



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 04:45 PM UTC

PDB ID : 8BVW / pdb_00008bvw
EMDB ID : EMD-16274
Title : RNA polymerase II pre-initiation complex with the distal +1 nucleosome (PIC-Nuc18W)
Authors : Abril-Garrido, J.; Dienemann, C.; Grabbe, F.; Velychko, T.; Lidschreiber, M.; Wang, H.; Cramer, P.
Deposited on : 2022-12-20
Resolution : 4.00 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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

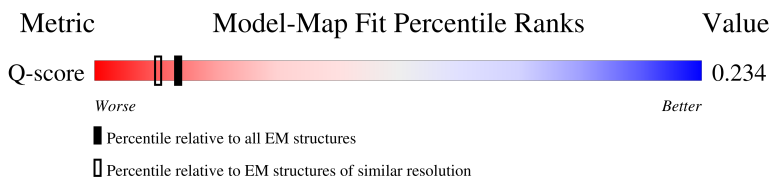
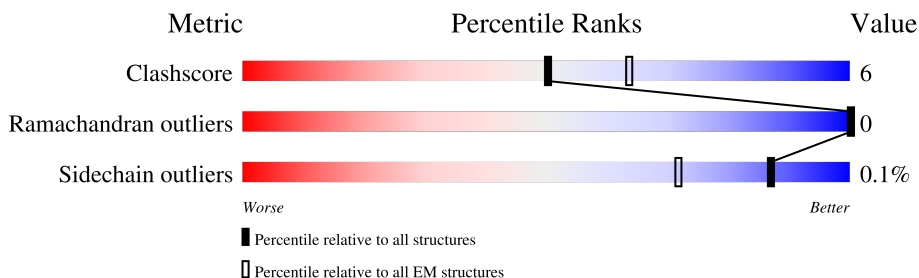
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	772	
2	1	760	
3	2	548	
4	3	462	

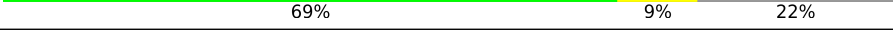
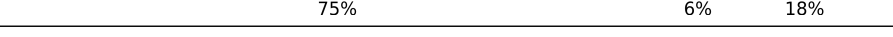
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	4	395	
6	5	308	
7	6	71	
8	7	309	
9	8	346	
10	9	323	
11	A	1970	
12	B	1174	
13	C	275	
14	D	142	
15	E	210	
16	F	127	
17	G	172	
18	H	150	
19	I	125	
20	J	67	
21	K	117	
22	L	58	
23	M	316	
24	N	218	
25	O	339	
26	Q	517	
27	R	249	
28	T	218	
29	U	376	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	V	109	
31	W	439	
32	X	291	
33	Y	8	
34	Z	19	
35	a	136	
35	e	136	
36	b	103	
36	f	103	
37	c	130	
37	g	130	
38	d	126	
38	h	126	

2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 84783 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 IIIH 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 IIIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	265	Total	C	N	O	S	0	0
			2167	1382	378	395	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	421	Total	C	N	O	S	0	0
			3337	2154	584	586	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	69	Total	C	N	O	S	0	0
			548	352	88	105	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	212	Total	C	N	O	S	0	0
			1724	1083	297	332	12		

- Molecule 9 is a protein called Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	299	Total	C	N	O	S	0	0
			2378	1535	406	426	11		

- Molecule 10 is a protein called Cyclin-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	287	Total	C	N	O	S	0	0
			2334	1493	402	422	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1423	Total	C	N	O	S	0	0
			11274	7092	2016	2094	72		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	THR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	TYR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	THR	deletion	UNP A0A7M4DUC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2

- Molecule 12 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	1136	Total	C	N	O	S	0	0
			9076	5739	1597	1676	64		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 14 is a protein called RNA polymerase II subunit D.

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

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

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

- Molecule 16 is a protein called DNA-directed RNA polymerase II subunit F.

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

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 18 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 19 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 20 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 21 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

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

- Molecule 22 is a protein called RNA polymerase II subunit K.

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

- Molecule 23 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	M	252	Total	C	N	O	S	0	0
			1953	1224	346	366	17		

- Molecule 24 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	206	Total	C	N	O	P	0	0
			4213	1998	774	1236	205		

- Molecule 25 is a protein called TATA-box-binding protein.

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

- Molecule 26 is a protein called General transcription factor IIF subunit 1.

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

- Molecule 27 is a protein called General transcription factor IIF subunit 2.

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

- Molecule 28 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	206	Total	C	N	O	P	0	0
			4227	2002	788	1232	205		

- Molecule 29 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	113	Total	C	N	O	S	0	0
			930	585	152	189	4		

- Molecule 30 is a protein called Transcription initiation factor IIA subunit 2.

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

- Molecule 31 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	202	Total	C	N	O	S	0	0
			1659	1042	299	307	11		

- Molecule 32 is a protein called Transcription initiation factor IIE subunit beta.

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

- Molecule 33 is a protein called Unassigned peptide, likely XPB.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Y	8	Total	C	N	O	0	0
			40	24	8	8		

- Molecule 34 is a protein called Unassigned peptide, likely TFIIE-beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	Z	19	Total	C	N	O	0	0
			95	57	19	19		

- Molecule 35 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a	97	Total	C	N	O	S	0	0
			802	506	155	138	3		
35	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 36 is a protein called Histone H4.

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

- Molecule 37 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	c	109	Total	C	N	O	0	0
			843	531	167	145		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
37	g	106	Total	C	N	O	0	0
			818	516	160	142		

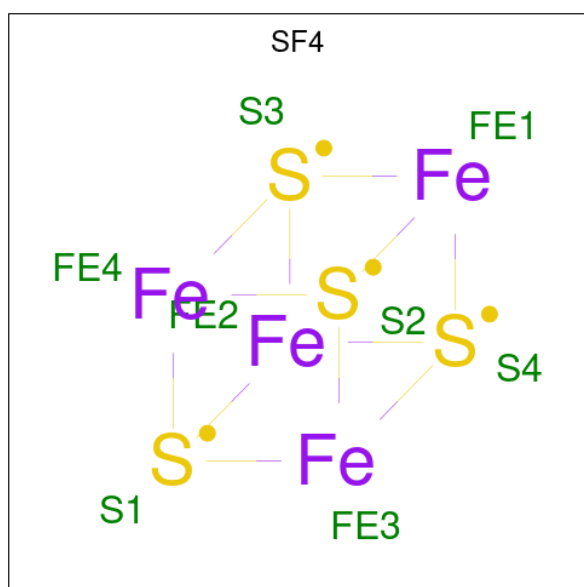
There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 38 is a protein called Histone H2B 1.1.

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

- Molecule 39 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
39	1	1	Total	Fe	S	0
			8	4	4	

- Molecule 40 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
40	4	3	Total 3	Zn 3	0
40	5	2	Total 2	Zn 2	0
40	7	2	Total 2	Zn 2	0
40	A	2	Total 2	Zn 2	0
40	B	1	Total 1	Zn 1	0
40	C	1	Total 1	Zn 1	0
40	I	2	Total 2	Zn 2	0
40	J	1	Total 1	Zn 1	0
40	L	1	Total 1	Zn 1	0
40	M	1	Total 1	Zn 1	0
40	W	1	Total 1	Zn 1	0

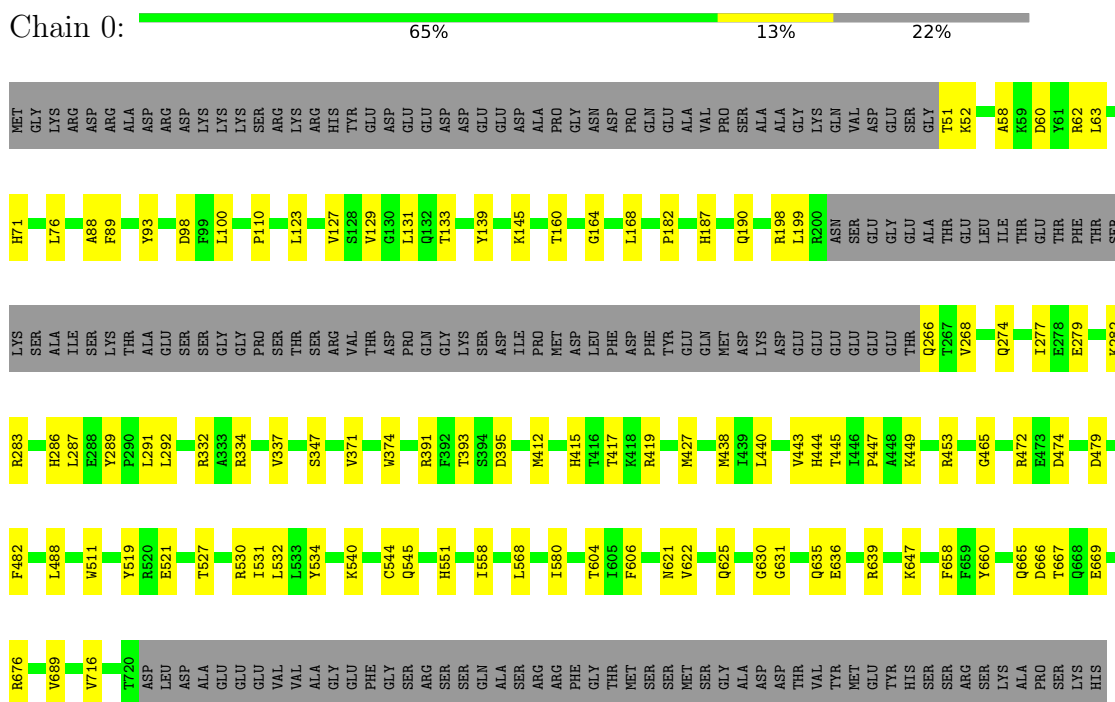
- Molecule 41 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

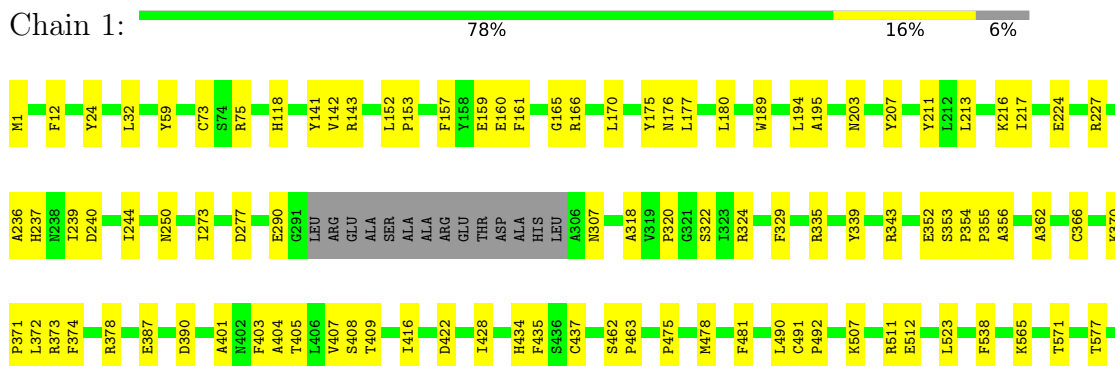
3 Residue-property plots

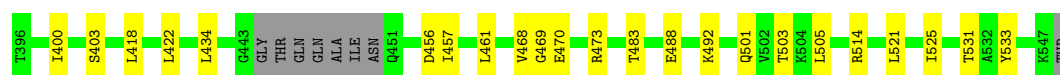
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

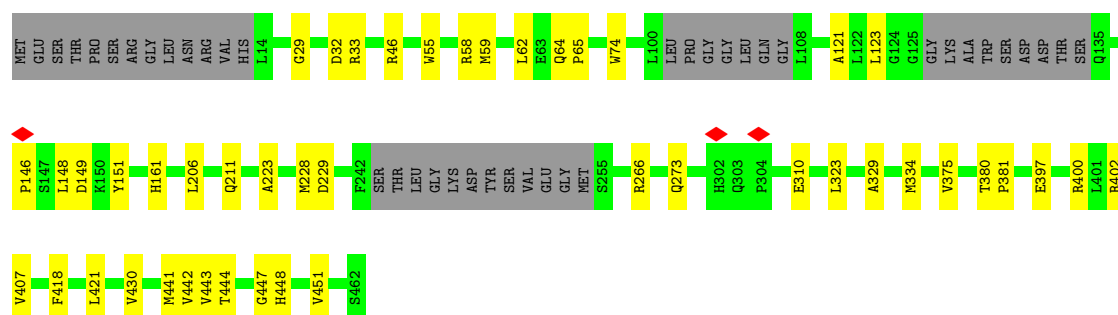


- Molecule 2: TFIIH basal transcription factor complex helicase XPD subunit

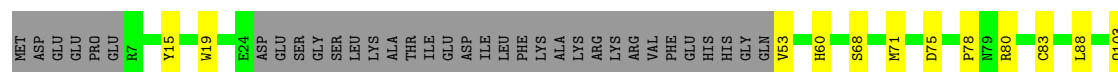


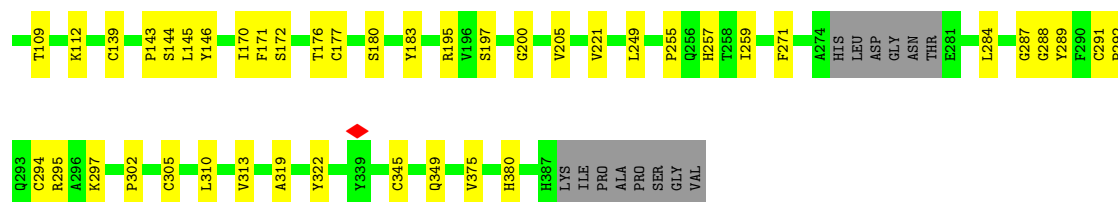


- Molecule 4: General transcription factor IIH subunit 4



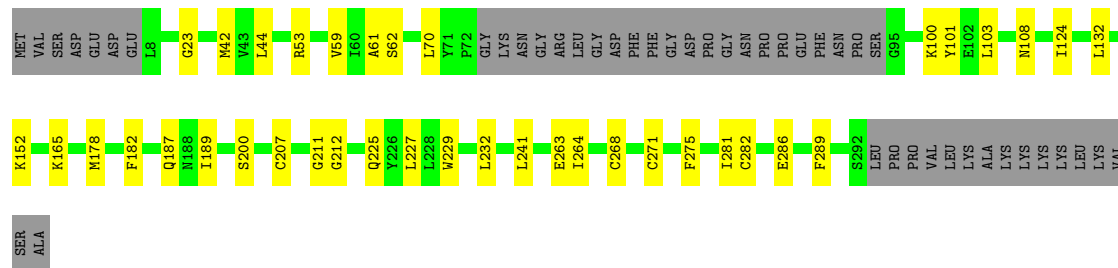
- Molecule 5: General transcription factor IIH subunit 2





• Molecule 6: General transcription factor IIH subunit 3

Chain 5: 73% 12% 15%



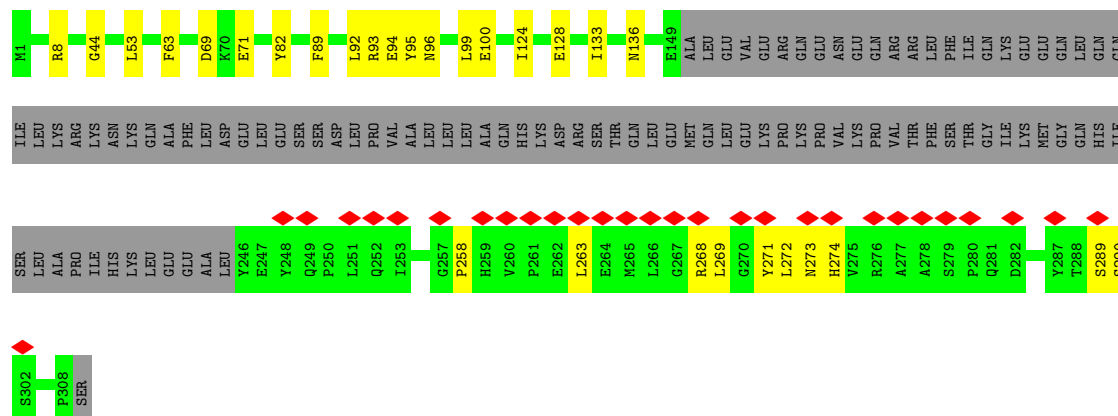
• Molecule 7: General transcription factor IIH subunit 5

Chain 6: 79% 18%



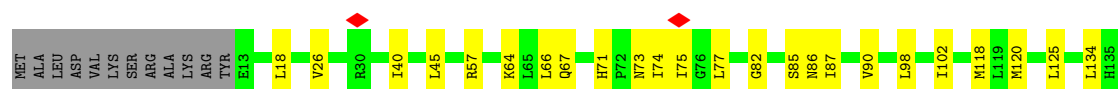
• Molecule 8: CDK-activating kinase assembly factor MAT1

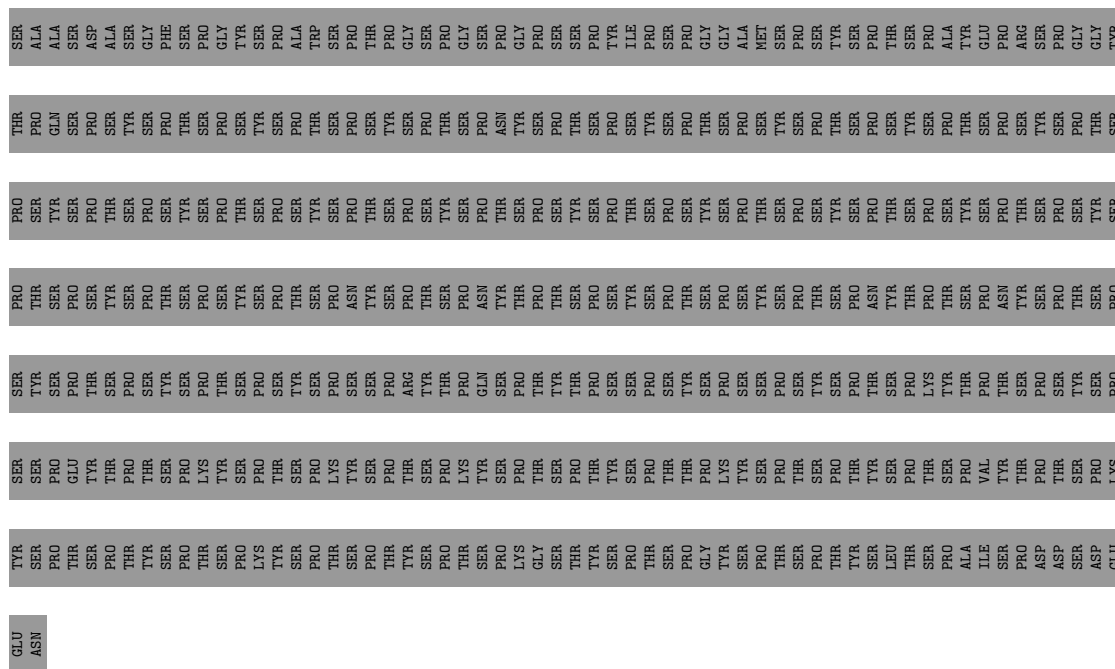
Chain 7: 11% 59% 10% 31%



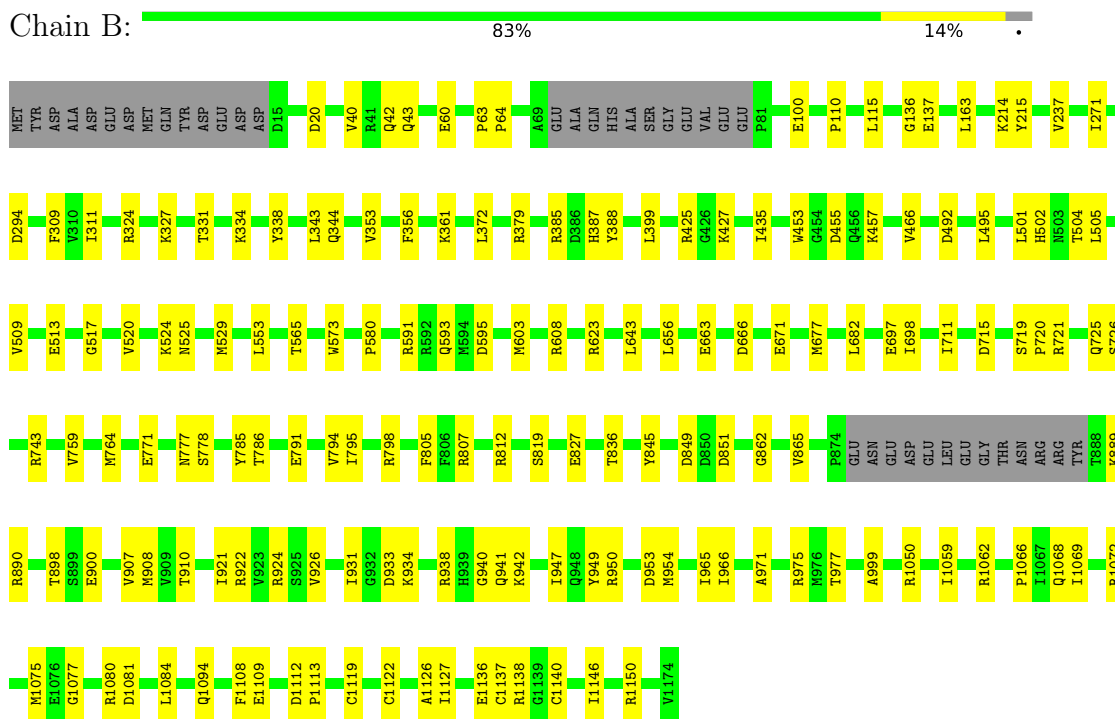
• Molecule 9: Cyclin-dependent kinase 7

Chain 8: 7% 72% 14% 14%

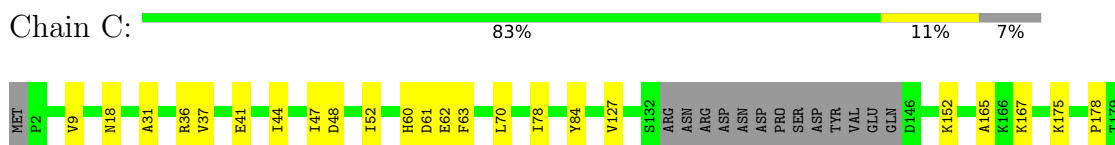




- Molecule 12: DNA-directed RNA polymerase subunit beta



- Molecule 13: DNA-directed RNA polymerase II subunit RPB3





- Molecule 14: RNA polymerase II subunit D

Chain D: 80% 11% 10%



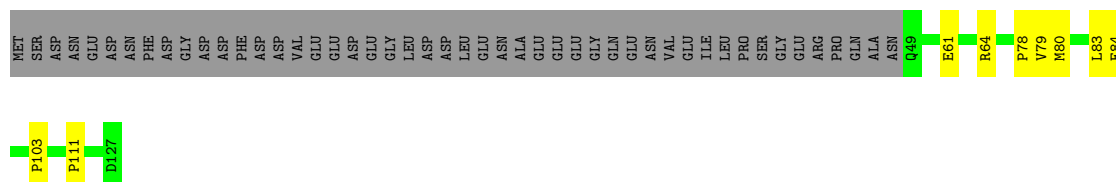
- Molecule 15: DNA-directed RNA polymerase II subunit E

Chain E: 81% 18%



- Molecule 16: DNA-directed RNA polymerase II subunit F

Chain F: 55% 7% 38%



- Molecule 17: DNA-directed RNA polymerase II subunit RPB7

Chain G: 87% 12%



- Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 87% 12%



- Molecule 19: DNA-directed RNA polymerase II subunit RPB9

Chain I: 75% 16% 9%



- Molecule 20: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 82% 13% .



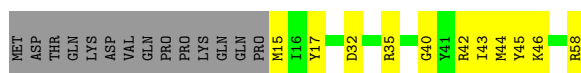
- Molecule 21: DNA-directed RNA polymerase II subunit RPB11-a

Chain K: 92% 6% .



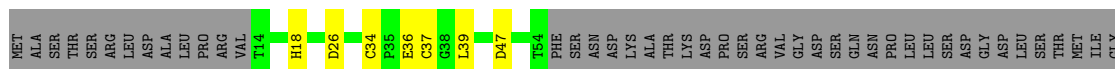
- Molecule 22: RNA polymerase II subunit K

Chain L: 57% 19% 24%



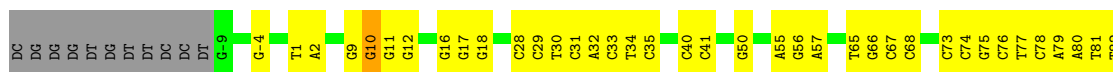
- Molecule 23: Transcription initiation factor IIB

Chain M: 72% 8% 20%



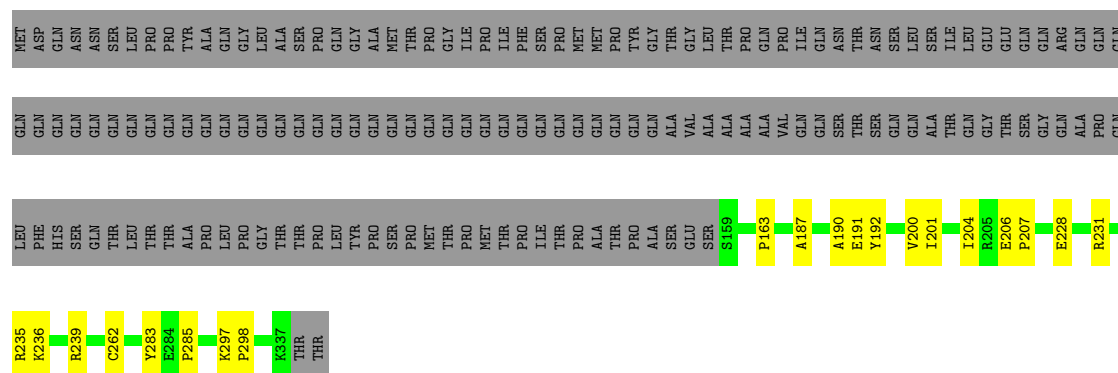
- Molecule 24: Non-template DNA

Chain N: 5% 60% 34% 6%

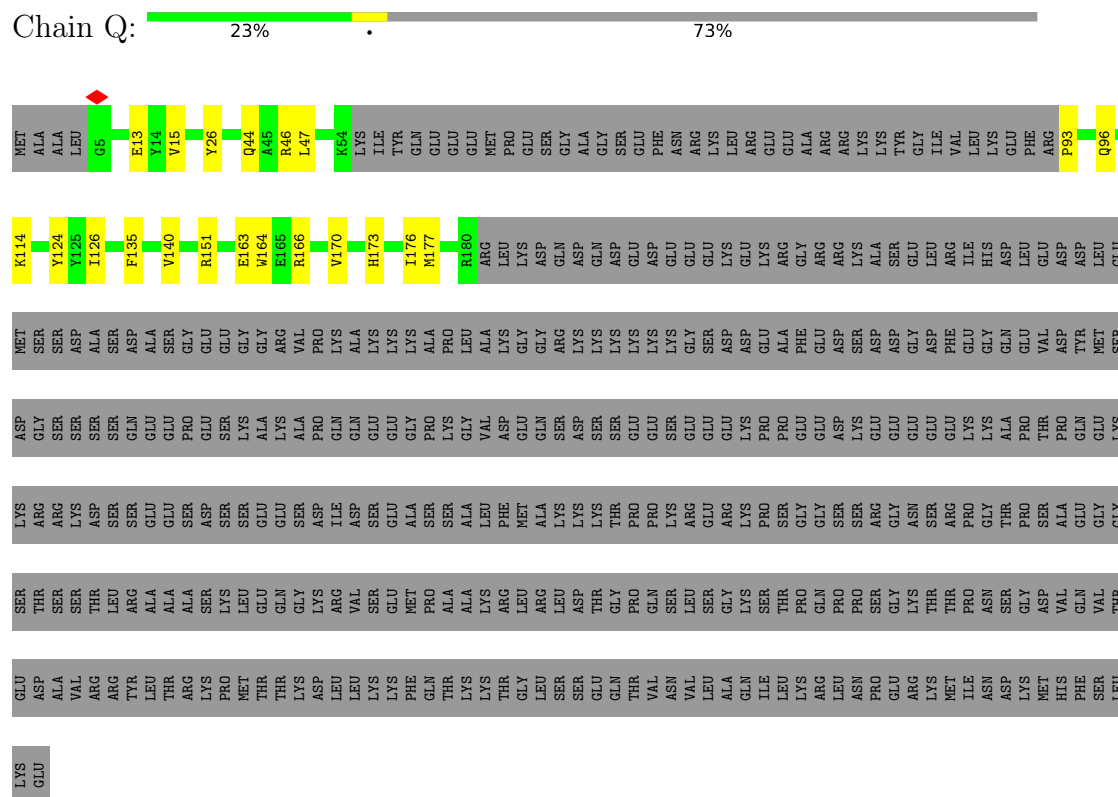


- Molecule 25: TATA-box-binding protein

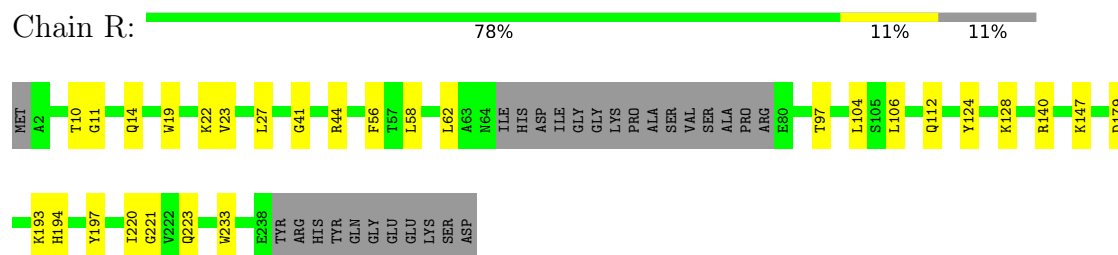
Chain O: 47% 6% 47%



- Molecule 26: General transcription factor IIF subunit 1

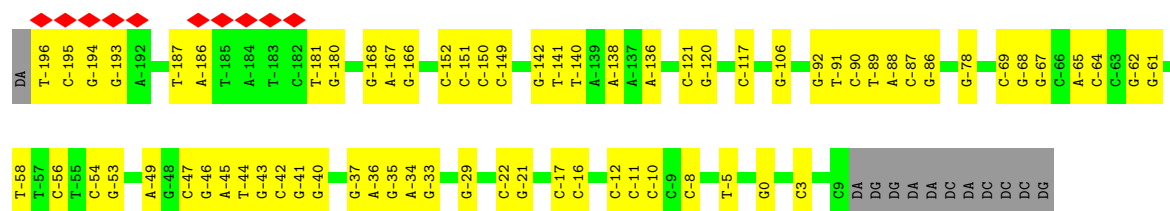


- Molecule 27: General transcription factor IIF subunit 2

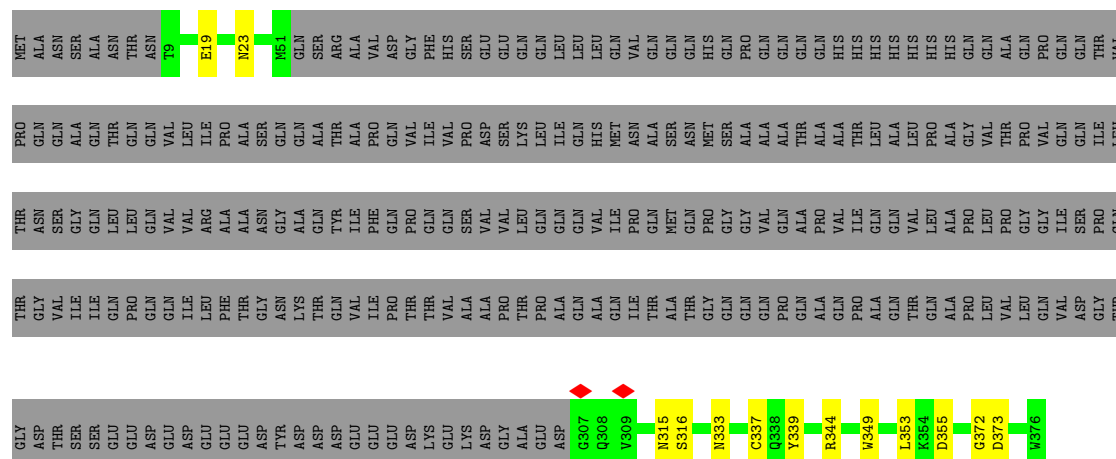


- Molecule 28: Template DNA

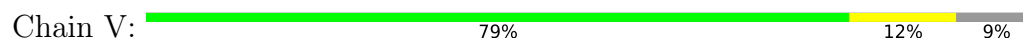




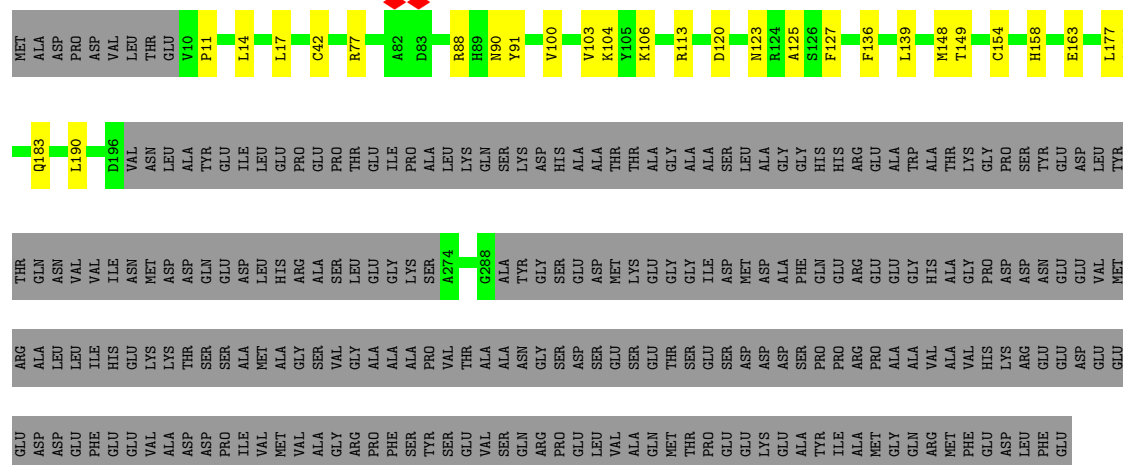
• Molecule 29: Transcription initiation factor IIA subunit 1



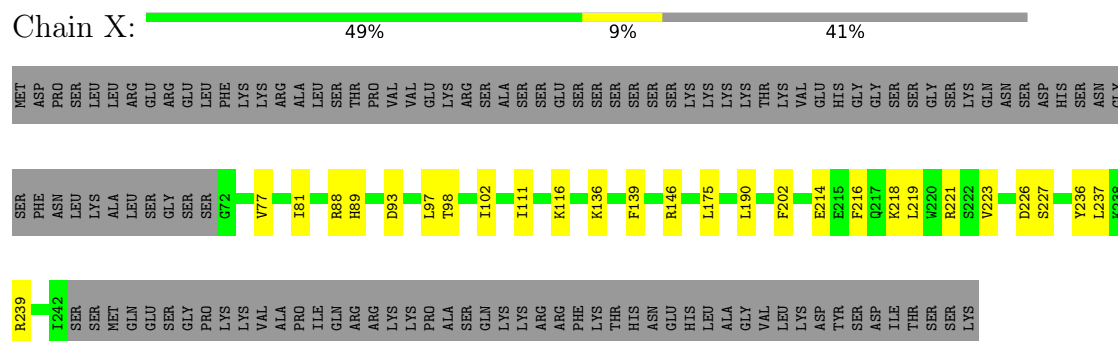
• Molecule 30: Transcription initiation factor IIA subunit 2



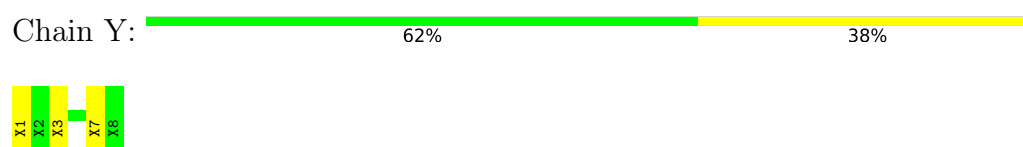
• Molecule 31: General transcription factor IIE subunit 1



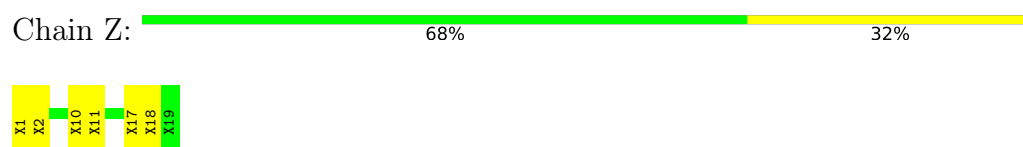
- Molecule 32: Transcription initiation factor IIE subunit beta



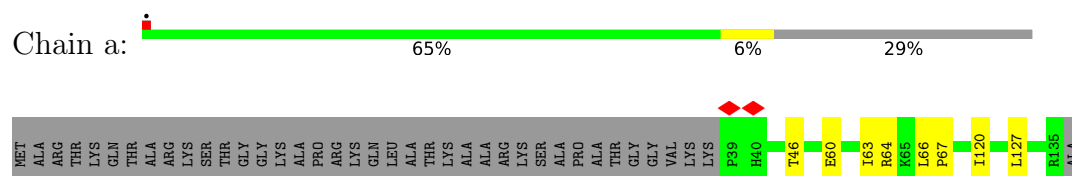
- Molecule 33: Unassigned peptide, likely XPB



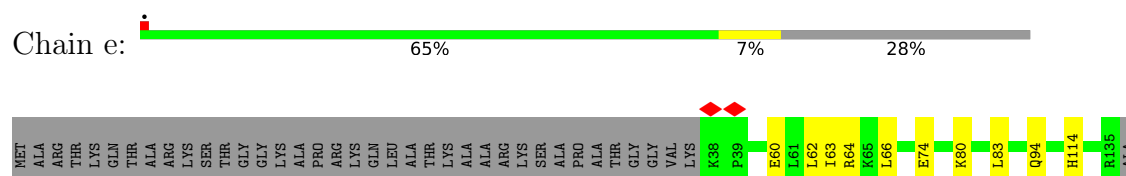
- Molecule 34: Unassigned peptide, likely TFIIE-beta



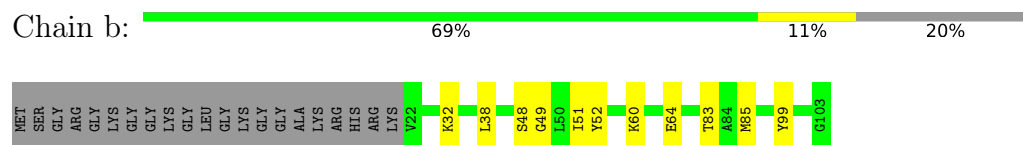
- Molecule 35: Histone H3.2



- Molecule 35: Histone H3.2

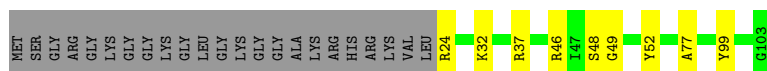


- Molecule 36: Histone H4



- Molecule 36: Histone H4

Chain f:  69% 9% 22%



- Molecule 37: Histone H2A type 1

Chain c:  78% 5% 16%



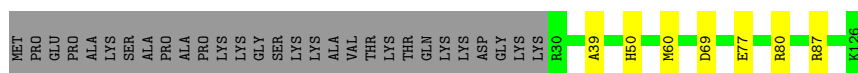
- Molecule 37: Histone H2A type 1

Chain g:  75% 6% 18%



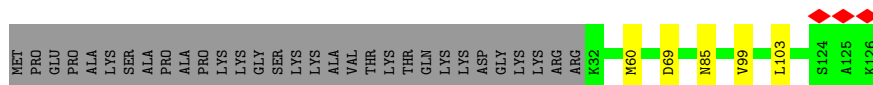
- Molecule 38: Histone H2B 1.1

Chain d:  71% 6% 23%



- Molecule 38: Histone H2B 1.1

Chain h:  71% 0% 25%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	188832	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41.58	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	44.013	Depositor
Minimum map value	-19.392	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SF4, 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	0.15	0/4994	0.51	0/6745
2	1	0.15	0/5875	0.53	0/7955
3	2	0.14	0/2210	0.48	0/2975
4	3	0.14	0/3411	0.50	0/4622
5	4	0.14	0/2793	0.50	0/3780
6	5	0.13	0/2103	0.47	0/2846
7	6	0.14	0/554	0.55	0/747
8	7	0.16	0/1756	0.53	0/2367
9	8	0.15	0/2437	0.52	0/3306
10	9	0.16	0/2384	0.55	0/3220
11	A	0.32	0/11479	0.60	0/15496
12	B	0.41	0/9257	0.63	0/12493
13	C	0.44	0/2102	0.63	0/2857
14	D	0.13	0/1064	0.48	0/1428
15	E	0.25	0/1752	0.52	0/2366
16	F	0.37	0/646	0.59	0/871
17	G	0.19	0/1382	0.50	0/1874
18	H	0.38	0/1207	0.60	0/1628
19	I	0.26	0/949	0.56	0/1284
20	J	0.51	0/516	0.71	0/696
21	K	0.41	0/939	0.58	0/1271
22	L	0.36	0/378	0.70	0/500
23	M	0.28	0/1983	0.58	0/2679
24	N	0.28	0/4724	0.71	1/7288 (0.0%)
25	O	0.18	0/1448	0.54	0/1948
26	Q	0.14	0/1167	0.47	0/1576
27	R	0.16	0/1817	0.45	0/2445
28	T	0.26	0/4744	0.67	0/7322
29	U	0.13	0/945	0.48	0/1274
30	V	0.14	0/816	0.49	0/1105
31	W	0.15	0/1686	0.50	0/2266
32	X	0.13	0/1427	0.47	0/1916

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	a	0.11	0/814	0.40	0/1092
35	e	0.10	0/823	0.40	0/1104
36	b	0.11	0/660	0.45	0/883
36	f	0.11	0/645	0.48	0/862
37	c	0.15	0/853	0.46	0/1149
37	g	0.15	0/828	0.47	0/1117
38	d	0.15	0/777	0.41	0/1041
38	h	0.19	0/755	0.43	0/1013
All	All	0.26	0/87100	0.56	1/119407 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	N	10	DG	C2'-C3'-O3'	-5.17	103.74	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	4890	0	4949	64	0
2	1	5751	0	5794	77	0
3	2	2167	0	2175	22	0
4	3	3337	0	3343	34	0
5	4	2732	0	2700	33	0
6	5	2066	0	2100	29	0
7	6	548	0	558	10	0
8	7	1724	0	1697	21	0
9	8	2378	0	2397	29	0
10	9	2334	0	2357	27	0
11	A	11274	0	11407	140	0
12	B	9076	0	9116	110	0
13	C	2059	0	2008	21	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	D	1050	0	1033	9	0
15	E	1721	0	1737	25	0
16	F	636	0	665	10	0
17	G	1351	0	1358	14	0
18	H	1186	0	1147	11	0
19	I	928	0	859	17	0
20	J	507	0	523	9	0
21	K	920	0	942	5	0
22	L	373	0	379	10	0
23	M	1953	0	1989	18	0
24	N	4213	0	2312	72	0
25	O	1422	0	1514	15	0
26	Q	1138	0	1103	16	0
27	R	1788	0	1819	18	0
28	T	4227	0	2310	76	0
29	U	930	0	888	12	0
30	V	806	0	818	8	0
31	W	1659	0	1665	19	0
32	X	1403	0	1428	19	0
33	Y	40	0	11	2	0
34	Z	95	0	28	3	0
35	a	802	0	841	7	0
35	e	811	0	853	8	0
36	b	653	0	696	9	0
36	f	638	0	676	10	0
37	c	843	0	908	6	0
37	g	818	0	877	6	0
38	d	766	0	797	5	0
38	h	744	0	771	4	0
39	1	8	0	0	0	0
40	4	3	0	0	0	0
40	5	2	0	0	0	0
40	7	2	0	0	0	0
40	A	2	0	0	0	0
40	B	1	0	0	0	0
40	C	1	0	0	0	0
40	I	2	0	0	0	0
40	J	1	0	0	0	0
40	L	1	0	0	0	0
40	M	1	0	0	0	0
40	W	1	0	0	0	0
41	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	84783	0	81548	894	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 6.

All (894) 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)
11:A:74:CYS:SG	11:A:84:HIS:CE1	2.57	0.98
28:T:-89:DT:H4'	28:T:-88:DA:H5'	1.53	0.90
12:B:953:ASP:OD1	13:C:36:ARG:NH2	2.10	0.84
20:J:6:ARG:HD2	20:J:13:ILE:HD13	1.58	0.84
14:D:44:ARG:NH1	14:D:47:GLN:OE1	2.12	0.83
28:T:-90:DC:H4'	28:T:-89:DT:H5'	1.61	0.81
18:H:58:LEU:HD11	18:H:143:LEU:HD11	1.63	0.80
2:1:372:LEU:HD11	2:1:404:ALA:HB1	1.64	0.79
11:A:1411:LEU:O	11:A:1421:ARG:NH2	2.17	0.78
37:g:30:ARG:HG3	37:g:33:ARG:HH21	1.47	0.78
12:B:388:TYR:OH	12:B:524:LYS:NZ	2.14	0.77
24:N:17:DG:N2	28:T:-17:DC:O2	2.18	0.76
15:E:46:ASP:O	15:E:52:ARG:NH1	2.18	0.76
11:A:1036:ASN:OD1	15:E:202:ARG:NH1	2.17	0.76
12:B:387:HIS:NE2	12:B:671:GLU:OE2	2.21	0.74
12:B:505:LEU:HD22	12:B:509:VAL:HB	1.69	0.74
11:A:811:ILE:HD12	19:I:79:PRO:HB3	1.68	0.74
34:Z:10:UNK:HA	34:Z:11:UNK:CB	2.19	0.72
11:A:1192:TRP:HZ3	11:A:1246:ILE:HG22	1.55	0.71
11:A:428:ASP:OD2	11:A:430:ARG:NH1	2.22	0.71
12:B:1109:GLU:OE1	12:B:1150:ARG:NH2	2.23	0.71
13:C:37:VAL:HG13	13:C:41:GLU:HB2	1.72	0.71
11:A:909:LEU:HD12	11:A:967:ARG:HD3	1.72	0.69
3:2:422:LEU:HD13	6:5:225:GLN:HE22	1.57	0.69
1:0:58:ALA:HB2	4:3:334:MET:HB3	1.74	0.69
1:0:198:ARG:NH1	1:0:199:LEU:O	2.26	0.68
12:B:343:LEU:O	12:B:361:LYS:NZ	2.27	0.68
15:E:77:PRO:O	15:E:107:GLN:NE2	2.25	0.68
13:C:78:ILE:HG21	13:C:127:VAL:HG22	1.75	0.68
1:0:635:GLN:HB3	1:0:676:ARG:HH22	1.59	0.67
12:B:836:THR:HB	12:B:889:LYS:HE2	1.76	0.67
2:1:372:LEU:HD23	2:1:408:SER:HB3	1.76	0.67
12:B:60:GLU:OE2	27:R:140:ARG:NH1	2.26	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:305:CYS:HB2	5:4:310:LEU:H	1.59	0.66
25:O:206:GLU:OE1	25:O:236:LYS:NZ	2.27	0.66
15:E:2:ASP:N	15:E:5:GLU:OE2	2.29	0.66
23:M:223:CYS:SG	27:R:147:LYS:NZ	2.69	0.66
11:A:460:ARG:HB2	11:A:501:MET:HE3	1.78	0.66
12:B:1059:ILE:O	12:B:1080:ARG:NH2	2.28	0.66
12:B:777:ASN:O	20:J:47:ARG:NH1	2.28	0.66
2:1:353:SER:HB2	2:1:356:ALA:HB3	1.77	0.65
11:A:727:PRO:HA	11:A:736:THR:HG21	1.78	0.65
11:A:659:GLU:OE2	11:A:985:ARG:NH1	2.29	0.65
12:B:677:MET:H	12:B:682:LEU:HG	1.62	0.65
4:3:148:LEU:HA	4:3:151:TYR:CZ	2.31	0.65
24:N:10:DG:H2"	24:N:11:DG:C8	2.32	0.64
12:B:910:THR:HG22	22:L:43:ILE:HA	1.77	0.64
11:A:1218:ARG:NH1	11:A:1250:ASP:OD1	2.30	0.64
23:M:248:ARG:HH21	23:M:287:GLN:HB3	1.63	0.64
6:5:165:LYS:HE2	6:5:200:SER:HB2	1.79	0.64
12:B:529:MET:HE1	12:B:698:ILE:HD12	1.80	0.64
27:R:10:THR:O	27:R:14:GLN:NE2	2.30	0.64
11:A:549:THR:O	11:A:589:LYS:NZ	2.27	0.64
1:0:472:ARG:NH2	1:0:474:ASP:OD2	2.31	0.63
11:A:1192:TRP:CZ3	11:A:1246:ILE:HG22	2.33	0.63
11:A:244:ARG:HB2	11:A:247:TRP:CD2	2.33	0.63
1:0:332:ARG:O	1:0:334:ARG:NH1	2.30	0.63
2:1:329:PHE:CD1	2:1:378:ARG:HG2	2.34	0.63
11:A:1178:ASP:OD1	11:A:1260:ARG:NH2	2.31	0.63
12:B:100:GLU:OE1	22:L:42:ARG:NH1	2.28	0.63
28:T:-167:DA:H5"	37:g:17:THR:HA	1.81	0.63
9:8:102:ILE:HD11	9:8:206:LEU:HD23	1.81	0.62
11:A:71:CYS:SG	11:A:74:CYS:HB2	2.39	0.62
28:T:-106:DG:OP1	35:a:64:ARG:NH1	2.28	0.62
15:E:172:ARG:NH1	15:E:210:GLN:OE1	2.31	0.62
24:N:56:DG:H1	28:T:-56:DC:H42	1.44	0.62
5:4:80:ARG:NH1	5:4:172:SER:OG	2.30	0.62
11:A:535:MET:O	11:A:669:TYR:OH	2.13	0.62
11:A:728:THR:H	11:A:736:THR:HG21	1.64	0.62
2:1:335:ARG:NH1	8:7:71:GLU:OE2	2.30	0.62
16:F:80:MET:HG3	16:F:103:PRO:HD3	1.81	0.62
11:A:1005:HIS:HD2	11:A:1006:PRO:HD2	1.64	0.62
12:B:425:ARG:HD2	12:B:427:LYS:HE3	1.82	0.61
36:b:60:LYS:NZ	36:b:64:GLU:OE2	2.28	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:W:88:ARG:NH1	31:W:90:ASN:OD1	2.33	0.61
12:B:294:ASP:OD2	12:B:379:ARG:NH1	2.31	0.61
24:N:193:DC:H5''	35:a:46:THR:HG23	1.82	0.61
2:1:244:ILE:HG23	2:1:437:CYS:HB3	1.82	0.61
2:1:462:SER:OG	2:1:463:PRO:HD2	2.00	0.61
3:2:531:THR:HG21	5:4:295:ARG:HG3	1.82	0.61
24:N:89:DA:H4'	24:N:90:DG:OP1	2.01	0.61
2:1:475:PRO:HG3	2:1:478:MET:HE2	1.82	0.60
5:4:78:PRO:HG2	5:4:83:CYS:HB2	1.83	0.60
24:N:1:DT:O2	28:T:0:DG:N2	2.34	0.60
24:N:35:DC:O2	28:T:-35:DG:N1	2.34	0.60
24:N:189:DA:H2''	24:N:190:DC:C6	2.36	0.60
12:B:933:ASP:OD2	12:B:1050:ARG:NH2	2.35	0.60
22:L:17:TYR:HB3	22:L:44:MET:HB3	1.83	0.60
6:5:44:LEU:HD22	6:5:227:LEU:HD13	1.85	0.59
11:A:1434:GLU:HG2	11:A:1437:ASP:HB2	1.84	0.59
5:4:60:HIS:CE1	5:4:103:GLN:HE21	2.20	0.59
11:A:805:ARG:NH2	12:B:671:GLU:O	2.35	0.59
2:1:160:GLU:HG2	2:1:189:TRP:HE1	1.66	0.59
35:e:63:ILE:O	35:e:94:GLN:NE2	2.36	0.59
25:O:192:TYR:HB2	25:O:200:VAL:HG22	1.84	0.59
6:5:282:CYS:O	6:5:286:GLU:N	2.32	0.59
24:N:192:DT:H2''	24:N:193:DC:C6	2.38	0.59
31:W:183:GLN:HG2	32:X:216:PHE:CE2	2.38	0.58
32:X:236:TYR:HA	32:X:239:ARG:HE	1.67	0.58
1:0:279:GLU:OE1	1:0:282:LYS:NZ	2.31	0.58
12:B:771:GLU:O	20:J:55:LEU:HD21	2.04	0.58
17:G:151:ARG:NH1	31:W:139:LEU:O	2.28	0.58
30:V:16:GLN:NE2	30:V:20:ASP:OD2	2.36	0.58
1:0:531:ILE:HA	1:0:534:TYR:CE2	2.39	0.58
11:A:620:HIS:O	18:H:97:TYR:OH	2.18	0.58
12:B:387:HIS:CD2	12:B:504:THR:HG21	2.38	0.58
25:O:297:LYS:HB3	25:O:298:PRO:HD3	1.85	0.58
11:A:472:HIS:NE2	11:A:492:TYR:OH	2.32	0.58
12:B:435:ILE:O	23:M:127:ARG:NH1	2.35	0.57
2:1:180:LEU:HD21	2:1:195:ALA:HB2	1.86	0.57
10:9:56:LEU:HD21	10:9:277:LEU:HD22	1.87	0.57
11:A:233:CYS:SG	11:A:244:ARG:NH1	2.78	0.57
4:3:402:ARG:NH1	7:6:11:GLU:OE2	2.35	0.57
4:3:206:LEU:O	4:3:211:GLN:NE2	2.38	0.57
9:8:67:GLN:HG2	9:8:77:LEU:HD23	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:9:238:LEU:HA	10:9:245:LEU:HD13	1.87	0.57
11:A:687:ILE:HD11	11:A:766:PHE:CD2	2.39	0.57
12:B:1069:ILE:HG23	23:M:47:ASP:HB2	1.87	0.57
10:9:56:LEU:HD23	10:9:96:VAL:HG11	1.87	0.57
12:B:643:LEU:HD11	12:B:656:LEU:HD11	1.87	0.57
32:X:146:ARG:HA	32:X:175:LEU:HB2	1.87	0.57
11:A:408:ARG:NH1	11:A:414:PRO:O	2.34	0.56
9:8:18:LEU:HB2	9:8:26:VAL:HG13	1.86	0.56
12:B:388:TYR:CZ	12:B:505:LEU:HD21	2.39	0.56
19:I:27:LYS:N	19:I:36:LEU:O	2.37	0.56
31:W:104:LYS:HE2	32:X:237:LEU:HD22	1.86	0.56
1:0:412:MET:O	1:0:419:ARG:NH1	2.36	0.56
2:1:507:LYS:O	2:1:511:ARG:N	2.37	0.56
2:1:589:GLU:OE1	5:4:183:TYR:OH	2.23	0.56
10:9:28:ARG:HH21	16:F:80:MET:C	2.13	0.56
30:V:82:ARG:NH1	30:V:83:GLU:O	2.38	0.56
14:D:59:GLU:N	14:D:59:GLU:OE1	2.34	0.56
1:0:568:LEU:HD11	1:0:606:PHE:HB3	1.88	0.56
9:8:57:ARG:NH1	10:9:119:ASN:OD1	2.36	0.56
11:A:1208:SER:HA	11:A:1266:GLU:HG3	1.87	0.56
11:A:963:ARG:O	11:A:967:ARG:HG2	2.06	0.56
27:R:179:ASP:OD1	27:R:179:ASP:N	2.38	0.56
1:0:266:GLN:N	33:Y:7:UNK:O	2.39	0.55
14:D:32:LEU:HD11	17:G:4:HIS:HB2	1.88	0.55
5:4:375:VAL:O	5:4:380:HIS:N	2.32	0.55
11:A:617:PRO:O	18:H:124:ARG:NH2	2.35	0.55
15:E:104:ILE:O	15:E:129:GLN:HA	2.07	0.55
24:N:10:DG:H1	28:T:-10:DC:H42	1.54	0.55
34:Z:1:UNK:O	34:Z:2:UNK:C	2.54	0.55
11:A:397:PHE:HE2	11:A:1486:ILE:HD11	1.71	0.55
11:A:421:ARG:HB2	11:A:425:ASP:OD1	2.06	0.55
28:T:-181:DT:H2"	28:T:-180:DG:C5	2.42	0.55
1:0:419:ARG:HH11	1:0:427:MET:HE1	1.71	0.55
12:B:764:MET:HE1	12:B:938:ARG:NH1	2.21	0.55
5:4:109:THR:CG2	5:4:144:SER:H	2.20	0.55
33:Y:1:UNK:O	33:Y:3:UNK:N	2.40	0.55
24:N:119:DA:N6	28:T:-120:DG:O6	2.39	0.55
24:N:177:DT:H2"	24:N:178:DG:C8	2.42	0.55
8:7:89:PHE:HB3	8:7:94:GLU:HB2	1.88	0.55
11:A:430:ARG:HH22	23:M:26:ASP:CG	2.14	0.55
6:5:101:TYR:CE2	6:5:103:LEU:HB3	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:324:ARG:NH1	8:7:100:GLU:OE1	2.38	0.54
12:B:941:GLN:NE2	12:B:977:THR:OG1	2.39	0.54
6:5:59:VAL:HG12	6:5:70:LEU:HD23	1.88	0.54
26:Q:26:TYR:HA	27:R:97:THR:HG22	1.90	0.54
32:X:89:HIS:HB2	32:X:139:PHE:CE1	2.42	0.54
35:a:63:ILE:HD11	36:b:38:LEU:HD11	1.90	0.54
12:B:743:ARG:O	12:B:922:ARG:NH1	2.40	0.54
26:Q:44:GLN:HE22	26:Q:46:ARG:HG3	1.73	0.54
1:0:164:GLY:H	1:0:292:LEU:HD11	1.73	0.54
12:B:715:ASP:N	12:B:715:ASP:OD1	2.41	0.54
12:B:851:ASP:OD2	22:L:17:TYR:OH	2.23	0.54
15:E:61:LEU:HB2	15:E:73:PHE:CE1	2.43	0.54
28:T:-141:DT:H2"	28:T:-140:DT:C6	2.43	0.54
29:U:372:GLY:HA3	30:V:58:PHE:CZ	2.42	0.54
2:1:354:PRO:HB2	2:1:355:PRO:HD3	1.90	0.54
4:3:223:ALA:HB1	4:3:228:MET:HB2	1.90	0.54
15:E:35:GLN:NE2	15:E:43:GLN:OE1	2.28	0.54
27:R:223:GLN:HB3	27:R:233:TRP:CE2	2.42	0.54
12:B:388:TYR:CE1	12:B:505:LEU:HD21	2.42	0.54
12:B:1066:PRO:HG2	12:B:1077:GLY:HA3	1.90	0.54
20:J:8:PHE:CD2	20:J:48:MET:HE1	2.42	0.54
22:L:32:ASP:OD1	22:L:32:ASP:N	2.39	0.54
11:A:497:ASP:O	12:B:942:LYS:HE2	2.07	0.53
3:2:434:LEU:HD13	6:5:229:TRP:HD1	1.73	0.53
11:A:408:ARG:HH12	11:A:413:TYR:C	2.16	0.53
28:T:-65:DA:H2"	28:T:-64:DC:C6	2.44	0.53
2:1:491:CYS:HB2	2:1:720:PHE:CE1	2.44	0.53
9:8:241:CYS:HA	9:8:246:TYR:CG	2.43	0.53
11:A:397:PHE:CE2	11:A:1486:ILE:HD11	2.43	0.53
11:A:295:GLN:HB3	32:X:218:LYS:HE2	1.91	0.53
11:A:465:HIS:ND1	11:A:467:MET:HE2	2.24	0.53
12:B:324:ARG:HH21	26:Q:164:TRP:HZ2	1.54	0.53
12:B:759:VAL:HG12	12:B:999:ALA:HB2	1.91	0.53
13:C:180:ALA:O	20:J:42:ARG:NH2	2.42	0.53
23:M:174:PRO:HD2	23:M:213:ASP:HB3	1.91	0.53
24:N:17:DG:N1	28:T:-17:DC:N3	2.40	0.53
31:W:127:PHE:O	31:W:136:PHE:N	2.33	0.53
11:A:465:HIS:CE1	11:A:467:MET:HE2	2.43	0.53
12:B:513:GLU:OE2	12:B:525:ASN:ND2	2.41	0.53
3:2:136:VAL:HG22	3:2:505:LEU:HG	1.90	0.53
1:0:625:GLN:OE1	1:0:639:ARG:NH1	2.36	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1242:ASP:HA	11:A:1262:MET:HE3	1.90	0.53
24:N:11:DG:H4'	24:N:12:DG:OP1	2.09	0.53
24:N:131:DC:H5''	36:f:48:SER:HA	1.91	0.53
2:1:211:TYR:HA	2:1:217:ILE:HD12	1.90	0.53
7:6:59:GLU:OE2	7:6:63:GLN:NE2	2.42	0.53
5:4:319:ALA:HA	5:4:322:TYR:CD2	2.44	0.53
8:7:263:LEU:HD21	8:7:272:LEU:HD21	1.91	0.53
28:T:-41:DG:H2'	28:T:-40:DG:C8	2.44	0.52
4:3:229:ASP:OD1	4:3:229:ASP:N	2.40	0.52
11:A:866:LYS:HE2	11:A:1416:ARG:HH22	1.73	0.52
2:1:143:ARG:NH1	2:1:159:GLU:OE1	2.37	0.52
11:A:350:VAL:HA	11:A:354:LEU:HD12	1.91	0.52
20:J:6:ARG:HD2	20:J:13:ILE:CD1	2.35	0.52
12:B:110:PRO:HG2	12:B:163:LEU:HD11	1.90	0.52
3:2:400:ILE:HG22	6:5:124:ILE:HD11	1.90	0.52
12:B:711:ILE:HG12	12:B:725:GLN:HG2	1.92	0.52
12:B:356:PHE:CZ	26:Q:114:LYS:HB3	2.45	0.52
12:B:721:ARG:NH1	12:B:940:GLY:O	2.42	0.52
8:7:8:ARG:NH2	31:W:177:LEU:HB3	2.25	0.52
24:N:128:DC:H2''	24:N:129:DC:C5	2.44	0.52
23:M:176:THR:N	23:M:179:GLU:OE1	2.41	0.52
25:O:204:ILE:HD12	25:O:207:PRO:HG2	1.92	0.52
6:5:268:CYS:SG	6:5:271:CYS:HB2	2.49	0.52
8:7:133:ILE:HA	8:7:136:ASN:ND2	2.24	0.52
11:A:458:PHE:HE2	11:A:484:LEU:HD11	1.75	0.52
18:H:130:ASN:HA	18:H:133:HIS:CE1	2.45	0.52
9:8:274:GLY:HA3	9:8:284:ILE:HD11	1.92	0.51
12:B:798:ARG:HB3	12:B:950:ARG:HA	1.93	0.51
16:F:79:VAL:HG11	16:F:83:LEU:HD23	1.92	0.51
24:N:82:DT:H2'	24:N:83:DG:C8	2.45	0.51
36:b:83:THR:HG22	36:b:85:MET:H	1.75	0.51
16:F:84:GLU:N	16:F:84:GLU:OE1	2.43	0.51
28:T:-69:DC:H2''	28:T:-68:DG:C8	2.46	0.51
36:b:99:TYR:OH	38:h:69:ASP:OD2	2.29	0.51
1:0:283:ARG:HG3	1:0:286:HIS:NE2	2.25	0.51
2:1:407:VAL:HG12	2:1:435:PHE:CE1	2.45	0.51
8:7:92:LEU:HA	8:7:95:TYR:CD2	2.45	0.51
24:N:11:DG:H1	28:T:-11:DC:H42	1.58	0.51
38:h:60:MET:HE3	38:h:60:MET:O	2.10	0.51
6:5:275:PHE:CZ	6:5:282:CYS:HB2	2.45	0.51
6:5:227:LEU:O	6:5:232:LEU:N	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:T:-78:DG:H5'	37:c:12:ARG:HH11	1.76	0.51
24:N:178:DG:H2''	24:N:179:DT:C5	2.46	0.51
2:1:705:ASN:HA	2:1:708:LEU:HG	1.93	0.51
5:4:146:TYR:CZ	5:4:180:SER:HB3	2.46	0.51
11:A:760:LEU:HD11	11:A:781:ILE:HG21	1.92	0.51
11:A:1228:MET:HE3	11:A:1228:MET:HA	1.93	0.51
11:A:1468:THR:HG22	16:F:64:ARG:HD2	1.93	0.51
12:B:331:THR:HG23	12:B:334:LYS:H	1.75	0.51
1:0:527:THR:O	1:0:530:ARG:HG2	2.11	0.50
5:4:302:PRO:HB3	5:4:313:VAL:HG23	1.94	0.50
11:A:889:LEU:O	11:A:890:ARG:NH1	2.37	0.50
24:N:179:DT:H2''	24:N:180:DC:C5	2.46	0.50
11:A:937:ASP:OD1	11:A:937:ASP:N	2.42	0.50
15:E:44:PHE:CB	15:E:52:ARG:HG3	2.42	0.50
24:N:90:DG:OP2	38:d:87:ARG:NH1	2.43	0.50
1:0:438:MET:HE2	1:0:440:LEU:HD21	1.92	0.50
3:2:457:ILE:HG23	3:2:461:LEU:HD13	1.94	0.50
12:B:385:ARG:NE	12:B:492:ASP:OD1	2.35	0.50
15:E:52:ARG:HD3	15:E:53:PRO:HD3	1.93	0.50
28:T:-88:DA:H2''	28:T:-87:DC:OP2	2.09	0.50
29:U:344:ARG:HD3	29:U:349:TRP:CZ2	2.46	0.50
31:W:17:LEU:HA	31:W:190:LEU:HD13	1.93	0.50
1:0:558:ILE:O	1:0:604:THR:HA	2.12	0.50
4:3:430:VAL:HG12	4:3:443:VAL:HB	1.93	0.50
27:R:194:HIS:HB3	27:R:197:TYR:CZ	2.45	0.50
2:1:373:ARG:NH1	2:1:409:THR:HG23	2.26	0.50
4:3:32:ASP:OD1	4:3:33:ARG:N	2.44	0.50
14:D:74:PHE:CZ	14:D:83:VAL:HG21	2.47	0.50
28:T:-21:DG:H5'	28:T:-21:DG:C8	2.47	0.50
3:2:514:ARG:HH12	3:2:521:LEU:HD22	1.75	0.50
14:D:70:ARG:HE	17:G:142:GLU:CD	2.20	0.50
1:0:133:THR:HB	1:0:160:THR:HG21	1.93	0.50
4:3:400:ARG:NH2	7:6:13:ASP:OD2	2.42	0.50
24:N:29:DC:H2'	24:N:30:DT:H71	1.92	0.50
19:I:91:HIS:CE1	19:I:93:GLU:HB3	2.47	0.50
7:6:34:ILE:HD13	7:6:45:VAL:HG12	1.93	0.50
11:A:253:LEU:HD21	11:A:317:MET:HE1	1.93	0.50
11:A:268:GLY:H	12:B:890:ARG:NH1	2.10	0.50
37:c:86:LEU:O	37:c:90:ASN:ND2	2.45	0.50
4:3:397:GLU:HA	4:3:400:ARG:HG2	1.94	0.49
5:4:292:PRO:HG3	6:5:264:ILE:HD11	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:467:MET:HE3	11:A:534:VAL:HG21	1.94	0.49
11:A:618:TYR:HB3	11:A:621:ILE:HG23	1.94	0.49
2:1:141:TYR:CZ	2:1:387:GLU:HG2	2.47	0.49
5:4:200:GLY:O	5:4:221:VAL:HA	2.12	0.49
9:8:125:LEU:HD21	9:8:138:LEU:HD11	1.94	0.49
11:A:763:TYR:OH	18:H:23:ASP:OD2	2.20	0.49
13:C:18:ASN:ND2	13:C:232:ASN:OD1	2.45	0.49
13:C:152:LYS:NZ	20:J:57:GLU:OE2	2.30	0.49
31:W:127:PHE:CD2	31:W:163:GLU:HB2	2.47	0.49
15:E:59:THR:HG22	15:E:75:PHE:HA	1.94	0.49
24:N:55:DA:H1'	24:N:56:DG:N1	2.27	0.49
28:T:-37:DG:H2''	28:T:-36:DA:C8	2.48	0.49
1:0:540:LYS:HZ1	1:0:669:GLU:CD	2.19	0.49
4:3:448:HIS:HA	4:3:451:VAL:HG12	1.95	0.49
6:5:229:TRP:CZ3	6:5:241:LEU:HD21	2.48	0.49
12:B:954:MET:HE1	12:B:966:ILE:HG13	1.94	0.49
19:I:39:CYS:SG	19:I:42:CYS:HB3	2.51	0.49
29:U:349:TRP:O	29:U:373:ASP:HA	2.12	0.49
31:W:120:ASP:HA	31:W:123:ASN:ND2	2.27	0.49
12:B:593:GLN:NE2	12:B:595:ASP:OD2	2.43	0.49
9:8:71:HIS:HE1	9:8:73:ASN:OD1	1.95	0.49
11:A:525:ILE:HA	11:A:535:MET:HE3	1.94	0.49
24:N:88:DT:H4'	24:N:89:DA:OP1	2.13	0.49
24:N:127:DT:H2''	24:N:128:DC:C5	2.48	0.49
28:T:-196:DT:H2''	28:T:-195:DC:H5'	1.95	0.49
2:1:390:ASP:N	2:1:390:ASP:OD1	2.45	0.49
4:3:55:TRP:HE1	4:3:74:TRP:HE3	1.61	0.49
28:T:-47:DC:N4	28:T:-46:DG:O6	2.46	0.49
2:1:354:PRO:HB2	2:1:355:PRO:CD	2.43	0.49
11:A:465:HIS:CE1	11:A:467:MET:HB2	2.48	0.49
12:B:1062:ARG:HD3	12:B:1081:ASP:O	2.13	0.49
13:C:44:ILE:HG21	13:C:178:PRO:HB3	1.94	0.49
24:N:57:DA:N7	28:T:-58:DT:N3	2.61	0.49
29:U:355:ASP:OD1	30:V:6:TYR:OH	2.30	0.49
1:0:447:PRO:HB2	1:0:472:ARG:NH2	2.26	0.49
9:8:120:MET:HE1	9:8:150:VAL:HA	1.95	0.49
11:A:118:LEU:HD12	11:A:148:CYS:HB3	1.93	0.49
28:T:-89:DT:H1'	28:T:-88:DA:C4	2.48	0.49
32:X:214:GLU:OE2	32:X:221:ARG:NH2	2.45	0.49
1:0:129:VAL:HG23	1:0:131:LEU:HG	1.94	0.48
11:A:1136:THR:O	11:A:1360:ASN:ND2	2.33	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:1112:ASP:OD1	12:B:1112:ASP:N	2.46	0.48
15:E:46:ASP:HB3	15:E:52:ARG:HB3	1.95	0.48
24:N:169:DC:H2'	24:N:170:DA:C5	2.48	0.48
11:A:909:LEU:CD1	11:A:967:ARG:HD3	2.41	0.48
24:N:141:DA:H2'	35:e:66:LEU:HD22	1.96	0.48
32:X:77:VAL:O	32:X:81:ILE:HG12	2.13	0.48
32:X:226:ASP:OD1	32:X:227:SER:N	2.46	0.48
1:O:139:TYR:CZ	5:4:19:TRP:HB2	2.48	0.48
11:A:963:ARG:NH2	11:A:967:ARG:NH2	2.62	0.48
24:N:18:DG:N2	28:T:-17:DC:O2	2.47	0.48
1:O:98:ASP:OD1	5:4:15:TYR:OH	2.25	0.48
2:1:176:ASN:O	2:1:180:LEU:N	2.39	0.48
2:1:511:ARG:NH1	2:1:512:GLU:OE1	2.47	0.48
2:1:722:ARG:NH2	5:4:75:ASP:OD2	2.46	0.48
23:M:18:HIS:ND1	23:M:36:GLU:HG3	2.28	0.48
6:5:42:MET:SD	6:5:108:ASN:HA	2.54	0.48
11:A:432:HIS:NE2	23:M:36:GLU:HA	2.29	0.48
12:B:926:VAL:HG21	13:C:62:GLU:HG3	1.94	0.48
15:E:73:PHE:CE2	15:E:99:ILE:HG13	2.48	0.48
19:I:69:ILE:HG22	19:I:71:ASP:H	1.79	0.48
4:3:448:HIS:NE2	7:6:4:VAL:HG21	2.29	0.48
11:A:757:GLN:NE2	11:A:778:LYS:O	2.47	0.48
25:O:283:TYR:CZ	25:O:285:PRO:HG3	2.49	0.48
1:O:519:TYR:HE2	1:O:666:ASP:HB2	1.79	0.48
1:O:665:GLN:O	1:O:667:THR:HG23	2.13	0.48
3:2:456:ASP:N	3:2:456:ASP:OD1	2.42	0.48
4:3:148:LEU:HA	4:3:151:TYR:CE1	2.48	0.48
11:A:360:ASP:OD1	12:B:1062:ARG:NE	2.34	0.48
11:A:498:GLY:HA3	12:B:934:LYS:HE2	1.94	0.48
19:I:91:HIS:HE1	19:I:93:GLU:HB3	1.77	0.48
24:N:11:DG:O6	28:T:-12:DC:N4	2.47	0.48
25:O:239:ARG:HG3	25:O:239:ARG:HH11	1.79	0.48
32:X:81:ILE:HG23	32:X:102:ILE:HG21	1.96	0.48
1:O:393:THR:HG22	1:O:395:ASP:H	1.79	0.48
19:I:65:LEU:HD23	19:I:68:ILE:HD12	1.95	0.48
29:U:19:GLU:O	29:U:23:ASN:ND2	2.39	0.48
4:3:266:ARG:NH2	4:3:273:GLN:OE1	2.45	0.48
5:4:257:HIS:HB2	5:4:289:TYR:CE2	2.49	0.48
12:B:908:MET:HB3	22:L:45:TYR:CE1	2.49	0.48
14:D:14:GLU:N	14:D:14:GLU:OE1	2.47	0.48
19:I:30:LYS:HA	19:I:33:ARG:NE	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:M:193:ARG:HH21	24:N:2:DA:P	2.37	0.48
24:N:28:DC:N4	28:T:-29:DG:O6	2.47	0.48
28:T:-42:DC:H2'	28:T:-41:DG:C8	2.49	0.48
2:1:322:SER:HB3	8:7:99:LEU:HD23	1.96	0.48
13:C:31:ALA:O	13:C:231:TYR:OH	2.29	0.48
24:N:73:DC:H2'	24:N:74:DC:C6	2.49	0.48
26:Q:47:LEU:HD23	27:R:104:LEU:HD22	1.96	0.48
1:0:337:VAL:O	1:0:488:LEU:N	2.45	0.47
8:7:274:HIS:CE1	10:9:175:LYS:HD2	2.48	0.47
10:9:165:ARG:HB3	10:9:166:PRO:HD3	1.95	0.47
12:B:455:ASP:OD2	12:B:457:LYS:NZ	2.31	0.47
15:E:88:LYS:HD2	15:E:91:CYS:SG	2.54	0.47
24:N:55:DA:H2''	24:N:56:DG:C6	2.49	0.47
26:Q:13:GLU:HA	27:R:44:ARG:HA	1.96	0.47
28:T:-88:DA:P	28:T:-88:DA:H3'	2.54	0.47
5:4:88:LEU:HD21	5:4:170:ILE:HD11	1.96	0.47
5:4:195:ARG:HH12	5:4:197:SER:HB3	1.80	0.47
11:A:379:GLY:HA2	11:A:475:ARG:O	2.14	0.47
8:7:82:TYR:CE1	8:7:124:ILE:HD13	2.49	0.47
11:A:502:ASN:HB3	12:B:1084:LEU:HD13	1.96	0.47
23:M:34:CYS:SG	23:M:37:CYS:HB3	2.53	0.47
10:9:110:PHE:CZ	10:9:114:LYS:HE3	2.49	0.47
24:N:11:DG:H2''	24:N:12:DG:N7	2.29	0.47
8:7:44:GLY:O	8:7:53:LEU:N	2.43	0.47
9:8:82:GLY:HA3	9:8:87:ILE:HA	1.96	0.47
12:B:794:VAL:HG13	12:B:965:ILE:HG23	1.96	0.47
24:N:139:DT:H2''	24:N:140:DA:C8	2.48	0.47
35:e:74:GLU:OE1	36:f:24:ARG:HB2	2.14	0.47
9:8:304:GLY:HA2	9:8:307:LEU:HD23	1.95	0.47
12:B:513:GLU:HG3	12:B:726:SER:HB3	1.97	0.47
24:N:131:DC:P	36:f:49:GLY:H	2.37	0.47
28:T:-5:DT:OP1	29:U:344:ARG:NH2	2.48	0.47
1:0:187:HIS:HA	1:0:190:GLN:HG2	1.97	0.47
2:1:571:THR:H	2:1:577:THR:CG2	2.27	0.47
10:9:77:ARG:HD3	10:9:164:TYR:CE1	2.50	0.47
11:A:246:GLU:HG2	11:A:247:TRP:CD1	2.50	0.47
11:A:618:TYR:HB3	11:A:621:ILE:O	2.14	0.47
11:A:732:THR:O	11:A:736:THR:HG23	2.15	0.47
19:I:100:HIS:O	19:I:100:HIS:CD2	2.68	0.47
27:R:58:LEU:HD11	27:R:62:LEU:HD23	1.96	0.47
28:T:-181:DT:H2''	28:T:-180:DG:C4	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:T:-117:DC:H5''	36:b:48:SER:HA	1.97	0.47
28:T:-91:DT:H1'	28:T:-90:DC:H5'	1.97	0.47
2:1:152:LEU:HD12	2:1:153:PRO:HD2	1.96	0.47
3:2:483:THR:OG1	3:2:492:LYS:NZ	2.26	0.47
8:7:269:LEU:HD22	8:7:290:SER:HB3	1.96	0.47
11:A:1005:HIS:CD2	11:A:1006:PRO:HD2	2.49	0.47
11:A:1182:GLN:O	11:A:1190:GLN:NE2	2.39	0.47
24:N:11:DG:H1	28:T:-11:DC:N4	2.13	0.47
24:N:77:DT:H2''	24:N:78:DC:C6	2.50	0.47
1:0:60:ASP:OD1	1:0:62:ARG:NH1	2.48	0.47
3:2:503:THR:HG21	3:2:533:TYR:CZ	2.50	0.47
5:4:291:CYS:HB3	5:4:294:CYS:HB2	1.97	0.47
24:N:34:DT:H4'	24:N:35:DC:OP1	2.15	0.47
1:0:532:LEU:HD22	1:0:716:VAL:HG13	1.97	0.47
5:4:288:GLY:N	5:4:297:LYS:HE2	2.30	0.47
6:5:281:ILE:HB	6:5:286:GLU:HA	1.96	0.47
14:D:106:GLU:OE2	14:D:138:ARG:NH1	2.47	0.47
2:1:422:ASP:H	2:1:428:ILE:CG2	2.29	0.46
4:3:29:GLY:O	4:3:33:ARG:NH2	2.48	0.46
5:4:345:CYS:O	5:4:349:GLN:N	2.46	0.46
11:A:365:THR:HG22	11:A:482:PHE:CE2	2.50	0.46
11:A:653:VAL:HG11	11:A:669:TYR:OH	2.15	0.46
11:A:1099:ALA:HA	11:A:1102:MET:SD	2.55	0.46
1:0:635:GLN:HB3	1:0:676:ARG:NH2	2.28	0.46
2:1:422:ASP:H	2:1:428:ILE:HG22	1.80	0.46
9:8:213:LEU:HD22	9:8:224:ARG:HB3	1.97	0.46
10:9:29:LYS:HE3	11:A:1481:LYS:HD3	1.97	0.46
24:N:9:DG:N2	28:T:-8:DC:O2	2.48	0.46
28:T:-22:DC:H2''	28:T:-21:DG:H5''	1.97	0.46
1:0:479:ASP:HA	1:0:482:PHE:CE2	2.50	0.46
9:8:64:LYS:NZ	10:9:115:VAL:O	2.32	0.46
9:8:136:ARG:O	9:8:174:VAL:HG22	2.15	0.46
32:X:89:HIS:HB2	32:X:139:PHE:CD1	2.50	0.46
35:a:60:GLU:N	35:a:60:GLU:OE1	2.48	0.46
2:1:32:LEU:HB3	2:1:59:TYR:CZ	2.51	0.46
3:2:373:ALA:HA	5:4:53:VAL:HA	1.96	0.46
9:8:40:ILE:HG12	9:8:90:VAL:HG22	1.96	0.46
12:B:42:GLN:H	12:B:42:GLN:CD	2.24	0.46
18:H:96:VAL:HG22	18:H:116:VAL:HG22	1.96	0.46
24:N:77:DT:H2''	24:N:78:DC:C5	2.50	0.46
1:0:371:VAL:HG12	1:0:391:ARG:HD2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:58:ARG:HD2	6:5:229:TRP:CE3	2.51	0.46
9:8:118:MET:HG3	9:8:203:LEU:HD13	1.97	0.46
12:B:214:LYS:HE2	12:B:215:TYR:CZ	2.51	0.46
12:B:453:TRP:NE1	12:B:466:VAL:HB	2.31	0.46
12:B:971:ALA:O	12:B:975:ARG:HD3	2.14	0.46
28:T:-151:DC:H2''	28:T:-150:DC:C5	2.50	0.46
28:T:-117:DC:P	36:b:49:GLY:H	2.39	0.46
1:0:415:HIS:NE2	1:0:417:THR:OG1	2.45	0.46
2:1:216:LYS:HB2	2:1:307:ASN:HB2	1.96	0.46
11:A:1178:ASP:HB3	11:A:1185:VAL:HG13	1.98	0.46
12:B:453:TRP:N	12:B:453:TRP:CD1	2.83	0.46
28:T:-44:DT:H2'	28:T:-43:DG:C8	2.51	0.46
4:3:161:HIS:NE2	4:3:323:LEU:HB2	2.31	0.46
4:3:444:THR:HG23	4:3:447:GLY:H	1.81	0.46
11:A:410:ASN:HD22	11:A:430:ARG:HB3	1.80	0.46
11:A:1218:ARG:NH2	11:A:1252:ALA:O	2.49	0.46
22:L:35:ARG:HG2	22:L:40:GLY:HA2	1.98	0.46
28:T:-166:DG:OP1	37:g:21:ARG:NH1	2.46	0.46
29:U:333:ASN:HB2	30:V:93:VAL:HG22	1.98	0.46
9:8:241:CYS:HA	9:8:246:TYR:CD2	2.50	0.46
10:9:96:VAL:HG13	10:9:101:PRO:HD3	1.98	0.46
11:A:189:PRO:HB3	11:A:202:TRP:CE2	2.50	0.46
11:A:495:ASP:OD1	11:A:495:ASP:O	2.34	0.46
14:D:87:LEU:HB3	14:D:97:LEU:HD22	1.97	0.46
19:I:41:ASN:HA	26:Q:177:MET:HE2	1.97	0.46
28:T:-141:DT:H2''	28:T:-140:DT:C5	2.51	0.46
36:f:77:ALA:HB2	38:h:85:ASN:HD21	1.81	0.46
2:1:401:ALA:O	2:1:405:THR:HG22	2.16	0.46
6:5:187:GLN:HB3	6:5:189:ILE:CD1	2.46	0.46
24:N:135:DG:O6	28:T:-136:DA:N6	2.49	0.46
29:U:344:ARG:HD3	29:U:349:TRP:CE2	2.51	0.46
2:1:320:PRO:HA	2:1:374:PHE:CG	2.51	0.46
2:1:362:ALA:O	2:1:366:CYS:HA	2.16	0.46
11:A:516:GLN:HA	11:A:520:MET:HG2	1.97	0.46
13:C:78:ILE:HG21	13:C:127:VAL:CG2	2.45	0.46
24:N:78:DC:OP2	37:c:33:ARG:HD3	2.16	0.46
24:N:81:DT:H2'	24:N:82:DT:C6	2.50	0.46
36:f:32:LYS:HE3	36:f:52:TYR:CZ	2.51	0.46
1:0:636:GLU:OE1	1:0:676:ARG:HD3	2.15	0.45
11:A:409:GLY:O	11:A:415:GLY:HA3	2.16	0.45
11:A:804:HIS:CE1	19:I:100:HIS:CD2	3.04	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:G:4:HIS:CE1	17:G:73:LYS:HD2	2.51	0.45
26:Q:126:ILE:HD11	26:Q:140:VAL:HG22	1.98	0.45
28:T:-62:DG:H2''	28:T:-61:DG:C8	2.51	0.45
30:V:67:PHE:HB2	30:V:72:TRP:CE3	2.51	0.45
1:O:544:CYS:SG	1:O:545:GLN:N	2.89	0.45
2:1:240:ASP:OD1	2:1:240:ASP:N	2.49	0.45
11:A:1483:GLY:O	11:A:1484:MET:HG3	2.17	0.45
12:B:778:SER:HG	12:B:805:PHE:HZ	1.63	0.45
31:W:11:PRO:HD2	31:W:14:LEU:HD12	1.98	0.45
31:W:148:MET:HG3	31:W:149:THR:HG23	1.98	0.45
1:O:622:VAL:HG22	1:O:658:PHE:HD2	1.81	0.45
3:2:400:ILE:HD12	3:2:400:ILE:H	1.81	0.45
12:B:795:ILE:HG12	12:B:947:ILE:HG22	1.98	0.45
25:O:206:GLU:HB3	25:O:207:PRO:HD3	1.99	0.45
1:O:123:LEU:O	1:O:127:VAL:HG23	2.16	0.45
10:9:86:TYR:OH	10:9:158:LEU:O	2.13	0.45
12:B:399:LEU:HB3	12:B:453:TRP:CZ3	2.51	0.45
24:N:88:DT:H2''	24:N:89:DA:C8	2.51	0.45
24:N:129:DC:H2''	24:N:130:DC:C6	2.51	0.45
25:O:228:GLU:CD	25:O:231:ARG:HH22	2.23	0.45
28:T:-168:DG:H3'	37:g:29:GLY:HA3	1.99	0.45
2:1:142:VAL:HG13	2:1:152:LEU:HD21	1.99	0.45
5:4:249:LEU:HD13	6:5:289:PHE:CD2	2.51	0.45
28:T:-54:DC:H2'	28:T:-53:DG:C8	2.52	0.45
7:6:13:ASP:OD1	7:6:13:ASP:N	2.49	0.45
10:9:95:SER:HB3	10:9:98:GLU:OE1	2.17	0.45
13:C:70:LEU:O	20:J:6:ARG:HD3	2.15	0.45
15:E:94:MET:O	15:E:98:ASN:N	2.49	0.45
17:G:144:ARG:NH2	17:G:167:TYR:HB3	2.32	0.45
18:H:37:MET:SD	18:H:127:GLY:HA3	2.56	0.45
24:N:89:DA:H1'	24:N:90:DG:C8	2.52	0.45
1:O:71:HIS:HA	1:O:145:LYS:HB2	1.99	0.45
3:2:305:LYS:HG2	3:2:309:HIS:CD2	2.52	0.45
4:3:59:MET:HA	4:3:62:LEU:HD23	1.97	0.45
10:9:28:ARG:NH1	11:A:1484:MET:SD	2.90	0.45
10:9:35:VAL:HG21	11:A:1484:MET:HE3	1.98	0.45
11:A:61:ARG:O	11:A:73:THR:HG21	2.16	0.45
24:N:50:DG:N2	28:T:-49:DA:N3	2.64	0.45
24:N:83:DG:H2'	24:N:84:DG:C8	2.51	0.45
28:T:-89:DT:H2''	28:T:-88:DA:C8	2.52	0.45
1:O:274:GLN:NE2	1:O:277:ILE:HD12	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Q:166:ARG:O	26:Q:170:VAL:N	2.50	0.45
2:1:462:SER:HB3	2:1:654:PHE:CE1	2.52	0.45
9:8:134:LEU:HG	9:8:162:PHE:CD1	2.52	0.45
11:A:1163:HIS:HB2	11:A:1301:ILE:O	2.17	0.45
17:G:89:VAL:HA	17:G:99:THR:HG22	1.99	0.45
24:N:191:DA:H2''	24:N:192:DT:C6	2.52	0.45
28:T:-12:DC:OP2	28:T:-12:DC:H3'	2.17	0.45
1:0:519:TYR:CE2	1:0:666:ASP:HB2	2.52	0.44
1:0:551:HIS:CB	1:0:558:ILE:HD11	2.47	0.44
1:0:631:GLY:HA2	1:0:676:ARG:HB2	1.98	0.44
3:2:483:THR:HB	3:2:488:GLU:OE1	2.18	0.44
11:A:668:PHE:CE1	11:A:672:ILE:HD11	2.52	0.44
12:B:666:ASP:OD1	12:B:666:ASP:C	2.60	0.44
12:B:759:VAL:CG1	12:B:999:ALA:HB2	2.47	0.44
13:C:260:GLN:HB2	21:K:91:ILE:HG21	1.98	0.44
17:G:39:THR:O	17:G:43:GLY:N	2.46	0.44
1:0:283:ARG:HA	1:0:286:HIS:CD2	2.52	0.44
11:A:30:GLU:O	11:A:34:MET:N	2.49	0.44
11:A:1468:THR:HG23	16:F:64:ARG:HB2	1.98	0.44
28:T:-68:DG:H1'	28:T:-67:DG:N7	2.32	0.44
32:X:236:TYR:HD1	32:X:239:ARG:CZ	2.31	0.44
1:0:88:ALA:HA	1:0:93:TYR:CD1	2.52	0.44
2:1:161:PHE:O	2:1:166:ARG:N	2.48	0.44
15:E:44:PHE:CG	15:E:52:ARG:HG3	2.51	0.44
28:T:-194:DG:H2''	28:T:-193:DG:C8	2.52	0.44
28:T:-121:DC:H2''	28:T:-120:DG:C8	2.52	0.44
28:T:-87:DC:OP2	28:T:-87:DC:H2'	2.18	0.44
32:X:88:ARG:NH2	32:X:93:ASP:OD2	2.50	0.44
1:0:630:GLY:O	1:0:676:ARG:NE	2.41	0.44
2:1:611:VAL:HG12	2:1:612:HIS:N	2.32	0.44
6:5:187:GLN:HB3	6:5:189:ILE:HD12	1.99	0.44
23:M:137:ARG:NE	23:M:171:GLU:OE2	2.50	0.44
26:Q:124:TYR:OH	27:R:22:LYS:HE2	2.16	0.44
31:W:106:LYS:HE3	32:X:223:VAL:HB	2.00	0.44
2:1:1:MET:O	2:1:12:PHE:N	2.50	0.44
2:1:490:LEU:HD12	2:1:492:PRO:HD3	1.99	0.44
5:4:171:PHE:HE2	5:4:205:VAL:HG21	1.82	0.44
1:0:449:LYS:O	1:0:453:ARG:NH1	2.51	0.44
11:A:400:ASP:OD1	11:A:401:ARG:N	2.49	0.44
28:T:-187:DT:H2''	28:T:-186:DA:C8	2.52	0.44
1:0:168:LEU:HB2	1:0:291:LEU:HD23	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:407:VAL:HG13	7:6:6:LYS:HE2	1.99	0.44
10:9:3:HIS:NE2	10:9:8:LYS:HG2	2.33	0.44
12:B:785:TYR:O	12:B:786:THR:HG22	2.16	0.44
15:E:74:VAL:HA	15:E:103:LEU:O	2.18	0.44
21:K:21:ILE:HG12	21:K:33:PHE:CD2	2.53	0.44
23:M:128:ILE:HG23	23:M:183:VAL:HG11	1.99	0.44
24:N:40:DC:H2''	24:N:41:DC:C6	2.52	0.44
2:1:290:GLU:HA	8:7:93:ARG:NH2	2.32	0.44
4:3:418:PHE:CE1	4:3:441:MET:HE2	2.53	0.44
5:4:68:SER:HB3	5:4:143:PRO:HD3	2.00	0.44
10:9:233:SER:HA	10:9:238:LEU:CB	2.48	0.44
11:A:972:THR:HG23	11:A:974:ASP:H	1.83	0.44
12:B:1068:GLN:O	12:B:1072:ARG:N	2.50	0.44
15:E:36:THR:OG1	15:E:38:GLU:OE2	2.31	0.44
24:N:80:DA:OP1	37:c:21:ARG:NH1	2.51	0.44
26:Q:163:GLU:HB3	26:Q:176:ILE:HD11	1.99	0.44
28:T:-69:DC:C2	28:T:-68:DG:C6	3.05	0.44
31:W:125:ALA:HB1	31:W:136:PHE:C	2.43	0.44
32:X:98:THR:HG23	32:X:136:LYS:HE3	1.99	0.44
1:0:182:PRO:HA	1:0:268:VAL:HG11	2.00	0.44
2:1:160:GLU:HG2	2:1:189:TRP:NE1	2.32	0.44
2:1:236:ALA:HB1	2:1:239:ILE:HB	1.99	0.44
2:1:612:HIS:HB3	2:1:673:ASP:HB2	2.00	0.44
5:4:259:ILE:HG22	5:4:287:GLY:HA3	2.00	0.44
9:8:226:PHE:CD1	9:8:232:PRO:HD3	2.53	0.44
11:A:1483:GLY:CA	16:F:80:MET:HA	2.48	0.44
17:G:38:CYS:HB2	17:G:44:PHE:CD2	2.53	0.44
27:R:220:ILE:HG13	27:R:221:GLY:H	1.83	0.44
1:0:347:SER:HA	1:0:374:TRP:CH2	2.53	0.43
11:A:485:ASN:O	11:A:488:VAL:HG22	2.18	0.43
12:B:719:SER:OG	12:B:720:PRO:HD3	2.18	0.43
12:B:862:GLY:HA3	12:B:898:THR:HA	2.00	0.43
13:C:60:HIS:CE1	13:C:63:PHE:HB2	2.53	0.43
17:G:81:LYS:HA	17:G:147:ILE:HG22	1.98	0.43
24:N:31:DC:H2''	24:N:32:DA:C8	2.53	0.43
2:1:176:ASN:OD1	2:1:177:LEU:N	2.49	0.43
2:1:224:GLU:CD	2:1:227:ARG:HE	2.25	0.43
2:1:403:PHE:CE1	2:1:407:VAL:HG11	2.53	0.43
2:1:613:HIS:HE1	2:1:614:TYR:CZ	2.36	0.43
9:8:210:VAL:HG13	9:8:211:PRO:HD2	2.00	0.43
12:B:20:ASP:OD1	12:B:20:ASP:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:O:239:ARG:NH2	29:U:315:ASN:OD1	2.50	0.43
26:Q:151:ARG:H	26:Q:151:ARG:HD3	1.82	0.43
31:W:77:ARG:HD3	31:W:91:TYR:CD1	2.54	0.43
35:a:120:ILE:HG13	36:b:51:ILE:HG13	2.00	0.43
10:9:36:ALA:HB2	17:G:20:PRO:CG	2.48	0.43
11:A:512:ARG:HH11	11:A:512:ARG:HB2	1.83	0.43
12:B:819:SER:H	12:B:827:GLU:CD	2.27	0.43
16:F:78:PRO:HG3	17:G:18:PHE:O	2.17	0.43
17:G:119:PHE:HB2	17:G:128:TYR:CE2	2.53	0.43
26:Q:15:VAL:O	26:Q:135:PHE:N	2.50	0.43
28:T:-167:DA:OP1	37:g:18:ARG:N	2.47	0.43
2:1:73:CYS:HA	2:1:207:TYR:O	2.19	0.43
2:1:339:TYR:OH	2:1:343:ARG:NH1	2.52	0.43
11:A:1067:TRP:CH2	11:A:1071:GLU:HG3	2.53	0.43
12:B:40:VAL:HG22	12:B:43:GLN:HB2	2.00	0.43
12:B:455:ASP:OD2	12:B:457:LYS:HG2	2.19	0.43
12:B:517:GLY:O	12:B:520:VAL:HG22	2.18	0.43
2:1:75:ARG:HH21	2:1:237:HIS:CD2	2.36	0.43
2:1:324:ARG:HE	8:7:96:ASN:ND2	2.16	0.43
4:3:46:ARG:NH2	6:5:53:ARG:HA	2.33	0.43
10:9:238:LEU:HA	10:9:245:LEU:CD1	2.48	0.43
11:A:59:ASP:CG	11:A:61:ARG:HE	2.25	0.43
11:A:1096:GLY:O	11:A:1100:THR:HG23	2.18	0.43
15:E:73:PHE:CD2	15:E:99:ILE:HG13	2.53	0.43
1:0:51:THR:HG23	1:0:52:LYS:N	2.34	0.43
1:0:511:TRP:CD1	1:0:689:VAL:HG13	2.53	0.43
6:5:207:CYS:O	6:5:211:GLY:N	2.51	0.43
8:7:268:ARG:HA	8:7:271:TYR:CE2	2.54	0.43
11:A:244:ARG:HB3	11:A:246:GLU:CD	2.43	0.43
11:A:1211:LEU:HD11	11:A:1258:ARG:HB3	2.01	0.43
13:C:9:VAL:HG11	21:K:105:PHE:CD1	2.54	0.43
13:C:84:TYR:CZ	13:C:167:LYS:HE2	2.54	0.43
24:N:172:DG:H2"	24:N:173:DC:C6	2.54	0.43
38:d:39:ALA:HA	38:d:60:MET:SD	2.58	0.43
5:4:109:THR:HG21	5:4:144:SER:H	1.83	0.43
7:6:24:ASP:OD1	7:6:25:GLU:N	2.51	0.43
11:A:346:LYS:HA	11:A:351:ARG:HB3	2.00	0.43
11:A:395:THR:CG2	11:A:396:PRO:HD2	2.49	0.43
11:A:1163:HIS:CD2	11:A:1302:GLU:HA	2.54	0.43
13:C:48:ASP:OD1	13:C:175:LYS:NZ	2.41	0.43
21:K:105:PHE:CE2	21:K:109:ILE:HD11	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:M:193:ARG:NH2	24:N:2:DA:OP2	2.39	0.43
31:W:42:CYS:SG	31:W:91:TYR:HB3	2.58	0.43
35:e:62:LEU:HD13	36:f:37:ARG:HB3	2.00	0.43
2:1:118:HIS:HA	2:1:157:PHE:HE2	1.84	0.43
2:1:407:VAL:HG12	2:1:435:PHE:CD1	2.54	0.43
2:1:565:LYS:HB3	2:1:595:ILE:HD11	2.01	0.43
2:1:688:ASP:OD2	2:1:689:LYS:NZ	2.44	0.43
5:4:145:LEU:HD12	5:4:176:THR:HG21	2.01	0.43
8:7:63:PHE:HB2	8:7:69:ASP:OD1	2.18	0.43
12:B:136:GLY:O	12:B:137:GLU:HG3	2.19	0.43
12:B:1122:CYS:HB3	12:B:1140:CYS:SG	2.58	0.43
13:C:52:ILE:HD12	13:C:61:ASP:HB3	2.01	0.43
6:5:152:LYS:H	6:5:152:LYS:HD2	1.82	0.43
6:5:178:MET:HG3	6:5:182:PHE:CE2	2.54	0.43
36:f:32:LYS:HE3	36:f:52:TYR:CE2	2.53	0.43
1:0:89:PHE:CD2	4:3:375:VAL:HG21	2.53	0.43
1:0:282:LYS:HG3	1:0:283:ARG:N	2.34	0.43
2:1:318:ALA:HB3	2:1:374:PHE:CZ	2.54	0.43
4:3:64:GLN:HG2	4:3:65:PRO:HD2	2.01	0.43
4:3:121:ALA:O	6:5:100:LYS:HE2	2.19	0.43
10:9:28:ARG:NH2	11:A:1483:GLY:HA2	2.34	0.43
11:A:57:LEU:HD22	11:A:280:LEU:HB3	2.01	0.43
11:A:479:TRP:CD1	12:B:931:ILE:HD12	2.53	0.43
19:I:12:VAL:HG23	19:I:13:GLY:H	1.83	0.43
25:O:163:PRO:HA	25:O:262:CYS:HB3	2.00	0.43
36:b:32:LYS:HG3	36:b:52:TYR:CE1	2.54	0.43
2:1:318:ALA:HB3	2:1:374:PHE:CE1	2.53	0.42
10:9:243:THR:HA	11:A:1008:LYS:HE3	2.01	0.42
11:A:239:GLU:HG3	11:A:241:ARG:HG2	2.00	0.42
12:B:786:THR:HG21	12:B:949:TYR:OH	2.18	0.42
25:O:191:GLU:HG3	25:O:201:ILE:HB	2.01	0.42
2:1:352:GLU:HA	2:1:416:ILE:O	2.19	0.42
2:1:370:LYS:HB2	2:1:371:PRO:HD3	2.01	0.42
3:2:468:VAL:HG21	3:2:525:ILE:HD11	2.01	0.42
8:7:273:ASN:HD21	8:7:289:SER:HB3	1.84	0.42
12:B:271:ILE:HD12	12:B:311:ILE:HD12	2.00	0.42
12:B:344:GLN:NE2	12:B:353:VAL:O	2.52	0.42
15:E:11:TRP:CE3	15:E:37:LEU:HB2	2.54	0.42
19:I:28:GLU:OE2	19:I:33:ARG:HD2	2.19	0.42
37:c:68:GLY:HA3	38:d:50:HIS:CD2	2.53	0.42
2:1:213:LEU:HD21	2:1:239:ILE:HD11	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:606:GLU:O	2:1:666:ARG:NH2	2.49	0.42
3:2:403:SER:HB3	6:5:23:GLY:HA3	2.01	0.42
4:3:146:PRO:HA	4:3:149:ASP:OD2	2.19	0.42
5:4:112:LYS:HG3	5:4:177:CYS:SG	2.59	0.42
8:7:124:ILE:HG12	8:7:128:GLU:HG3	2.01	0.42
24:N:32:DA:H2"	24:N:33:DC:C6	2.54	0.42
3:2:193:ILE:HB	3:2:221:TRP:NE1	2.35	0.42
3:2:470:GLU:OE1	3:2:473:ARG:NH2	2.42	0.42
9:8:66:LEU:HD23	9:8:77:LEU:HB2	2.01	0.42
11:A:872:MET:HG2	11:A:873:VAL:N	2.33	0.42
23:M:283:VAL:HG22	23:M:286:ARG:NH2	2.35	0.42
24:N:65:DT:C4	24:N:66:DG:C6	3.07	0.42
32:X:190:LEU:HB2	32:X:202:PHE:HB2	2.02	0.42
2:1:170:LEU:HD11	2:1:175:TYR:CZ	2.55	0.42
8:7:273:ASN:ND2	8:7:289:SER:HB3	2.35	0.42
10:9:27:ASN:ND2	10:9:48:LEU:O	2.43	0.42
12:B:1069:ILE:CG2	23:M:47:ASP:HB2	2.50	0.42
25:O:204:ILE:HG13	25:O:207:PRO:HD2	2.01	0.42
2:1:161:PHE:CE1	2:1:194:LEU:HA	2.55	0.42
11:A:230:ASP:N	11:A:230:ASP:OD1	2.53	0.42
11:A:875:TYR:OH	16:F:61:GLU:OE2	2.28	0.42
12:B:385:ARG:CZ	12:B:495:LEU:HD22	2.49	0.42
12:B:807:ARG:HH12	22:L:58:ARG:C	2.27	0.42
15:E:167:GLU:O	15:E:208:LEU:HD22	2.20	0.42
27:R:11:GLY:HA3	27:R:106:LEU:O	2.19	0.42
28:T:-117:DC:OP1	36:b:49:GLY:N	2.51	0.42
28:T:-92:DG:H2"	28:T:-91:DT:H5'	2.01	0.42
37:c:101:VAL:HG11	36:f:99:TYR:CE2	2.54	0.42
38:d:77:GLU:OE1	38:d:80:ARG:NH1	2.52	0.42
1:0:76:LEU:HD11	1:0:100:LEU:HD21	2.01	0.42
2:1:538:PHE:HA	2:1:598:SER:O	2.19	0.42
3:2:136:VAL:O	3:2:501:GLN:HB3	2.19	0.42
11:A:256:PRO:HG2	11:A:276:LEU:HD23	2.02	0.42
11:A:865:ILE:O	11:A:869:GLU:HB2	2.20	0.42
12:B:924:ARG:NH2	13:C:62:GLU:OE1	2.52	0.42
13:C:268:GLN:HA	13:C:271:VAL:HG12	2.02	0.42
18:H:35:PHE:HB2	18:H:37:MET:HG2	2.00	0.42
24:N:148:DA:H2"	24:N:149:DG:C8	2.55	0.42
28:T:-142:DG:H2"	28:T:-141:DT:C5	2.54	0.42
32:X:111:ILE:O	32:X:116:LYS:NZ	2.47	0.42
38:d:69:ASP:OD2	36:f:99:TYR:OH	2.29	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:211:TYR:HA	2:1:217:ILE:CD1	2.50	0.42
2:1:250:ASN:CG	2:1:434:HIS:HD1	2.28	0.42
6:5:62:SER:OG	6:5:132:LEU:O	2.35	0.42
9:8:298:ARG:HA	9:8:299:PRO:C	2.45	0.42
10:9:98:GLU:HG2	10:9:99:TYR:CD2	2.55	0.42
11:A:469:MET:SD	12:B:1094:GLN:NE2	2.78	0.42
11:A:477:LEU:HD23	11:A:477:LEU:HA	1.87	0.42
12:B:608:ARG:HE	19:I:100:HIS:CE1	2.37	0.42
12:B:1126:ALA:HB3	12:B:1146:ILE:HD11	2.02	0.42
18:H:102:ASP:OD1	18:H:110:THR:N	2.52	0.42
27:R:193:LYS:HB3	27:R:197:TYR:OH	2.19	0.42
28:T:-92:DG:H2''	28:T:-91:DT:C5'	2.50	0.42
31:W:154:CYS:O	31:W:158:HIS:N	2.53	0.42
32:X:88:ARG:HG2	32:X:97:LEU:HD11	2.01	0.42
37:g:25:GLN:N	37:g:57:GLU:OE1	2.45	0.42
1:0:551:HIS:HB2	1:0:558:ILE:HD11	2.02	0.42
15:E:103:LEU:HD11	15:E:130:PHE:CD2	2.55	0.42
24:N:57:DA:N7	28:T:-58:DT:C4	2.88	0.42
24:N:138:DT:H2''	24:N:139:DT:C5	2.54	0.42
25:O:235:ARG:NH2	29:U:316:SER:OG	2.42	0.42
26:Q:93:PRO:HA	26:Q:96:GLN:CD	2.44	0.42
3:2:469:GLY:O	3:2:473:ARG:HG3	2.20	0.42
11:A:425:ASP:HB2	23:M:39:LEU:CD1	2.50	0.42
18:H:20:LYS:HE2	18:H:22:PHE:O	2.20	0.42
31:W:100:VAL:HA	31:W:103:VAL:HG22	2.01	0.42
11:A:364:ARG:HD2	11:A:502:ASN:OD1	2.20	0.41
12:B:553:LEU:HD21	12:B:573:TRP:CE2	2.55	0.41
24:N:150:DG:H2''	24:N:151:DG:C8	2.55	0.41
25:O:191:GLU:CG	25:O:201:ILE:HB	2.50	0.41
35:e:80:LYS:HB3	35:e:83:LEU:HD11	2.01	0.41
4:3:442:VAL:HG11	7:6:9:LEU:HD13	2.01	0.41
8:7:8:ARG:NH1	31:W:178:ALA:HA	2.35	0.41
11:A:140:ARG:NH1	11:A:234:PHE:O	2.42	0.41
11:A:526:VAL:HA	11:A:533:PRO:HA	2.03	0.41
11:A:532:ARG:HH11	11:A:532:ARG:HG3	1.84	0.41
12:B:1127:ILE:HG12	12:B:1136:GLU:O	2.20	0.41
24:N:160:DC:H2''	24:N:161:DC:C5	2.55	0.41
30:V:80:GLU:HG3	30:V:89:LYS:HE2	2.02	0.41
2:1:523:LEU:HD13	2:1:710:VAL:HG13	2.01	0.41
8:7:258:PRO:HD2	8:7:301:PHE:O	2.19	0.41
9:8:74:ILE:HG23	9:8:156:PHE:CZ	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:1119:CYS:HB2	12:B:1137:CYS:SG	2.59	0.41
5:4:71:MET:HB2	5:4:139:CYS:SG	2.61	0.41
7:6:17:LYS:HE3	7:6:39:ASP:O	2.20	0.41
11:A:969:ILE:C	11:A:971:PRO:HD3	2.45	0.41
12:B:623:ARG:NH2	12:B:697:GLU:OE2	2.38	0.41
12:B:907:VAL:HG22	12:B:921:ILE:HG12	2.02	0.41
24:N:16:DG:H1	28:T:-16:DC:H42	1.68	0.41
28:T:-12:DC:H4'	28:T:-11:DC:OP1	2.21	0.41
1:0:52:LYS:HE2	1:0:63:LEU:HD12	2.02	0.41
1:0:444:HIS:CE1	1:0:445:THR:HG23	2.56	0.41
2:1:273:ILE:O	2:1:277:ASP:N	2.54	0.41
3:2:127:LEU:HD13	3:2:127:LEU:HA	1.95	0.41
4:3:64:GLN:NE2	4:3:65:PRO:O	2.54	0.41
10:9:151:ILE:HG23	10:9:158:LEU:HD11	2.02	0.41
12:B:591:ARG:NH2	12:B:663:GLU:OE1	2.52	0.41
12:B:812:ARG:NH1	12:B:900:GLU:OE2	2.44	0.41
12:B:845:TYR:CE1	12:B:865:VAL:HG21	2.56	0.41
24:N:151:DG:H2''	24:N:152:DG:C8	2.55	0.41
1:0:658:PHE:HB3	1:0:660:TYR:CE1	2.56	0.41
2:1:681:ASP:HB3	2:1:684:PHE:CD2	2.55	0.41
9:8:175:THR:O	9:8:179:ARG:N	2.54	0.41
9:8:220:ASP:O	9:8:224:ARG:HG2	2.20	0.41
9:8:267:ASP:OD1	9:8:267:ASP:N	2.53	0.41
11:A:496:PHE:CD2	12:B:791:GLU:HB2	2.56	0.41
11:A:1248:ASN:ND2	11:A:1254:LYS:O	2.47	0.41
15:E:11:TRP:HB2	15:E:40:PHE:CD2	2.55	0.41
35:e:60:GLU:OE1	35:e:60:GLU:N	2.52	0.41
11:A:34:MET:HA	12:B:1138:ARG:HB3	2.02	0.41
11:A:87:HIS:HA	11:A:253:LEU:O	2.21	0.41
11:A:90:LEU:HD12	11:A:250:VAL:O	2.21	0.41
11:A:1201:ASP:C	11:A:1203:ASP:H	2.29	0.41
12:B:565:THR:HG21	12:B:580:PRO:HG3	2.02	0.41
15:E:9:ARG:HD3	15:E:132:GLN:NE2	2.35	0.41
25:O:187:ALA:HB3	25:O:190:ALA:HB2	2.03	0.41
28:T:-89:DT:P	28:T:-89:DT:H3'	2.60	0.41
28:T:-87:DC:H2''	28:T:-86:DG:C8	2.55	0.41
1:0:580:ILE:N	1:0:606:PHE:O	2.49	0.41
2:1:161:PHE:CD1	2:1:165:GLY:HA3	2.55	0.41
4:3:329:ALA:HB2	4:3:334:MET:SD	2.61	0.41
11:A:479:TRP:HB2	11:A:483:ARG:NH2	2.36	0.41
11:A:621:ILE:HG23	11:A:621:ILE:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:841:MET:HE3	12:B:501:LEU:O	2.19	0.41
11:A:1128:ILE:HB	11:A:1414:ILE:HG13	2.02	0.41
11:A:1226:LEU:HD23	11:A:1230:GLN:HE21	1.86	0.41
11:A:1227:THR:H	11:A:1230:GLN:NE2	2.18	0.41
14:D:131:LEU:O	14:D:135:GLN:HG2	2.20	0.41
24:N:41:DC:O2	28:T:-40:DG:N2	2.54	0.41
28:T:-45:DA:H2'	28:T:-44:DT:C6	2.56	0.41
34:Z:17:UNK:HA	34:Z:18:UNK:HA	1.64	0.41
35:a:127:LEU:HD22	35:e:114:HIS:CG	2.55	0.41
4:3:380:THR:HA	4:3:381:PRO:C	2.46	0.41
5:4:255:PRO:HA	6:5:263:GLU:OE2	2.21	0.41
5:4:271:PHE:HD1	5:4:284:LEU:HA	1.86	0.41
9:8:98:LEU:HD21	9:8:206:LEU:HD21	2.02	0.41
10:9:129:LEU:O	10:9:136:GLN:NE2	2.51	0.41
11:A:362:SER:HA	11:A:503:LEU:O	2.21	0.41
11:A:369:PRO:HB3	11:A:496:PHE:CE2	2.56	0.41
11:A:1097:GLU:HB3	11:A:1098:PRO:HD3	2.02	0.41
12:B:603:MET:HE2	12:B:603:MET:HB2	1.90	0.41
12:B:1108:PHE:CE1	12:B:1113:PRO:HA	2.56	0.41
24:N:-4:DG:O6	28:T:3:DC:N4	2.54	0.41
24:N:131:DC:H4'	36:f:46:ARG:CZ	2.50	0.41
3:2:418:LEU:HD21	4:3:123:LEU:HD11	2.02	0.41
4:3:421:LEU:HD21	4:3:451:VAL:HG21	2.03	0.41
11:A:981:CYS:HB3	11:A:986:MET:HE1	2.03	0.41
12:B:63:PRO:HA	12:B:64:PRO:HD3	1.97	0.41
12:B:849:ASP:HB3	22:L:15:MET:HE1	2.02	0.41
22:L:46:LYS:HB3	22:L:46:LYS:HE3	1.90	0.41
24:N:107:DT:O2	28:T:-106:DG:N2	2.54	0.41
28:T:-152:DC:H2''	28:T:-151:DC:C6	2.56	0.41
28:T:-68:DG:H4'	28:T:-67:DG:O5'	2.21	0.41
31:W:113:ARG:HD2	32:X:219:LEU:CD1	2.50	0.41
38:h:99:VAL:HG13	38:h:103:LEU:HD12	2.03	0.41
2:1:24:TYR:HA	2:1:481:PHE:CZ	2.56	0.40
2:1:161:PHE:CZ	2:1:194:LEU:HA	2.56	0.40
12:B:237:VAL:HG12	12:B:372:LEU:HD22	2.04	0.40
13:C:193:ARG:HA	13:C:193:ARG:HD3	1.87	0.40
19:I:40:ARG:CZ	26:Q:173:HIS:HB2	2.52	0.40
20:J:9:THR:OG1	20:J:47:ARG:NH2	2.52	0.40
23:M:120:GLU:HG3	23:M:124:MET:HE2	2.03	0.40
24:N:78:DC:H2''	24:N:79:DA:C8	2.56	0.40
27:R:23:VAL:HB	27:R:27:LEU:HD23	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:R:124:TYR:O	27:R:128:LYS:HG2	2.22	0.40
28:T:-138:DA:H5''	35:e:64:ARG:NH2	2.36	0.40
35:a:66:LEU:HB3	35:a:67:PRO:HD3	2.02	0.40
1:0:443:VAL:HG11	1:0:465:GLY:HA3	2.04	0.40
9:8:45:LEU:HB2	9:8:85:SER:HA	2.02	0.40
10:9:175:LYS:HE2	10:9:184:PRO:HD2	2.03	0.40
11:A:268:GLY:H	12:B:890:ARG:HH11	1.68	0.40
11:A:1235:ILE:HG13	11:A:1296:MET:HE1	2.02	0.40
17:G:88:VAL:HA	17:G:141:ASP:O	2.22	0.40
27:R:41:GLY:HA3	27:R:56:PHE:CZ	2.57	0.40
2:1:587:ALA:HB3	2:1:594:ALA:HB2	2.04	0.40
15:E:3:ASP:OD1	15:E:48:PRO:HG2	2.22	0.40
17:G:89:VAL:HB	17:G:138:GLN:O	2.22	0.40
18:H:118:TYR:HB2	18:H:121:LEU:HB2	2.02	0.40
19:I:57:LYS:HB3	19:I:57:LYS:HE3	1.94	0.40
24:N:67:DC:H2''	24:N:68:DC:C6	2.55	0.40
26:Q:164:TRP:CD1	26:Q:164:TRP:C	3.00	0.40
27:R:19:TRP:CG	27:R:112:GLN:HB3	2.56	0.40
28:T:-150:DC:H2''	28:T:-149:DC:C5	2.56	0.40
28:T:-68:DG:C4	28:T:-67:DG:C6	3.09	0.40
29:U:339:TYR:HA	29:U:353:LEU:HA	2.04	0.40
30:V:62:LEU:HD21	30:V:65:TYR:HB3	2.04	0.40
1:0:110:PRO:HB2	4:3:310:GLU:OE1	2.21	0.40
1:0:287:LEU:HD23	1:0:289:TYR:HD2	1.86	0.40
6:5:61:ALA:HB2	6:5:70:LEU:HD21	2.03	0.40
6:5:207:CYS:O	6:5:212:GLY:N	2.54	0.40
9:8:66:LEU:HD21	9:8:75:ILE:HG23	2.03	0.40
11:A:874:LYS:HB3	16:F:111:PRO:HG3	2.02	0.40
12:B:115:LEU:HD23	12:B:115:LEU:HA	1.94	0.40
12:B:309:PHE:CZ	19:I:40:ARG:HB3	2.56	0.40
12:B:1068:GLN:HG3	12:B:1075:MET:HB3	2.03	0.40
13:C:47:ILE:HA	13:C:165:ALA:HA	2.03	0.40
24:N:75:DG:C5	24:N:76:DC:C4	3.10	0.40
28:T:-88:DA:C2'	28:T:-87:DC:H5'	2.50	0.40
28:T:-34:DA:H2'	28:T:-33:DG:C8	2.57	0.40
1:0:621:ASN:OD1	1:0:647:LYS:HE2	2.20	0.40
11:A:583:ARG:HA	11:A:584:PRO:HD3	1.98	0.40
12:B:327:LYS:HB3	12:B:338:TYR:CE2	2.57	0.40
12:B:502:HIS:CE1	12:B:504:THR:HG23	2.55	0.40
21:K:1:MET:HG3	21:K:2:ASN:N	2.35	0.40
29:U:337:CYS:SG	29:U:353:LEU:HD13	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	601/772 (78%)	581 (97%)	20 (3%)	0	100	100
2	1	710/760 (93%)	679 (96%)	31 (4%)	0	100	100
3	2	253/548 (46%)	246 (97%)	7 (3%)	0	100	100
4	3	413/462 (89%)	398 (96%)	15 (4%)	0	100	100
5	4	341/395 (86%)	330 (97%)	11 (3%)	0	100	100
6	5	259/308 (84%)	245 (95%)	14 (5%)	0	100	100
7	6	67/71 (94%)	66 (98%)	1 (2%)	0	100	100
8	7	208/309 (67%)	191 (92%)	17 (8%)	0	100	100
9	8	297/346 (86%)	286 (96%)	11 (4%)	0	100	100
10	9	285/323 (88%)	278 (98%)	7 (2%)	0	100	100
11	A	1413/1970 (72%)	1375 (97%)	38 (3%)	0	100	100
12	B	1130/1174 (96%)	1093 (97%)	37 (3%)	0	100	100
13	C	253/275 (92%)	246 (97%)	7 (3%)	0	100	100
14	D	126/142 (89%)	123 (98%)	3 (2%)	0	100	100
15	E	207/210 (99%)	204 (99%)	3 (1%)	0	100	100
16	F	77/127 (61%)	76 (99%)	1 (1%)	0	100	100
17	G	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
18	H	146/150 (97%)	144 (99%)	2 (1%)	0	100	100
19	I	112/125 (90%)	104 (93%)	8 (7%)	0	100	100
20	J	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
21	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
22	L	42/58 (72%)	40 (95%)	2 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	M	248/316 (78%)	239 (96%)	9 (4%)	0	100	100
25	O	177/339 (52%)	175 (99%)	2 (1%)	0	100	100
26	Q	134/517 (26%)	129 (96%)	5 (4%)	0	100	100
27	R	218/249 (88%)	214 (98%)	4 (2%)	0	100	100
29	U	109/376 (29%)	107 (98%)	2 (2%)	0	100	100
30	V	97/109 (89%)	92 (95%)	5 (5%)	0	100	100
31	W	198/439 (45%)	196 (99%)	2 (1%)	0	100	100
32	X	169/291 (58%)	161 (95%)	8 (5%)	0	100	100
35	a	95/136 (70%)	94 (99%)	1 (1%)	0	100	100
35	e	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
36	b	80/103 (78%)	80 (100%)	0	0	100	100
36	f	78/103 (76%)	77 (99%)	1 (1%)	0	100	100
37	c	107/130 (82%)	105 (98%)	2 (2%)	0	100	100
37	g	104/130 (80%)	102 (98%)	2 (2%)	0	100	100
38	d	95/126 (75%)	94 (99%)	1 (1%)	0	100	100
38	h	93/126 (74%)	91 (98%)	2 (2%)	0	100	100
All	All	9382/12507 (75%)	9090 (97%)	292 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	536/678 (79%)	535 (100%)	1 (0%)	87	87
2	1	624/664 (94%)	623 (100%)	1 (0%)	87	87
3	2	241/484 (50%)	241 (100%)	0	100	100
4	3	351/399 (88%)	351 (100%)	0	100	100
5	4	311/352 (88%)	311 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	5	234/272 (86%)	234 (100%)	0	100	100
7	6	62/64 (97%)	62 (100%)	0	100	100
8	7	194/283 (69%)	194 (100%)	0	100	100
9	8	259/299 (87%)	258 (100%)	1 (0%)	84	84
10	9	259/296 (88%)	259 (100%)	0	100	100
11	A	1254/1749 (72%)	1253 (100%)	1 (0%)	88	89
12	B	994/1027 (97%)	994 (100%)	0	100	100
13	C	234/252 (93%)	234 (100%)	0	100	100
14	D	118/126 (94%)	117 (99%)	1 (1%)	73	77
15	E	191/192 (100%)	191 (100%)	0	100	100
16	F	69/111 (62%)	69 (100%)	0	100	100
17	G	152/153 (99%)	152 (100%)	0	100	100
18	H	129/131 (98%)	129 (100%)	0	100	100
19	I	103/112 (92%)	103 (100%)	0	100	100
20	J	53/56 (95%)	53 (100%)	0	100	100
21	K	104/106 (98%)	104 (100%)	0	100	100
22	L	41/55 (74%)	41 (100%)	0	100	100
23	M	215/268 (80%)	215 (100%)	0	100	100
25	O	154/293 (53%)	154 (100%)	0	100	100
26	Q	121/448 (27%)	121 (100%)	0	100	100
27	R	196/218 (90%)	196 (100%)	0	100	100
29	U	105/324 (32%)	105 (100%)	0	100	100
30	V	90/98 (92%)	90 (100%)	0	100	100
31	W	182/373 (49%)	182 (100%)	0	100	100
32	X	154/261 (59%)	154 (100%)	0	100	100
35	a	85/111 (77%)	85 (100%)	0	100	100
35	e	86/111 (78%)	86 (100%)	0	100	100
36	b	67/79 (85%)	67 (100%)	0	100	100
36	f	65/79 (82%)	65 (100%)	0	100	100
37	c	86/101 (85%)	86 (100%)	0	100	100
37	g	84/101 (83%)	84 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	d	83/106 (78%)	83 (100%)	0	100	100
38	h	81/106 (76%)	81 (100%)	0	100	100
All	All	8367/10938 (76%)	8362 (100%)	5 (0%)	87	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	521	GLU
2	1	203	ASN
9	8	86	ASN
11	A	512	ARG
14	D	129	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	181	HIS
1	0	274	GLN
1	0	714	GLN
2	1	148	HIS
2	1	201	HIS
2	1	351	GLN
2	1	560	ASN
2	1	590	ASN
2	1	613	HIS
2	1	723	GLN
4	3	54	ASN
4	3	68	GLN
4	3	97	HIS
4	3	211	GLN
5	4	103	GLN
6	5	46	ASN
6	5	108	ASN
6	5	145	HIS
6	5	155	GLN
6	5	205	GLN
6	5	225	GLN
6	5	258	HIS
8	7	24	ASN
9	8	71	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	8	105	ASN
10	9	10	HIS
10	9	288	ASN
11	A	459	ASN
11	A	507	GLN
11	A	620	HIS
11	A	671	ASN
11	A	765	ASN
11	A	905	ASN
11	A	1042	ASN
11	A	1093	GLN
12	B	117	ASN
12	B	312	GLN
12	B	486	ASN
12	B	537	GLN
12	B	593	GLN
12	B	642	GLN
12	B	654	GLN
12	B	1009	GLN
12	B	1030	ASN
13	C	66	HIS
13	C	114	HIS
13	C	190	ASN
13	C	217	GLN
14	D	129	GLN
15	E	189	GLN
18	H	133	HIS
19	I	100	HIS
25	O	189	ASN
26	Q	10	ASN
30	V	39	GLN
32	X	177	ASN
37	c	25	GLN
37	c	111	ASN
38	d	68	ASN
37	g	25	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
39	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
39	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.

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.

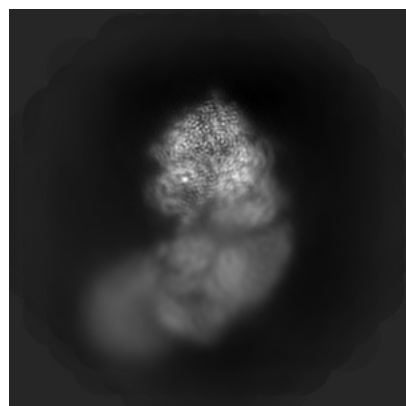
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16274. These allow visual inspection of the internal detail of the map and identification of artifacts.

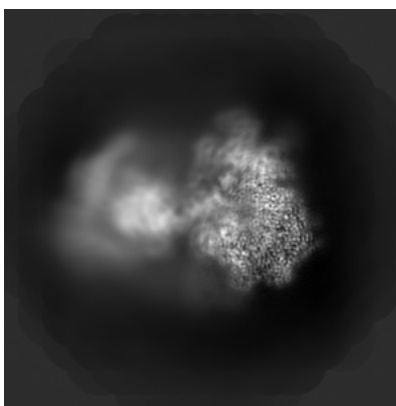
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

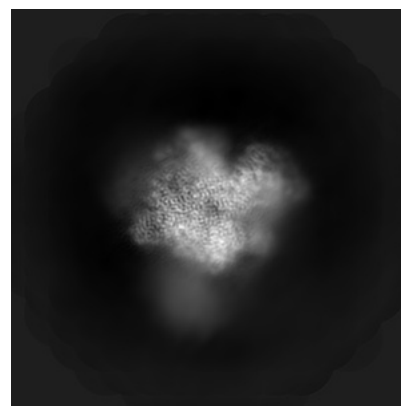
6.1.1 Primary map



X

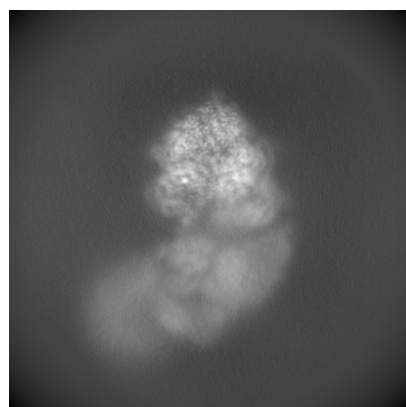


Y

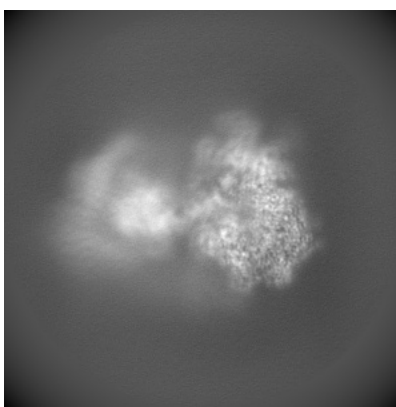


Z

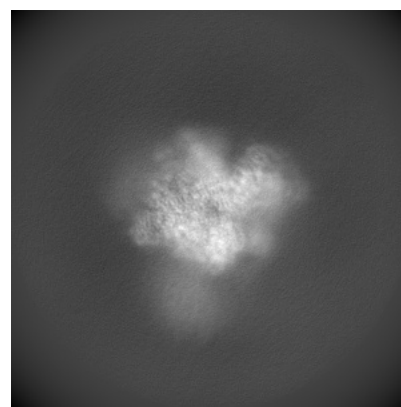
6.1.2 Raw map



X



Y

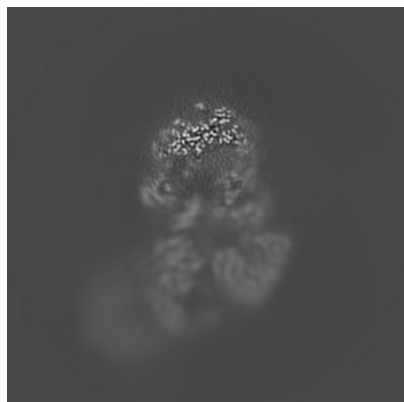


Z

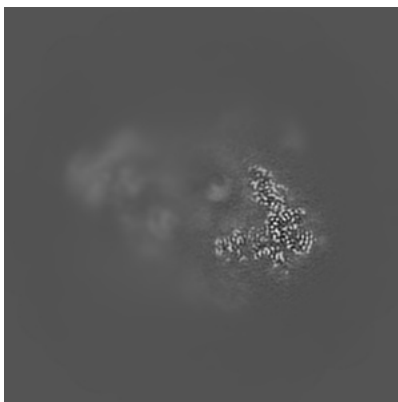
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

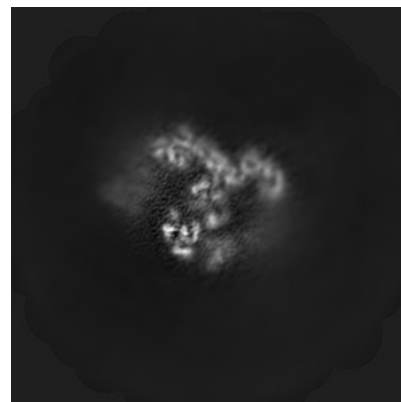
6.2.1 Primary map



X Index: 200

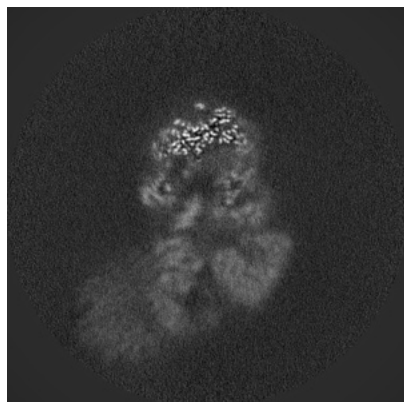


Y Index: 200

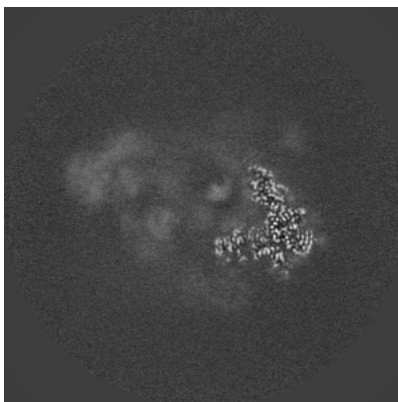


Z Index: 200

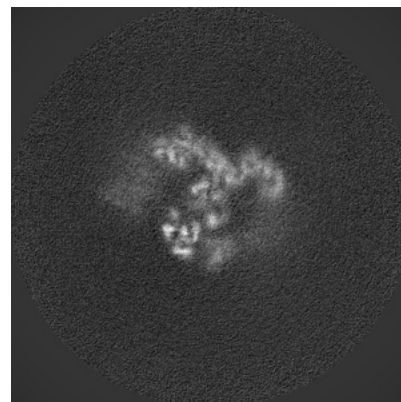
6.2.2 Raw map



X Index: 200



Y Index: 200

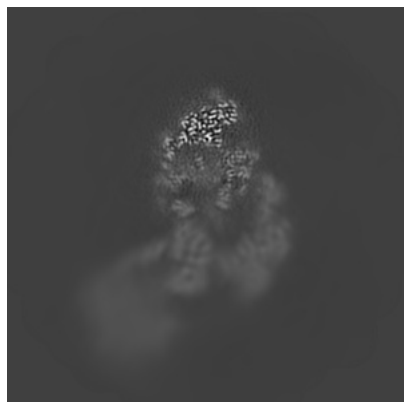


Z Index: 200

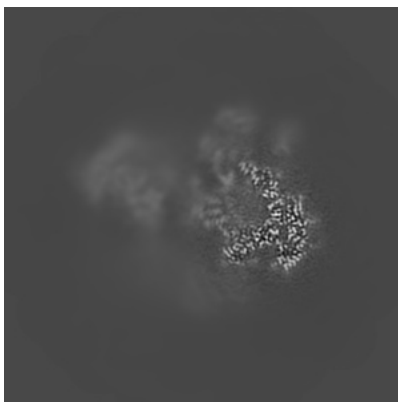
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

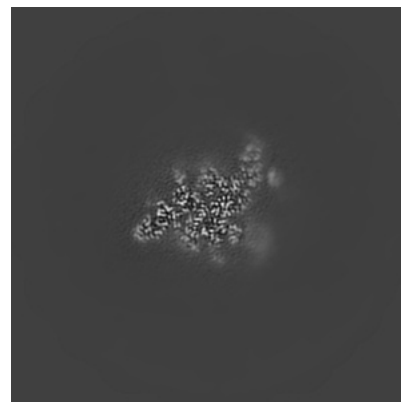
6.3.1 Primary map



X Index: 183

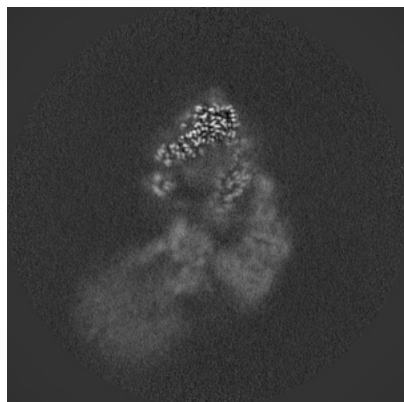


Y Index: 213

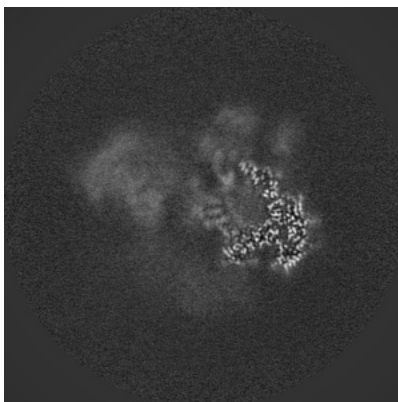


Z Index: 265

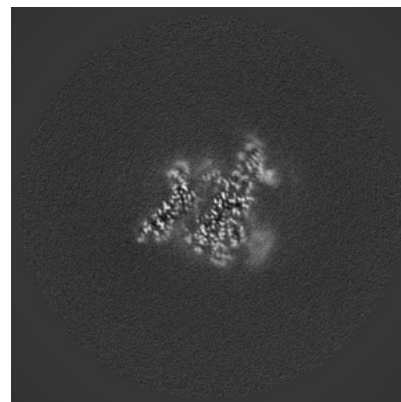
6.3.2 Raw map



X Index: 190



Y Index: 213

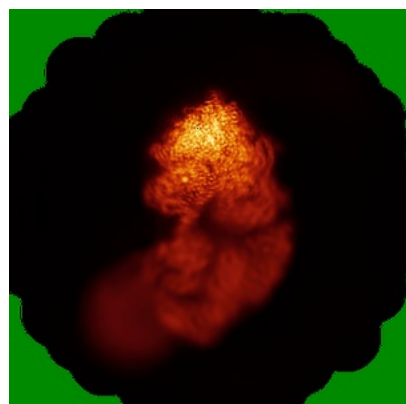


Z Index: 260

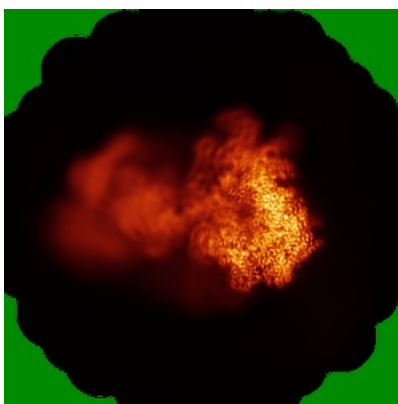
The images above show the largest variance slices of the map in three orthogonal directions.

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

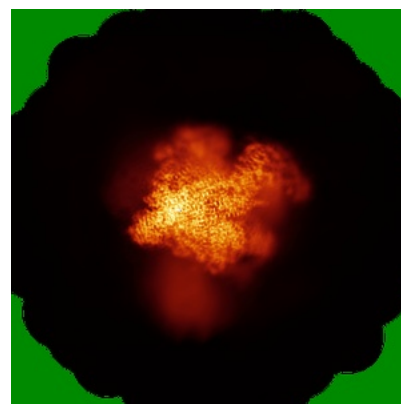
6.4.1 Primary map



X

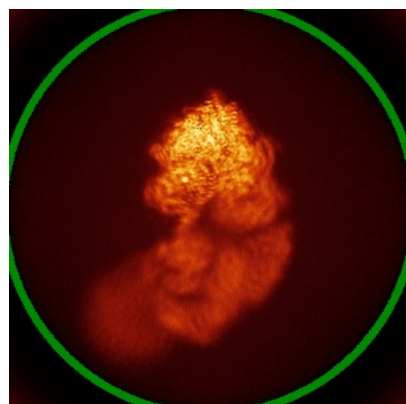


Y

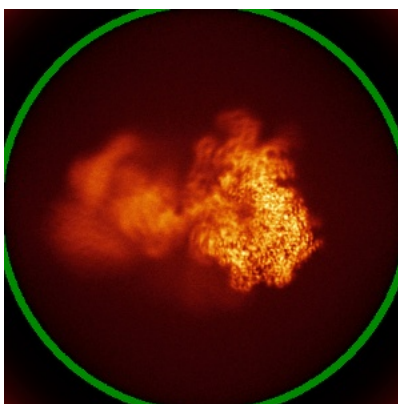


Z

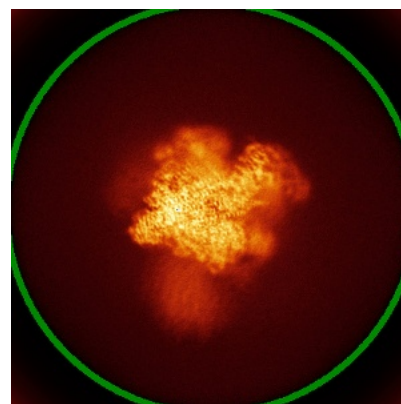
6.4.2 Raw map



X



Y

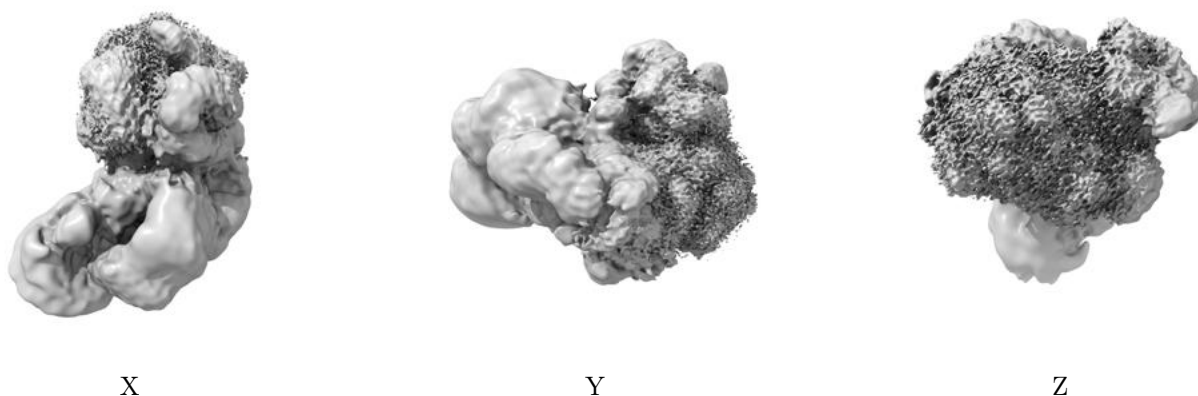


Z

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.

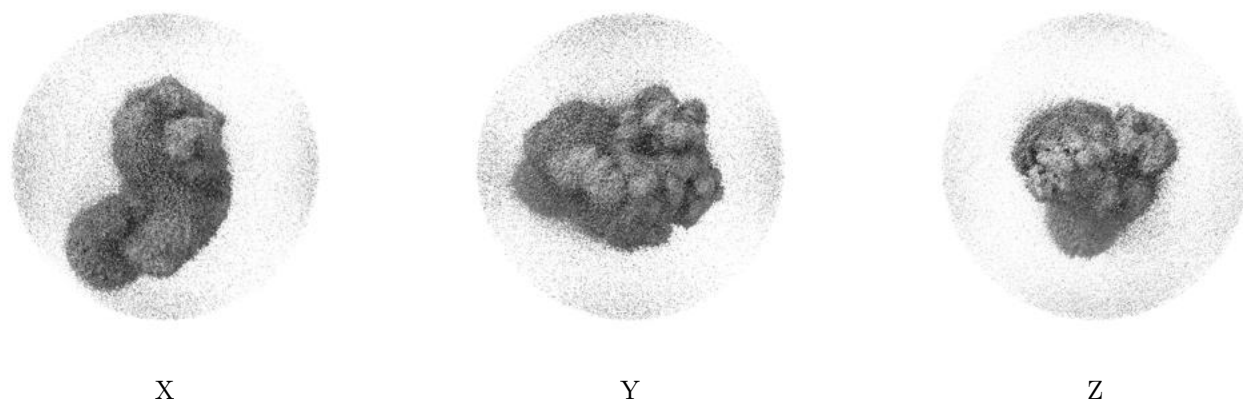
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.5. 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



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.

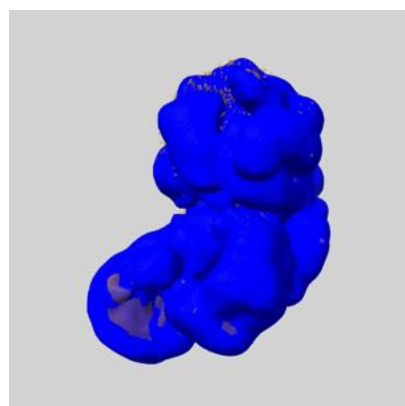
6.6 Mask visualisation [i](#)

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

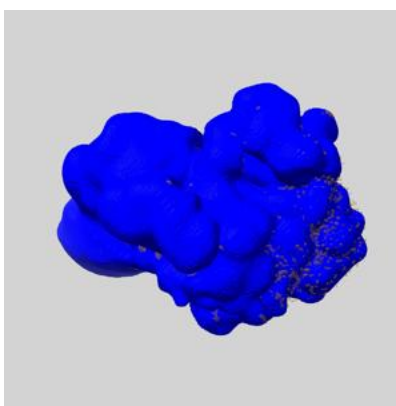
A mask typically either:

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

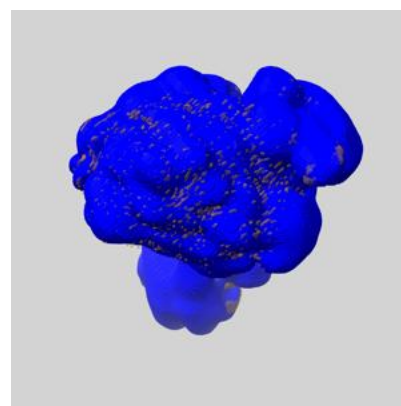
6.6.1 emd_16274_msk_1.map [i](#)



X



Y

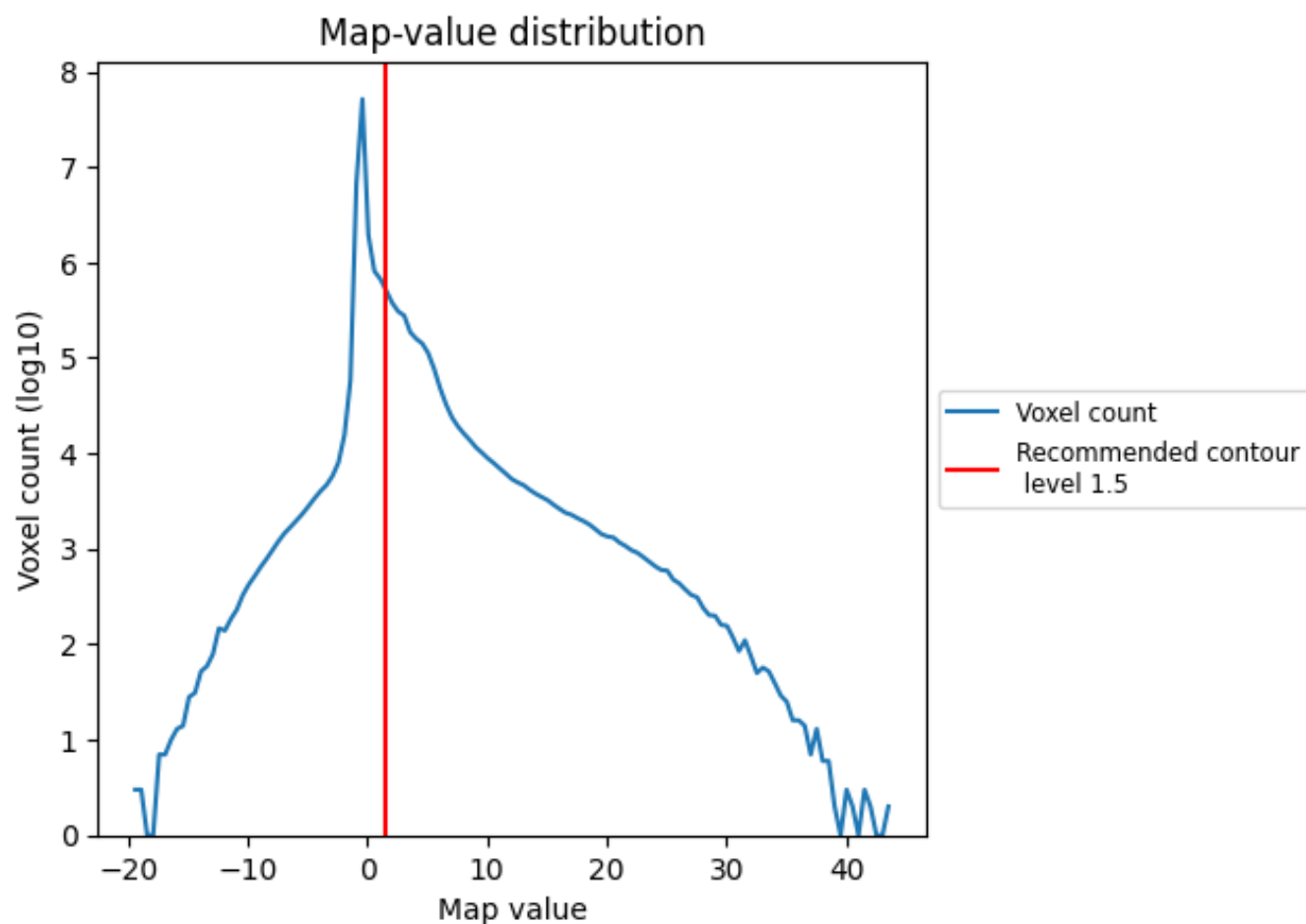


Z

7 Map analysis [i](#)

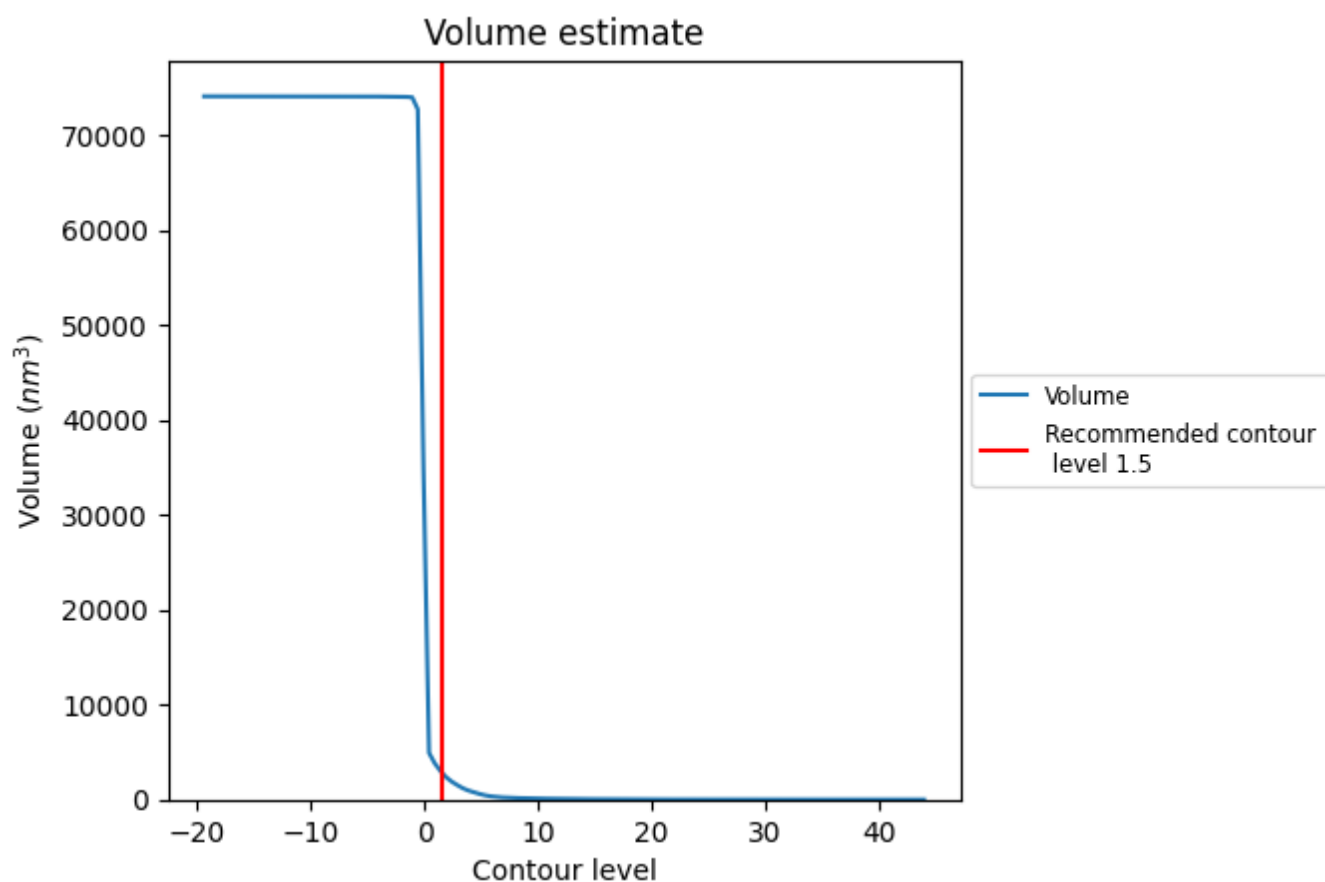
This section contains the results of statistical analysis of the map.

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.

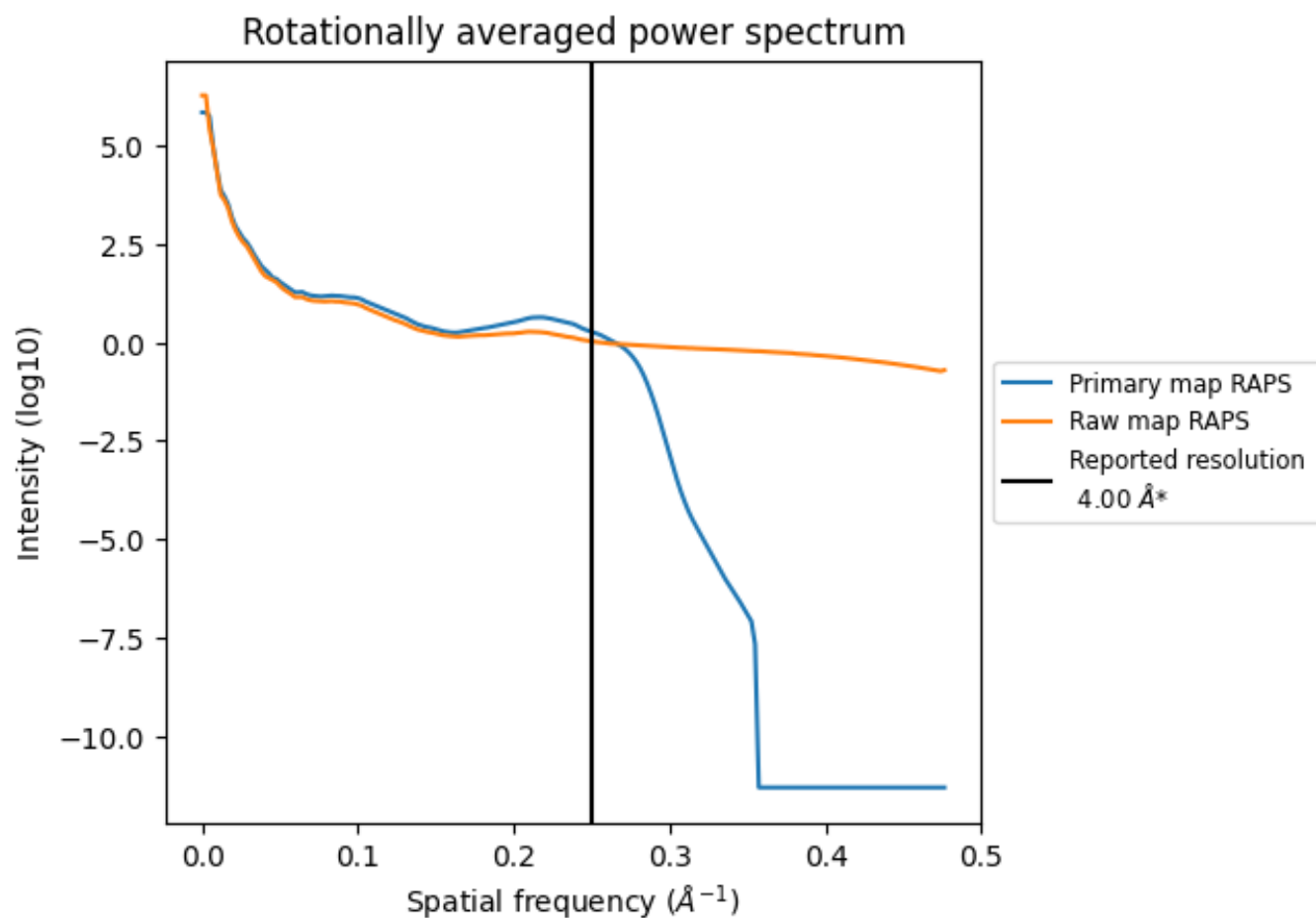
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2912 nm^3 ; this corresponds to an approximate mass of 2631 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 ⓘ

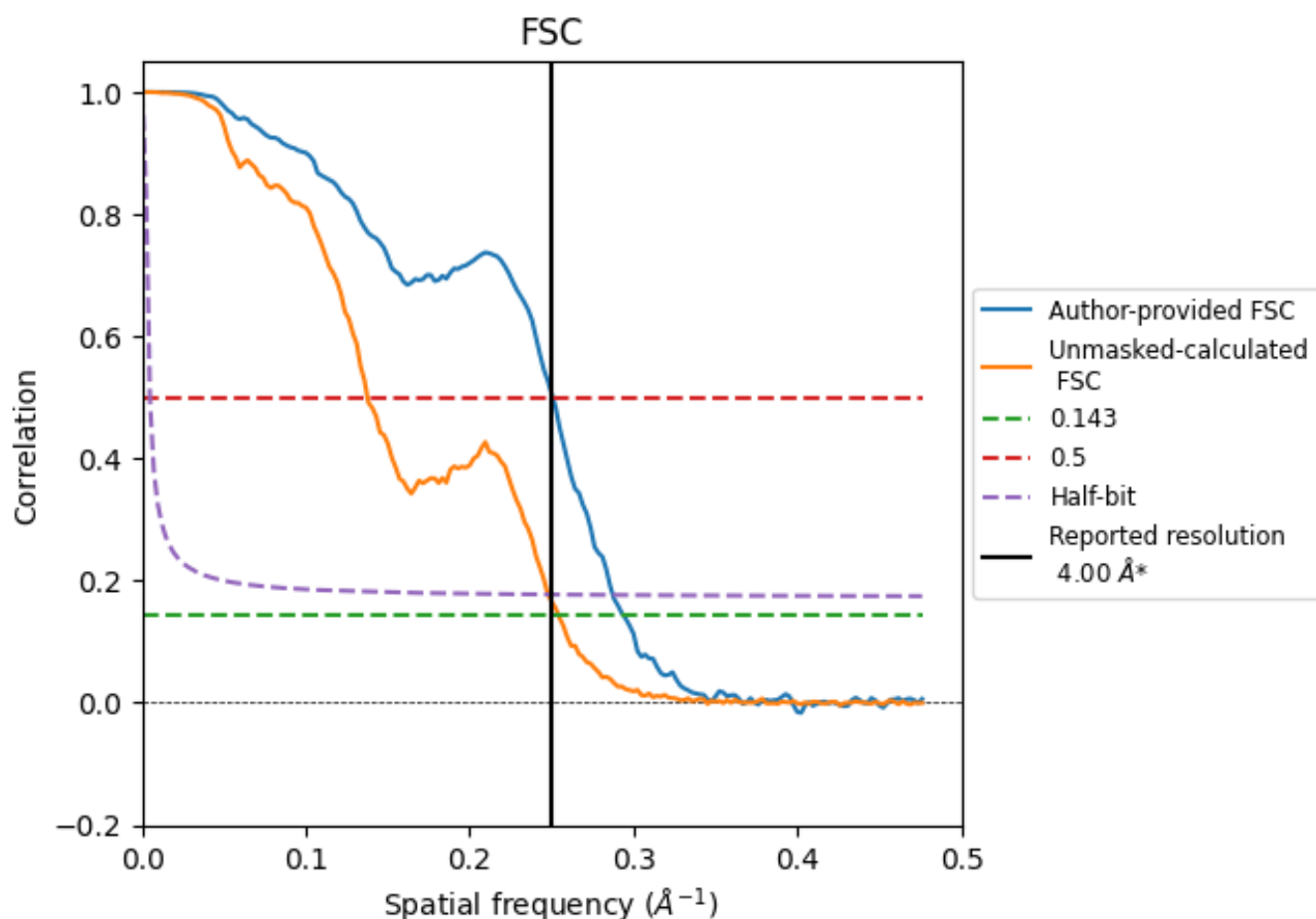


*Reported resolution corresponds to spatial frequency of 0.250 $\text{\AA}^{-1}$

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 0.250 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

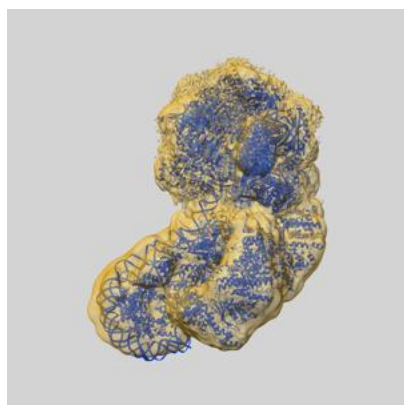
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.40	3.99	3.48
Unmasked-calculated*	3.93	7.27	4.04

*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 3.40 differs from the reported value 4.0 by more than 10 %

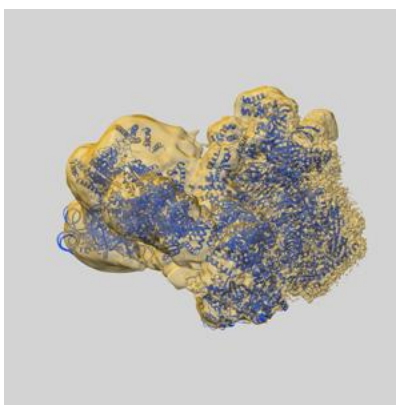
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16274 and PDB model 8BVW. Per-residue inclusion information can be found in section [3](#) on page [13](#).

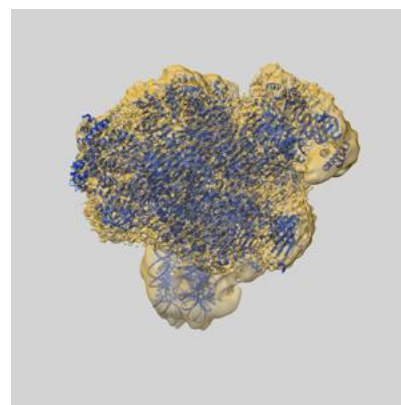
9.1 Map-model overlay [i](#)



X



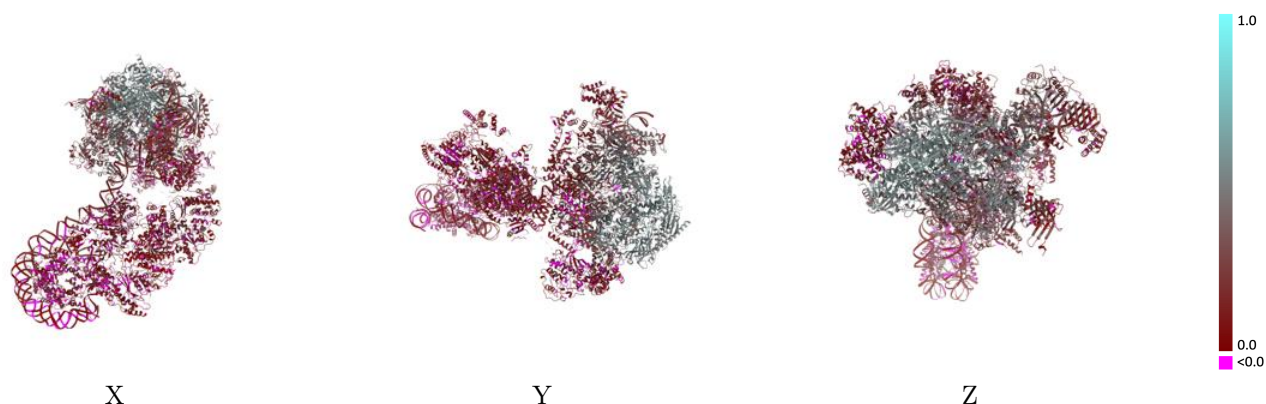
Y



Z

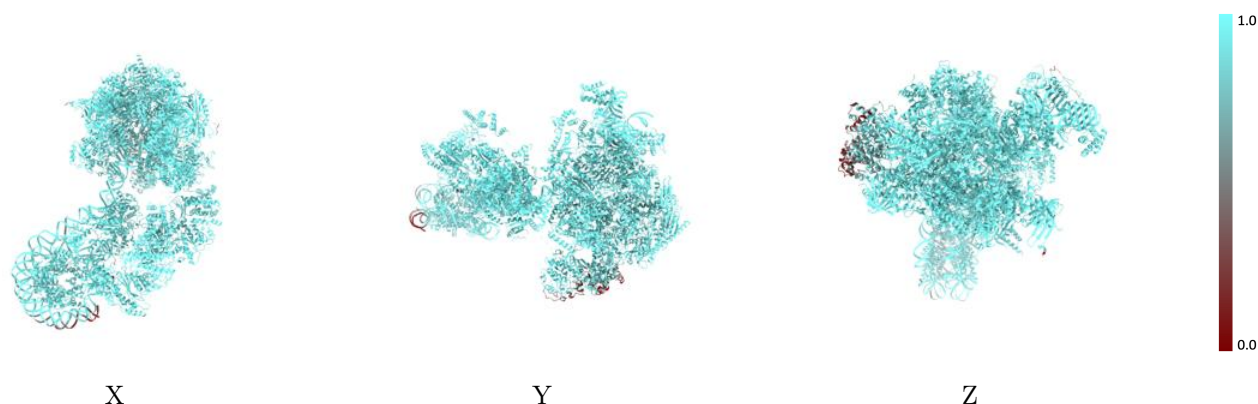
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



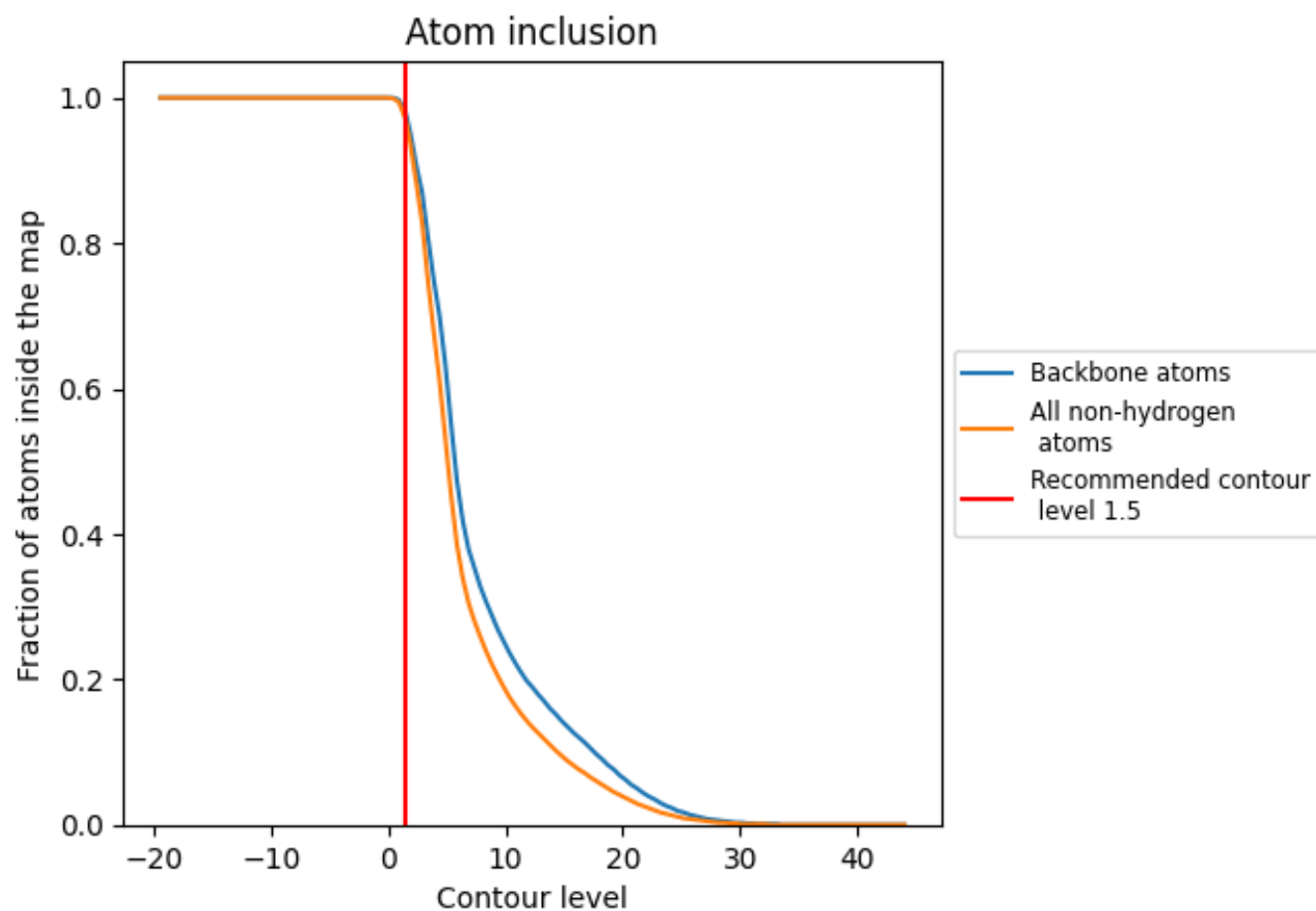
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 97% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9700	 0.2340
0	 0.9990	 0.1090
1	 1.0000	 0.1240
2	 0.9970	 0.0750
3	 0.9910	 0.0850
4	 0.9970	 0.1070
5	 0.9990	 0.0820
6	 1.0000	 0.1000
7	 0.8290	 0.1100
8	 0.8600	 0.0850
9	 0.6860	 0.1290
A	 0.9900	 0.4010
B	 0.9940	 0.4740
C	 0.9960	 0.5080
D	 0.9960	 0.1830
E	 0.9920	 0.3460
F	 0.9950	 0.4830
G	 0.9980	 0.2590
H	 0.9930	 0.4830
I	 0.9970	 0.3870
J	 1.0000	 0.5280
K	 0.9950	 0.5110
L	 0.9970	 0.4690
M	 0.9870	 0.3920
N	 0.9230	 0.1080
O	 0.9950	 0.2900
Q	 0.9780	 0.2450
R	 0.9930	 0.2160
T	 0.9130	 0.1080
U	 0.9860	 0.1570
V	 1.0000	 0.1780
W	 0.9900	 0.1360
X	 0.9960	 0.1540
Y	 1.0000	 0.0750
Z	 1.0000	 0.0600



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
a	 0.9820	 0.0580
b	 1.0000	 0.0440
c	 0.9950	 0.0220
d	 1.0000	 0.0450
e	 0.9830	 0.0430
f	 1.0000	 0.0550
g	 0.9840	 0.0480
h	 0.9750	 0.0810