	1	Total 1	Zn 1	0
37	I	2	Total 2	Zn 2	0
37	J	1	Total 1	Zn 1	0
37	L	1	Total 1	Zn 1	0
37	M	1	Total 1	Zn 1	0
37	W	1	Total 1	Zn 1	0

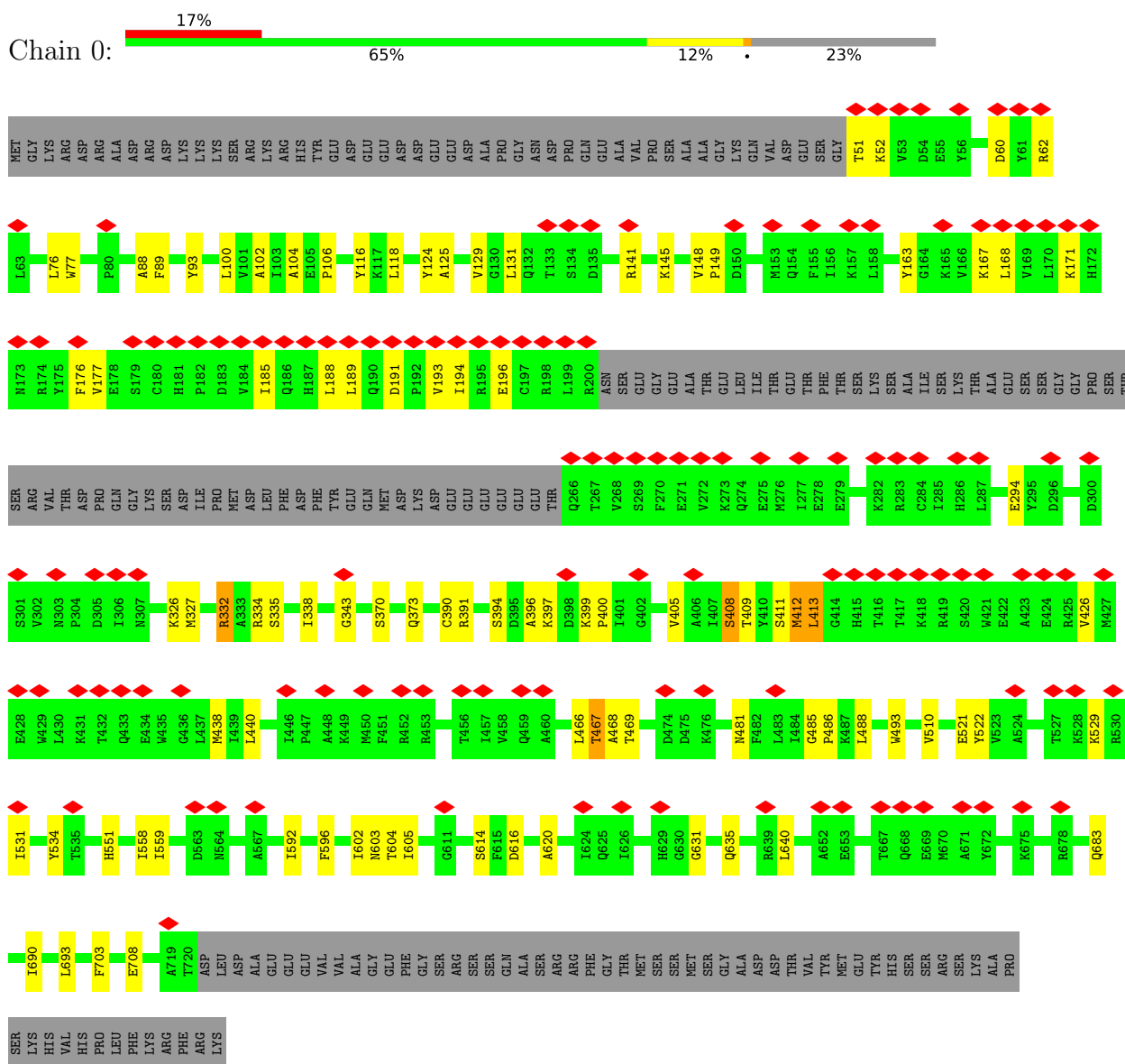
- Molecule 38 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

3 Residue-property plots

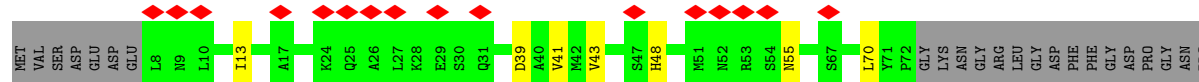
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

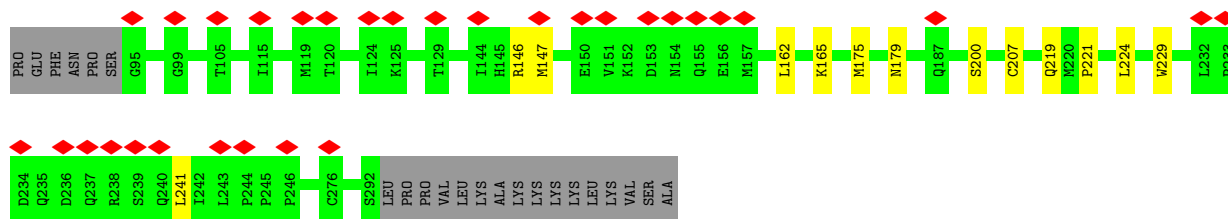
- Molecule 1: General transcription and DNA repair factor IIH helicase subunit XPB



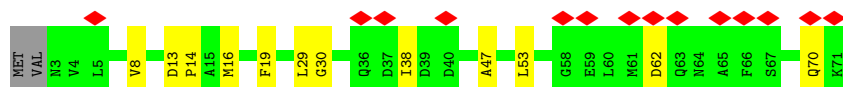
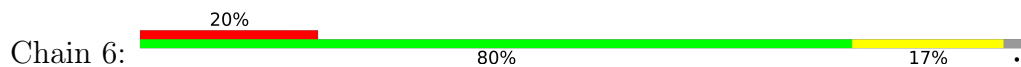
- Molecule 2: TFIIH basal transcription factor complex helicase XPD subunit



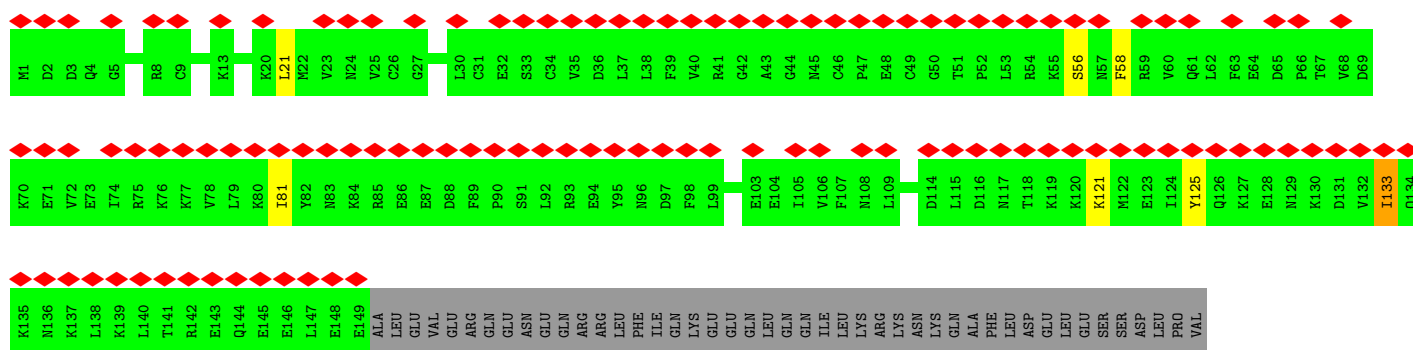




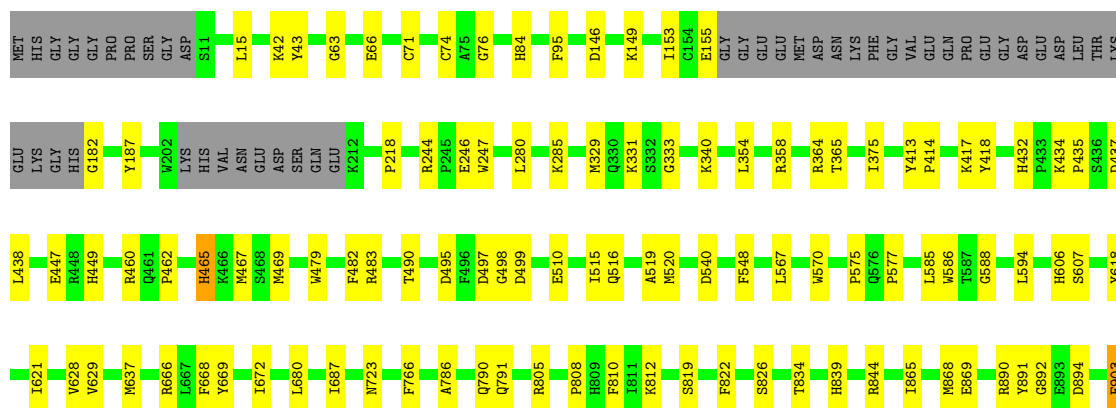
- Molecule 7: General transcription factor IIH subunit 5

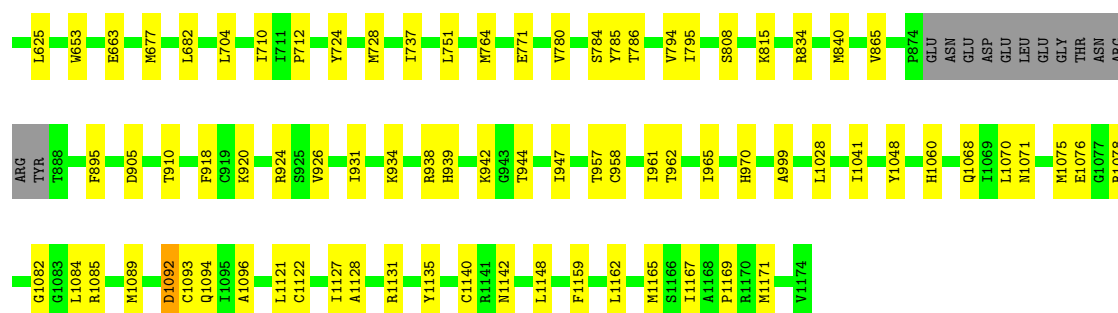


- Molecule 8: CDK-activating kinase assembly factor MAT1



- Molecule 9: DNA-directed RNA polymerase subunit





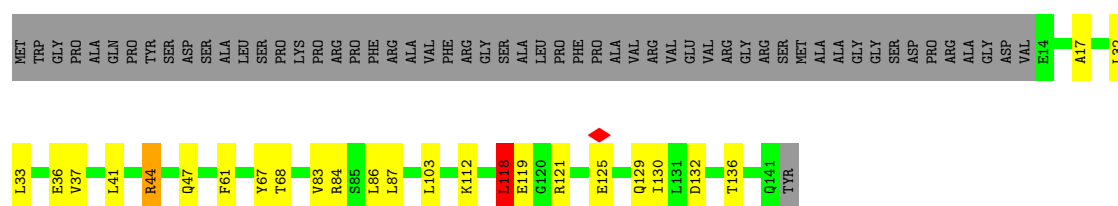
- Molecule 11: DNA-directed RNA polymerase II subunit RPB3

Chain C: 83% 10% 7%



- Molecule 12: RNA polymerase II subunit D

Chain D: 56% 12% 30%



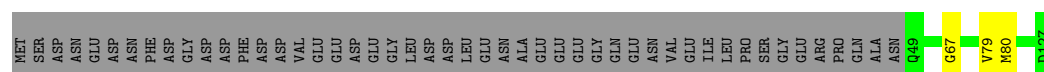
- Molecule 13: DNA-directed RNA polymerase II subunit E

Chain E: 89% 9%



- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 60% 38%



- Molecule 15: DNA-directed RNA polymerase II subunit RPB7

Chain G: 87% 13%



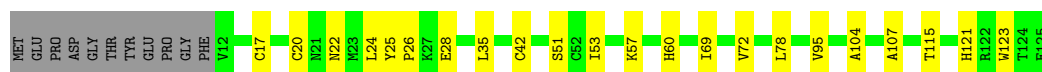
- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 86% 12% ..



- Molecule 17: DNA-directed RNA polymerase II subunit RPB9

Chain I: 74% 18% 9%



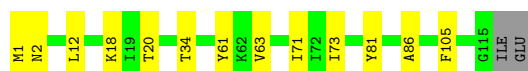
- Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 85% 10% .



- Molecule 19: DNA-directed RNA polymerase II subunit RPB11-a

Chain K: 87% 11% .



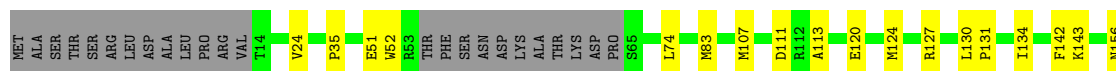
- Molecule 20: RNA polymerase II subunit K

Chain L: 59% 17% 24%

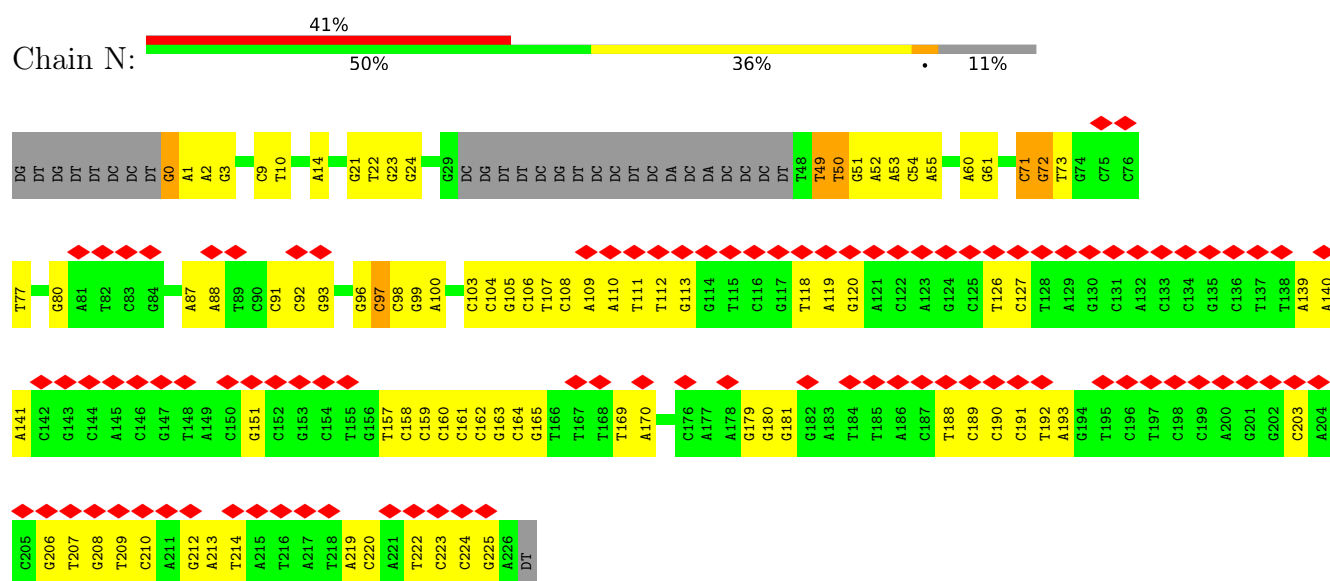


- Molecule 21: Transcription initiation factor IIB

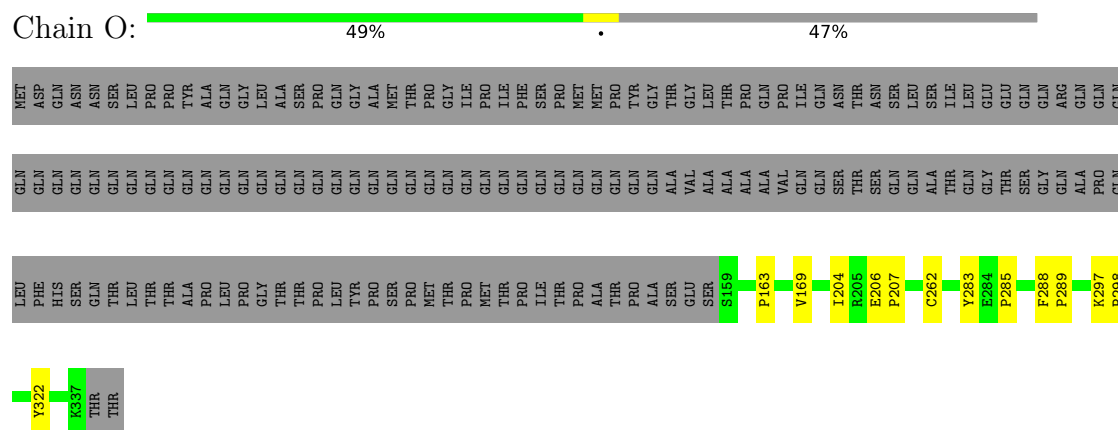
Chain M: 83% 10% 8%



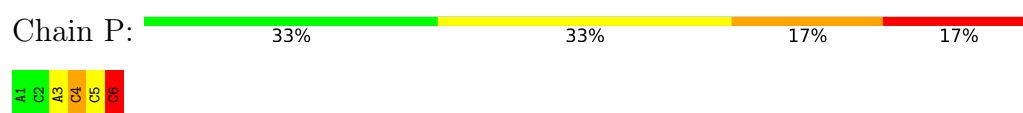
- Molecule 22: Non-template DNA



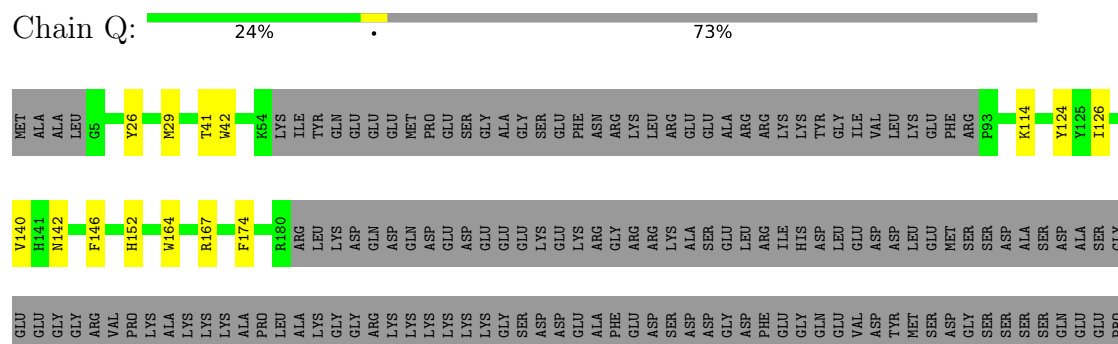
- Molecule 23: TATA-box-binding protein

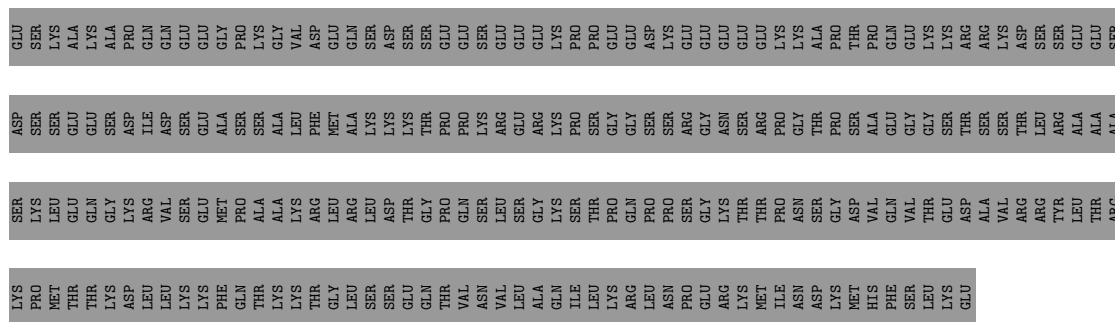


- Molecule 24: RNA (5'-R(P*AP*CP*AP*CP*CP*C)-3')

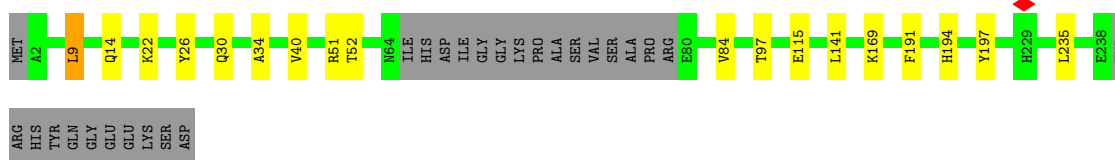
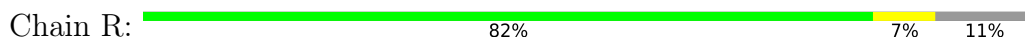


- Molecule 25: General transcription factor IIF subunit 1

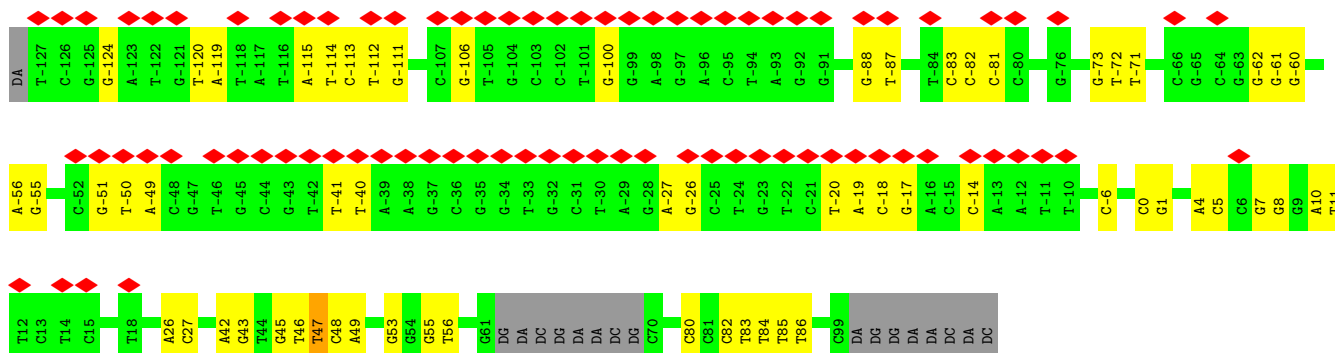




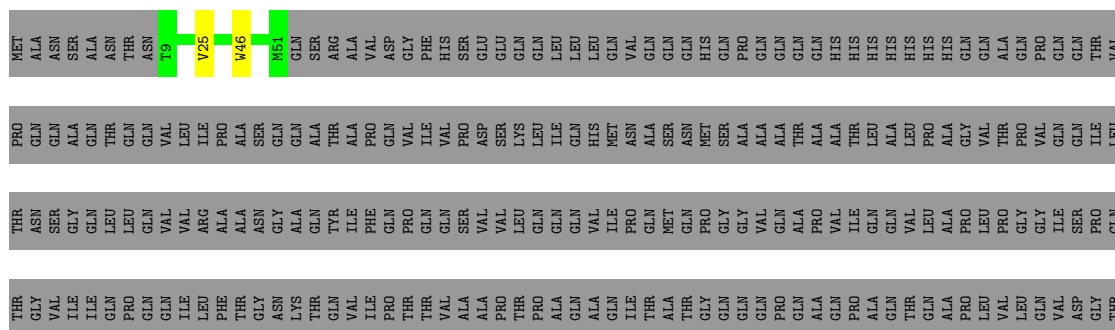
- Molecule 26: General transcription factor IIF subunit 2

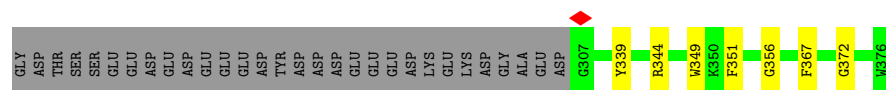


- Molecule 27: Template DNA

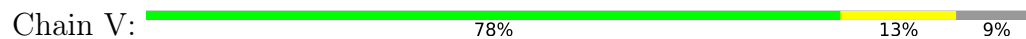


- Molecule 28: Transcription initiation factor IIA subunit 1

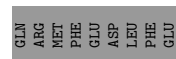
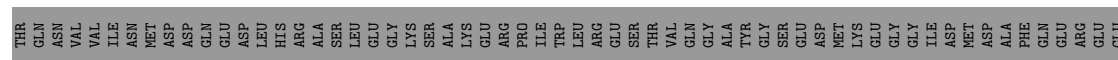
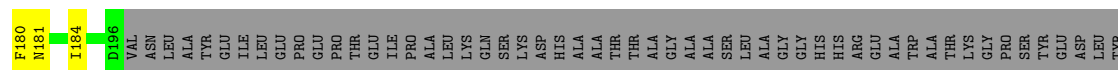
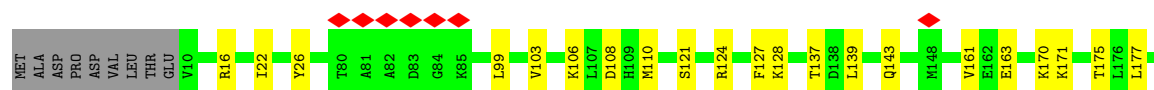
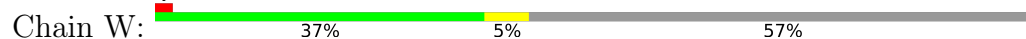




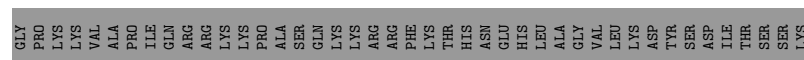
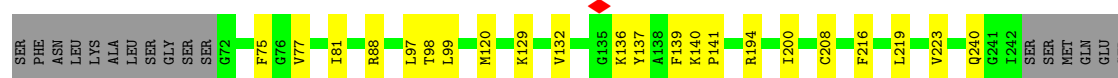
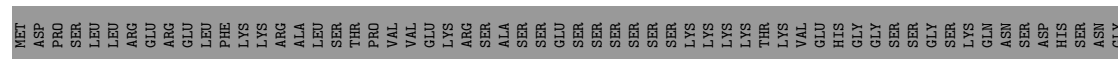
- Molecule 29: Transcription initiation factor IIA subunit 2



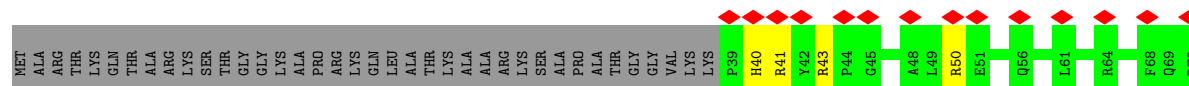
- Molecule 30: General transcription factor IIE subunit 1

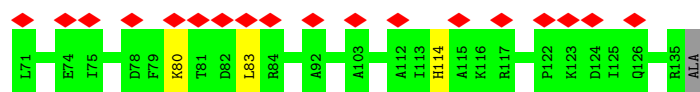


- Molecule 31: Transcription initiation factor IIE subunit beta

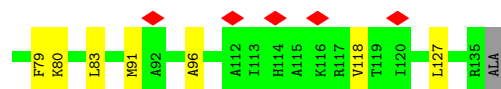
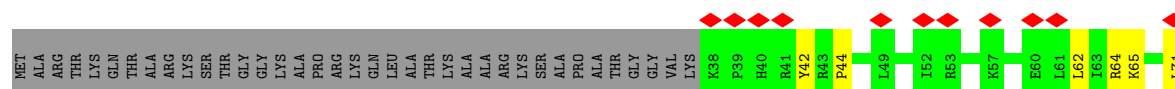


- Molecule 32: Histone H3.2

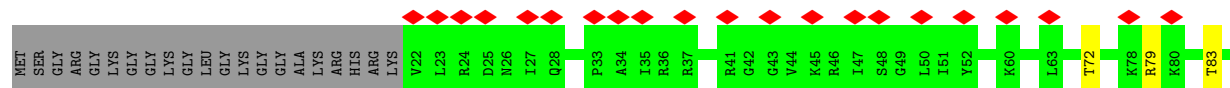
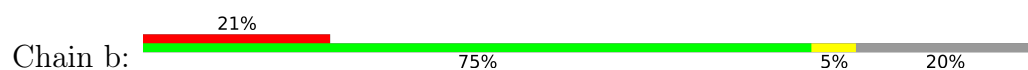




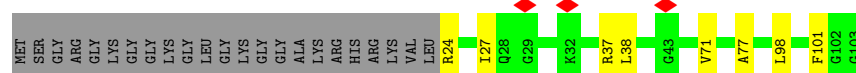
• Molecule 32: Histone H3.2



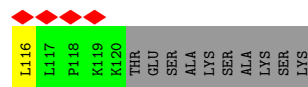
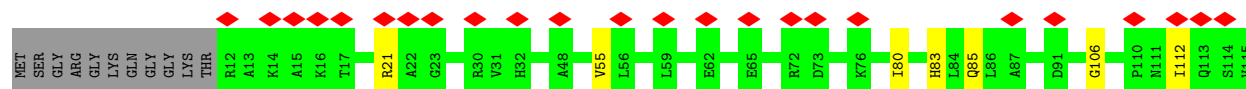
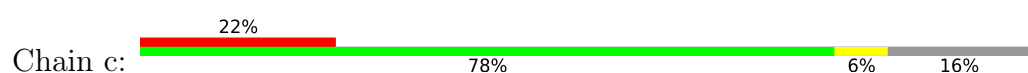
• Molecule 33: Histone H4



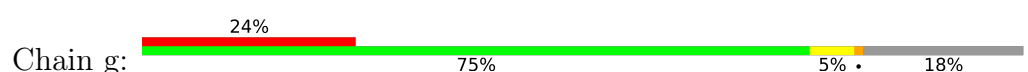
• Molecule 33: Histone H4

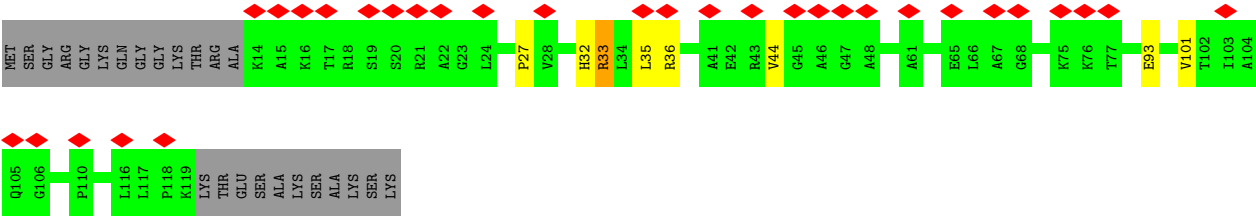


• Molecule 34: Histone H2A type 1

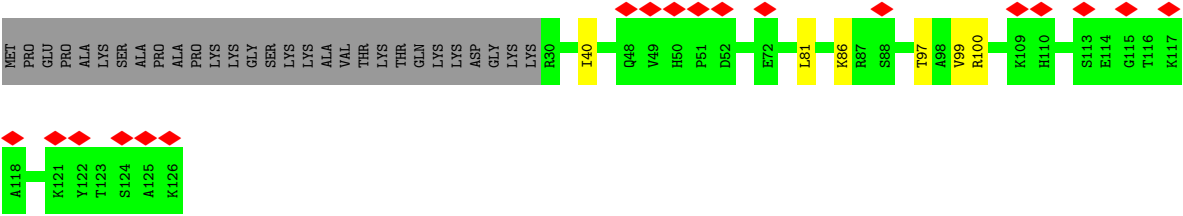


• Molecule 34: Histone H2A type 1

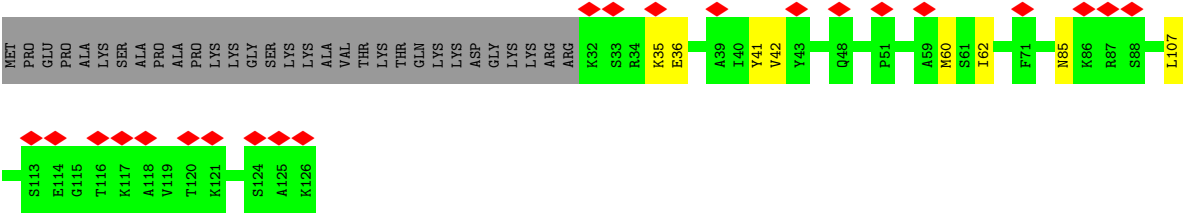




• Molecule 35: Histone H2B 1.1



• Molecule 35: Histone H2B 1.1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40410	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 ($e^-/\text{\AA}^2$)	40.00	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.110	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 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	0	0.28	0/4994	0.94	17/6745 (0.3%)
2	1	0.26	0/5875	0.79	3/7955 (0.0%)
3	2	0.25	0/3073	0.70	0/4132
4	3	0.25	0/3412	0.71	0/4622
5	4	0.28	0/2793	0.84	0/3780
6	5	0.24	0/2103	0.69	0/2846
7	6	0.23	0/555	0.81	0/747
8	7	0.30	0/1241	0.82	0/1665
9	A	0.31	0/11462	0.78	0/15473
10	B	0.34	0/9149	0.76	0/12349
11	C	0.33	0/2102	0.71	0/2857
12	D	0.29	0/1064	0.96	2/1428 (0.1%)
13	E	0.25	0/1752	0.70	0/2366
14	F	0.31	0/646	0.69	0/871
15	G	0.27	0/1382	0.75	0/1874
16	H	0.28	0/1207	0.63	0/1628
17	I	0.30	0/949	0.74	0/1284
18	J	0.32	0/516	0.72	0/696
19	K	0.34	0/939	0.67	0/1271
20	L	0.32	0/378	0.86	0/500
21	M	0.28	0/2287	0.73	0/3084
22	N	0.36	0/4819	0.94	13/7434 (0.2%)
23	O	0.27	0/1448	0.70	0/1948
24	P	0.55	0/137	1.32	1/210 (0.5%)
25	Q	0.26	0/1167	0.80	0/1576
26	R	0.23	0/1817	0.66	0/2445
27	T	0.33	0/5030	0.85	2/7761 (0.0%)
28	U	0.21	0/946	0.72	0/1274
29	V	0.24	0/816	0.67	0/1105
30	W	0.25	0/1560	0.72	0/2097
31	X	0.23	0/1427	0.74	0/1916
32	a	0.30	0/814	0.83	0/1092

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	e	0.26	0/823	0.79	1/1104 (0.1%)
33	b	0.24	0/660	0.75	0/883
33	f	0.27	0/645	0.89	0/862
34	c	0.25	0/853	0.80	0/1149
34	g	0.24	0/828	0.77	0/1117
35	d	0.24	0/777	0.70	0/1041
35	h	0.27	0/755	0.78	1/1013 (0.1%)
All	All	0.29	0/83201	0.79	40/114200 (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
1	0	0	1
2	1	0	1
9	A	0	1
11	C	0	2
12	D	0	2
13	E	0	2
20	L	0	2
21	M	0	1
32	a	0	1
33	f	0	1
34	c	0	1
34	g	0	1
35	d	0	1
All	All	0	17

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	49	DT	OP1-P-O3'	-13.14	68.58	108.00
22	N	49	DT	OP2-P-O3'	-11.76	72.71	108.00
22	N	49	DT	O3'-P-O5'	11.04	120.57	104.00
22	N	49	DT	P-O3'-C3'	9.96	135.14	120.20
1	0	605	ILE	N-CA-C	-8.99	95.06	108.46
1	0	390	CYS	N-CA-C	8.26	122.72	108.76
1	0	604	THR	CA-C-N	7.74	133.70	122.94
1	0	604	THR	C-N-CA	7.74	133.70	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	T	46	DT	OP2-P-O3'	7.24	129.72	108.00
22	N	80	DG	O4'-C1'-N9	7.16	119.14	108.40
2	1	353	SER	N-CA-C	6.53	124.25	109.81
1	0	408	SER	CA-C-N	6.32	133.61	121.54
1	0	408	SER	C-N-CA	6.32	133.61	121.54
22	N	50	DT	O5'-P-OP2	-6.30	89.09	108.00
12	D	125	GLU	N-CA-C	6.21	118.98	111.40
1	0	411	SER	N-CA-C	6.19	118.95	111.40
22	N	97	DC	O5'-C5'-C4'	6.00	119.81	110.80
1	0	391	ARG	CA-C-N	-5.93	111.30	122.27
1	0	391	ARG	C-N-CA	-5.93	111.30	122.27
1	0	396	ALA	CA-C-N	5.79	138.52	122.15
1	0	396	ALA	C-N-CA	5.79	138.52	122.15
2	1	117	ILE	N-CA-C	5.75	121.31	109.34
1	0	413	LEU	N-CA-C	5.70	119.04	111.75
27	T	47	DT	OP1-P-OP2	-5.64	103.08	120.00
1	0	466	LEU	CA-C-N	5.64	131.35	122.21
1	0	466	LEU	C-N-CA	5.64	131.35	122.21
22	N	50	DT	OP1-P-OP2	5.61	136.81	120.00
22	N	0	DG	C2'-C3'-O3'	5.58	119.86	111.50
22	N	71	DC	P-O3'-C3'	5.47	128.41	120.20
22	N	50	DT	P-O5'-C5'	5.46	128.19	120.00
24	P	6	C	C5'-C4'-C3'	-5.38	107.94	116.00
35	h	36	GLU	N-CA-C	5.34	117.43	108.73
1	0	391	ARG	N-CA-C	-5.30	102.43	110.28
32	e	64	ARG	CA-CB-CG	-5.30	103.50	114.10
22	N	72	DG	N9-C1'-C2'	5.29	121.44	113.50
22	N	80	DG	C1'-O4'-C4'	-5.24	101.84	109.70
1	0	467	THR	N-CA-C	-5.17	101.43	109.24
12	D	118	LEU	N-CA-C	5.12	118.99	112.34
1	0	412	MET	N-CA-C	5.12	117.98	111.69
2	1	724	MET	N-CA-C	5.09	120.60	113.02

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	332	ARG	Sidechain
2	1	345	ARG	Sidechain
9	A	483	ARG	Sidechain
11	C	118	ARG	Sidechain
11	C	35	ARG	Sidechain

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Mol	Chain	Res	Type	Group
12	D	121	ARG	Sidechain
12	D	44	ARG	Sidechain
13	E	195	ARG	Sidechain
13	E	9	ARG	Sidechain
20	L	37	ARG	Sidechain
20	L	58	ARG	Sidechain
21	M	248	ARG	Sidechain
32	a	41	ARG	Sidechain
34	c	21	ARG	Sidechain
35	d	100	ARG	Sidechain
33	f	24	ARG	Sidechain
34	g	33	ARG	Sidechain

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	0	4890	0	4949	58	0
2	1	5751	0	5798	42	0
3	2	3016	0	3065	17	0
4	3	3338	0	3343	16	0
5	4	2732	0	2705	28	0
6	5	2066	0	2102	10	0
7	6	549	0	558	10	0
8	7	1225	0	1228	3	0
9	A	11257	0	11398	121	0
10	B	8971	0	8999	108	0
11	C	2059	0	2007	17	0
12	D	1050	0	1033	15	0
13	E	1721	0	1737	12	0
14	F	636	0	665	3	0
15	G	1351	0	1358	20	0
16	H	1186	0	1147	14	0
17	I	928	0	864	16	0
18	J	507	0	523	6	0
19	K	920	0	942	9	0
20	L	373	0	379	4	0
21	M	2253	0	2271	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	N	4293	0	2341	79	0
23	O	1422	0	1514	9	0
24	P	124	0	66	4	0
25	Q	1138	0	1103	16	0
26	R	1788	0	1819	13	0
27	T	4487	0	2462	48	0
28	U	931	0	888	9	0
29	V	806	0	818	11	0
30	W	1535	0	1541	17	0
31	X	1403	0	1428	17	0
32	a	802	0	841	6	0
32	e	811	0	853	12	0
33	b	653	0	696	5	0
33	f	638	0	676	7	0
34	c	843	0	908	5	0
34	g	818	0	877	8	0
35	d	766	0	797	5	0
35	h	744	0	771	7	0
36	1	8	0	0	0	0
37	4	4	0	0	0	0
37	5	1	0	0	0	0
37	7	2	0	0	0	0
37	A	2	0	0	0	0
37	B	1	0	0	0	0
37	C	1	0	0	0	0
37	I	2	0	0	0	0
37	J	1	0	0	0	0
37	L	1	0	0	0	0
37	M	1	0	0	0	0
37	W	1	0	0	0	0
38	A	1	0	0	0	0
All	All	80807	0	77470	703	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 4.

All (703) 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)
1:0:529:LYS:HE3	22:N:77:DT:H5"	1.48	0.95
1:0:631:GLY:HA2	1:0:635:GLN:HB3	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:497:ASP:OD2	24:P:6:C:O3'	1.95	0.84
22:N:157:DT:H2''	22:N:158:DC:C5	2.21	0.76
2:1:565:LYS:HB3	2:1:595:ILE:HD11	1.68	0.76
2:1:611:VAL:HG23	2:1:669:ARG:HG2	1.66	0.76
1:0:408:SER:HA	1:0:412:MET:HB3	1.69	0.74
5:4:320:ARG:HA	5:4:323:HIS:CD2	2.27	0.70
22:N:158:DC:H2''	22:N:159:DC:C5	2.27	0.70
25:Q:114:LYS:HZ2	25:Q:142:ASN:HD21	1.40	0.69
16:H:92:MET:HE1	16:H:121:LEU:HD12	1.75	0.68
17:I:42:CYS:HB3	25:Q:152:HIS:CE1	2.29	0.68
17:I:26:PRO:HB3	17:I:53:ILE:HD13	1.76	0.68
25:Q:114:LYS:NZ	25:Q:142:ASN:HD21	1.92	0.67
22:N:189:DC:H2''	22:N:190:DC:C5	2.31	0.66
21:M:127:ARG:HD2	21:M:183:VAL:HG13	1.78	0.66
35:d:86:LYS:HD3	35:h:35:LYS:HD2	1.76	0.66
10:B:1068:GLN:HG3	10:B:1075:MET:HB3	1.78	0.66
22:N:207:DT:H2''	22:N:208:DG:C8	2.31	0.65
9:A:499:ASP:OD1	24:P:6:C:O2'	2.13	0.65
16:H:58:LEU:HD11	16:H:143:LEU:HD11	1.77	0.65
19:K:12:LEU:HD11	19:K:18:LYS:HE2	1.79	0.65
22:N:209:DT:H2''	22:N:210:DC:C5	2.32	0.65
10:B:356:PHE:CE2	25:Q:114:LYS:HD3	2.32	0.65
9:A:1216:LEU:HD13	9:A:1228:MET:HE1	1.79	0.64
15:G:104:MET:HG2	15:G:105:SER:N	2.13	0.64
6:5:219:GLN:HG3	6:5:221:PRO:HD2	1.79	0.63
9:A:903:PHE:CZ	9:A:976:LYS:HE3	2.34	0.63
27:T:-20:DT:H4'	27:T:-19:DA:H5'	1.81	0.63
16:H:130:ASN:HA	16:H:133:HIS:CE1	2.34	0.62
1:0:334:ARG:O	1:0:338:ILE:HG13	2.00	0.62
9:A:469:MET:HE3	10:B:1094:GLN:HE21	1.63	0.62
27:T:0:DC:H2''	27:T:1:DG:C8	2.34	0.62
22:N:23:DG:H2'	22:N:24:DG:C8	2.34	0.62
17:I:42:CYS:HB3	25:Q:152:HIS:HE1	1.62	0.62
1:0:125:ALA:HB2	1:0:486:PRO:HB2	1.82	0.62
22:N:0:DG:H1'	22:N:1:DA:C8	2.35	0.62
22:N:219:DA:H2''	22:N:220:DC:C6	2.35	0.62
10:B:1122:CYS:HB3	10:B:1140:CYS:SG	2.39	0.62
1:0:167:LYS:HE2	1:0:332:ARG:HD3	1.82	0.62
16:H:96:VAL:HG23	16:H:116:VAL:HG22	1.81	0.61
9:A:629:VAL:HG12	9:A:637:MET:HG2	1.81	0.61
22:N:222:DT:H2''	22:N:223:DC:C6	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:221:VAL:HG22	5:4:222:ILE:H	1.65	0.61
9:A:465:HIS:CD2	9:A:467:MET:HE2	2.35	0.61
27:T:-124:DG:H21	32:a:40:HIS:HB2	1.65	0.61
1:0:596:PHE:HA	1:0:602:ILE:HG23	1.81	0.61
28:U:372:GLY:HA3	29:V:58:PHE:CZ	2.36	0.61
9:A:244:ARG:HB2	9:A:247:TRP:CE2	2.36	0.60
3:2:422:LEU:HD21	6:5:224:LEU:HD23	1.83	0.60
9:A:668:PHE:CZ	9:A:672:ILE:HD11	2.35	0.60
9:A:1486:ILE:HD13	14:F:79:VAL:H	1.65	0.60
10:B:1060:HIS:HB3	10:B:1078:ARG:HG2	1.84	0.60
22:N:188:DT:H2''	22:N:189:DC:C6	2.36	0.60
9:A:1485:GLU:HB3	9:A:1487:PRO:HD2	1.84	0.60
22:N:224:DC:H2''	22:N:225:DG:C8	2.38	0.59
10:B:1121:LEU:HD12	10:B:1142:ASN:HD21	1.66	0.59
27:T:47:DT:OP2	27:T:47:DT:H6	1.85	0.59
1:0:104:ALA:HB2	1:0:118:LEU:HD23	1.84	0.59
28:U:344:ARG:HD3	28:U:349:TRP:CE2	2.37	0.59
9:A:1039:LEU:O	9:A:1043:ILE:HG12	2.02	0.59
22:N:60:DA:H2''	22:N:61:DG:C8	2.38	0.59
22:N:96:DG:H2''	22:N:97:DC:C5	2.37	0.59
11:C:84:TYR:CZ	11:C:167:LYS:HE2	2.37	0.59
2:1:637:LEU:HD21	2:1:648:GLU:HB2	1.85	0.59
10:B:550:MET:HE1	10:B:574:VAL:HG12	1.85	0.59
9:A:365:THR:HG22	9:A:482:PHE:CD2	2.37	0.58
9:A:1393:VAL:HG13	9:A:1398:LEU:HD21	1.85	0.58
34:c:55:VAL:HG21	35:d:99:VAL:HG21	1.86	0.58
5:4:162:HIS:ND1	5:4:250:ILE:HD12	2.18	0.58
1:0:409:THR:O	1:0:413:LEU:HD13	2.04	0.58
1:0:531:ILE:HA	1:0:534:TYR:CE2	2.38	0.58
34:g:35:LEU:HD13	34:g:44:VAL:HG11	1.85	0.58
8:7:81:ILE:HD12	8:7:121:LYS:HE3	1.84	0.58
31:X:194:ARG:HD2	31:X:200:ILE:HD11	1.86	0.58
22:N:106:DC:H2''	22:N:107:DT:C5	2.38	0.58
2:1:462:SER:OG	2:1:463:PRO:HD2	2.03	0.58
17:I:17:CYS:HB2	17:I:24:LEU:HD21	1.86	0.58
25:Q:26:TYR:HA	26:R:97:THR:HG22	1.86	0.58
27:T:4:DA:H2''	27:T:5:DC:C6	2.39	0.58
9:A:469:MET:HE2	10:B:1093:CYS:HB3	1.86	0.57
9:A:1209:PRO:HG3	17:I:28:GLU:OE2	2.05	0.57
10:B:724:TYR:HB3	10:B:728:MET:HE3	1.86	0.57
21:M:290:ARG:HH21	21:M:316:LEU:HD11	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:N:169:DT:H2''	22:N:170:DA:C8	2.39	0.57
27:T:84:DT:H2'	27:T:85:DT:C6	2.38	0.57
23:O:163:PRO:HA	23:O:262:CYS:HB3	1.85	0.57
8:7:56:SER:HB2	8:7:58:PHE:CE2	2.39	0.57
10:B:1159:PHE:HE2	10:B:1171:MET:SD	2.28	0.57
26:R:9:LEU:HD23	26:R:9:LEU:H	1.70	0.57
9:A:1036:ASN:HD22	13:E:202:ARG:HB3	1.69	0.57
22:N:208:DG:H2''	22:N:209:DT:C5	2.40	0.57
23:O:297:LYS:HB3	23:O:298:PRO:HD3	1.85	0.57
10:B:33:TYR:HD2	10:B:653:TRP:CZ2	2.23	0.57
1:0:343:GLY:HA3	1:0:640:LEU:HD23	1.85	0.57
9:A:1099:ALA:HA	9:A:1102:MET:HE1	1.87	0.57
34:c:85:GLN:HG2	34:c:106:GLY:HA3	1.85	0.57
12:D:112:LYS:HB3	12:D:118:LEU:HD13	1.87	0.56
10:B:1076:GLU:O	10:B:1082:GLY:HA3	2.05	0.56
10:B:1167:ILE:O	10:B:1169:PRO:HD3	2.05	0.56
15:G:7:LEU:HB2	15:G:72:TYR:CZ	2.40	0.56
15:G:15:PRO:HA	15:G:18:PHE:CZ	2.40	0.56
27:T:-41:DT:H2''	27:T:-40:DT:C5	2.40	0.56
13:E:73:PHE:CE2	13:E:99:ILE:HG13	2.41	0.56
17:I:104:ALA:HB3	17:I:107:ALA:HB2	1.88	0.56
22:N:108:DC:H2''	22:N:109:DA:C8	2.41	0.56
27:T:-14:DC:H5'	27:T:-14:DC:C6	2.40	0.56
32:a:80:LYS:HB3	32:a:83:LEU:HD11	1.86	0.56
27:T:-82:DC:H2''	27:T:-81:DC:C5	2.41	0.56
9:A:986:MET:HE1	9:A:1072:ILE:HA	1.88	0.56
22:N:159:DC:H2''	22:N:160:DC:C5	2.41	0.56
9:A:375:ILE:HD11	9:A:666:ARG:HA	1.89	0.55
3:2:481:VAL:HG23	3:2:483:THR:HG23	1.89	0.55
9:A:892:GLY:C	9:A:894:ASP:H	2.15	0.55
26:R:194:HIS:HB3	26:R:197:TYR:CZ	2.42	0.55
17:I:95:VAL:HG23	17:I:115:THR:HG22	1.87	0.55
27:T:-72:DT:H2''	27:T:-71:DT:C6	2.42	0.55
31:X:98:THR:HG23	31:X:136:LYS:HE3	1.88	0.55
4:3:444:THR:HG23	4:3:447:GLY:H	1.72	0.55
11:C:60:HIS:NE2	11:C:63:PHE:HB2	2.22	0.55
4:3:335:LEU:HD21	7:6:70:GLN:HB3	1.89	0.55
15:G:44:PHE:CE2	15:G:157:ILE:HG22	2.42	0.55
9:A:1093:GLN:HE22	10:B:1096:ALA:HB2	1.72	0.54
23:O:283:TYR:CZ	23:O:285:PRO:HG3	2.42	0.54
22:N:9:DC:H2'	22:N:10:DT:H72	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1279:MET:HE3	9:A:1284:PHE:HA	1.88	0.54
1:O:185:ILE:HG23	1:O:189:LEU:HD13	1.89	0.54
9:A:865:ILE:HD13	10:B:1092:ASP:OD2	2.07	0.54
1:O:373:GLN:OE1	1:O:616:ASP:HA	2.08	0.54
9:A:74:CYS:HB2	10:B:1128:ALA:O	2.08	0.54
10:B:834:ARG:HA	10:B:840:MET:SD	2.48	0.54
22:N:21:DG:H2'	22:N:22:DT:H71	1.90	0.54
28:U:344:ARG:HD3	28:U:349:TRP:CZ2	2.42	0.54
2:1:118:HIS:O	2:1:121:VAL:HG22	2.08	0.54
9:A:84:HIS:CE1	10:B:1127:ILE:HG23	2.43	0.54
2:1:488:VAL:HG23	2:1:724:MET:HE3	1.90	0.54
9:A:432:HIS:CE1	9:A:437:ASP:HB2	2.42	0.54
29:V:3:TYR:HB3	29:V:5:LEU:HD13	1.90	0.54
1:O:76:LEU:HD11	1:O:100:LEU:HD21	1.90	0.53
10:B:592:ARG:HE	10:B:663:GLU:CD	2.16	0.53
22:N:213:DA:H2'	22:N:214:DT:H71	1.90	0.53
9:A:868:MET:SD	9:A:1092:ALA:HB2	2.49	0.53
19:K:81:TYR:CE2	19:K:86:ALA:HB2	2.44	0.53
1:O:438:MET:HE2	1:O:440:LEU:HD21	1.90	0.53
22:N:49:DT:H2''	22:N:50:DT:H5'	1.90	0.53
22:N:104:DC:H2''	22:N:105:DG:C8	2.43	0.53
10:B:1089:MET:HG3	27:T:53:DG:H4'	1.91	0.53
9:A:479:TRP:CG	10:B:931:ILE:HD12	2.44	0.53
22:N:72:DG:H2''	22:N:73:DT:C6	2.44	0.53
11:C:56:SER:HB2	11:C:158:GLU:H	1.73	0.53
17:I:26:PRO:HB3	17:I:53:ILE:CD1	2.39	0.53
1:O:326:LYS:HE3	1:O:488:LEU:HB3	1.89	0.52
10:B:42:GLN:H	10:B:42:GLN:CD	2.17	0.52
21:M:131:PRO:HD2	21:M:134:ILE:HD12	1.91	0.52
31:X:88:ARG:HG2	31:X:97:LEU:HD11	1.90	0.52
21:M:107:MET:HE2	21:M:111:ASP:HB3	1.92	0.52
10:B:399:LEU:HB3	10:B:453:TRP:CZ3	2.45	0.52
25:Q:29:MET:HG3	25:Q:146:PHE:CE1	2.43	0.52
9:A:810:PHE:CZ	9:A:819:SER:HA	2.45	0.52
16:H:10:PHE:CE2	16:H:32:SER:HB3	2.45	0.52
12:D:83:VAL:HG13	12:D:87:LEU:HD12	1.92	0.52
35:h:42:VAL:HB	35:h:60:MET:HE1	1.91	0.52
6:5:48:HIS:CD2	6:5:55:ASN:HB3	2.45	0.52
9:A:890:ARG:HH21	9:A:1023:VAL:HA	1.75	0.52
9:A:1375:ARG:NE	13:E:195:ARG:HH12	2.08	0.52
31:X:99:LEU:HB2	31:X:120:MET:SD	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:T:48:DC:H1'	27:T:49:DA:C8	2.45	0.51
9:A:791:GLN:HE22	9:A:839:HIS:HA	1.74	0.51
30:W:128:LYS:H	30:W:161:VAL:HG13	1.75	0.51
9:A:1020:LEU:HD22	9:A:1076:PHE:CD1	2.45	0.51
9:A:1224:ARG:HB2	9:A:1226:LEU:HD11	1.93	0.51
17:I:57:LYS:HD3	17:I:60:HIS:HA	1.93	0.51
21:M:74:LEU:HB3	21:M:143:LYS:HD2	1.92	0.51
27:T:-18:DC:H2''	27:T:-17:DG:C8	2.45	0.51
4:3:403:PHE:CZ	7:6:53:LEU:HD22	2.46	0.51
11:C:39:ILE:HG23	11:C:177:ASN:ND2	2.26	0.51
22:N:1:DA:H1'	22:N:2:DA:H5''	1.93	0.51
22:N:50:DT:H1'	22:N:51:DG:C8	2.46	0.51
22:N:107:DT:H2''	22:N:108:DC:C5	2.45	0.51
8:7:125:TYR:CD1	8:7:133:ILE:HD13	2.46	0.51
1:0:141:ARG:HA	1:0:149:PRO:HG2	1.93	0.51
22:N:190:DC:H2''	22:N:191:DC:C5	2.46	0.51
30:W:106:LYS:HE3	31:X:223:VAL:HB	1.92	0.51
10:B:99:TRP:CE2	10:B:105:PRO:HB3	2.45	0.51
10:B:96:PRO:HG2	10:B:120:TYR:CZ	2.46	0.51
22:N:97:DC:H2''	22:N:98:DC:C2	2.46	0.50
9:A:146:ASP:HA	9:A:149:LYS:HE3	1.93	0.50
10:B:677:MET:H	10:B:682:LEU:HG	1.76	0.50
9:A:928:ARG:HD3	16:H:106:THR:HB	1.92	0.50
10:B:910:THR:HG22	20:L:43:ILE:HA	1.91	0.50
9:A:155:GLU:HA	9:A:182:GLY:O	2.12	0.50
9:A:687:ILE:HD11	9:A:766:PHE:CZ	2.47	0.50
2:1:718:LYS:HA	2:1:721:LEU:HD12	1.94	0.50
2:1:57:MET:HE2	2:1:57:MET:HA	1.94	0.50
10:B:156:LEU:HD22	10:B:184:TYR:CZ	2.47	0.50
2:1:414:PHE:CD2	2:1:437:CYS:HB2	2.46	0.50
3:2:531:THR:HG21	5:4:295:ARG:HG3	1.94	0.50
10:B:1028:LEU:HD12	10:B:1041:ILE:HB	1.93	0.50
15:G:5:ILE:HD11	15:G:76:VAL:HG21	1.94	0.50
2:1:487:ARG:HG2	2:1:724:MET:HE1	1.94	0.50
2:1:720:PHE:C	2:1:722:ARG:H	2.19	0.50
9:A:1278:LYS:HG3	9:A:1279:MET:H	1.77	0.50
11:C:101:PHE:CE2	11:C:122:SER:HB3	2.47	0.50
1:0:592:ILE:HG22	1:0:596:PHE:HB2	1.94	0.50
9:A:340:LYS:HG3	9:A:1436:VAL:HG21	1.92	0.50
22:N:49:DT:H1'	22:N:50:DT:H5'	1.94	0.49
22:N:179:DG:H2''	22:N:180:DG:N7	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:1075:MET:HG3	10:B:1075:MET:O	2.12	0.49
12:D:32:LEU:HD11	15:G:4:HIS:HB2	1.94	0.49
1:0:631:GLY:CA	1:0:635:GLN:HB3	2.35	0.49
9:A:365:THR:HG22	9:A:482:PHE:CE2	2.47	0.49
9:A:865:ILE:HD13	10:B:1092:ASP:CG	2.36	0.49
16:H:103:GLU:HB3	16:H:109:ALA:HB2	1.93	0.49
2:1:536:VAL:HG21	2:1:610:PHE:CE2	2.47	0.49
15:G:95:VAL:HG11	30:W:127:PHE:CZ	2.48	0.49
19:K:63:VAL:HG12	19:K:71:ILE:HG22	1.93	0.49
1:0:510:VAL:HA	1:0:690:ILE:O	2.13	0.49
2:1:82:LYS:NZ	2:1:613:HIS:CE1	2.81	0.49
9:A:1224:ARG:HB2	9:A:1226:LEU:CD1	2.43	0.49
2:1:48:LYS:HE2	2:1:234:ASP:OD1	2.13	0.49
2:1:269:THR:HG21	2:1:386:LEU:HD21	1.94	0.49
10:B:117:ASN:HA	10:B:189:GLY:HA3	1.95	0.49
10:B:934:LYS:HG2	10:B:944:THR:HG22	1.95	0.49
13:E:59:THR:HG23	13:E:74:VAL:O	2.13	0.49
22:N:169:DT:H2''	22:N:170:DA:N7	2.28	0.49
1:0:106:PRO:HG3	1:0:116:TYR:CE2	2.48	0.49
9:A:244:ARG:HB2	9:A:247:TRP:CD2	2.48	0.49
10:B:215:TYR:CG	10:B:238:SER:HB3	2.48	0.49
10:B:712:PRO:O	10:B:939:HIS:HE1	1.96	0.49
17:I:35:LEU:HD23	17:I:51:SER:HA	1.94	0.49
22:N:119:DA:H2''	22:N:120:DG:C8	2.48	0.49
27:T:-83:DC:H2''	27:T:-82:DC:C6	2.48	0.49
5:4:56:GLY:O	5:4:238:PRO:HB2	2.13	0.48
22:N:49:DT:C4'	22:N:50:DT:OP1	2.61	0.48
26:R:34:ALA:HB3	26:R:40:VAL:HG12	1.95	0.48
9:A:1254:LYS:HE2	9:A:1254:LYS:HA	1.94	0.48
19:K:61:TYR:HB2	19:K:73:ILE:HG12	1.96	0.48
27:T:85:DT:H2'	27:T:86:DT:C6	2.48	0.48
32:e:91:MET:HB3	33:f:101:PHE:CZ	2.48	0.48
1:0:124:TYR:HB3	1:0:163:TYR:CZ	2.47	0.48
2:1:49:THR:HG23	2:1:72:TYR:CZ	2.49	0.48
7:6:16:MET:HA	7:6:19:PHE:CD1	2.48	0.48
22:N:107:DT:H2''	22:N:108:DC:C6	2.48	0.48
4:3:348:ARG:HH12	7:6:62:ASP:HA	1.77	0.48
4:3:376:MET:HE2	4:3:382:VAL:HG12	1.94	0.48
27:T:83:DT:H2'	27:T:84:DT:C6	2.48	0.48
1:0:370:SER:HB2	1:0:614:SER:OG	2.14	0.48
17:I:104:ALA:CB	17:I:107:ALA:HB2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:114:HIS:CG	32:e:127:LEU:HD22	2.48	0.48
9:A:331:LYS:HA	21:M:83:MET:SD	2.53	0.48
9:A:1443:ALA:HB2	10:B:1167:ILE:HG23	1.95	0.48
10:B:712:PRO:O	10:B:939:HIS:CE1	2.66	0.48
11:C:78:ILE:HG21	11:C:127:VAL:HG22	1.96	0.48
2:1:579:VAL:HG13	2:1:583:LYS:HE2	1.94	0.48
2:1:668:ILE:HD11	2:1:677:MET:SD	2.54	0.48
15:G:15:PRO:HA	15:G:18:PHE:CE1	2.49	0.48
22:N:97:DC:H2''	22:N:98:DC:C4	2.49	0.48
33:f:77:ALA:HB2	35:h:85:ASN:ND2	2.29	0.48
2:1:422:ASP:HA	2:1:432:ILE:HG21	1.96	0.47
9:A:917:GLU:HA	9:A:956:PHE:CZ	2.49	0.47
12:D:67:TYR:CE2	15:G:101:ILE:HA	2.48	0.47
22:N:111:DT:H2'	22:N:112:DT:C6	2.49	0.47
10:B:356:PHE:CD1	25:Q:114:LYS:HB3	2.49	0.47
31:X:139:PHE:O	31:X:141:PRO:HD3	2.14	0.47
9:A:577:PRO:HB3	9:A:586:TRP:CE2	2.49	0.47
9:A:993:ILE:HG23	9:A:994:PHE:CD2	2.50	0.47
10:B:1162:LEU:HA	10:B:1165:MET:HE3	1.96	0.47
20:L:35:ARG:HG2	20:L:40:GLY:HA2	1.95	0.47
22:N:55:DA:C2	27:T:45:DG:C2	3.02	0.47
2:1:73:CYS:HA	2:1:207:TYR:O	2.13	0.47
12:D:118:LEU:HG	12:D:119:GLU:N	2.27	0.47
22:N:161:DC:H2''	22:N:162:DC:C6	2.50	0.47
29:V:5:LEU:HD11	29:V:98:CYS:SG	2.54	0.47
1:0:193:VAL:O	1:0:196:GLU:HG3	2.14	0.47
2:1:12:PHE:CG	2:1:13:PRO:HD2	2.49	0.47
22:N:162:DC:H2''	22:N:163:DG:C8	2.49	0.47
26:R:51:ARG:HE	26:R:52:THR:H	1.63	0.47
1:0:60:ASP:OD1	1:0:62:ARG:HG2	2.15	0.47
20:L:17:TYR:HB3	20:L:44:MET:HB3	1.96	0.47
22:N:151:DG:C2	27:T:-51:DG:N2	2.82	0.47
22:N:159:DC:H2''	22:N:160:DC:C6	2.50	0.47
22:N:164:DC:H2''	22:N:165:DG:C8	2.49	0.47
27:T:26:DA:H2''	27:T:27:DC:C5	2.49	0.47
30:W:177:LEU:O	30:W:180:PHE:HB3	2.14	0.47
5:4:232:LEU:HA	5:4:236:VAL:HB	1.96	0.47
9:A:434:LYS:O	9:A:438:LEU:HD13	2.15	0.47
32:e:80:LYS:HB3	32:e:83:LEU:HD11	1.96	0.47
9:A:891:TYR:CZ	9:A:1396:ARG:HB3	2.49	0.47
27:T:-73:DG:H2''	27:T:-72:DT:C5	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:90:TYR:C	13:E:94:MET:HE3	2.40	0.47
15:G:38:CYS:HB2	15:G:44:PHE:CD1	2.50	0.47
2:1:460:THR:HG21	2:1:665:GLY:HA3	1.96	0.46
25:Q:126:ILE:HD11	25:Q:140:VAL:HG22	1.96	0.46
27:T:8:DG:H8	27:T:8:DG:OP2	1.98	0.46
34:g:35:LEU:HB3	34:g:44:VAL:HG21	1.97	0.46
5:4:149:LEU:HD23	5:4:167:VAL:HG21	1.97	0.46
5:4:323:HIS:CE1	6:5:179:ASN:OD1	2.68	0.46
11:C:60:HIS:CD2	11:C:63:PHE:HB2	2.50	0.46
17:I:25:TYR:HB2	25:Q:174:PHE:CZ	2.50	0.46
27:T:-61:DG:H2''	27:T:-60:DG:N7	2.31	0.46
1:0:168:LEU:HA	1:0:177:VAL:HG22	1.96	0.46
21:M:142:PHE:HE2	21:M:159:ILE:HG23	1.80	0.46
22:N:103:DC:H2'	22:N:104:DC:C6	2.50	0.46
27:T:-113:DC:H2''	27:T:-112:DT:C6	2.50	0.46
2:1:237:HIS:HB3	2:1:458:SER:HB3	1.97	0.46
3:2:488:GLU:HB3	5:4:158:HIS:CD2	2.50	0.46
5:4:162:HIS:CG	5:4:163:THR:N	2.84	0.46
9:A:498:GLY:HA3	10:B:934:LYS:HE2	1.96	0.46
21:M:51:GLU:H	21:M:51:GLU:CD	2.23	0.46
21:M:286:ARG:HD2	22:N:3:DG:H3'	1.97	0.46
3:2:462:LYS:HE3	5:4:282:PRO:HG2	1.97	0.46
10:B:453:TRP:NE1	10:B:466:VAL:HB	2.31	0.46
21:M:172:GLY:C	21:M:174:PRO:HD3	2.40	0.46
32:e:65:LYS:HE3	32:e:91:MET:SD	2.55	0.46
2:1:82:LYS:HZ2	2:1:613:HIS:CE1	2.34	0.46
9:A:606:HIS:CG	9:A:607:SER:N	2.83	0.46
23:O:204:ILE:HG13	23:O:207:PRO:HD2	1.97	0.46
1:0:703:PHE:HA	1:0:708:GLU:HB2	1.98	0.46
10:B:710:ILE:HA	10:B:764:MET:HE2	1.95	0.46
15:G:108:ILE:HD11	15:G:145:LEU:HD22	1.98	0.46
27:T:83:DT:C5	27:T:84:DT:H73	2.51	0.46
33:b:99:TYR:CE2	34:g:101:VAL:HG11	2.50	0.46
1:0:188:LEU:HD23	1:0:194:ILE:HG21	1.97	0.46
1:0:467:THR:C	1:0:469:THR:H	2.23	0.46
2:1:12:PHE:CD1	2:1:13:PRO:HD2	2.51	0.46
7:6:13:ASP:HB2	7:6:14:PRO:HD2	1.97	0.46
9:A:76:GLY:HA2	10:B:1131:ARG:NH2	2.31	0.46
12:D:86:LEU:HD21	12:D:130:ILE:HG23	1.98	0.46
25:Q:114:LYS:NZ	25:Q:142:ASN:ND2	2.63	0.46
2:1:445:LYS:HB3	2:1:446:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:628:VAL:HA	9:A:637:MET:O	2.16	0.46
9:A:786:ALA:O	9:A:826:SER:HB3	2.16	0.46
27:T:-120:DT:H2''	27:T:-119:DA:C8	2.51	0.46
28:U:372:GLY:HA3	29:V:58:PHE:CE1	2.51	0.46
35:h:60:MET:HE3	35:h:60:MET:O	2.16	0.46
9:A:479:TRP:CD1	10:B:931:ILE:HD12	2.51	0.46
9:A:791:GLN:HE22	9:A:839:HIS:CA	2.29	0.46
29:V:64:THR:HB	29:V:75:VAL:HB	1.98	0.46
2:1:727:PRO:HG3	5:4:235:HIS:ND1	2.31	0.45
9:A:63:GLY:HA2	9:A:71:CYS:SG	2.56	0.45
9:A:1179:PRO:HA	9:A:1209:PRO:HB3	1.98	0.45
10:B:446:TYR:CE1	10:B:450:THR:HG21	2.51	0.45
10:B:728:MET:HE2	10:B:942:LYS:HD2	1.98	0.45
9:A:992:LYS:HA	9:A:992:LYS:HE3	1.98	0.45
10:B:388:TYR:CE1	10:B:505:LEU:HD21	2.51	0.45
10:B:957:THR:HG22	10:B:958:CYS:N	2.31	0.45
13:E:2:ASP:O	13:E:5:GLU:HG3	2.15	0.45
22:N:0:DG:H1'	22:N:1:DA:N7	2.31	0.45
23:O:206:GLU:HB3	23:O:207:PRO:HD3	1.99	0.45
9:A:1193:VAL:HG13	9:A:1197:TYR:CD2	2.52	0.45
9:A:1207:ILE:HD12	9:A:1207:ILE:O	2.16	0.45
9:A:1302:GLU:CD	9:A:1302:GLU:H	2.23	0.45
10:B:1068:GLN:OE1	10:B:1071:ASN:HB3	2.16	0.45
25:Q:41:THR:HG23	25:Q:42:TRP:HD1	1.82	0.45
25:Q:124:TYR:OH	26:R:22:LYS:HE2	2.17	0.45
26:R:84:VAL:HG23	26:R:115:GLU:HB3	1.99	0.45
27:T:80:DC:H5'	27:T:80:DC:C6	2.52	0.45
1:0:77:TRP:CE2	1:0:145:LYS:HE3	2.51	0.45
7:6:30:GLY:O	22:N:157:DT:H5''	2.17	0.45
10:B:1165:MET:HB3	10:B:1165:MET:HE2	1.83	0.45
12:D:41:LEU:HD12	12:D:68:THR:HG21	1.97	0.45
1:0:171:LYS:HB3	1:0:176:PHE:CE1	2.51	0.45
3:2:194:GLU:HA	3:2:197:PHE:CE2	2.51	0.45
4:3:155:ARG:O	4:3:158:VAL:HG22	2.16	0.45
9:A:417:LYS:HG2	9:A:449:HIS:NE2	2.32	0.45
10:B:795:ILE:HG12	10:B:947:ILE:HG22	1.98	0.45
17:I:69:ILE:O	17:I:72:VAL:HG12	2.17	0.45
27:T:-100:DG:H3'	34:g:33:ARG:CZ	2.47	0.45
1:0:397:LYS:C	1:0:400:PRO:HD3	2.41	0.45
5:4:80:ARG:O	5:4:84:THR:HG23	2.17	0.45
9:A:540:ASP:OD1	10:B:970:HIS:CE1	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:577:PRO:HA	9:A:586:TRP:CD1	2.51	0.45
2:1:368:GLN:OE1	2:1:371:PRO:HG2	2.16	0.45
3:2:488:GLU:CD	5:4:158:HIS:CD2	2.94	0.45
19:K:81:TYR:HE2	19:K:86:ALA:HB2	1.81	0.45
27:T:10:DA:H1'	27:T:11:DT:O4'	2.16	0.45
1:0:493:TRP:CG	1:0:683:GLN:HE21	2.35	0.45
6:5:229:TRP:CH2	6:5:241:LEU:HD21	2.52	0.45
9:A:413:TYR:HA	9:A:414:PRO:C	2.42	0.45
10:B:356:PHE:CD2	25:Q:114:LYS:HD3	2.52	0.45
11:C:99:VAL:HG13	11:C:123:ASN:OD1	2.16	0.45
22:N:23:DG:H2'	22:N:24:DG:H8	1.80	0.45
5:4:319:ALA:HB1	6:5:175:MET:HE1	1.98	0.45
10:B:171:LEU:HD13	10:B:178:PRO:HA	1.99	0.45
10:B:204:THR:HB	10:B:206:TYR:CZ	2.52	0.45
31:X:129:LYS:HE3	31:X:139:PHE:CZ	2.52	0.45
4:3:334:MET:HG2	4:3:344:ALA:HB2	1.99	0.45
5:4:220:HIS:HD2	5:4:235:HIS:NE2	2.15	0.45
6:5:13:ILE:HD13	6:5:41:VAL:HG13	1.99	0.45
9:A:15:LEU:HA	10:B:1148:LEU:O	2.17	0.45
10:B:53:MET:SD	26:R:141:LEU:HD22	2.57	0.45
12:D:41:LEU:HD22	12:D:61:PHE:CE2	2.52	0.45
15:G:95:VAL:HG22	30:W:163:GLU:OE2	2.17	0.45
31:X:120:MET:HE3	31:X:137:TYR:CD2	2.51	0.45
32:e:96:ALA:HB2	33:f:98:LEU:HD22	1.99	0.45
4:3:431:LEU:HD21	4:3:434:GLU:CG	2.47	0.44
9:A:548:PHE:CZ	9:A:588:GLY:HA2	2.52	0.44
10:B:1060:HIS:CB	10:B:1078:ARG:HG2	2.48	0.44
5:4:267:ALA:HB1	5:4:269:PRO:HD3	1.99	0.44
12:D:37:VAL:HG21	15:G:2:PHE:CG	2.52	0.44
13:E:104:ILE:O	13:E:129:GLN:HA	2.17	0.44
3:2:481:VAL:HB	5:4:158:HIS:HB2	1.98	0.44
9:A:1480:CYS:HB3	15:G:19:GLY:CA	2.48	0.44
22:N:53:DA:H2''	22:N:54:DC:C6	2.52	0.44
22:N:157:DT:H2''	22:N:158:DC:C6	2.52	0.44
27:T:82:DC:H3'	27:T:83:DT:H71	1.99	0.44
34:c:116:LEU:HD22	32:e:118:VAL:HG22	2.00	0.44
1:0:102:ALA:O	1:0:125:ALA:HB3	2.17	0.44
1:0:529:LYS:HE3	22:N:77:DT:C5'	2.33	0.44
2:1:628:THR:HA	2:1:633:LEU:HD13	1.99	0.44
9:A:892:GLY:C	9:A:894:ASP:N	2.76	0.44
10:B:307:GLU:HG3	25:Q:167:ARG:NE	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:587:LEU:HD13	10:B:603:MET:HG2	1.99	0.44
10:B:905:ASP:HB2	10:B:924:ARG:HB2	2.00	0.44
19:K:1:MET:HG3	19:K:2:ASN:N	2.33	0.44
1:0:481:ASN:HA	1:0:485:GLY:O	2.18	0.44
2:1:493:MET:O	2:1:678:VAL:HA	2.17	0.44
4:3:208:THR:HB	4:3:209:PRO:HD3	1.99	0.44
27:T:-112:DT:H2''	27:T:-111:DG:C5	2.53	0.44
27:T:84:DT:H2'	27:T:85:DT:C5	2.52	0.44
30:W:108:ASP:HB3	31:X:240:GLN:NE2	2.32	0.44
5:4:166:GLU:HA	5:4:195:ARG:O	2.17	0.44
9:A:95:PHE:CE2	9:A:218:PRO:HG3	2.53	0.44
9:A:285:LYS:HE2	9:A:285:LYS:HB3	1.82	0.44
10:B:384:ASP:OD1	10:B:387:HIS:HB2	2.17	0.44
10:B:780:VAL:HG21	10:B:1048:TYR:CE1	2.52	0.44
11:C:68:LEU:HD23	11:C:71:ILE:HD12	2.00	0.44
21:M:113:ALA:HB1	21:M:156:ASN:HD21	1.83	0.44
21:M:225:PRO:HD2	21:M:228:VAL:HG21	2.00	0.44
22:N:180:DG:H2''	22:N:181:DG:N7	2.31	0.44
1:0:405:VAL:HG22	1:0:426:VAL:HG13	2.00	0.44
9:A:921:ARG:O	9:A:1052:ARG:NH1	2.48	0.44
13:E:130:PHE:HB3	13:E:135:LEU:HD11	1.99	0.44
16:H:37:MET:CE	16:H:127:GLY:HA3	2.48	0.44
22:N:126:DT:H2''	22:N:127:DC:C6	2.51	0.44
26:R:191:PHE:CE2	31:X:75:PHE:HB3	2.52	0.44
9:A:981:CYS:HB3	9:A:986:MET:SD	2.58	0.44
1:0:51:THR:HG23	1:0:52:LYS:N	2.33	0.44
1:0:408:SER:HA	1:0:412:MET:CB	2.45	0.44
2:1:522:ASN:C	2:1:522:ASN:HD22	2.26	0.44
5:4:205:VAL:CG1	5:4:207:VAL:HG12	2.47	0.44
9:A:515:ILE:HG23	9:A:519:ALA:HB3	1.99	0.44
9:A:1239:PHE:CZ	9:A:1292:MET:HG2	2.52	0.44
10:B:1076:GLU:OE2	21:M:52:TRP:HA	2.18	0.44
22:N:112:DT:H2'	22:N:113:DG:C8	2.52	0.44
22:N:224:DC:P	32:a:43:ARG:HE	2.41	0.44
27:T:-82:DC:H2''	27:T:-81:DC:C6	2.53	0.44
27:T:-26:DG:OP1	33:b:83:THR:HG21	2.17	0.44
30:W:110:MET:SD	31:X:219:LEU:HG	2.58	0.44
32:e:79:PHE:HB2	33:f:71:VAL:HG11	1.99	0.44
9:A:1240:GLY:HA2	9:A:1243:LEU:O	2.18	0.43
30:W:181:ASN:HA	30:W:184:ILE:HG22	2.00	0.43
1:0:559:ILE:HG13	1:0:620:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:244:ARG:HB3	9:A:246:GLU:CD	2.44	0.43
27:T:-120:DT:C5'	32:a:50:ARG:HG2	2.47	0.43
30:W:99:LEU:O	30:W:103:VAL:HG23	2.18	0.43
2:1:693:LEU:HG	2:1:694:PRO:HD2	2.01	0.43
9:A:1480:CYS:HB3	15:G:19:GLY:C	2.43	0.43
11:C:245:VAL:HG11	19:K:105:PHE:CE2	2.53	0.43
19:K:61:TYR:CB	19:K:73:ILE:HG12	2.48	0.43
32:e:62:LEU:HD12	33:f:38:LEU:HD23	2.00	0.43
7:6:29:LEU:HD23	7:6:29:LEU:HA	1.90	0.43
10:B:815:LYS:HB2	10:B:918:PHE:CZ	2.53	0.43
10:B:521:GLY:O	10:B:524:LYS:HE2	2.18	0.43
2:1:571:THR:H	2:1:577:THR:CG2	2.32	0.43
9:A:516:GLN:HA	9:A:520:MET:HG2	2.00	0.43
10:B:1070:LEU:HD23	10:B:1070:LEU:C	2.44	0.43
31:X:120:MET:HG3	31:X:137:TYR:CE2	2.53	0.43
27:T:-14:DC:H5'	27:T:-14:DC:H6	1.83	0.43
29:V:28:ILE:HD12	29:V:32:LEU:HD23	2.00	0.43
31:X:140:LYS:HA	31:X:141:PRO:HD3	1.89	0.43
2:1:72:TYR:HE1	2:1:74:SER:HG	1.67	0.43
10:B:286:GLU:HB3	10:B:558:PRO:HG2	2.01	0.43
16:H:92:MET:HE2	16:H:92:MET:HB3	1.85	0.43
1:0:529:LYS:HA	22:N:77:DT:OP1	2.19	0.43
3:2:10:LEU:HD23	3:2:26:LEU:HD13	2.01	0.43
4:3:228:MET:HA	4:3:228:MET:HE2	2.00	0.43
4:3:413:LEU:HD23	4:3:413:LEU:H	1.82	0.43
9:A:358:ARG:HA	10:B:1085:ARG:HA	2.01	0.43
9:A:618:TYR:HB3	9:A:621:ILE:O	2.19	0.43
9:A:1480:CYS:HB3	15:G:19:GLY:O	2.18	0.43
22:N:87:DA:H1'	22:N:88:DA:N7	2.34	0.43
26:R:169:LYS:HE2	26:R:169:LYS:HB3	1.84	0.43
9:A:434:LYS:HA	9:A:435:PRO:HD3	1.89	0.43
27:T:55:DG:H2'	27:T:56:DT:C6	2.54	0.43
5:4:100:PRO:O	5:4:311:THR:HB	2.19	0.42
6:5:165:LYS:HE2	6:5:200:SER:HB2	2.00	0.42
9:A:575:PRO:HG3	9:A:594:LEU:HD11	2.01	0.42
15:G:47:ALA:H	15:G:75:ILE:HG13	1.85	0.42
21:M:235:ILE:HG13	21:M:236:ALA:N	2.33	0.42
22:N:98:DC:H1'	22:N:99:DG:N7	2.34	0.42
27:T:-62:DG:H21	32:e:44:PRO:HG3	1.83	0.42
30:W:121:SER:HA	30:W:124:ARG:HG2	2.01	0.42
5:4:171:PHE:CG	5:4:174:LEU:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:805:ARG:CZ	9:A:808:PRO:HA	2.48	0.42
9:A:1395:TYR:HA	9:A:1398:LEU:HD23	2.00	0.42
10:B:33:TYR:HB2	10:B:653:TRP:CZ3	2.54	0.42
10:B:207:VAL:HG11	10:B:375:ALA:CB	2.49	0.42
10:B:785:TYR:O	10:B:786:THR:HG22	2.19	0.42
24:P:3:A:H5"	24:P:4:C:OP2	2.19	0.42
2:1:459:GLY:C	2:1:460:THR:HG1	2.27	0.42
18:J:47:ARG:CZ	18:J:48:MET:HE3	2.50	0.42
35:d:81:LEU:HD13	35:d:97:THR:HB	2.01	0.42
3:2:481:VAL:HB	5:4:158:HIS:CB	2.50	0.42
9:A:1315:ASP:HA	9:A:1318:LYS:HB3	2.01	0.42
22:N:118:DT:H2"	22:N:119:DA:C8	2.54	0.42
27:T:-124:DG:H21	32:a:40:HIS:CB	2.30	0.42
28:U:25:VAL:HG11	29:V:36:VAL:HG13	2.02	0.42
34:c:112:ILE:HG23	34:c:116:LEU:HD12	2.01	0.42
34:g:93:GLU:CD	35:h:107:LEU:HG	2.45	0.42
1:0:467:THR:O	1:0:468:ALA:HB3	2.20	0.42
5:4:55:LEU:HA	5:4:240:PRO:HA	2.01	0.42
9:A:418:TYR:HB2	9:A:447:GLU:HB2	2.01	0.42
23:O:297:LYS:CB	23:O:298:PRO:HD3	2.49	0.42
27:T:-72:DT:H2"	27:T:-71:DT:C5	2.55	0.42
28:U:349:TRP:HB3	28:U:351:PHE:CZ	2.54	0.42
30:W:22:ILE:HA	30:W:26:TYR:CD1	2.55	0.42
1:0:394:SER:HA	1:0:397:LYS:NZ	2.34	0.42
1:0:558:ILE:O	1:0:603:ASN:O	2.38	0.42
9:A:435:PRO:HA	9:A:438:LEU:HB2	2.02	0.42
9:A:983:LEU:HD22	9:A:983:LEU:H	1.84	0.42
10:B:751:LEU:HD12	10:B:808:SER:HB3	2.02	0.42
21:M:130:LEU:HD22	21:M:134:ILE:HD13	2.00	0.42
21:M:235:ILE:HG22	21:M:300:PHE:HA	2.01	0.42
30:W:124:ARG:HB2	30:W:170:LYS:HE2	2.01	0.42
32:e:62:LEU:HD22	33:f:37:ARG:HE	1.84	0.42
7:6:8:VAL:HG23	7:6:47:ALA:HA	2.02	0.42
9:A:510:GLU:HA	14:F:67:GLY:HA3	2.01	0.42
10:B:136:GLY:O	10:B:137:GLU:HG3	2.19	0.42
10:B:737:ILE:HD12	10:B:737:ILE:HA	1.86	0.42
10:B:962:THR:O	18:J:9:THR:HG23	2.20	0.42
21:M:120:GLU:HG3	21:M:124:MET:HE2	2.01	0.42
32:e:71:LEU:HD13	33:f:27:ILE:HA	2.02	0.42
9:A:865:ILE:O	9:A:869:GLU:HB3	2.20	0.42
10:B:225:LEU:HG	10:B:226:GLU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:515:PRO:O	10:B:520:VAL:HA	2.19	0.42
22:N:49:DT:H2''	22:N:50:DT:H2'	2.01	0.42
22:N:99:DG:C5	22:N:100:DA:C6	3.08	0.42
30:W:127:PHE:HD2	30:W:161:VAL:HG11	1.84	0.42
2:1:354:PRO:HB2	2:1:355:PRO:HD3	2.01	0.42
9:A:924:TYR:CZ	9:A:949:GLN:HB3	2.55	0.42
10:B:99:TRP:NE1	10:B:105:PRO:HB3	2.35	0.42
11:C:190:ASN:ND2	11:C:193:ARG:HD3	2.35	0.42
12:D:44:ARG:NH1	12:D:47:GLN:OE1	2.53	0.42
26:R:26:TYR:O	26:R:30:GLN:HG2	2.20	0.42
26:R:191:PHE:HB2	26:R:235:LEU:HD23	2.02	0.42
27:T:-56:DA:C6	27:T:-55:DG:C6	3.07	0.42
27:T:-27:DA:H3'	33:b:79:ARG:CD	2.50	0.42
6:5:146:ARG:NH1	6:5:147:MET:HA	2.35	0.42
9:A:1141:VAL:HB	9:A:1336:LEU:HB2	2.02	0.42
9:A:1153:ARG:O	9:A:1157:ILE:HG12	2.20	0.42
9:A:1243:LEU:HD13	9:A:1261:ILE:HA	2.01	0.42
10:B:65:ILE:HG23	10:B:416:ARG:HG2	2.02	0.42
12:D:103:LEU:HD22	15:G:144:ARG:HD2	2.02	0.42
27:T:42:DA:H2''	27:T:43:DG:C8	2.55	0.42
1:0:148:VAL:N	1:0:149:PRO:CD	2.84	0.41
1:0:467:THR:C	1:0:469:THR:N	2.78	0.41
3:2:218:LYS:HA	3:2:221:TRP:CE3	2.55	0.41
5:4:169:ILE:HG21	5:4:171:PHE:CE1	2.55	0.41
7:6:16:MET:O	7:6:19:PHE:HB2	2.20	0.41
7:6:38:ILE:H	7:6:38:ILE:HD12	1.85	0.41
9:A:567:LEU:HD23	9:A:570:TRP:HB2	2.02	0.41
10:B:363:TYR:CG	10:B:553:LEU:HD23	2.55	0.41
10:B:553:LEU:HD12	10:B:575:GLY:HA2	2.01	0.41
10:B:865:VAL:HG22	10:B:895:PHE:CD2	2.55	0.41
33:b:100:GLY:HA2	35:h:62:ILE:HG13	2.03	0.41
9:A:834:THR:HG23	10:B:677:MET:HE3	2.02	0.41
10:B:590:LEU:HD23	10:B:590:LEU:HA	1.86	0.41
12:D:17:ALA:HB2	15:G:80:PHE:HB2	2.02	0.41
19:K:20:THR:OG1	19:K:34:THR:HB	2.20	0.41
22:N:192:DT:H2''	22:N:193:DA:C8	2.55	0.41
34:g:27:PRO:HD3	35:h:41:TYR:CD1	2.56	0.41
1:0:510:VAL:HG11	1:0:693:LEU:CD1	2.51	0.41
3:2:299:SER:O	3:2:303:ILE:HG12	2.20	0.41
9:A:577:PRO:HB3	9:A:586:TRP:CD2	2.55	0.41
10:B:380:ARG:CZ	10:B:609:GLU:HG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:52:ILE:HD12	11:C:61:ASP:HB3	2.02	0.41
21:M:24:VAL:HG23	21:M:35:PRO:HB3	2.01	0.41
22:N:139:DA:H2''	22:N:140:DA:C8	2.55	0.41
29:V:72:TRP:CE3	29:V:74:PHE:CZ	3.09	0.41
30:W:137:THR:HG22	30:W:139:LEU:H	1.84	0.41
5:4:55:LEU:HD22	5:4:238:PRO:O	2.20	0.41
9:A:153:ILE:HD12	9:A:187:TYR:HA	2.03	0.41
9:A:791:GLN:HE22	9:A:839:HIS:N	2.18	0.41
10:B:961:ILE:CG1	18:J:42:ARG:HD2	2.50	0.41
12:D:33:LEU:O	12:D:37:VAL:HG23	2.21	0.41
22:N:51:DG:H2''	22:N:52:DA:C8	2.55	0.41
1:0:129:VAL:HG23	1:0:131:LEU:HG	2.02	0.41
1:0:399:LYS:H	1:0:400:PRO:HD3	1.85	0.41
10:B:369:VAL:O	10:B:373:LEU:HG	2.20	0.41
10:B:1068:GLN:CG	10:B:1075:MET:HB3	2.49	0.41
23:O:322:TYR:N	23:O:322:TYR:CD1	2.86	0.41
2:1:664:VAL:HG11	2:1:679:PHE:CZ	2.56	0.41
2:1:711:ASP:O	2:1:715:GLN:HG2	2.20	0.41
10:B:385:ARG:O	10:B:391:LYS:HE3	2.21	0.41
10:B:603:MET:HE2	10:B:603:MET:HB2	1.86	0.41
13:E:88:LYS:O	13:E:92:GLN:HG2	2.21	0.41
16:H:121:LEU:HD23	16:H:121:LEU:HA	1.83	0.41
17:I:121:HIS:CD2	17:I:123:TRP:CE3	3.09	0.41
22:N:203:DC:OP2	22:N:203:DC:H2'	2.21	0.41
27:T:-115:DA:H2'	27:T:-114:DT:H71	2.01	0.41
28:U:46:TRP:CD1	29:V:15:LEU:HB2	2.55	0.41
34:g:32:HIS:CD2	34:g:36:ARG:HE	2.39	0.41
1:0:88:ALA:HA	1:0:93:TYR:CD1	2.55	0.41
1:0:510:VAL:HG22	1:0:690:ILE:HB	2.02	0.41
2:1:82:LYS:HD2	2:1:613:HIS:CE1	2.56	0.41
9:A:994:PHE:CE2	9:A:1064:ALA:HA	2.56	0.41
9:A:1484:MET:HG3	14:F:80:MET:C	2.45	0.41
10:B:115:LEU:O	10:B:920:LYS:HE3	2.21	0.41
10:B:204:THR:HB	10:B:206:TYR:OH	2.20	0.41
10:B:926:VAL:HG21	11:C:62:GLU:HG3	2.02	0.41
20:L:19:CYS:O	20:L:23:HIS:HA	2.20	0.41
22:N:71:DC:H1'	22:N:72:DG:O5'	2.20	0.41
22:N:109:DA:H2''	22:N:110:DA:C8	2.55	0.41
22:N:188:DT:H2''	22:N:189:DC:C5	2.55	0.41
28:U:356:GLY:HA3	28:U:367:PHE:CZ	2.56	0.41
1:0:327:MET:HG3	1:0:335:SER:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:460:ARG:HG2	9:A:462:PRO:HD2	2.03	0.41
9:A:812:LYS:HB2	17:I:78:LEU:HD23	2.03	0.41
9:A:1143:LEU:HB2	9:A:1148:ALA:HB2	2.03	0.41
11:C:78:ILE:HG21	11:C:127:VAL:CG2	2.51	0.41
15:G:18:PHE:N	15:G:18:PHE:CD1	2.86	0.41
26:R:9:LEU:H	26:R:9:LEU:CD2	2.31	0.41
27:T:-88:DG:C6	27:T:-87:DT:C4	3.09	0.41
27:T:-6:DC:H3'	35:d:40:ILE:CD1	2.51	0.41
34:c:80:ILE:HG12	34:c:83:HIS:CE1	2.55	0.41
1:0:294:GLU:HB3	1:0:332:ARG:HB3	2.03	0.41
1:0:551:HIS:CB	1:0:558:ILE:HD11	2.50	0.41
3:2:483:THR:HG21	3:2:492:LYS:HE2	2.01	0.41
3:2:488:GLU:CD	5:4:158:HIS:HD2	2.29	0.41
4:3:90:LEU:HG	4:3:95:ILE:HD12	2.03	0.41
4:3:109:ILE:CG1	4:3:115:ARG:HH22	2.33	0.41
4:3:431:LEU:HD21	4:3:434:GLU:HG2	2.02	0.41
6:5:39:ASP:O	6:5:43:VAL:HG23	2.21	0.41
9:A:42:LYS:HE3	9:A:43:TYR:CZ	2.55	0.41
9:A:1245:CYS:HA	9:A:1258:ARG:O	2.21	0.41
10:B:206:TYR:HB3	10:B:208:PHE:CZ	2.56	0.41
10:B:625:LEU:HD23	10:B:625:LEU:HA	1.82	0.41
10:B:712:PRO:HB3	10:B:999:ALA:HB3	2.02	0.41
22:N:14:DA:H2	23:O:169:VAL:HG21	1.86	0.41
22:N:164:DC:H4'	32:e:42:TYR:CE2	2.56	0.41
23:O:288:PHE:CD1	23:O:289:PRO:HD2	2.55	0.41
25:Q:164:TRP:NE1	25:Q:167:ARG:HH22	2.18	0.41
29:V:71:VAL:HG13	29:V:98:CYS:SG	2.61	0.41
31:X:77:VAL:O	31:X:81:ILE:HG12	2.20	0.41
1:0:89:PHE:CG	4:3:375:VAL:HG21	2.56	0.41
3:2:47:TYR:HB3	3:2:100:LEU:HD23	2.03	0.41
9:A:621:ILE:CD1	16:H:124:ARG:HB2	2.50	0.41
10:B:1127:ILE:O	10:B:1135:TYR:HA	2.21	0.41
12:D:132:ASP:O	12:D:136:THR:HG23	2.21	0.41
13:E:173:ILE:HG23	13:E:209:VAL:HA	2.03	0.41
22:N:212:DG:H1'	22:N:213:DA:N7	2.36	0.41
34:g:32:HIS:CE1	34:g:36:ARG:HE	2.39	0.41
1:0:51:THR:HG23	1:0:52:LYS:H	1.85	0.40
9:A:680:LEU:HD21	10:B:784:SER:HB3	2.03	0.40
10:B:764:MET:HE1	10:B:938:ARG:NH1	2.36	0.40
17:I:20:CYS:SG	17:I:22:ASN:HB2	2.60	0.40
22:N:49:DT:C2'	22:N:50:DT:H5'	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:N:93:DG:C2	27:T:7:DG:N2	2.89	0.40
27:T:-50:DT:H1'	27:T:-49:DA:C8	2.55	0.40
33:b:72:THR:HG22	35:d:97:THR:HG23	2.02	0.40
1:0:522:TYR:CD1	1:0:522:TYR:C	2.99	0.40
1:0:631:GLY:HA2	1:0:635:GLN:CB	2.41	0.40
10:B:93:LEU:HD12	10:B:123:PRO:O	2.21	0.40
11:C:84:TYR:CE1	11:C:167:LYS:HG2	2.56	0.40
12:D:36:GLU:OE2	12:D:84:ARG:NH2	2.54	0.40
24:P:3:A:C6	24:P:4:C:C4	3.09	0.40
30:W:171:LYS:O	30:W:175:THR:HG23	2.21	0.40
31:X:132:VAL:HG22	31:X:137:TYR:CD1	2.56	0.40
2:1:489:CYS:HA	2:1:724:MET:SD	2.61	0.40
9:A:495:ASP:OD1	9:A:495:ASP:O	2.40	0.40
10:B:1092:ASP:OD1	10:B:1092:ASP:C	2.64	0.40
16:H:92:MET:HE2	16:H:118:TYR:HB3	2.02	0.40
18:J:16:ASN:OD1	18:J:17:LYS:HG3	2.21	0.40
22:N:53:DA:H2''	22:N:54:DC:H6	1.86	0.40
22:N:91:DC:H2''	22:N:92:DC:C5	2.56	0.40
22:N:206:DG:C2	27:T:-106:DG:C2	3.09	0.40
28:U:339:TYR:CZ	29:V:99:ASP:HB3	2.56	0.40
30:W:16:ARG:HG3	31:X:208:CYS:SG	2.61	0.40
2:1:460:THR:HG23	2:1:696:TRP:CZ2	2.56	0.40
2:1:571:THR:H	2:1:577:THR:HG22	1.86	0.40
3:2:486:LEU:O	3:2:489:LYS:HG2	2.21	0.40
4:3:90:LEU:HD22	4:3:96:TRP:CH2	2.56	0.40
5:4:220:HIS:HD2	5:4:235:HIS:CD2	2.38	0.40
10:B:331:THR:HG23	10:B:334:LYS:H	1.87	0.40
10:B:771:GLU:O	18:J:55:LEU:HD21	2.21	0.40
11:C:54:ALA:O	11:C:159:LEU:HD12	2.21	0.40
13:E:9:ARG:HG3	13:E:136:LEU:HD21	2.04	0.40
18:J:47:ARG:HD2	18:J:47:ARG:C	2.46	0.40
22:N:9:DC:H2''	22:N:10:DT:C6	2.55	0.40
30:W:180:PHE:HB2	31:X:216:PHE:CE1	2.56	0.40
3:2:498:GLU:O	3:2:502:VAL:HG13	2.22	0.40
9:A:329:MET:SD	9:A:333:GLY:HA2	2.61	0.40
9:A:364:ARG:HB2	10:B:1084:LEU:HD11	2.03	0.40
9:A:790:GLN:HA	9:A:822:PHE:HA	2.03	0.40
9:A:844:ARG:NH2	10:B:501:LEU:HD13	2.36	0.40
9:A:932:ARG:HD2	16:H:106:THR:O	2.21	0.40
10:B:528:LEU:HG	10:B:704:LEU:O	2.21	0.40
10:B:794:VAL:HG13	10:B:965:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:44:ILE:HG21	11:C:178:PRO:HB3	2.02	0.40
13:E:11:TRP:HB2	13:E:40:PHE:CD2	2.56	0.40
16:H:95:LYS:HD3	16:H:138:ASP:HA	2.03	0.40
22:N:140:DA:H2"	22:N:141:DA:C8	2.57	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	0	601/782 (77%)	566 (94%)	35 (6%)	0	100	100
2	1	710/760 (93%)	673 (95%)	35 (5%)	2 (0%)	36	72
3	2	359/548 (66%)	346 (96%)	13 (4%)	0	100	100
4	3	413/462 (89%)	393 (95%)	20 (5%)	0	100	100
5	4	341/395 (86%)	318 (93%)	23 (7%)	0	100	100
6	5	259/308 (84%)	248 (96%)	11 (4%)	0	100	100
7	6	67/71 (94%)	63 (94%)	4 (6%)	0	100	100
8	7	147/309 (48%)	137 (93%)	10 (7%)	0	100	100
9	A	1411/1984 (71%)	1350 (96%)	61 (4%)	0	100	100
10	B	1111/1300 (86%)	1079 (97%)	32 (3%)	0	100	100
11	C	253/275 (92%)	247 (98%)	6 (2%)	0	100	100
12	D	126/184 (68%)	121 (96%)	5 (4%)	0	100	100
13	E	207/210 (99%)	204 (99%)	3 (1%)	0	100	100
14	F	77/127 (61%)	75 (97%)	2 (3%)	0	100	100
15	G	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
16	H	146/150 (97%)	144 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	I	112/125 (90%)	105 (94%)	7 (6%)	0	100	100
18	J	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
19	K	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
20	L	42/58 (72%)	41 (98%)	1 (2%)	0	100	100
21	M	288/316 (91%)	277 (96%)	11 (4%)	0	100	100
23	O	177/339 (52%)	175 (99%)	2 (1%)	0	100	100
25	Q	134/517 (26%)	127 (95%)	7 (5%)	0	100	100
26	R	218/249 (88%)	214 (98%)	4 (2%)	0	100	100
28	U	109/376 (29%)	106 (97%)	3 (3%)	0	100	100
29	V	97/109 (89%)	93 (96%)	4 (4%)	0	100	100
30	W	185/439 (42%)	185 (100%)	0	0	100	100
31	X	169/291 (58%)	163 (96%)	6 (4%)	0	100	100
32	a	95/136 (70%)	94 (99%)	1 (1%)	0	100	100
32	e	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
33	b	80/103 (78%)	79 (99%)	1 (1%)	0	100	100
33	f	78/103 (76%)	75 (96%)	3 (4%)	0	100	100
34	c	107/130 (82%)	106 (99%)	1 (1%)	0	100	100
34	g	104/130 (80%)	102 (98%)	2 (2%)	0	100	100
35	d	95/126 (75%)	94 (99%)	1 (1%)	0	100	100
35	h	93/126 (74%)	93 (100%)	0	0	100	100
All	All	8851/12030 (74%)	8522 (96%)	327 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	671	LYS
2	1	721	LEU

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	0	536/688 (78%)	534 (100%)	2 (0%)	84	84
2	1	624/664 (94%)	615 (99%)	9 (1%)	59	72
3	2	333/484 (69%)	331 (99%)	2 (1%)	78	83
4	3	351/399 (88%)	347 (99%)	4 (1%)	65	76
5	4	311/352 (88%)	306 (98%)	5 (2%)	55	70
6	5	234/272 (86%)	231 (99%)	3 (1%)	61	74
7	6	62/64 (97%)	62 (100%)	0	100	100
8	7	143/283 (50%)	141 (99%)	2 (1%)	59	72
9	A	1252/1763 (71%)	1238 (99%)	14 (1%)	65	76
10	B	985/1127 (87%)	983 (100%)	2 (0%)	87	87
11	C	234/252 (93%)	234 (100%)	0	100	100
12	D	118/160 (74%)	116 (98%)	2 (2%)	53	69
13	E	191/192 (100%)	190 (100%)	1 (0%)	81	83
14	F	69/111 (62%)	69 (100%)	0	100	100
15	G	152/153 (99%)	152 (100%)	0	100	100
16	H	129/131 (98%)	128 (99%)	1 (1%)	73	80
17	I	103/112 (92%)	103 (100%)	0	100	100
18	J	53/56 (95%)	53 (100%)	0	100	100
19	K	104/106 (98%)	104 (100%)	0	100	100
20	L	41/55 (74%)	40 (98%)	1 (2%)	43	64
21	M	247/268 (92%)	247 (100%)	0	100	100
23	O	154/293 (53%)	154 (100%)	0	100	100
25	Q	121/448 (27%)	121 (100%)	0	100	100
26	R	196/218 (90%)	194 (99%)	2 (1%)	68	78
28	U	105/324 (32%)	105 (100%)	0	100	100
29	V	90/98 (92%)	90 (100%)	0	100	100
30	W	169/373 (45%)	168 (99%)	1 (1%)	78	83
31	X	154/261 (59%)	154 (100%)	0	100	100
32	a	85/111 (77%)	85 (100%)	0	100	100
32	e	86/111 (78%)	86 (100%)	0	100	100
33	b	67/79 (85%)	67 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	f	65/79 (82%)	65 (100%)	0	100	100
34	c	86/101 (85%)	86 (100%)	0	100	100
34	g	84/101 (83%)	84 (100%)	0	100	100
35	d	83/106 (78%)	83 (100%)	0	100	100
35	h	81/106 (76%)	81 (100%)	0	100	100
All	All	7898/10501 (75%)	7847 (99%)	51 (1%)	76	83

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	191	ASP
1	0	521	GLU
2	1	40	LEU
2	1	194	LEU
2	1	203	ASN
2	1	227	ARG
2	1	377	GLU
2	1	430	ASN
2	1	473	PHE
2	1	673	ASP
2	1	728	PHE
3	2	9	LEU
3	2	536	LEU
4	3	32	ASP
4	3	335	LEU
4	3	370	THR
4	3	434	GLU
5	4	230	GLU
5	4	311	THR
5	4	338	GLU
5	4	375	VAL
5	4	379	LEU
6	5	70	LEU
6	5	162	LEU
6	5	207	CYS
8	7	21	LEU
8	7	133	ILE
9	A	66	GLU
9	A	280	LEU
9	A	354	LEU

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Mol	Chain	Res	Type
9	A	465	HIS
9	A	490	THR
9	A	585	LEU
9	A	669	TYR
9	A	723	ASN
9	A	903	PHE
9	A	983	LEU
9	A	1158	LEU
9	A	1249	ASP
9	A	1291	ASN
9	A	1398	LEU
10	B	40	VAL
10	B	1092	ASP
12	D	118	LEU
12	D	129	GLN
13	E	135	LEU
16	H	96	VAL
20	L	31	ARG
26	R	9	LEU
26	R	14	GLN
30	W	143	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	154	GLN
1	0	181	HIS
1	0	366	ASN
1	0	497	GLN
1	0	714	GLN
2	1	97	GLN
2	1	114	ASN
2	1	148	HIS
2	1	164	HIS
2	1	430	ASN
2	1	522	ASN
2	1	560	ASN
2	1	585	GLN
2	1	613	HIS
3	2	64	GLN
3	2	76	ASN
3	2	309	HIS

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Mol	Chain	Res	Type
3	2	375	ASN
3	2	384	HIS
3	2	402	ASN
3	2	496	ASN
4	3	15	GLN
4	3	68	GLN
4	3	211	GLN
4	3	390	GLN
5	4	158	HIS
5	4	220	HIS
5	4	324	HIS
5	4	340	ASN
5	4	387	HIS
6	5	9	ASN
6	5	48	HIS
6	5	55	ASN
8	7	57	ASN
8	7	136	ASN
9	A	77	ASN
9	A	143	HIS
9	A	313	HIS
9	A	439	HIS
9	A	516	GLN
9	A	529	GLN
9	A	599	HIS
9	A	673	GLN
9	A	723	ASN
9	A	731	ASN
9	A	742	ASN
9	A	792	ASN
9	A	905	ASN
9	A	947	HIS
9	A	1005	HIS
9	A	1032	GLN
9	A	1036	ASN
9	A	1251	ASN
9	A	1291	ASN
10	B	56	GLN
10	B	265	GLN
10	B	312	GLN
10	B	420	GLN
10	B	452	ASN

Continued on next page...

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Mol	Chain	Res	Type
10	B	582	GLN
10	B	593	GLN
10	B	642	GLN
10	B	654	GLN
10	B	741	HIS
10	B	913	GLN
10	B	1094	GLN
10	B	1120	ASN
10	B	1142	ASN
11	C	190	ASN
11	C	217	GLN
12	D	38	HIS
13	E	92	GLN
13	E	95	GLN
13	E	133	GLN
14	F	49	GLN
15	G	28	GLN
16	H	133	HIS
19	K	89	ASN
21	M	140	ASN
21	M	156	ASN
23	O	166	GLN
23	O	242	GLN
23	O	277	HIS
23	O	278	GLN
25	Q	10	ASN
25	Q	142	ASN
25	Q	152	HIS
26	R	14	GLN
26	R	81	HIS
26	R	182	HIS
28	U	48	ASN
28	U	347	ASN
29	V	4	GLN
29	V	35	GLN
31	X	144	ASN
31	X	177	ASN
31	X	188	GLN
32	a	69	GLN
32	a	109	ASN
35	d	68	ASN
34	g	25	GLN

Continued on next page...

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Mol	Chain	Res	Type
35	h	50	HIS
35	h	85	ASN
35	h	110	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	P	5/6 (83%)	3 (60%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
24	P	4	C
24	P	5	C
24	P	6	C

There are no RNA pucker outliers to report.

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 19 ligands modelled in this entry, 18 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	SF4	1	1000	2	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	SF4	1	1000	2	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

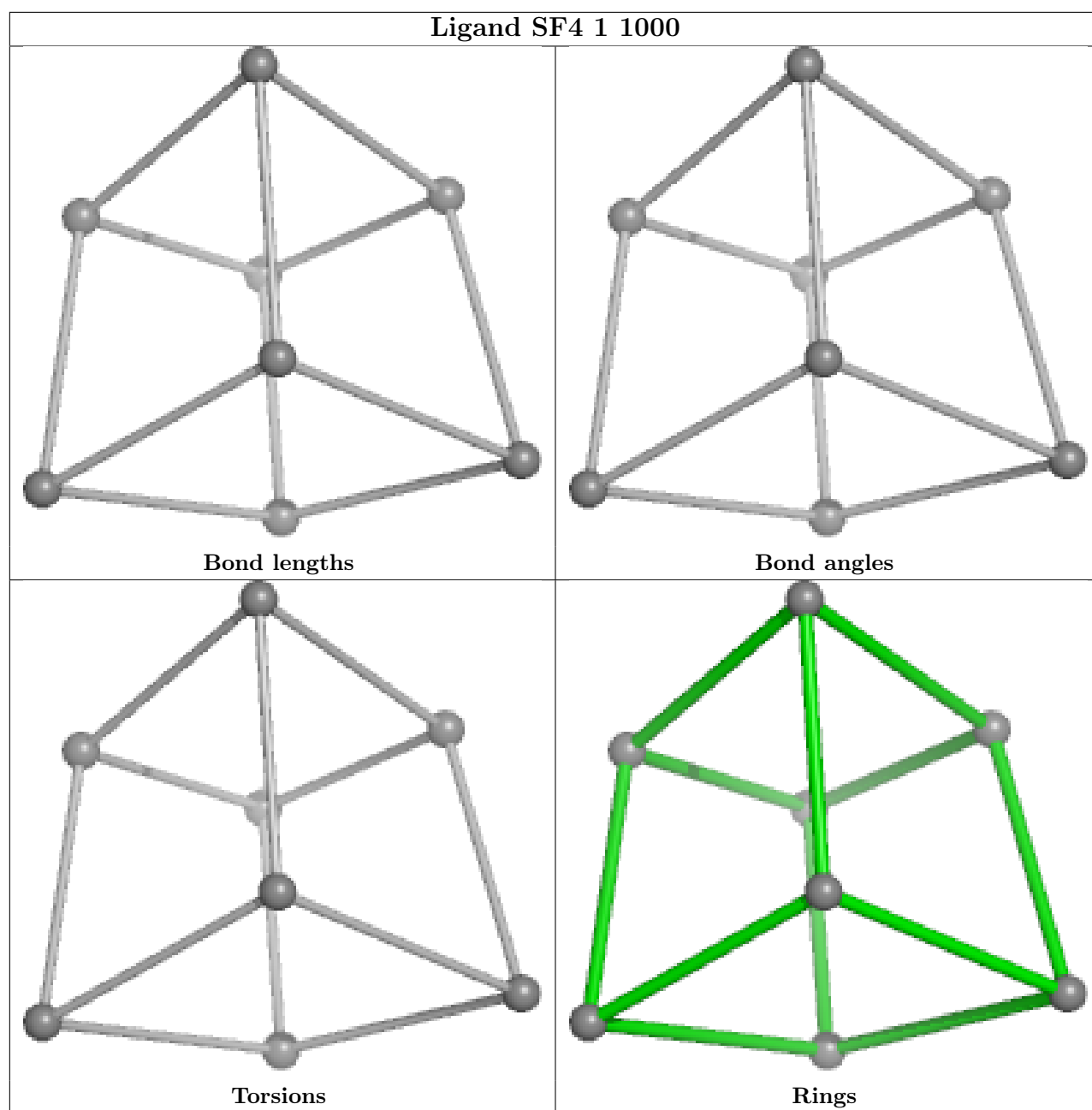
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

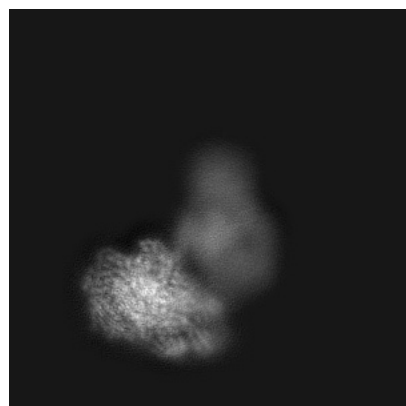
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57693. These allow visual inspection of the internal detail of the map and identification of artifacts.

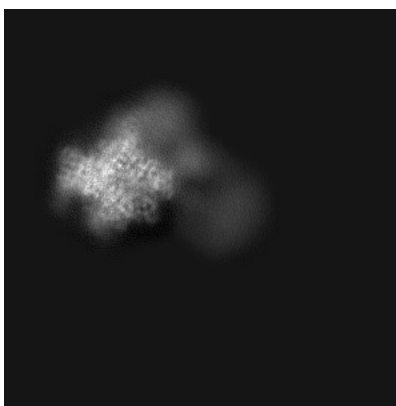
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

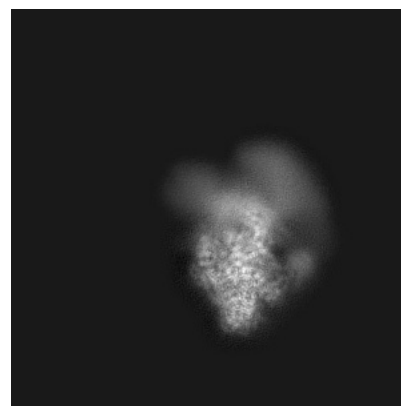
6.1.1 Primary map



X

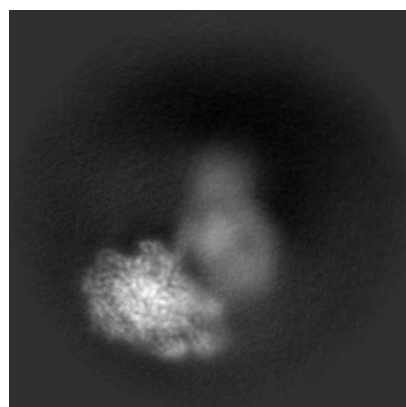


Y

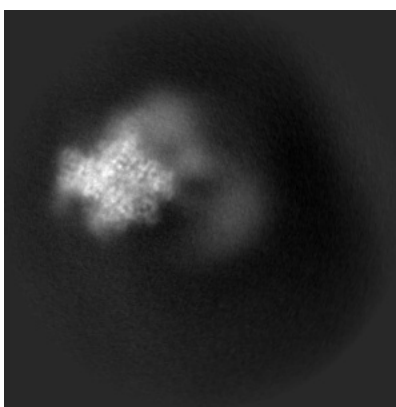


Z

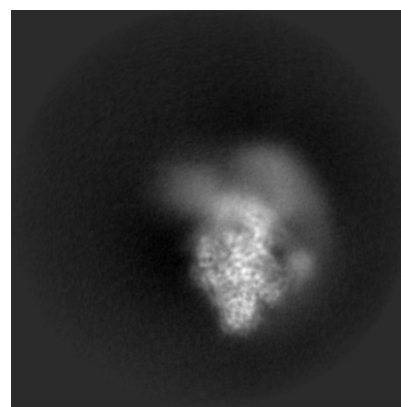
6.1.2 Raw map



X



Y

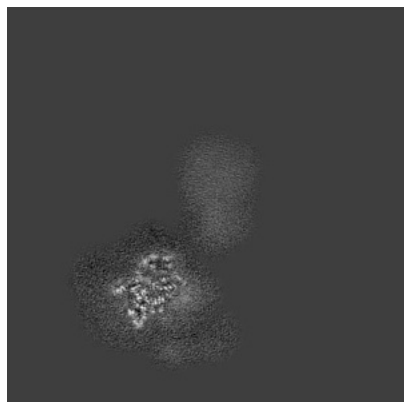


Z

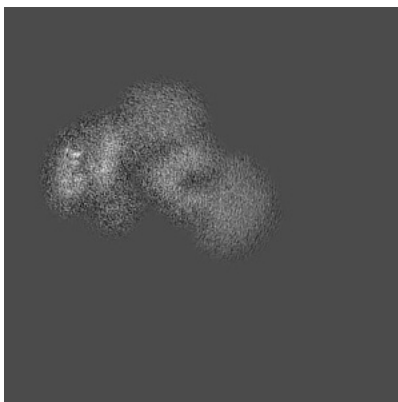
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

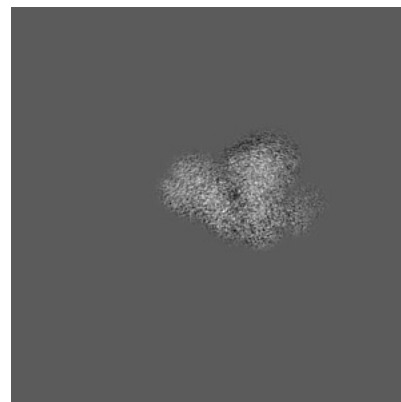
6.2.1 Primary map



X Index: 240

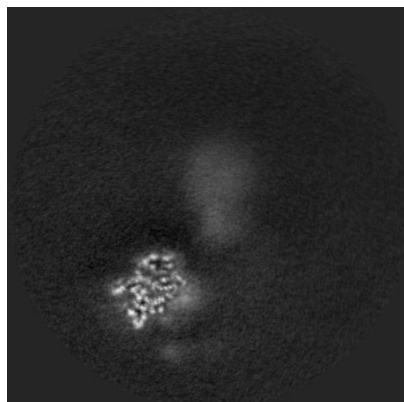


Y Index: 240

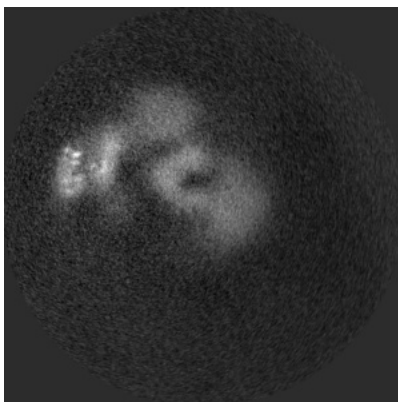


Z Index: 240

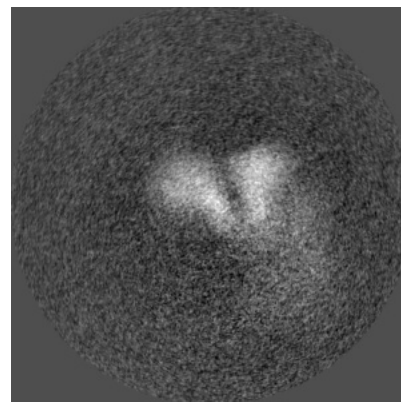
6.2.2 Raw map



X Index: 240



Y Index: 240

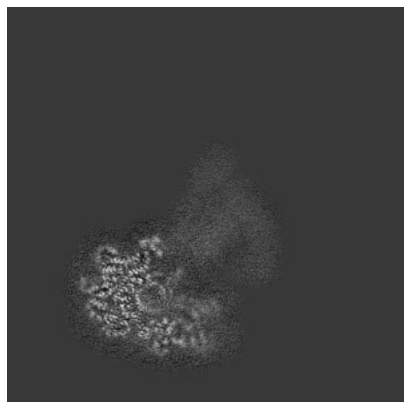


Z Index: 240

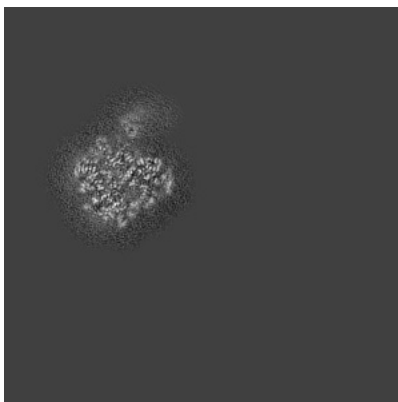
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

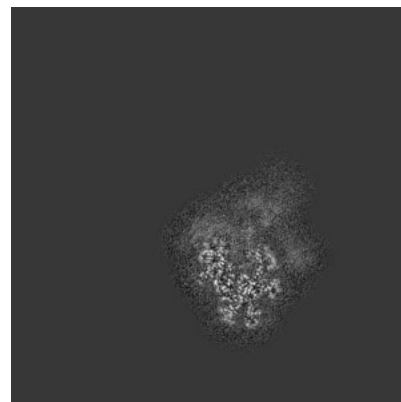
6.3.1 Primary map



X Index: 281

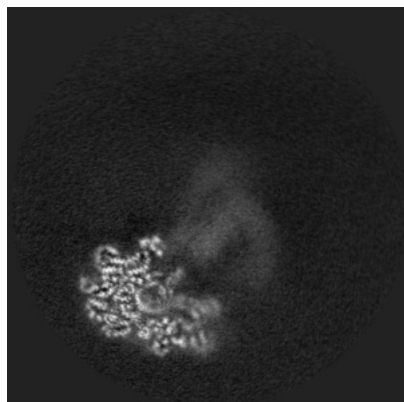


Y Index: 159

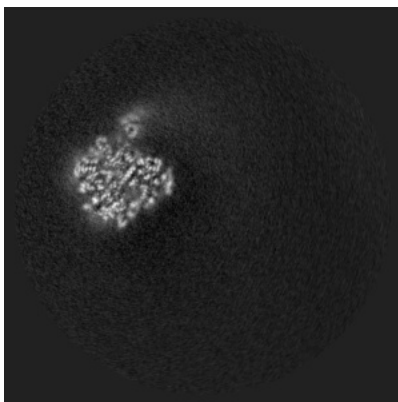


Z Index: 129

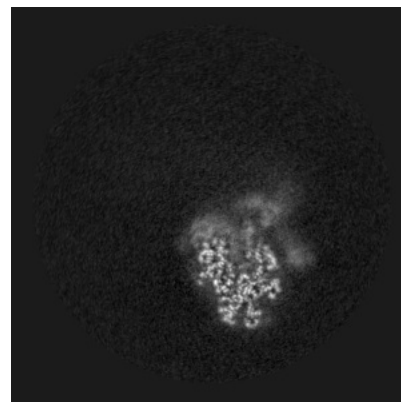
6.3.2 Raw map



X Index: 281



Y Index: 159

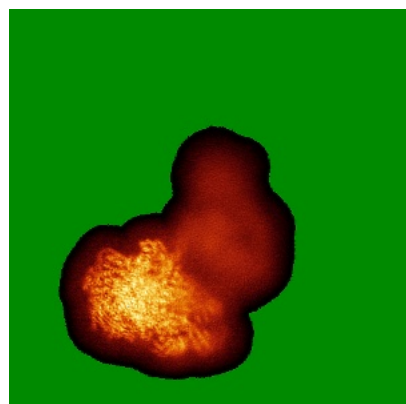


Z Index: 129

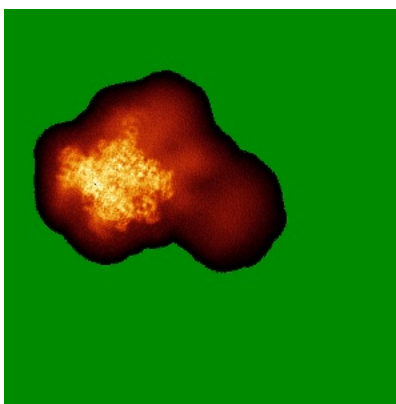
The images above show the largest variance slices of the map in three orthogonal directions.

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

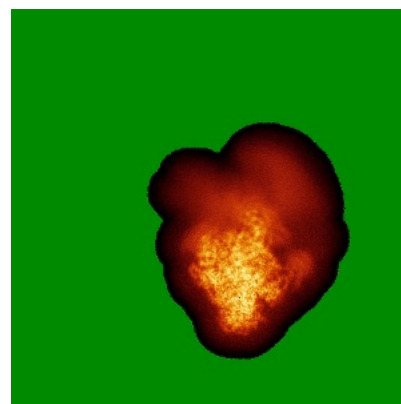
6.4.1 Primary map



X

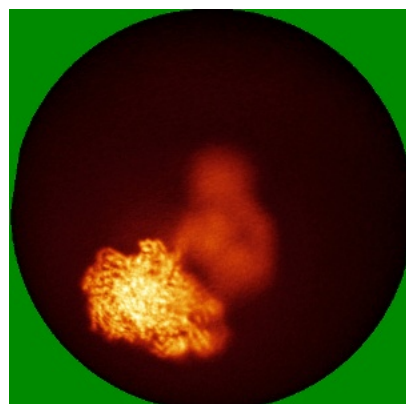


Y

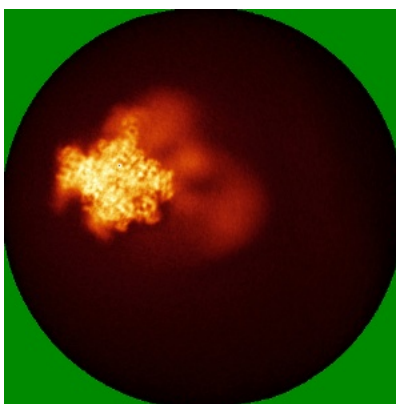


Z

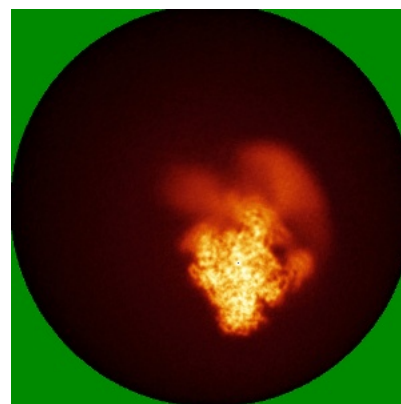
6.4.2 Raw map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

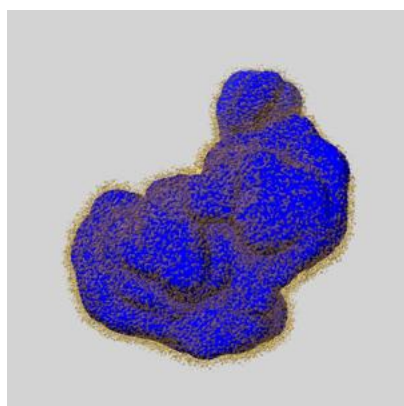
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

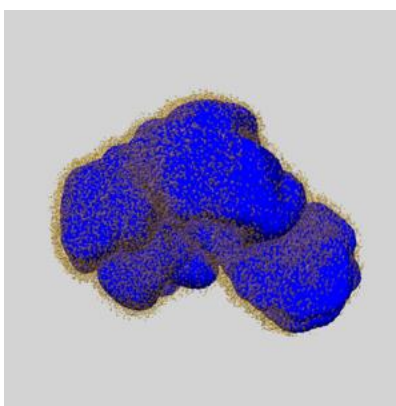
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

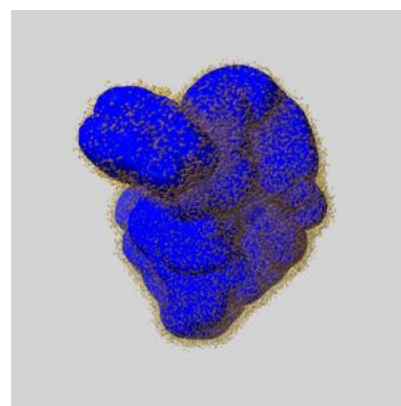
6.6.1 emd_57693_msk_1.map [i](#)



X



Y

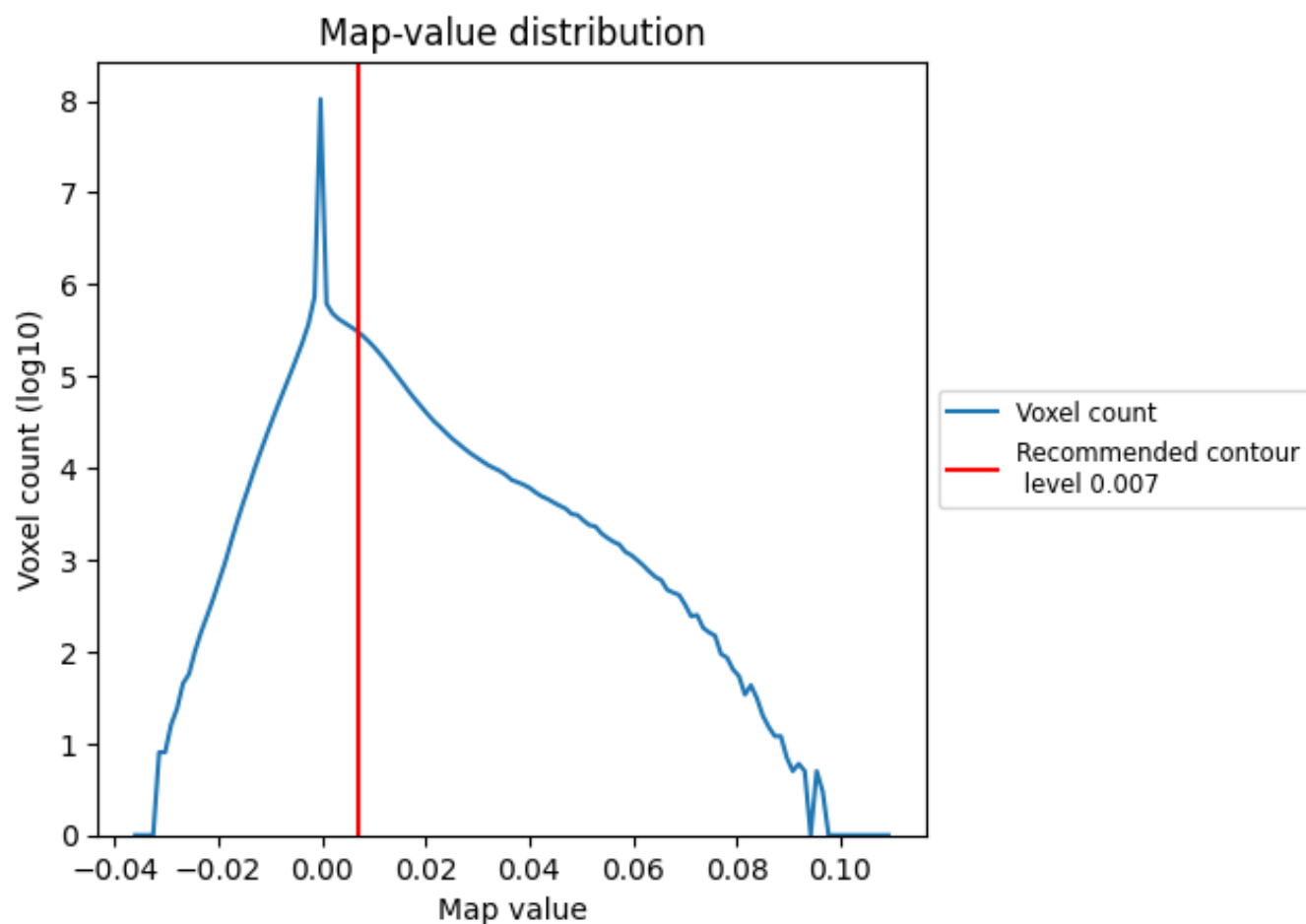


Z

7 Map analysis [i](#)

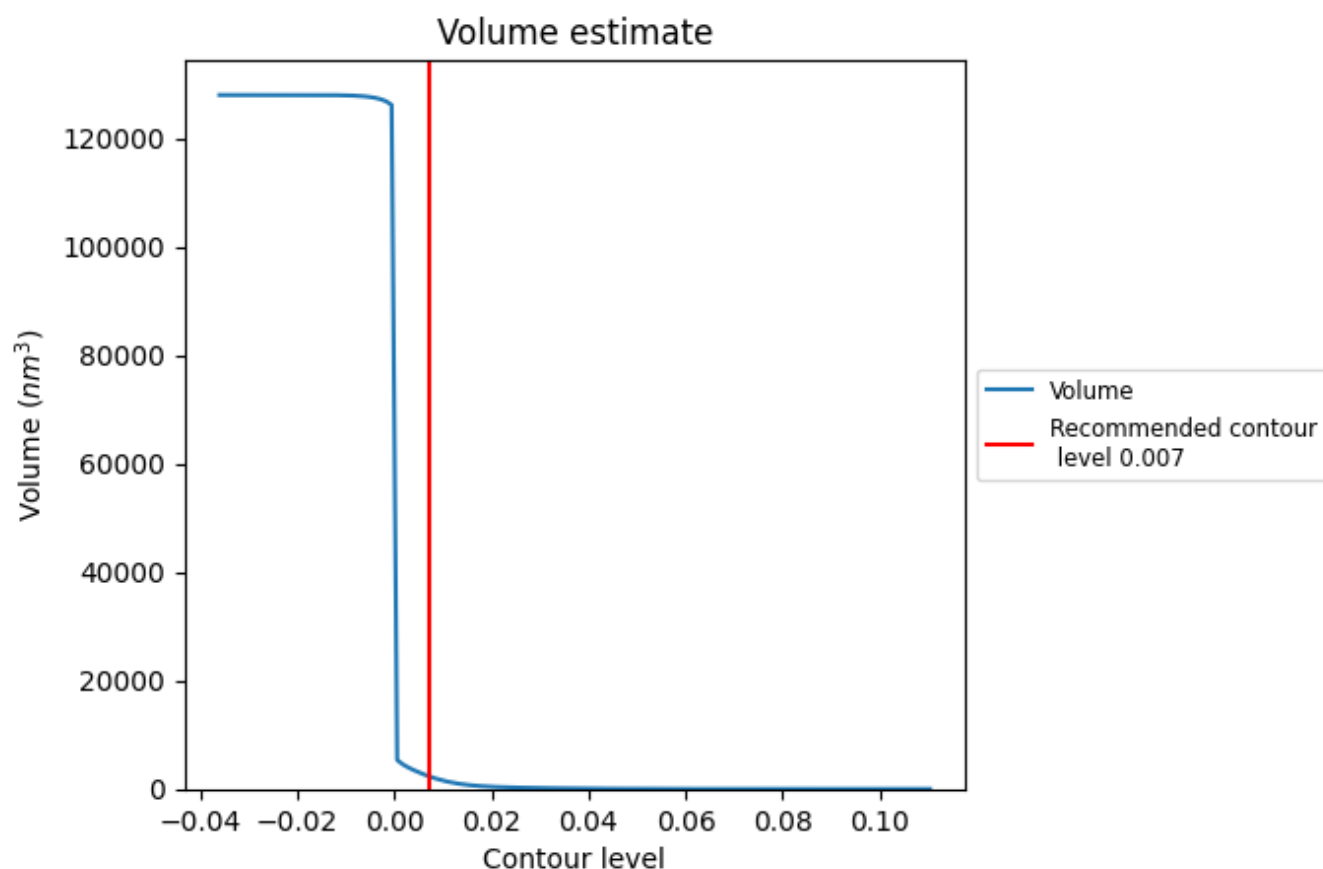
This section contains the results of statistical analysis of the map.

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.

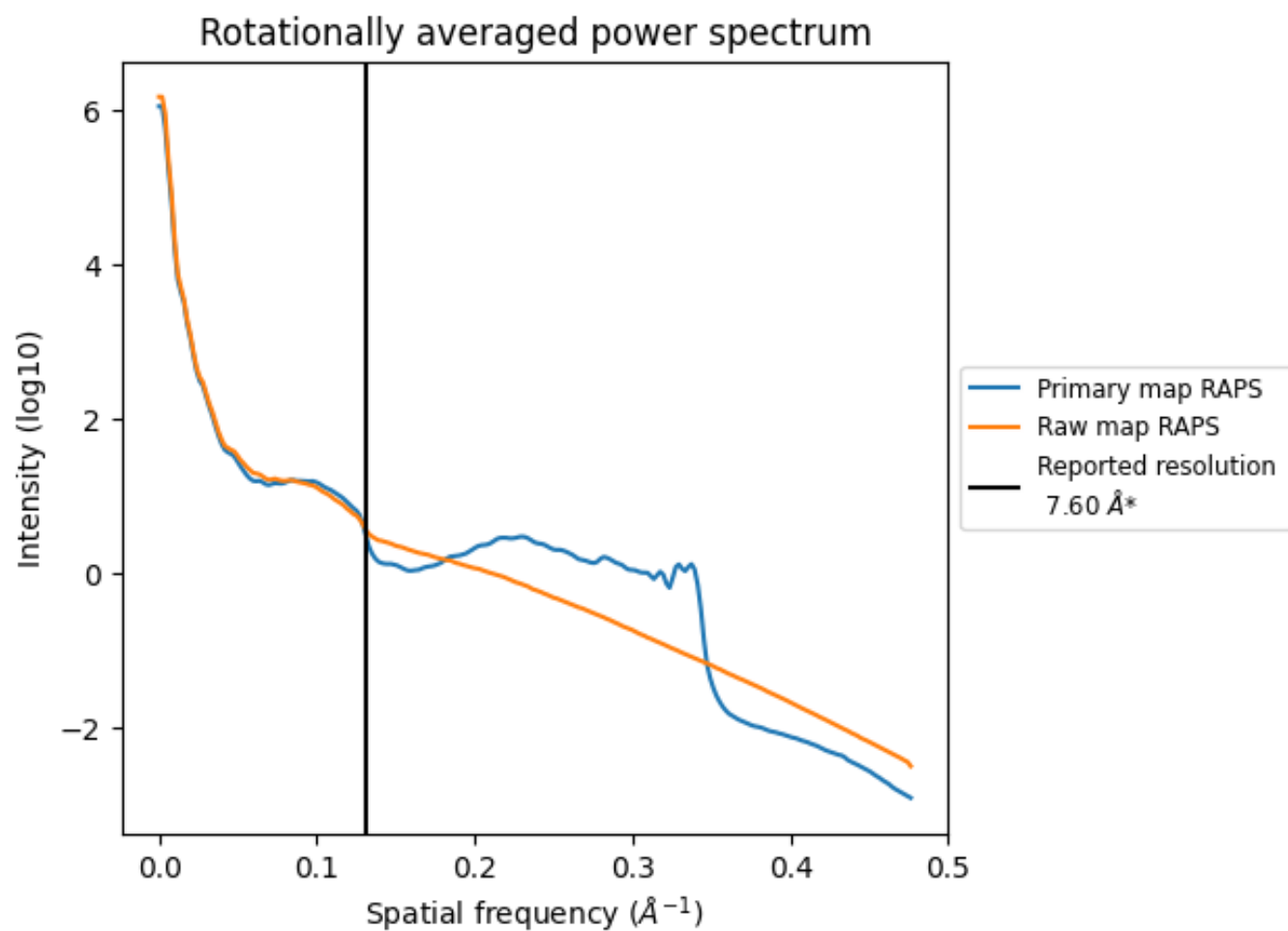
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2385 nm^3 ; this corresponds to an approximate mass of 2154 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 ⓘ

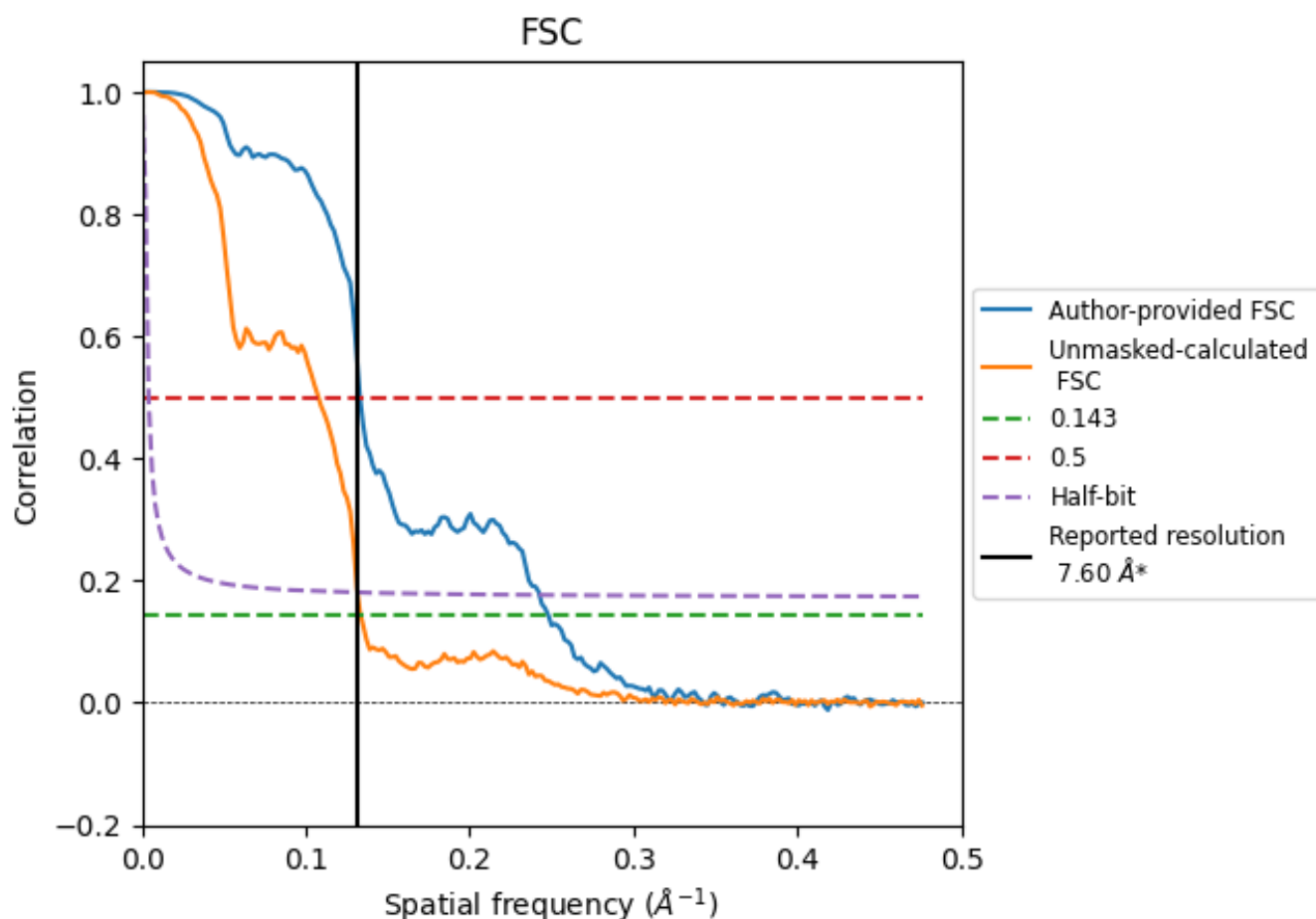


*Reported resolution corresponds to spatial frequency of 0.132 Å⁻¹

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 0.132 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

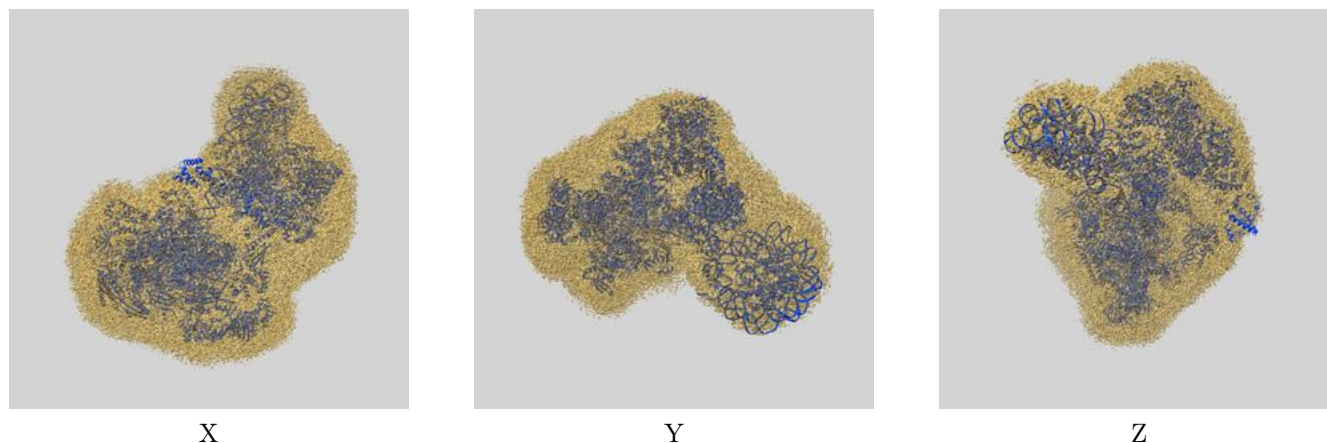
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.60	-	-
Author-provided FSC curve	4.03	7.52	4.12
Unmasked-calculated*	7.49	9.29	7.62

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.03 differs from the reported value 7.6 by more than 10 %

9 Map-model fit [i](#)

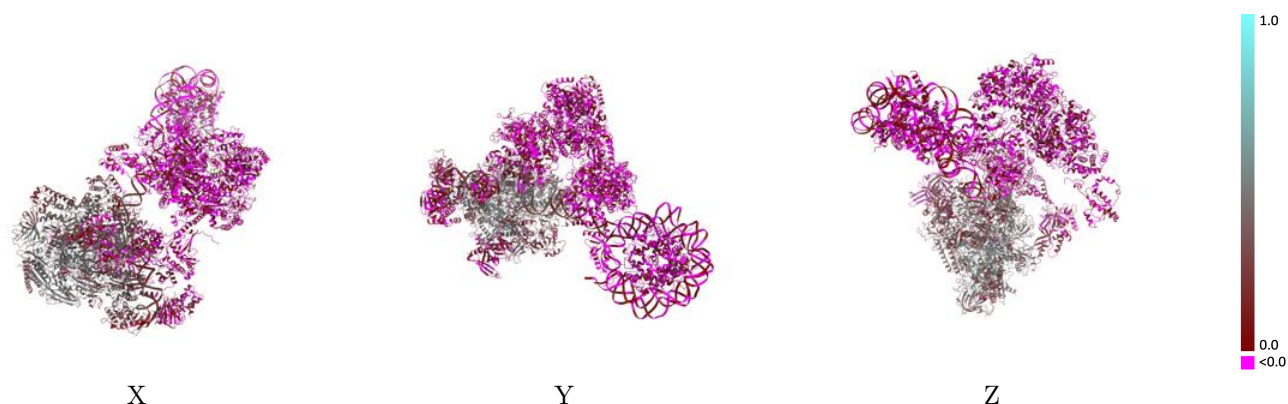
This section contains information regarding the fit between EMDB map EMD-57693 and PDB model 30FH. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



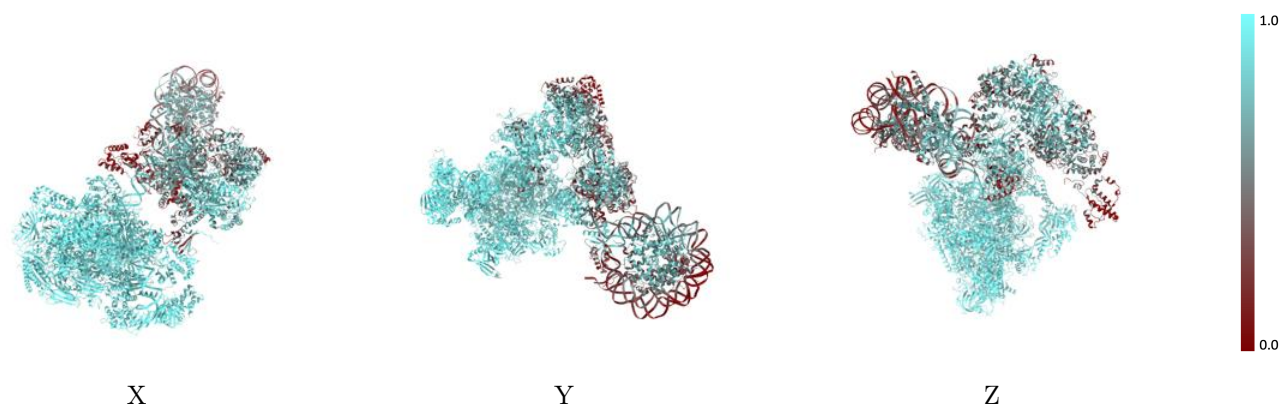
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



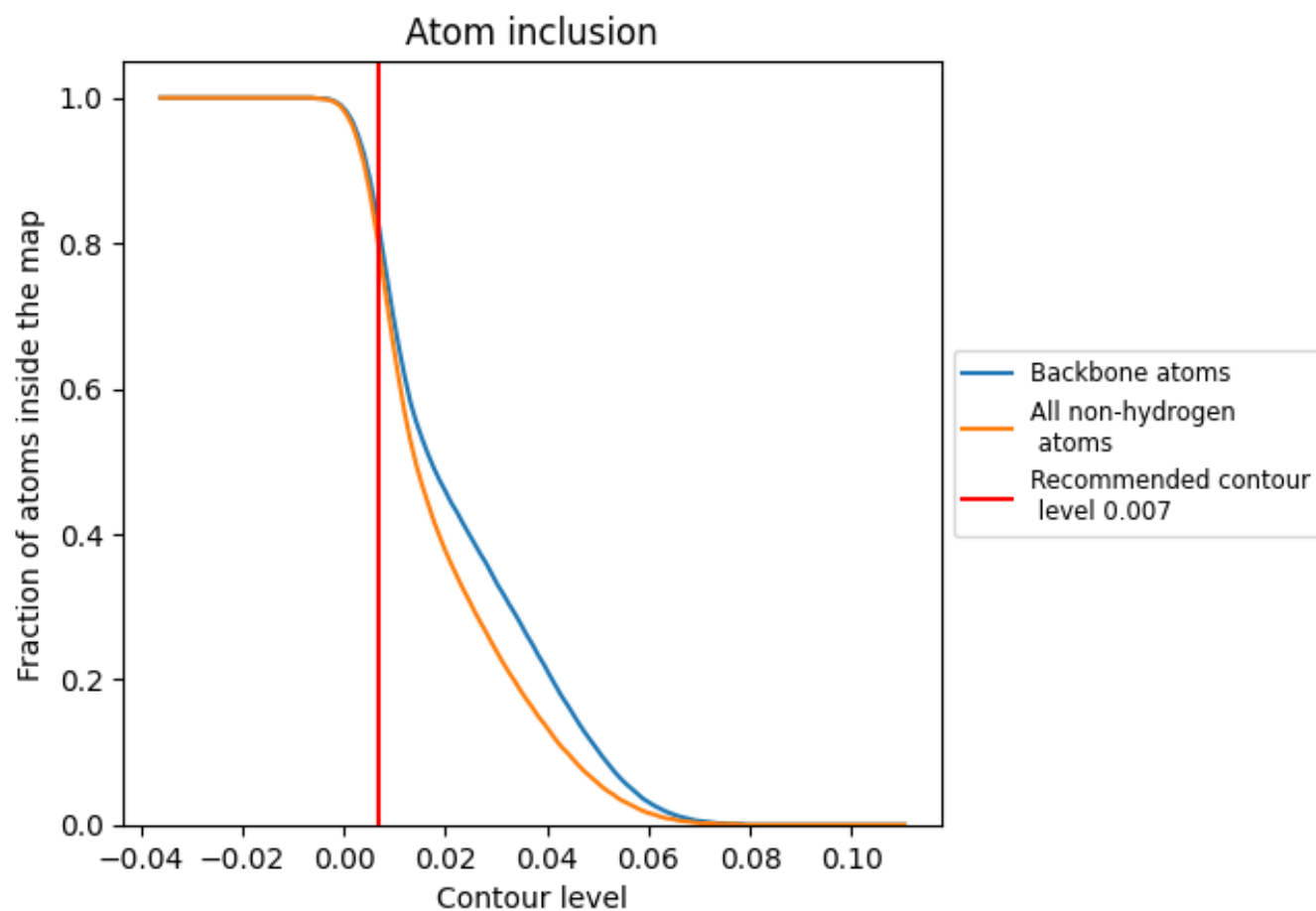
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 79% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7930	 0.1610
0	 0.6540	 -0.0100
1	 0.6300	 0.0160
2	 0.6290	 -0.0050
3	 0.5430	 -0.0060
4	 0.8200	 0.0130
5	 0.6700	 0.0030
6	 0.6790	 0.0270
7	 0.2000	 0.0180
A	 0.9700	 0.3670
B	 0.9800	 0.4090
C	 0.9830	 0.4220
D	 0.9270	 0.0410
E	 0.9520	 0.3140
F	 0.9890	 0.3700
G	 0.9480	 0.1470
H	 0.9780	 0.3580
I	 0.9710	 0.3010
J	 0.9880	 0.4250
K	 0.9780	 0.3860
L	 0.9780	 0.2800
M	 0.9620	 0.2700
N	 0.5260	 0.0560
O	 0.9570	 0.1600
P	 1.0000	 0.3540
Q	 0.9510	 0.0740
R	 0.9440	 0.0890
T	 0.5600	 0.0740
U	 0.9260	 0.0420
V	 0.9330	 0.0530
W	 0.8980	 0.0450
X	 0.9490	 0.0270
a	 0.5270	 -0.0230
b	 0.5600	 -0.0080
c	 0.5740	 0.0050



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Chain	Atom inclusion	Q-score
d	 0.5870	 -0.0220
e	 0.6700	 -0.0190
f	 0.7710	 -0.0030
g	 0.5890	 -0.0060
h	 0.5940	 0.0180