



## wwPDB EM Validation Summary Report ⓘ

Sep 28, 2024 – 07:50 pm BST

PDB ID : 6GCS  
EMDB ID : EMD-4384  
Title : Cryo-EM structure of respiratory complex I from *Yarrowia lipolytica*  
Authors : Parey, K.; Vonck, J.  
Deposited on : 2018-04-19  
Resolution : 4.32 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

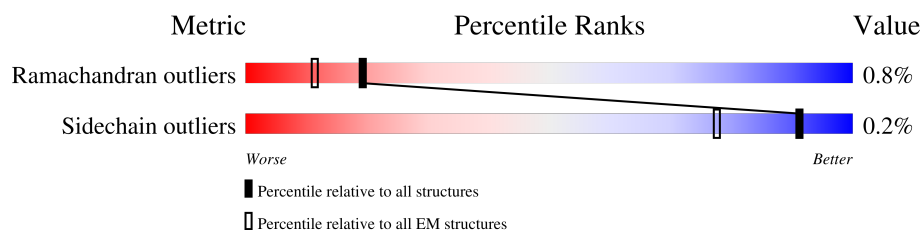
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance

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

The reported resolution of this entry is 4.32 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	728	<div> <div>34%</div> <div>94%</div> <div>5%</div> </div>
2	B	488	<div> <div>39%</div> <div>90%</div> <div>9%</div> </div>
3	C	466	<div> <div>33%</div> <div>87%</div> <div>11%</div> </div>
4	D	87	<div> <div>39%</div> <div>91%</div> <div>8%</div> </div>
5	E	375	<div> <div>37%</div> <div>83%</div> <div>15%</div> </div>
6	F	144	<div> <div>26%</div> <div>81%</div> <div>17%</div> </div>
7	G	281	<div> <div>14%</div> <div>78%</div> <div>17%</div> </div>
8	H	243	<div> <div>30%</div> <div>74%</div> <div>24%</div> </div>
9	I	229	<div> <div>18%</div> <div>77%</div> <div>21%</div> </div>

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Mol	Chain	Length	Quality of chain
10	J	198	
11	K	210	
12	L	86	
13	M	136	
14	O	109	
15	P	124	
16	Q	132	
17	R	109	
18	S	159	
19	U	172	
20	W	123	
21	X	169	
22	Y	161	
23	Z	137	
24	a	100	
25	b	64	
26	c	60	
27	d	92	
28	e	45	
29	f	87	
30	g	63	
31	h	138	
32	i	53	
33	j	93	
34	n	93	

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Mol	Chain	Length	Quality of chain
35	1	341	<div> <div>50%</div> <div>96%</div> <div>.</div> </div>
36	2	469	<div> <div>23%</div> <div>94%</div> <div>..</div> </div>
37	3	128	<div> <div>57%</div> <div>84%</div> <div>.. 14%</div> </div>
38	4	486	<div> <div>33%</div> <div>95%</div> <div>..</div> </div>
39	5	655	<div> <div>41%</div> <div>95%</div> <div>..</div> </div>
40	6	185	<div> <div>52%</div> <div>98%</div> <div>..</div> </div>
41	8	99	<div> <div>53%</div> <div>82%</div> <div>. 17%</div> </div>
42	9	89	<div> <div>22%</div> <div>66%</div> <div>34%</div> </div>

## 2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 55137 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 75-KDA PROTEIN (NUAM).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	689	Total	C	N	O	S	0	0
			5236	3251	921	1035	29		

- Molecule 2 is a protein called 51-KDA PROTEIN (NUBM).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	443	Total	C	N	O	S	0	0
			3380	2132	595	630	23		

- Molecule 3 is a protein called 49-KDA PROTEIN (NUCM).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	416	Total	C	N	O	S	0	0
			3190	2032	548	589	21		

- Molecule 4 is a protein called NIMM SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	80	Total	C	N	O	S	0	0
			559	352	103	101	3		

- Molecule 5 is a protein called NUEM SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	318	Total	C	N	O	S	0	0
			2546	1621	445	471	9		

- Molecule 6 is a protein called NUFM SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	119	Total	C	N	O	S	0	0
			915	578	155	181	1		

- Molecule 7 is a protein called 30-KDA PROTEIN (NUGM).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	232	Total	C	N	O	S	0	0
			1680	1069	294	313	4		

- Molecule 8 is a protein called 24-KDA SUBUNIT (NUHM).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	185	Total	C	N	O	S	0	0
			1385	870	232	266	17		

- Molecule 9 is a protein called TYKY SUBUNIT (NUIM).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	180	Total	C	N	O	S	0	0
			1441	915	240	276	10		

- Molecule 10 is a protein called NUJM SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	140	Total	C	N	O	S	0	0
			961	612	174	170	5		

- Molecule 11 is a protein called PSST SUBUNIT (NUKM).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	169	Total	C	N	O	S	0	0
			1339	852	235	238	14		

- Molecule 12 is a protein called ND4L SUBUNIT (NULM).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	86	Total	C	N	O	S	0	0
			668	447	106	112	3		

- Molecule 13 is a protein called NUMM SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	105	Total	C	N	O	S	0	0
			726	449	136	136	5		

- Molecule 14 is a protein called ACPM1 SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	77	Total	C	N	O	0	0
			591	373	93	125		

- Molecule 15 is a protein called NB4M SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	116	Total	C	N	O	S	0	0
			982	633	170	177	2		

- Molecule 16 is a protein called ACPM2 SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	85	Total	C	N	O	S	0	0
			648	405	103	138	2		

- Molecule 17 is a protein called NI2M SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	102	Total	C	N	O	S	0	0
			820	517	159	142	2		

- Molecule 18 is a protein called NESM SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	S	159	Total	C	N	O	0	0
			796	477	159	160		

- Molecule 19 is a protein called NUPM SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	158	Total	C	N	O	S	0	0
			1141	707	205	219	10		

- Molecule 20 is a protein called NB6M SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	118	Total	C	N	O	S	0	0
			929	590	174	160	5		

- Molecule 21 is a protein called NUXM SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	117	Total	C	N	O	S	0	0
			638	392	124	121	1		

- Molecule 22 is a protein called NUYM SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	115	Total	C	N	O	S	0	0
			957	610	173	172	2		

- Molecule 23 is a protein called NUZM SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	Z	137	Total	C	N	O	0	0
			686	411	137	138		

- Molecule 24 is a protein called NIAM SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	a	100	Total	C	N	O	0	0
			501	300	100	101		

- Molecule 25 is a protein called NEBM SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	b	64	Total	C	N	O	0	0
			321	192	64	65		

- Molecule 26 is a protein called NB2M SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	c	42	Total	C	N	O	0	0
			251	163	43	45		

- Molecule 27 is a protein called NIDM SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	89	Total	C	N	O	S	0	0
			752	467	136	146	3		

- Molecule 28 is a protein called NUUM SUBUNIT.



Mol	Chain	Residues	Atoms				AltConf	Trace
28	e	45	Total	C	N	O	0	0
			226	135	45	46		

- Molecule 29 is a protein called NI8M SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	80	Total	C	N	O	S	0
			629	394	119	115	1	0

- Molecule 30 is a protein called NI9M SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	g	60	Total	C	N	O		0
			492	328	88	76		0

- Molecule 31 is a protein called N7BM SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	h	130	Total	C	N	O	S	0
			1081	697	184	198	2	0

- Molecule 32 is a protein called UNKNOWN SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	i	53	Total	C	N	O		0
			266	159	53	54		0

- Molecule 33 is a protein called NB5M SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	j	73	Total	C	N	O		0
			436	266	87	83		0

- Molecule 34 is a protein called NUNM SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	n	93	Total	C	N	O		0
			466	279	93	94		0

- Molecule 35 is a protein called ND1 SUBUNIT (NU1M).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1	340	Total	C	N	O	S	0	0
			2608	1766	390	445	7		

- Molecule 36 is a protein called ND2 SUBUNIT (NU2M).

Mol	Chain	Residues	Atoms					AltConf	Trace
36	2	452	Total	C	N	O	S	0	0
			3376	2263	511	590	12		

- Molecule 37 is a protein called ND3 SUBUNIT (NU3M).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	3	110	Total	C	N	O	S	0	0
			871	600	129	140	2		

- Molecule 38 is a protein called ND4 SUBUNIT (NU4M).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	4	475	Total	C	N	O	S	0	0
			3312	2188	533	581	10		

- Molecule 39 is a protein called ND5 SUBUNIT (NU5M).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	5	639	Total	C	N	O	S	0	0
			4599	3032	723	817	27		

- Molecule 40 is a protein called ND6 SUBUNIT (NU6M).

Mol	Chain	Residues	Atoms					AltConf	Trace
40	6	183	Total	C	N	O	S	0	0
			1211	812	189	203	7		

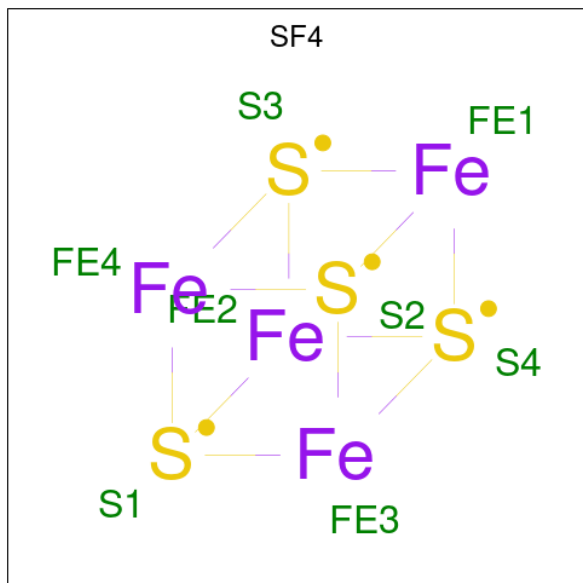
- Molecule 41 is a protein called NB8M SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	8	82	Total	C	N	O	S	0	0
			672	426	122	116	8		

- Molecule 42 is a protein called NIPM SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	9	59	Total	C	N	O	S	0	0
			468	290	85	87	6		

- Molecule 43 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



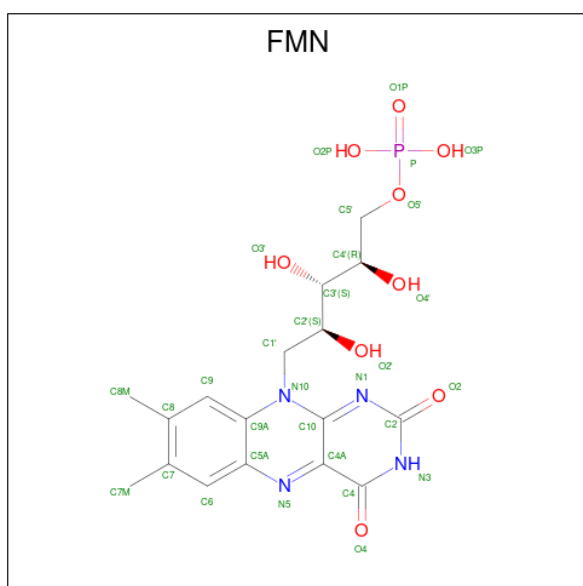
Mol	Chain	Residues	Atoms			AltConf
43	A	1	Total	Fe	S	0
			8	4	4	
43	A	1	Total	Fe	S	0
			8	4	4	
43	B	1	Total	Fe	S	0
			8	4	4	
43	I	1	Total	Fe	S	0
			8	4	4	
43	I	1	Total	Fe	S	0
			8	4	4	
43	K	1	Total	Fe	S	0
			8	4	4	

- Molecule 44 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).

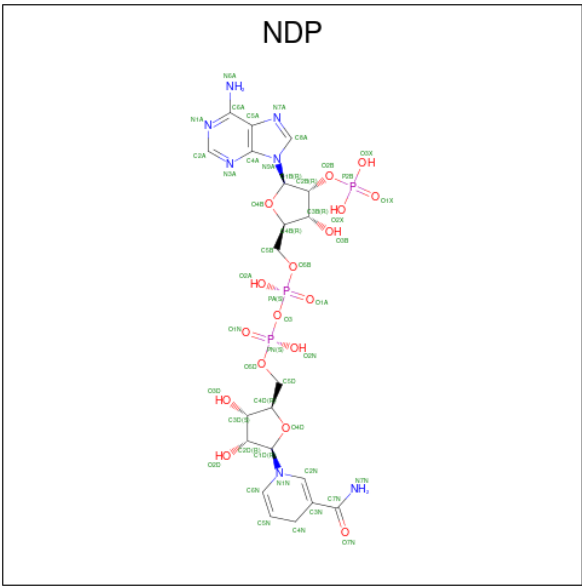


Mol	Chain	Residues	Atoms			AltConf
44	A	1	Total	Fe	S	0
			4	2	2	
44	H	1	Total	Fe	S	0
			4	2	2	

- Molecule 45 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).

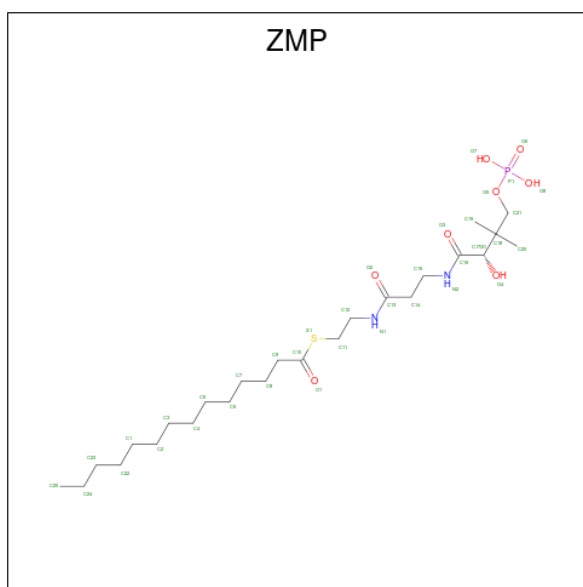


Mol	Chain	Residues	Atoms					AltConf
46	E	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 47 is ZINC ION (three-letter code: ZN) (formula: Zn).

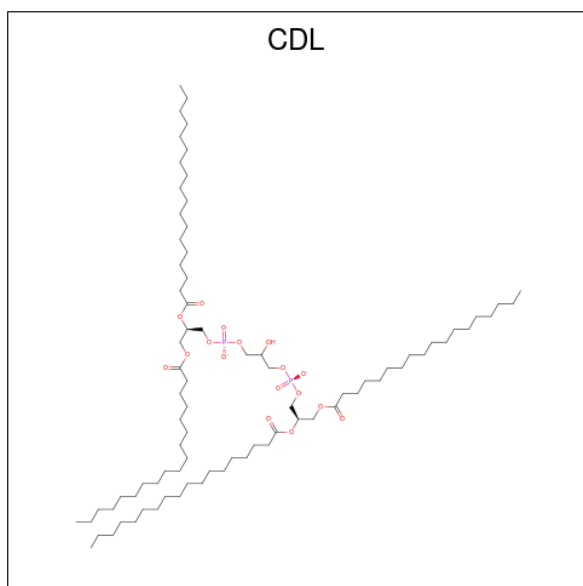
Mol	Chain	Residues	Atoms		AltConf
47	M	1	Total	Zn	0
			1	1	

- Molecule 48 is S-[2-( {N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>8</sub>PS).



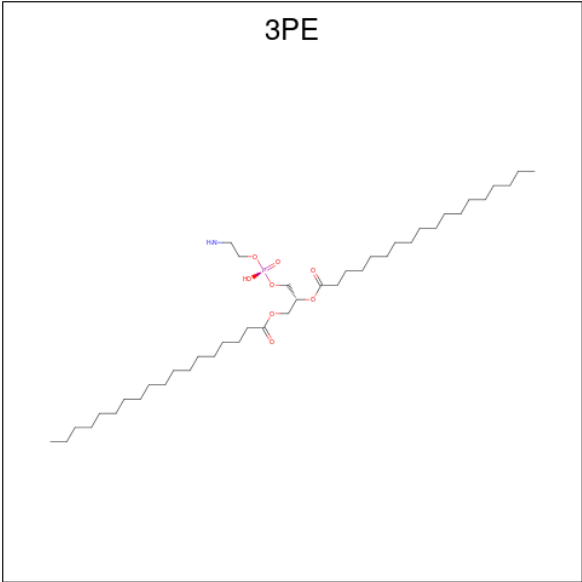
Mol	Chain	Residues	Atoms						AltConf
48	O	1	Total	C	N	O	P	S	0
			29	18	2	7	1	1	

- Molecule 49 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				AltConf
49	g	1	Total	C	O	P	
			83	64	17	2	0

- Molecule 50 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).

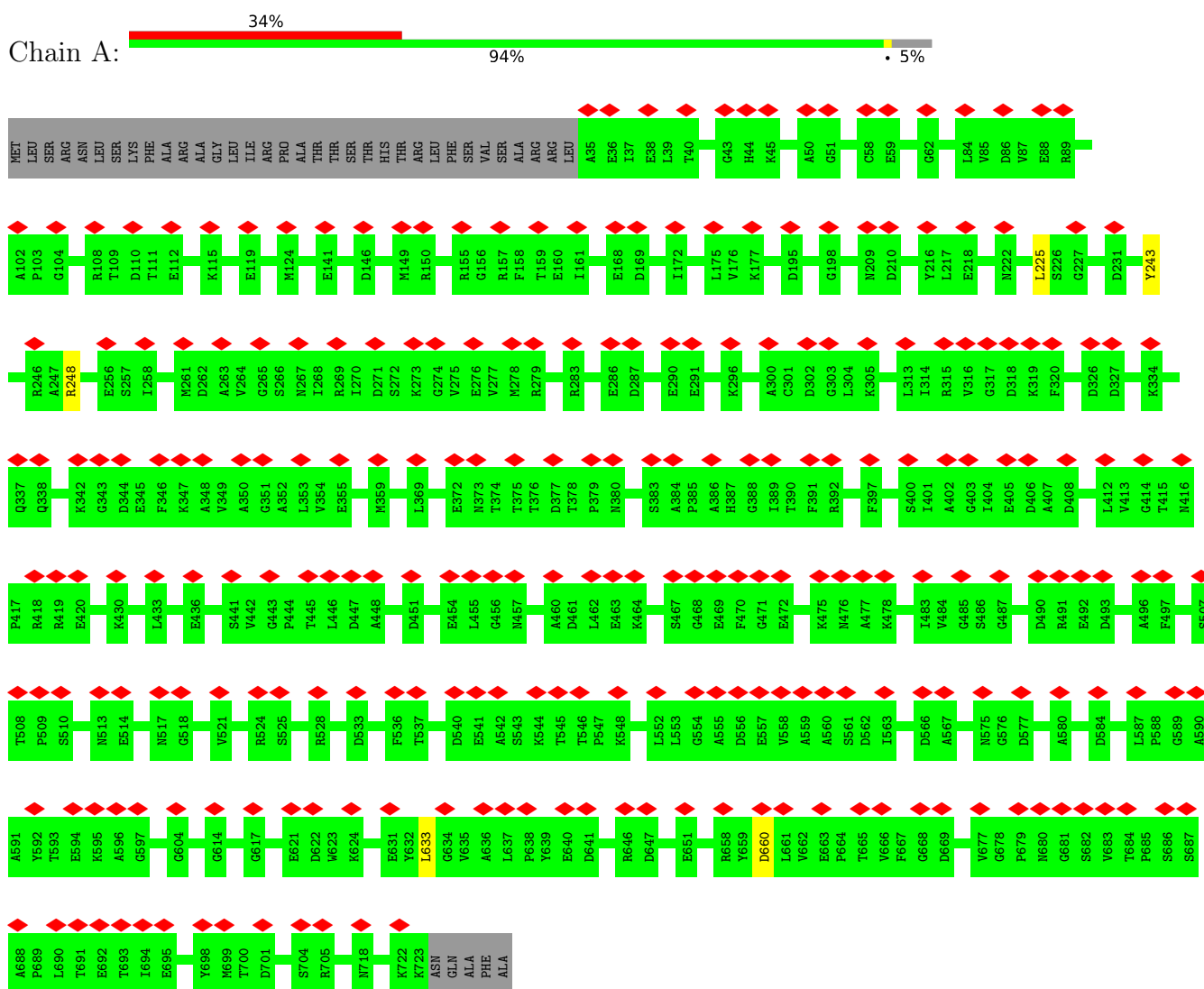


Mol	Chain	Residues	Atoms					AltConf
50	g	1	Total	C	N	O	P	0
			43	33	1	8	1	
50	1	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	4	1	Total	C	N	O	P	0
			43	33	1	8	1	

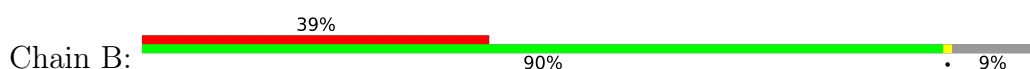
### 3 Residue-property plots

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

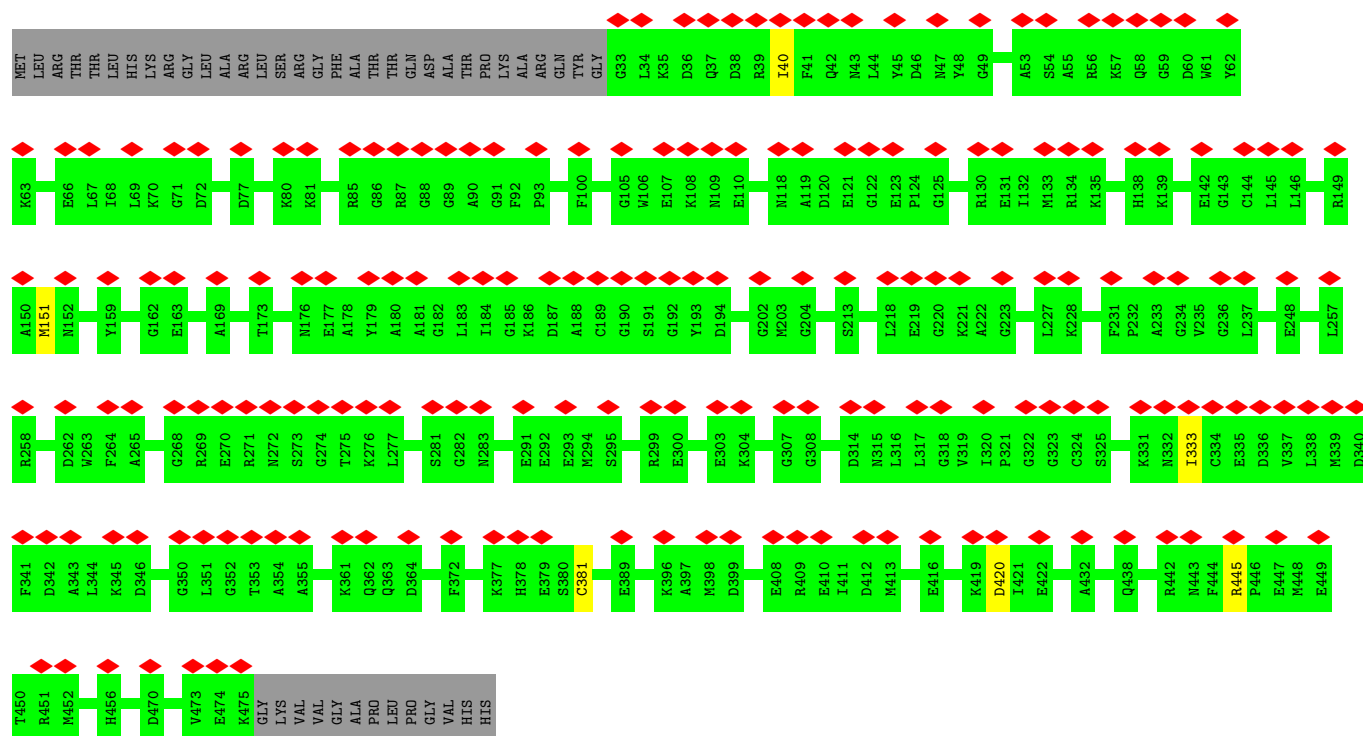
#### • Molecule 1: 75-KDA PROTEIN (NUAM)



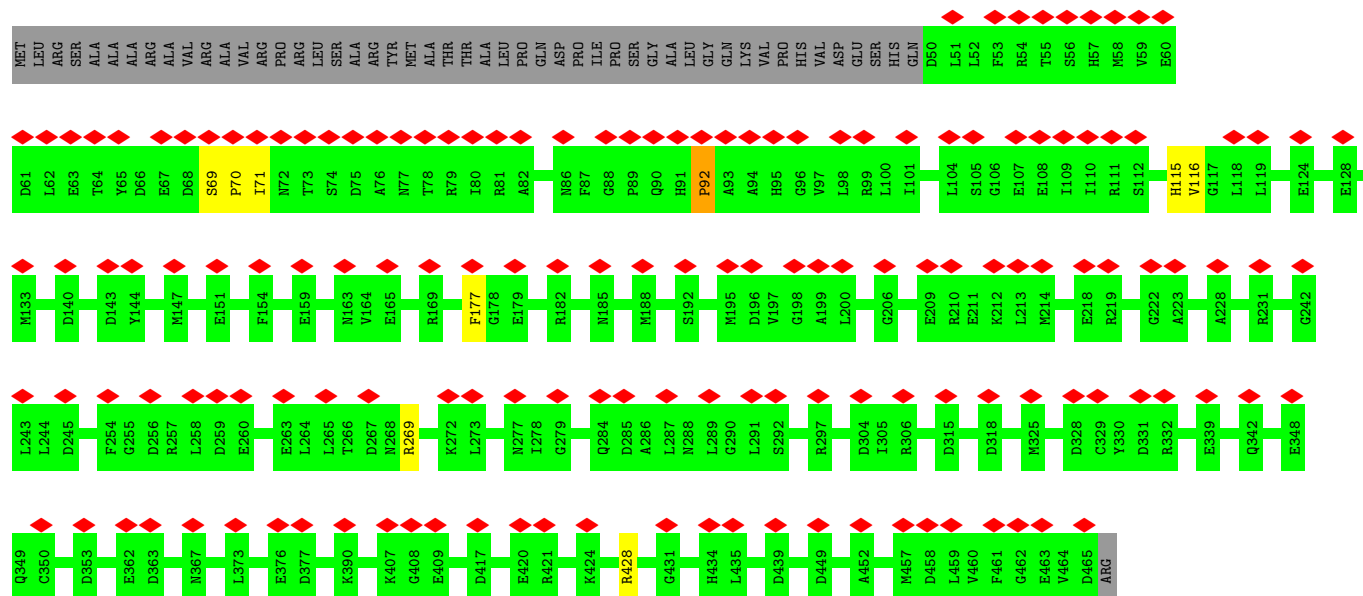
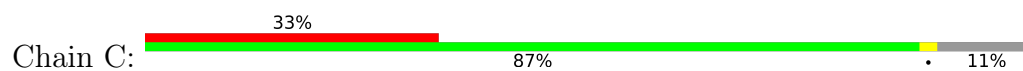
#### • Molecule 2: 51-KDA PROTEIN (NUBM)



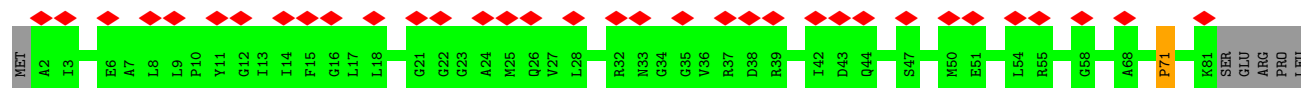
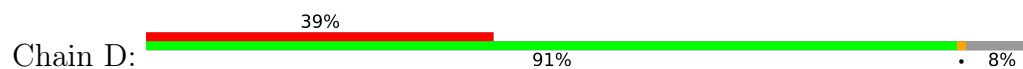




• Molecule 3: 49-KDA PROTEIN (NUCM)




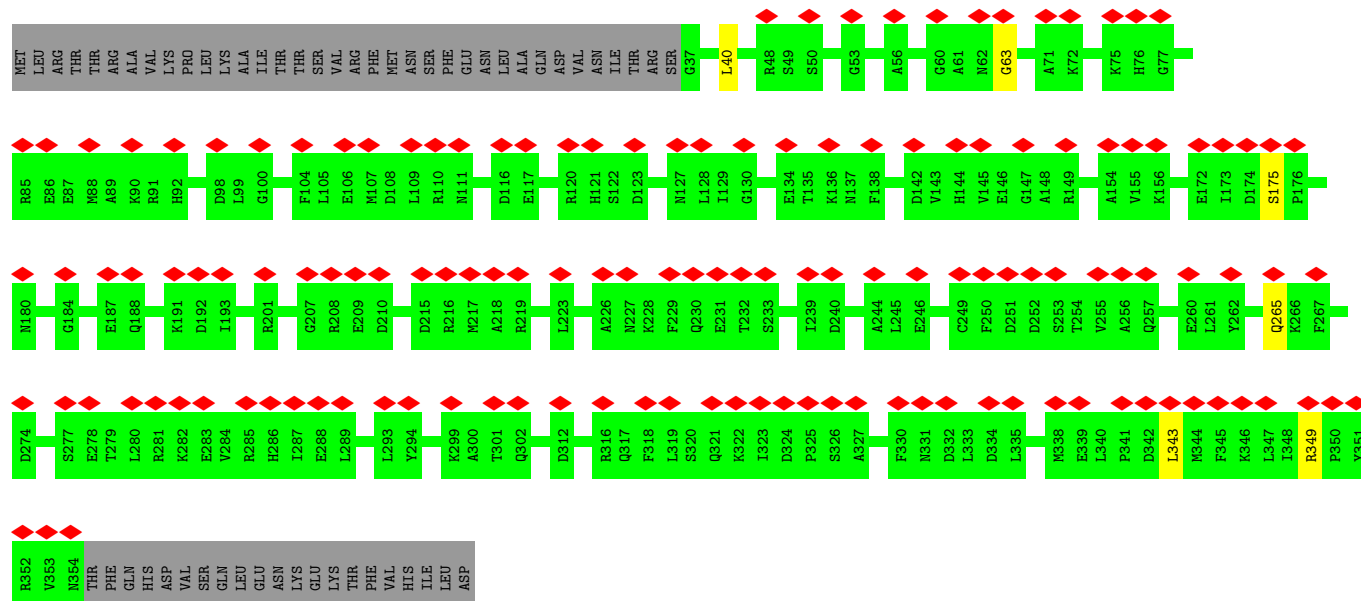
• Molecule 4: NIMM SUBUNIT




ILE

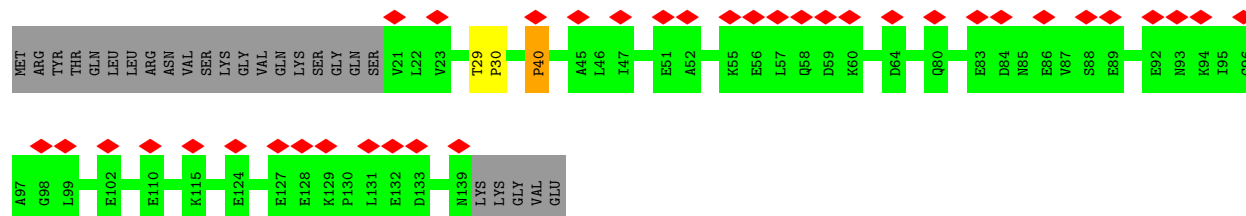
- Molecule 5: NUEM SUBUNIT

Chain E: 




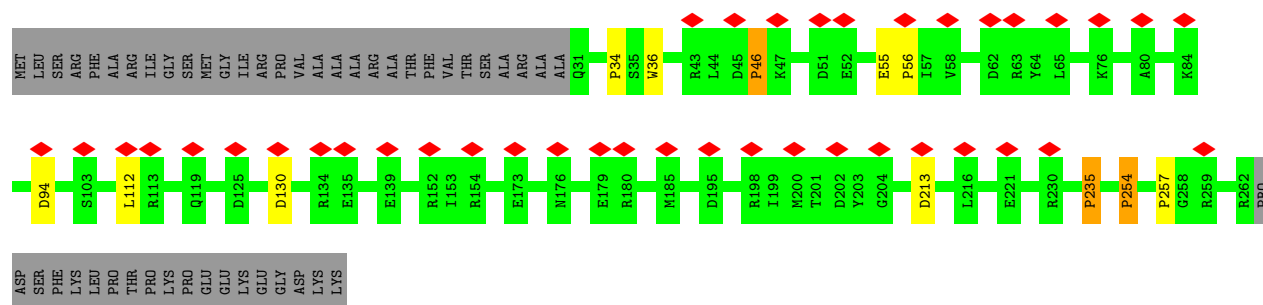
- Molecule 6: NUFM SUBUNIT

Chain F: 

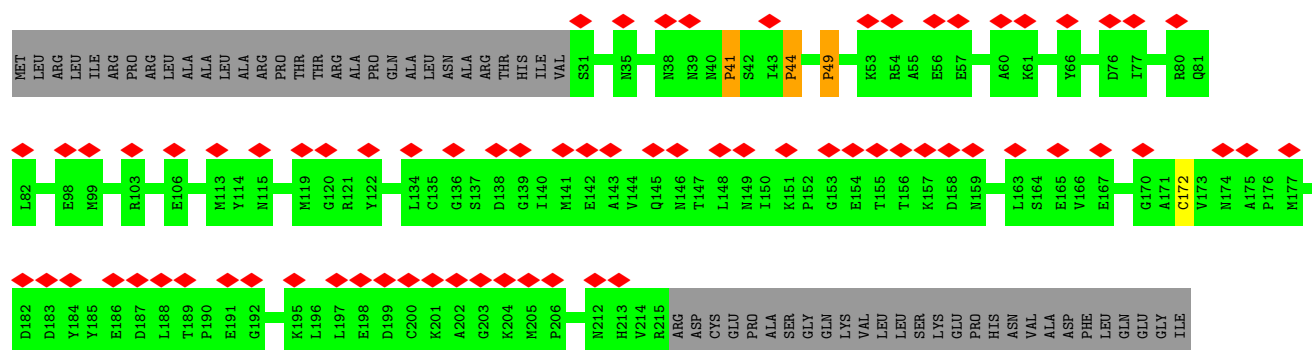
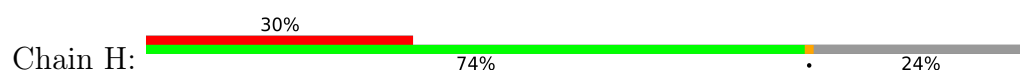


- Molecule 7: 30-KDA PROTEIN (NUGM)

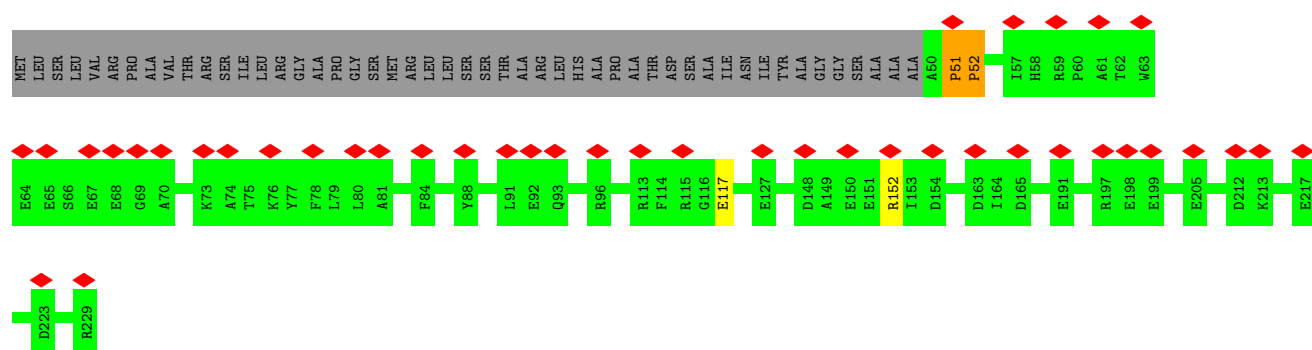
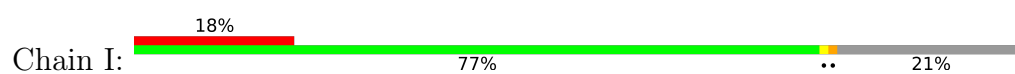
Chain G: 



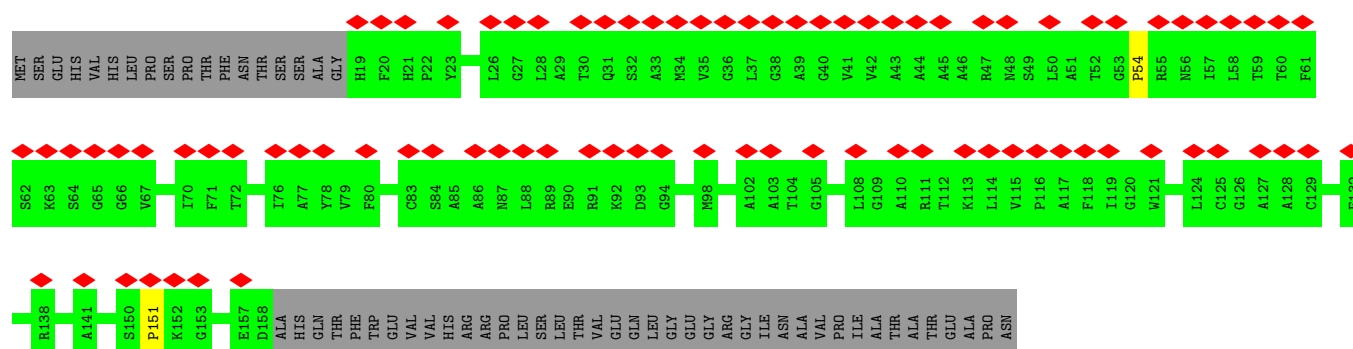
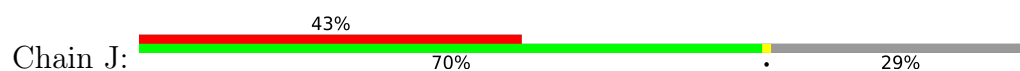
- Molecule 8: 24-KDA SUBUNIT (NUHM)



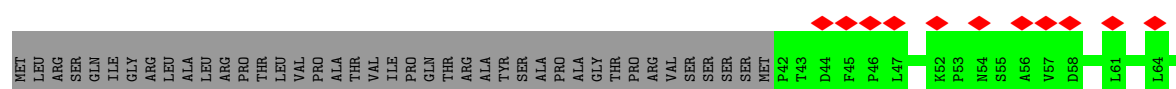
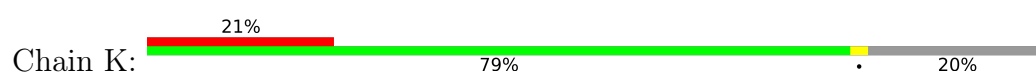
• Molecule 9: TYKY SUBUNIT (NUIM)

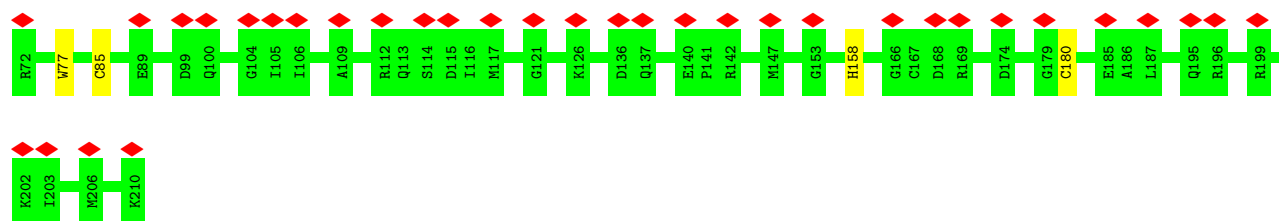


• Molecule 10: NUJM SUBUNIT

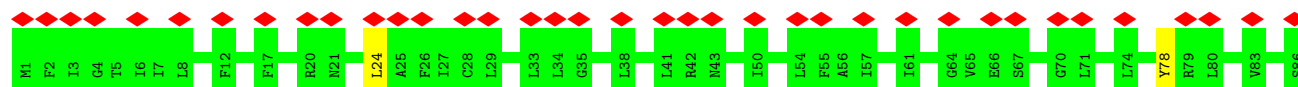
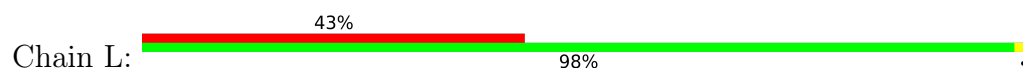


• Molecule 11: PSST SUBUNIT (NUKM)

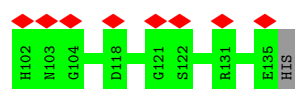
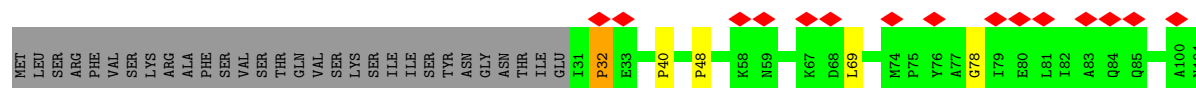
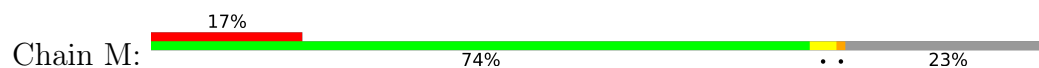




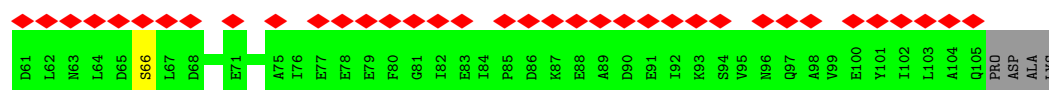
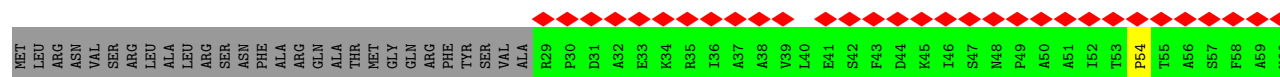
• Molecule 12: ND4L SUBUNIT (NULM)



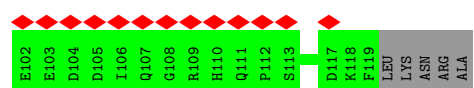
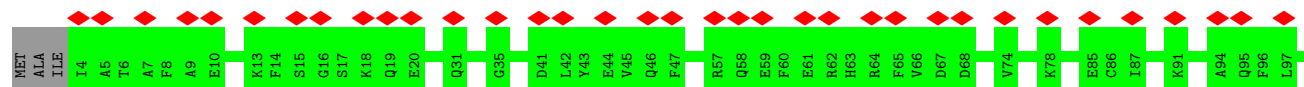
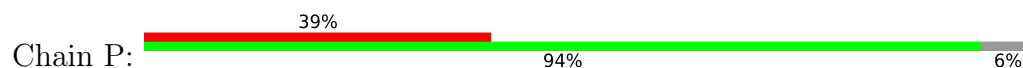
• Molecule 13: NUMM SUBUNIT



• Molecule 14: ACPM1 SUBUNIT

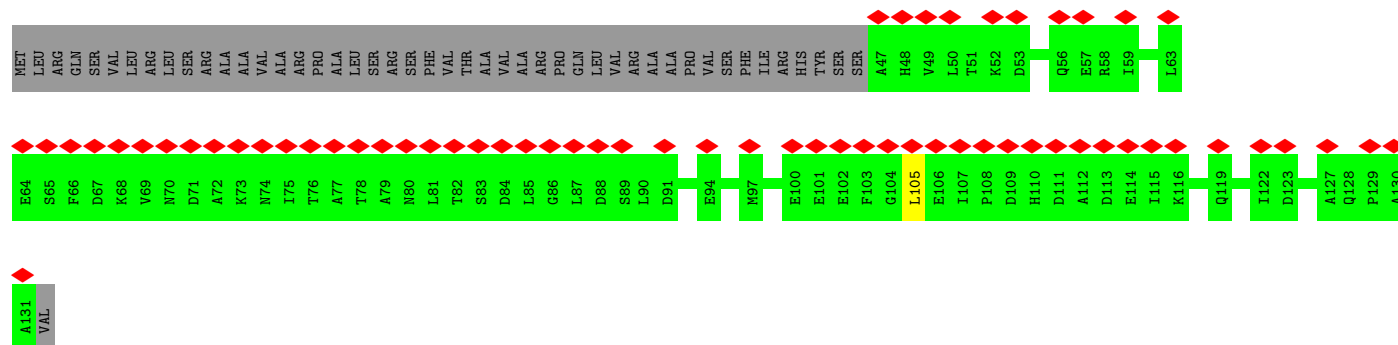


• Molecule 15: NB4M SUBUNIT



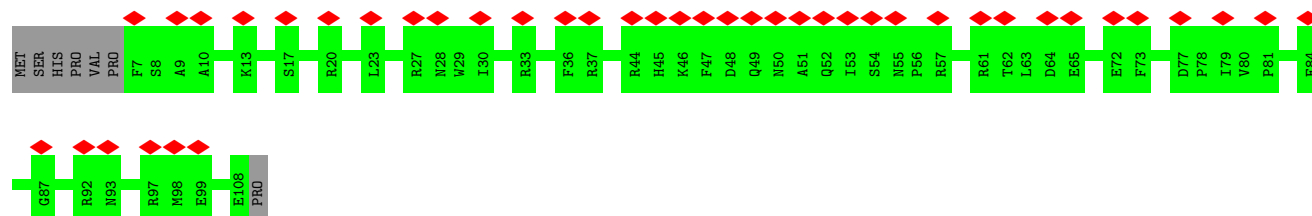
• Molecule 16: ACPM2 SUBUNIT

Chain Q: 



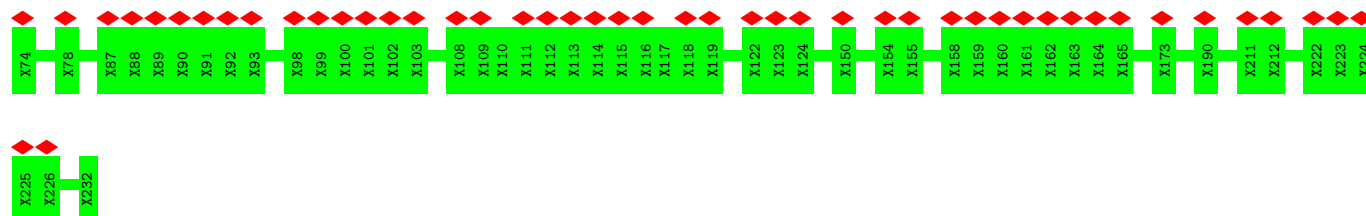
• Molecule 17: NI2M SUBUNIT

Chain R: 




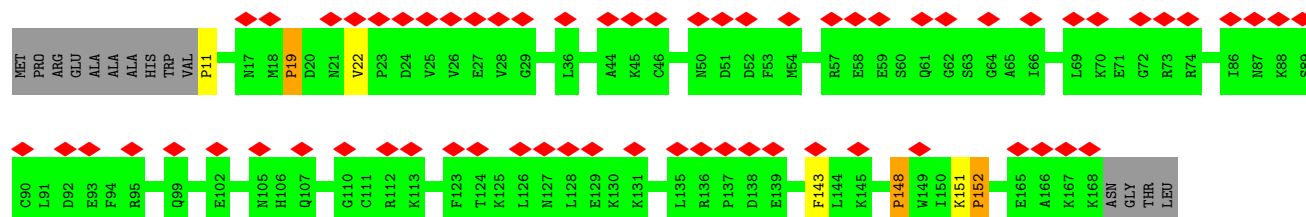
• Molecule 18: NESM SUBUNIT

Chain S: 



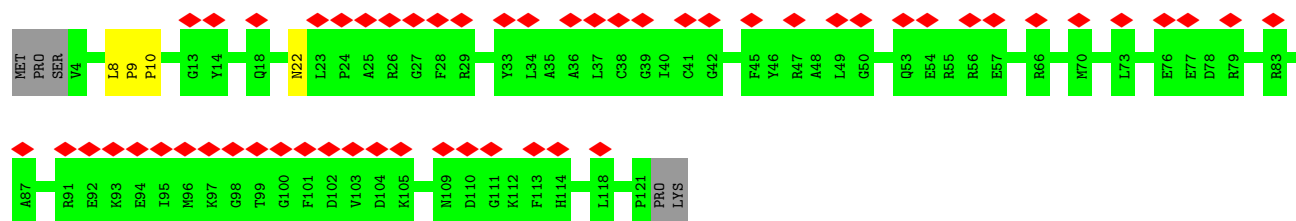
• Molecule 19: NUPM SUBUNIT

Chain U: 

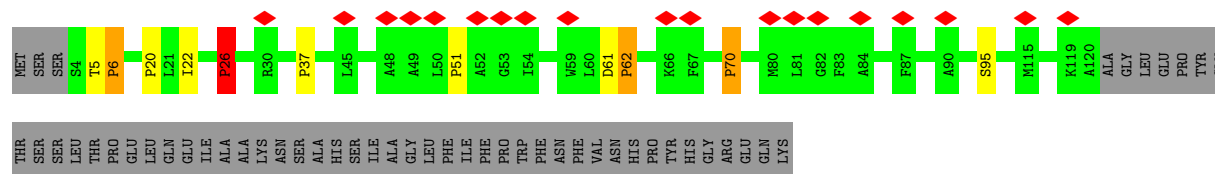


• Molecule 20: NB6M SUBUNIT

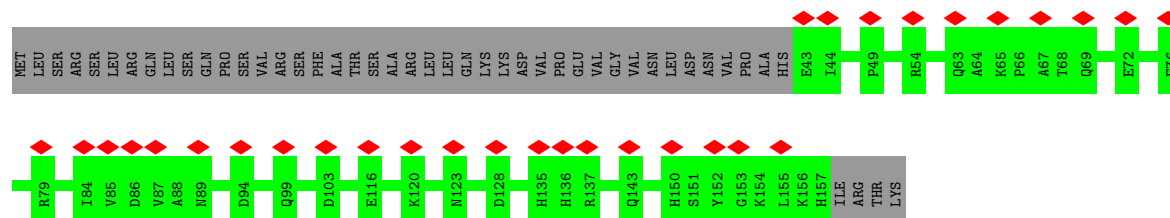
Chain W: 



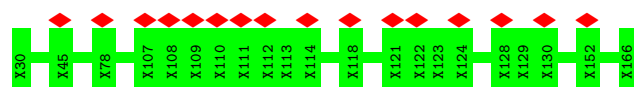
• Molecule 21: NUXM SUBUNIT



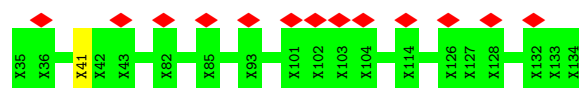
• Molecule 22: NUYM SUBUNIT



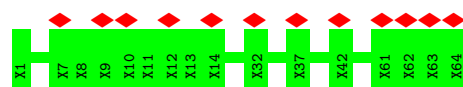
• Molecule 23: NUZM SUBUNIT



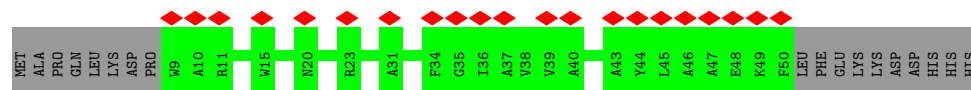
• Molecule 24: NIAM SUBUNIT



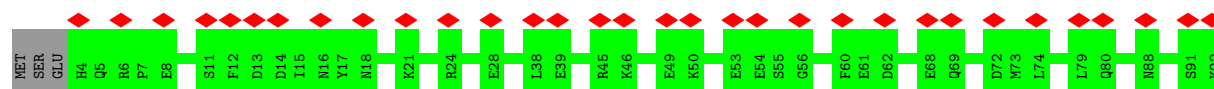
• Molecule 25: NEBM SUBUNIT



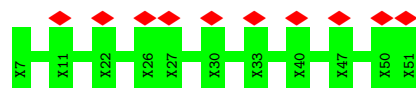
- Molecule 26: NB2M SUBUNIT



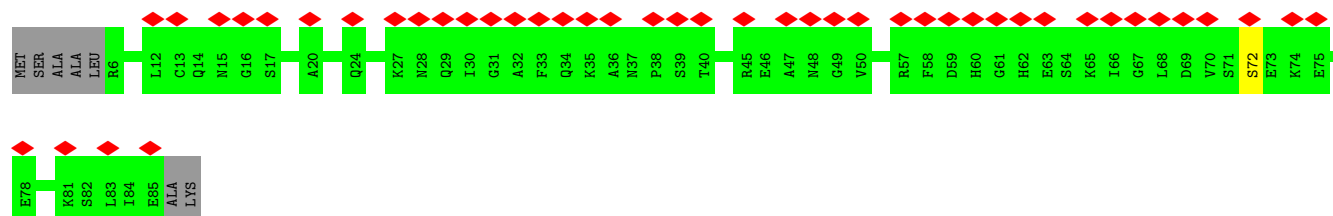
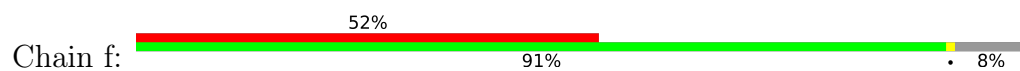
- Molecule 27: NIDM SUBUNIT



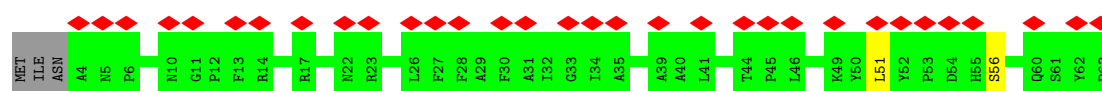
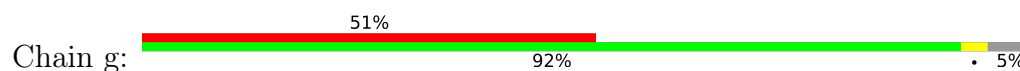
- Molecule 28: NUUM SUBUNIT



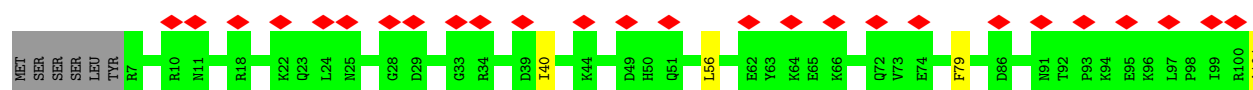
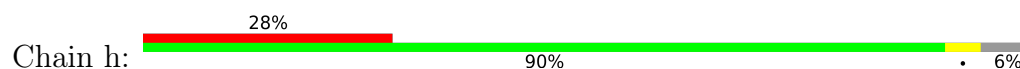
- Molecule 29: NI8M SUBUNIT



- Molecule 30: NI9M SUBUNIT

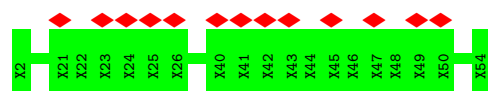


- Molecule 31: N7BM SUBUNIT

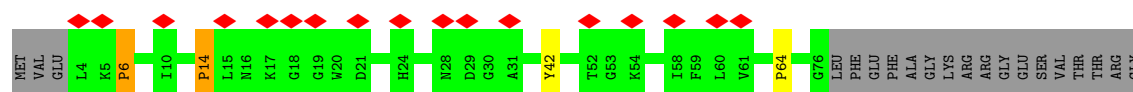
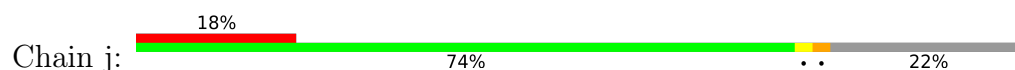




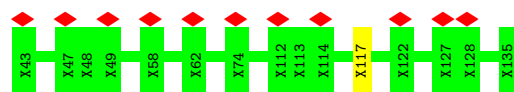
- Molecule 32: UNKNOWN SUBUNIT



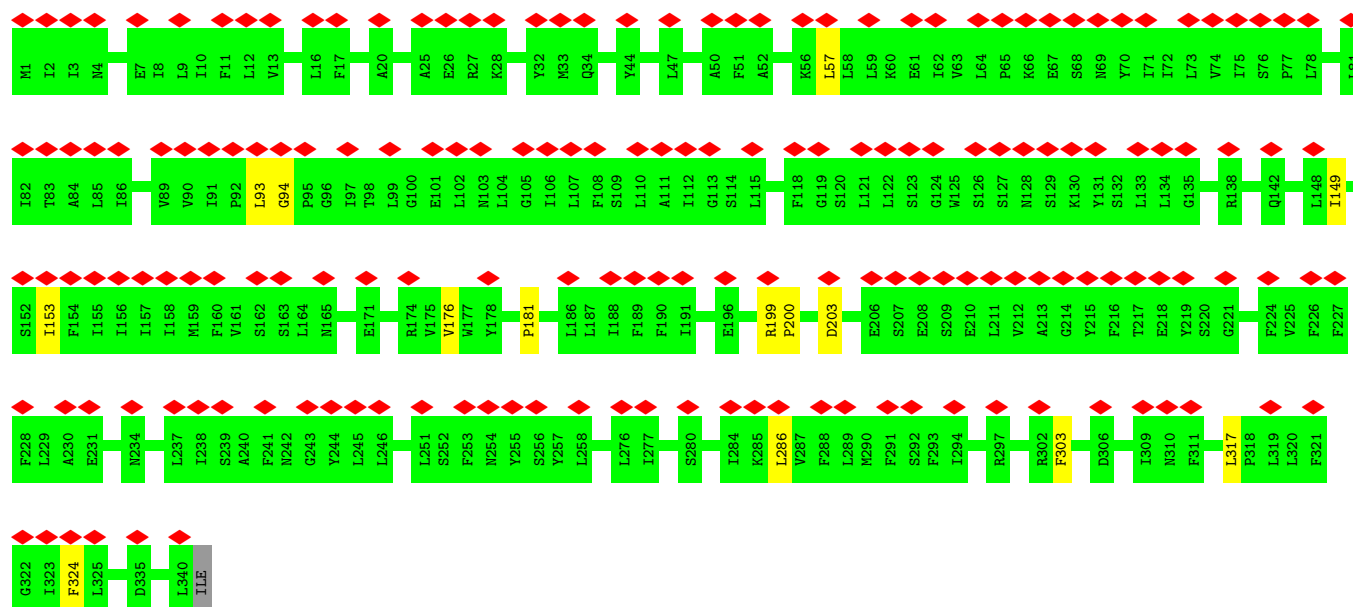
- Molecule 33: NB5M SUBUNIT



- Molecule 34: NUNM SUBUNIT

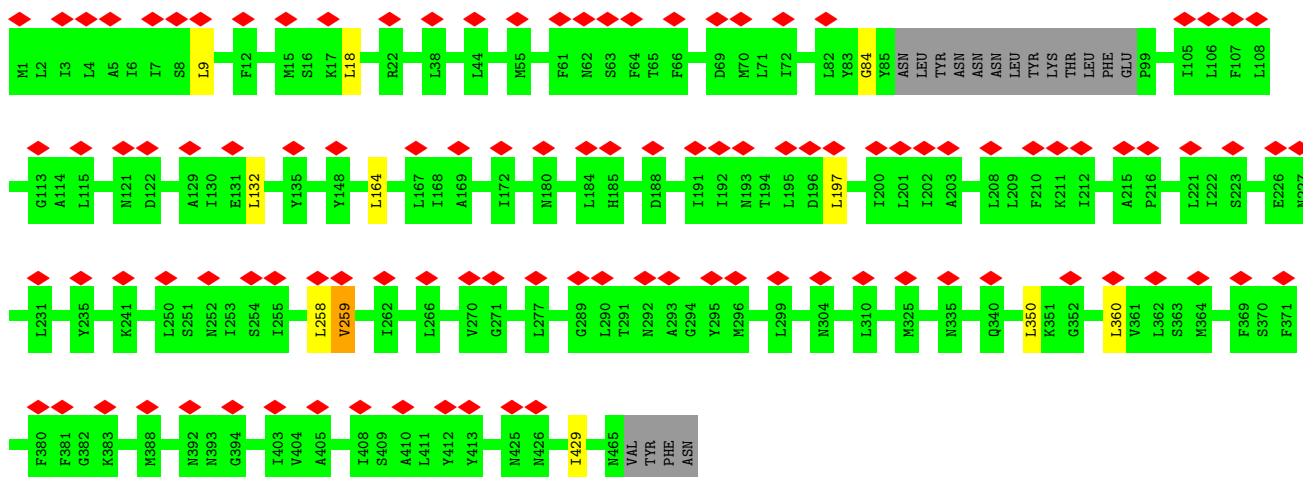


- Molecule 35: ND1 SUBUNIT (NU1M)

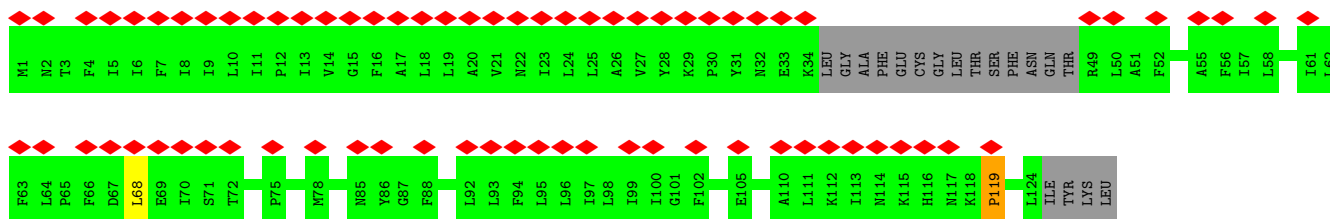
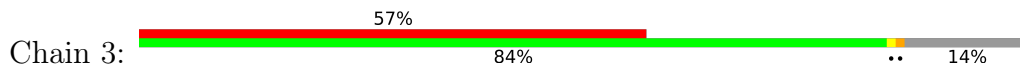


- Molecule 36: ND2 SUBUNIT (NU2M)

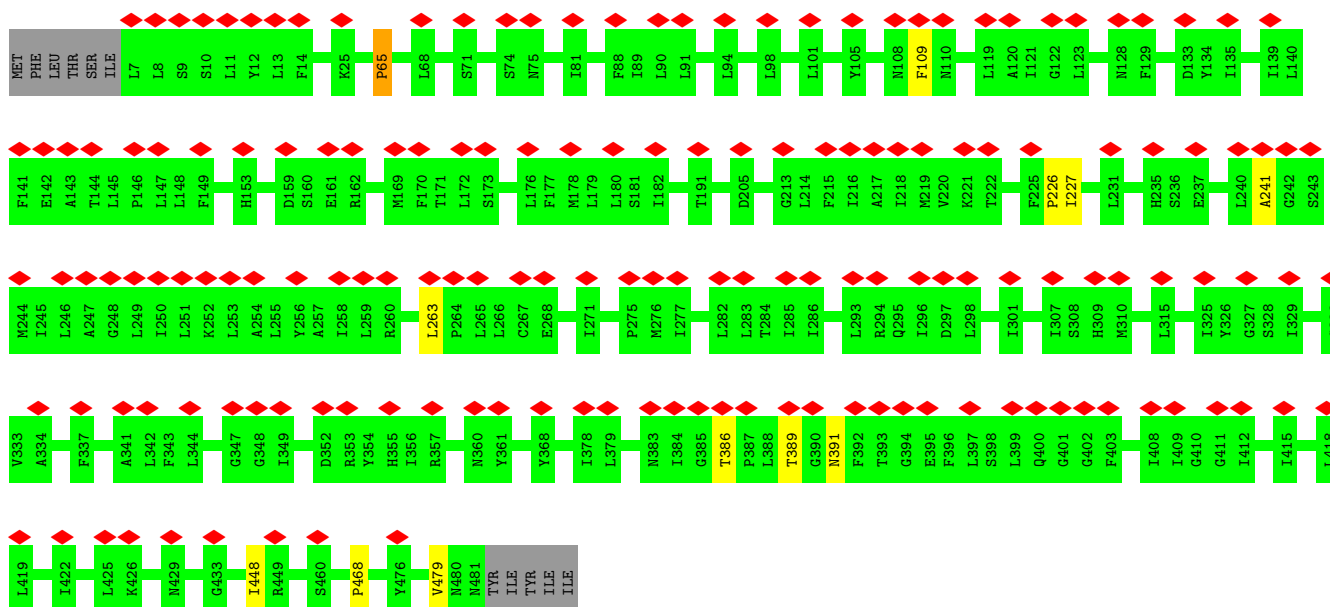




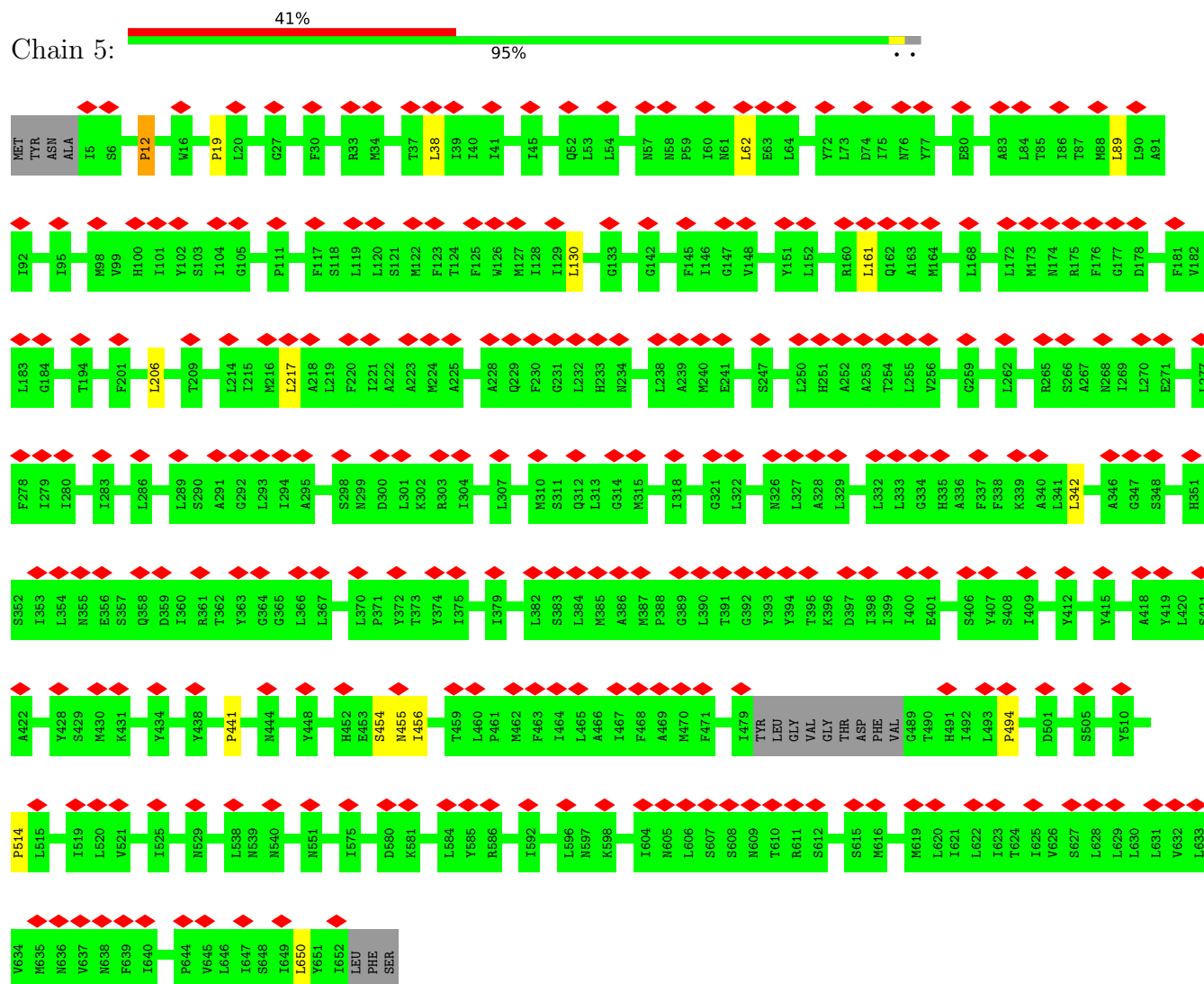
• Molecule 37: ND3 SUBUNIT (NU3M)

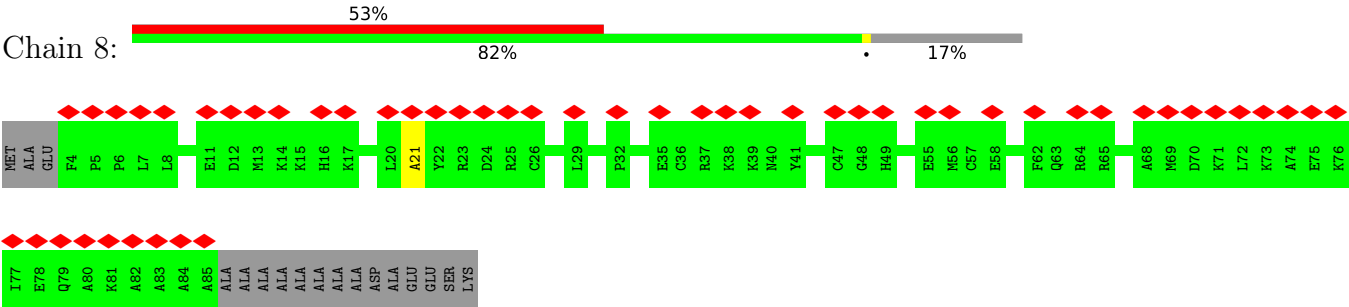


• Molecule 38: ND4 SUBUNIT (NU4M)

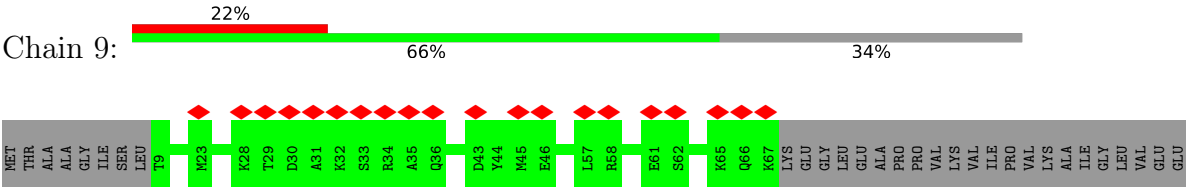


• Molecule 39: ND5 SUBUNIT (NU5M)





● Molecule 42: NIPM SUBUNIT



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	124626	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60.5	Depositor
Minimum defocus (nm)	-1.5	Depositor
Maximum defocus (nm)	-3.0	Depositor
Magnification	45872	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.256	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	497.04, 497.04, 497.04	wwPDB
Map dimensions	456, 456, 456	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, ZMP, SF4, CDL, FMN, NDP, ZN, FES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.46	0/5329	0.65	2/7232 (0.0%)
2	B	0.42	0/3451	0.66	2/4660 (0.0%)
3	C	0.54	0/3260	0.71	3/4421 (0.1%)
4	D	0.43	0/568	0.71	1/770 (0.1%)
5	E	0.44	0/2604	0.68	1/3529 (0.0%)
6	F	0.40	0/932	0.67	2/1265 (0.2%)
7	G	0.57	0/1721	0.81	8/2356 (0.3%)
8	H	0.43	0/1411	0.69	3/1919 (0.2%)
9	I	0.60	0/1475	0.76	2/1998 (0.1%)
10	J	0.36	0/983	0.67	1/1343 (0.1%)
11	K	0.59	0/1377	0.70	0/1872
12	L	0.49	0/676	0.80	1/913 (0.1%)
13	M	0.44	0/741	0.73	4/1009 (0.4%)
14	O	0.37	0/598	0.58	0/813
15	P	0.47	0/1007	0.63	0/1355
16	Q	0.33	0/654	0.64	1/890 (0.1%)
17	R	0.34	0/840	0.53	0/1136
19	U	0.37	0/1157	0.77	4/1568 (0.3%)
20	W	0.41	0/948	0.68	2/1275 (0.2%)
21	X	0.35	0/641	0.81	7/881 (0.8%)
22	Y	0.52	0/985	0.63	0/1330
26	c	0.30	0/255	0.53	0/349
27	d	0.41	0/768	0.66	0/1031
29	f	0.43	0/639	0.68	0/856
30	g	0.43	0/516	0.67	1/707 (0.1%)
31	h	0.49	0/1118	0.74	3/1522 (0.2%)
33	j	0.37	0/444	0.71	3/611 (0.5%)
35	1	0.50	0/2674	0.81	4/3656 (0.1%)
36	2	0.54	0/3440	0.78	8/4696 (0.2%)
37	3	0.46	0/890	0.88	3/1213 (0.2%)
38	4	0.49	0/3373	0.75	3/4630 (0.1%)
39	5	0.43	0/4692	0.73	14/6430 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
40	6	0.43	0/1229	0.69	1/1686 (0.1%)
41	8	0.38	0/686	0.58	0/918
42	9	0.38	0/477	0.57	0/637
All	All	0.47	0/52559	0.71	84/71477 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	B	0	2
5	E	0	5
7	G	0	2
9	I	0	1
10	J	0	1
11	K	0	1
12	L	0	1
19	U	0	2
20	W	0	1
21	X	0	2
24	a	0	1
29	f	0	1
30	g	0	1
31	h	0	1
33	j	0	1
34	n	0	1
35	1	0	9
36	2	0	2
38	4	0	3
39	5	0	1
41	8	0	1
All	All	0	43

There are no bond length outliers.

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	94	ASP	CB-CG-OD1	10.06	127.36	118.30
37	3	68	LEU	CA-CB-CG	9.54	137.24	115.30
31	h	56	LEU	CA-CB-CG	8.15	134.04	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	U	19	PRO	N-CA-CB	7.71	112.55	103.30
39	5	206	LEU	CB-CG-CD1	-7.49	98.27	111.00

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	TYR	Peptide
1	A	248	ARG	Peptide
1	A	633	LEU	Peptide
2	B	151	MET	Peptide
2	B	445	ARG	Peptide

## 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 [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	687/728 (94%)	604 (88%)	83 (12%)	0	100	100
2	B	441/488 (90%)	391 (89%)	49 (11%)	1 (0%)	44	78
3	C	414/466 (89%)	371 (90%)	39 (9%)	4 (1%)	13	48
4	D	78/87 (90%)	66 (85%)	11 (14%)	1 (1%)	10	41
5	E	316/375 (84%)	261 (83%)	55 (17%)	0	100	100
6	F	117/144 (81%)	101 (86%)	14 (12%)	2 (2%)	7	36
7	G	230/281 (82%)	180 (78%)	45 (20%)	5 (2%)	5	30
8	H	183/243 (75%)	151 (82%)	29 (16%)	3 (2%)	8	37
9	I	178/229 (78%)	148 (83%)	28 (16%)	2 (1%)	12	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	138/198 (70%)	123 (89%)	15 (11%)	0	100	100
11	K	167/210 (80%)	143 (86%)	23 (14%)	1 (1%)	22	59
12	L	84/86 (98%)	69 (82%)	15 (18%)	0	100	100
13	M	103/136 (76%)	84 (82%)	17 (16%)	2 (2%)	6	33
14	O	75/109 (69%)	68 (91%)	6 (8%)	1 (1%)	10	41
15	P	114/124 (92%)	103 (90%)	11 (10%)	0	100	100
16	Q	83/132 (63%)	70 (84%)	13 (16%)	0	100	100
17	R	100/109 (92%)	90 (90%)	10 (10%)	0	100	100
19	U	156/172 (91%)	128 (82%)	24 (15%)	4 (3%)	4	26
20	W	116/123 (94%)	104 (90%)	11 (10%)	1 (1%)	14	50
21	X	115/169 (68%)	81 (70%)	27 (24%)	7 (6%)	1	13
22	Y	113/161 (70%)	95 (84%)	18 (16%)	0	100	100
26	c	40/60 (67%)	35 (88%)	5 (12%)	0	100	100
27	d	87/92 (95%)	78 (90%)	9 (10%)	0	100	100
29	f	78/87 (90%)	66 (85%)	12 (15%)	0	100	100
30	g	58/63 (92%)	42 (72%)	16 (28%)	0	100	100
31	h	128/138 (93%)	103 (80%)	24 (19%)	1 (1%)	16	53
33	j	71/93 (76%)	62 (87%)	7 (10%)	2 (3%)	4	25
35	1	338/341 (99%)	291 (86%)	46 (14%)	1 (0%)	37	72
36	2	448/469 (96%)	400 (89%)	46 (10%)	2 (0%)	30	67
37	3	106/128 (83%)	87 (82%)	18 (17%)	1 (1%)	14	50
38	4	473/486 (97%)	394 (83%)	72 (15%)	7 (2%)	8	39
39	5	635/655 (97%)	554 (87%)	78 (12%)	3 (0%)	25	63
40	6	181/185 (98%)	162 (90%)	19 (10%)	0	100	100
41	8	80/99 (81%)	71 (89%)	9 (11%)	0	100	100
42	9	57/89 (64%)	52 (91%)	5 (9%)	0	100	100
All	All	6788/7755 (88%)	5828 (86%)	909 (13%)	51 (1%)	19	53

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	116	VAL
4	D	71	PRO

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Mol	Chain	Res	Type
6	F	29	THR
7	G	34	PRO
7	G	46	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	563/595 (95%)	563 (100%)	0	100	100
2	B	340/389 (87%)	339 (100%)	1 (0%)	91	92
3	C	320/394 (81%)	317 (99%)	3 (1%)	75	83
4	D	44/69 (64%)	44 (100%)	0	100	100
5	E	275/329 (84%)	275 (100%)	0	100	100
6	F	89/129 (69%)	89 (100%)	0	100	100
7	G	143/245 (58%)	143 (100%)	0	100	100
8	H	144/212 (68%)	143 (99%)	1 (1%)	81	87
9	I	148/187 (79%)	147 (99%)	1 (1%)	81	87
10	J	80/147 (54%)	80 (100%)	0	100	100
11	K	146/180 (81%)	144 (99%)	2 (1%)	62	76
12	L	75/75 (100%)	75 (100%)	0	100	100
13	M	60/115 (52%)	60 (100%)	0	100	100
14	O	65/91 (71%)	64 (98%)	1 (2%)	60	75
15	P	104/110 (94%)	104 (100%)	0	100	100
16	Q	72/111 (65%)	72 (100%)	0	100	100
17	R	84/100 (84%)	84 (100%)	0	100	100
19	U	110/148 (74%)	110 (100%)	0	100	100
20	W	89/102 (87%)	89 (100%)	0	100	100
21	X	17/133 (13%)	17 (100%)	0	100	100
22	Y	98/140 (70%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	c	11/45 (24%)	11 (100%)	0	100	100
27	d	82/85 (96%)	82 (100%)	0	100	100
29	f	69/73 (94%)	69 (100%)	0	100	100
30	g	49/52 (94%)	49 (100%)	0	100	100
31	h	115/123 (94%)	114 (99%)	1 (1%)	75	83
33	j	17/73 (23%)	17 (100%)	0	100	100
35	1	272/302 (90%)	272 (100%)	0	100	100
36	2	340/433 (78%)	340 (100%)	0	100	100
37	3	93/114 (82%)	93 (100%)	0	100	100
38	4	295/434 (68%)	295 (100%)	0	100	100
39	5	426/580 (73%)	426 (100%)	0	100	100
40	6	88/167 (53%)	88 (100%)	0	100	100
41	8	69/76 (91%)	69 (100%)	0	100	100
42	9	49/76 (64%)	49 (100%)	0	100	100
All	All	5041/6634 (76%)	5031 (100%)	10 (0%)	91	94

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	85	CYS
14	O	66	SER
31	h	79	PHE
3	C	428	ARG
8	H	172	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	103	ASN
39	5	233	HIS
19	U	50	ASN
38	4	103	ASN
15	P	95	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	$\# Z  > 2$
43	SF4	A	802	1	0,12,12	-	-	-		
43	SF4	A	801	1	0,12,12	-	-	-		
43	SF4	I	301	9	0,12,12	-	-	-		
43	SF4	I	302	9	0,12,12	-	-	-		
50	3PE	g	202	-	42,42,50	0.93	4 (9%)	45,47,55	1.11	2 (4%)
44	FES	H	301	8	0,4,4	-	-	-		
48	ZMP	O	201	14	22,28,36	2.01	6 (27%)	27,35,45	2.13	9 (33%)
45	FMN	B	502	-	33,33,33	2.57	10 (30%)	48,50,50	1.55	9 (18%)
50	3PE	1	401	-	50,50,50	0.85	3 (6%)	53,55,55	1.15	2 (3%)
49	CDL	g	201	-	82,82,99	0.95	7 (8%)	88,94,111	1.16	5 (5%)
46	NDP	E	401	-	45,52,52	4.06	20 (44%)	53,80,80	2.25	11 (20%)
43	SF4	K	301	11	0,12,12	-	-	-		
50	3PE	4	501	-	42,42,50	0.95	4 (9%)	45,47,55	1.13	3 (6%)
44	FES	A	803	1	0,4,4	-	-	-		
43	SF4	B	501	2	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	SF4	A	802	1	-	-	0/6/5/5
50	3PE	g	202	-	-	24/46/46/54	-
43	SF4	A	801	1	-	-	0/6/5/5
43	SF4	B	501	2	-	-	0/6/5/5
43	SF4	I	301	9	-	-	0/6/5/5
43	SF4	I	302	9	-	-	0/6/5/5
48	ZMP	O	201	14	-	5/33/35/43	-
45	FMN	B	502	-	-	12/18/18/18	0/3/3/3
50	3PE	1	401	-	-	28/54/54/54	-
44	FES	H	301	8	-	-	0/1/1/1
49	CDL	g	201	-	-	43/93/93/110	-
43	SF4	K	301	11	-	-	0/6/5/5
50	3PE	4	501	-	-	22/46/46/54	-
44	FES	A	803	1	-	-	0/1/1/1
46	NDP	E	401	-	-	5/30/77/77	0/5/5/5

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	E	401	NDP	O4B-C1B	14.81	1.61	1.41
46	E	401	NDP	C6N-C5N	12.17	1.55	1.33
46	E	401	NDP	O4D-C1D	8.02	1.61	1.42
46	E	401	NDP	C2D-C1D	-7.37	1.29	1.53
46	E	401	NDP	O4D-C4D	-6.95	1.29	1.45

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	E	401	NDP	C5A-C6A-N6A	9.75	135.16	120.35
46	E	401	NDP	N6A-C6A-N1A	-7.33	103.35	118.57
48	O	201	ZMP	C9-C10-S1	6.68	121.24	113.46
46	E	401	NDP	N3A-C2A-N1A	-6.19	119.01	128.68
50	1	401	3PE	O21-C21-C22	4.67	121.56	111.50

There are no chirality outliers.

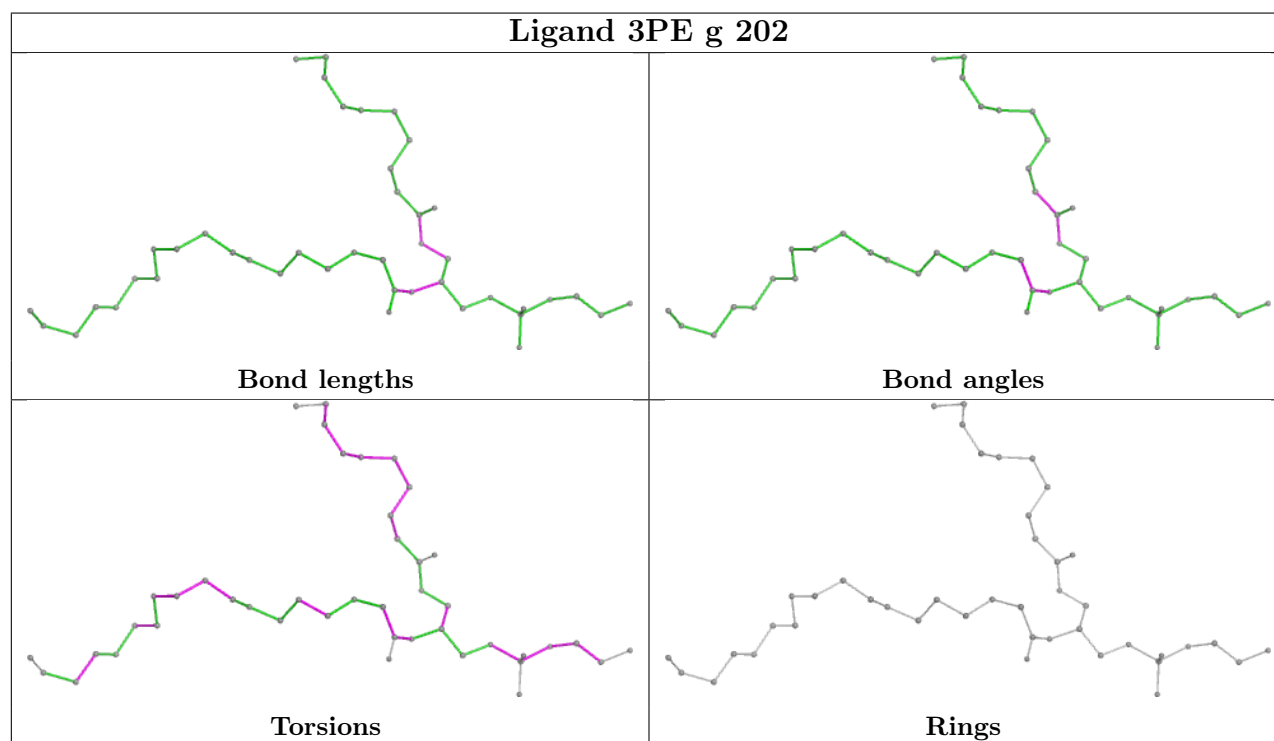
5 of 139 torsion outliers are listed below:

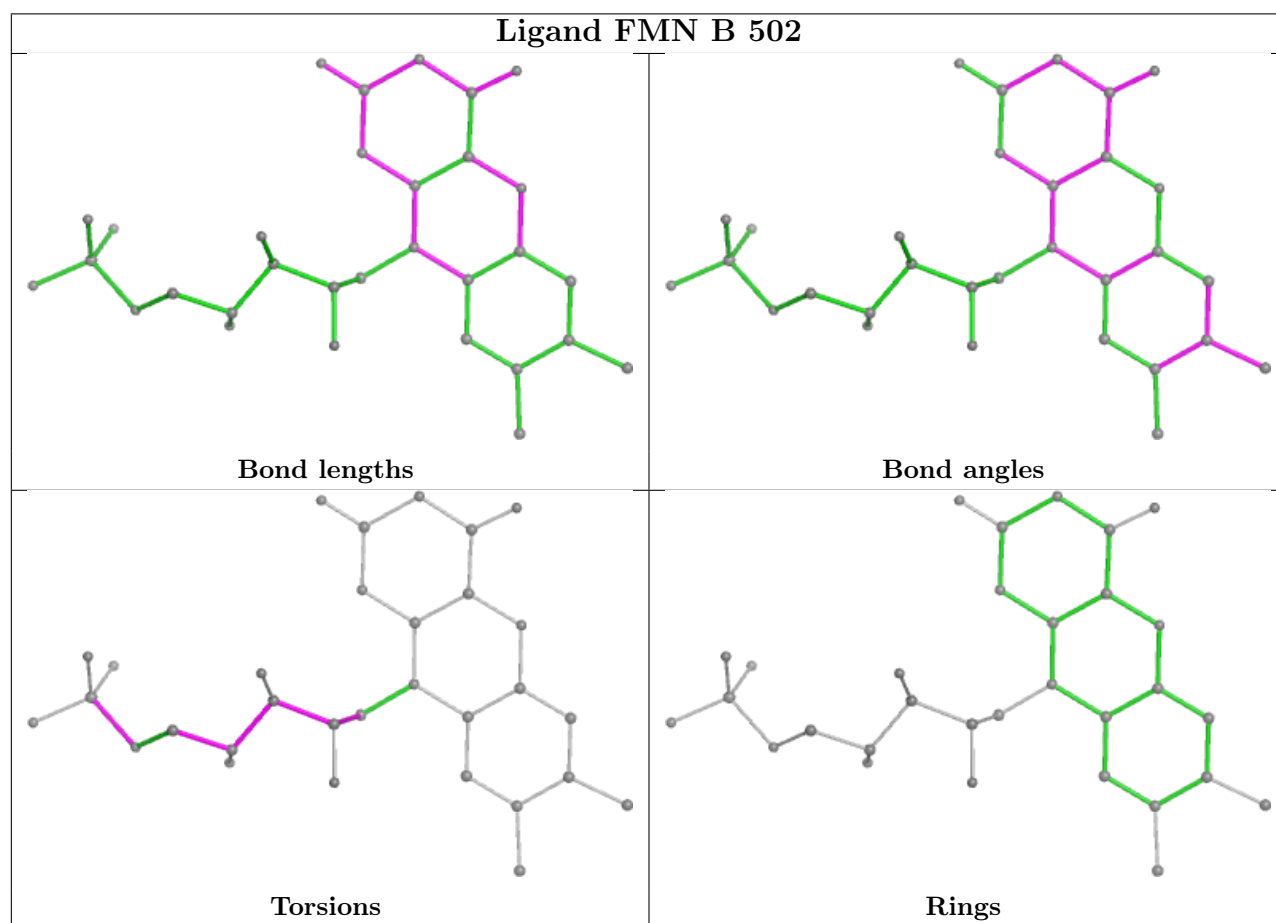
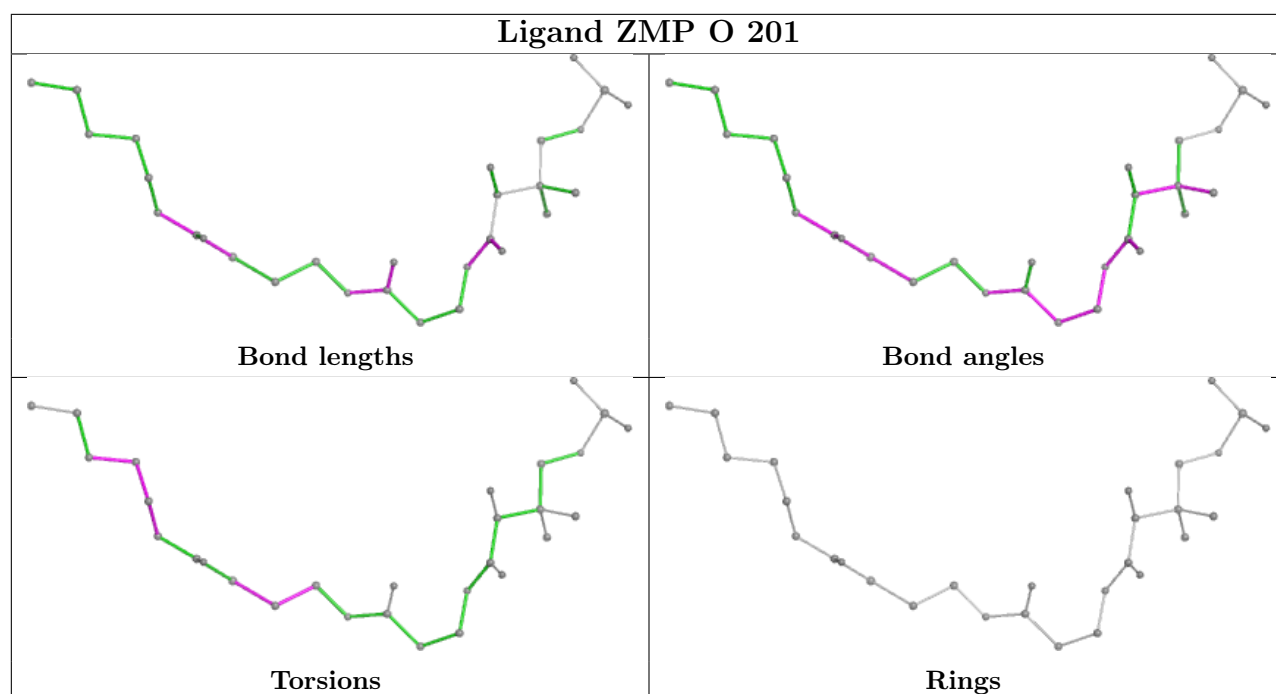
Mol	Chain	Res	Type	Atoms
45	B	502	FMN	N10-C1'-C2'-O2'
45	B	502	FMN	N10-C1'-C2'-C3'
45	B	502	FMN	C1'-C2'-C3'-O3'
45	B	502	FMN	C1'-C2'-C3'-C4'
45	B	502	FMN	O2'-C2'-C3'-C4'

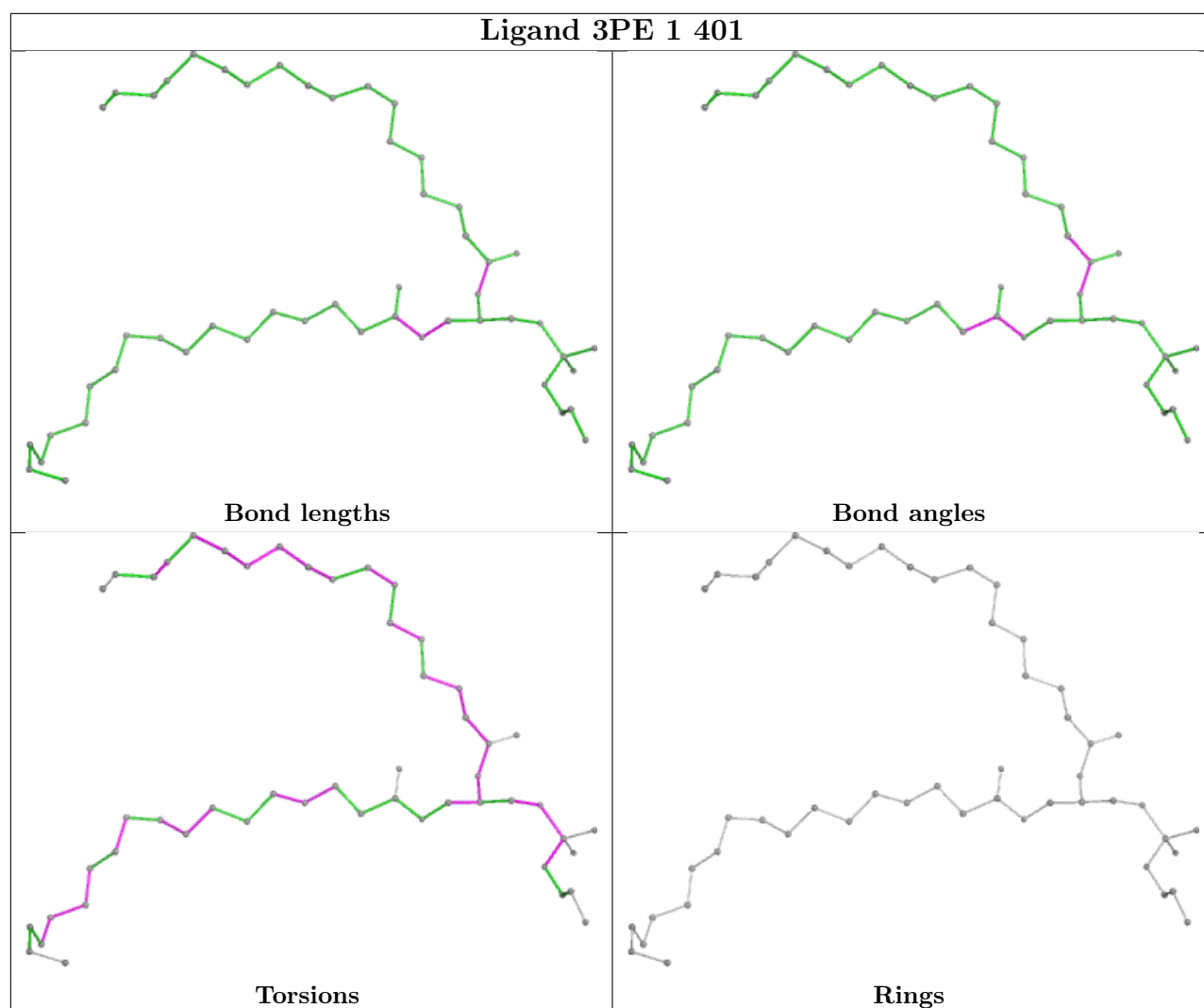
There are no ring outliers.

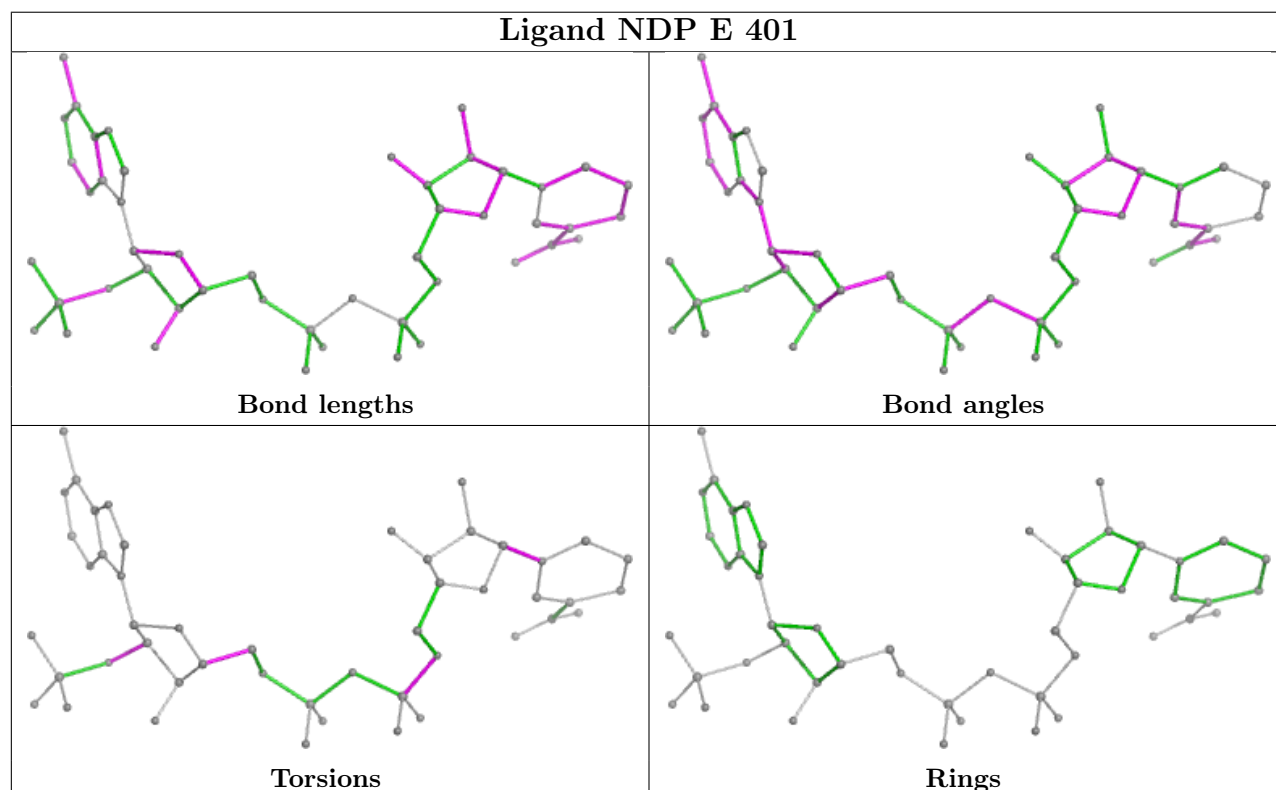
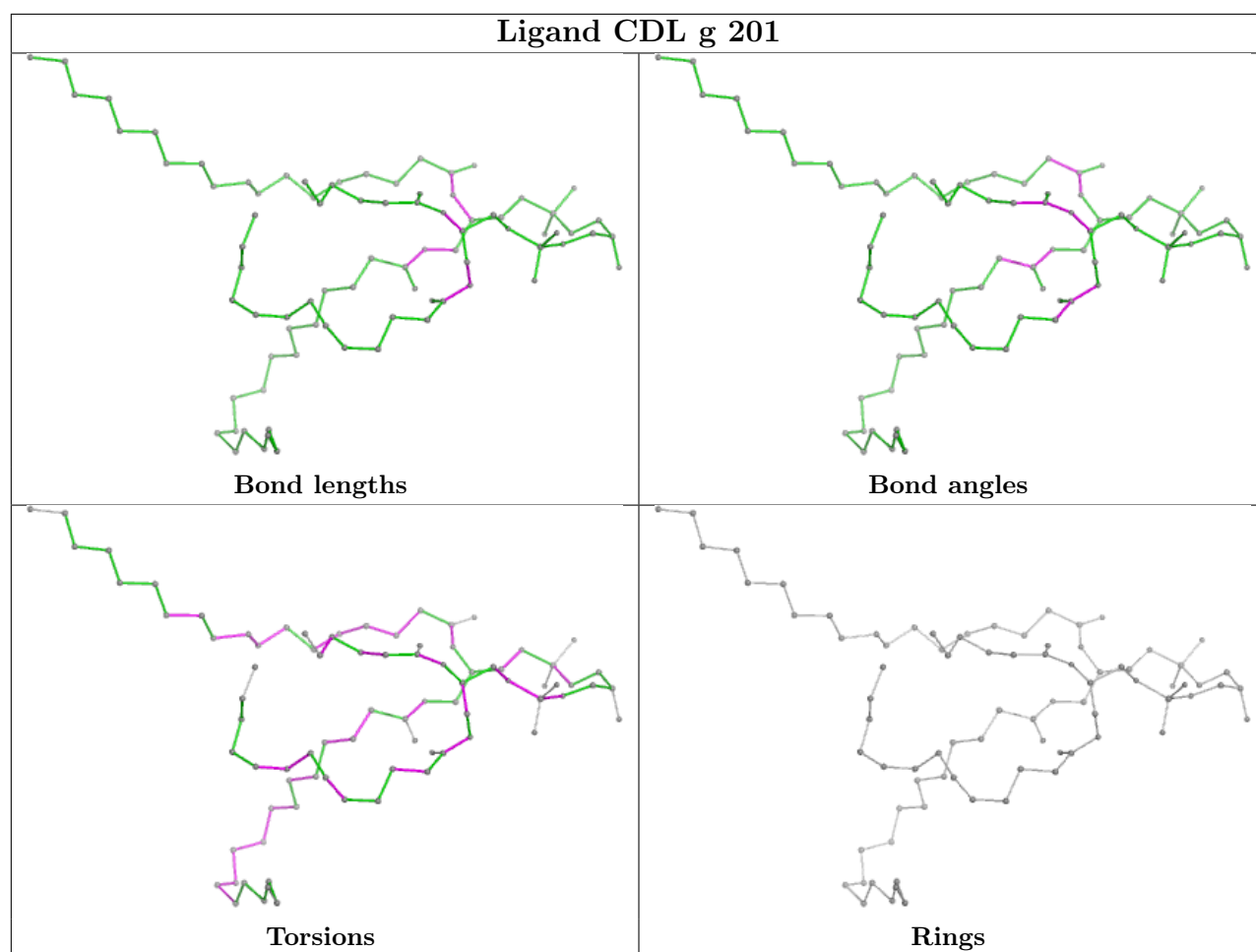
No monomer is involved in short contacts.

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

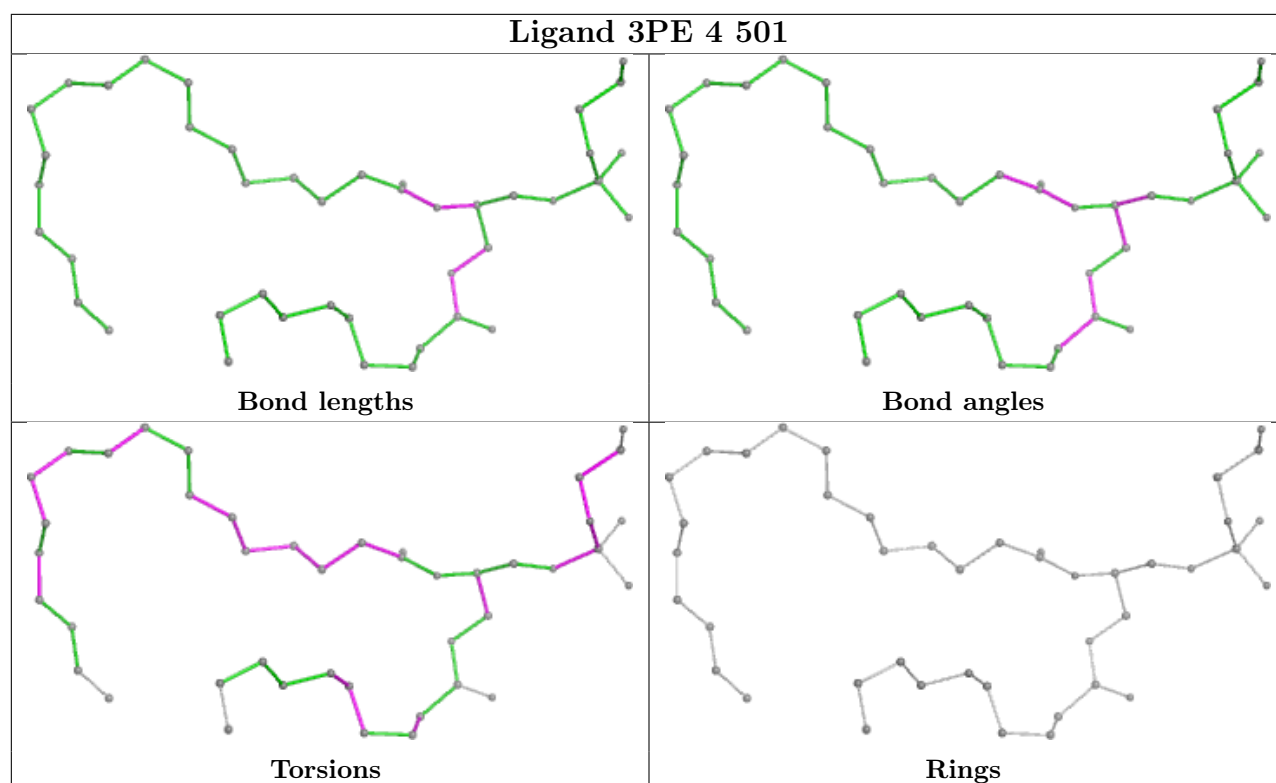












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

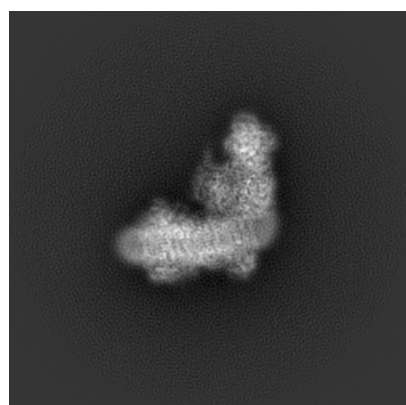
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4384. These allow visual inspection of the internal detail of the map and identification of artifacts.

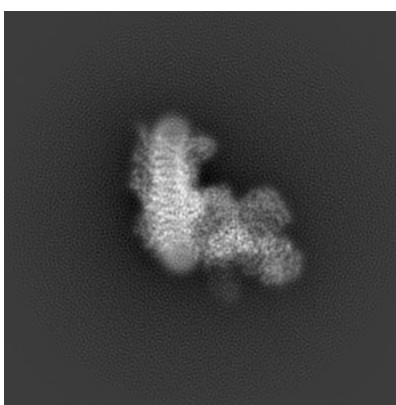
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

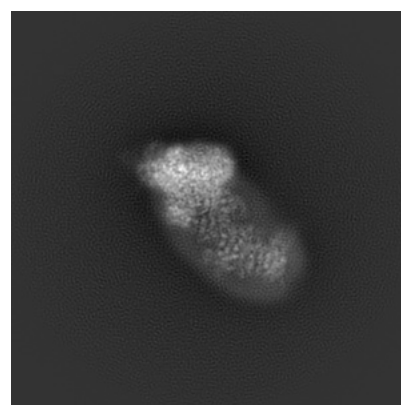
#### 6.1.1 Primary map



X



Y

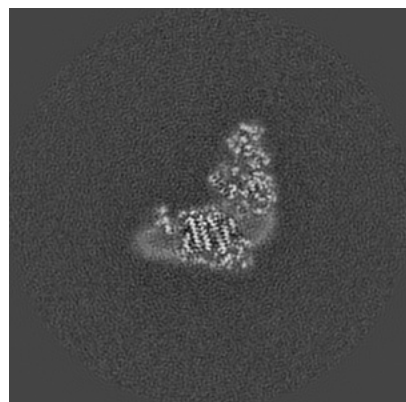


Z

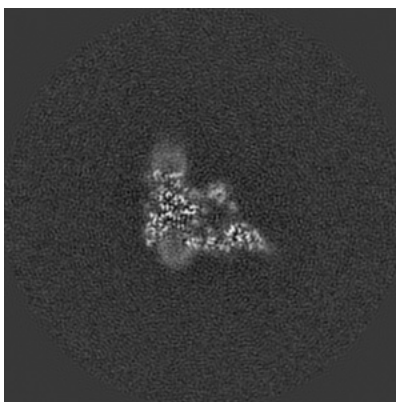
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

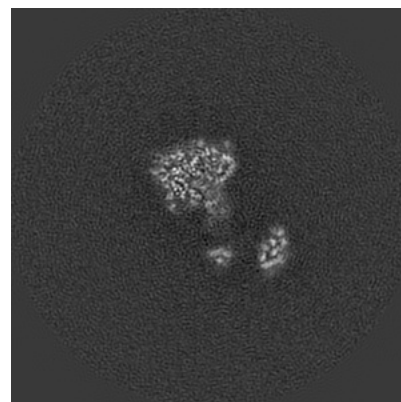
#### 6.2.1 Primary map



X Index: 228



Y Index: 228

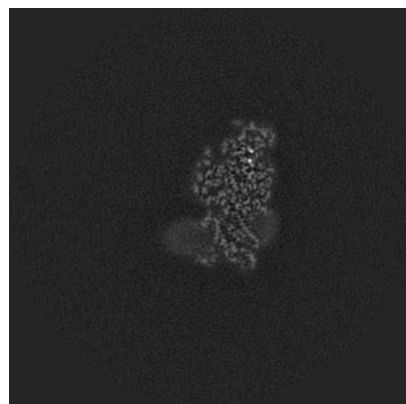


Z Index: 228

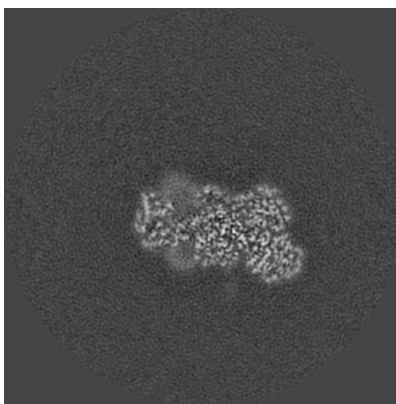
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

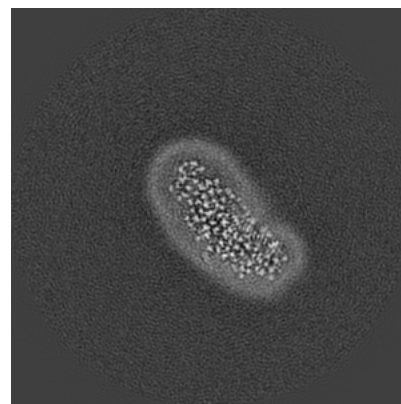
### 6.3.1 Primary map



X Index: 192



Y Index: 268

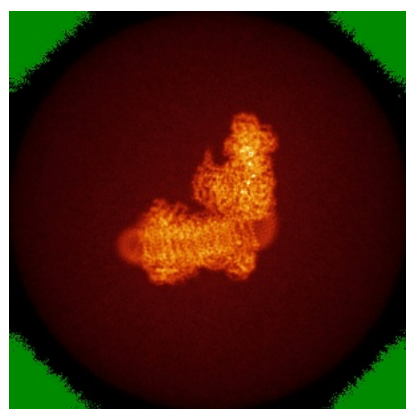


Z Index: 201

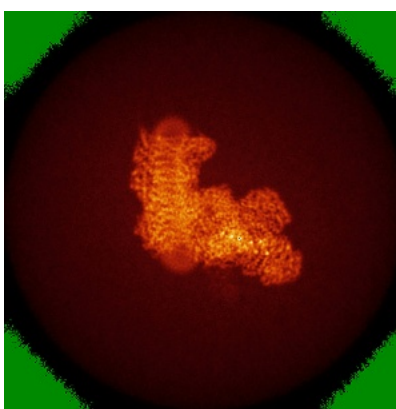
The images above show the largest variance slices of the map in three orthogonal directions.

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

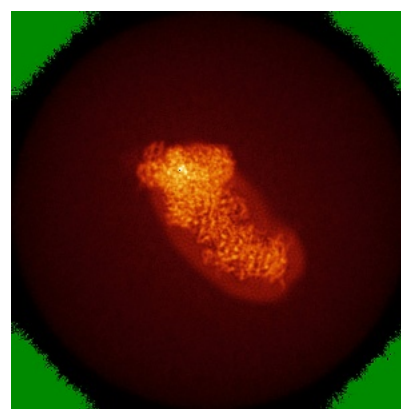
### 6.4.1 Primary map



X



Y

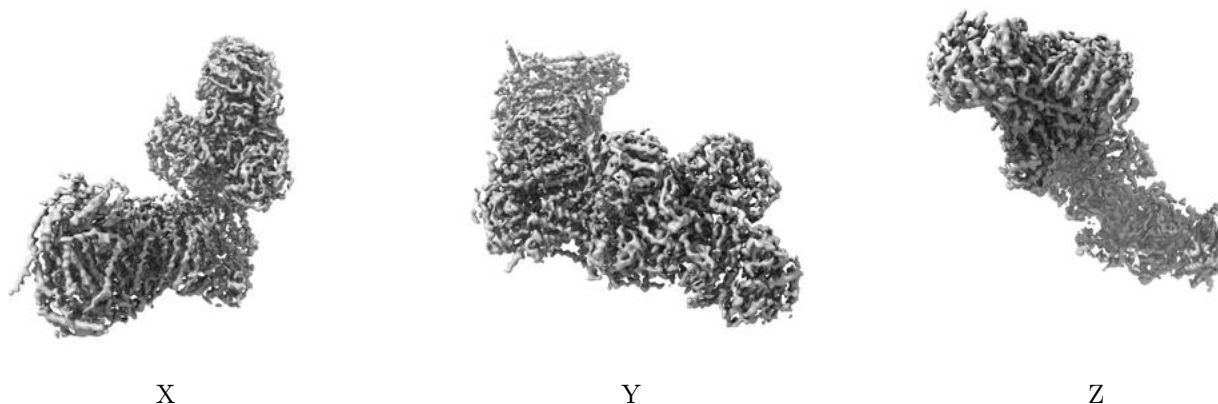


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

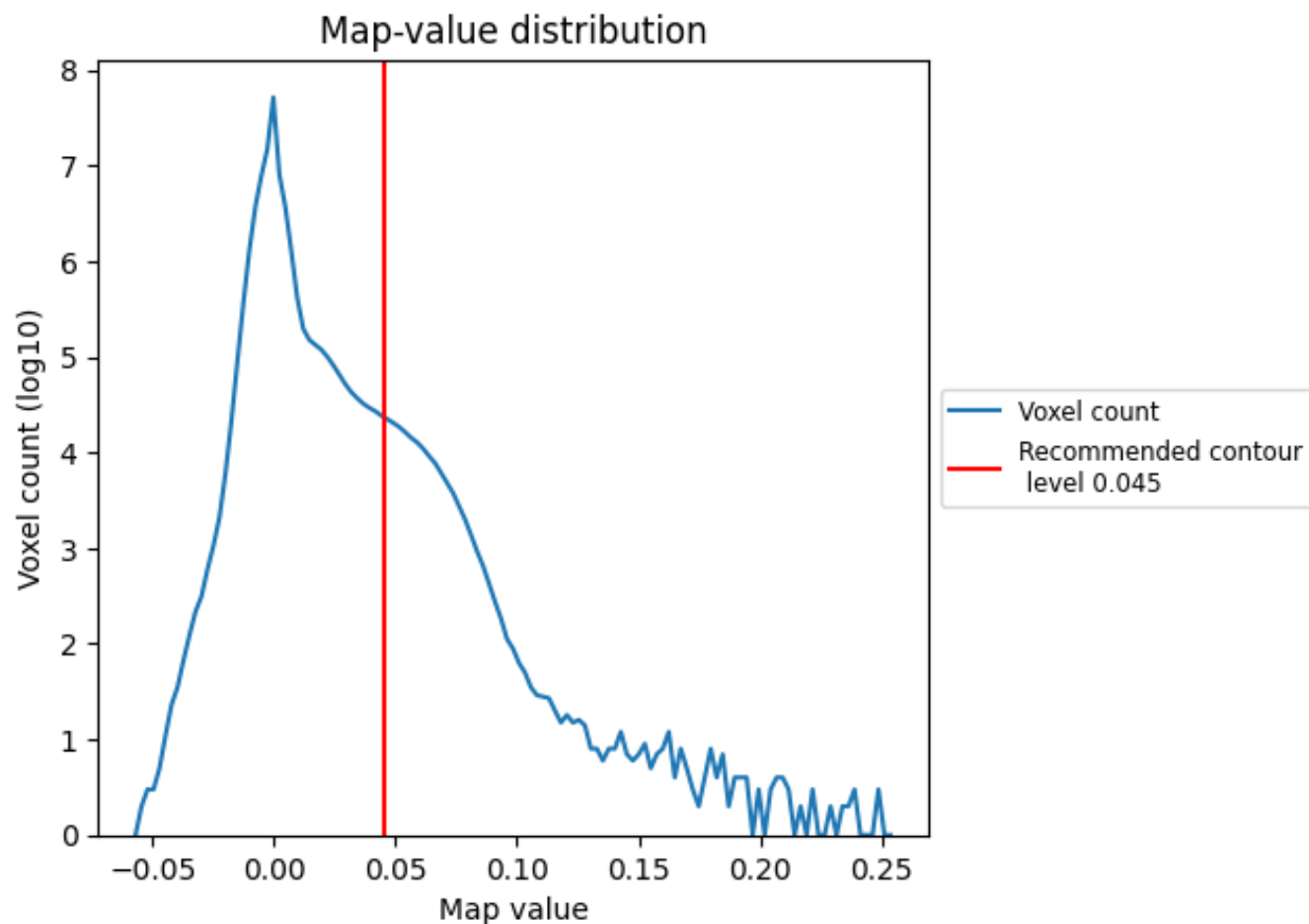
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

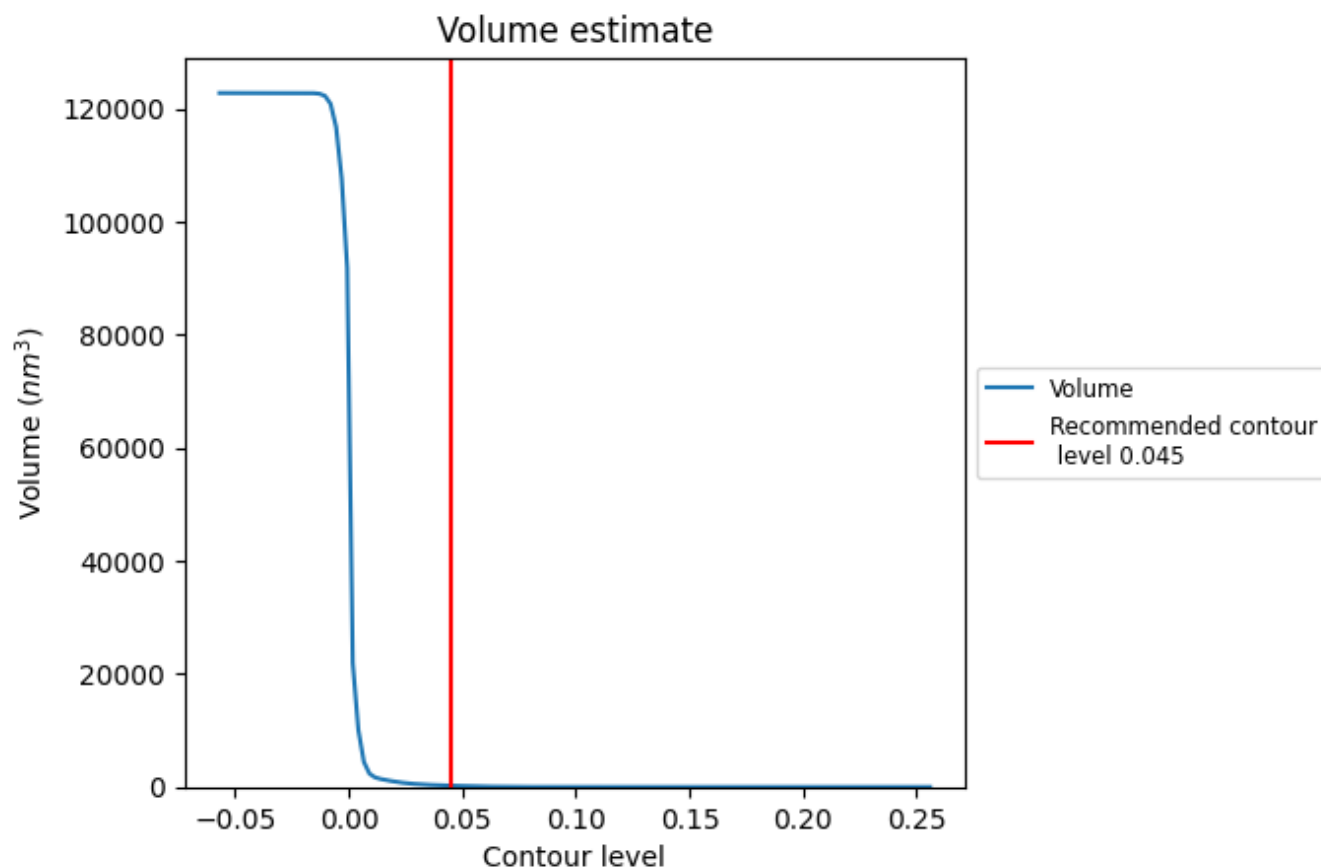
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

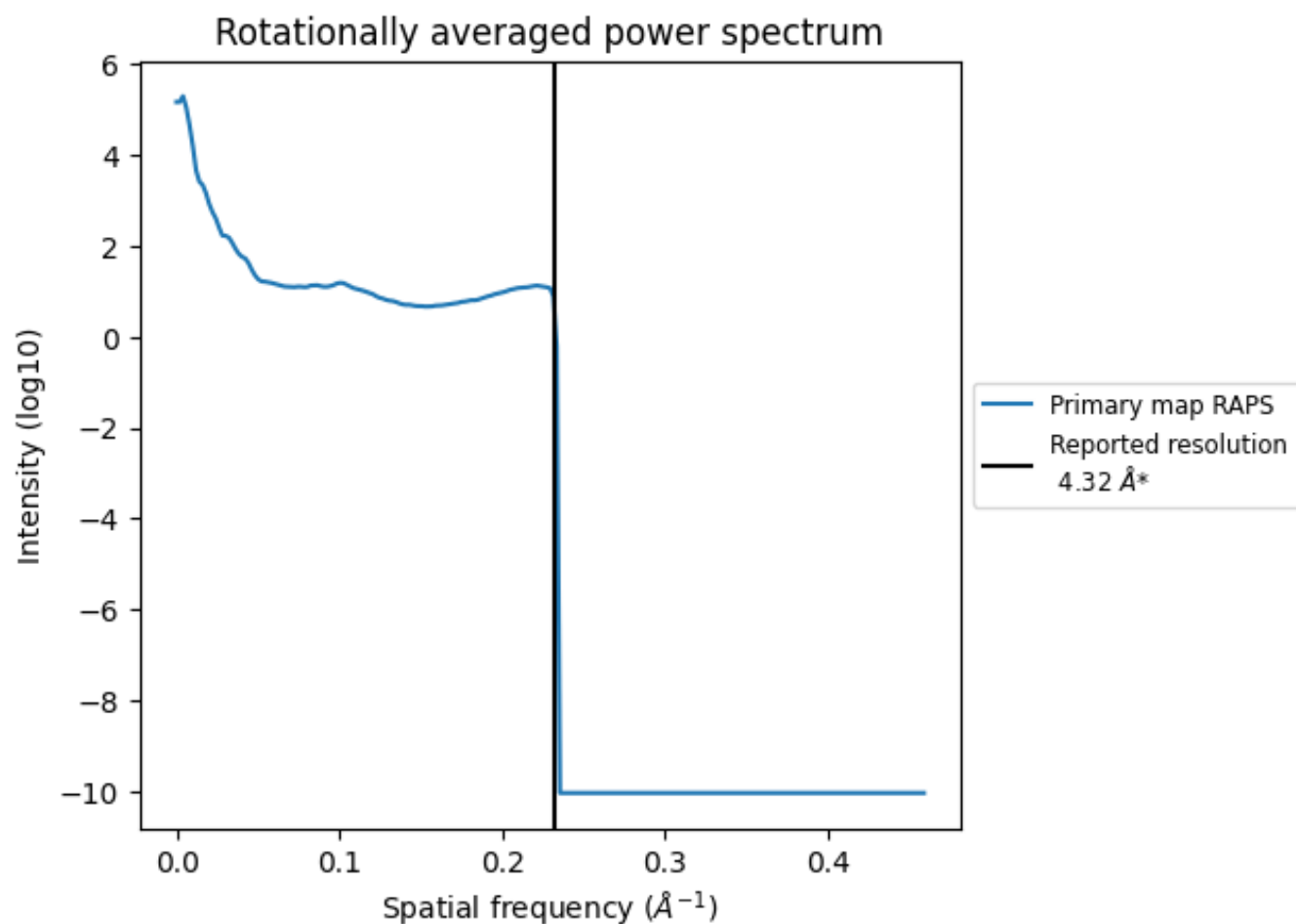
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 223 nm<sup>3</sup>; this corresponds to an approximate mass of 202 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

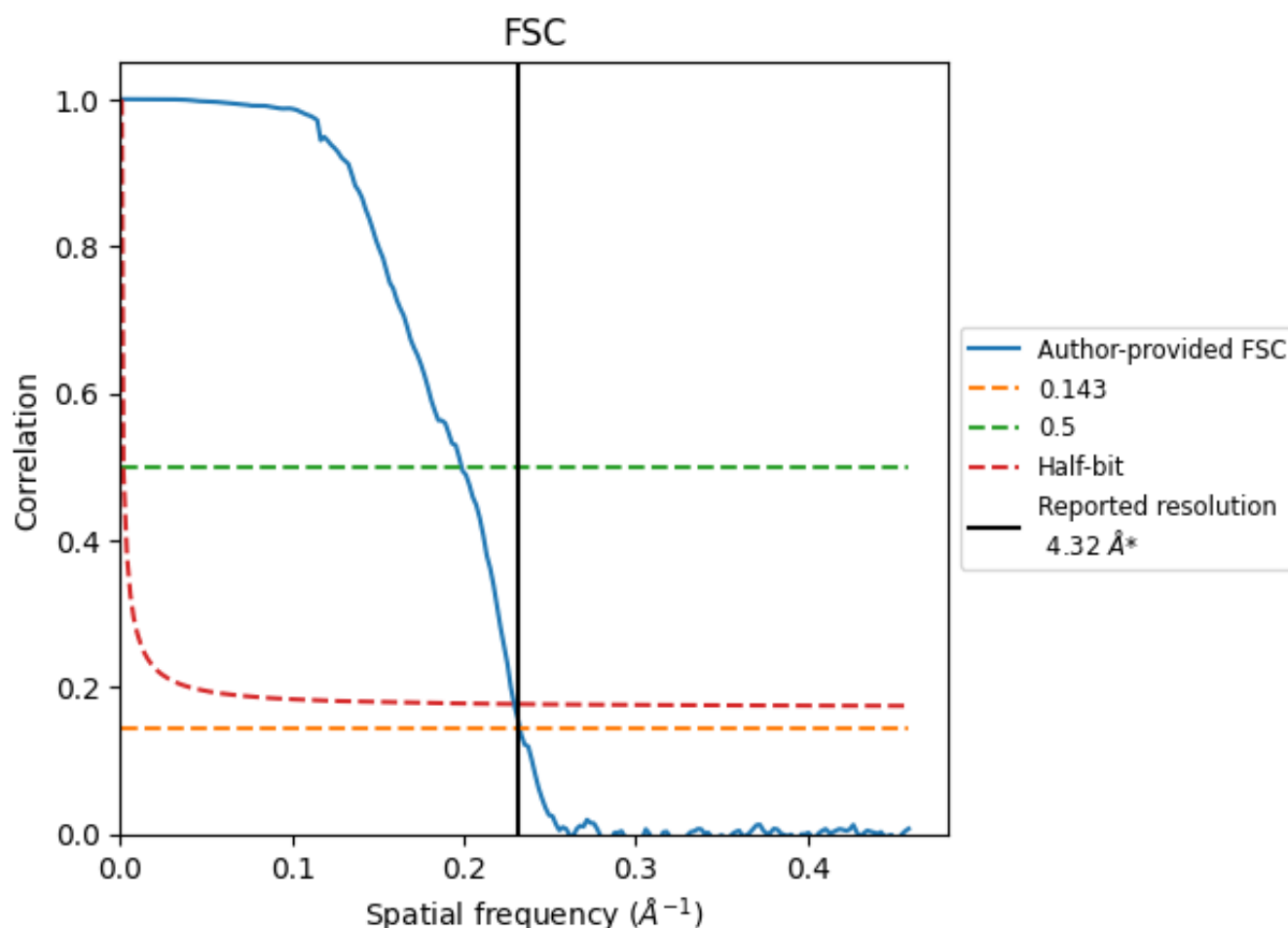


\*Reported resolution corresponds to spatial frequency of 0.231 Å<sup>-1</sup>

## 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 0.231 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

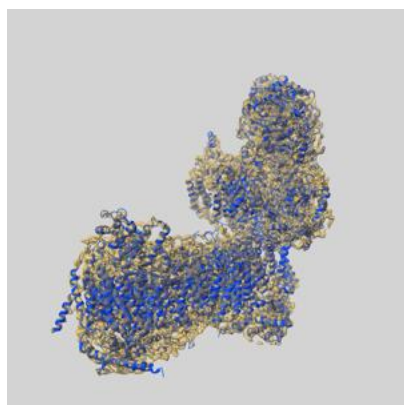
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.32	-	-
Author-provided FSC curve	4.30	5.04	4.36
Unmasked-calculated*	-	-	-

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

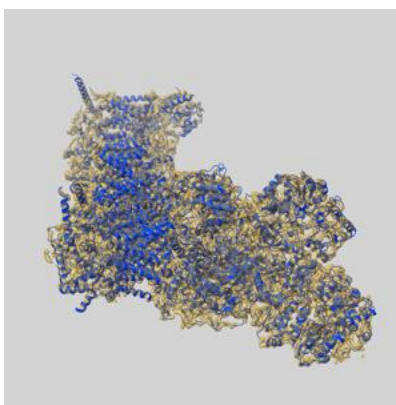
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4384 and PDB model 6GCS. Per-residue inclusion information can be found in section 3 on page 16.

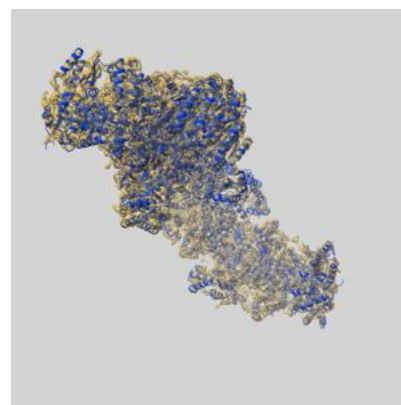
### 9.1 Map-model overlay [i](#)



X



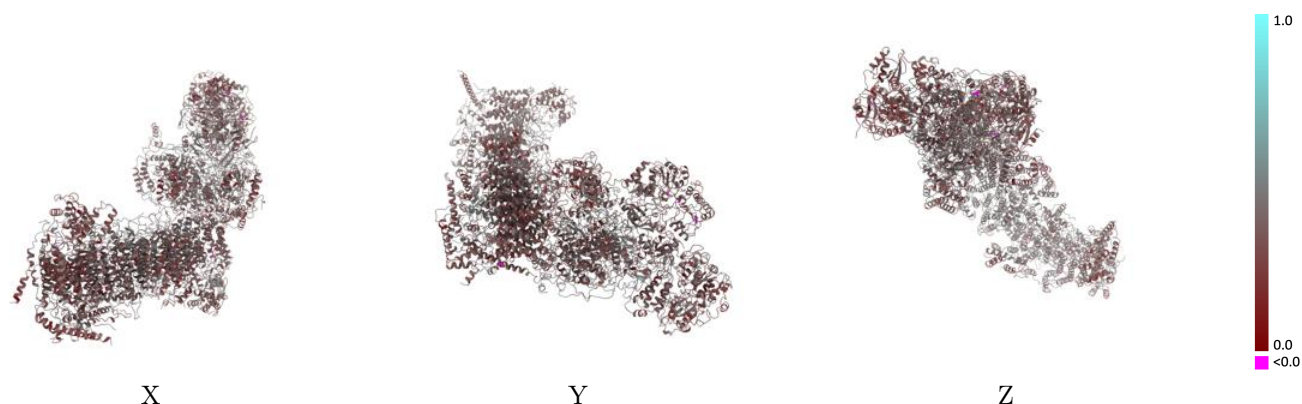
Y



Z

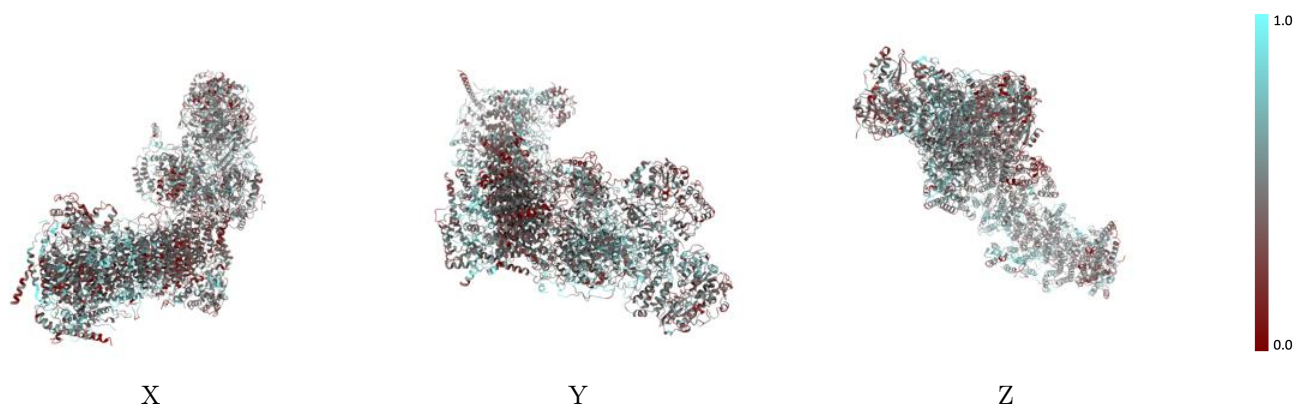
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



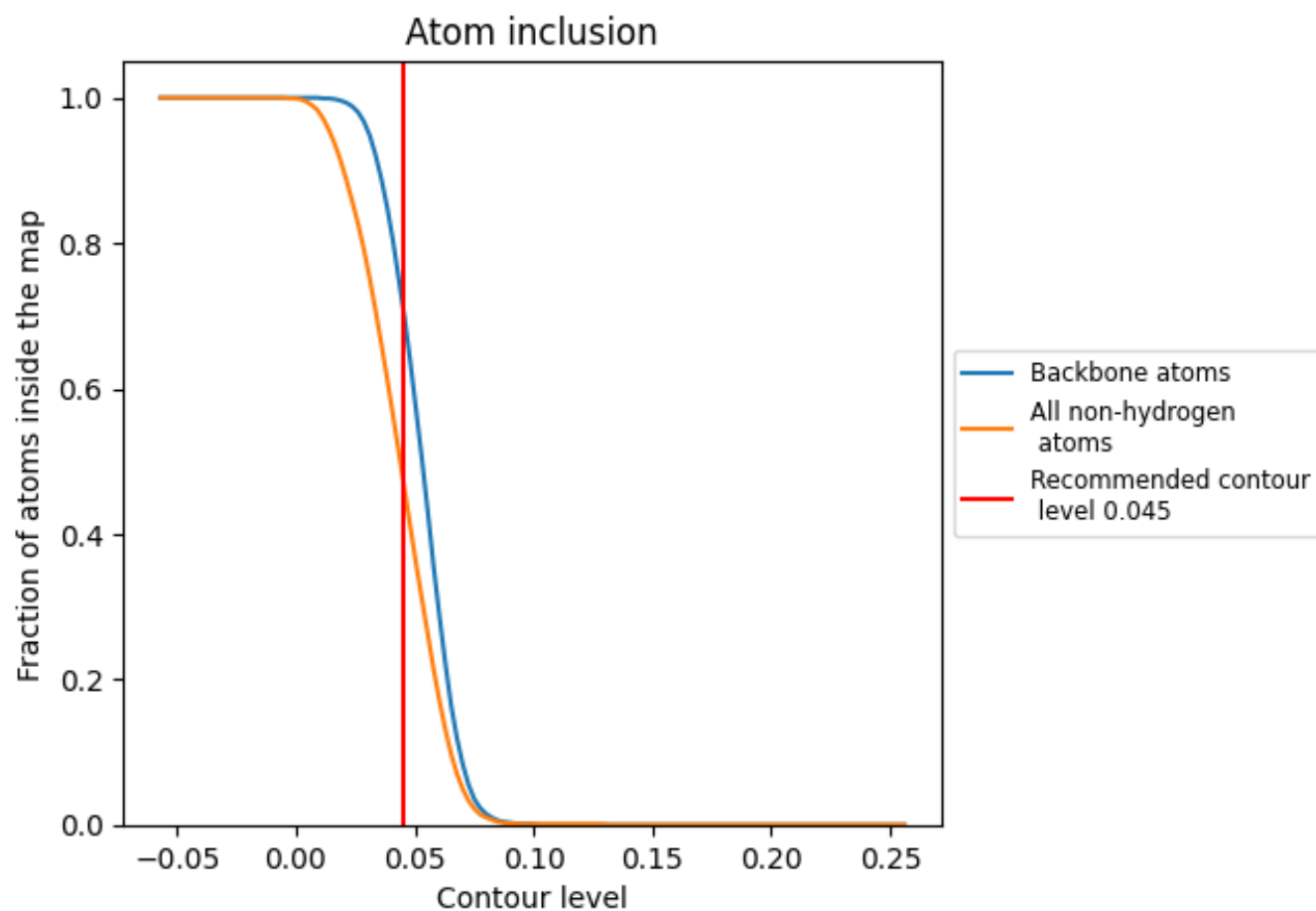
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 71% of all backbone atoms, 48% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4760	 0.3710
1	 0.4040	 0.3510
2	 0.5170	 0.3900
3	 0.3210	 0.3650
4	 0.4920	 0.3770
5	 0.4510	 0.3460
6	 0.3990	 0.3890
8	 0.3540	 0.3110
9	 0.4630	 0.3350
A	 0.4730	 0.3650
B	 0.4500	 0.3440
C	 0.4780	 0.3900
D	 0.4820	 0.3780
E	 0.4480	 0.3640
F	 0.4970	 0.3730
G	 0.5750	 0.4070
H	 0.4820	 0.3450
I	 0.5320	 0.3770
J	 0.3470	 0.3500
K	 0.5320	 0.3860
L	 0.4240	 0.3750
M	 0.5720	 0.4050
O	 0.2150	 0.3280
P	 0.4490	 0.3790
Q	 0.2880	 0.3160
R	 0.4530	 0.3550
S	 0.6020	 0.3880
U	 0.4660	 0.3660
W	 0.4460	 0.3610
X	 0.6380	 0.4220
Y	 0.4960	 0.3990
Z	 0.7390	 0.4500
a	 0.6890	 0.4510
b	 0.6510	 0.3740
c	 0.4160	 0.3580



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Chain	Atom inclusion	Q-score
d	 0.4810	 0.3480
e	 0.6280	 0.4130
f	 0.3840	 0.3520
g	 0.3760	 0.3870
h	 0.5030	 0.3900
i	 0.6350	 0.3870
j	 0.5920	 0.4240
n	 0.7100	 0.4180