



Full wwPDB EM Validation Report ⓘ

Oct 26, 2022 – 01:30 PM JST

PDB ID : 8GXQ
EMDB ID : EMD-34359
Title : PIC-Mediator in complex with +1 nucleosome (T40N) in MH-binding state
Authors : Chen, X.; Wang, X.; Liu, W.; Ren, Y.; Qu, X.; Li, J.; Yin, X.; Xu, Y.
Deposited on : 2022-09-21
Resolution : 5.04 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:

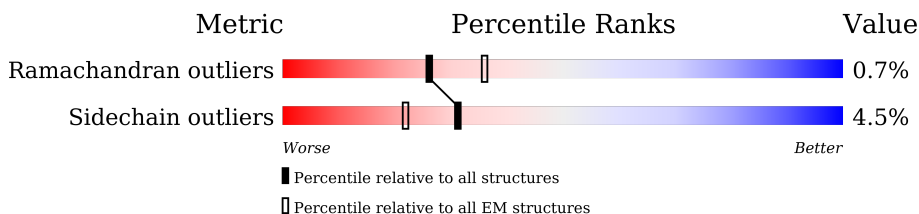
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 5.04 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.










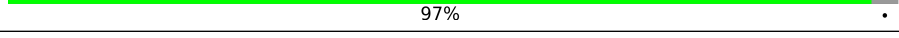
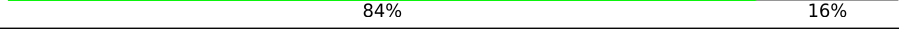
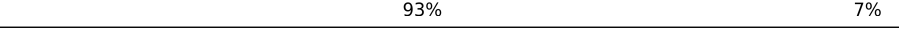
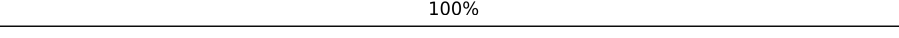
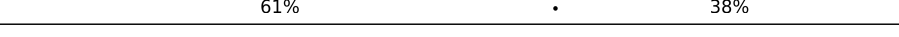
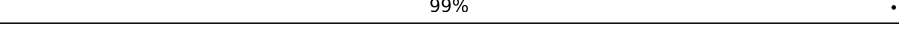
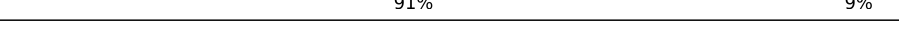
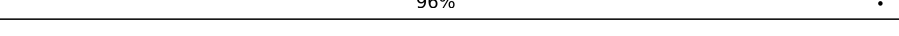
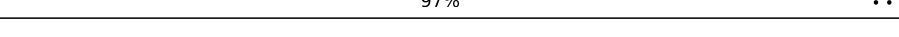
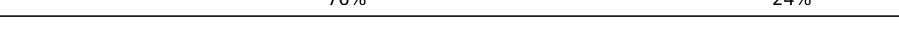

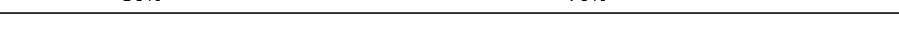






Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	
2	Y	228	
3	BA	316	
4	DA	1872	
5	EA	439	
6	FA	517	
7	HA	760	
8	NA	136	
8	NE	136	




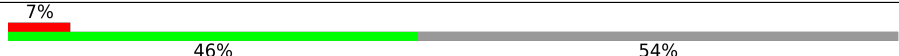
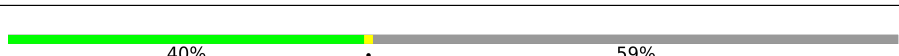
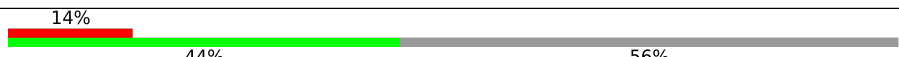
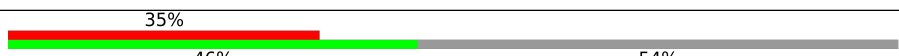

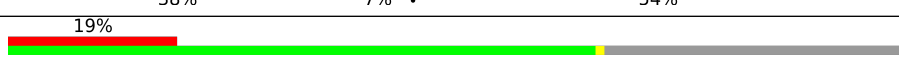


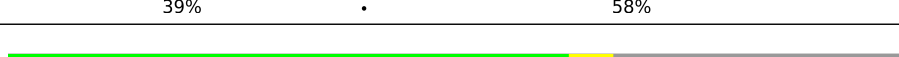

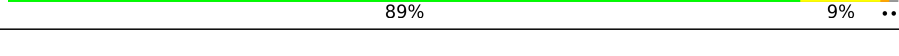
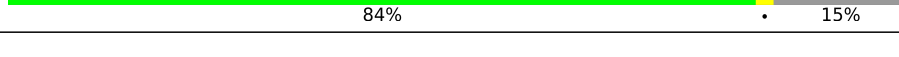


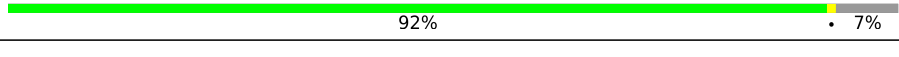

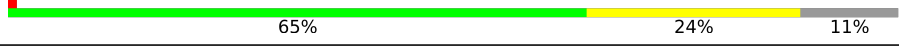
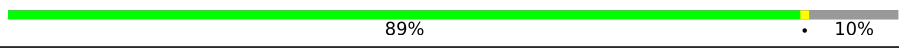
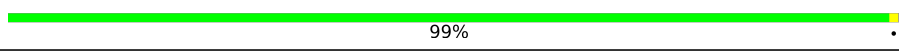



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Mol	Chain	Length	Quality of chain
9	PA	1970	 74% 25%
10	DB	1199	 79% 20%
11	EB	291	 58% 41%
12	FB	249	 88% 11%
13	HB	548	 48% 52%
14	NB	103	 78% 22%
14	NF	103	 81% 17%
15	PB	1174	 97%
16	HC	462	 84% 16%
17	PC	275	 93% 7%
18	PE	210	 100%
19	PF	127	 61% 38%
20	PH	150	 99%
21	PI	125	 91% 9%
22	PJ	67	 96%
23	PK	117	 97%
24	PL	58	 76% 24%
25	DP	339	 53% 47%
26	DQ	376	 30% 70%
27	DO	109	 89% 9%
28	Dc	929	 5% 13% 86%
29	DD	1085	 14% 85%
29	Dd	1085	 9% 15% 85%
30	DE	800	 66% 32%
30	De	800	 21% 67% 33%



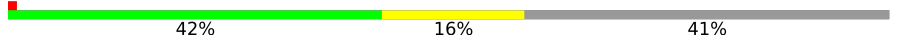







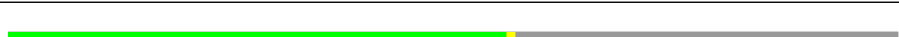


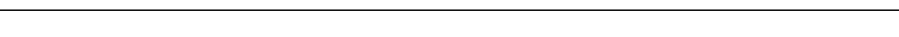
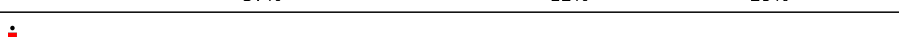
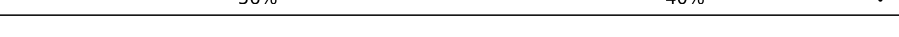



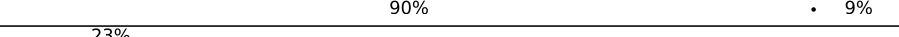
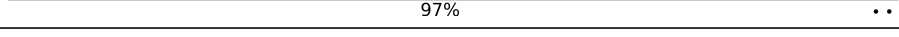




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Mol	Chain	Length	Quality of chain
31	DF	677	
31	Df	677	
32	DI	264	
32	Di	264	
33	DJ	218	
33	Dj	218	
34	Dk	211	
35	DL	161	
35	Dl	161	
36	Dm	124	
37	DG	349	
38	DH	310	
39	HD	309	
40	HE	308	
41	HG	395	
42	HH	782	
43	HF	71	
44	HI	346	
45	HJ	323	
46	PD	142	
47	PG	172	
48	g	233	
49	j	135	
50	n	1454	
51	s	244	


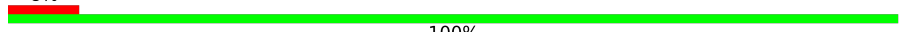
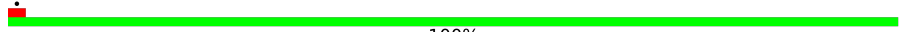
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Mol	Chain	Length	Quality of chain
52	u	144	 76% 19%
53	a	1581	 23% 5% 72%
54	d	270	 42% 16% 41%
55	f	246	 59% 8% 32%
56	i	146	 5% 40% 10% 50%
57	m	131	 85% 15%
58	q	651	 73% 12% 15%
59	z	600	 14% 84%
60	b	200	 52% 6% 42%
61	c	311	 80% 15%
62	e	178	 56% 43%
63	l	178	 71% 29%
64	o	788	 19% 80%
65	h	268	 57% 12% 29%
66	k	117	 56% 40% 4%
67	r	208	 78% 13% 8%
68	t	212	 72% 19% 9%
69	v	200	 48% 18% 33%
70	p	841	 90% 9%
71	w	1368	 23% 97%
72	x	989	 89% 9%
73	y	747	 28% 72%
74	NC	128	 78% 20%
74	NG	128	 80% 16%
75	ND	126	 75% 25%

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Mol	Chain	Length	Quality of chain
75	NH	126	 75% 25%
76	NX	162	 8% 100%
77	NY	162	 100%

2 Entry composition [i](#)

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
			Total	C	N	O	P		
1	X	67	1387	652	275	394	66	0	0

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

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

- Molecule 3 is a protein called Transcription initiation factor IIB.

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

- Molecule 4 is a protein called Transcription initiation factor TFIID subunit 1.

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

- Molecule 5 is a protein called General transcription factor IIE subunit 1.

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

- Molecule 6 is a protein called General transcription factor IIF subunit 1.

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

- Molecule 7 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPD.

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

- Molecule 8 is a protein called Histone H3.

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

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

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

- Molecule 10 is a protein called Transcription initiation factor TFIID subunit 2.

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

- Molecule 11 is a protein called Transcription initiation factor IIE subunit beta.

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

- Molecule 12 is a protein called General transcription factor IIF subunit 2.

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

- Molecule 13 is a protein called General transcription factor IIIH subunit 1.

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

- Molecule 14 is a protein called Histone H4.

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

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

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

- Molecule 16 is a protein called General transcription factor IIH subunit 4.

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

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 18 is a protein called DNA-directed RNA polymerase II subunit E.

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

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

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

- Molecule 20 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 21 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 22 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 23 is a protein called RNA_pol_L_2 domain-containing protein.

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

- Molecule 24 is a protein called RPB12.

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

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

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

- Molecule 26 is a protein called Transcription initiation factor IIA subunit 1.

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

- Molecule 27 is a protein called Transcription initiation factor IIA subunit 2.

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

- Molecule 28 is a protein called Transcription initiation factor TFIID subunit 3.

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

- Molecule 29 is a protein called Transcription initiation factor TFIID subunit 4.

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

- Molecule 30 is a protein called Transcription initiation factor TFIID subunit 5.

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

- Molecule 31 is a protein called Transcription initiation factor TFIID subunit 6.

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

- Molecule 32 is a protein called Transcription initiation factor TFIID subunit 9.

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

- Molecule 33 is a protein called Transcription initiation factor TFIID subunit 10.

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

- Molecule 34 is a protein called Transcription initiation factor TFIID subunit 11.

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

- Molecule 35 is a protein called Transcription initiation factor TFIID subunit 12.

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

- Molecule 36 is a protein called Transcription initiation factor TFIID subunit 13.

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

- Molecule 37 is a protein called Transcription initiation factor TFIID subunit 7.

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

- Molecule 38 is a protein called Transcription initiation factor TFIID subunit 8.

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

- Molecule 39 is a protein called CDK-activating kinase assembly factor MAT1.

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

- Molecule 40 is a protein called General transcription factor IIH subunit 3.

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

- Molecule 41 is a protein called General transcription factor IIIH subunit 2.

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

- Molecule 42 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPB.

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

- Molecule 43 is a protein called General transcription factor IIIH subunit 5.

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

- Molecule 44 is a protein called Cyclin-dependent kinase 7.

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

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 45 is a protein called Cyclin-H.

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

- Molecule 46 is a protein called DNA-directed RNA polymerase II subunit RPB4.

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

- Molecule 47 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 48 is a protein called Mediator of RNA polymerase II transcription subunit 7.

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

- Molecule 49 is a protein called Mediator of RNA polymerase II transcription subunit 10.

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

- Molecule 50 is a protein called Mediator of RNA polymerase II transcription subunit 14.

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

- Molecule 51 is a protein called Mediator of RNA polymerase II transcription subunit 19.

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

- Molecule 52 is a protein called Mediator of RNA polymerase II transcription subunit 21.

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

- Molecule 53 is a protein called Mediator of RNA polymerase II transcription subunit 1.

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

- Molecule 54 is a protein called Mediator of RNA polymerase II transcription subunit 4.

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

- Molecule 55 is a protein called Mediator of RNA polymerase II transcription subunit 6.

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

- Molecule 56 is a protein called Mediator of RNA polymerase II transcription subunit 9.

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

- Molecule 57 is a protein called Mediator of RNA polymerase II transcription subunit 31.

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

- Molecule 58 is a protein called Mediator of RNA polymerase II transcription subunit 17.

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

- Molecule 59 is a protein called Mediator of RNA polymerase II transcription subunit 26.

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

- Molecule 60 is a protein called Mediator of RNA polymerase II transcription subunit 29.

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

- Molecule 61 is a protein called Mediator of RNA polymerase II transcription subunit 27.

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

- Molecule 62 is a protein called Mediator of RNA polymerase II transcription subunit 28.

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

- Molecule 63 is a protein called Mediator of RNA polymerase II transcription subunit 30.

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

- Molecule 64 is a protein called Mediator of RNA polymerase II transcription subunit 15.

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

- Molecule 65 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 8.

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

- Molecule 66 is a protein called Mediator of RNA polymerase II transcription subunit 11.

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

- Molecule 67 is a protein called Mediator of RNA polymerase II transcription subunit 18.

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

- Molecule 68 is a protein called Mediator of RNA polymerase II transcription subunit 20.

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

- Molecule 69 is a protein called Mediator of RNA polymerase II transcription subunit 22.

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

- Molecule 70 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 16.

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

- Molecule 71 is a protein called Mediator of RNA polymerase II transcription subunit 23.

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

- Molecule 72 is a protein called Mediator of RNA polymerase II transcription subunit 24.

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

- Molecule 73 is a protein called Mediator of RNA polymerase II transcription subunit 25.

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

- Molecule 74 is a protein called HISTONE H2A.Z.

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

- Molecule 75 is a protein called Histone H2B.

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

- Molecule 76 is a DNA chain called DNA (162-mer).

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

- Molecule 77 is a DNA chain called DNA (162-mer).

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

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

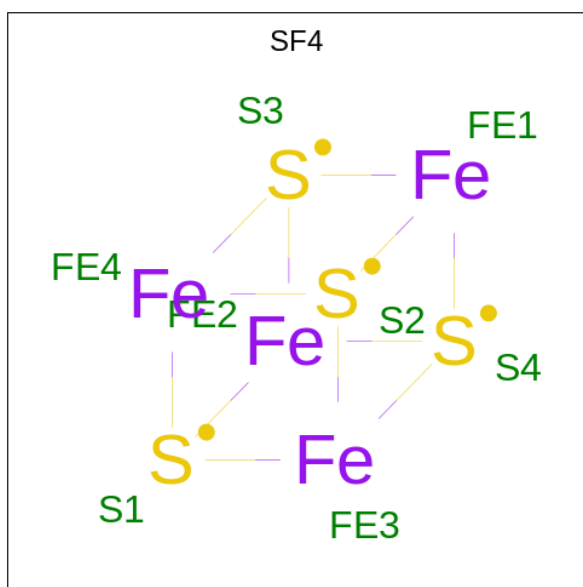
Mol	Chain	Residues	Atoms		AltConf
78	BA	1	Total	Zn	0
			1	1	
78	EA	1	Total	Zn	0
			1	1	
78	PA	2	Total	Zn	0
			2	2	
78	PB	1	Total	Zn	0
			1	1	
78	PC	1	Total	Zn	0
			1	1	
78	PI	2	Total	Zn	0
			2	2	
78	PJ	1	Total	Zn	0
			1	1	
78	PL	1	Total	Zn	0
			1	1	
78	HD	2	Total	Zn	0
			2	2	
78	HE	2	Total	Zn	0
			2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

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Mol	Chain	Residues	Atoms		AltConf
78	HG	3	Total 3	Zn 3	0
78	c	1	Total 1	Zn 1	0
78	p	1	Total 1	Zn 1	0

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



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

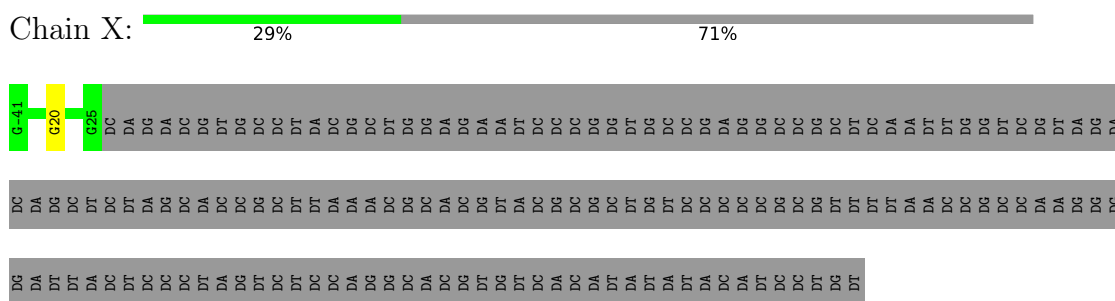
- Molecule 80 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

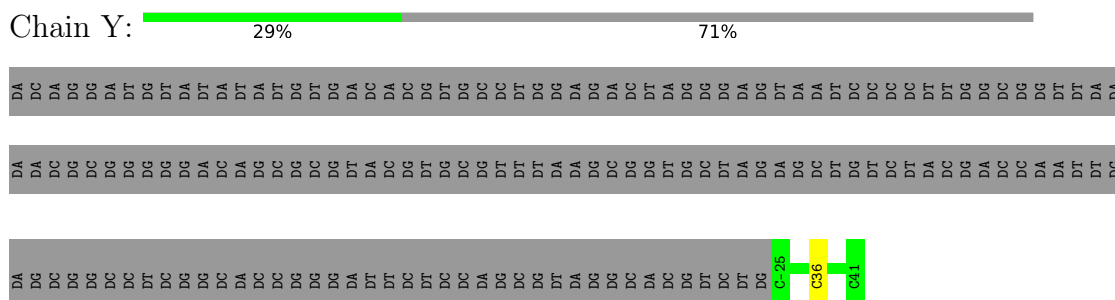
3 Residue-property plots [i](#)

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

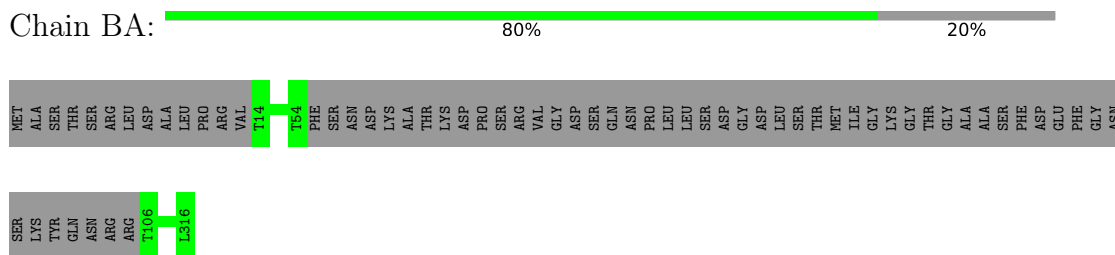
- Molecule 1: DNA (228-mer)



- Molecule 2: DNA (228-mer)

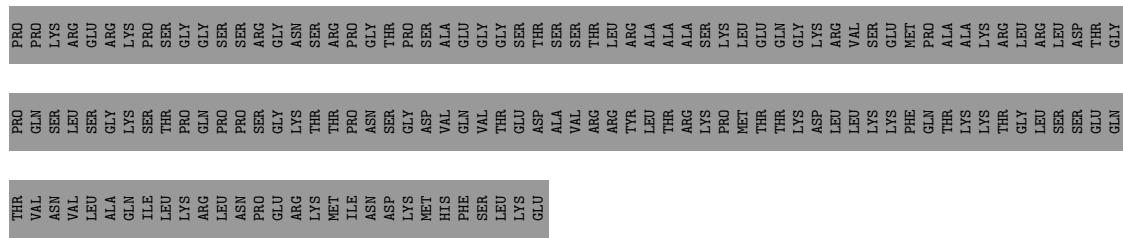


- Molecule 3: Transcription initiation factor IIB



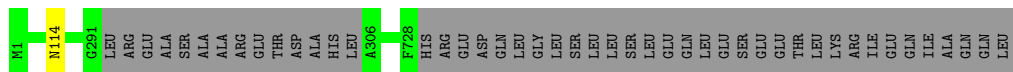
- Molecule 4: Transcription initiation factor TFIID subunit 1





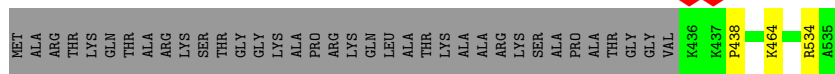
• Molecule 7: General transcription and DNA repair factor IIIH helicase subunit XPD

Chain HA:



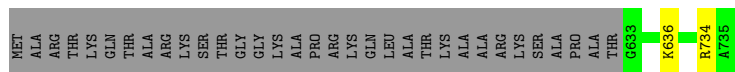
• Molecule 8: Histone H3

Chain NA:



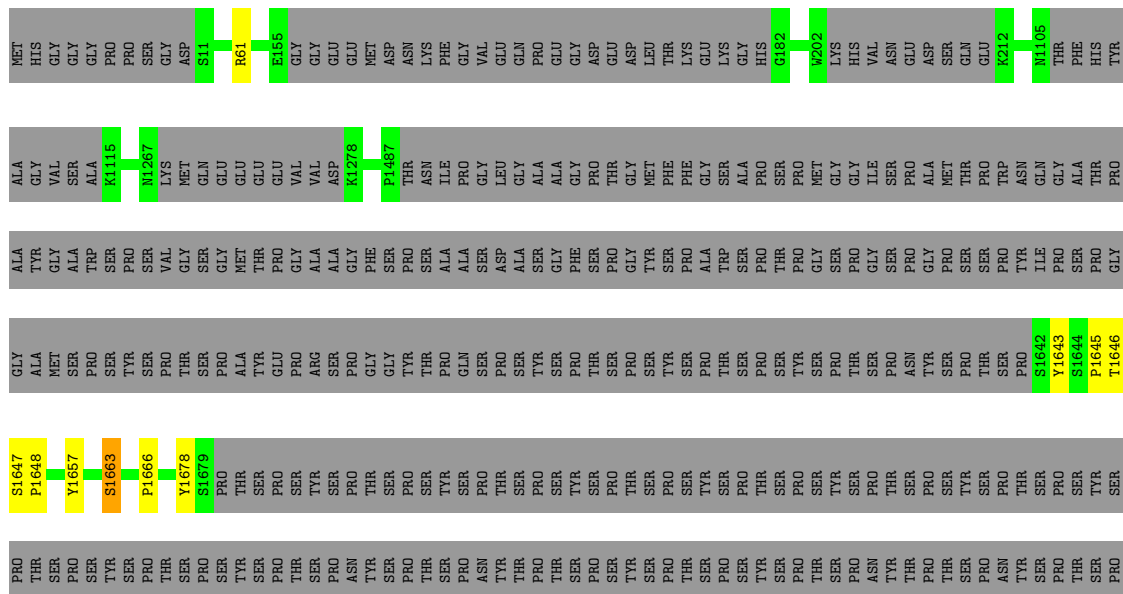
• Molecule 8: Histone H3

Chain NE:



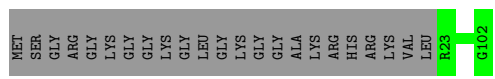
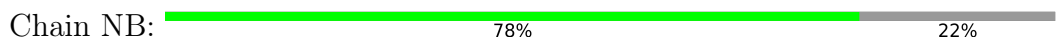
• Molecule 9: DNA-directed RNA polymerase subunit

Chain PA:

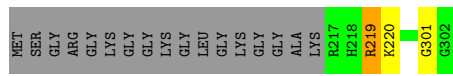
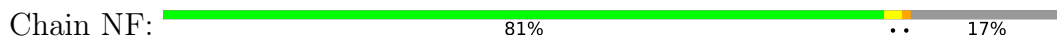




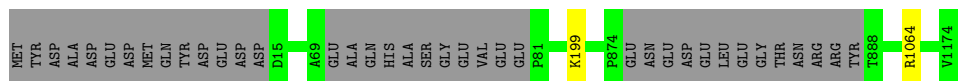
• Molecule 14: Histone H4



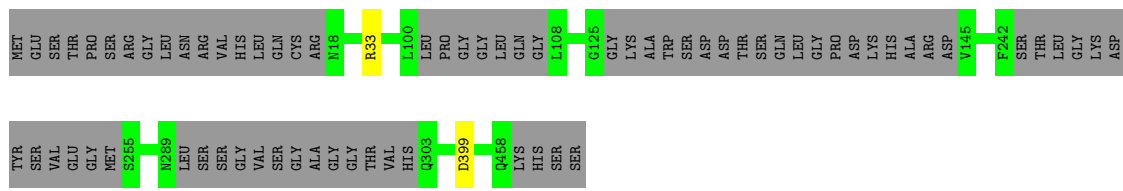
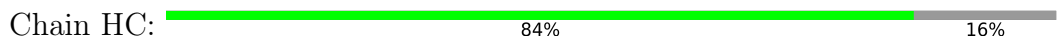
• Molecule 14: Histone H4



• Molecule 15: DNA-directed RNA polymerase subunit beta

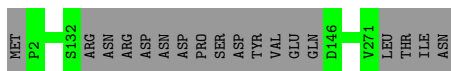


• Molecule 16: General transcription factor IIH subunit 4



• Molecule 17: DNA-directed RNA polymerase II subunit RPB3

Chain PC:  93% 7%



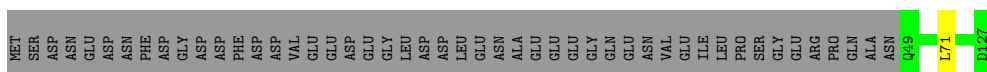
- Molecule 18: DNA-directed RNA polymerase II subunit E

Chain PE:  100%



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

Chain PF:  61% 38%




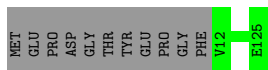
- Molecule 20: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain PH:  99%



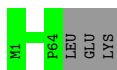
- Molecule 21: DNA-directed RNA polymerase II subunit RPB9

Chain PI:  91% 9%



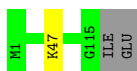
- Molecule 22: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain PJ:  96%

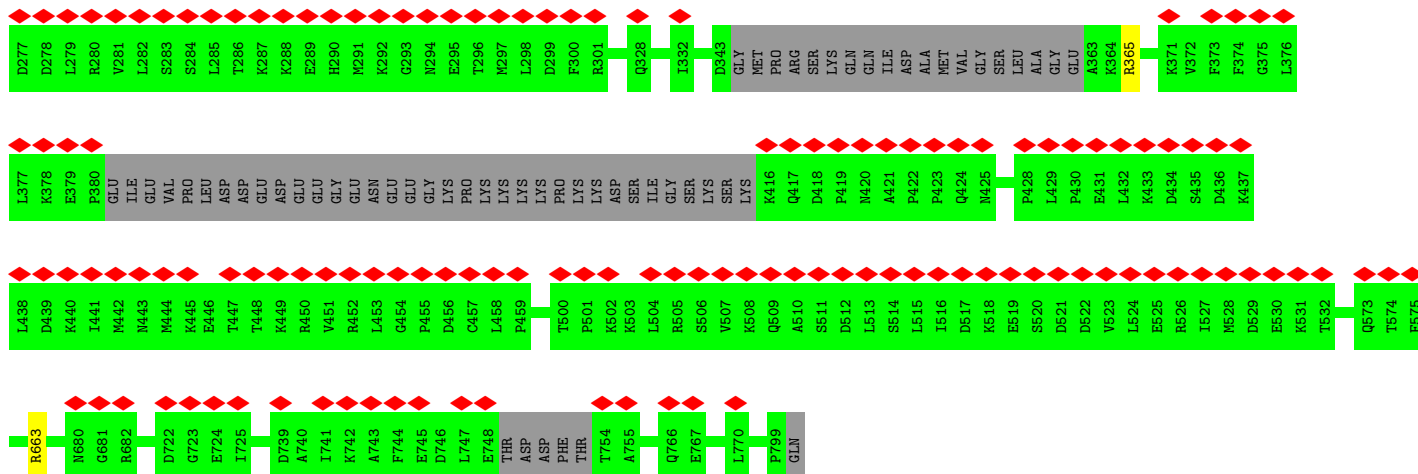


- Molecule 23: RNA_pol_L_2 domain-containing protein

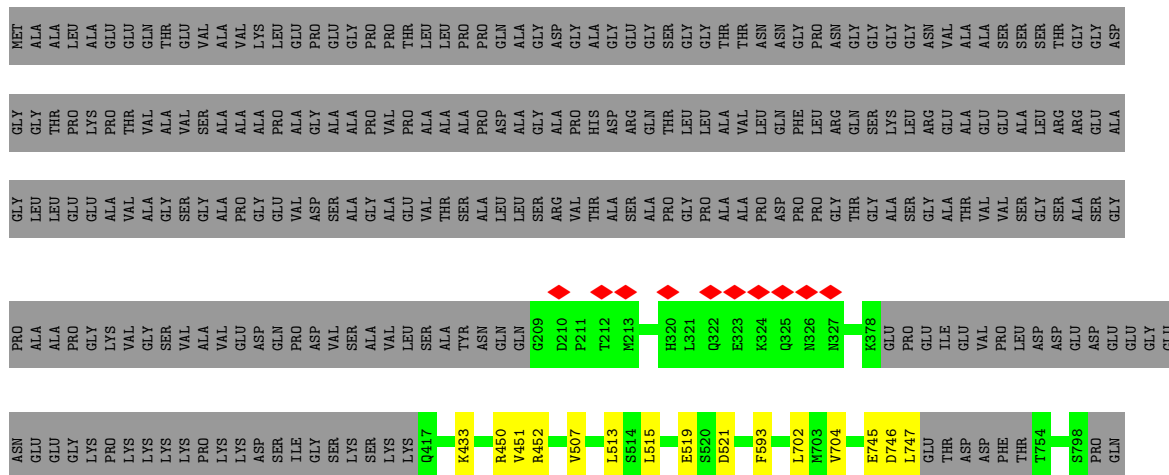
Chain PK:  97%



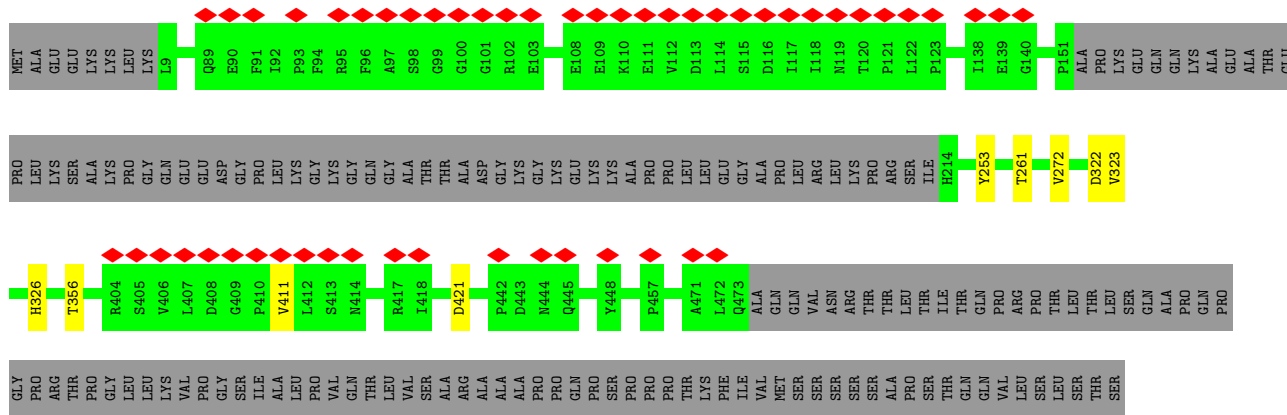
- Molecule 24: RPB12

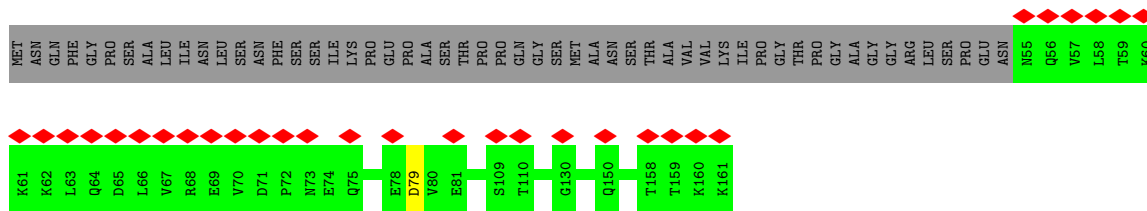


• Molecule 30: Transcription initiation factor TFIID subunit 5

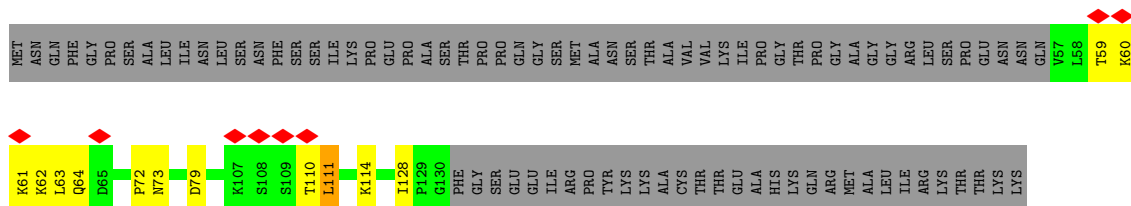
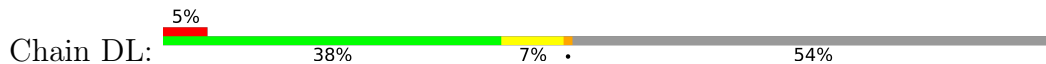


• Molecule 31: Transcription initiation factor TFIID subunit 6

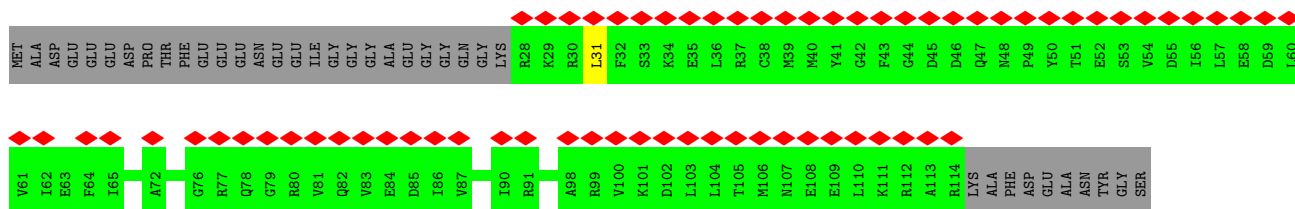
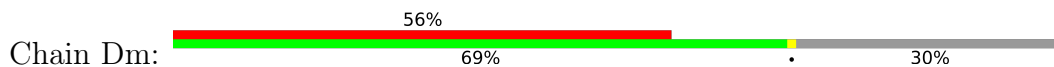




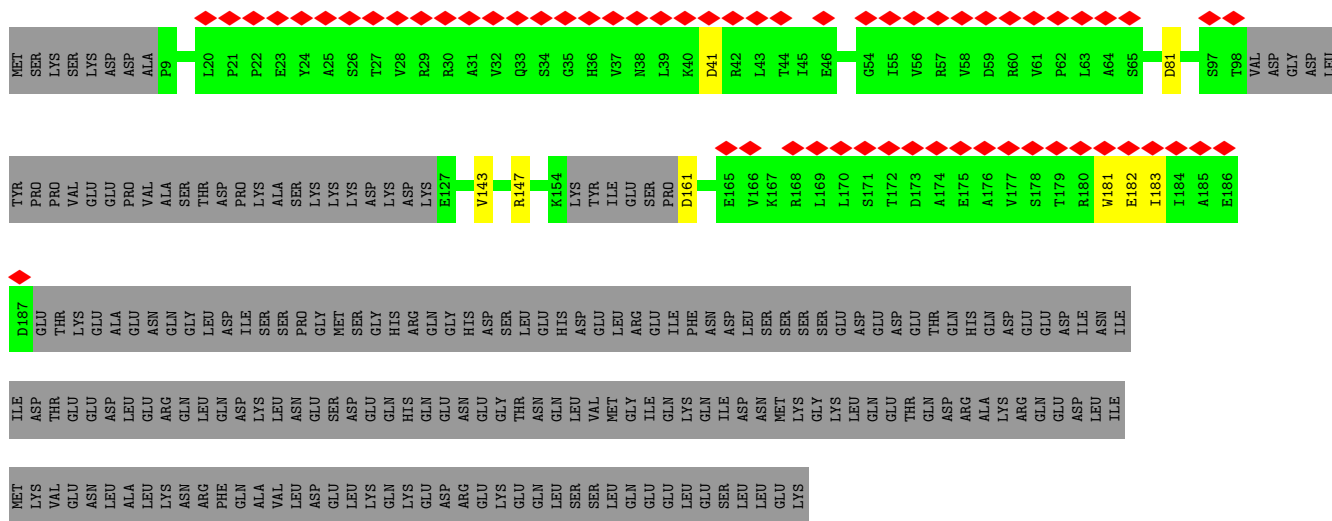
• Molecule 35: Transcription initiation factor TFIID subunit 12



• Molecule 36: Transcription initiation factor TFIID subunit 13

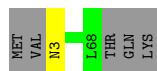


• Molecule 37: Transcription initiation factor TFIID subunit 7



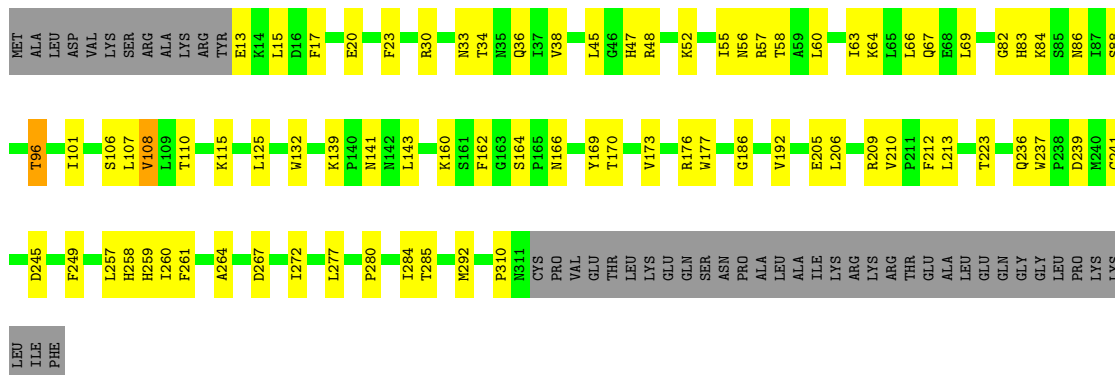
• Molecule 38: Transcription initiation factor TFIID subunit 8

Chain HF:  92% • 7%



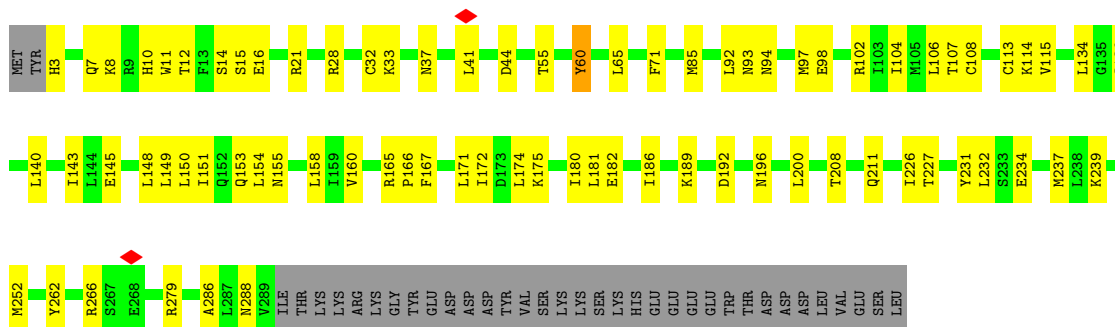
• Molecule 44: Cyclin-dependent kinase 7

Chain HI:  64% • 22% • 14%



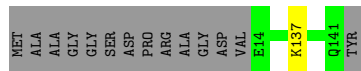
• Molecule 45: Cyclin-H

Chain HJ:  65% • 24% • 11%



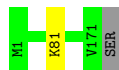
• Molecule 46: DNA-directed RNA polymerase II subunit RPB4

Chain PD:  89% • 10%



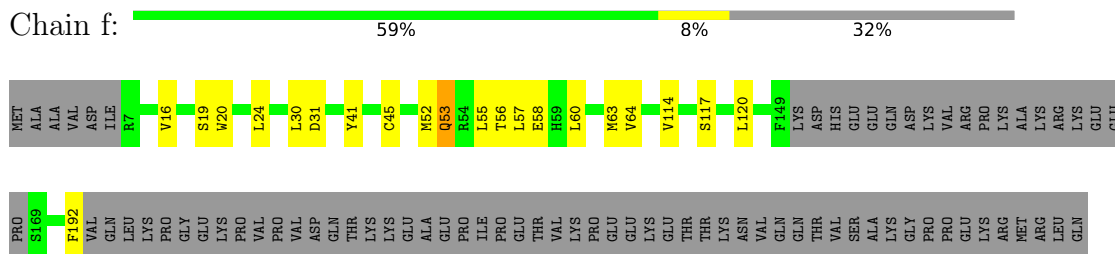
• Molecule 47: DNA-directed RNA polymerase II subunit RPB7

Chain PG:  99%

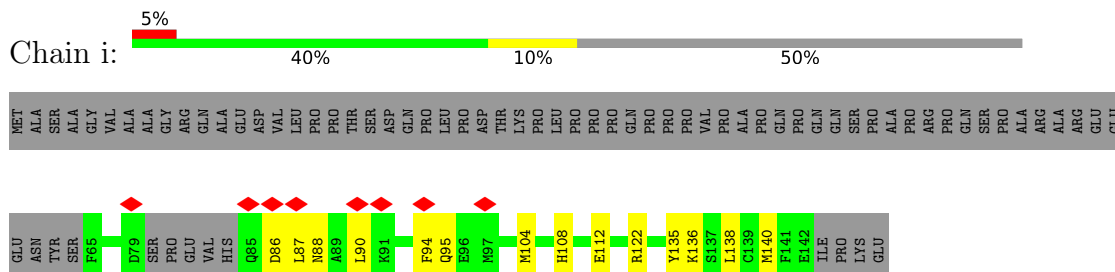


• Molecule 48: Mediator of RNA polymerase II transcription subunit 7

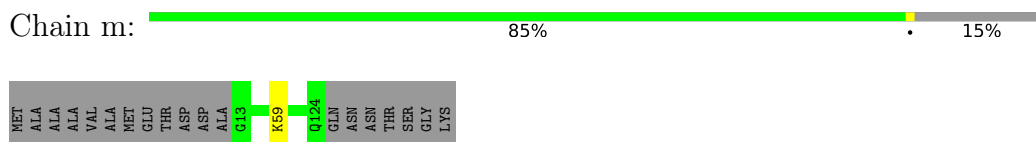
- Molecule 55: Mediator of RNA polymerase II transcription subunit 6



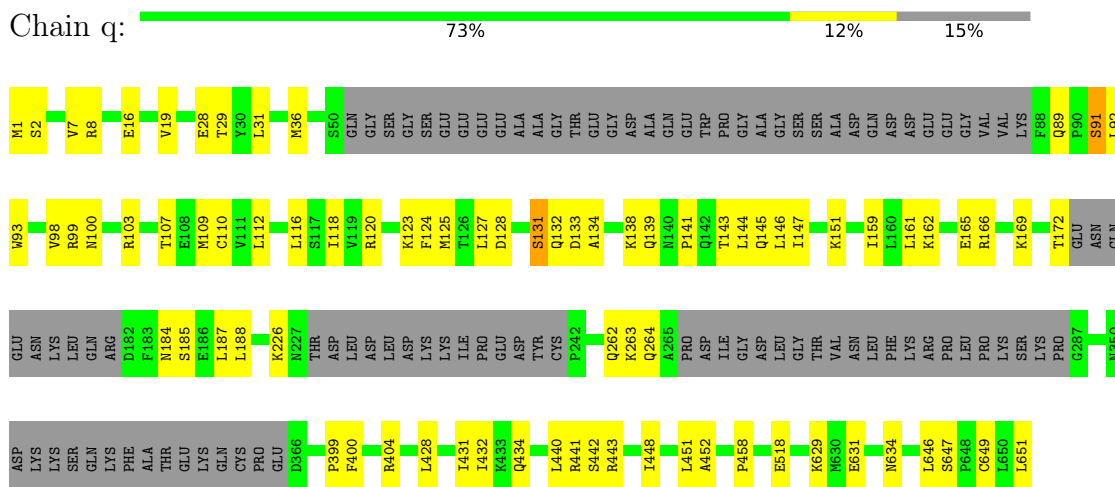
- Molecule 56: Mediator of RNA polymerase II transcription subunit 9



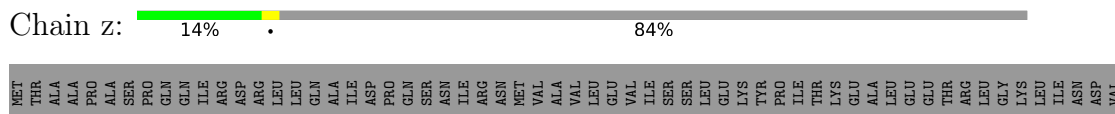
- Molecule 57: Mediator of RNA polymerase II transcription subunit 31

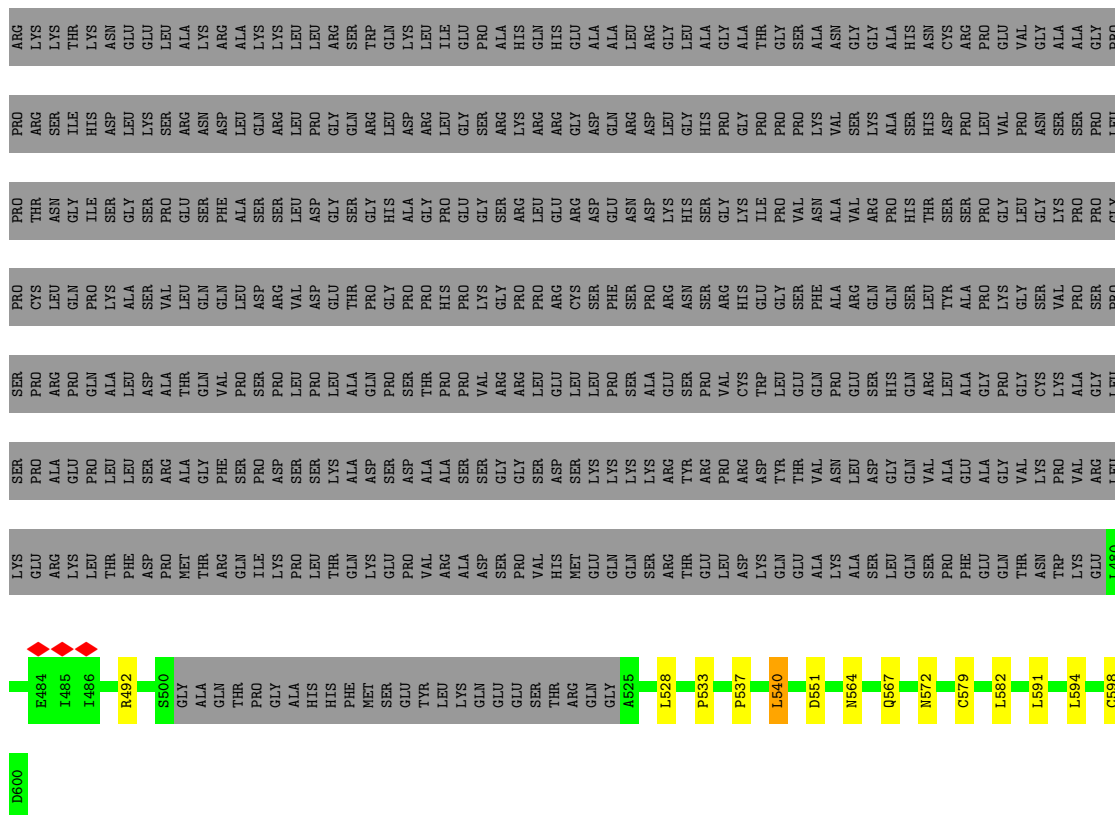


- Molecule 58: Mediator of RNA polymerase II transcription subunit 17

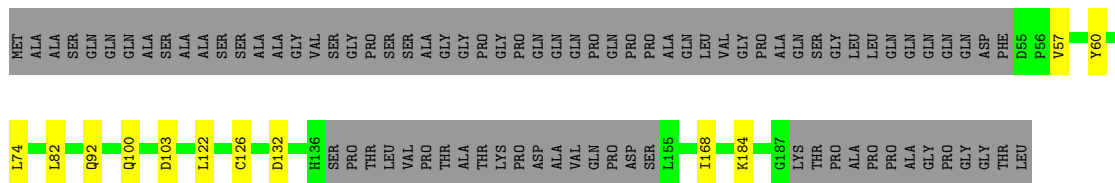


- Molecule 59: Mediator of RNA polymerase II transcription subunit 26

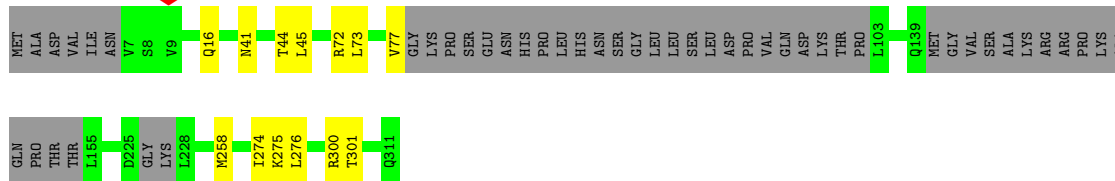
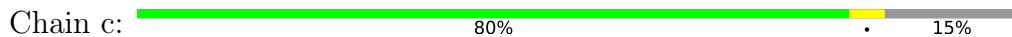




• Molecule 60: Mediator of RNA polymerase II transcription subunit 29

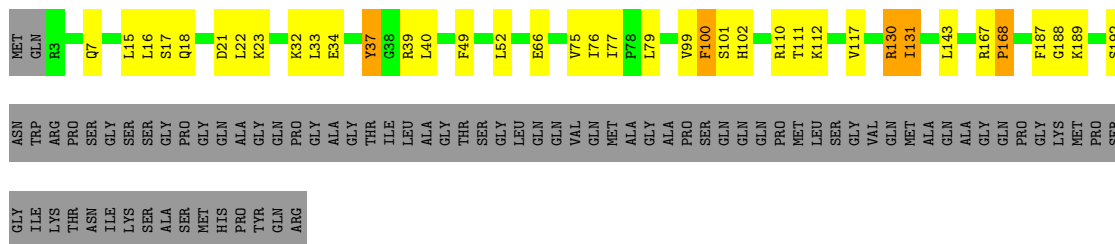


• Molecule 61: Mediator of RNA polymerase II transcription subunit 27

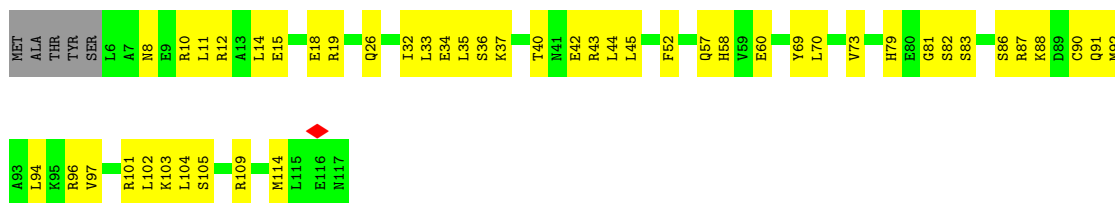


• Molecule 62: Mediator of RNA polymerase II transcription subunit 28

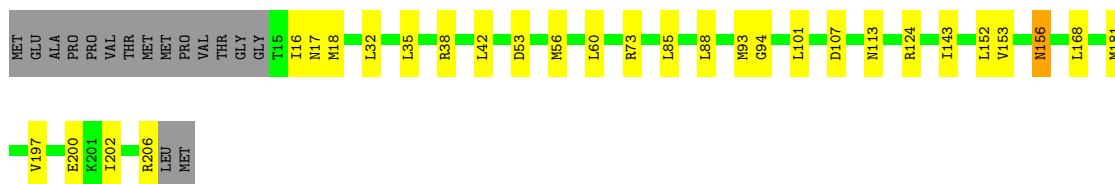
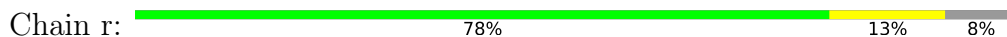




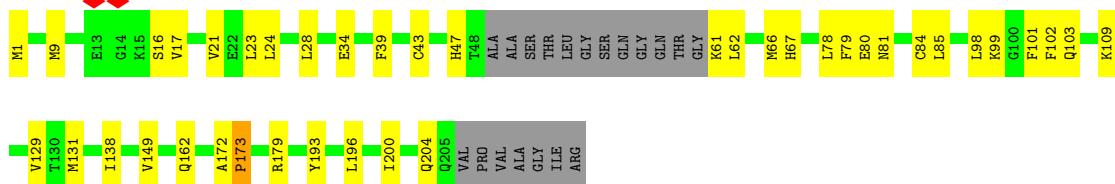
- Molecule 66: Mediator of RNA polymerase II transcription subunit 11



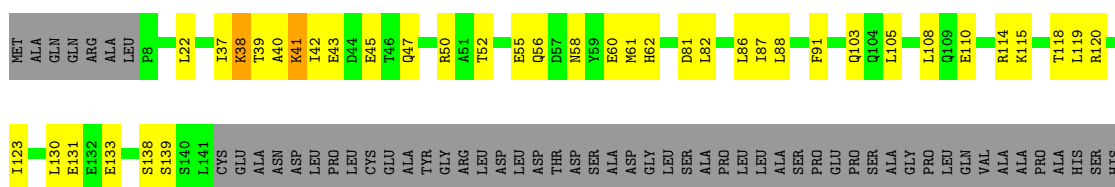
- Molecule 67: Mediator of RNA polymerase II transcription subunit 18



- Molecule 68: Mediator of RNA polymerase II transcription subunit 20



- Molecule 69: Mediator of RNA polymerase II transcription subunit 22



ALA
GLY
GLY
PRO
PRO
GLY
GLY
PRO
THR
GLU
HIS
ALA

- Molecule 70: Isoform 2 of Mediator of RNA polymerase II transcription subunit 16

Chain p: 90% 9%

MET
CYS
ASP
LEU
LEU
ARG
ARG
PRO
PRO
ALA
ALA
GLY
GLY
M12
M13
V162
L170
D289
L295
E314
GLY
LEU
PRO
VAL
ASN
ASN
ASN
ILE
PHE
GLN
GLN
ILE
ILE
SER
PRO
PRO
VAL
VAL
VAL
ASP
GLY
LYS
GLN
GLN
PRO
T335
T401
S408
ALA
ALA
PRO
PRO
ARG
PRO
VAL
VAL
ASP
GLU
PRO
ALA
ALA
LYS

ARG
PRO
THR
ALA
GLY
PRO
ALA
V429
L443
L564
R634
GLN
GLY
SER
LEU
L639
C699
E703
P705
D710
P727
P756
THR
LEU
PRO
PRO
GLY
SER
VAL
ALA
ALA
THR
LEU
LEU
GLN
LEU
ASP
GLY
LEU
ALA
ARG
ALA
ALA
PRO
GLY
GLN
G777
P841

- Molecule 71: Mediator of RNA polymerase II transcription subunit 23

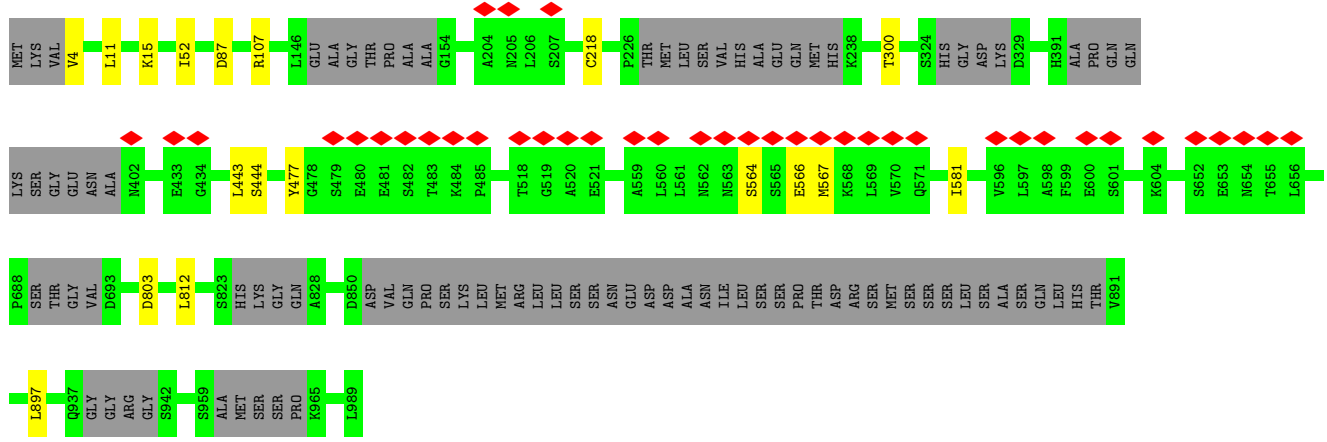
Chain w: 23% 97%

M1
E2
T3
Q4
S7
E11
F22
D32
I38
S39
G42
A43
F44
R45
Q46
G49
G50
L51
S52
Q53
E54
S55
H56
A84
M85
A86
V87
E88
T89
G90
L91
P94
R95
L96
V97
C98
E99
I102
N103
S104
D105
V122
R123
K124
I125
I126
G127
G128
V129
D130
Y131
K132
G133
V134
R135
D136
L137
L138
K139
V140
I141
E142
K143
K144
I145
L146
T147
A163
V166
I167
A168
Y169
I170
L171
E172
R173
M174
A175
C176
L177
L178
L178
P179
A180
Y181
F182
A183
V184
T185
E186
I187
R188
K189
L190
Y191
P192
E193
G194
K195
L196
P197
V205
F208
V209
T210
T211
F212
D244
P245
A246
T247
L255
Q292
K294
Q295
R296
C297
M425
Q460
R463
M464
K465
S466
G503
I504
M505
R506
T666
R667
F668
L669
S670
D671
P672
K673
D705
S706
I707
Q708
G709
T710
W711
C712
D713
K714
D714
I715
L716
Q717
T718
I719
M720
S721
F722
I723
P724
H725
M726
W727
A728
S729
G737
P738
L739
Q740
A741
F742
F743
K744
M746
M747
V748
P749
Q750
E751
S752
R753
F754
M755
L756
K757
K758
M759
V760
E761
E762
E763
Y764
R765
K766
W767
K768
M770
S771
N772
E773
N774
D775
I776
I777
T778
H779
M782
Q783
G784
S785
P786
L792
K795
M796
L797
L798
E799
T800
D801
H802
V941
D942
P943
P944
V945
Q946
I947
Q948
K1050
N1054
A1055
R1056
E1057
E1058
N1059
A1116
T1194
A1195
C1196
M1203
Q1261
T1264
R1265
L1279
N1280
V1281
D1282
Q1283
M1284
S1285
C1286
H1287
L1288
M1291
D1292
C1295
D1296
F1297
L1298
Y1299
K1302
Y1303
G1307
D1308
S1309
V1310
K1311
E1312
Q1313
V1314
E1315
K1316
I1317
I1318
C1319
M1320
L1321
L1322
P1323
A1324
L1325
K1326
L1327
L1328
L1329
R1330
F1331
I1332
T1333
H1334
ILE
SER
LYS
MET
GLU
PRO
ALA
ALA
VAL
PRO
PRO
GLN
ALA
MET
SER
SER
GLY
SER
PRO
ALA
PRO
GLN
SER
ASN
GLN
VAL
PRO
VAL
VAL
SER
SER
LEU
PRO
VAL
THR

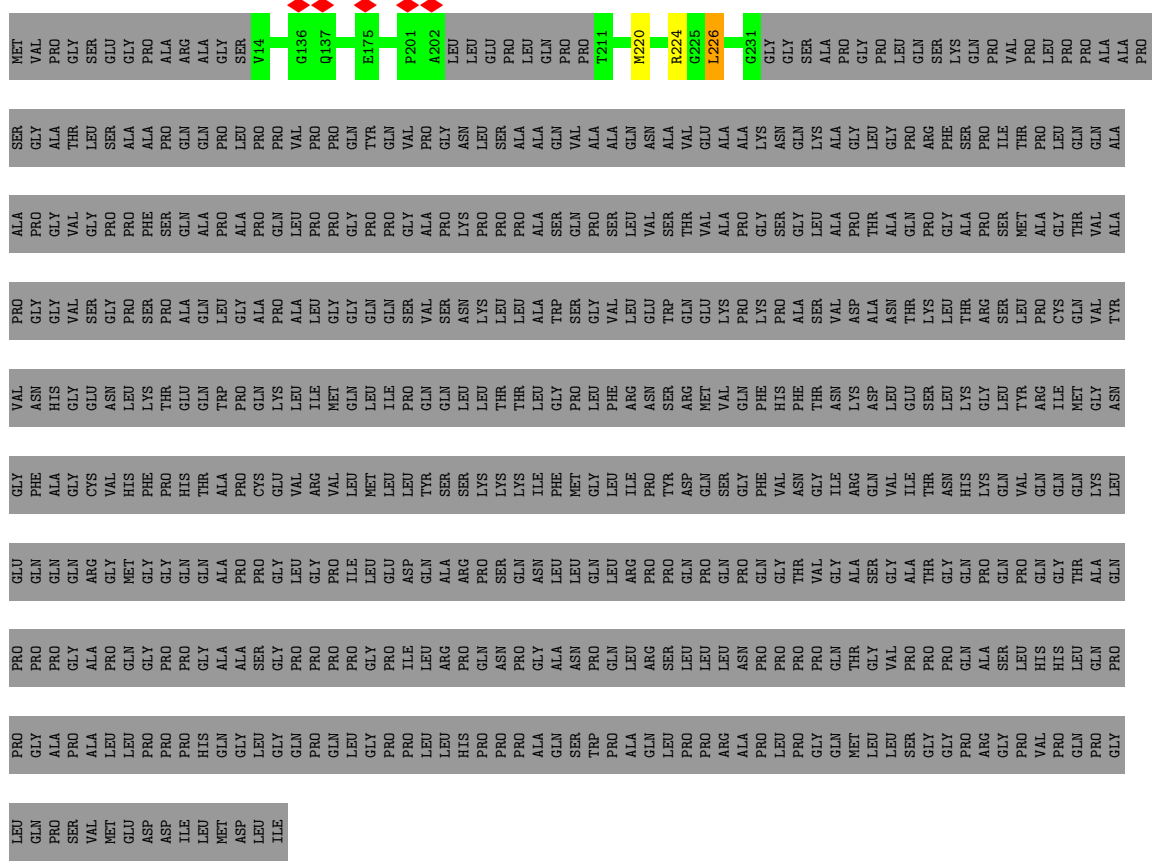
GLN

- Molecule 72: Mediator of RNA polymerase II transcription subunit 24

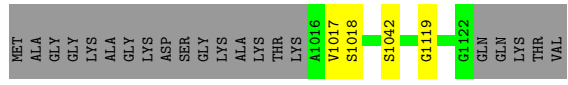
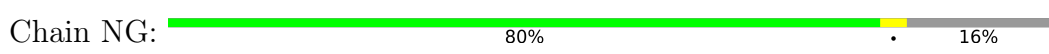
Chain x: 89% 9%



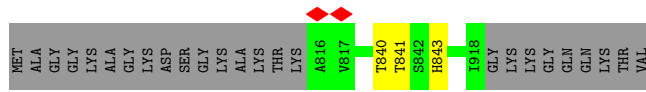
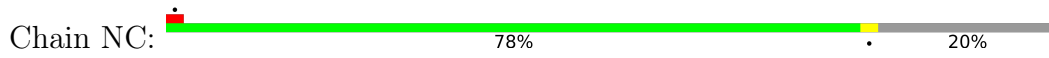
• Molecule 73: Mediator of RNA polymerase II transcription subunit 25



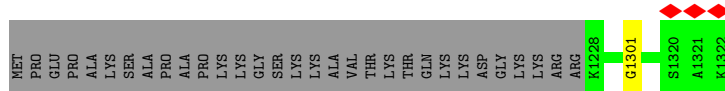
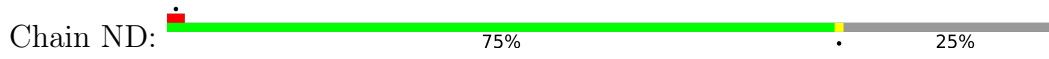
• Molecule 74: HISTONE H2A.Z



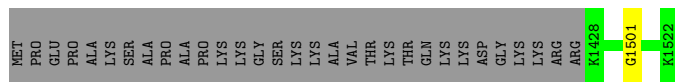
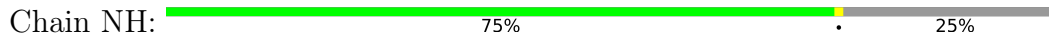
• Molecule 74: HISTONE H2A.Z



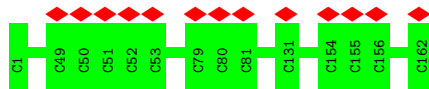
• Molecule 75: Histone H2B



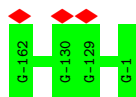
• Molecule 75: Histone H2B



• Molecule 76: DNA (162-mer)



• Molecule 77: DNA (162-mer)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26458	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	2.678	Depositor
Minimum map value	-1.034	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.079	Depositor
Recommended contour level	0.156	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.56	0/1561	0.82	1/2411 (0.0%)
2	Y	0.67	1/1516 (0.1%)	0.92	0/2334
3	BA	0.25	0/1983	0.40	0/2679
4	DA	0.51	0/4679	0.62	1/6320 (0.0%)
5	EA	0.33	0/1560	0.51	0/2097
6	FA	0.24	0/1167	0.41	0/1576
7	HA	0.25	0/5875	0.41	0/7955
8	NA	0.68	0/497	0.82	1/693 (0.1%)
8	NE	0.77	0/510	0.88	0/710
9	PA	0.27	0/11851	0.43	0/16014
10	DB	0.47	1/7993 (0.0%)	0.61	0/10836
11	EB	0.28	0/1427	0.46	0/1916
12	FB	0.26	0/1817	0.41	0/2445
13	HB	0.25	0/2210	0.40	0/2975
14	NB	0.76	0/390	0.84	0/539
14	NF	0.85	0/420	0.97	1/581 (0.2%)
15	PB	0.25	0/9257	0.42	0/12493
16	HC	0.28	0/3230	0.43	0/4376
17	PC	0.24	0/2102	0.42	0/2857
18	PE	0.24	0/1752	0.41	0/2366
19	PF	0.27	0/646	0.41	0/871
20	PH	0.24	0/1207	0.43	0/1628
21	PI	0.24	0/949	0.44	0/1284
22	PJ	0.26	0/516	0.41	0/696
23	PK	0.26	0/939	0.40	0/1271
24	PL	0.26	0/378	0.41	0/500
25	DP	0.25	0/1448	0.42	0/1948
26	DQ	0.25	0/945	0.42	0/1274
27	DO	0.25	0/816	0.43	0/1105
28	Dc	0.40	0/1035	0.54	0/1406
29	DD	0.42	0/1343	0.53	0/1795
29	Dd	0.29	0/1321	0.49	0/1772

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	DE	0.39	0/4469	0.56	0/6050
30	De	0.33	0/4433	0.55	0/6004
31	DF	0.50	0/3167	0.69	1/4303 (0.0%)
31	Df	0.42	0/3140	0.63	0/4268
32	DI	0.43	0/981	0.56	0/1332
32	Di	0.31	0/989	0.49	0/1343
33	DJ	0.30	0/736	0.49	1/998 (0.1%)
33	Dj	0.30	0/775	0.52	0/1049
34	Dk	0.31	0/799	0.48	0/1070
35	DL	0.44	0/613	0.65	1/829 (0.1%)
35	Dl	0.41	0/888	0.54	1/1194 (0.1%)
36	Dm	0.31	0/733	0.52	0/977
37	DG	0.52	0/1199	0.63	0/1612
38	DH	0.37	0/1673	0.58	1/2285 (0.0%)
39	HD	0.49	0/2436	0.68	3/3286 (0.1%)
40	HE	0.32	0/2103	0.47	0/2846
41	HG	0.25	0/2793	0.41	0/3780
42	HH	0.25	0/4994	0.40	0/6745
43	HF	0.27	0/529	0.49	1/714 (0.1%)
44	HI	0.67	0/2433	0.96	0/3302
45	HJ	0.73	0/2356	0.97	1/3185 (0.0%)
46	PD	0.30	0/1064	0.42	0/1428
47	PG	0.27	0/1382	0.45	0/1874
48	g	0.57	0/911	0.86	2/1219 (0.2%)
49	j	0.37	0/849	0.54	0/1150
50	n	0.36	0/7901	0.57	14/10731 (0.1%)
51	s	0.64	0/741	0.75	1/1002 (0.1%)
52	u	0.54	0/895	0.75	2/1215 (0.2%)
53	a	0.61	0/3507	0.78	1/4760 (0.0%)
54	d	0.62	0/1281	0.65	0/1718
55	f	0.55	0/1402	0.67	1/1905 (0.1%)
56	i	0.68	0/612	0.75	1/815 (0.1%)
57	m	0.27	0/1010	0.38	0/1359
58	q	0.49	1/4456 (0.0%)	0.56	0/6019
59	z	0.64	0/781	0.86	0/1067
60	b	0.51	0/911	0.63	0/1229
61	c	0.43	0/2172	0.56	0/2935
62	e	0.28	0/840	0.40	0/1128
63	l	0.26	0/1048	0.43	0/1405
64	o	0.41	0/1256	0.65	0/1724
65	h	0.63	0/1485	0.73	1/2008 (0.0%)
66	k	0.66	0/885	0.67	0/1190
67	r	0.59	0/1565	0.73	0/2106

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
68	t	0.70	0/1530	0.87	0/2066
69	v	0.66	0/1092	0.74	0/1468
70	p	0.65	0/6116	0.69	0/8311
71	w	0.56	0/11056	0.60	0/15023
72	x	0.58	0/7191	0.64	1/9728 (0.0%)
73	y	0.57	0/1645	0.64	0/2240
74	NC	0.80	0/505	0.86	0/700
74	NG	0.68	0/523	0.90	1/724 (0.1%)
75	ND	0.76	0/470	0.83	0/654
75	NH	0.66	0/470	0.85	0/654
76	NX	0.35	0/3401	0.84	0/5180
77	NY	0.40	0/4046	0.77	0/6310
All	All	0.45	3/190578 (0.0%)	0.60	39/259940 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
39	HD	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	q	452	ALA	C-N	5.60	1.47	1.34
2	Y	36	DC	O3'-P	5.14	1.67	1.61
10	DB	494	SER	CA-CB	-5.06	1.45	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	g	128	PRO	N-CA-C	-7.74	91.97	112.10
50	n	1351	PRO	N-CA-CB	7.36	112.13	103.30
48	g	128	PRO	CA-N-CD	-7.30	101.28	111.50
50	n	1343	PRO	N-CA-CB	7.26	112.01	103.30
31	DF	320	ARG	CB-CG-CD	7.09	130.03	111.60
50	n	1355	PRO	N-CA-CB	6.84	111.51	103.30
50	n	1352	PRO	N-CA-CB	6.33	110.89	103.30
50	n	1326	PRO	N-CA-CB	6.19	110.72	103.30
4	DA	498	PRO	N-CA-CB	5.99	110.48	103.30
53	a	412	ARG	CB-CA-C	5.99	122.37	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	s	107	ASN	N-CA-C	-5.86	95.18	111.00
50	n	1255	PRO	N-CA-CB	5.86	110.33	103.30
50	n	1237	PRO	N-CA-CB	5.82	110.29	103.30
50	n	1348	PRO	N-CA-CB	5.77	110.22	103.30
74	NG	1119	GLY	N-CA-C	5.77	127.53	113.10
52	u	64	ARG	CB-CA-C	-5.76	98.87	110.40
50	n	1344	PRO	N-CA-CB	5.74	110.19	103.30
50	n	288	PRO	N-CA-C	5.74	127.02	112.10
50	n	74	PRO	N-CA-CB	5.71	110.15	103.30
38	DH	110	TYR	CB-CA-C	-5.70	98.99	110.40
43	HF	3	ASN	CB-CA-C	-5.62	99.17	110.40
39	HD	220	PRO	N-CA-CB	5.61	110.03	103.30
1	X	20	DG	P-O3'-C3'	5.61	126.43	119.70
50	n	1347	PRO	N-CA-CB	5.50	109.90	103.30
39	HD	237	PRO	N-CA-CB	5.39	109.77	103.30
39	HD	217	PRO	N-CA-CB	5.39	109.77	103.30
50	n	591	PHE	CB-CA-C	5.31	121.03	110.40
65	h	168	PRO	N-CA-CB	5.25	109.61	103.30
50	n	676	ASP	CB-CG-OD2	5.23	123.01	118.30
45	HJ	60	TYR	CB-CA-C	5.23	120.86	110.40
14	NF	219	ARG	N-CA-C	5.19	125.00	111.00
35	DI	79	ASP	CB-CG-OD2	5.18	122.96	118.30
33	DJ	118	ASP	CB-CG-OD2	5.14	122.92	118.30
35	DL	79	ASP	CB-CG-OD2	5.10	122.89	118.30
52	u	75	SER	N-CA-CB	-5.09	102.87	110.50
55	f	31	ASP	CB-CG-OD2	5.09	122.88	118.30
56	i	135	TYR	CB-CA-C	5.08	120.55	110.40
72	x	581	ILE	CG1-CB-CG2	-5.03	100.33	111.40
8	NA	464	LYS	N-CA-C	5.03	124.58	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
39	HD	126	GLN	Mainchain

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	
3	BA	248/316 (78%)	246 (99%)	2 (1%)	0	100	100
4	DA	542/1872 (29%)	524 (97%)	15 (3%)	3 (1%)	25	65
5	EA	185/439 (42%)	183 (99%)	1 (0%)	1 (0%)	29	68
6	FA	134/517 (26%)	129 (96%)	5 (4%)	0	100	100
7	HA	710/760 (93%)	682 (96%)	28 (4%)	0	100	100
8	NA	98/136 (72%)	94 (96%)	2 (2%)	2 (2%)	7	39
8	NE	101/136 (74%)	96 (95%)	3 (3%)	2 (2%)	7	39
9	PA	1457/1970 (74%)	1406 (96%)	47 (3%)	4 (0%)	41	76
10	DB	959/1199 (80%)	910 (95%)	49 (5%)	0	100	100
11	EB	169/291 (58%)	164 (97%)	5 (3%)	0	100	100
12	FB	218/249 (88%)	213 (98%)	4 (2%)	1 (0%)	29	68
13	HB	253/548 (46%)	245 (97%)	8 (3%)	0	100	100
14	NB	78/103 (76%)	78 (100%)	0	0	100	100
14	NF	84/103 (82%)	77 (92%)	4 (5%)	3 (4%)	3	28
15	PB	1130/1174 (96%)	1093 (97%)	37 (3%)	0	100	100
16	HC	380/462 (82%)	363 (96%)	17 (4%)	0	100	100
17	PC	253/275 (92%)	241 (95%)	12 (5%)	0	100	100
18	PE	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
19	PF	77/127 (61%)	76 (99%)	1 (1%)	0	100	100
20	PH	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
21	PI	112/125 (90%)	104 (93%)	8 (7%)	0	100	100
22	PJ	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
23	PK	113/117 (97%)	112 (99%)	1 (1%)	0	100	100
24	PL	42/58 (72%)	40 (95%)	2 (5%)	0	100	100
25	DP	177/339 (52%)	175 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	DQ	109/376 (29%)	102 (94%)	7 (6%)	0	100	100
27	DO	97/109 (89%)	95 (98%)	2 (2%)	0	100	100
28	Dc	125/929 (14%)	116 (93%)	9 (7%)	0	100	100
29	DD	153/1085 (14%)	146 (95%)	5 (3%)	2 (1%)	12	48
29	Dd	154/1085 (14%)	150 (97%)	4 (3%)	0	100	100
30	DE	540/800 (68%)	505 (94%)	33 (6%)	2 (0%)	34	72
30	De	531/800 (66%)	484 (91%)	47 (9%)	0	100	100
31	DF	404/677 (60%)	376 (93%)	21 (5%)	7 (2%)	9	43
31	Df	399/677 (59%)	378 (95%)	20 (5%)	1 (0%)	41	76
32	DI	118/264 (45%)	113 (96%)	3 (2%)	2 (2%)	9	43
32	Di	119/264 (45%)	115 (97%)	4 (3%)	0	100	100
33	DJ	86/218 (39%)	82 (95%)	4 (5%)	0	100	100
33	Dj	91/218 (42%)	89 (98%)	2 (2%)	0	100	100
34	Dk	96/211 (46%)	91 (95%)	5 (5%)	0	100	100
35	DL	72/161 (45%)	62 (86%)	6 (8%)	4 (6%)	2	20
35	DI	105/161 (65%)	101 (96%)	4 (4%)	0	100	100
36	Dm	85/124 (68%)	79 (93%)	6 (7%)	0	100	100
37	DG	139/349 (40%)	135 (97%)	4 (3%)	0	100	100
38	DH	207/310 (67%)	190 (92%)	13 (6%)	4 (2%)	8	40
39	HD	304/309 (98%)	267 (88%)	27 (9%)	10 (3%)	4	29
40	HE	259/308 (84%)	252 (97%)	7 (3%)	0	100	100
41	HG	341/395 (86%)	329 (96%)	12 (4%)	0	100	100
42	HH	601/782 (77%)	575 (96%)	26 (4%)	0	100	100
43	HF	64/71 (90%)	62 (97%)	2 (3%)	0	100	100
44	HI	297/346 (86%)	267 (90%)	18 (6%)	12 (4%)	3	25
45	HJ	285/323 (88%)	268 (94%)	14 (5%)	3 (1%)	14	52
46	PD	126/142 (89%)	122 (97%)	4 (3%)	0	100	100
47	PG	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
48	g	104/233 (45%)	99 (95%)	4 (4%)	1 (1%)	15	54
49	j	120/135 (89%)	117 (98%)	1 (1%)	2 (2%)	9	43
50	n	993/1454 (68%)	894 (90%)	80 (8%)	19 (2%)	8	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	s	91/244 (37%)	82 (90%)	7 (8%)	2 (2%)	6	37
52	u	113/144 (78%)	105 (93%)	5 (4%)	3 (3%)	5	33
53	a	430/1581 (27%)	386 (90%)	39 (9%)	5 (1%)	13	50
54	d	154/270 (57%)	143 (93%)	9 (6%)	2 (1%)	12	48
55	f	163/246 (66%)	149 (91%)	12 (7%)	2 (1%)	13	50
56	i	69/146 (47%)	65 (94%)	2 (3%)	2 (3%)	4	31
57	m	110/131 (84%)	106 (96%)	4 (4%)	0	100	100
58	q	543/651 (83%)	484 (89%)	52 (10%)	7 (1%)	12	48
59	z	93/600 (16%)	84 (90%)	6 (6%)	3 (3%)	4	30
60	b	111/200 (56%)	109 (98%)	1 (1%)	1 (1%)	17	56
61	c	255/311 (82%)	241 (94%)	14 (6%)	0	100	100
62	e	98/178 (55%)	92 (94%)	4 (4%)	2 (2%)	7	39
63	l	120/178 (67%)	115 (96%)	5 (4%)	0	100	100
64	o	152/788 (19%)	136 (90%)	12 (8%)	4 (3%)	5	34
65	h	188/268 (70%)	165 (88%)	15 (8%)	8 (4%)	2	24
66	k	110/117 (94%)	96 (87%)	12 (11%)	2 (2%)	8	41
67	r	190/208 (91%)	180 (95%)	6 (3%)	4 (2%)	7	38
68	t	189/212 (89%)	169 (89%)	16 (8%)	4 (2%)	7	38
69	v	132/200 (66%)	116 (88%)	10 (8%)	6 (4%)	2	24
70	p	756/841 (90%)	704 (93%)	50 (7%)	2 (0%)	41	76
71	w	1332/1368 (97%)	1262 (95%)	66 (5%)	4 (0%)	41	76
72	x	877/989 (89%)	828 (94%)	44 (5%)	5 (1%)	25	65
73	y	206/747 (28%)	196 (95%)	9 (4%)	1 (0%)	29	68
74	NC	101/128 (79%)	93 (92%)	5 (5%)	3 (3%)	4	31
74	NG	105/128 (82%)	94 (90%)	8 (8%)	3 (3%)	4	31
75	ND	93/126 (74%)	91 (98%)	1 (1%)	1 (1%)	14	52
75	NH	93/126 (74%)	89 (96%)	3 (3%)	1 (1%)	14	52
All	All	22102/36357 (61%)	20865 (94%)	1075 (5%)	162 (1%)	26	62

All (162) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	DA	498	PRO

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Mol	Chain	Res	Type
4	DA	1158	SER
8	NA	534	ARG
9	PA	1666	PRO
12	FB	229	HIS
29	DD	876	ALA
30	DE	452	ARG
31	DF	68	THR
31	DF	69	SER
31	DF	442	PRO
38	DH	115	GLN
38	DH	141	PRO
35	DL	73	ASN
39	HD	54	ARG
39	HD	214	LYS
39	HD	220	PRO
39	HD	237	PRO
49	j	31	PRO
50	n	154	ILE
50	n	363	GLU
50	n	1351	PRO
50	n	1355	PRO
53	a	502	MET
54	d	187	LEU
55	f	53	GLN
58	q	131	SER
65	h	100	PHE
65	h	130	ARG
65	h	167	ARG
65	h	168	PRO
68	t	173	PRO
69	v	91	PHE
70	p	705	PRO
72	x	15	LYS
72	x	567	MET
8	NE	636	LYS
74	NG	1017	VAL
74	NC	841	THR
75	ND	1301	GLY
75	NH	1501	GLY
9	PA	1645	PRO
9	PA	1663	SER
29	DD	898	VAL

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Mol	Chain	Res	Type
30	DE	704	VAL
38	DH	129	VAL
35	DL	111	LEU
35	DL	114	LYS
39	HD	233	ILE
39	HD	234	SER
44	HI	96	THR
44	HI	108	VAL
44	HI	192	VAL
44	HI	236	GLN
44	HI	239	ASP
44	HI	310	PRO
50	n	169	LEU
50	n	254	VAL
50	n	1343	PRO
52	u	32	PRO
52	u	76	LEU
53	a	164	PRO
53	a	334	PRO
56	i	108	HIS
56	i	138	LEU
58	q	399	PRO
62	e	146	ILE
64	o	714	ASP
65	h	37	TYR
65	h	131	ILE
68	t	99	LYS
69	v	40	ALA
69	v	41	LYS
69	v	42	ILE
69	v	139	SER
70	p	727	PRO
71	w	1196	CYS
72	x	444	SER
72	x	564	SER
74	NC	843	HIS
31	DF	321	PRO
39	HD	56	SER
39	HD	289	SER
44	HI	106	SER
44	HI	277	LEU
45	HJ	237	MET

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Mol	Chain	Res	Type
50	n	150	PRO
50	n	153	ALA
50	n	1237	PRO
51	s	129	SER
52	u	84	ALA
53	a	487	LEU
54	d	170	GLY
58	q	91	SER
58	q	458	PRO
64	o	709	LYS
67	r	156	ASN
69	v	38	LYS
71	w	1203	MET
74	NC	840	THR
5	EA	153	ARG
31	DF	66	LEU
38	DH	137	GLY
32	DI	62	LYS
44	HI	264	ALA
45	HJ	286	ALA
49	j	34	GLN
50	n	165	SER
50	n	265	LEU
50	n	1255	PRO
51	s	105	LEU
53	a	208	VAL
58	q	127	LEU
58	q	134	ALA
59	z	533	PRO
60	b	100	GLN
62	e	147	ASN
67	r	113	ASN
68	t	172	ALA
72	x	566	GLU
73	y	226	LEU
14	NF	220	LYS
14	NF	301	GLY
74	NG	1042	SER
8	NA	438	PRO
31	DF	64	GLN
31	DF	440	PRO
39	HD	225	THR

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Mol	Chain	Res	Type
39	HD	265	MET
45	HJ	16	GLU
48	g	127	ARG
50	n	264	ALA
50	n	286	GLU
50	n	524	ASN
50	n	1352	PRO
55	f	55	LEU
59	z	540	LEU
64	o	721	LEU
66	k	79	HIS
66	k	81	GLY
68	t	129	VAL
71	w	32	ASP
74	NG	1018	SER
4	DA	506	ASP
31	Df	411	VAL
35	DL	72	PRO
44	HI	82	GLY
44	HI	212	PHE
50	n	164	GLY
58	q	89	GLN
65	h	188	GLY
71	w	1194	THR
8	NE	734	ARG
14	NF	219	ARG
59	z	537	PRO
67	r	94	GLY
67	r	153	VAL
50	n	528	HIS
9	PA	1648	PRO
44	HI	186	GLY
64	o	716	PRO
65	h	99	VAL
32	DI	85	SER

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	
3	BA	215/268 (80%)	215 (100%)	0	100	100
4	DA	495/1665 (30%)	460 (93%)	35 (7%)	14	41
5	EA	169/373 (45%)	167 (99%)	2 (1%)	71	84
6	FA	121/448 (27%)	119 (98%)	2 (2%)	60	78
7	HA	624/664 (94%)	623 (100%)	1 (0%)	93	96
9	PA	1302/1749 (74%)	1294 (99%)	8 (1%)	86	92
10	DB	876/1083 (81%)	859 (98%)	17 (2%)	57	75
11	EB	154/261 (59%)	153 (99%)	1 (1%)	86	92
12	FB	196/218 (90%)	195 (100%)	1 (0%)	88	93
13	HB	241/484 (50%)	241 (100%)	0	100	100
15	PB	994/1027 (97%)	992 (100%)	2 (0%)	93	96
16	HC	342/399 (86%)	340 (99%)	2 (1%)	86	92
17	PC	234/252 (93%)	234 (100%)	0	100	100
18	PE	191/192 (100%)	191 (100%)	0	100	100
19	PF	69/111 (62%)	68 (99%)	1 (1%)	67	81
20	PH	129/131 (98%)	129 (100%)	0	100	100
21	PI	103/112 (92%)	103 (100%)	0	100	100
22	PJ	53/56 (95%)	53 (100%)	0	100	100
23	PK	104/106 (98%)	103 (99%)	1 (1%)	76	86
24	PL	41/55 (74%)	41 (100%)	0	100	100
25	DP	154/293 (53%)	154 (100%)	0	100	100
26	DQ	105/324 (32%)	105 (100%)	0	100	100
27	DO	90/98 (92%)	88 (98%)	2 (2%)	52	71
28	Dc	113/833 (14%)	111 (98%)	2 (2%)	59	77
29	DD	144/815 (18%)	136 (94%)	8 (6%)	21	47
29	Dd	146/815 (18%)	146 (100%)	0	100	100
30	DE	478/657 (73%)	465 (97%)	13 (3%)	44	65
30	De	475/657 (72%)	473 (100%)	2 (0%)	91	94
31	DF	324/574 (56%)	300 (93%)	24 (7%)	13	40
31	Df	322/574 (56%)	314 (98%)	8 (2%)	47	68
32	DI	106/235 (45%)	99 (93%)	7 (7%)	16	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	Di	107/235 (46%)	107 (100%)	0	100	100
33	DJ	79/154 (51%)	78 (99%)	1 (1%)	69	82
33	Dj	83/154 (54%)	83 (100%)	0	100	100
34	Dk	87/182 (48%)	87 (100%)	0	100	100
35	DL	69/141 (49%)	60 (87%)	9 (13%)	4	20
35	DI	98/141 (70%)	98 (100%)	0	100	100
36	Dm	80/106 (76%)	79 (99%)	1 (1%)	69	82
37	DG	133/322 (41%)	125 (94%)	8 (6%)	19	46
38	DH	181/270 (67%)	172 (95%)	9 (5%)	24	50
39	HD	251/283 (89%)	232 (92%)	19 (8%)	13	39
40	HE	234/272 (86%)	229 (98%)	5 (2%)	53	72
41	HG	311/352 (88%)	310 (100%)	1 (0%)	92	95
42	HH	536/688 (78%)	533 (99%)	3 (1%)	86	92
43	HF	59/64 (92%)	59 (100%)	0	100	100
44	HI	258/298 (87%)	189 (73%)	69 (27%)	0	3
45	HJ	252/296 (85%)	177 (70%)	75 (30%)	0	2
46	PD	118/126 (94%)	117 (99%)	1 (1%)	81	89
47	PG	152/153 (99%)	151 (99%)	1 (1%)	84	90
48	g	102/216 (47%)	94 (92%)	8 (8%)	12	38
49	j	66/124 (53%)	65 (98%)	1 (2%)	65	80
50	n	807/1271 (64%)	784 (97%)	23 (3%)	42	64
51	s	83/208 (40%)	73 (88%)	10 (12%)	5	22
52	u	95/119 (80%)	92 (97%)	3 (3%)	39	61
53	a	393/1391 (28%)	318 (81%)	75 (19%)	1	9
54	d	139/230 (60%)	95 (68%)	44 (32%)	0	2
55	f	149/223 (67%)	130 (87%)	19 (13%)	4	20
56	i	71/133 (53%)	60 (84%)	11 (16%)	2	15
57	m	102/115 (89%)	101 (99%)	1 (1%)	76	86
58	q	491/577 (85%)	416 (85%)	75 (15%)	2	15
59	z	89/512 (17%)	76 (85%)	13 (15%)	3	17
60	b	102/163 (63%)	91 (89%)	11 (11%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
61	c	238/280 (85%)	225 (94%)	13 (6%)	21	48
62	e	94/152 (62%)	94 (100%)	0	100	100
63	l	116/155 (75%)	116 (100%)	0	100	100
64	o	141/697 (20%)	138 (98%)	3 (2%)	53	72
65	h	161/225 (72%)	127 (79%)	34 (21%)	1	7
66	k	94/98 (96%)	49 (52%)	45 (48%)	0	0
67	r	169/183 (92%)	143 (85%)	26 (15%)	2	15
68	t	166/178 (93%)	128 (77%)	38 (23%)	1	5
69	v	122/173 (70%)	87 (71%)	35 (29%)	0	3
70	p	681/736 (92%)	671 (98%)	10 (2%)	65	80
71	w	1203/1232 (98%)	1200 (100%)	3 (0%)	93	96
72	x	789/864 (91%)	777 (98%)	12 (2%)	65	80
73	y	175/601 (29%)	172 (98%)	3 (2%)	60	78
All	All	19036/30622 (62%)	18179 (96%)	857 (4%)	31	53

All (857) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	DA	347	ARG
4	DA	353	LEU
4	DA	357	GLU
4	DA	396	LEU
4	DA	397	LEU
4	DA	401	ASN
4	DA	403	LEU
4	DA	405	VAL
4	DA	464	TRP
4	DA	468	PHE
4	DA	470	ILE
4	DA	474	ASP
4	DA	482	ASP
4	DA	491	MET
4	DA	496	GLU
4	DA	500	LEU
4	DA	502	LEU
4	DA	503	ASP
4	DA	511	LEU

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Mol	Chain	Res	Type
4	DA	574	TYR
4	DA	639	LEU
4	DA	661	GLU
4	DA	667	THR
4	DA	711	ASP
4	DA	727	THR
4	DA	730	PHE
4	DA	828	GLU
4	DA	943	LYS
4	DA	970	ASN
4	DA	1052	ARG
4	DA	1058	HIS
4	DA	1059	GLN
4	DA	1062	TYR
4	DA	1165	LEU
4	DA	1203	GLU
5	EA	152	PHE
5	EA	185	GLU
6	FA	44	GLN
6	FA	151	ARG
7	HA	114	ASN
9	PA	61	ARG
9	PA	1643	TYR
9	PA	1646	THR
9	PA	1647	SER
9	PA	1657	TYR
9	PA	1663	SER
9	PA	1678	TYR
9	PA	1794	SER
10	DB	21	GLU
10	DB	24	ARG
10	DB	71	ARG
10	DB	140	GLU
10	DB	184	ASN
10	DB	225	TYR
10	DB	262	MET
10	DB	266	THR
10	DB	293	GLU
10	DB	431	LEU
10	DB	488	PHE
10	DB	559	LYS
10	DB	603	LYS

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Mol	Chain	Res	Type
10	DB	638	ARG
10	DB	640	VAL
10	DB	771	VAL
10	DB	818	THR
11	EB	114	LYS
12	FB	230	LYS
15	PB	199	LYS
15	PB	1064	ARG
16	HC	33	ARG
16	HC	399	ASP
19	PF	71	LEU
23	PK	47	LYS
27	DO	51	ARG
27	DO	82	ARG
28	Dc	24	ASP
28	Dc	106	VAL
30	De	365	ARG
30	De	663	ARG
31	Df	253	TYR
31	Df	261	THR
31	Df	272	VAL
31	Df	322	ASP
31	Df	323	VAL
31	Df	326	HIS
31	Df	356	THR
31	Df	421	ASP
29	DD	891	ILE
29	DD	894	LEU
29	DD	897	ASP
29	DD	924	LYS
29	DD	955	LYS
29	DD	958	LYS
29	DD	1006	LEU
29	DD	1009	LEU
36	Dm	31	LEU
30	DE	433	LYS
30	DE	450	ARG
30	DE	451	VAL
30	DE	507	VAL
30	DE	513	LEU
30	DE	515	LEU
30	DE	519	GLU

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Mol	Chain	Res	Type
30	DE	521	ASP
30	DE	593	PHE
30	DE	702	LEU
30	DE	745	GLU
30	DE	746	ASP
30	DE	747	LEU
31	DF	55	LEU
31	DF	60	MET
31	DF	62	LYS
31	DF	64	GLN
31	DF	66	LEU
31	DF	111	GLU
31	DF	114	LEU
31	DF	118	ILE
31	DF	120	THR
31	DF	209	LYS
31	DF	211	ARG
31	DF	258	ARG
31	DF	261	THR
31	DF	271	VAL
31	DF	280	ILE
31	DF	301	VAL
31	DF	319	LEU
31	DF	320	ARG
31	DF	339	GLN
31	DF	348	THR
31	DF	354	ARG
31	DF	391	LEU
31	DF	397	GLN
31	DF	427	LEU
37	DG	41	ASP
37	DG	81	ASP
37	DG	143	VAL
37	DG	147	ARG
37	DG	161	ASP
37	DG	181	TRP
37	DG	182	GLU
37	DG	183	ILE
38	DH	50	PHE
38	DH	116	ARG
38	DH	132	LYS
38	DH	135	THR

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Mol	Chain	Res	Type
38	DH	159	TYR
38	DH	160	ILE
38	DH	161	LYS
38	DH	164	THR
38	DH	169	VAL
32	DI	31	TYR
32	DI	32	GLU
32	DI	34	ARG
32	DI	63	LYS
32	DI	69	ASP
32	DI	82	SER
32	DI	83	PHE
33	DJ	192	LYS
35	DL	59	THR
35	DL	60	LYS
35	DL	61	LYS
35	DL	62	LYS
35	DL	63	LEU
35	DL	64	GLN
35	DL	110	THR
35	DL	111	LEU
35	DL	128	ILE
39	HD	10	LYS
39	HD	11	THR
39	HD	28	HIS
39	HD	41	ARG
39	HD	251	LEU
39	HD	252	GLN
39	HD	254	GLU
39	HD	263	LEU
39	HD	268	ARG
39	HD	272	LEU
39	HD	275	VAL
39	HD	276	ARG
39	HD	287	TYR
39	HD	288	THR
39	HD	293	CYS
39	HD	295	ARG
39	HD	304	LEU
39	HD	305	PHE
39	HD	306	TRP
40	HE	62	SER

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Mol	Chain	Res	Type
40	HE	64	ILE
40	HE	222	SER
40	HE	257	CYS
40	HE	258	HIS
41	HG	343	ARG
42	HH	198	ARG
42	HH	266	GLN
42	HH	692	LYS
44	HI	13	GLU
44	HI	15	LEU
44	HI	17	PHE
44	HI	20	GLU
44	HI	23	PHE
44	HI	30	ARG
44	HI	33	ASN
44	HI	34	THR
44	HI	36	GLN
44	HI	38	VAL
44	HI	45	LEU
44	HI	47	HIS
44	HI	48	ARG
44	HI	52	LYS
44	HI	55	ILE
44	HI	56	ASN
44	HI	57	ARG
44	HI	58	THR
44	HI	60	LEU
44	HI	63	ILE
44	HI	64	LYS
44	HI	66	LEU
44	HI	67	GLN
44	HI	69	LEU
44	HI	83	HIS
44	HI	84	LYS
44	HI	86	ASN
44	HI	88	SER
44	HI	96	THR
44	HI	101	ILE
44	HI	107	LEU
44	HI	108	VAL
44	HI	110	THR
44	HI	115	LYS

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Mol	Chain	Res	Type
44	HI	125	LEU
44	HI	132	TRP
44	HI	139	LYS
44	HI	141	ASN
44	HI	143	LEU
44	HI	160	LYS
44	HI	162	PHE
44	HI	164	SER
44	HI	166	ASN
44	HI	169	TYR
44	HI	170	THR
44	HI	173	VAL
44	HI	176	ARG
44	HI	177	TRP
44	HI	205	GLU
44	HI	206	LEU
44	HI	209	ARG
44	HI	210	VAL
44	HI	213	LEU
44	HI	223	THR
44	HI	237	TRP
44	HI	241	CYS
44	HI	245	ASP
44	HI	249	PHE
44	HI	257	LEU
44	HI	258	HIS
44	HI	259	HIS
44	HI	260	ILE
44	HI	261	PHE
44	HI	267	ASP
44	HI	272	ILE
44	HI	280	PRO
44	HI	284	ILE
44	HI	285	THR
44	HI	292	MET
45	HJ	3	HIS
45	HJ	7	GLN
45	HJ	8	LYS
45	HJ	10	HIS
45	HJ	11	TRP
45	HJ	12	THR
45	HJ	14	SER

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Mol	Chain	Res	Type
45	HJ	15	SER
45	HJ	21	ARG
45	HJ	28	ARG
45	HJ	32	CYS
45	HJ	33	LYS
45	HJ	37	ASN
45	HJ	41	LEU
45	HJ	44	ASP
45	HJ	55	THR
45	HJ	60	TYR
45	HJ	65	LEU
45	HJ	71	PHE
45	HJ	85	MET
45	HJ	92	LEU
45	HJ	93	ASN
45	HJ	94	ASN
45	HJ	97	MET
45	HJ	98	GLU
45	HJ	102	ARG
45	HJ	104	ILE
45	HJ	106	LEU
45	HJ	107	THR
45	HJ	108	CYS
45	HJ	113	CYS
45	HJ	114	LYS
45	HJ	115	VAL
45	HJ	134	LEU
45	HJ	136	GLN
45	HJ	140	LEU
45	HJ	143	ILE
45	HJ	145	GLU
45	HJ	148	LEU
45	HJ	149	LEU
45	HJ	150	LEU
45	HJ	151	ILE
45	HJ	153	GLN
45	HJ	154	LEU
45	HJ	155	ASN
45	HJ	158	LEU
45	HJ	160	VAL
45	HJ	165	ARG
45	HJ	166	PRO

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Mol	Chain	Res	Type
45	HJ	167	PHE
45	HJ	171	LEU
45	HJ	172	ILE
45	HJ	174	LEU
45	HJ	175	LYS
45	HJ	180	ILE
45	HJ	181	LEU
45	HJ	182	GLU
45	HJ	186	ILE
45	HJ	189	LYS
45	HJ	192	ASP
45	HJ	196	ASN
45	HJ	200	LEU
45	HJ	208	THR
45	HJ	211	GLN
45	HJ	226	ILE
45	HJ	227	THR
45	HJ	231	TYR
45	HJ	232	LEU
45	HJ	234	GLU
45	HJ	239	LYS
45	HJ	252	MET
45	HJ	262	TYR
45	HJ	266	ARG
45	HJ	279	ARG
45	HJ	288	ASN
46	PD	137	LYS
47	PG	81	LYS
48	g	72	PHE
48	g	126	TYR
48	g	130	GLN
48	g	132	ARG
48	g	137	VAL
48	g	155	LYS
48	g	159	ARG
48	g	171	LEU
49	j	82	LYS
50	n	154	ILE
50	n	159	ASP
50	n	166	TYR
50	n	168	ARG
50	n	169	LEU

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Mol	Chain	Res	Type
50	n	212	LEU
50	n	226	VAL
50	n	227	GLU
50	n	252	ILE
50	n	253	LEU
50	n	254	VAL
50	n	255	GLU
50	n	261	ASP
50	n	265	LEU
50	n	266	VAL
50	n	267	HIS
50	n	283	PHE
50	n	289	LEU
50	n	363	GLU
50	n	371	GLN
50	n	528	HIS
50	n	589	GLN
50	n	634	MET
51	s	90	GLU
51	s	93	TYR
51	s	105	LEU
51	s	109	LEU
51	s	112	LEU
51	s	116	ILE
51	s	127	LEU
51	s	128	ARG
51	s	131	ILE
51	s	137	LEU
52	u	49	ASN
52	u	76	LEU
52	u	79	GLU
53	a	58	LEU
53	a	62	LEU
53	a	66	GLN
53	a	70	LYS
53	a	71	VAL
53	a	72	THR
53	a	74	LEU
53	a	77	MET
53	a	78	THR
53	a	80	ARG
53	a	83	SER

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Mol	Chain	Res	Type
53	a	86	ARG
53	a	87	GLN
53	a	93	HIS
53	a	106	ASP
53	a	107	MET
53	a	108	PHE
53	a	109	TYR
53	a	111	GLU
53	a	128	HIS
53	a	131	ASN
53	a	133	VAL
53	a	145	LYS
53	a	148	ASP
53	a	160	LEU
53	a	162	ASN
53	a	167	ASN
53	a	168	LYS
53	a	173	MET
53	a	201	ASP
53	a	214	ARG
53	a	226	VAL
53	a	232	LEU
53	a	244	GLU
53	a	246	ASN
53	a	253	MET
53	a	254	ASN
53	a	258	THR
53	a	259	ILE
53	a	267	LYS
53	a	278	HIS
53	a	288	PHE
53	a	297	VAL
53	a	305	LEU
53	a	309	GLN
53	a	324	CYS
53	a	325	THR
53	a	327	ILE
53	a	329	LEU
53	a	332	THR
53	a	333	GLN
53	a	335	THR
53	a	339	LEU

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Mol	Chain	Res	Type
53	a	348	LEU
53	a	357	LEU
53	a	367	LEU
53	a	373	CYS
53	a	378	LYS
53	a	384	ASP
53	a	388	LEU
53	a	391	THR
53	a	400	HIS
53	a	414	GLN
53	a	421	ILE
53	a	427	ARG
53	a	432	GLU
53	a	433	ASP
53	a	437	LEU
53	a	438	LEU
53	a	441	GLU
53	a	443	CYS
53	a	501	CYS
53	a	502	MET
53	a	504	ILE
53	a	509	ARG
54	d	28	GLU
54	d	30	LEU
54	d	63	ASN
54	d	64	GLN
54	d	66	LEU
54	d	67	GLU
54	d	69	LEU
54	d	70	ILE
54	d	71	HIS
54	d	72	ARG
54	d	73	ASP
54	d	78	GLU
54	d	79	LEU
54	d	80	MET
54	d	81	LYS
54	d	82	LEU
54	d	85	ASN
54	d	91	HIS
54	d	92	GLU
54	d	98	LYS

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Mol	Chain	Res	Type
54	d	101	GLU
54	d	106	ASP
54	d	107	ILE
54	d	108	GLN
54	d	110	LEU
54	d	114	LEU
54	d	115	LYS
54	d	116	GLU
54	d	119	GLN
54	d	121	LEU
54	d	126	TYR
54	d	127	GLN
54	d	129	LYS
54	d	130	GLU
54	d	131	LYS
54	d	132	LEU
54	d	133	LYS
54	d	135	ILE
54	d	173	ARG
54	d	181	GLU
54	d	184	SER
54	d	186	LEU
54	d	187	LEU
54	d	189	GLN
55	f	16	VAL
55	f	19	SER
55	f	20	TRP
55	f	24	LEU
55	f	30	LEU
55	f	41	TYR
55	f	45	CYS
55	f	52	MET
55	f	53	GLN
55	f	56	THR
55	f	57	LEU
55	f	58	GLU
55	f	60	LEU
55	f	63	MET
55	f	64	VAL
55	f	114	VAL
55	f	117	SER
55	f	120	LEU

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Mol	Chain	Res	Type
55	f	192	PHE
56	i	86	ASP
56	i	87	LEU
56	i	88	ASN
56	i	90	LEU
56	i	94	PHE
56	i	95	GLN
56	i	104	MET
56	i	112	GLU
56	i	122	ARG
56	i	136	LYS
56	i	140	MET
57	m	59	LYS
58	q	1	MET
58	q	2	SER
58	q	7	VAL
58	q	8	ARG
58	q	16	GLU
58	q	19	VAL
58	q	28	GLU
58	q	29	THR
58	q	31	LEU
58	q	36	MET
58	q	91	SER
58	q	92	LEU
58	q	93	TRP
58	q	98	VAL
58	q	99	ARG
58	q	100	ASN
58	q	103	ARG
58	q	107	THR
58	q	109	MET
58	q	110	CYS
58	q	112	LEU
58	q	116	LEU
58	q	118	ILE
58	q	120	ARG
58	q	123	LYS
58	q	124	PHE
58	q	125	MET
58	q	128	ASP
58	q	131	SER

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Mol	Chain	Res	Type
58	q	132	GLN
58	q	133	ASP
58	q	138	LYS
58	q	139	GLN
58	q	141	PRO
58	q	143	THR
58	q	144	LEU
58	q	145	GLN
58	q	146	LEU
58	q	147	ILE
58	q	151	LYS
58	q	159	ILE
58	q	161	LEU
58	q	162	LYS
58	q	165	GLU
58	q	166	ARG
58	q	169	LYS
58	q	172	THR
58	q	184	ASN
58	q	185	SER
58	q	187	LEU
58	q	188	LEU
58	q	226	LYS
58	q	262	GLN
58	q	263	LYS
58	q	264	GLN
58	q	400	PHE
58	q	404	ARG
58	q	428	LEU
58	q	431	ILE
58	q	432	ILE
58	q	434	GLN
58	q	440	LEU
58	q	441	ARG
58	q	442	SER
58	q	443	ARG
58	q	448	ILE
58	q	451	LEU
58	q	518	GLU
58	q	629	LYS
58	q	631	GLU
58	q	634	ASN

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Mol	Chain	Res	Type
58	q	646	LEU
58	q	647	SER
58	q	649	CYS
58	q	651	LEU
59	z	492	ARG
59	z	528	LEU
59	z	540	LEU
59	z	551	ASP
59	z	564	ASN
59	z	567	GLN
59	z	572	ASN
59	z	579	CYS
59	z	582	LEU
59	z	591	LEU
59	z	594	LEU
59	z	598	CYS
59	z	599	LEU
60	b	57	VAL
60	b	60	TYR
60	b	74	LEU
60	b	82	LEU
60	b	92	GLN
60	b	103	ASP
60	b	122	LEU
60	b	126	CYS
60	b	132	ASP
60	b	168	ILE
60	b	184	LYS
61	c	16	GLN
61	c	41	ASN
61	c	44	THR
61	c	45	LEU
61	c	72	ARG
61	c	73	LEU
61	c	77	VAL
61	c	258	MET
61	c	274	ILE
61	c	275	LYS
61	c	276	LEU
61	c	300	ARG
61	c	301	THR
64	o	635	ASN

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Mol	Chain	Res	Type
64	o	697	HIS
64	o	704	VAL
65	h	7	GLN
65	h	15	LEU
65	h	16	LEU
65	h	17	SER
65	h	18	GLN
65	h	21	ASP
65	h	22	LEU
65	h	23	LYS
65	h	32	LYS
65	h	33	LEU
65	h	34	GLU
65	h	37	TYR
65	h	39	ARG
65	h	40	LEU
65	h	49	PHE
65	h	52	LEU
65	h	66	GLU
65	h	75	VAL
65	h	76	ILE
65	h	77	ILE
65	h	79	LEU
65	h	100	PHE
65	h	101	SER
65	h	102	HIS
65	h	110	ARG
65	h	111	THR
65	h	112	LYS
65	h	117	VAL
65	h	130	ARG
65	h	131	ILE
65	h	143	LEU
65	h	187	PHE
65	h	189	LYS
65	h	192	SER
66	k	8	ASN
66	k	10	ARG
66	k	11	LEU
66	k	12	ARG
66	k	14	LEU
66	k	15	GLU

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Mol	Chain	Res	Type
66	k	18	GLU
66	k	19	ARG
66	k	26	GLN
66	k	32	ILE
66	k	33	LEU
66	k	34	GLU
66	k	35	LEU
66	k	36	SER
66	k	37	LYS
66	k	40	THR
66	k	42	GLU
66	k	43	ARG
66	k	44	LEU
66	k	45	LEU
66	k	52	PHE
66	k	57	GLN
66	k	58	HIS
66	k	60	GLU
66	k	69	TYR
66	k	70	LEU
66	k	73	VAL
66	k	82	SER
66	k	83	SER
66	k	86	SER
66	k	87	ARG
66	k	88	LYS
66	k	90	CYS
66	k	91	GLN
66	k	92	MET
66	k	94	LEU
66	k	96	ARG
66	k	97	VAL
66	k	101	ARG
66	k	102	LEU
66	k	103	LYS
66	k	104	LEU
66	k	105	SER
66	k	109	ARG
66	k	114	MET
67	r	16	ILE
67	r	17	ASN
67	r	18	MET

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Mol	Chain	Res	Type
67	r	32	LEU
67	r	35	LEU
67	r	38	ARG
67	r	42	LEU
67	r	53	ASP
67	r	56	MET
67	r	60	LEU
67	r	73	ARG
67	r	85	LEU
67	r	88	LEU
67	r	93	MET
67	r	101	LEU
67	r	107	ASP
67	r	124	ARG
67	r	143	ILE
67	r	152	LEU
67	r	156	ASN
67	r	168	LEU
67	r	181	MET
67	r	197	VAL
67	r	200	GLU
67	r	202	ILE
67	r	206	ARG
68	t	1	MET
68	t	9	MET
68	t	16	SER
68	t	17	VAL
68	t	21	VAL
68	t	23	LEU
68	t	24	LEU
68	t	28	LEU
68	t	34	GLU
68	t	39	PHE
68	t	43	CYS
68	t	47	HIS
68	t	61	LYS
68	t	62	LEU
68	t	66	MET
68	t	67	HIS
68	t	78	LEU
68	t	79	PHE
68	t	80	GLU

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Mol	Chain	Res	Type
68	t	81	ASN
68	t	84	CYS
68	t	85	LEU
68	t	98	LEU
68	t	101	PHE
68	t	102	PHE
68	t	103	GLN
68	t	109	LYS
68	t	110	ILE
68	t	131	MET
68	t	138	ILE
68	t	149	VAL
68	t	162	GLN
68	t	173	PRO
68	t	179	ARG
68	t	193	TYR
68	t	196	LEU
68	t	200	ILE
68	t	204	GLN
69	v	22	LEU
69	v	37	ILE
69	v	38	LYS
69	v	39	THR
69	v	41	LYS
69	v	43	GLU
69	v	45	GLU
69	v	47	GLN
69	v	50	ARG
69	v	52	THR
69	v	55	GLU
69	v	56	GLN
69	v	58	ASN
69	v	60	GLU
69	v	61	MET
69	v	62	HIS
69	v	81	ASP
69	v	82	LEU
69	v	86	LEU
69	v	87	ILE
69	v	88	LEU
69	v	103	GLN
69	v	105	LEU

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Mol	Chain	Res	Type
69	v	108	LEU
69	v	110	GLU
69	v	114	ARG
69	v	115	LYS
69	v	118	THR
69	v	119	LEU
69	v	120	ARG
69	v	123	ILE
69	v	130	LEU
69	v	131	GLU
69	v	133	GLU
69	v	138	SER
70	p	13	MET
70	p	162	VAL
70	p	170	LEU
70	p	289	ASP
70	p	295	LEU
70	p	401	THR
70	p	443	LEU
70	p	564	LEU
70	p	699	CYS
70	p	710	ASP
71	w	22	PHE
71	w	425	MET
71	w	726	ASN
72	x	4	VAL
72	x	11	LEU
72	x	52	ILE
72	x	87	ASP
72	x	107	ARG
72	x	218	CYS
72	x	300	THR
72	x	443	LEU
72	x	477	TYR
72	x	803	ASP
72	x	812	LEU
72	x	897	LEU
73	y	220	MET
73	y	224	ARG
73	y	226	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (257) such sidechains are listed below:

Mol	Chain	Res	Type
4	DA	401	ASN
4	DA	409	HIS
4	DA	860	ASN
4	DA	896	GLN
4	DA	1073	GLN
5	EA	142	ASN
10	DB	30	HIS
10	DB	176	HIS
10	DB	183	GLN
10	DB	184	ASN
10	DB	235	HIS
10	DB	272	GLN
10	DB	348	GLN
10	DB	432	HIS
10	DB	439	HIS
10	DB	450	GLN
10	DB	509	ASN
10	DB	576	ASN
10	DB	750	GLN
10	DB	813	ASN
10	DB	908	GLN
10	DB	916	ASN
11	EB	89	HIS
12	FB	229	HIS
15	PB	1101	GLN
16	HC	352	GLN
16	HC	410	ASN
29	Dd	912	ASN
29	Dd	1069	ASN
30	De	246	HIS
30	De	294	ASN
30	De	320	HIS
30	De	336	HIS
30	De	424	GLN
30	De	616	HIS
31	Df	325	ASN
32	Di	81	GLN
34	Dk	186	HIS
35	DI	73	ASN
35	DI	105	HIS
29	DD	922	GLN
29	DD	925	ASN
29	DD	936	GLN

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Mol	Chain	Res	Type
29	DD	1053	GLN
29	DD	1075	HIS
36	Dm	107	ASN
30	DE	254	ASN
30	DE	268	HIS
30	DE	327	ASN
30	DE	351	GLN
30	DE	509	GLN
30	DE	616	HIS
30	DE	636	HIS
30	DE	640	ASN
31	DF	119	ASN
31	DF	214	HIS
31	DF	270	ASN
31	DF	273	GLN
31	DF	275	ASN
31	DF	316	GLN
31	DF	326	HIS
37	DG	48	HIS
38	DH	145	HIS
38	DH	173	GLN
32	DI	21	GLN
32	DI	38	GLN
32	DI	60	HIS
32	DI	81	GLN
32	DI	98	GLN
33	DJ	160	GLN
33	DJ	173	HIS
35	DL	117	GLN
35	DL	123	GLN
39	HD	24	ASN
39	HD	136	ASN
39	HD	294	HIS
39	HD	298	GLN
40	HE	65	GLN
40	HE	225	GLN
43	HF	36	GLN
44	HI	56	ASN
44	HI	67	GLN
44	HI	83	HIS
44	HI	86	ASN
44	HI	131	HIS

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Mol	Chain	Res	Type
44	HI	135	HIS
44	HI	166	ASN
45	HJ	7	GLN
45	HJ	37	ASN
45	HJ	100	HIS
45	HJ	128	ASN
45	HJ	211	GLN
45	HJ	275	GLN
45	HJ	288	ASN
46	PD	66	ASN
46	PD	76	ASN
46	PD	141	GLN
47	PG	124	ASN
48	g	120	HIS
48	g	130	GLN
49	j	92	ASN
50	n	201	HIS
50	n	211	GLN
50	n	267	HIS
50	n	330	HIS
50	n	410	HIS
50	n	411	GLN
50	n	507	GLN
50	n	521	GLN
50	n	532	ASN
50	n	651	ASN
50	n	668	HIS
50	n	841	ASN
50	n	880	ASN
50	n	909	GLN
51	s	82	ASN
51	s	88	ASN
52	u	49	ASN
52	u	56	GLN
52	u	86	GLN
52	u	97	ASN
53	a	87	GLN
53	a	131	ASN
53	a	146	ASN
53	a	254	ASN
53	a	333	GLN
53	a	359	HIS

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Mol	Chain	Res	Type
53	a	377	ASN
53	a	413	HIS
53	a	439	GLN
53	a	459	ASN
54	d	63	ASN
54	d	64	GLN
54	d	71	HIS
54	d	85	ASN
54	d	111	GLN
54	d	113	GLN
54	d	119	GLN
54	d	127	GLN
54	d	191	ASN
55	f	84	GLN
55	f	107	GLN
55	f	127	GLN
56	i	70	HIS
56	i	85	GLN
56	i	108	HIS
56	i	117	GLN
57	m	80	GLN
57	m	90	ASN
57	m	106	GLN
57	m	116	GLN
58	q	139	GLN
58	q	262	GLN
58	q	310	GLN
58	q	321	GLN
58	q	394	HIS
58	q	402	HIS
58	q	411	GLN
58	q	434	GLN
58	q	437	HIS
58	q	461	GLN
58	q	496	ASN
58	q	506	HIS
58	q	519	GLN
58	q	533	GLN
58	q	539	GLN
58	q	547	GLN
58	q	565	ASN
58	q	611	GLN

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Mol	Chain	Res	Type
58	q	626	GLN
59	z	527	GLN
59	z	529	HIS
59	z	549	GLN
59	z	556	GLN
59	z	567	GLN
59	z	585	HIS
59	z	592	ASN
60	b	66	GLN
60	b	92	GLN
60	b	129	GLN
60	b	136	HIS
61	c	10	ASN
61	c	41	ASN
61	c	237	GLN
61	c	245	HIS
61	c	306	HIS
62	e	97	GLN
62	e	132	HIS
62	e	140	GLN
63	l	72	GLN
63	l	102	ASN
63	l	151	GLN
64	o	697	HIS
64	o	701	ASN
64	o	753	HIS
64	o	778	GLN
65	h	18	GLN
65	h	55	GLN
65	h	60	ASN
65	h	65	HIS
65	h	102	HIS
65	h	171	GLN
66	k	41	ASN
66	k	66	GLN
66	k	77	GLN
66	k	79	HIS
66	k	91	GLN
67	r	156	ASN
68	t	8	GLN
68	t	103	GLN
68	t	178	ASN

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Mol	Chain	Res	Type
68	t	204	GLN
69	v	16	GLN
69	v	32	ASN
69	v	62	HIS
69	v	103	GLN
70	p	63	HIS
70	p	80	HIS
70	p	225	ASN
70	p	272	ASN
70	p	282	HIS
70	p	387	HIS
70	p	400	GLN
70	p	435	GLN
70	p	598	ASN
70	p	619	GLN
70	p	751	GLN
71	w	203	ASN
71	w	378	GLN
71	w	421	HIS
71	w	513	ASN
71	w	726	ASN
71	w	783	GLN
71	w	822	HIS
71	w	851	ASN
71	w	874	HIS
71	w	921	HIS
71	w	923	ASN
71	w	925	HIS
71	w	972	HIS
71	w	1059	ASN
71	w	1134	GLN
71	w	1300	HIS
71	w	1320	ASN
72	x	8	GLN
72	x	49	GLN
72	x	179	HIS
72	x	217	GLN
72	x	356	ASN
72	x	361	ASN
72	x	380	ASN
72	x	402	ASN
72	x	404	GLN

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Mol	Chain	Res	Type
72	x	472	ASN
72	x	502	HIS
72	x	544	HIS
73	y	134	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 monosaccharides 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	7	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
79	SF4	HA	1000	7	-	-	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.

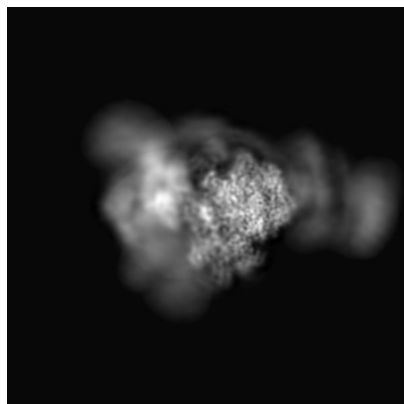
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34359. These allow visual inspection of the internal detail of the map and identification of artifacts.

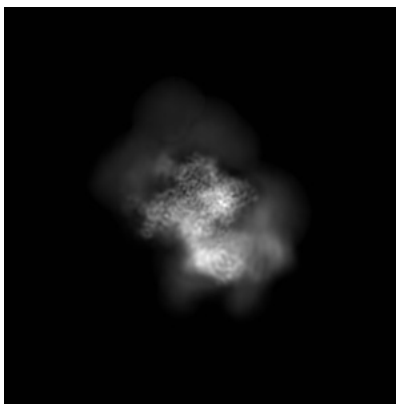
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

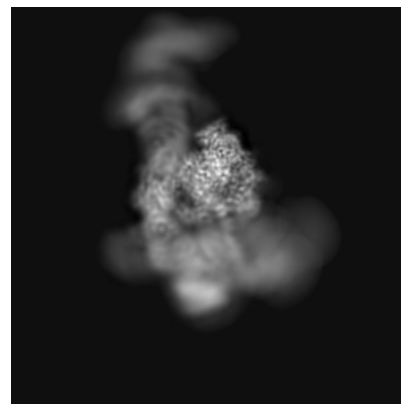
6.1.1 Primary map



X

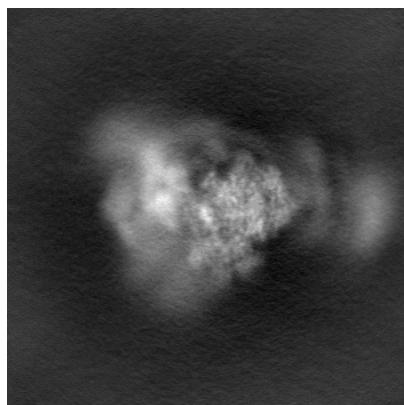


Y

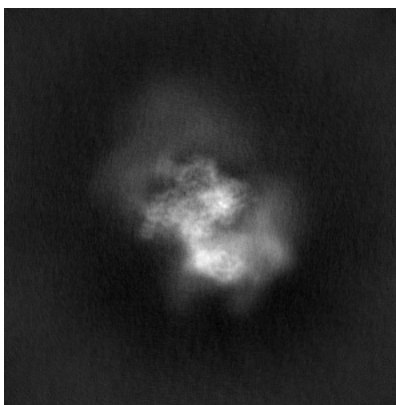


Z

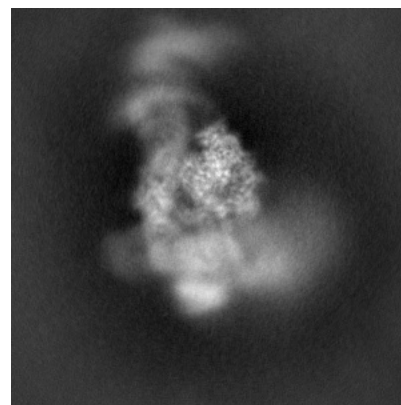
6.1.2 Raw map



X



Y

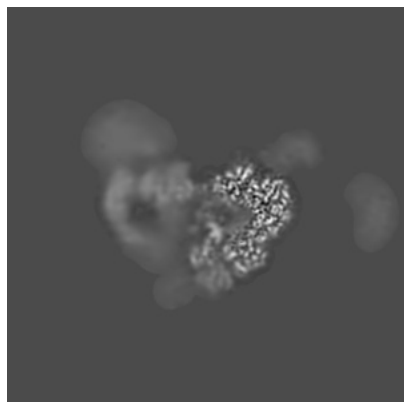


Z

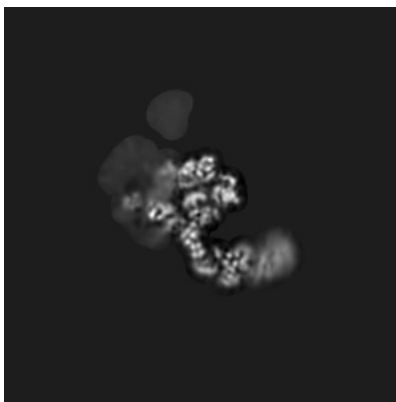
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

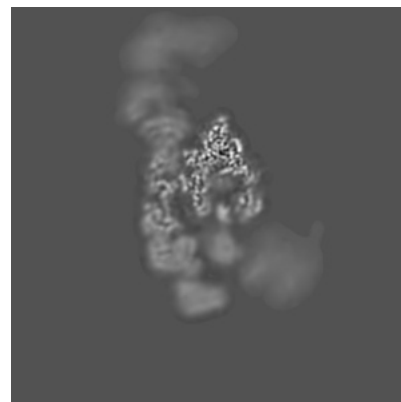
6.2.1 Primary map



X Index: 210

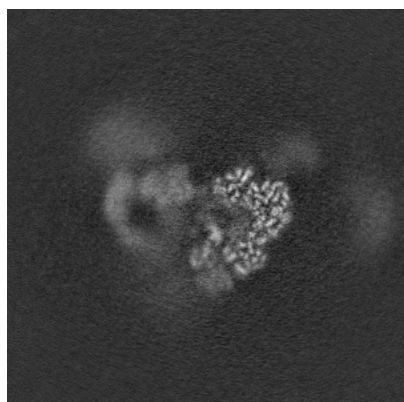


Y Index: 210

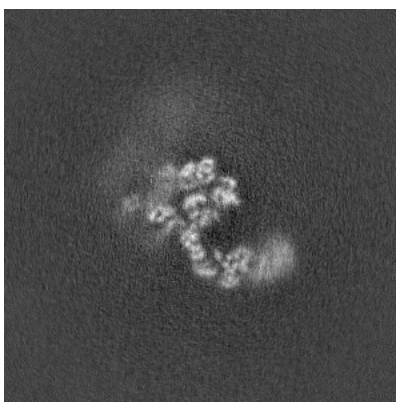


Z Index: 210

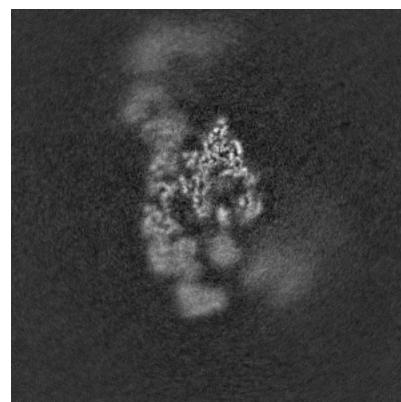
6.2.2 Raw map



X Index: 210



Y Index: 210

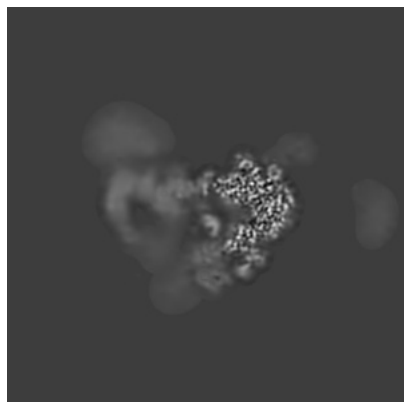


Z Index: 210

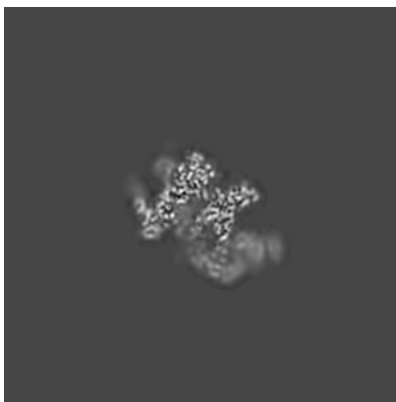
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

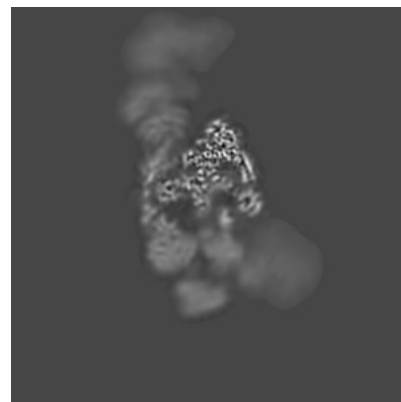
6.3.1 Primary map



X Index: 215

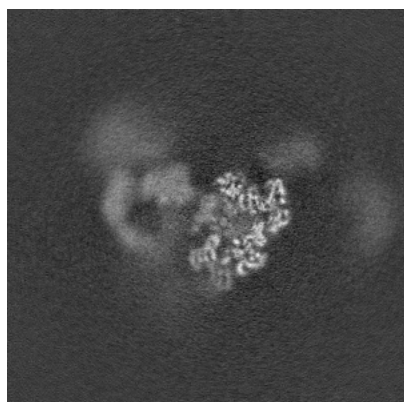


Y Index: 246

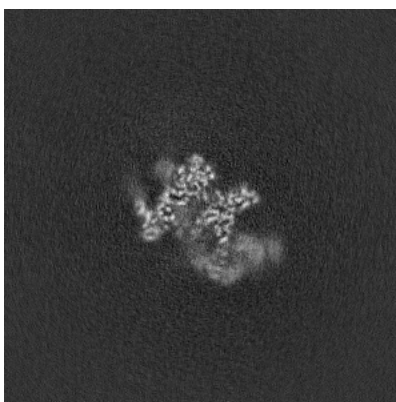


Z Index: 216

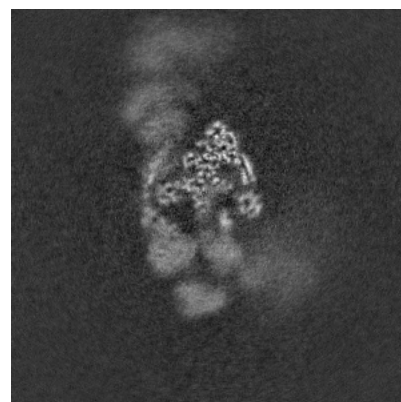
6.3.2 Raw map



X Index: 206



Y Index: 246

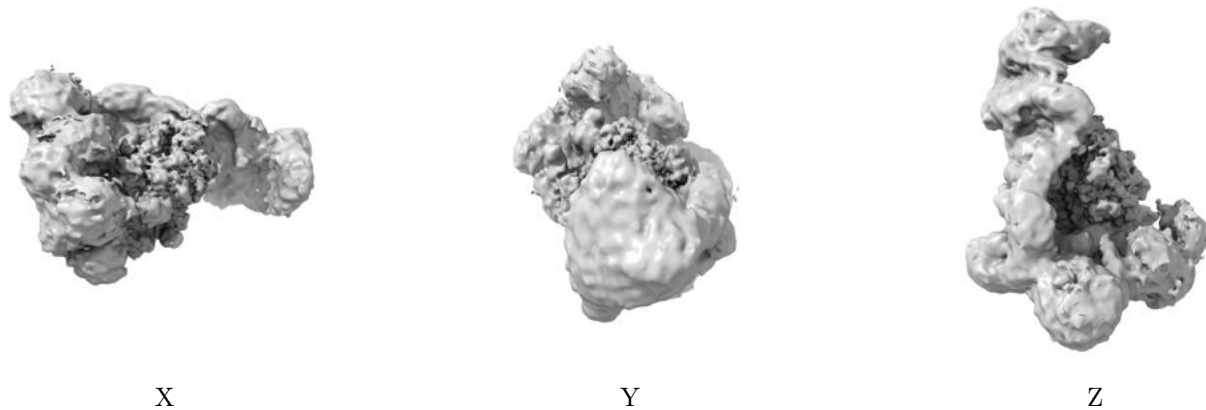


Z Index: 216

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

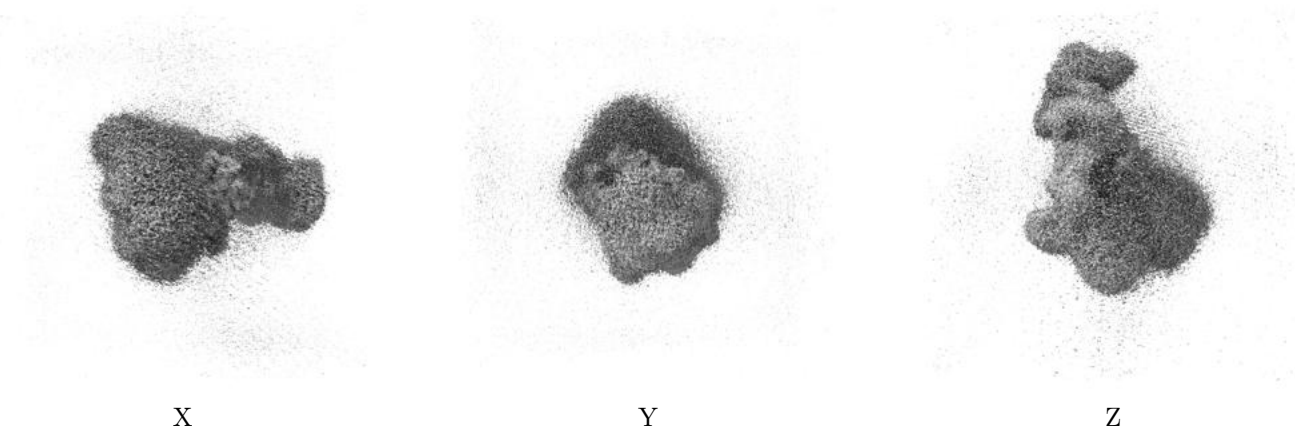
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.156. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

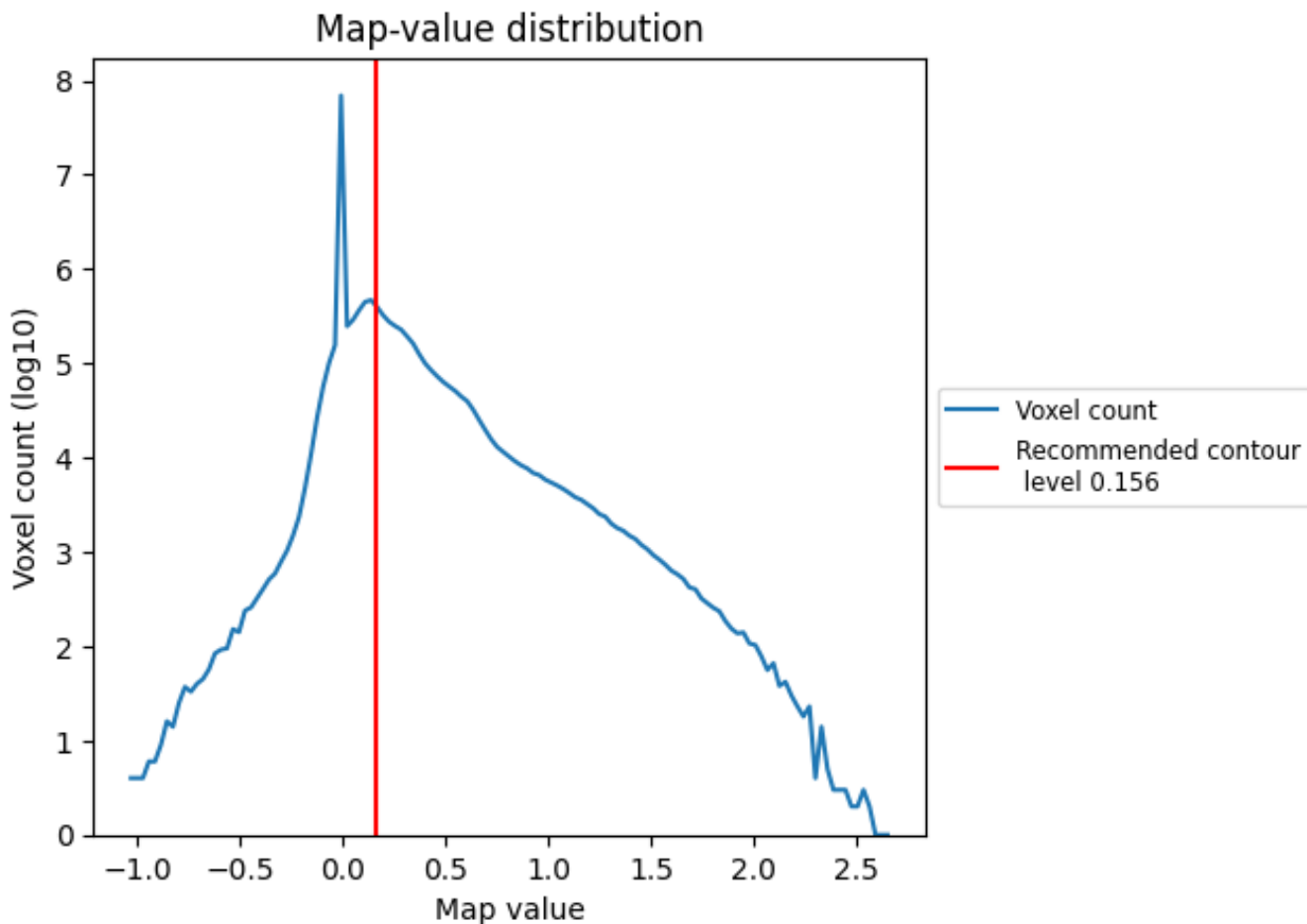
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

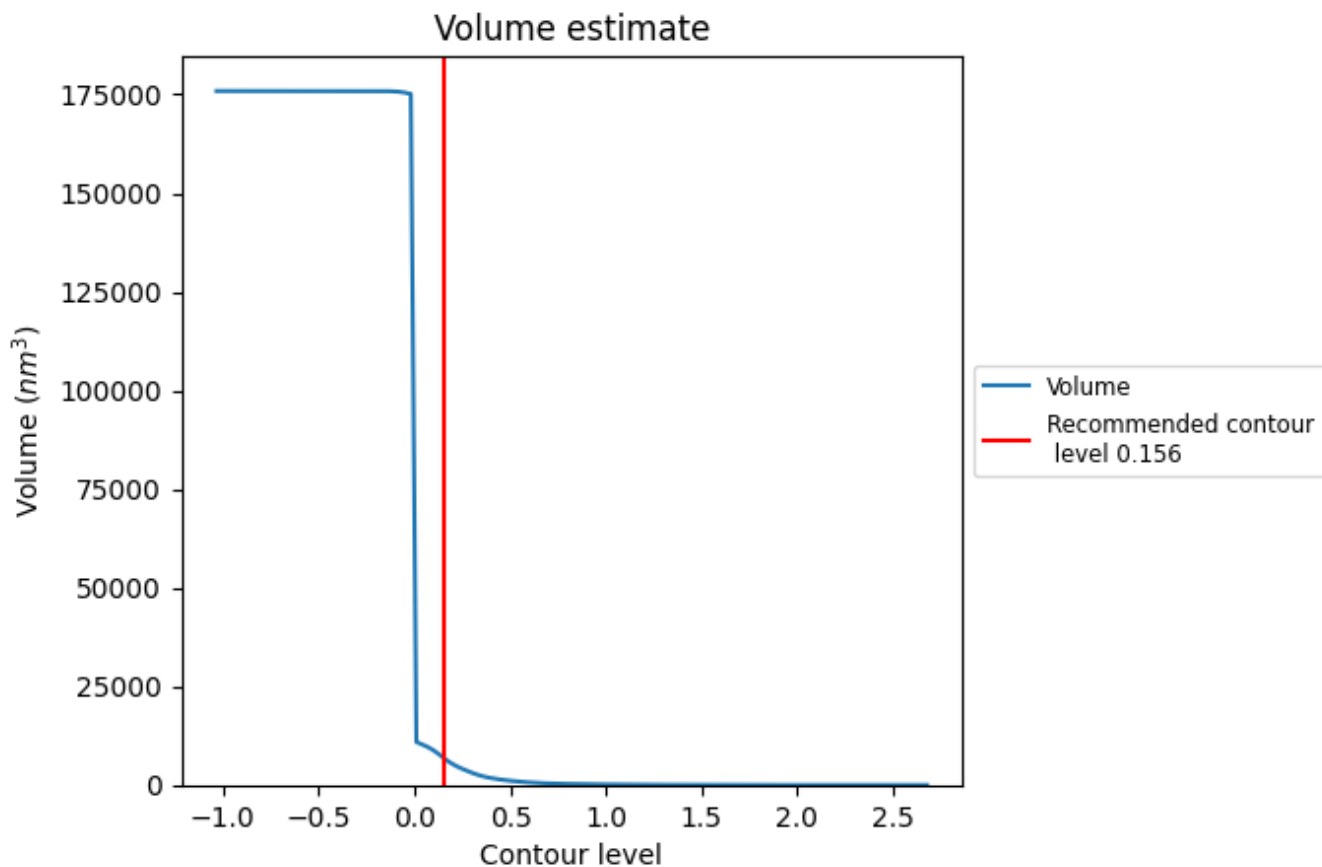
This section contains the results of statistical analysis of the map.

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.

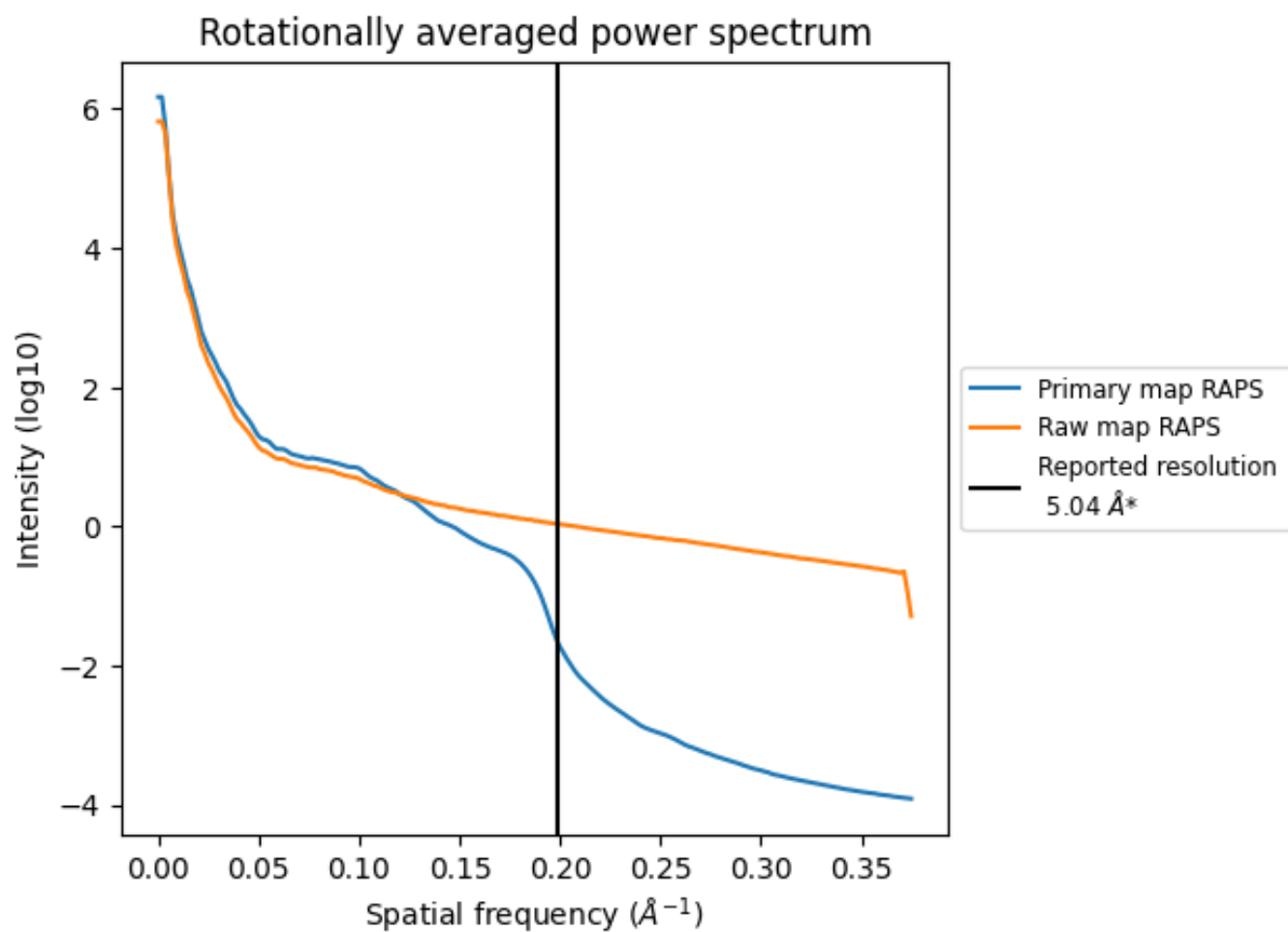
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 6707 nm^3 ; this corresponds to an approximate mass of 6058 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 i

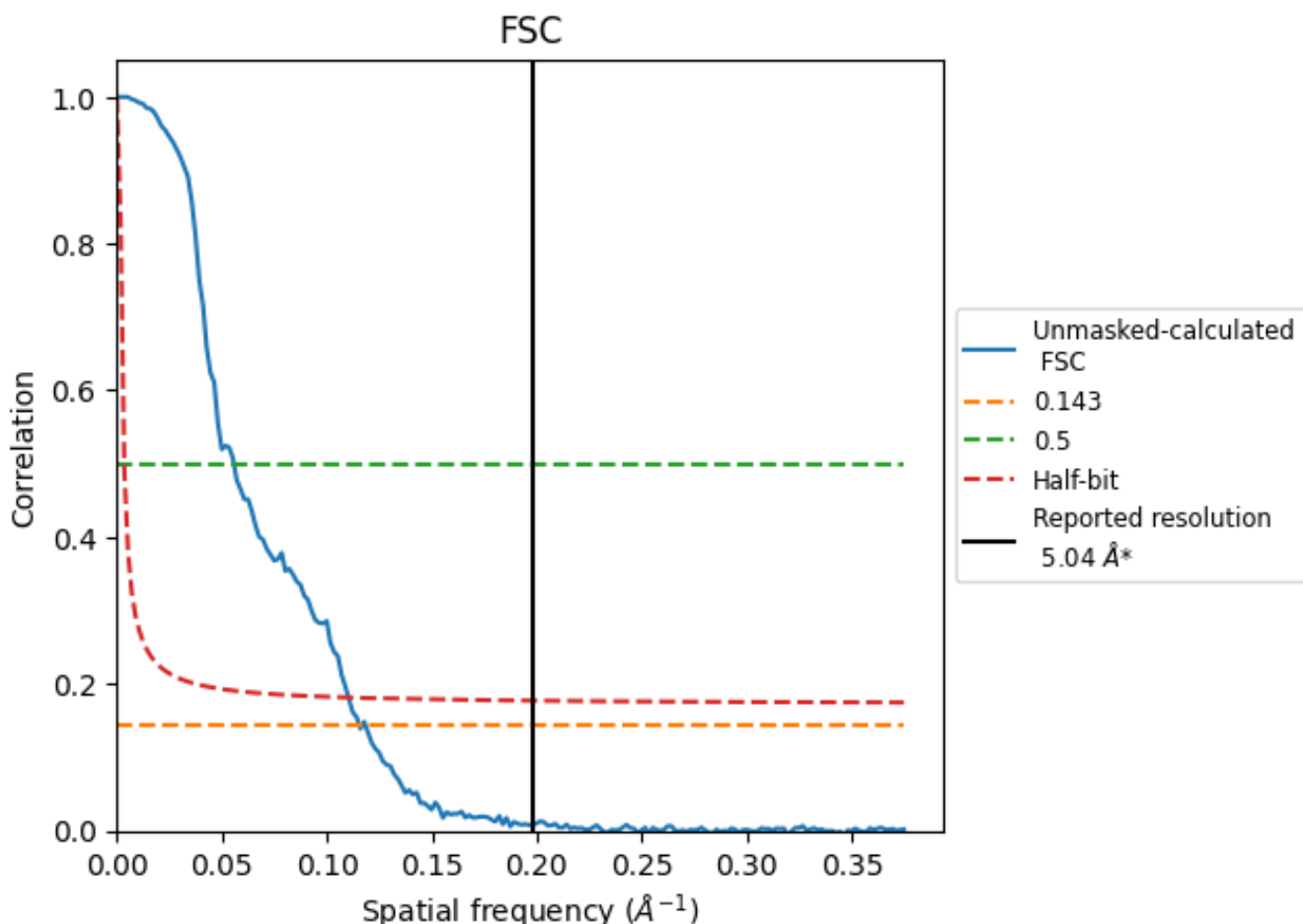


*Reported resolution corresponds to spatial frequency of 0.198 Å⁻¹

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 0.198 Å⁻¹

8.2 Resolution estimates [i](#)

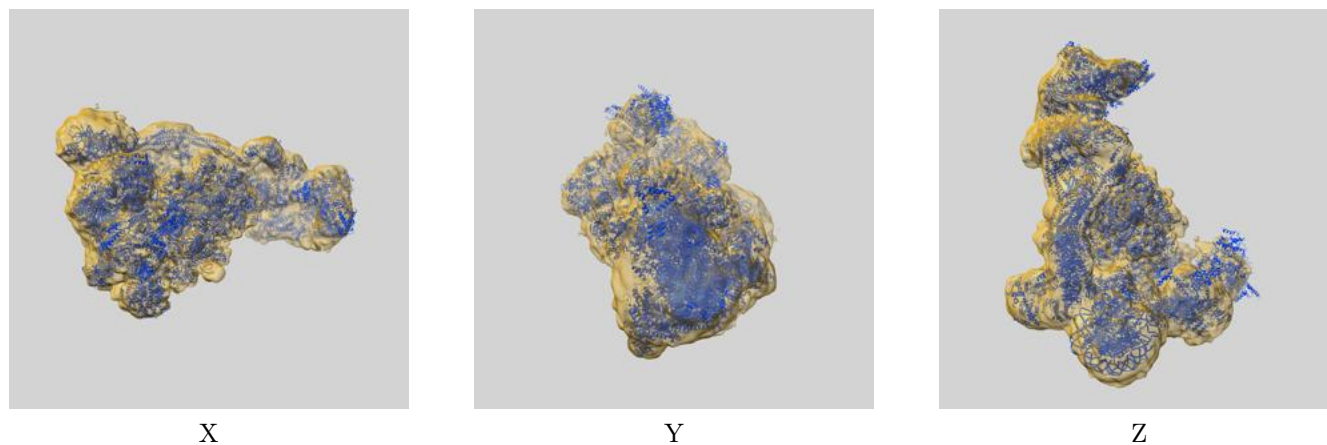
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.04	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.66	17.92	9.07

*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 8.66 differs from the reported value 5.04 by more than 10 %

9 Map-model fit [i](#)

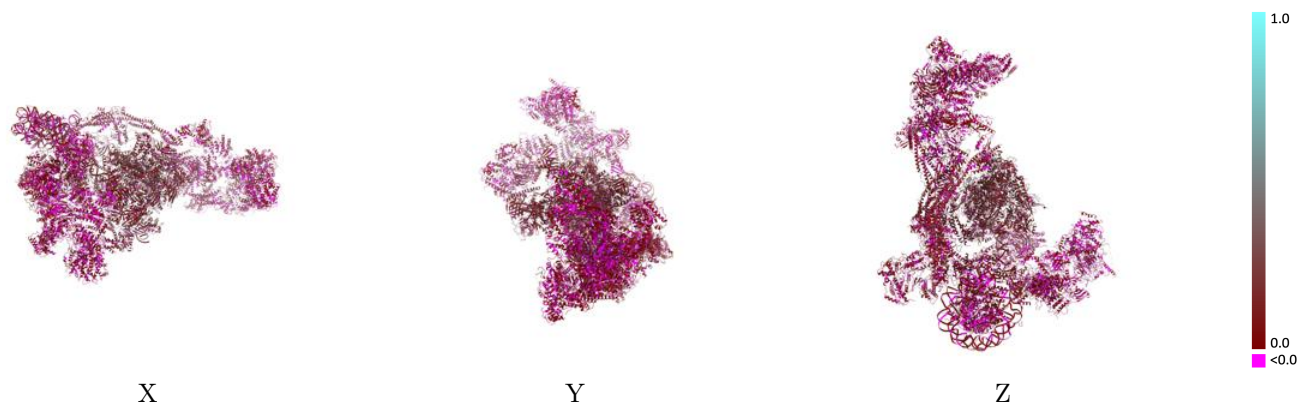
This section contains information regarding the fit between EMDB map EMD-34359 and PDB model 8GXQ. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



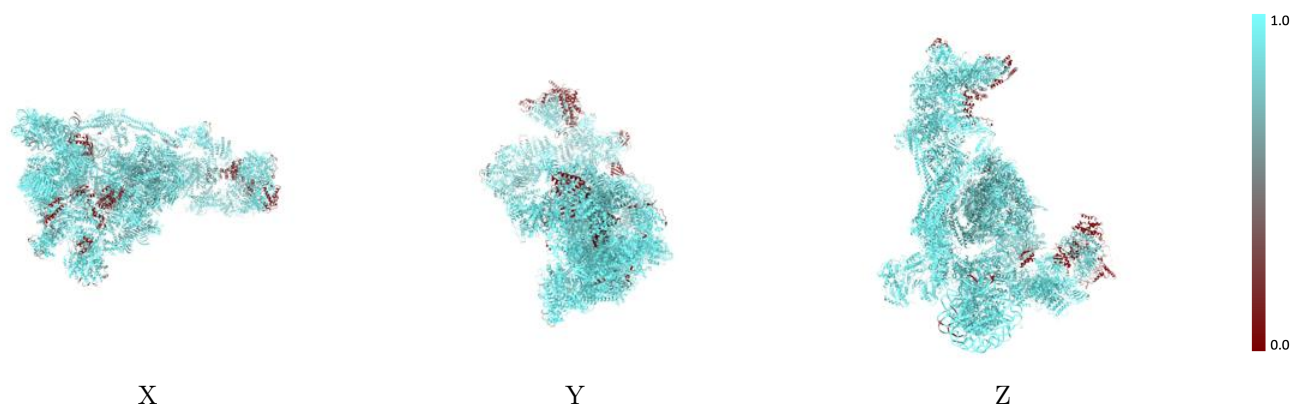
The images above show the 3D surface view of the map at the recommended contour level 0.156 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



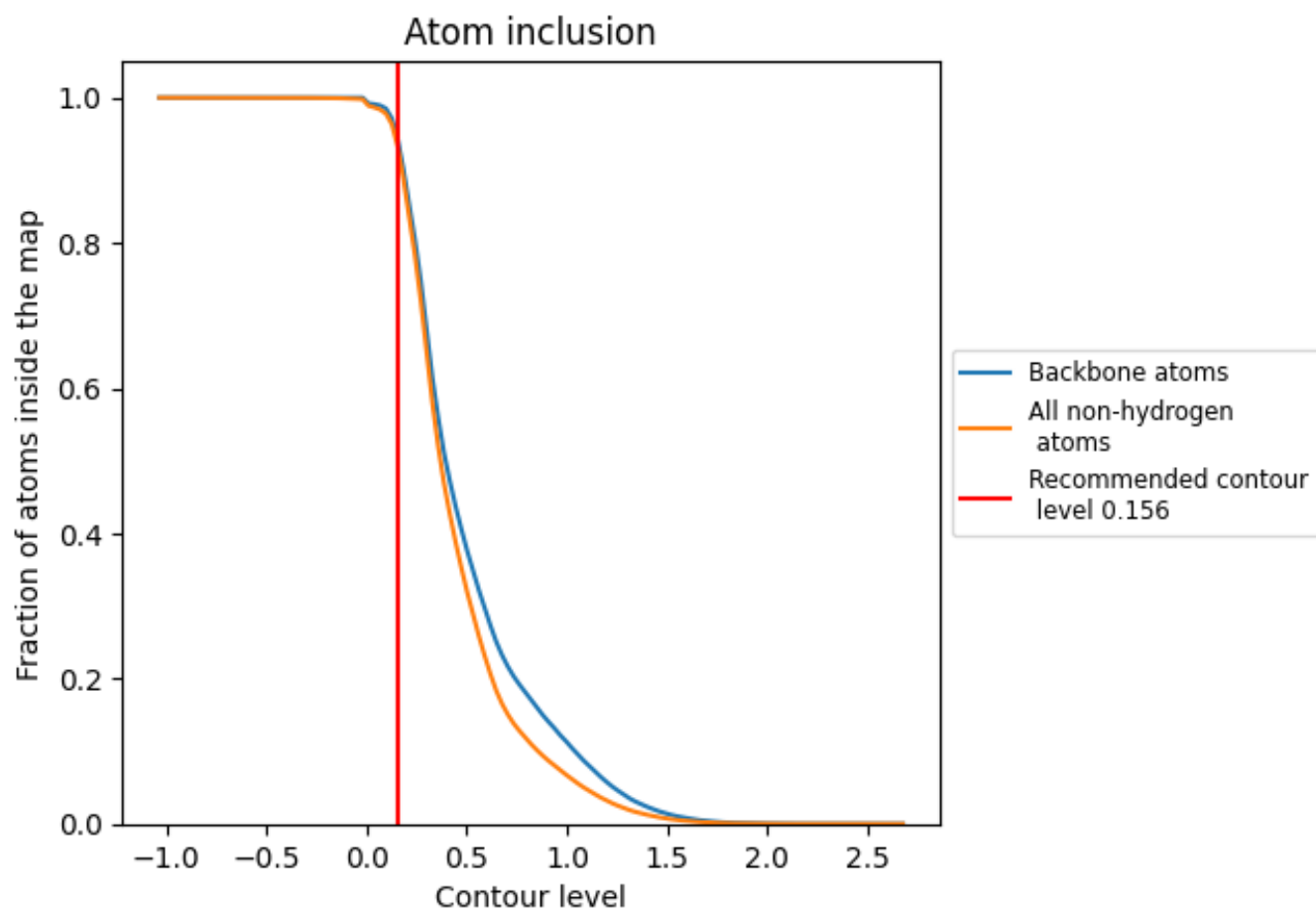
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.156).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (0.156) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9325	 0.0840
BA	 0.9712	 0.1780
DA	 0.8720	 0.0300
DB	 0.9937	 0.0440
DD	 0.9022	 0.0440
DE	 0.9785	 0.0430
DF	 0.9614	 0.0410
DG	 0.5765	 0.0150
DH	 0.9975	 0.0490
DI	 0.9198	 0.0360
DJ	 0.9958	 0.0450
DL	 0.8454	 0.0330
DO	 0.9734	 0.1060
DP	 0.9827	 0.1390
DQ	 0.9683	 0.1190
Dc	 0.6202	 0.0290
Dd	 0.3482	 0.0030
De	 0.6778	 0.0240
Df	 0.8639	 0.0370
Di	 0.8367	 0.0200
Dj	 0.6604	 0.0400
Dk	 0.2266	 -0.0000
DI	 0.6636	 0.0310
Dm	 0.2123	 0.0040
EA	 0.9498	 0.1120
EB	 0.9899	 0.1230
FA	 0.9874	 0.1360
FB	 0.9863	 0.1460
HA	 0.9975	 0.1150
HB	 0.9976	 0.0670
HC	 0.9968	 0.0860
HD	 0.9873	 0.1130
HE	 0.9976	 0.0490
HF	 1.0000	 0.0790
HG	 0.9989	 0.0690

























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Chain	Atom inclusion	Q-score
HH	 0.9944	 0.0730
HI	 0.9979	 0.0630
HJ	 0.9832	 0.0630
NA	 0.9799	 0.0770
NB	 1.0000	 0.0420
NC	 0.9842	 0.0110
ND	 0.9703	 0.0500
NE	 0.9941	 0.0710
NF	 1.0000	 0.0330
NG	 1.0000	 0.0430
NH	 1.0000	 0.0020
NX	 0.9068	 0.0340
NY	 0.9396	 0.0460
PA	 0.9563	 0.1830
PB	 0.9531	 0.2030
PC	 0.9628	 0.2080
PD	 0.9633	 0.1720
PE	 0.9786	 0.1790
PF	 0.9287	 0.2020
PG	 0.9722	 0.1580
PH	 0.9603	 0.1920
PI	 0.9780	 0.1840
PJ	 0.9535	 0.1870
PK	 0.9452	 0.2030
PL	 0.9804	 0.2110
X	 1.0000	 0.1830
Y	 0.9993	 0.1940
a	 0.9249	 0.0510
b	 0.9966	 0.0400
c	 0.9890	 0.0500
d	 0.9726	 0.0590
e	 0.9988	 0.0910
f	 0.9992	 0.1300
g	 1.0000	 0.1080
h	 0.9875	 0.1470
i	 0.8662	 0.0960
j	 1.0000	 0.0750
k	 0.9883	 0.1390
l	 1.0000	 0.0690
m	 1.0000	 0.0690
n	 0.9879	 0.0610
o	 0.9967	 0.0280

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Chain	Atom inclusion	Q-score
p	 0.9963	 0.0430
q	 0.9970	 0.0780
r	 0.9947	 0.1020
s	 1.0000	 0.0400
t	 0.9865	 0.0680
u	 1.0000	 0.0900
v	 0.9840	 0.1110
w	 0.7509	 0.0240
x	 0.9498	 0.0400
y	 0.9747	 0.0310
z	 0.9478	 0.0340