



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 05:12 AM JST

PDB ID : 8GXS
EMDB ID : EMD-34360
Title : PIC-Mediator in complex with +1 nucleosome (T40N) in H-binding state
Authors : Chen, X.; Wang, X.; Liu, W.; Ren, Y.; Qu, X.; Li, J.; Yin, X.
Deposited on : 2022-09-21
Resolution : 4.16 Å(reported)

This is a wwPDB EM Validation Summary 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

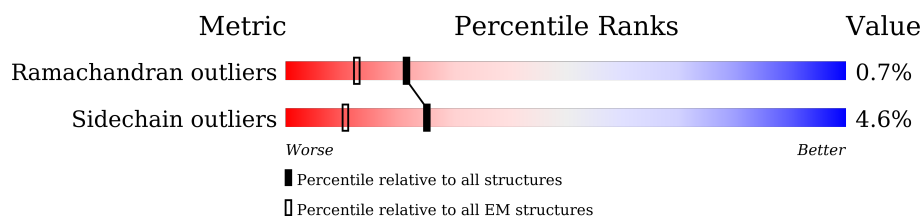
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.16 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.










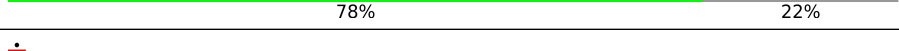
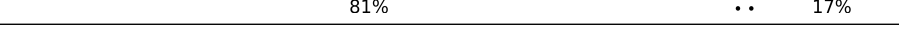
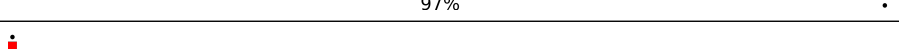
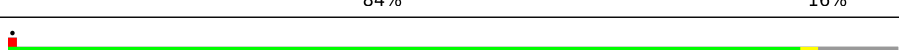


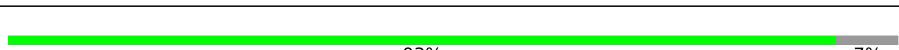
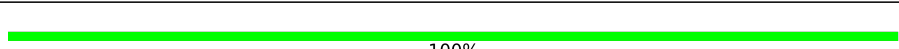

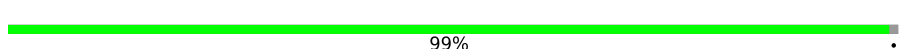
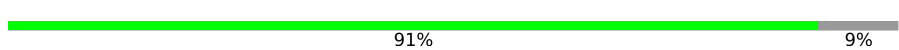
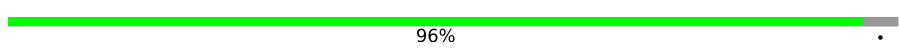
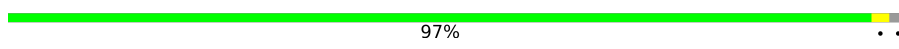
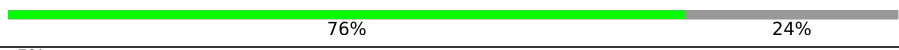
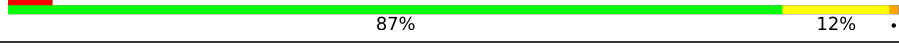



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	X	228	 27% 71%
2	Y	228	 29% 71%
3	NX	162	 17% 99%
4	NY	162	 17% 100%
5	BA	316	 80% 20%
6	DA	1872	 8% 28% 70%
7	EA	439	 42% 57%
8	FA	517	 26% 73%
9	HA	760	 94% 6%























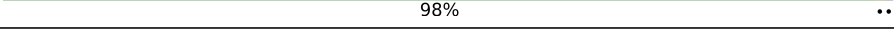
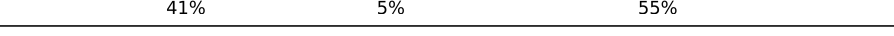

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Mol	Chain	Length	Quality of chain
10	NA	136	
10	NE	136	
11	PA	1970	
12	DB	1199	
13	EB	291	
14	FB	249	
15	HB	548	
16	NB	103	
16	NF	103	
17	PB	1174	
18	HC	462	
19	DO	109	
20	DP	339	
21	DQ	376	
22	PC	275	
23	PE	210	
24	PF	127	
25	PH	150	
26	PI	125	
27	PJ	67	
28	PK	117	
29	PL	58	
30	HD	309	
31	HG	395	
32	HE	308	





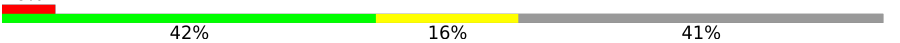






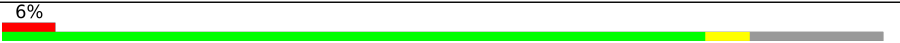




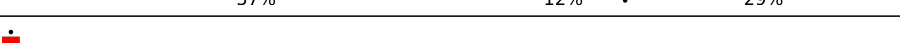
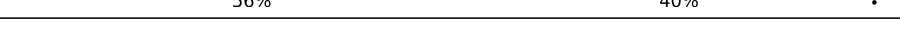



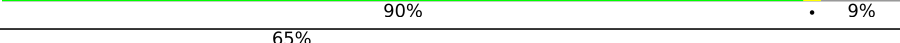
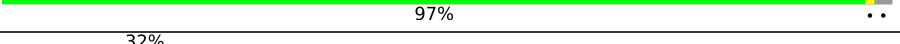


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Mol	Chain	Length	Quality of chain
33	HF	71	
34	HH	782	
35	DD	1085	
35	Dd	1085	
36	DE	800	
36	De	800	
37	DF	677	
37	Df	677	
38	DG	349	
39	DH	310	
40	DI	264	
40	Di	264	
41	DL	161	
41	Dl	161	
42	Dc	929	
43	DJ	218	
43	Dj	218	
44	Dk	211	
45	Dm	124	
46	HI	346	
47	HJ	323	
48	PD	142	
49	PG	172	
50	g	233	
51	j	135	


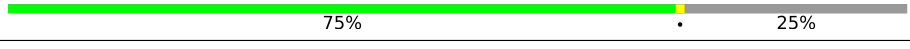
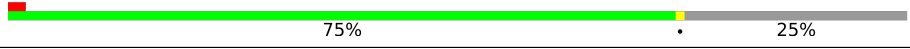
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Mol	Chain	Length	Quality of chain
52	n	1454	
53	s	244	
54	u	144	
55	a	1581	
56	d	270	
57	f	246	
58	i	146	
59	m	131	
60	q	651	
61	z	600	
62	b	200	
63	c	311	
64	e	178	
65	l	178	
66	o	788	
67	h	268	
68	k	117	
69	r	208	
70	t	212	
71	v	200	
72	p	841	
73	w	1368	
74	x	989	
75	y	747	
76	NC	128	

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Mol	Chain	Length	Quality of chain
76	NG	128	 80% 16%
77	ND	126	 75% 25%
77	NH	126	 75% 25%

2 Entry composition

There are 80 unique types of molecules in this entry. The entry contains 185972 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 DNA chain called DNA (228-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	67	Total	C	N	O	P	0	0
			1387	652	275	394	66		

- Molecule 2 is a DNA chain called DNA (228-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Y	67	Total	C	N	O	P	0	0
			1357	643	239	408	67		

- Molecule 3 is a DNA chain called DNA (162-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	NX	162	Total	C	N	O	P	0	0
			3078	1458	486	972	162		

- Molecule 4 is a DNA chain called DNA (162-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	NY	162	Total	C	N	O	P	0	0
			3561	1620	810	970	161		

- Molecule 5 is a protein called Transcription initiation factor IIB.

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

- Molecule 6 is a protein called Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	DA	558	Total	C	N	O	S	0	0
			4563	2913	791	832	27		

- Molecule 7 is a protein called General transcription factor IIE subunit 1.

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

- Molecule 8 is a protein called General transcription factor IIF subunit 1.

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

- Molecule 9 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD.

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

- Molecule 10 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	NA	100	Total	C	N	O		0	0
			498	298	100	100			
10	NE	103	Total	C	N	O		0	0
			511	305	103	103			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	PA	1471	Total	C	N	O	S	0	0
			11628	7314	2064	2178	72		

- Molecule 12 is a protein called Transcription initiation factor TFIID subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	DB	963	Total	C	N	O	S	0	0
			7796	5011	1315	1412	58		

- Molecule 13 is a protein called Transcription initiation factor IIE subunit beta.

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

- Molecule 14 is a protein called General transcription factor IIF subunit 2.

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

- Molecule 15 is a protein called General transcription factor IIH subunit 1.

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

- Molecule 16 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	NB	80	Total	C	N	O	0	0
			391	231	80	80		
16	NF	86	Total	C	N	O	0	0
			421	249	86	86		

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

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

- Molecule 18 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	HC	390	Total	C	N	O	S	0	0
			3158	2050	545	551	12		

- Molecule 19 is a protein called Transcription initiation factor IIA subunit 2.

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

- Molecule 20 is a protein called TATA-box-binding protein.

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

- Molecule 21 is a protein called Transcription initiation factor IIA subunit 1.

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

- Molecule 22 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 23 is a protein called DNA-directed RNA polymerase II subunit E.

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

- Molecule 24 is a protein called DNA-directed RNA polymerase II subunit F.

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

- Molecule 25 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 26 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 27 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 28 is a protein called RNA_pol_L_2 domain-containing protein.

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

- Molecule 29 is a protein called RPB12.

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

- Molecule 30 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	HD	306	Total	C	N	O	S	0	0
			2400	1498	424	465	13		

- Molecule 31 is a protein called General transcription factor IIH subunit 2.

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

- Molecule 32 is a protein called General transcription factor IIH subunit 3.

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

- Molecule 33 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	HF	66	Total	C	N	O	S	0	0
			523	337	83	100	3		

- Molecule 34 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

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

- Molecule 35 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	DD	159	Total	C	N	O	S	0	0
			1330	830	248	249	3		
35	Dd	158	Total	C	N	O	S	0	0
			1307	814	238	252	3		

- Molecule 36 is a protein called Transcription initiation factor TFIID subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	DE	546	Total	C	N	O	S	0	0
			4364	2766	757	820	21		
36	De	539	Total	C	N	O	S	0	0
			4327	2746	748	814	19		

- Molecule 37 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	DF	408	Total	C	N	O	S	0	0
			3109	1970	542	579	18		
37	Df	403	Total	C	N	O	S	0	0
			3081	1954	533	576	18		

- Molecule 38 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	DG	145	Total	C	N	O	S	0	0
			1180	748	217	211	4		

- Molecule 39 is a protein called Transcription initiation factor TFIID subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	DH	209	Total	C	N	O	S	0	0
			1633	1034	283	311	5		

- Molecule 40 is a protein called Transcription initiation factor TFIID subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	DI	120	Total	C	N	O	S	0	0
			959	610	166	177	6		
40	Di	121	Total	C	N	O	S	0	0
			967	615	167	178	7		

- Molecule 41 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	DL	74	Total	C	N	O	S	0	0
			605	379	105	118	3		
41	Dl	107	Total	C	N	O	S	0	0
			876	547	158	166	5		

- Molecule 42 is a protein called Transcription initiation factor TFIID subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Dc	127	Total	C	N	O	S	0	0
			1011	638	174	193	6		

- Molecule 43 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Dj	95	Total	C	N	O	S	0	0
			759	488	124	143	4		
43	DJ	90	Total	C	N	O	S	0	0
			720	466	115	135	4		

- Molecule 44 is a protein called Transcription initiation factor TFIID subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Dk	98	Total	C	N	O	S	0	0
			785	499	142	139	5		

- Molecule 45 is a protein called Transcription initiation factor TFIID subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Dm	87	Total	C	N	O	S	0	0
			724	456	131	131	6		

- Molecule 46 is a protein called Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	HI	299	Total	C	N	O	S	0	0
			2374	1532	405	426	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
HI	41	ALA	LYS	engineered mutation	UNP P50613

- Molecule 47 is a protein called Cyclin-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	HJ	287	Total	C	N	O	S	0	0
			2307	1477	398	417	15		

- Molecule 48 is a protein called DNA-directed RNA polymerase II subunit RPB4.

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

- Molecule 49 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 50 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	g	106	Total	C	N	O	S	0	0
			898	569	166	157	6		

- Molecule 51 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	j	122	Total	C	N	O	S	0	0
			840	527	151	159	3		

- Molecule 52 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	n	1015	Total	C	N	O	S	0	0
			7751	4941	1363	1405	42		

- Molecule 53 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	s	93	Total	C	N	O	S	0	0
			723	463	121	135	4		

- Molecule 54 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	117	Total	C	N	O	S	0	0
			886	552	146	184	4		

- Molecule 55 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	a	438	Total	C	N	O	S	0	0
			3430	2190	584	632	24		

- Molecule 56 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	d	158	Total	C	N	O	S	0	0
			1268	791	228	243	6		

- Molecule 57 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	f	167	Total	C	N	O	S	0	0
			1365	882	235	243	5		

- Molecule 58 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	i	73	Total	C	N	O	S	0	0
			605	382	107	110	6		

- Molecule 59 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	m	112	Total	C	N	O	S	0	0
			983	641	172	165	5		

- Molecule 60 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	q	555	Total	C	N	O	S	0	0
			4373	2765	783	805	20		

- Molecule 61 is a protein called Mediator of RNA polymerase II transcription subunit 26.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	z	97	Total	C	N	O	S	0	0
			765	472	136	154	3		

- Molecule 62 is a protein called Mediator of RNA polymerase II transcription subunit 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	b	115	Total	C	N	O	S	0	0
			899	563	155	172	9		

- Molecule 63 is a protein called Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	c	263	Total	C	N	O	S	0	0
			2131	1356	379	385	11		

- Molecule 64 is a protein called Mediator of RNA polymerase II transcription subunit 28.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	e	102	Total	C	N	O	S	0	0
			832	520	146	163	3		

- Molecule 65 is a protein called Mediator of RNA polymerase II transcription subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	l	126	Total	C	N	O	S	0	0
			1040	649	191	193	7		

- Molecule 66 is a protein called Mediator of RNA polymerase II transcription subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	o	156	Total	C	N	O	S	0	0
			1221	780	212	222	7		

- Molecule 67 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	h	190	Total	C	N	O	S	0	0
			1465	913	259	289	4		

- Molecule 68 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	k	112	Total	C	N	O	S	0	0
			879	537	163	175	4		

- Molecule 69 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	r	192	Total	C	N	O	S	0	0
			1535	973	271	276	15		

- Molecule 70 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	t	193	Total	C	N	O	S	0	0
			1499	955	247	280	17		

- Molecule 71 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	v	134	Total	C	N	O	S	0	0
			1083	668	185	226	4		

- Molecule 72 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	p	766	Total	C	N	O	S	0	0
			5983	3816	1026	1092	49		

- Molecule 73 is a protein called Mediator of RNA polymerase II transcription subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	w	1334	Total	C	N	O	S	0	0
			10774	6967	1827	1909	71		

- Molecule 74 is a protein called Mediator of RNA polymerase II transcription subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	x	897	Total	C	N	O	S	0	0
			7061	4524	1190	1293	54		

- Molecule 75 is a protein called Mediator of RNA polymerase II transcription subunit 25.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	y	210	Total	C	N	O	S	0	0
			1605	1030	264	302	9		

- Molecule 76 is a protein called HISTONE H2A.Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	NC	103	Total	C	N	O		0	0
			506	300	103	103			
76	NG	107	Total	C	N	O		0	0
			524	310	107	107			

- Molecule 77 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	ND	95	Total	C	N	O		0	0
			471	281	95	95			
77	NH	95	Total	C	N	O		0	0
			471	281	95	95			

- Molecule 78 is ZINC ION (three-letter code: ZN) (formula: Zn).

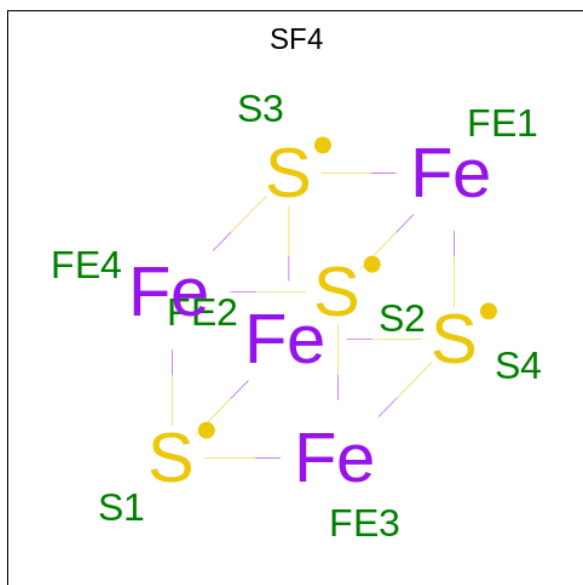
Mol	Chain	Residues	Atoms		AltConf
78	BA	1	Total	Zn	0
			1	1	
78	EA	1	Total	Zn	0
			1	1	
78	PA	2	Total	Zn	0
			2	2	
78	PB	1	Total	Zn	0
			1	1	
78	PC	1	Total	Zn	0
			1	1	
78	PI	2	Total	Zn	0
			2	2	
78	PJ	1	Total	Zn	0
			1	1	
78	PL	1	Total	Zn	0
			1	1	
78	HD	2	Total	Zn	0
			2	2	
78	HG	3	Total	Zn	0
			3	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
78	HE	2	Total	Zn	0
			2	2	
78	c	1	Total	Zn	0
			1	1	
78	p	1	Total	Zn	0
			1	1	

- Molecule 79 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 80 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
80	PA	1	Total	Mg	0
			1	1	

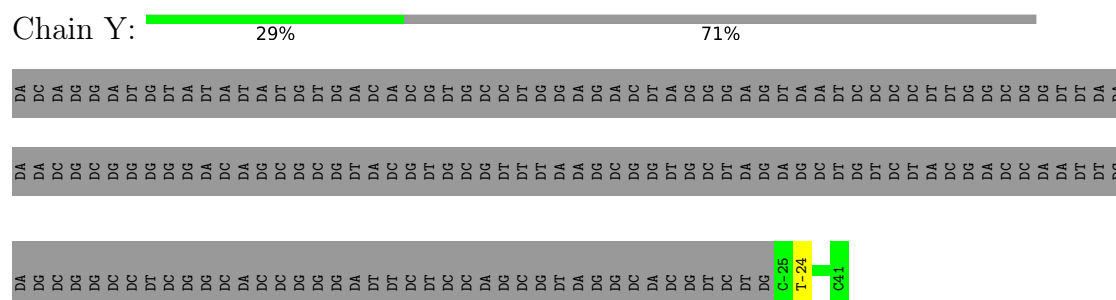
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

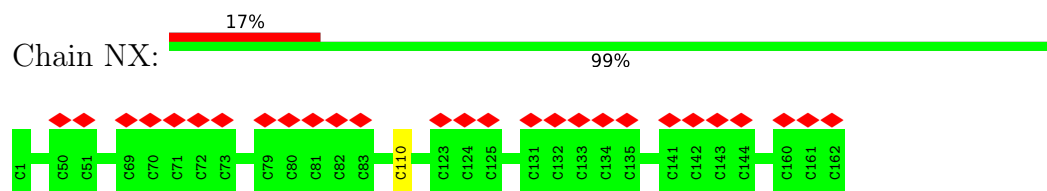
• Molecule 1: DNA (228-mer)



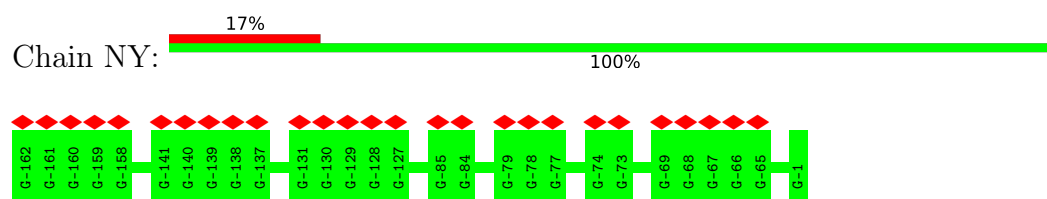
• Molecule 2: DNA (228-mer)



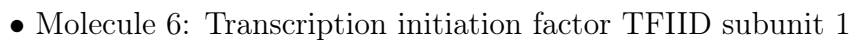
• Molecule 3: DNA (162-mer)

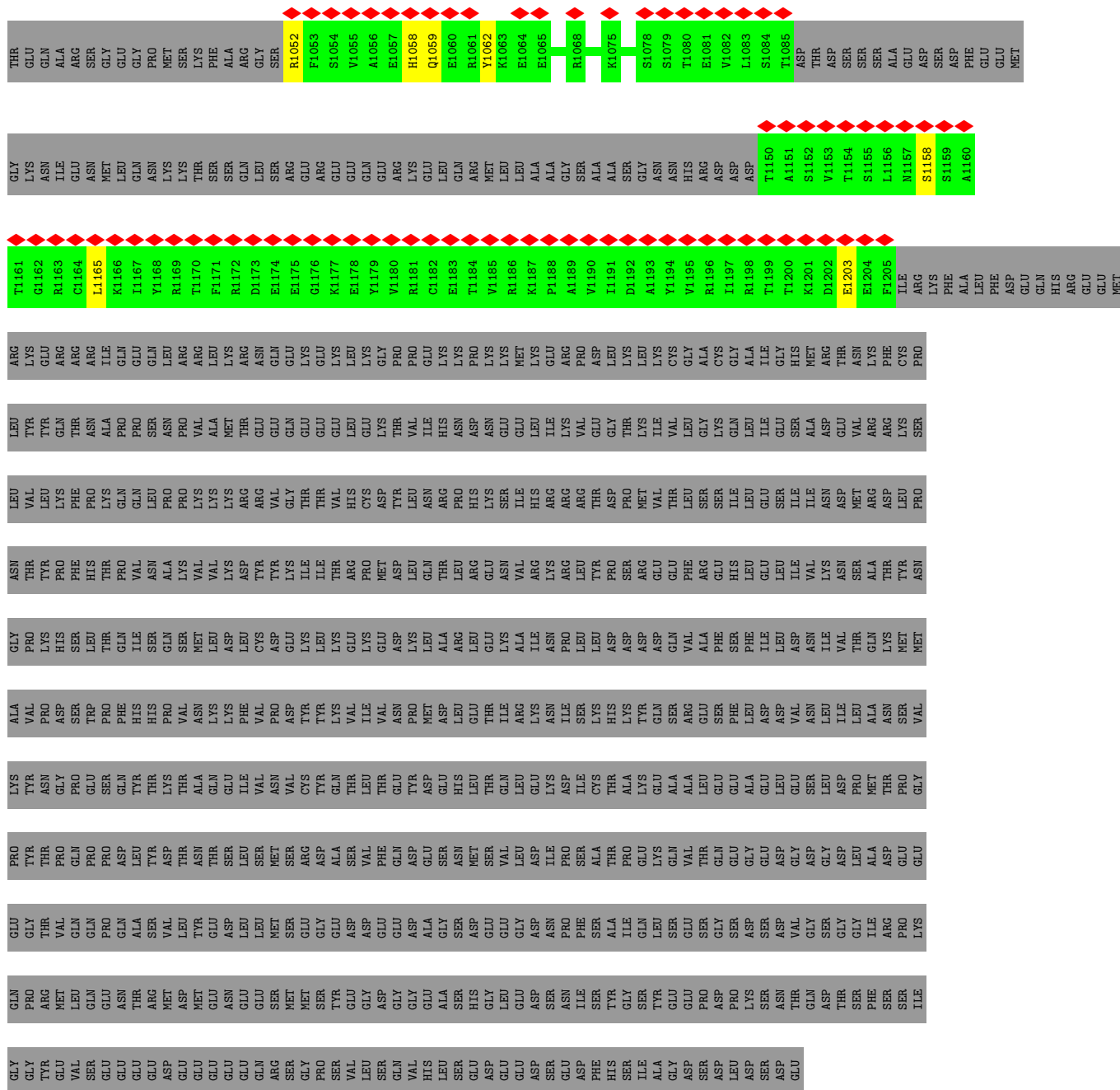


• Molecule 4: DNA (162-mer)

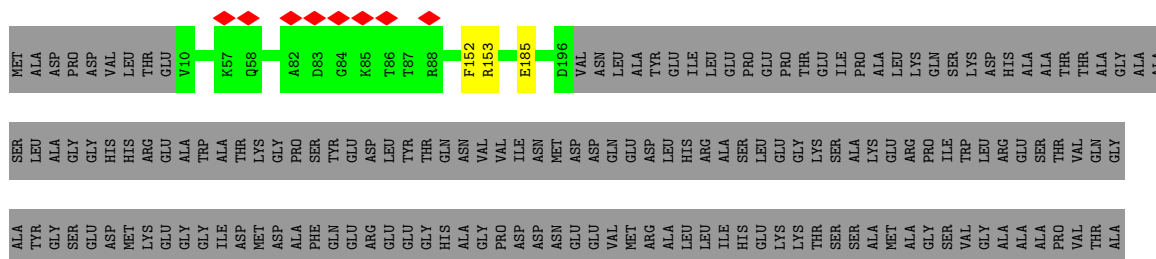


Chain BA: 80% 20%





- Molecule 7: General transcription factor IIE subunit 1



ALA	ASN	GLN	ARG	PRO	GLY	LEU	VAL	GLN	ALA	GLN	GLY	THR	PRO	GLY	GLY	ASP	ASP	ASP	GLY	GLY	GLY	ASP	ASP	GLY	GLY	GLY	VAL	ALA	ALA	GLY	ARG	PRO	PHE	SER	TYR	SER	GLY	VAL									
ALA	ASP	SER	GLY	VAL	GLN	THR	GLY	GLY	ASP	ASP	GLY	GLY	PRO	PRO	ARG	VAL	ALA	ALA	VAL	HIS	LYS	ARG	GLY	GLY	GLY	ASP	ASP	ASP	GLY	PHE	GLY	GLY	GLY	GLY	VAL	VAL	VAL	VAL	GLY	ARG	PRO	PHE	SER	TYR	SER	GLY	VAL

- Molecule 8: General transcription factor IIF subunit 1

Chain FA:

[illegible]

- Molecule 9: General transcription and DNA repair factor IIH helicase subunit XPD

Chain HA: 

NI
 NI114
 G291
 LEU
 ARG
 GLU
 ALA
 SER
 ALA
 ALA
 ARG
 GLU
 THR
 ASP
 ALA
 HIS
 LEU
 A306
 P426
 Q572
 F728
 HIS
 ARG
 GLU
 ASP
 GLN
 LEU
 GLY
 LEU
 SER
 LEU
 SER
 LEU
 LEU
 GLU
 GLN
 LEU
 GLU
 SER
 GLU
 GLU
 THR
 LEU
 LYS
 ARG
 TLE
 GLU
 GLN
 TLE
 ALA
 GLN
 LEU
 LEU

- Molecule 10: Histone H3

Chain NA: 71% 0% 26%

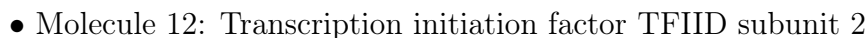
MET	ALA	ARG	THR	LYS	GLN	THR	ALA	ARG	LYS	SER	THR	THR	GLY	GLY	LYS	ALA	PRO	ARG	LYS	GLN	LEU	ALA	LEU	THR	LYS	LYS	ALA	ALA	ARG	LYS	SER	ALA	PRO	VAL	K436	K437	P438	H439	R440	Y441		K464		R534	I535	
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- Molecule 10: Histone H3

Chain NE: 74% . 24%

MET	ALA	ARG	THR	LYS	GLN	THR	ALA	ARG	LYS	SER	THR	GLY	GLY	LYS	ALA	ALA	PRO	ARG	LYS	GLN	LEU	ALA	ALA	THR	LYS	ALA	ALA	ALA	ARG	LYS	SER	ALA	ALA	PRO	ALA	ALA	THR	6633	6634	6635	6636	6637	6638	6639	6640	6641	6642	6643	6644	6645	6646	6647	6648	6649	6650	6651	6652	6653	6654	6655	6656	6657	6658	6659	6660	6661	6662	6663	6664	6665	6666	6667	6668	6669	6670	6671	6672	6673	6674	6675	6676	6677	6678	6679	6680	6681	6682	6683	6684	6685	6686	6687	6688	6689	6690	6691	6692	6693	6694	6695	6696	6697	6698	6699	6700	6701	6702	6703	6704	6705	6706	6707	6708	6709	6710	6711	6712	6713	6714	6715	6716	6717	6718	6719	6720	6721	6722	6723	6724	6725	6726	6727	6728	6729	6730	6731	6732	6733	6734	6735	6736	6737	6738	6739	6740	6741	6742	6743	6744	6745	6746	6747	6748	6749	6750	6751	6752	6753	6754	6755	6756	6757	6758	6759	6760	6761	6762	6763	6764	6765	6766	6767	6768	6769	6770	6771	6772	6773	6774	6775	6776	6777	6778	6779	6780	6781	6782	6783	6784	6785	6786	6787	6788	6789	6790	6791	6792	6793	6794	6795	6796	6797	6798	6799	6800	6801	6802	6803	6804	6805	6806	6807	6808	6809	6810	6811	6812	6813	6814	6815	6816	6817	6818	6819	6820	6821	6822	6823	6824	6825	6826	6827	6828	6829	6830	6831	6832	6833	6834	6835	6836	6837	6838	6839	6840	6841	6842	6843	6844	6845	6846	6847	6848	6849	6850	6851	6852	6853	6854	6855	6856	6857	6858	6859	6860	6861	6862	6863	6864	6865	6866	6867	6868	6869	6870	6871	6872	6873	6874	6875	6876	6877	6878	6879	6880	6881	6882	6883	6884	6885	6886	6887	6888	6889	6890	6891	6892	6893	6894	6895	6896	6897	6898	6899	6900	6901	6902	6903	6904	6905	6906	6907	6908	6909	6910	6911	6912	6913	6914	6915	6916	6917	6918	6919	6920	6921	6922	6923	6924	6925	6926	6927	6928	6929	6930	6931	6932	6933	6934	6935	6936	6937	6938	6939	6940	6941	6942	6943	6944	6945	6946	6947	6948	6949	6950	6951	6952	6953	6954	6955	6956	6957	6958	6959	6960	6961	6962	6963	6964	6965	6966	6967	6968	6969	6970	6971	6972	6973	6974	6975	6976	6977	6978	6979	6980	6981	6982	6983	6984	6985	6986	6987	6988	6989	6990	6991	6992	6993	6994	6995	6996	6997	6998	6999	7000	7001	7002	7003	7004	7005	7006	7007	7008	7009	7010	7011	7012	7013	7014	7015	7016	7017	7018	7019	7020	7021	7022	7023	7024	7025	7026	7027	7028	7029	7030	7031	7032	7033	7034	7035	7036	7037	7038	7039	7040	7041	7042	7043	7044	7045	7046	7047	7048	7049	7050	7051	7052	7053	7054	7055	7056	7057	7058	7059	706
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74% • 25%



79% 20%



- Molecule 13: Transcription initiation factor IIE subunit beta

Chain EB: 58% 41%

MET	ASP	PRO	SER	SER	LEU	LEU	ARG	GLU	GLU	ARG	ARG	GLU	GLU	PHE	LYS	LYS	ARG	ALA	ALA	LEU	SER	THR	THR	PRO	VAL	VAL	VAL	GLU	LYS	ARG	SER	SER	SER	SER	GLU	GLU	SER	SER	SER	SER	SER	LYS	LYS	LYS	LYS	LYS	THR	THR	LYS	VAL	GLU	GLY	GLY	GLY	GLY	SER	SER	SER	SER	GLN	ASN	SER	ASP	SER	HIS	HIS	SER	ASN	GLY
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SER PHE ASN LEU LYS ALA LEU SER GLY SER SER G72 K114 E189 T242 SER MET GIN GLU SER GLY PRO PRO LYS VAL ALA PRO ILE GLN ARG ARG LYS LYS PRO PRO ALA SER GLN LYS LYS THR HIS ASN HIS GLI HIS LEU ALA GLY VAL LEU ASP

SER
ASP
ILE
THR
SER
SER
LYS

- Molecule 14: General transcription factor IIF subunit 2

Chain FB: 88% • 11%

MET
 A2
 N64
 ILE
 HIS
 ASP
 ILE
 GLY
 GLY
 LYS
 PRO
 ALA
 SER
 VAL
 SER
 ALA
 PRO
 ARG
 E60
 H229
 K230
 E238
 TYR
 ARG
 HIS
 TYR
 GLN
 GLY
 GLU
 GLU
 LYS
 SER
 ASP

- Molecule 15: General transcription factor IIH subunit 1

Chain HB:

MET	ALA	THR	SER	SER	GLU	GLU	VAL	LEU	LEU	ILE	VAL	LYS	LYS	VAL	ARG	GLN	LYS	LYS	GLN	ASP	GLY	GLY	ALA	ALA	LEU	TYR	LEU	MET	MET	ALA	GLU	ARG	ILE	ALA	ALA	TRP	ALA	ALA	ALA	PRO	GLY	GLU	GLY	LYS	ASP	ASP	ARG	ARG	PHE	THR	THR	ILE	LYS	SER	SER	HIS	MET	MET	TYR	ALA	ALA	LYS	LYS	ILE	ILE	GLU	GLU	PRO	SER	LYS	GLY	LYS
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[illegible][illegible]

LVS	GLY	LEU	LVS	THR	MET	VAL	SER	LEU	GLY	VAL	LVS	ASN	PRO	LEU	LEU	LEU	ASP	ASP	LVS	PRO	LEU	ASP	GLY	GLY	THR	GLY	ILE	SER	SER	SER	ASN	LVS	SER	ILE	E297	K321	GLN	GLU	GLU	GLN	ASN	THR	SER	GLU	PRO
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[illegible]

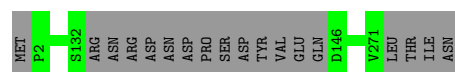
K547
THR

- Molecule 16: Histone H4

Chain NB: 78% 22%



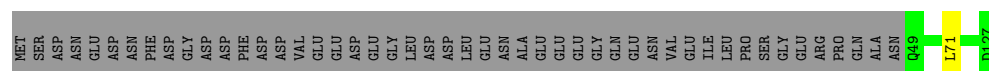
- Chain PC: 93% 7%



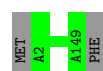
- Chain PE: 100%



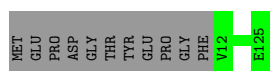
- Chain PF:  61% 38%



- Chain PH: 99%



- Chain PI:  91% 9%



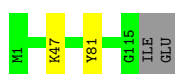
- Molecule 27: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain PJ: 96%



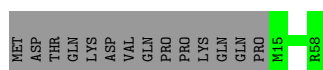
- Molecule 28: RNA_pol_L_2 domain-containing protein

Chain PK: 97%



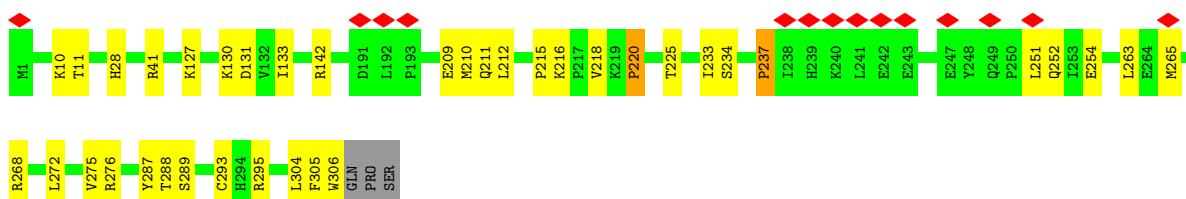
- Molecule 29: RPB12

Chain PL: 76% 24%



- Molecule 30: CDK-activating kinase assembly factor MAT1

Chain HD: 5% 87% 12%



- Molecule 31: General transcription factor IIH subunit 2

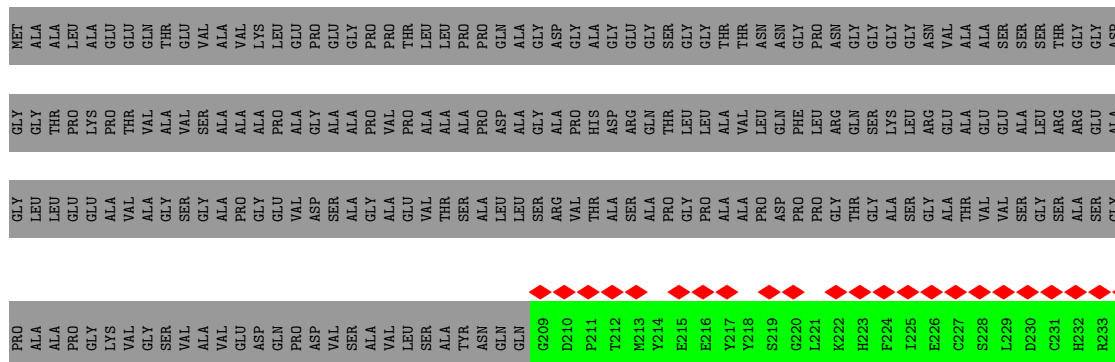
Chain HG: 88% 12%

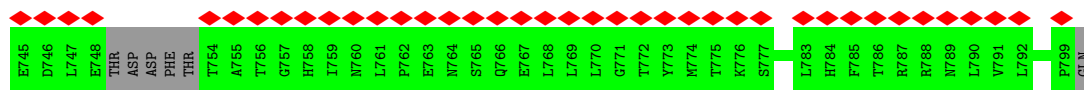


- Molecule 32: General transcription factor IIH subunit 3

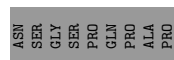
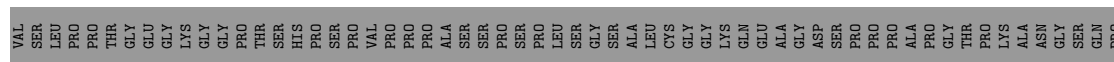
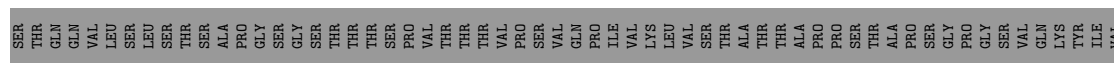
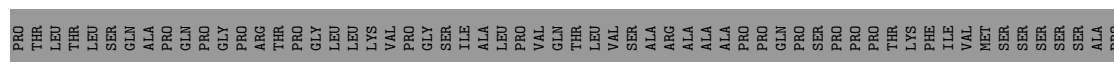
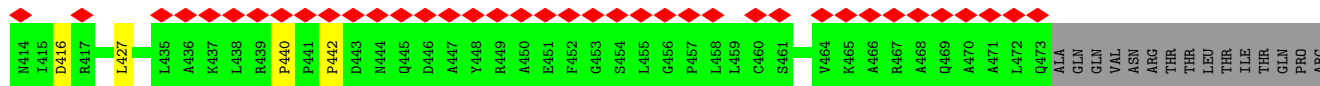
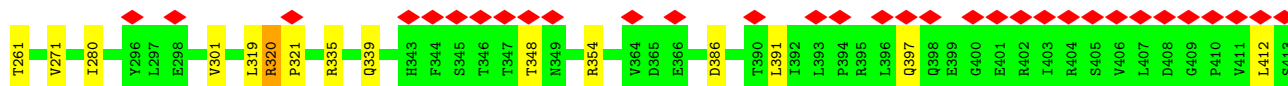
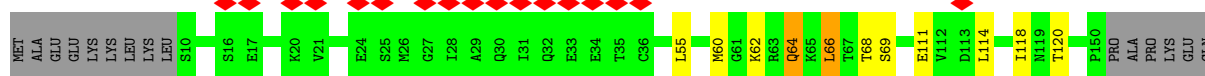
Chain HE: 84% 15%

- Molecule 36: Transcription initiation factor TFIID subunit 5

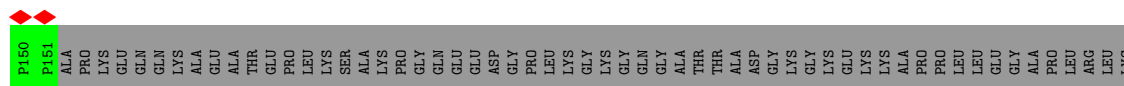
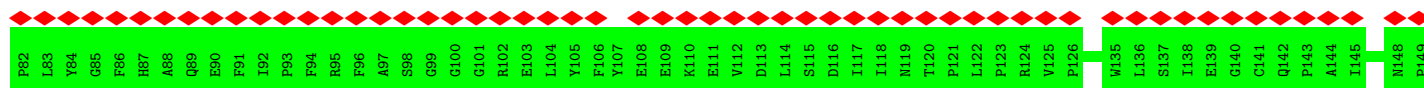
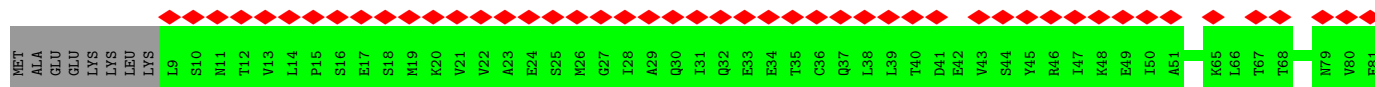


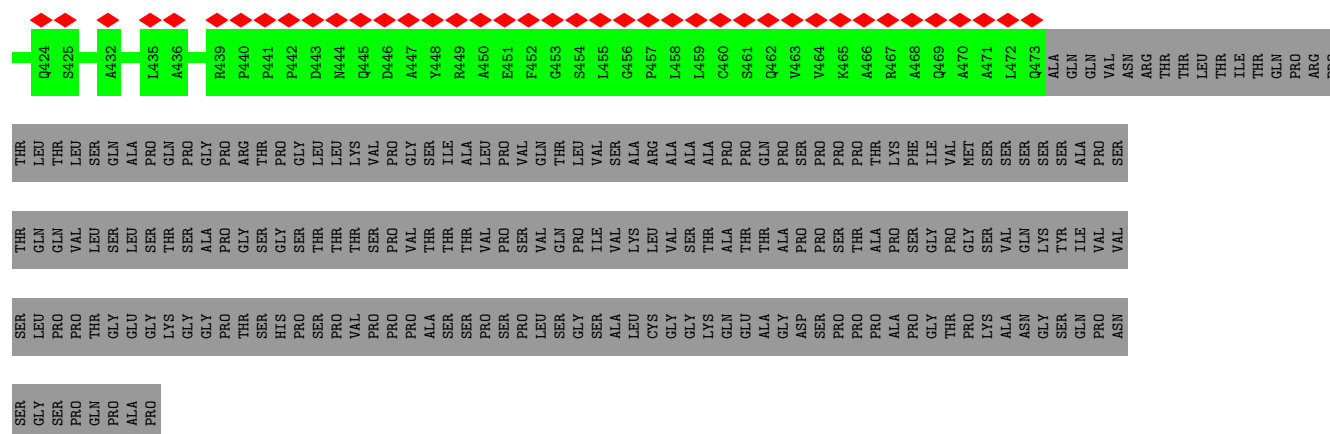


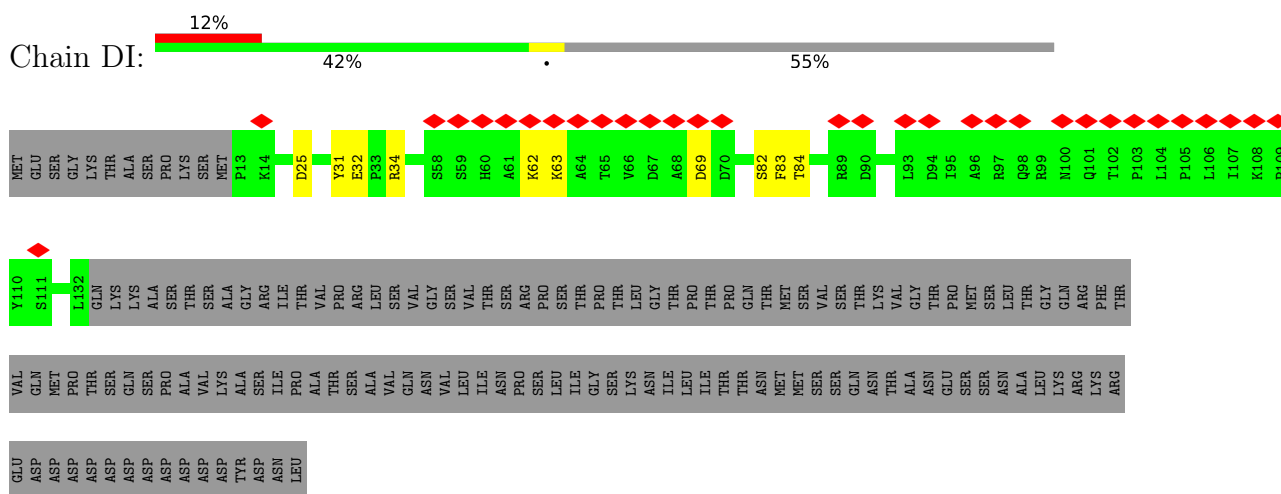
• Molecule 37: Transcription initiation factor TFIID subunit 6



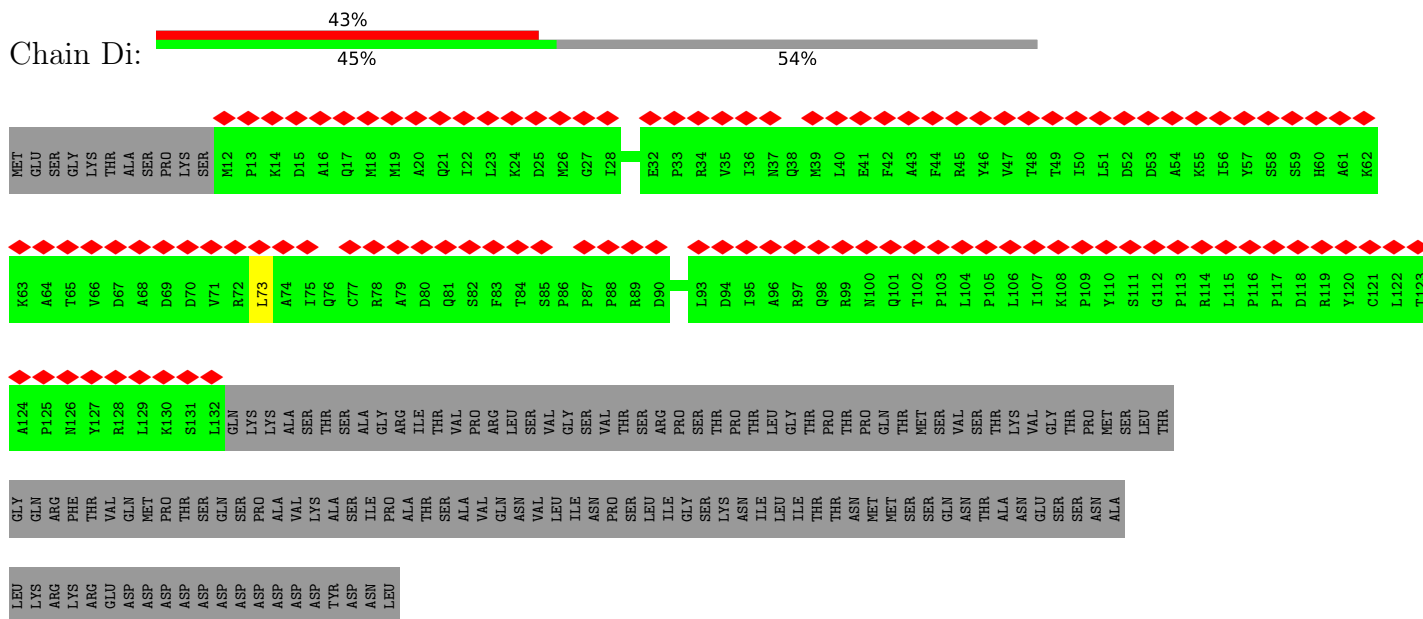
• Molecule 37: Transcription initiation factor TFIID subunit 6



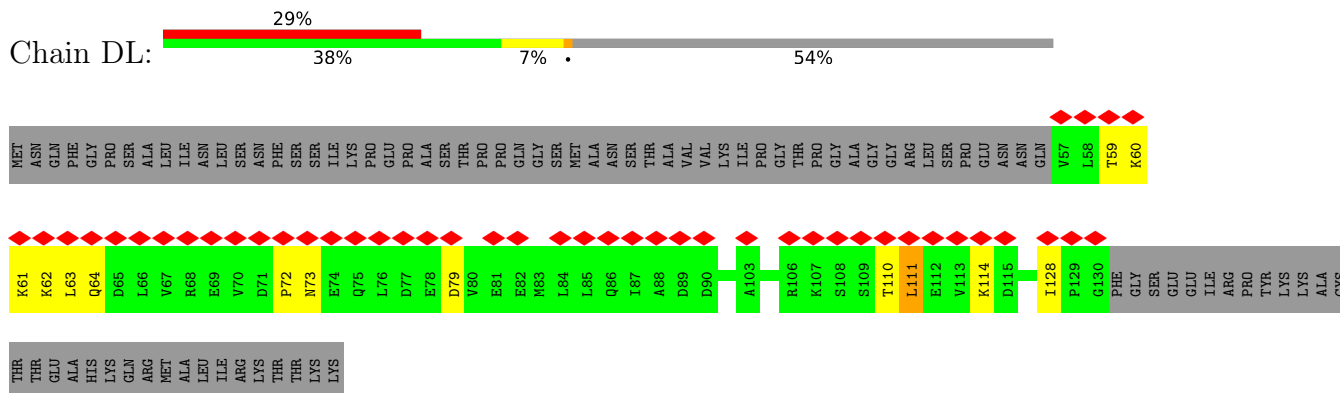




- Molecule 40: Transcription initiation factor TFIID subunit 9



- Molecule 41: Transcription initiation factor TFIID subunit 12



- Molecule 41: Transcription initiation factor TFIID subunit 12

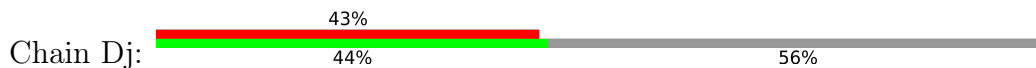
Chain D1:

Chain Dc:

[illegible]

TRP	PHE	VAL	VAL	PRO	LYS
CYS	THR	THR	THR	SER	ARG
PRO	GLU	GLU	GLU	ASN	GLU
LYS	THR	THR	THR	ARG	ARG
CYS	VAL	VAL	VAL	PRO	LYS
ALA	SER	SER	SER	LYS	ARG
ASN	THR	THR	THR	THR	GLU
LYS	TYR	TYR	TYR	PRO	LYS
LYS	VAL	VAL	VAL	PRO	GLU
ASP	ILE	ILE	ILE	PRO	LYS
LYS	ARG	ARG	ARG	ALA	GLU
LYS	ASP	ASP	ASP	PRO	LYS
LYS	GLU	GLU	GLU	ALA	HIS
HIS	TRP	TRP	TRP	PRO	LYS
	LYS	LYS	LYS	HIS	HIS
	ARG	ARG	ARG	ALA	HIS
	ALA	ALA	ALA	GLY	GLY
	HIS	ILE	ILE	PRO	ILE
		TRP	TRP	MET	LYS
		ILE	ILE	LEU	VAL
		CYS	CYS	VAL	GLU
		PRO	PRO	SER	PRO
		GLY	GLY	PRO	VAL
		CYS	CYS	ALA	ALA
		ASN	ASN	PRO	LEU
		LYS	LYS	VAL	ALA
		PRO	PRO	PRO	PRO
		ASP	ASP	LEU	SER
		ASP	ASP	PRO	PRO
		GLY	GLY	LEU	VAL
		SER	SER	LEU	ILE
		PRO	PRO	ALA	PRO
		MET	MET	GLN	ARG
		ILE	ILE	ALA	LEU
		GLY	GLY	ALA	THR
		CYS	CYS	ALA	LEU
		ASP	ASP	GLY	ARG
		ASP	ASP	PRO	VAL
		TYR	TYR	GLY	GLY
		HIS	HIS	PRO	GLN
		THR	THR	GLY	LYS
		PRO	PRO	ILE	VAL
		CYS	CYS	ALA	ILE
		VAL	VAL	ALA	SER
		GLY	GLY	GLY	LYS
		ILE	ILE	SER	VAL
		MET	MET	ALA	VAL
		THR	THR	SER	PRO
		ALA	ALA	ALA	ALA
		PRO	PRO	LYS	PRO
		GLU	GLU	ALA	GLU
		GLY	GLY	PRO	ALA
		VAL	VAL	VAL	LYS
		MET	MET	PRO	PRO
		GLN	GLN	SER	ALA

- Molecule 43: Transcription initiation factor TFIID subunit 10

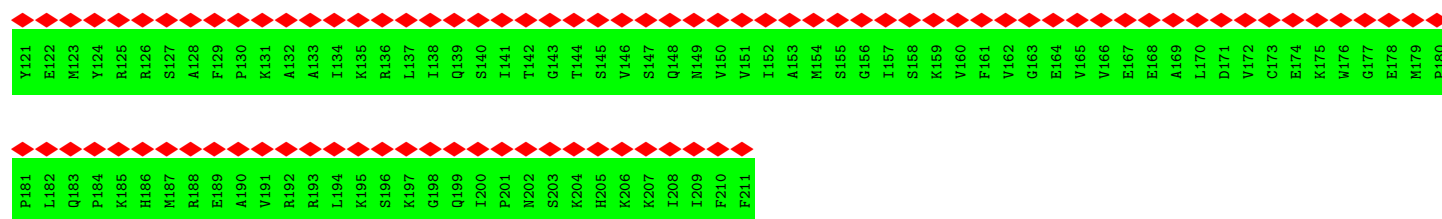
[illegible]

- Molecule 43: Transcription initiation factor TFIID subunit 10

[illegible]

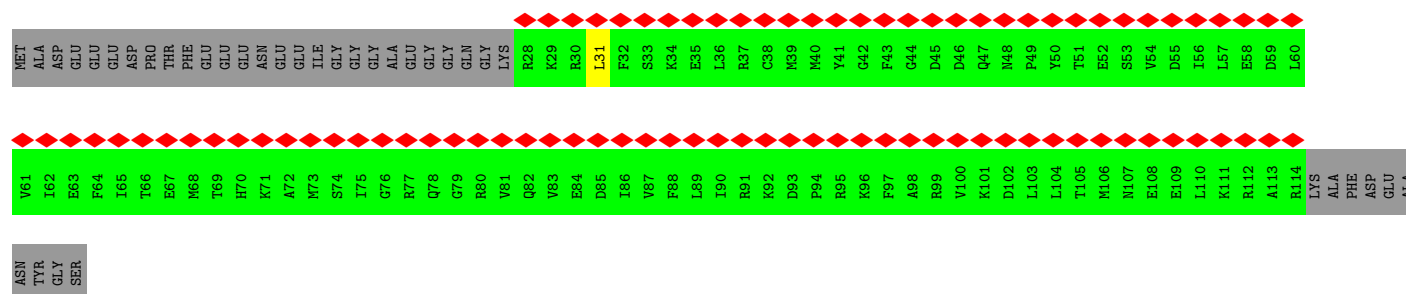
- Molecule 44: Transcription initiation factor TFIID subunit 11

[illegible]



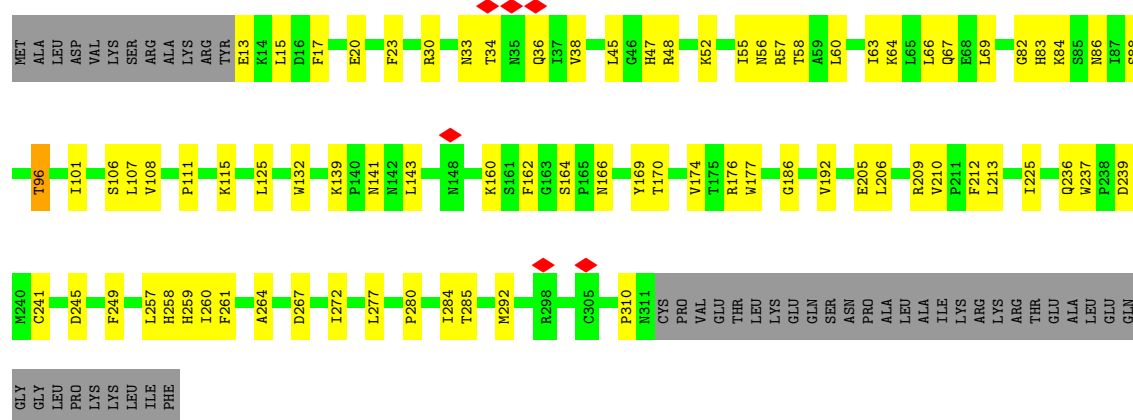
- Molecule 45: Transcription initiation factor TFIID subunit 13

Chain Dm: 70% 69% 30%



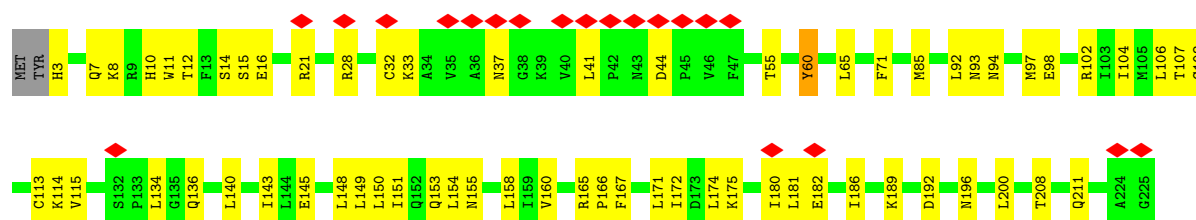
- Molecule 46: Cyclin-dependent kinase 7

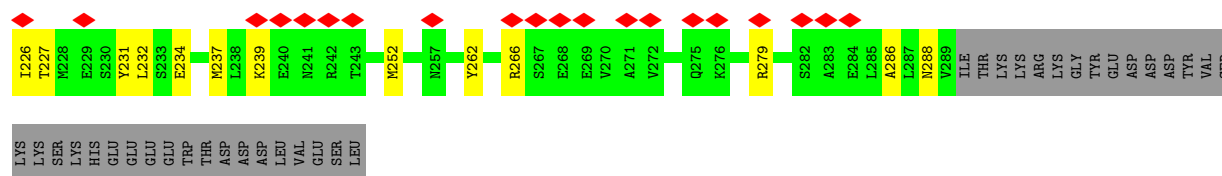
Chain HI: 64% 23% 14%



- Molecule 47: Cyclin-H

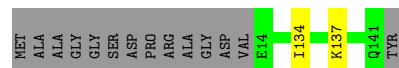
Chain HJ: 12% 65% 24% 11%





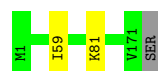
- Molecule 48: DNA-directed RNA polymerase II subunit RPB4

Chain PD: 89% 10%



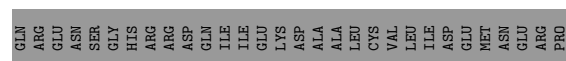
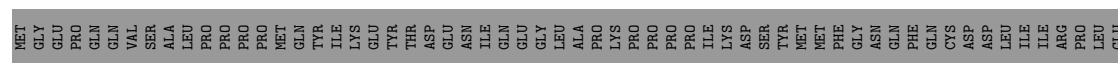
- Molecule 49: DNA-directed RNA polymerase II subunit RPB7

Chain PG: 98% ..



- Molecule 50: Mediator of RNA polymerase II transcription subunit 7

Chain g: 41% 5% 55%



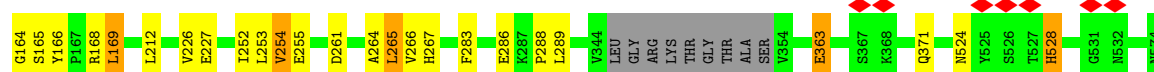
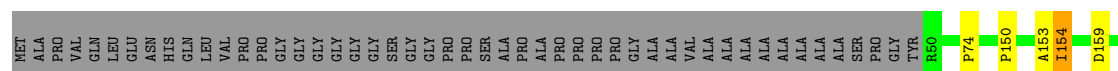
- Molecule 51: Mediator of RNA polymerase II transcription subunit 10

Chain j: 88% 10%



- Molecule 52: Mediator of RNA polymerase II transcription subunit 14

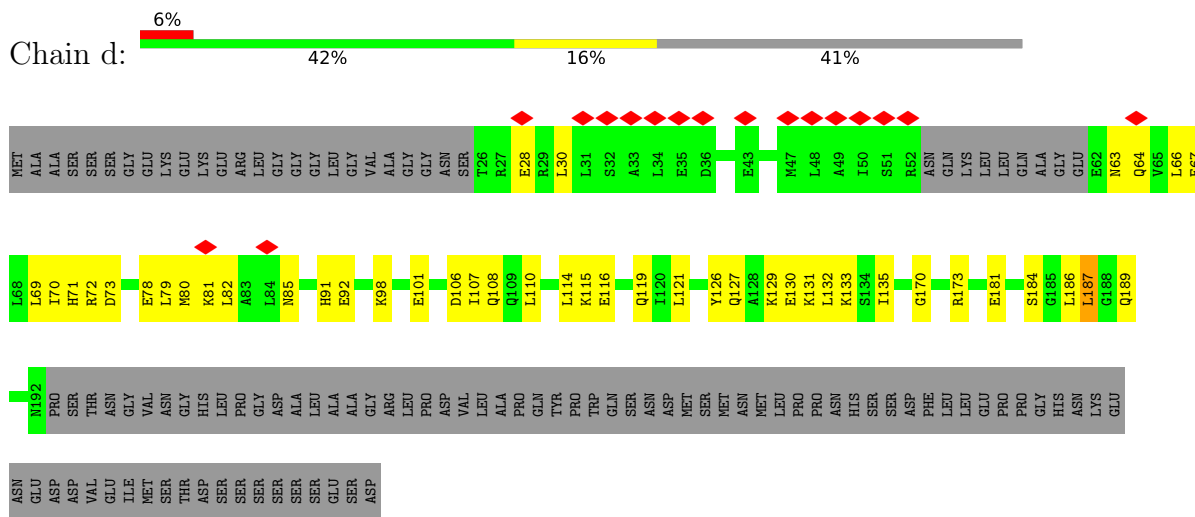
Chain n: 6% 67% 30%



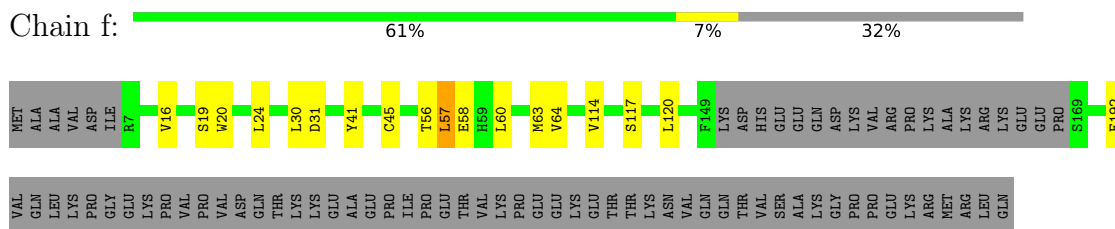


[illegible]

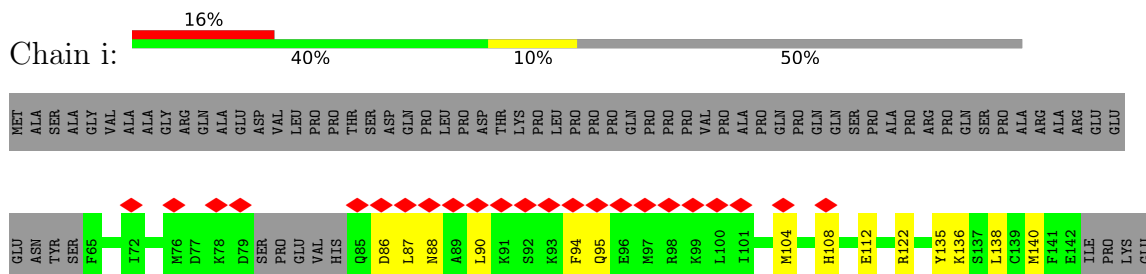
- Molecule 56: Mediator of RNA polymerase II transcription subunit 4



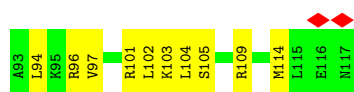
- Molecule 57: Mediator of RNA polymerase II transcription subunit 6



- Molecule 58: Mediator of RNA polymerase II transcription subunit 9

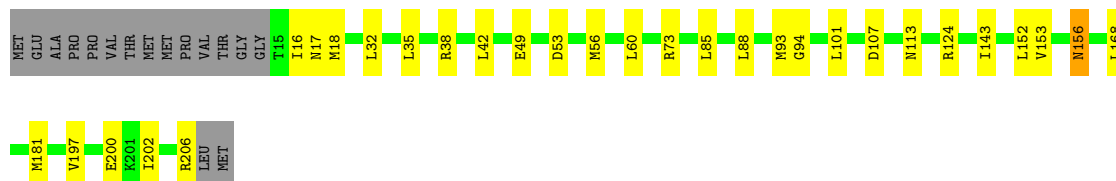






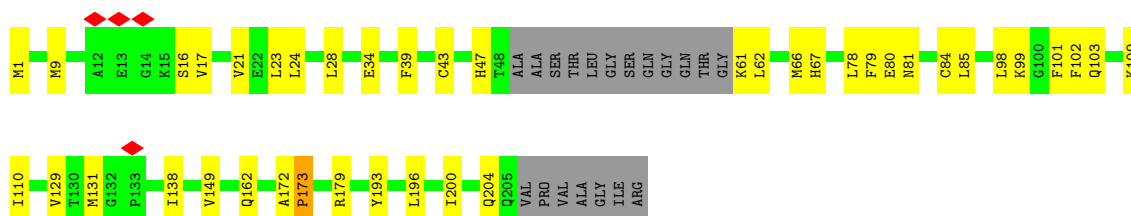
- Molecule 69: Mediator of RNA polymerase II transcription subunit 18

Chain r: 78% 14% 8%



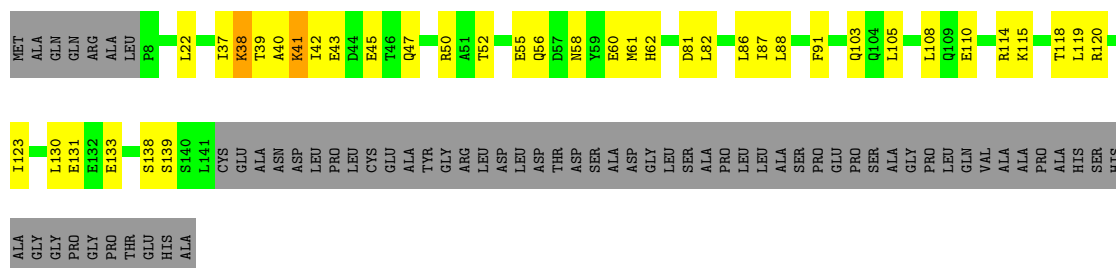
- Molecule 70: Mediator of RNA polymerase II transcription subunit 20

Chain t: 72% 19% 9%



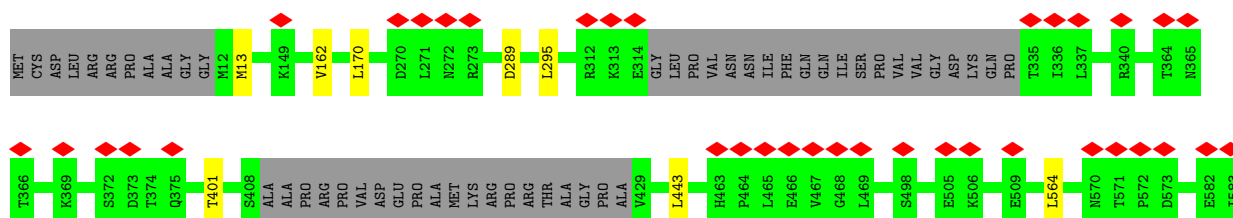
- Molecule 71: Mediator of RNA polymerase II transcription subunit 22

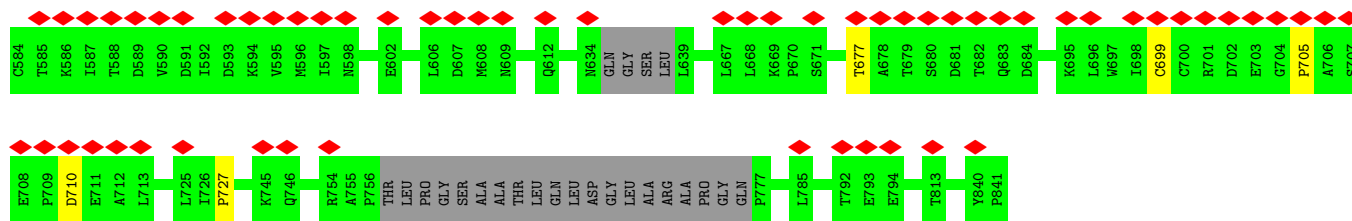
Chain v: 48% 18% 33%



- Molecule 72: Isoform 2 of Mediator of RNA polymerase II transcription subunit 16

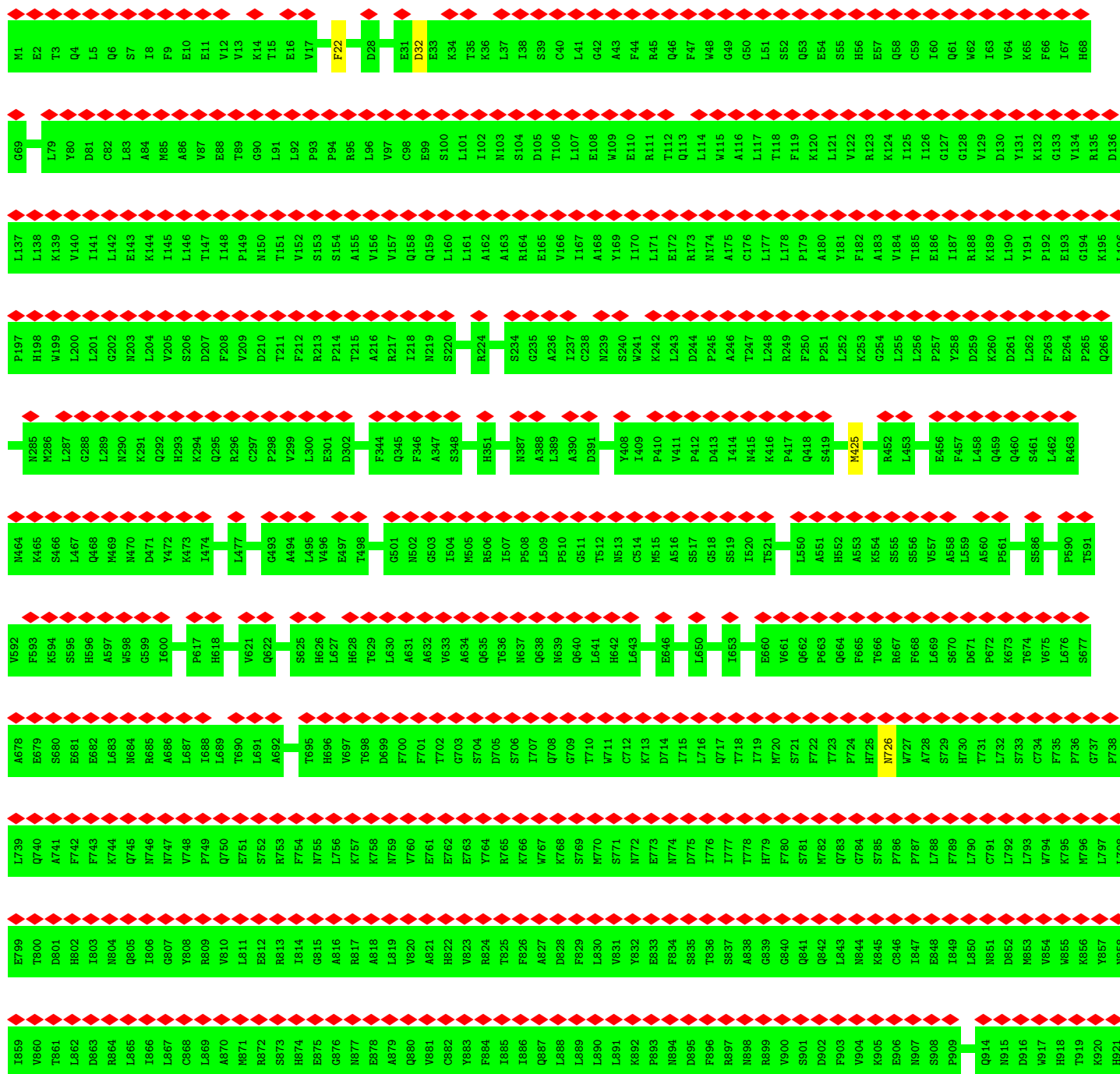
Chain p: 11% 90% 9%





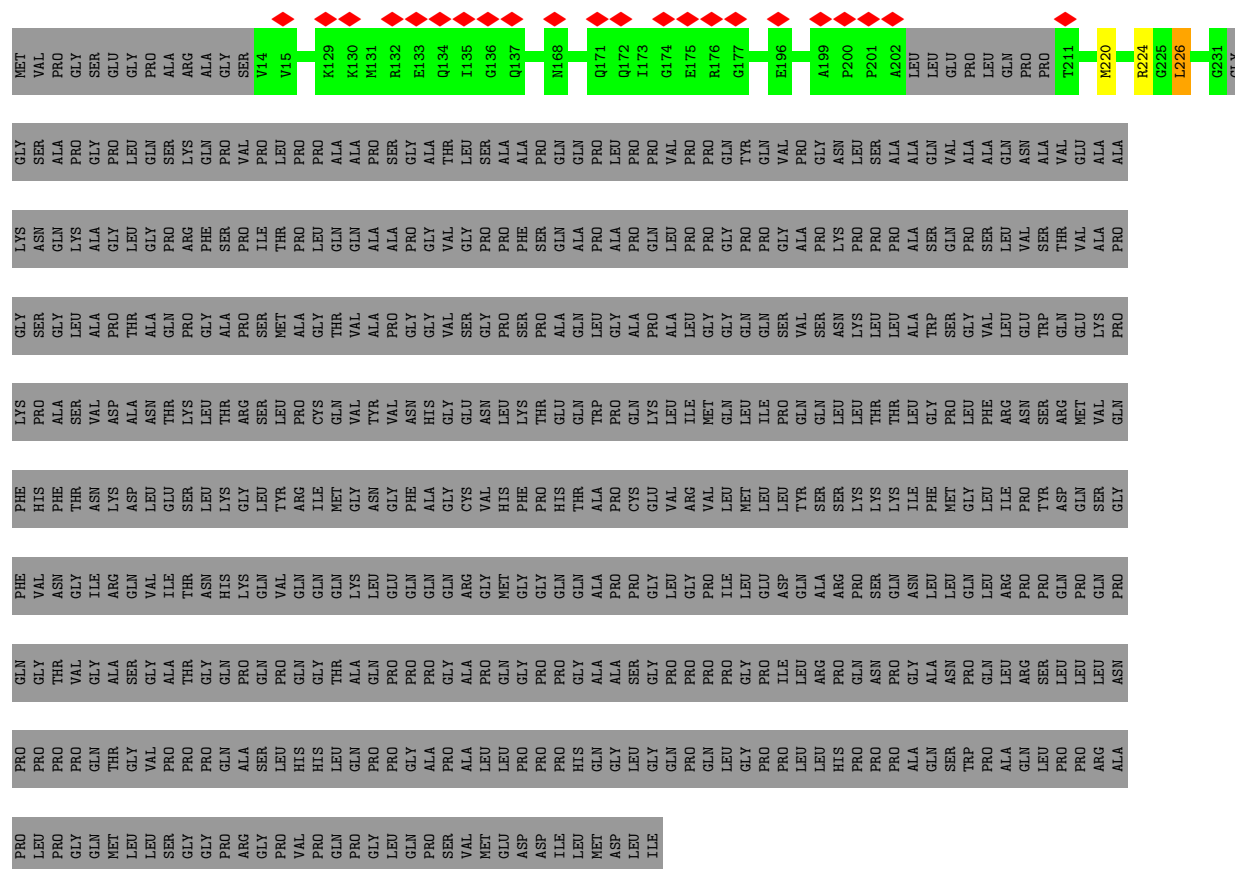
• Molecule 73: Mediator of RNA polymerase II transcription subunit 23


Chain w: 65% 97%





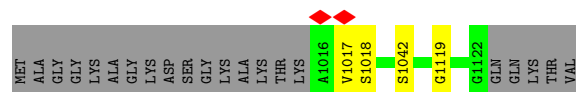
- Chain γ :  28% 72%



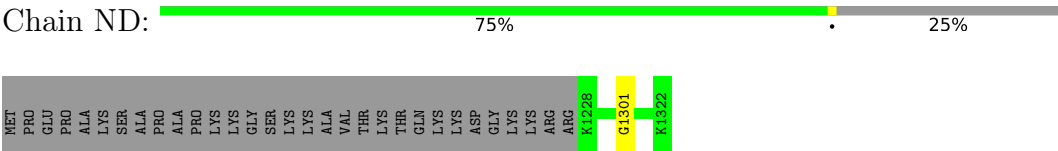
- Chain NC:  78% • 20%



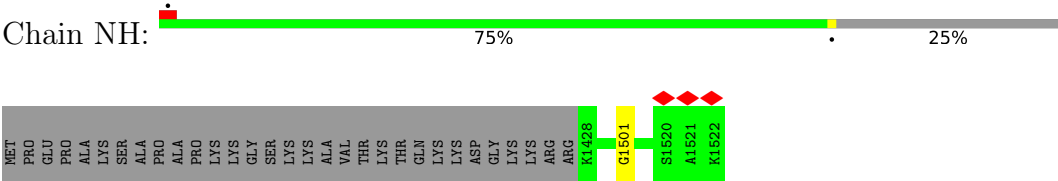
- Chain NG: 80% 16%



● Molecule 77: Histone H2B



● Molecule 77: Histone H2B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29473	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.762	Depositor
Minimum map value	-1.277	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.205	Depositor
Map size (\AA)	560.27997, 560.27997, 560.27997	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.3339999, 1.3339999, 1.3339999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, SF4

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	X	0.63	5/1561 (0.3%)	0.83	1/2411 (0.0%)
2	Y	0.67	1/1516 (0.1%)	0.92	0/2334
3	NX	0.34	1/3401 (0.0%)	0.82	0/5180
4	NY	0.38	0/4046	0.76	0/6310
5	BA	0.25	0/1983	0.41	0/2679
6	DA	0.51	0/4679	0.62	1/6320 (0.0%)
7	EA	0.34	0/1560	0.51	0/2097
8	FA	0.25	0/1167	0.41	0/1576
9	HA	0.26	0/5875	0.41	0/7955
10	NA	0.68	0/497	0.82	1/693 (0.1%)
10	NE	0.76	0/510	0.88	0/710
11	PA	0.28	0/11851	0.44	0/16014
12	DB	0.47	1/7993 (0.0%)	0.61	0/10836
13	EB	0.28	0/1427	0.46	0/1916
14	FB	0.26	0/1817	0.41	0/2445
15	HB	0.25	0/2210	0.40	0/2975
16	NB	0.76	0/390	0.84	0/539
16	NF	0.85	0/420	0.97	1/581 (0.2%)
17	PB	0.25	0/9257	0.42	0/12493
18	HC	0.28	0/3230	0.43	0/4376
19	DO	0.25	0/816	0.43	0/1105
20	DP	0.25	0/1448	0.42	0/1948
21	DQ	0.25	0/945	0.42	0/1274
22	PC	0.24	0/2102	0.42	0/2857
23	PE	0.25	0/1752	0.41	0/2366
24	PF	0.28	0/646	0.42	0/871
25	PH	0.24	0/1207	0.43	0/1628
26	PI	0.25	0/949	0.44	0/1284
27	PJ	0.26	0/516	0.41	0/696
28	PK	0.26	0/939	0.40	0/1271
29	PL	0.26	0/378	0.41	0/500
30	HD	0.50	0/2436	0.67	2/3286 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	HG	0.25	0/2793	0.42	0/3780
32	HE	0.31	0/2103	0.46	0/2846
33	HF	0.27	0/529	0.49	1/714 (0.1%)
34	HH	0.25	0/4994	0.41	0/6745
35	DD	0.42	0/1343	0.52	0/1795
35	Dd	0.29	0/1321	0.49	0/1772
36	DE	0.39	0/4469	0.56	0/6050
36	De	0.33	0/4433	0.55	0/6004
37	DF	0.51	0/3167	0.69	1/4303 (0.0%)
37	Df	0.42	0/3140	0.63	0/4268
38	DG	0.52	0/1199	0.63	0/1612
39	DH	0.37	0/1673	0.58	1/2285 (0.0%)
40	DI	0.43	0/981	0.58	0/1332
40	Di	0.31	0/989	0.48	0/1343
41	DL	0.44	0/613	0.65	1/829 (0.1%)
41	DI	0.41	0/888	0.54	1/1194 (0.1%)
42	Dc	0.40	0/1035	0.54	0/1406
43	DJ	0.30	0/736	0.49	1/998 (0.1%)
43	Dj	0.30	0/775	0.52	0/1049
44	Dk	0.31	0/799	0.48	0/1070
45	Dm	0.32	0/733	0.52	0/977
46	HI	0.67	0/2433	0.96	0/3302
47	HJ	0.74	0/2356	0.97	1/3185 (0.0%)
48	PD	0.29	0/1064	0.44	0/1428
49	PG	0.27	0/1382	0.44	0/1874
50	g	0.57	0/911	0.86	2/1219 (0.2%)
51	j	0.37	0/849	0.54	0/1150
52	n	0.36	0/7901	0.57	14/10731 (0.1%)
53	s	0.64	0/741	0.76	1/1002 (0.1%)
54	u	0.54	0/895	0.75	2/1215 (0.2%)
55	a	0.62	0/3507	0.78	1/4760 (0.0%)
56	d	0.62	0/1281	0.65	0/1718
57	f	0.56	0/1402	0.68	1/1905 (0.1%)
58	i	0.68	0/612	0.76	1/815 (0.1%)
59	m	0.28	0/1010	0.38	0/1359
60	q	0.49	1/4456 (0.0%)	0.56	0/6019
61	z	0.64	0/781	0.86	0/1067
62	b	0.51	0/911	0.63	0/1229
63	c	0.43	0/2172	0.58	1/2935 (0.0%)
64	e	0.29	0/840	0.40	0/1128
65	l	0.26	0/1048	0.43	0/1405
66	o	0.41	0/1256	0.65	0/1724
67	h	0.63	0/1485	0.73	1/2008 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
68	k	0.66	0/885	0.67	0/1190
69	r	0.60	0/1565	0.73	0/2106
70	t	0.70	0/1530	0.87	0/2066
71	v	0.66	0/1092	0.74	0/1468
72	p	0.65	0/6116	0.69	0/8311
73	w	0.57	0/11056	0.60	0/15023
74	x	0.58	0/7191	0.64	0/9728
75	y	0.57	0/1645	0.64	0/2240
76	NC	0.80	0/505	0.86	0/700
76	NG	0.68	0/523	0.90	1/724 (0.1%)
77	ND	0.76	0/470	0.83	0/654
77	NH	0.65	0/470	0.85	0/654
All	All	0.45	9/190578 (0.0%)	0.60	38/259940 (0.0%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	q	452	ALA	C-N	5.60	1.47	1.34
1	X	3	DG	O3'-P	5.58	1.67	1.61
1	X	17	DC	O3'-P	5.55	1.67	1.61
1	X	19	DA	O3'-P	5.46	1.67	1.61
1	X	-33	DC	O3'-P	5.28	1.67	1.61

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	g	128	PRO	N-CA-C	-7.63	92.27	112.10
50	g	128	PRO	CA-N-CD	-7.39	101.15	111.50
52	n	1351	PRO	N-CA-CB	7.36	112.14	103.30
52	n	1343	PRO	N-CA-CB	7.25	112.01	103.30
52	n	1355	PRO	N-CA-CB	6.89	111.57	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
5	BA	248/316 (78%)	246 (99%)	2 (1%)	0	100	100
6	DA	542/1872 (29%)	524 (97%)	15 (3%)	3 (1%)	22	59
7	EA	185/439 (42%)	183 (99%)	1 (0%)	1 (0%)	25	62
8	FA	134/517 (26%)	129 (96%)	5 (4%)	0	100	100
9	HA	710/760 (93%)	682 (96%)	28 (4%)	0	100	100
10	NA	98/136 (72%)	94 (96%)	2 (2%)	2 (2%)	6	34
10	NE	101/136 (74%)	96 (95%)	3 (3%)	2 (2%)	6	34
11	PA	1457/1970 (74%)	1406 (96%)	47 (3%)	4 (0%)	37	72
12	DB	959/1199 (80%)	910 (95%)	49 (5%)	0	100	100
13	EB	169/291 (58%)	164 (97%)	5 (3%)	0	100	100
14	FB	218/249 (88%)	213 (98%)	4 (2%)	1 (0%)	25	62
15	HB	253/548 (46%)	245 (97%)	8 (3%)	0	100	100
16	NB	78/103 (76%)	78 (100%)	0	0	100	100
16	NF	84/103 (82%)	77 (92%)	4 (5%)	3 (4%)	3	23
17	PB	1130/1174 (96%)	1093 (97%)	37 (3%)	0	100	100
18	HC	380/462 (82%)	363 (96%)	17 (4%)	0	100	100
19	DO	97/109 (89%)	95 (98%)	2 (2%)	0	100	100
20	DP	177/339 (52%)	175 (99%)	2 (1%)	0	100	100
21	DQ	109/376 (29%)	102 (94%)	7 (6%)	0	100	100
22	PC	253/275 (92%)	241 (95%)	12 (5%)	0	100	100
23	PE	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
24	PF	77/127 (61%)	76 (99%)	1 (1%)	0	100	100
25	PH	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
26	PI	112/125 (90%)	104 (93%)	8 (7%)	0	100	100
27	PJ	62/67 (92%)	60 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	PK	113/117 (97%)	112 (99%)	1 (1%)	0	100	100
29	PL	42/58 (72%)	40 (95%)	2 (5%)	0	100	100
30	HD	304/309 (98%)	265 (87%)	29 (10%)	10 (3%)	3	25
31	HG	341/395 (86%)	329 (96%)	12 (4%)	0	100	100
32	HE	259/308 (84%)	253 (98%)	6 (2%)	0	100	100
33	HF	64/71 (90%)	62 (97%)	2 (3%)	0	100	100
34	HH	601/782 (77%)	573 (95%)	27 (4%)	1 (0%)	44	77
35	DD	153/1085 (14%)	146 (95%)	5 (3%)	2 (1%)	10	43
35	Dd	154/1085 (14%)	150 (97%)	4 (3%)	0	100	100
36	DE	540/800 (68%)	506 (94%)	32 (6%)	2 (0%)	30	67
36	De	531/800 (66%)	484 (91%)	47 (9%)	0	100	100
37	DF	404/677 (60%)	377 (93%)	20 (5%)	7 (2%)	7	37
37	Df	399/677 (59%)	378 (95%)	20 (5%)	1 (0%)	37	72
38	DG	139/349 (40%)	135 (97%)	4 (3%)	0	100	100
39	DH	207/310 (67%)	191 (92%)	12 (6%)	4 (2%)	6	35
40	DI	118/264 (45%)	113 (96%)	4 (3%)	1 (1%)	16	54
40	Di	119/264 (45%)	115 (97%)	4 (3%)	0	100	100
41	DL	72/161 (45%)	62 (86%)	6 (8%)	4 (6%)	1	17
41	Dl	105/161 (65%)	101 (96%)	4 (4%)	0	100	100
42	Dc	125/929 (14%)	116 (93%)	9 (7%)	0	100	100
43	DJ	86/218 (39%)	82 (95%)	4 (5%)	0	100	100
43	Dj	91/218 (42%)	89 (98%)	2 (2%)	0	100	100
44	Dk	96/211 (46%)	91 (95%)	5 (5%)	0	100	100
45	Dm	85/124 (68%)	79 (93%)	6 (7%)	0	100	100
46	HI	297/346 (86%)	265 (89%)	20 (7%)	12 (4%)	2	21
47	HJ	285/323 (88%)	268 (94%)	14 (5%)	3 (1%)	12	46
48	PD	126/142 (89%)	122 (97%)	4 (3%)	0	100	100
49	PG	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
50	g	104/233 (45%)	99 (95%)	4 (4%)	1 (1%)	13	48
51	j	120/135 (89%)	117 (98%)	1 (1%)	2 (2%)	7	37
52	n	993/1454 (68%)	894 (90%)	80 (8%)	19 (2%)	6	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	s	91/244 (37%)	81 (89%)	8 (9%)	2 (2%)	5	32
54	u	113/144 (78%)	104 (92%)	5 (4%)	4 (4%)	3	24
55	a	430/1581 (27%)	387 (90%)	38 (9%)	5 (1%)	11	44
56	d	154/270 (57%)	143 (93%)	9 (6%)	2 (1%)	10	43
57	f	163/246 (66%)	150 (92%)	12 (7%)	1 (1%)	22	59
58	i	69/146 (47%)	65 (94%)	2 (3%)	2 (3%)	3	27
59	m	110/131 (84%)	106 (96%)	4 (4%)	0	100	100
60	q	543/651 (83%)	486 (90%)	50 (9%)	7 (1%)	10	43
61	z	93/600 (16%)	83 (89%)	7 (8%)	3 (3%)	3	25
62	b	111/200 (56%)	109 (98%)	1 (1%)	1 (1%)	14	50
63	c	255/311 (82%)	239 (94%)	15 (6%)	1 (0%)	30	67
64	e	98/178 (55%)	92 (94%)	4 (4%)	2 (2%)	6	34
65	l	120/178 (67%)	115 (96%)	5 (4%)	0	100	100
66	o	152/788 (19%)	135 (89%)	13 (9%)	4 (3%)	4	29
67	h	188/268 (70%)	165 (88%)	15 (8%)	8 (4%)	2	21
68	k	110/117 (94%)	96 (87%)	12 (11%)	2 (2%)	7	36
69	r	190/208 (91%)	180 (95%)	6 (3%)	4 (2%)	5	33
70	t	189/212 (89%)	169 (89%)	16 (8%)	4 (2%)	5	33
71	v	132/200 (66%)	116 (88%)	10 (8%)	6 (4%)	2	20
72	p	756/841 (90%)	707 (94%)	47 (6%)	2 (0%)	37	72
73	w	1332/1368 (97%)	1262 (95%)	66 (5%)	4 (0%)	37	72
74	x	877/989 (89%)	828 (94%)	44 (5%)	5 (1%)	22	59
75	y	206/747 (28%)	196 (95%)	9 (4%)	1 (0%)	25	62
76	NC	101/128 (79%)	93 (92%)	5 (5%)	3 (3%)	3	26
76	NG	105/128 (82%)	94 (90%)	8 (8%)	3 (3%)	3	27
77	ND	93/126 (74%)	91 (98%)	1 (1%)	1 (1%)	12	46
77	NH	93/126 (74%)	89 (96%)	3 (3%)	1 (1%)	12	46
All	All	22102/36357 (61%)	20863 (94%)	1076 (5%)	163 (1%)	21	56

5 of 163 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	DA	498	PRO

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Mol	Chain	Res	Type
6	DA	1158	SER
10	NA	534	ARG
11	PA	1666	PRO
14	FB	229	HIS

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	
5	BA	215/268 (80%)	215 (100%)	0	100	100
6	DA	495/1665 (30%)	460 (93%)	35 (7%)	12	35
7	EA	169/373 (45%)	167 (99%)	2 (1%)	67	78
8	FA	121/448 (27%)	119 (98%)	2 (2%)	56	72
9	HA	624/664 (94%)	622 (100%)	2 (0%)	91	92
11	PA	1302/1749 (74%)	1294 (99%)	8 (1%)	84	88
12	DB	876/1083 (81%)	859 (98%)	17 (2%)	52	69
13	EB	154/261 (59%)	153 (99%)	1 (1%)	84	88
14	FB	196/218 (90%)	195 (100%)	1 (0%)	86	90
15	HB	241/484 (50%)	241 (100%)	0	100	100
17	PB	994/1027 (97%)	992 (100%)	2 (0%)	92	94
18	HC	342/399 (86%)	340 (99%)	2 (1%)	84	88
19	DO	90/98 (92%)	88 (98%)	2 (2%)	47	65
20	DP	154/293 (53%)	154 (100%)	0	100	100
21	DQ	105/324 (32%)	105 (100%)	0	100	100
22	PC	234/252 (93%)	234 (100%)	0	100	100
23	PE	191/192 (100%)	191 (100%)	0	100	100
24	PF	69/111 (62%)	68 (99%)	1 (1%)	62	75
25	PH	129/131 (98%)	129 (100%)	0	100	100
26	PI	103/112 (92%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	PJ	53/56 (95%)	53 (100%)	0	100	100
28	PK	104/106 (98%)	102 (98%)	2 (2%)	52	69
29	PL	41/55 (74%)	41 (100%)	0	100	100
30	HD	251/283 (89%)	223 (89%)	28 (11%)	5	20
31	HG	311/352 (88%)	310 (100%)	1 (0%)	91	92
32	HE	234/272 (86%)	230 (98%)	4 (2%)	56	72
33	HF	59/64 (92%)	59 (100%)	0	100	100
34	HH	536/688 (78%)	531 (99%)	5 (1%)	75	83
35	DD	144/815 (18%)	135 (94%)	9 (6%)	15	38
35	Dd	146/815 (18%)	146 (100%)	0	100	100
36	DE	478/657 (73%)	465 (97%)	13 (3%)	40	60
36	De	475/657 (72%)	473 (100%)	2 (0%)	89	91
37	DF	324/574 (56%)	296 (91%)	28 (9%)	8	29
37	Df	322/574 (56%)	314 (98%)	8 (2%)	42	62
38	DG	133/322 (41%)	125 (94%)	8 (6%)	16	40
39	DH	181/270 (67%)	172 (95%)	9 (5%)	20	44
40	DI	106/235 (45%)	97 (92%)	9 (8%)	8	30
40	Di	107/235 (46%)	106 (99%)	1 (1%)	75	83
41	DL	69/141 (49%)	60 (87%)	9 (13%)	3	17
41	DI	98/141 (70%)	98 (100%)	0	100	100
42	Dc	113/833 (14%)	111 (98%)	2 (2%)	54	71
43	DJ	79/154 (51%)	78 (99%)	1 (1%)	65	76
43	Dj	83/154 (54%)	83 (100%)	0	100	100
44	Dk	87/182 (48%)	87 (100%)	0	100	100
45	Dm	80/106 (76%)	79 (99%)	1 (1%)	65	76
46	HI	258/298 (87%)	190 (74%)	68 (26%)	0	3
47	HJ	252/296 (85%)	177 (70%)	75 (30%)	0	2
48	PD	118/126 (94%)	116 (98%)	2 (2%)	56	72
49	PG	152/153 (99%)	150 (99%)	2 (1%)	65	76
50	g	102/216 (47%)	93 (91%)	9 (9%)	8	28
51	j	66/124 (53%)	65 (98%)	1 (2%)	60	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	n	807/1271 (64%)	784 (97%)	23 (3%)	37	58
53	s	83/208 (40%)	73 (88%)	10 (12%)	4	18
54	u	95/119 (80%)	92 (97%)	3 (3%)	34	55
55	a	393/1391 (28%)	318 (81%)	75 (19%)	1	8
56	d	139/230 (60%)	95 (68%)	44 (32%)	0	2
57	f	149/223 (67%)	132 (89%)	17 (11%)	4	19
58	i	71/133 (53%)	60 (84%)	11 (16%)	2	13
59	m	102/115 (89%)	101 (99%)	1 (1%)	73	81
60	q	491/577 (85%)	414 (84%)	77 (16%)	2	13
61	z	89/512 (17%)	76 (85%)	13 (15%)	2	14
62	b	102/163 (63%)	91 (89%)	11 (11%)	5	21
63	c	238/280 (85%)	223 (94%)	15 (6%)	15	38
64	e	94/152 (62%)	94 (100%)	0	100	100
65	l	116/155 (75%)	116 (100%)	0	100	100
66	o	141/697 (20%)	138 (98%)	3 (2%)	48	66
67	h	161/225 (72%)	128 (80%)	33 (20%)	1	6
68	k	94/98 (96%)	49 (52%)	45 (48%)	0	0
69	r	169/183 (92%)	142 (84%)	27 (16%)	2	12
70	t	166/178 (93%)	128 (77%)	38 (23%)	0	4
71	v	122/173 (70%)	87 (71%)	35 (29%)	0	2
72	p	681/736 (92%)	670 (98%)	11 (2%)	58	73
73	w	1203/1232 (98%)	1200 (100%)	3 (0%)	92	94
74	x	789/864 (91%)	777 (98%)	12 (2%)	60	74
75	y	175/601 (29%)	172 (98%)	3 (2%)	56	72
All	All	19036/30622 (62%)	18154 (95%)	882 (5%)	25	47

5 of 882 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
55	a	373	CYS
60	q	109	MET
74	x	897	LEU
70	t	84	CYS
55	a	441	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 254 such sidechains are listed below:

Mol	Chain	Res	Type
54	u	86	GLN
72	p	751	GLN
58	i	117	GLN
72	p	598	ASN
73	w	1134	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 20 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	$\# Z > 2$
79	SF4	HA	1000	9	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
79	SF4	HA	1000	9	-	-	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.

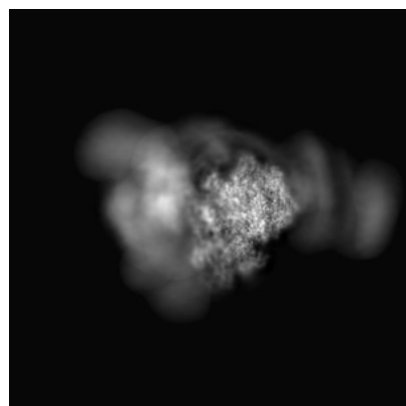
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34360. These allow visual inspection of the internal detail of the map and identification of artifacts.

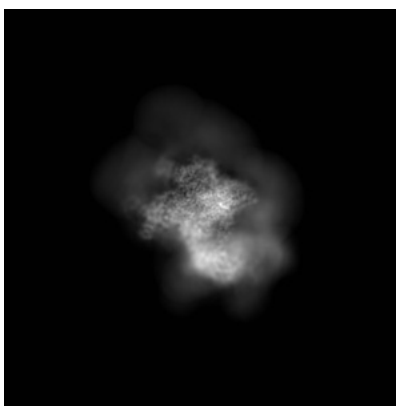
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

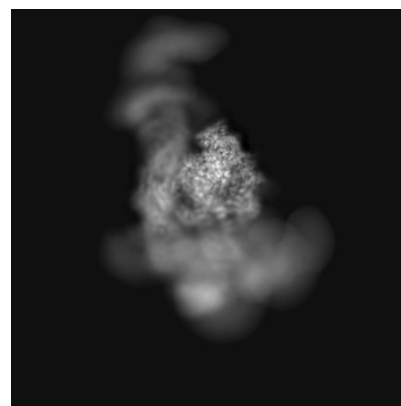
6.1.1 Primary map



X

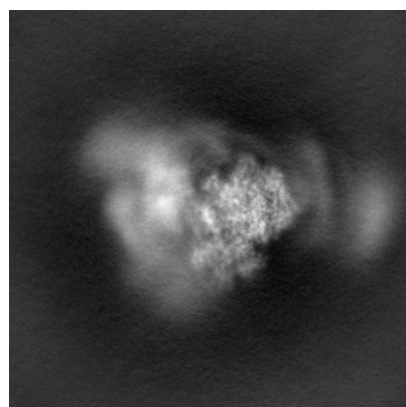


Y

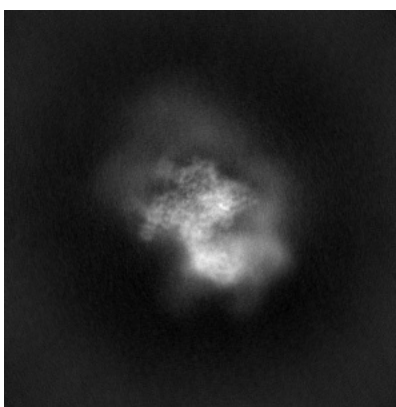


Z

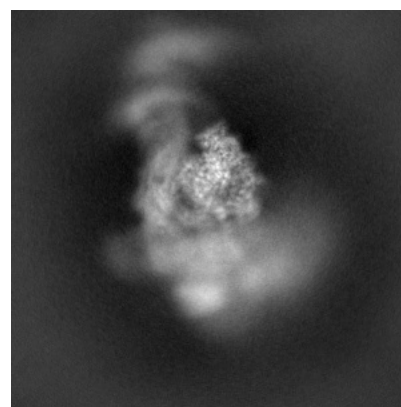
6.1.2 Raw map



X



Y

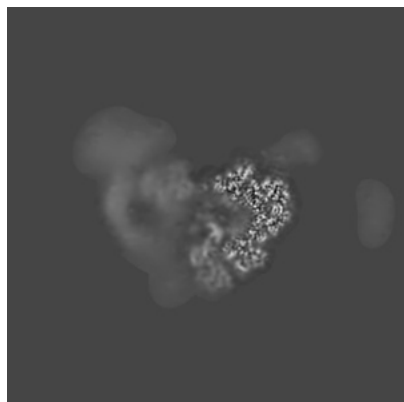


Z

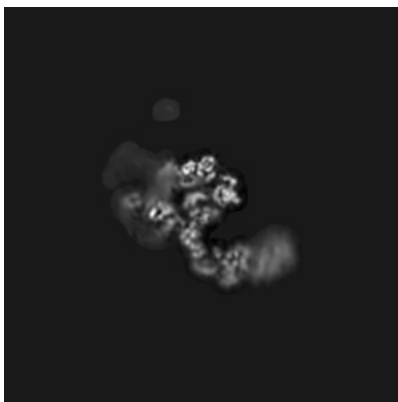
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

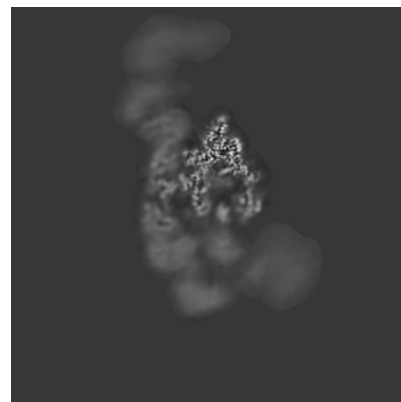
6.2.1 Primary map



X Index: 210

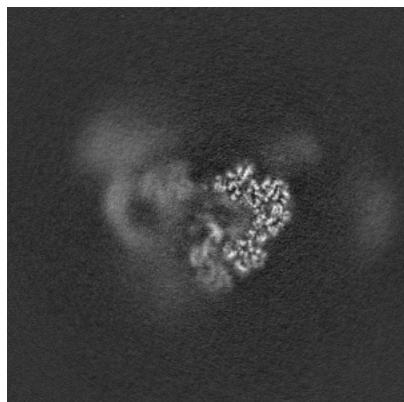


Y Index: 210

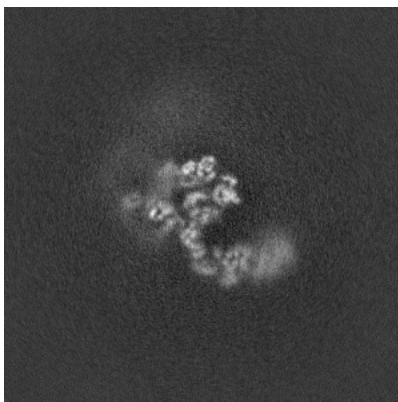


Z Index: 210

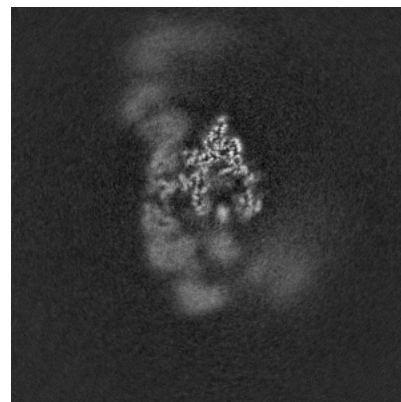
6.2.2 Raw map



X Index: 210



Y Index: 210

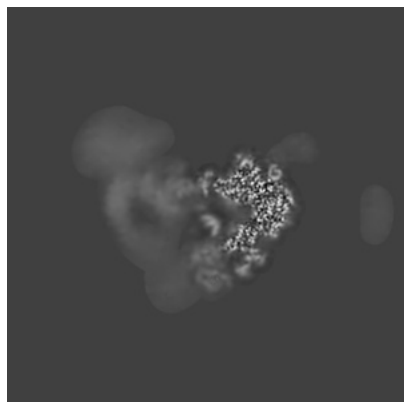


Z Index: 210

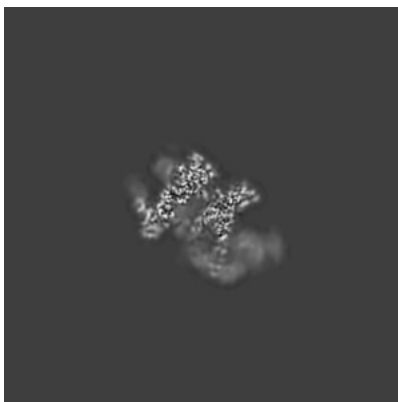
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

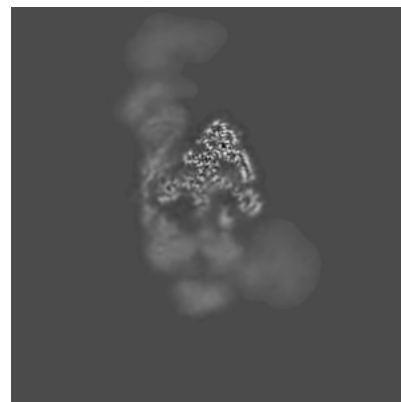
6.3.1 Primary map



X Index: 215

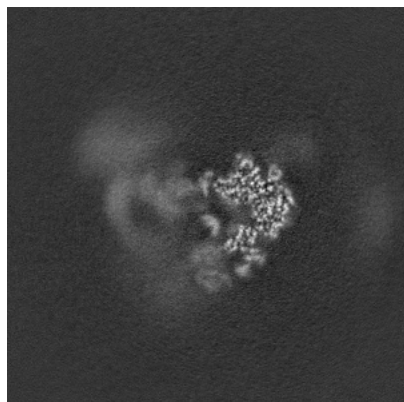


Y Index: 246

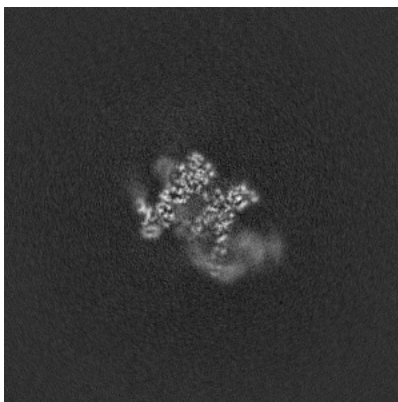


Z Index: 217

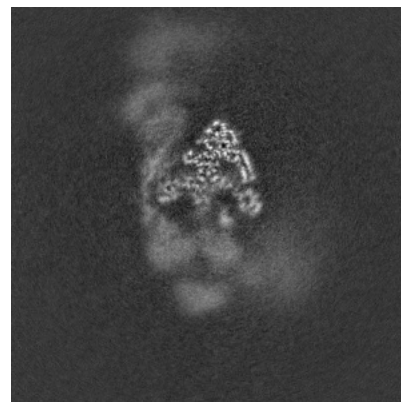
6.3.2 Raw map



X Index: 215



Y Index: 245

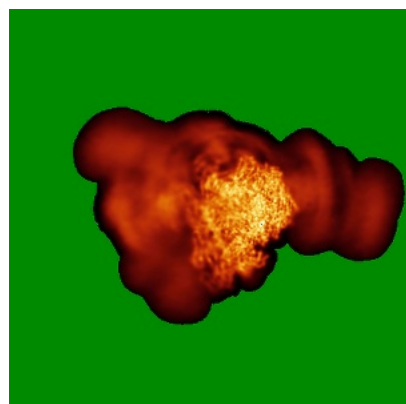


Z Index: 217

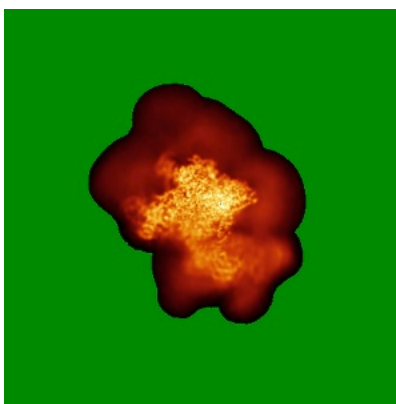
The images above show the largest variance slices of the map in three orthogonal directions.

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

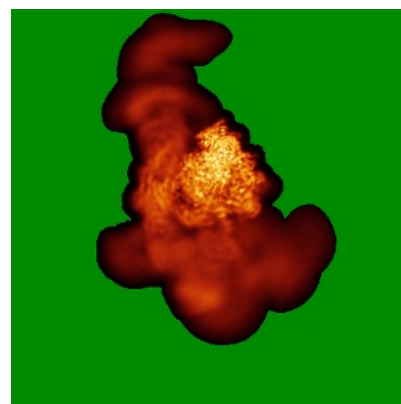
6.4.1 Primary map



X

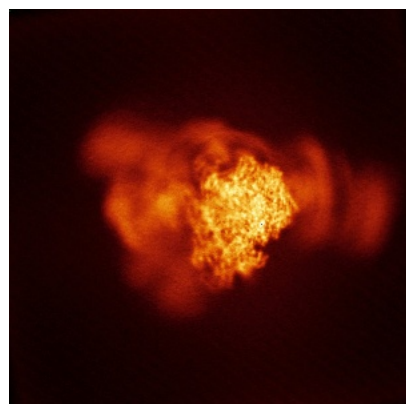


Y

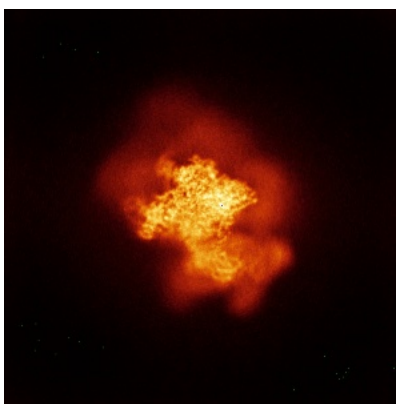


Z

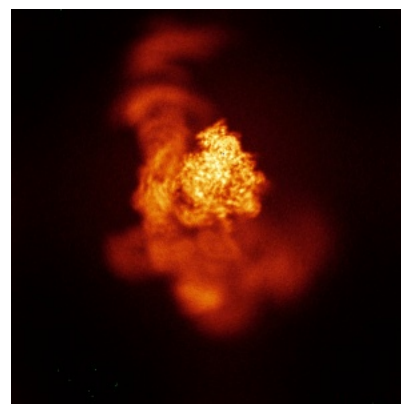
6.4.2 Raw map



X



Y

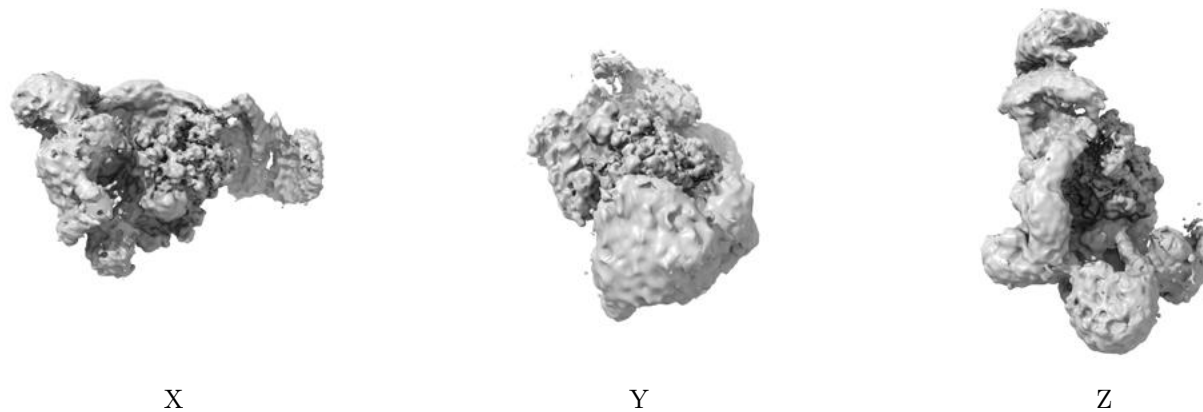


Z

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.

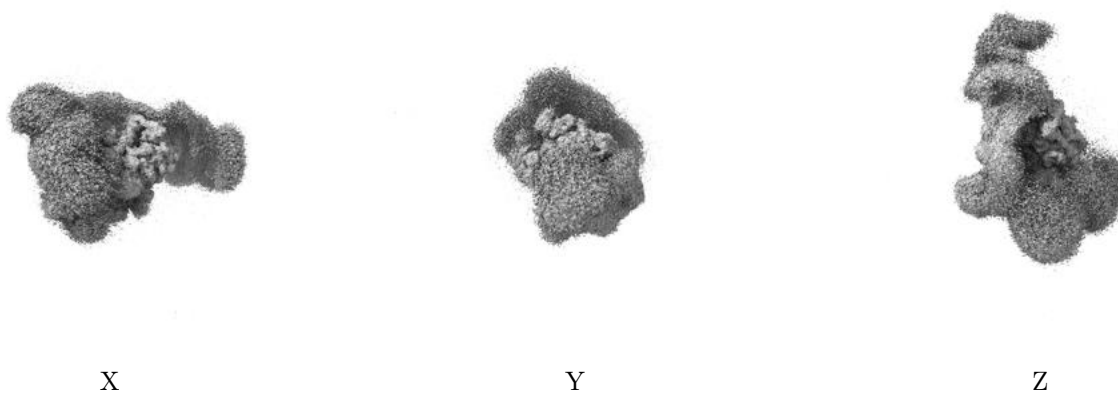
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.205. 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.

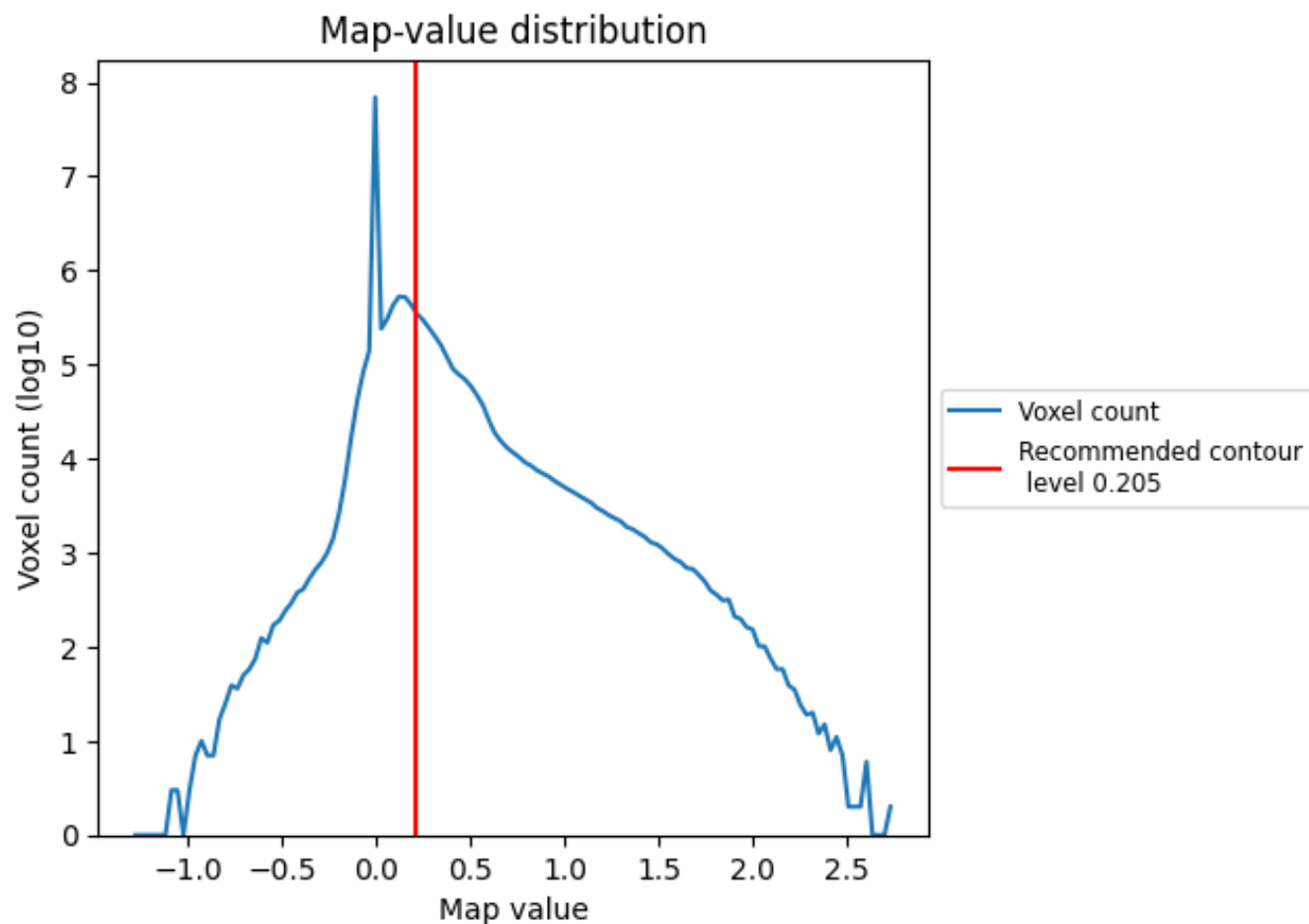
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

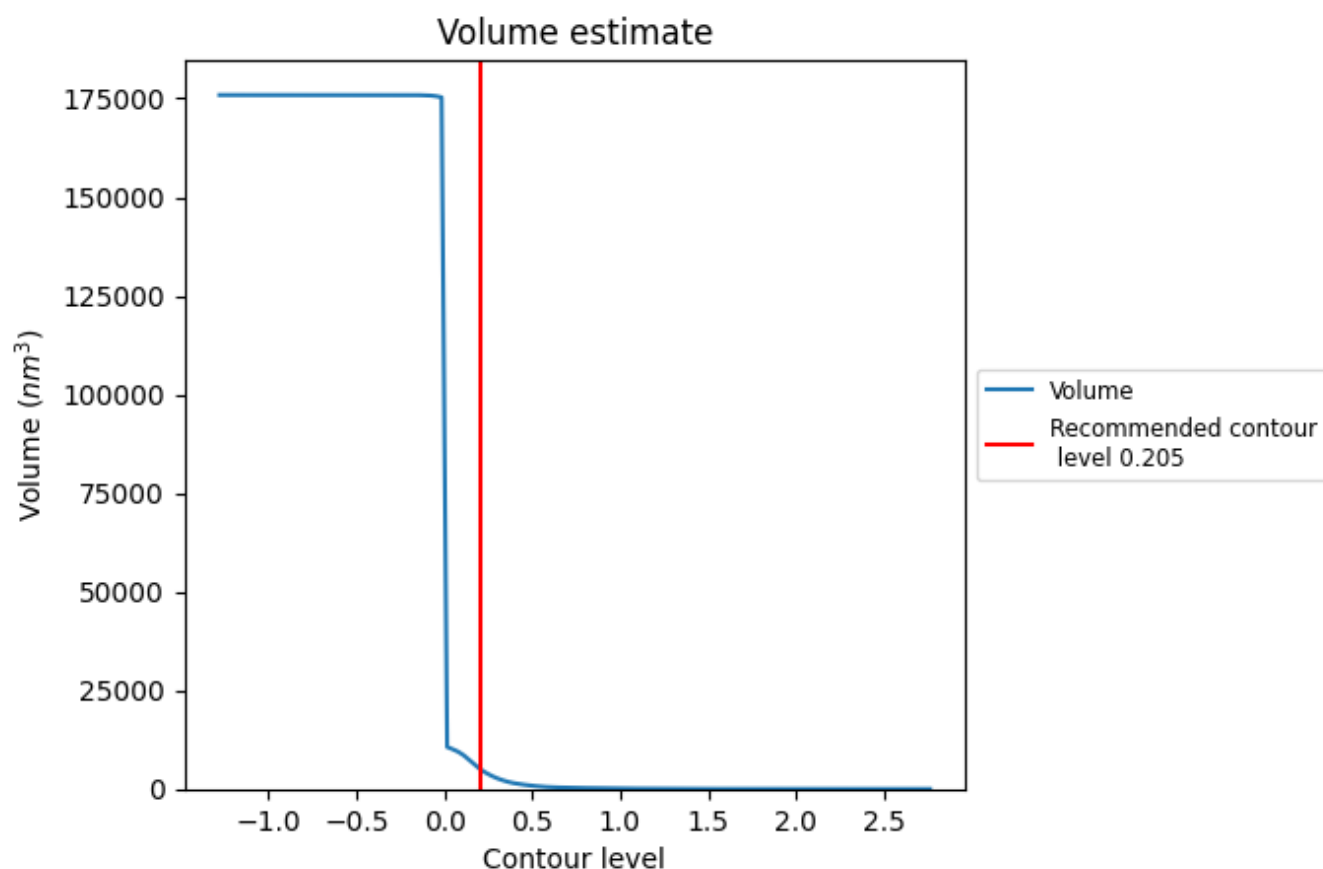
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

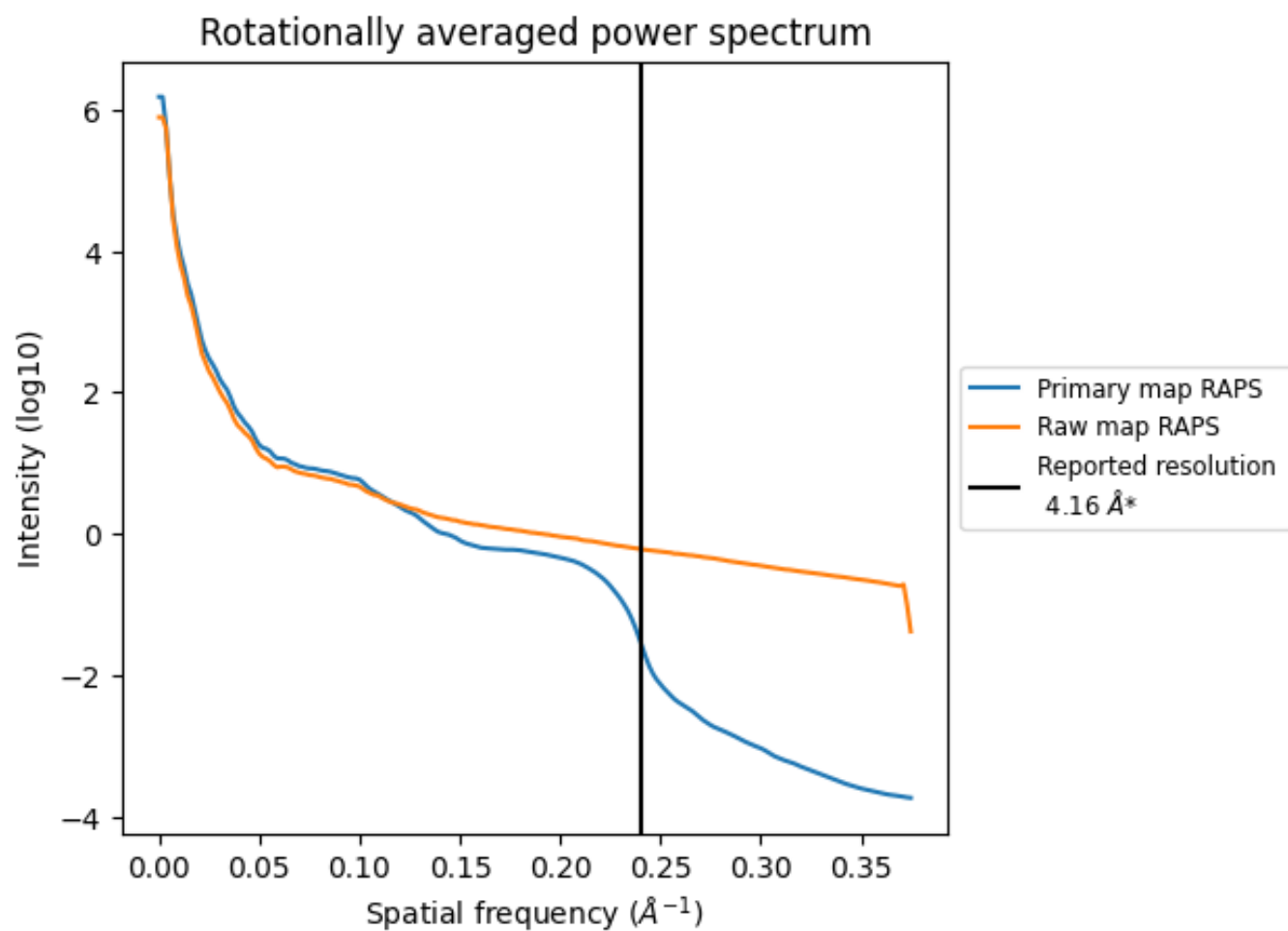
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4986 nm^3 ; this corresponds to an approximate mass of 4504 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 ⓘ

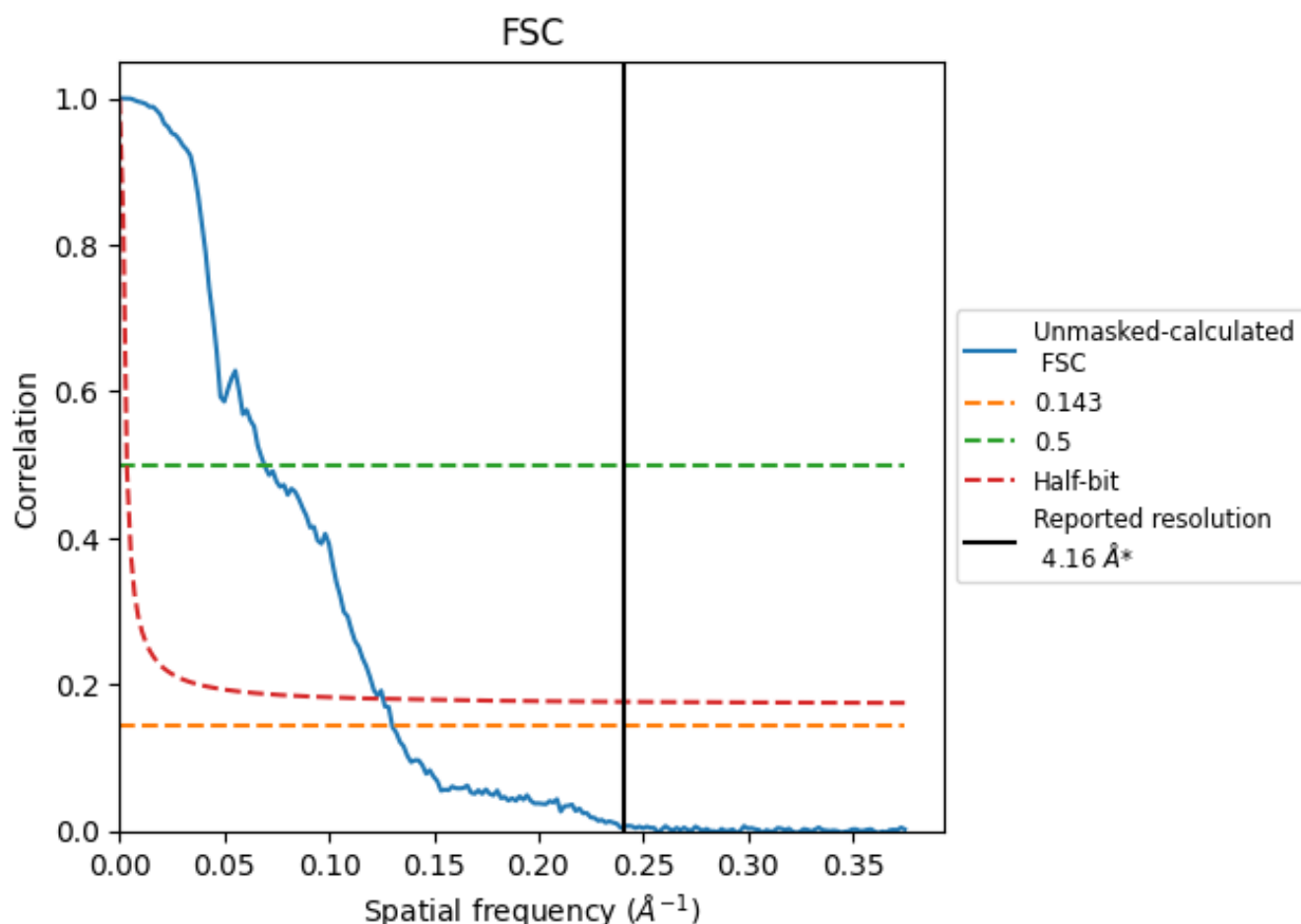


*Reported resolution corresponds to spatial frequency of 0.240 Å⁻¹

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 0.240 Å⁻¹

8.2 Resolution estimates [i](#)

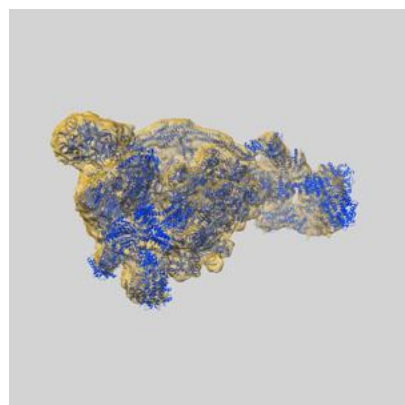
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.16	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.68	14.47	7.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.68 differs from the reported value 4.16 by more than 10 %

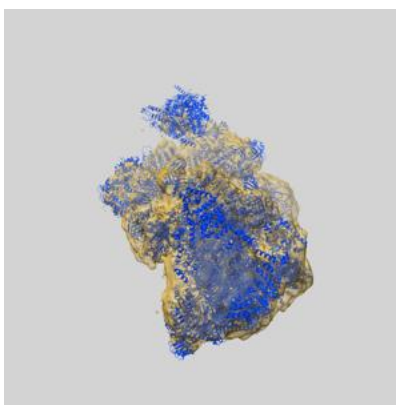
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34360 and PDB model 8GXS. Per-residue inclusion information can be found in section 3 on page 20.

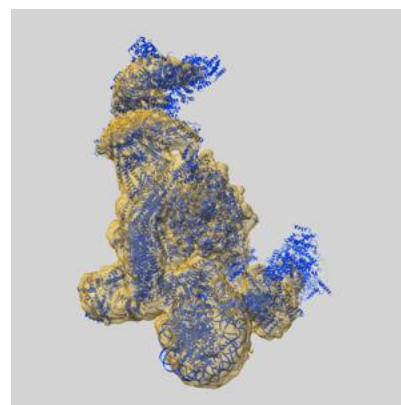
9.1 Map-model overlay [i](#)



X



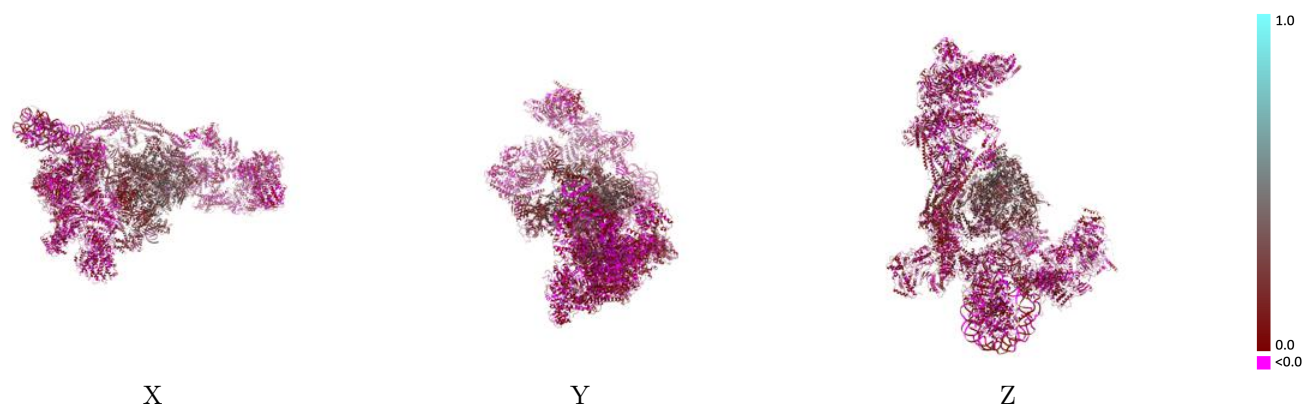
Y



Z

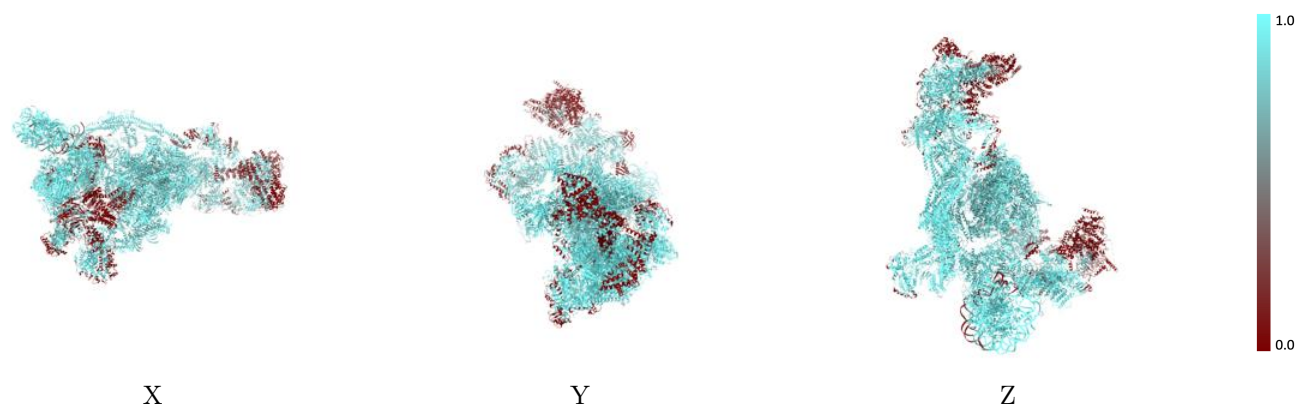
The images above show the 3D surface view of the map at the recommended contour level 0.205 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



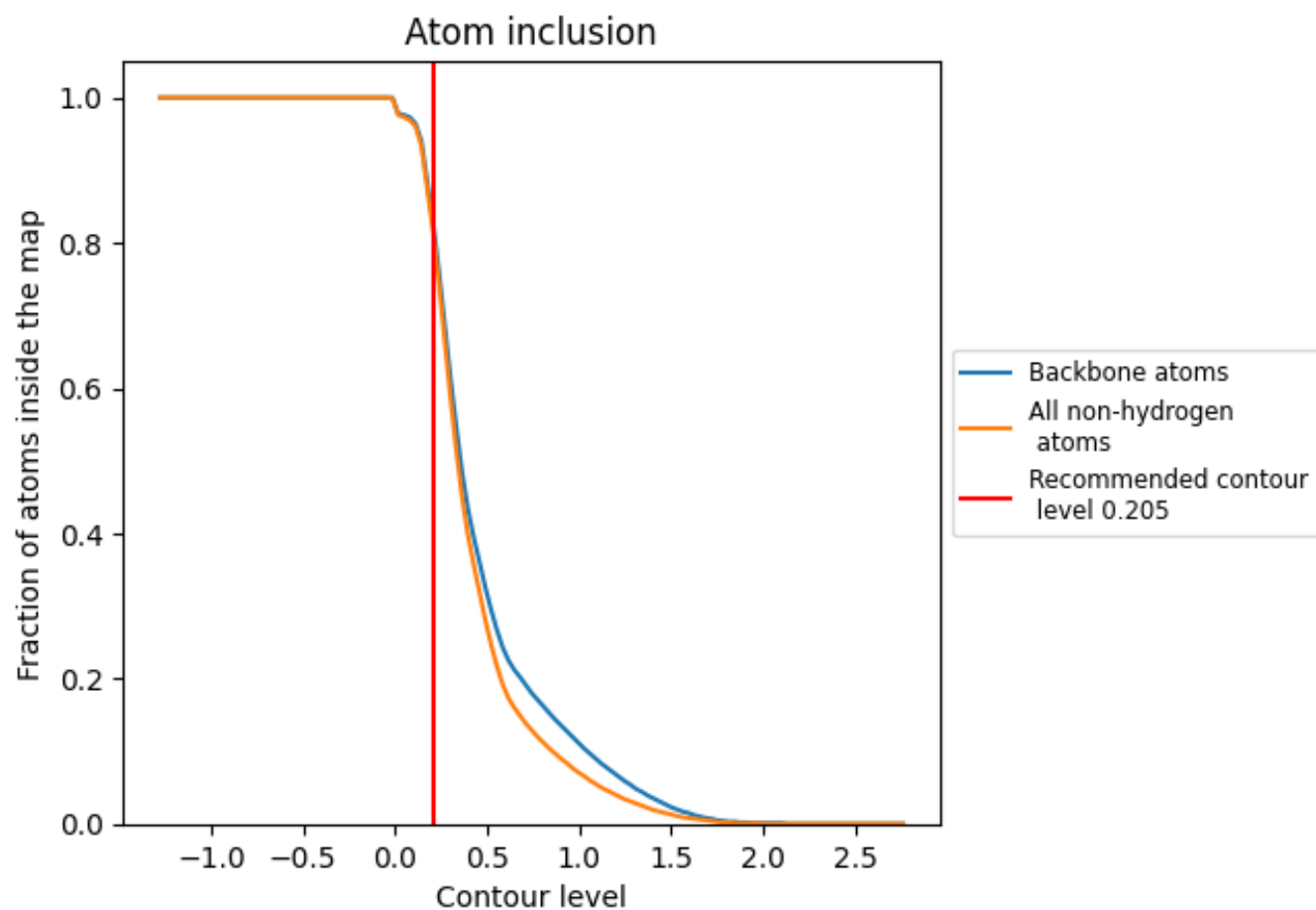
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.205).







































































9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.205) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8180	 0.0930
BA	 0.9700	 0.2280
DA	 0.7100	 0.0220
DB	 0.9430	 0.0400
DD	 0.6540	 0.0380
DE	 0.8400	 0.0360
DF	 0.7870	 0.0420
DG	 0.3760	 0.0250
DH	 0.9100	 0.0420
DI	 0.7220	 0.0330
DJ	 0.8810	 0.0270
DL	 0.3730	 0.0400
DO	 0.9520	 0.1340
DP	 0.9860	 0.1680
DQ	 0.9410	 0.1180
Dc	 0.0650	 0.0310
Dd	 0.0020	 0.0010
De	 0.1900	 0.0150
Df	 0.5500	 0.0330
Di	 0.0590	 0.0290
Dj	 0.0170	 0.0500
Dk	 0.0000	 -0.0140
DI	 0.0000	 -0.0070
Dm	 0.0000	 -0.0090
EA	 0.9340	 0.1170
EB	 0.9760	 0.1150
FA	 0.9710	 0.1500
FB	 0.9780	 0.1680
HA	 0.9890	 0.0880
HB	 0.9870	 0.0480
HC	 0.9830	 0.0680
HD	 0.9190	 0.1020
HE	 0.9820	 0.0530
HF	 1.0000	 0.0510
HG	 0.9890	 0.0560

























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Chain	Atom inclusion	Q-score
HH	 0.9900	 0.0720
HI	 0.9670	 0.0600
HJ	 0.8510	 0.0620
NA	 0.9420	 0.0310
NB	 1.0000	 0.0490
NC	 1.0000	 0.0050
ND	 1.0000	 0.0090
NE	 0.9770	 0.0330
NF	 0.9720	 0.0480
NG	 0.9850	 0.0410
NH	 0.9640	 0.0380
NX	 0.8070	 0.0300
NY	 0.7950	 0.0250
PA	 0.9580	 0.2510
PB	 0.9670	 0.3080
PC	 0.9740	 0.3060
PD	 0.9710	 0.1790
PE	 0.9610	 0.2250
PF	 0.9290	 0.2910
PG	 0.9770	 0.1770
PH	 0.9740	 0.2790
PI	 0.9770	 0.2320
PJ	 0.9720	 0.3180
PK	 0.9570	 0.3000
PL	 0.9640	 0.3100
X	 0.9990	 0.1960
Y	 0.9970	 0.2010
a	 0.6860	 0.0430
b	 0.8340	 0.0330
c	 0.9130	 0.0440
d	 0.8600	 0.0710
e	 0.9870	 0.0840
f	 0.9930	 0.1270
g	 1.0000	 0.0910
h	 0.9850	 0.1250
i	 0.6570	 0.0630
j	 0.9780	 0.0830
k	 0.9760	 0.1280
l	 0.9910	 0.0600
m	 1.0000	 0.0720
n	 0.9280	 0.0510
o	 0.8830	 0.0320

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Chain	Atom inclusion	Q-score
p	 0.8590	 0.0390
q	 0.9980	 0.0750
r	 0.9910	 0.0850
s	 0.9920	 0.0460
t	 0.9650	 0.0660
u	 1.0000	 0.0740
v	 0.9850	 0.1190
w	 0.3200	 0.0150
x	 0.6380	 0.0290
y	 0.8770	 0.0350
z	 0.9320	 0.0350