wwPDB EM Validation Summary Report ⓘ

Dec 18, 2022 – 03:42 am GMT

PDB ID	:	7A24
EMDB ID	:	EMD-11615
Title	:	Assembly intermediate of the plant mitochondrial complex I
Authors	:	Soufari, H.; Waltz, F.; Hashem, Y.
Deposited on	:	2020-08-16
Resolution	:	3.80 Å(reported)

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

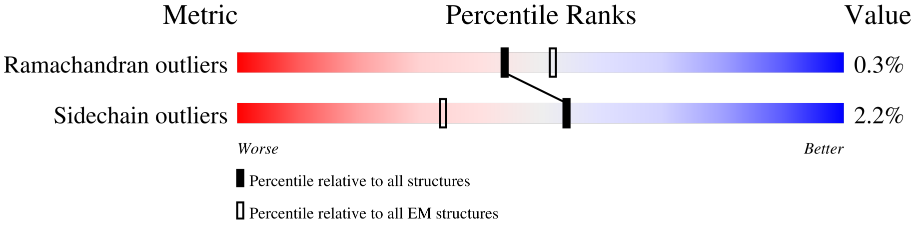
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

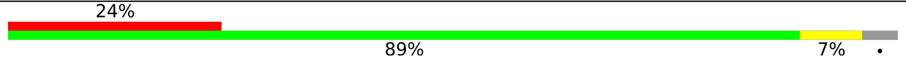
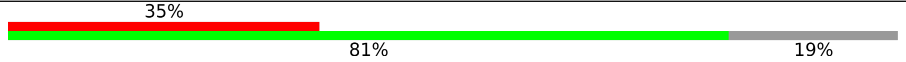
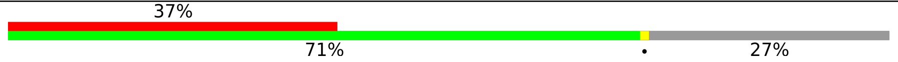
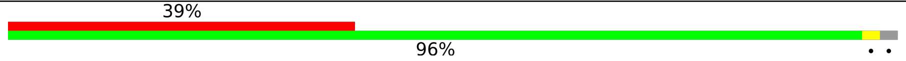
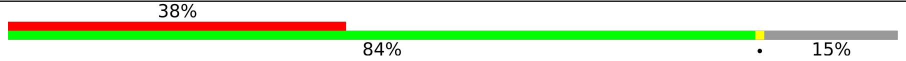
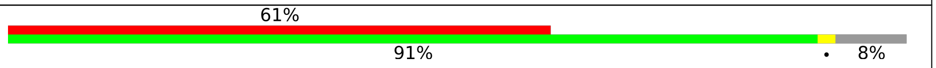
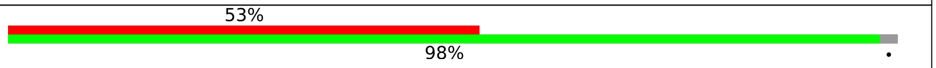
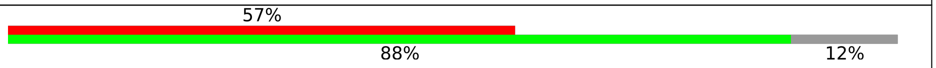
The reported resolution of this entry is 3.80 Å.

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.



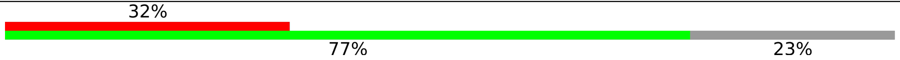
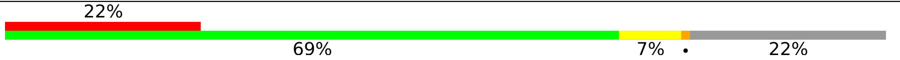
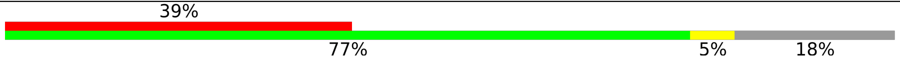
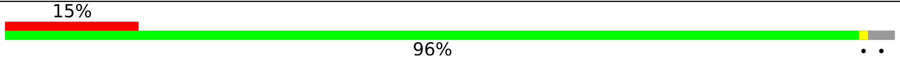
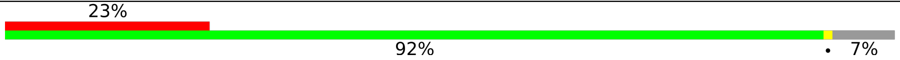
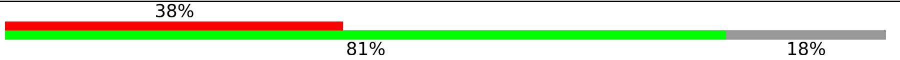
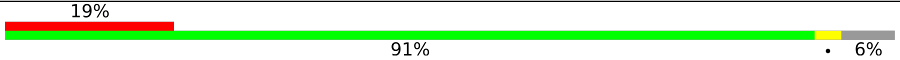
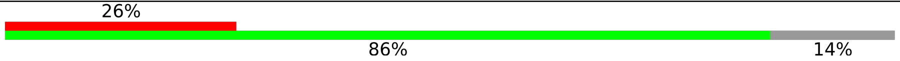
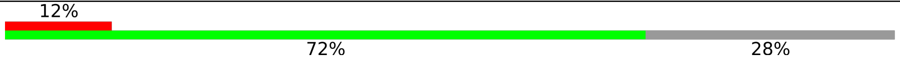
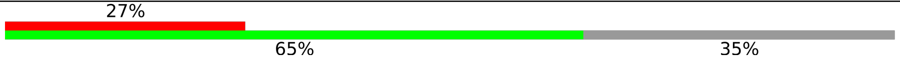
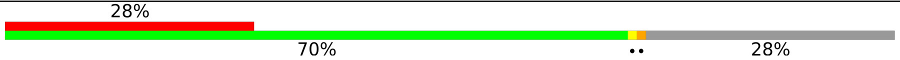
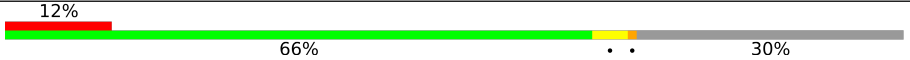
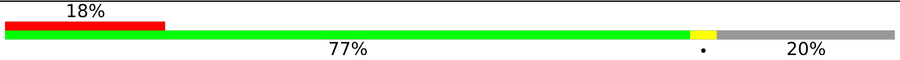
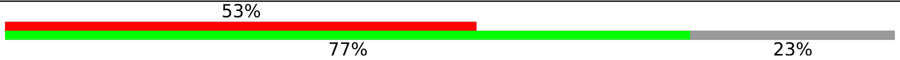
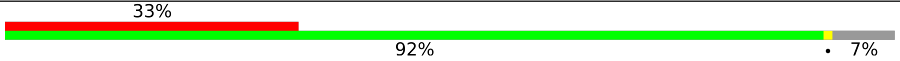
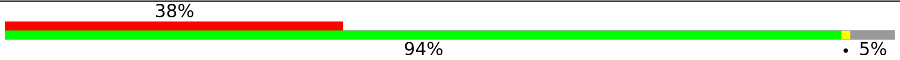
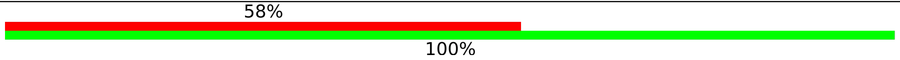
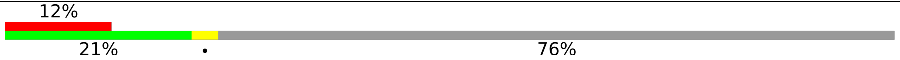
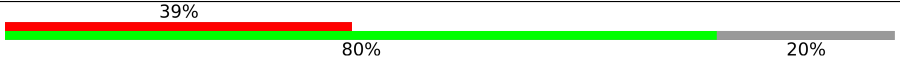
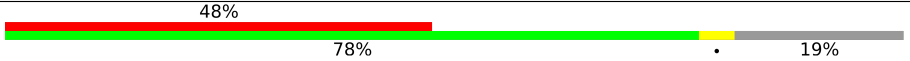
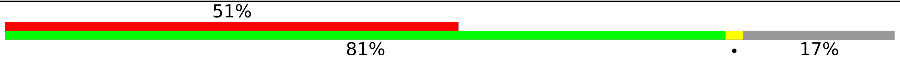
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	486	
2	I	499	
3	J	119	
4	N	205	
5	H	325	
6	K	100	
7	Y	106	
8	Z	143	
9	V	65	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	W	65	
11	S	131	
12	i	81	
13	j	83	
14	G	394	
15	C	748	
16	T	402	
17	F	190	
18	B	255	
19	O	154	
20	P	110	
21	R	169	
22	U	159	
23	E	218	
24	D	222	
25	X	133	
26	c	106	
27	Q	97	
28	k	122	
29	r	24	
30	n	113	
31	o	252	
32	p	275	
32	q	275	
33	z	610	

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 49497 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 51kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	429	3328	2100	593	610	25	0	0

- Molecule 2 is a protein called Nad2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	I	481	3754	2525	569	633	27	0	0

- Molecule 3 is a protein called Nad3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	96	800	559	112	126	3	0	0

- Molecule 4 is a protein called Nad6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	N	149	1201	810	194	189	8	0	0

- Molecule 5 is a protein called Nad1m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	318	2493	1691	378	409	15	0	0

- Molecule 6 is a protein called Nad4Lm.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	K	85	667	450	101	110	6	0	0

- Molecule 7 is a protein called PGIV.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	98	Total	C	N	O	S	0	0
			774	484	133	145	12		

- Molecule 8 is a protein called B16.6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	140	Total	C	N	O	S	0	0
			1103	701	195	199	8		

- Molecule 9 is a protein called MWFE.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	57	Total	C	N	O	S	0	0
			461	296	82	78	5		

- Molecule 10 is a protein called B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	37	Total	C	N	O	S	0	0
			273	179	45	46	3		

- Molecule 11 is a protein called B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	101	Total	C	N	O	S	0	0
			821	513	143	161	4		

- Molecule 12 is a protein called B14.5b.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	i	63	Total	C	N	O	S	0	0
			492	319	87	81	5		

- Molecule 13 is a protein called 15kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	j	68	Total	C	N	O	S	0	0
			582	359	113	103	7		

- Molecule 14 is a protein called Nad7m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	G	382	3049	1939	535	551	24	0	0

- Molecule 15 is a protein called 75kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	C	693	5288	3315	926	1008	39	0	0

- Molecule 16 is a protein called 39kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	T	328	2535	1628	433	459	15	0	0

- Molecule 17 is a protein called Nad9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	F	178	1518	979	262	272	5	0	0

- Molecule 18 is a protein called 24kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	B	219	1702	1081	286	323	12	0	0

- Molecule 19 is a protein called 18kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	O	111	874	561	150	162	1	0	0

- Molecule 20 is a protein called 13kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	P	71	554	348	97	103	6	0	0

- Molecule 21 is a protein called B13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	121	Total 977	C 614	N 165	O 193	S 5	0	0

- Molecule 22 is a protein called B17.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	122	Total 1011	C 643	N 184	O 183	S 1	0	0

- Molecule 23 is a protein called PSST.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	E	153	Total 1215	C 779	N 212	O 210	S 14	0	0

- Molecule 24 is a protein called TYKY.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	D	177	Total 1438	C 901	N 239	O 287	S 11	0	0

- Molecule 25 is a protein called B14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	103	Total 843	C 537	N 151	O 152	S 3	0	0

- Molecule 26 is a protein called MNLL.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	99	Total 744	C 479	N 121	O 140	S 4	0	0

- Molecule 27 is a protein called B8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Q	92	Total 722	C 456	N 128	O 132	S 6	0	0

- Molecule 28 is a protein called ACPM1.

Mol	Chain	Residues	Atoms	AltConf	Trace
28	k	78	Total C N O S 614 390 94 127 3	0	0

- Molecule 29 is a protein called Unk1.

Mol	Chain	Residues	Atoms	AltConf	Trace
29	r	24	Total C N O 120 72 24 24	0	0

- Molecule 30 is a protein called P2.

Mol	Chain	Residues	Atoms	AltConf	Trace
30	n	27	Total C N O 205 133 35 37	0	0

- Molecule 31 is a protein called CAL1.

Mol	Chain	Residues	Atoms	AltConf	Trace
31	o	202	Total C N O S 1568 1006 270 287 5	0	0

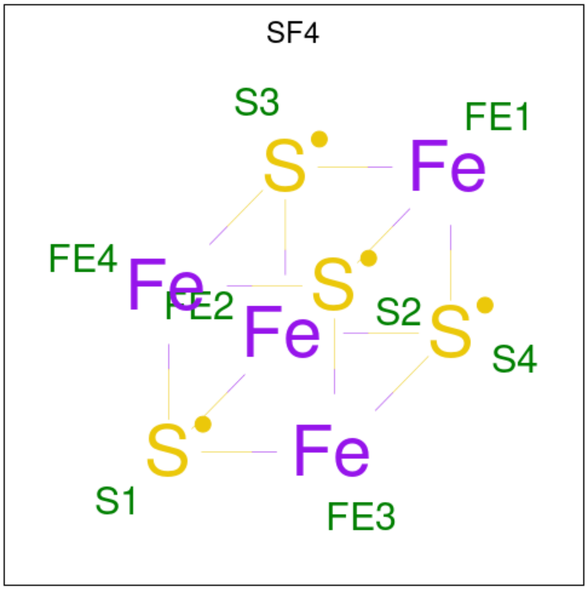
- Molecule 32 is a protein called CA1.

Mol	Chain	Residues	Atoms	AltConf	Trace
32	q	228	Total C N O S 1736 1088 318 324 6	0	0
32	p	224	Total C N O S 1705 1068 311 320 6	0	0

- Molecule 33 is a protein called GLDH.

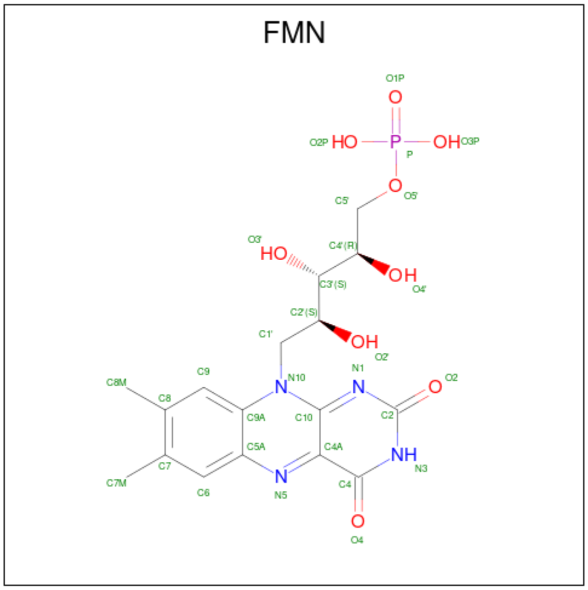
Mol	Chain	Residues	Atoms	AltConf	Trace
33	z	499	Total C N O S 3992 2527 700 754 11	0	0

- Molecule 34 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



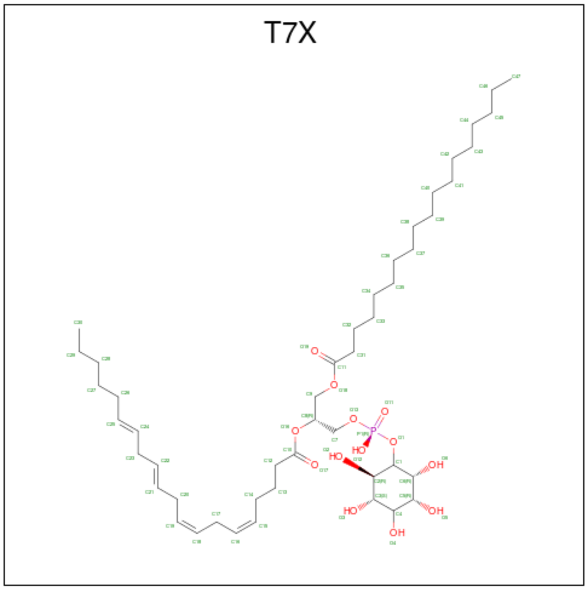
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
34	A	1	8	4	4	0
			Total	Fe	S	
34	C	1	16	8	8	0
			Total	Fe	S	
34	C	1	16	8	8	0
			Total	Fe	S	
34	E	1	8	4	4	0
			Total	Fe	S	
34	D	1	16	8	8	0
			Total	Fe	S	
34	D	1	16	8	8	0

- Molecule 35 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



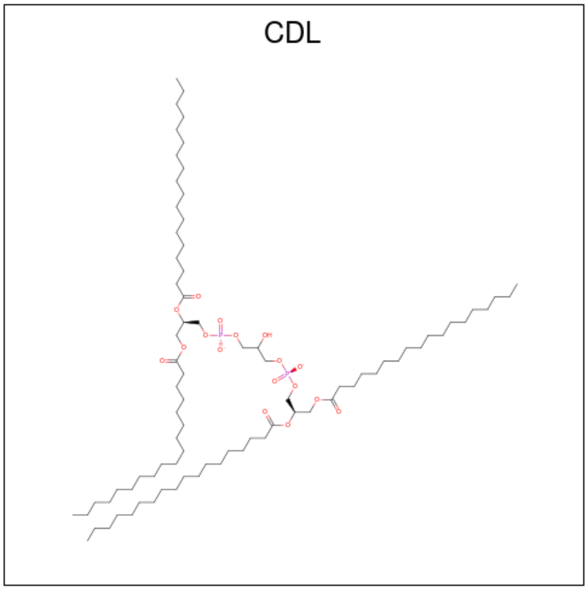
Mol	Chain	Residues	Atoms	AltConf
35	A	1	Total C N O P 31 17 4 9 1	0

- Molecule 36 is Phosphatidylinositol (three-letter code: T7X) (formula: $C_{47}H_{83}O_{13}P$).



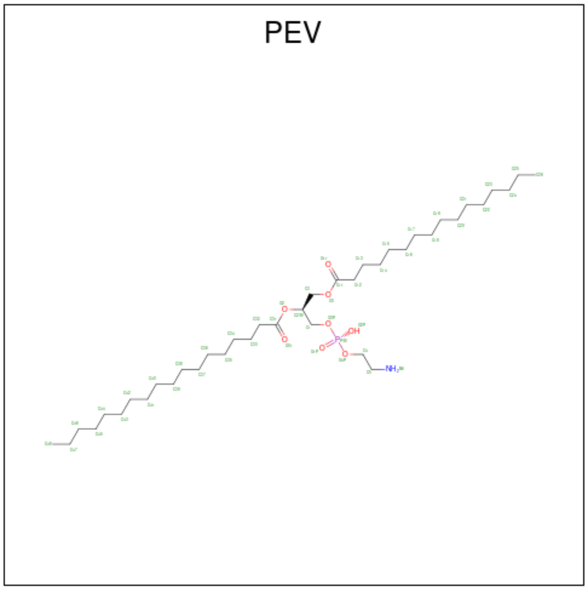
Mol	Chain	Residues	Atoms	AltConf
36	I	1	Total C O P 42 28 13 1	0
36	c	1	Total C O P 37 23 13 1	0

- Molecule 37 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



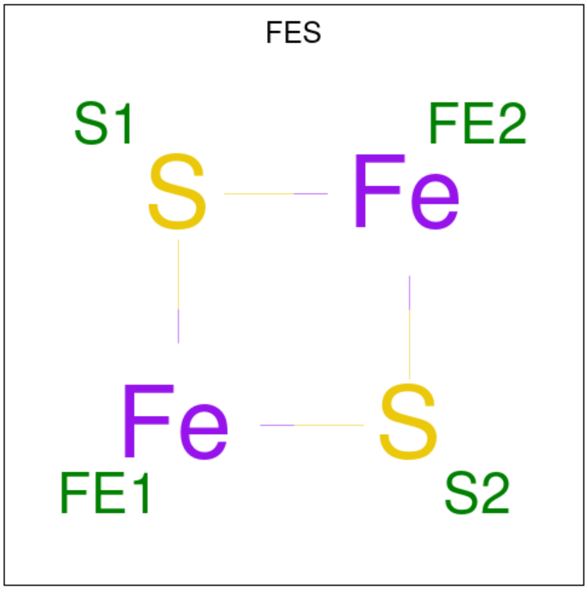
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
37	i	1	90	71	17	2	0

- Molecule 38 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PEV) (formula: $C_{39}H_{78}NO_8P$).



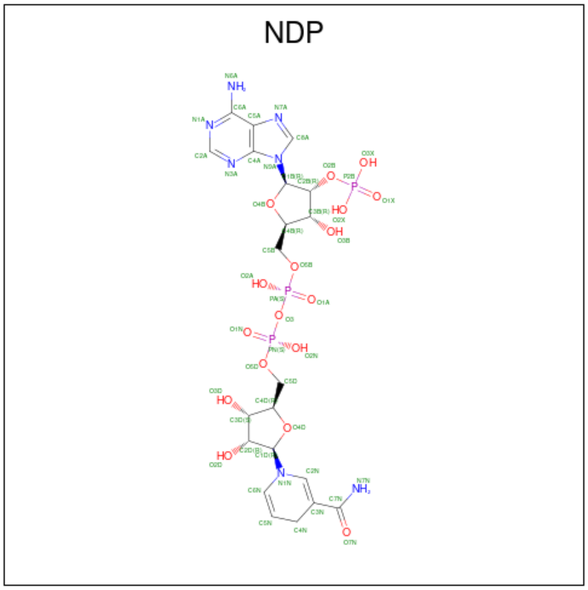
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
38	G	1	28	18	1	8	1	0

- Molecule 39 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	AltConf
39	C	1	Total Fe S 4 2 2	0
39	B	1	Total Fe S 4 2 2	0

- Molecule 40 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_{7}O_{17}P_{3}$).

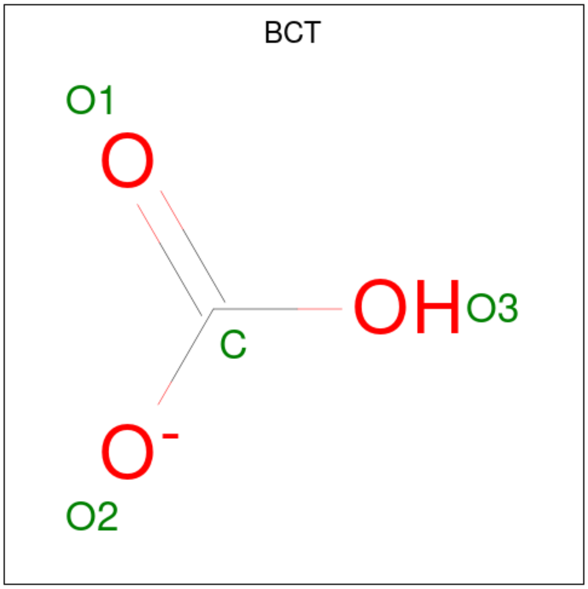


Mol	Chain	Residues	Atoms	AltConf
40	T	1	Total C N O P 48 21 7 17 3	0

- Molecule 41 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
41	P	1	Total Zn 1 1	0
41	q	1	Total Zn 1 1	0

- Molecule 42 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



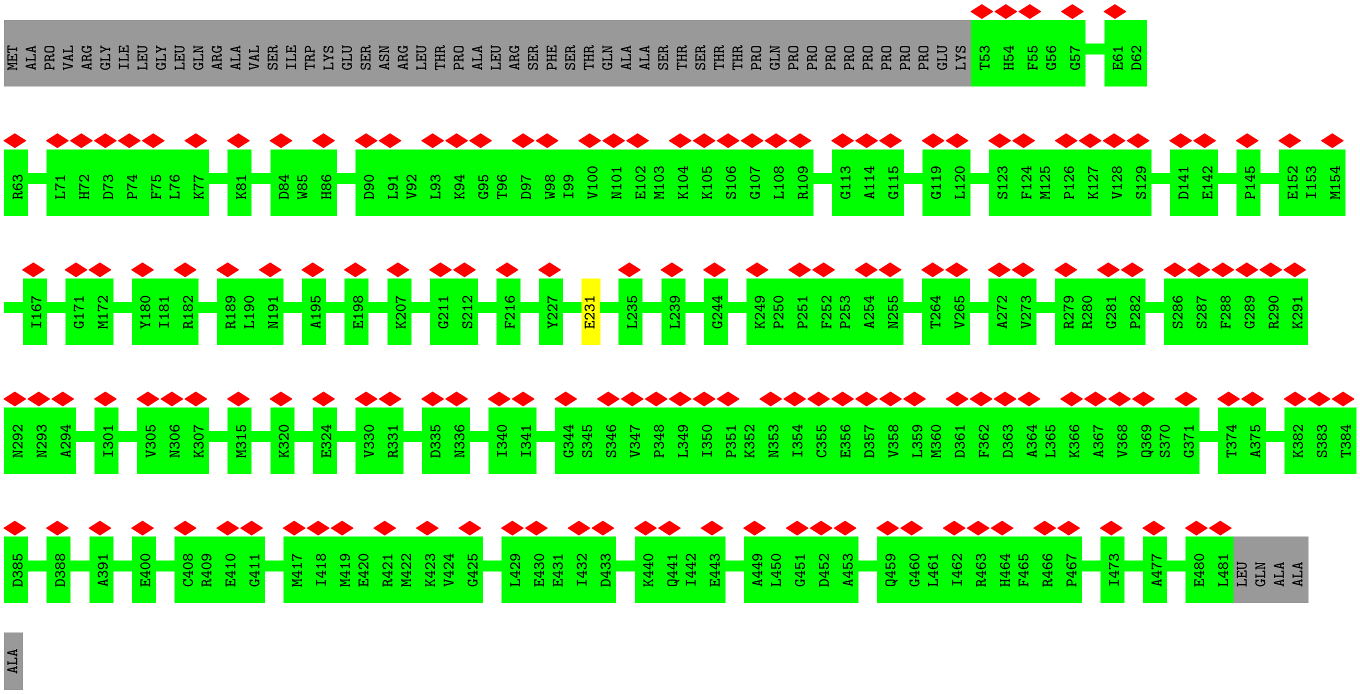
Mol	Chain	Residues	Atoms	AltConf
42	q	1	Total C O 4 1 3	0

3 Residue-property plots ⓘ

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

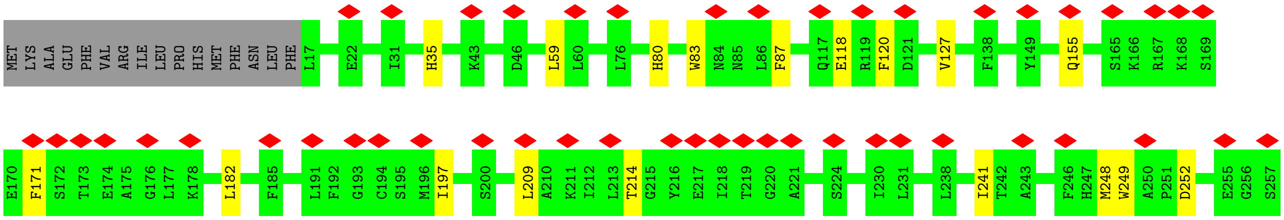
- Molecule 1: 51kDa

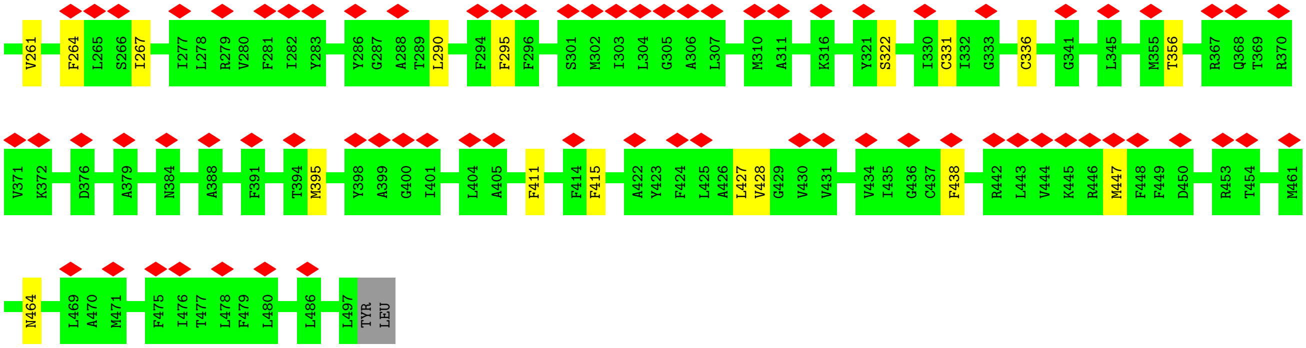
Chain A:



- Molecule 2: Nad2m

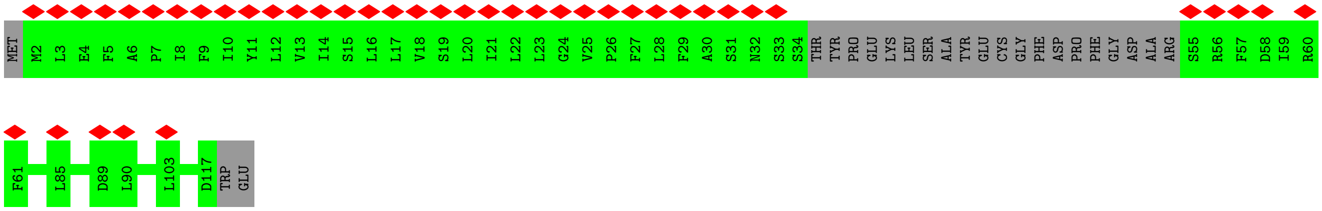
Chain I:





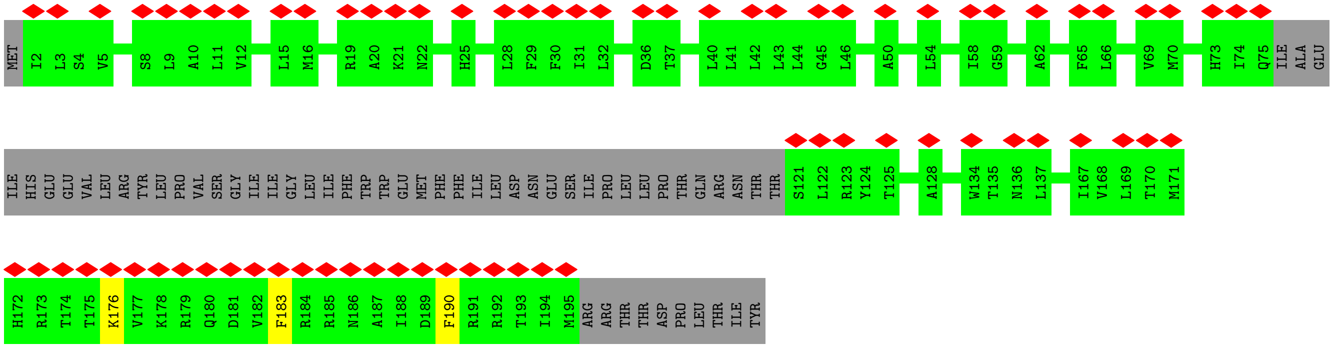
- Molecule 3: Nad3m

Chain J:



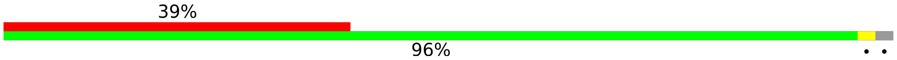
- Molecule 4: Nad6m

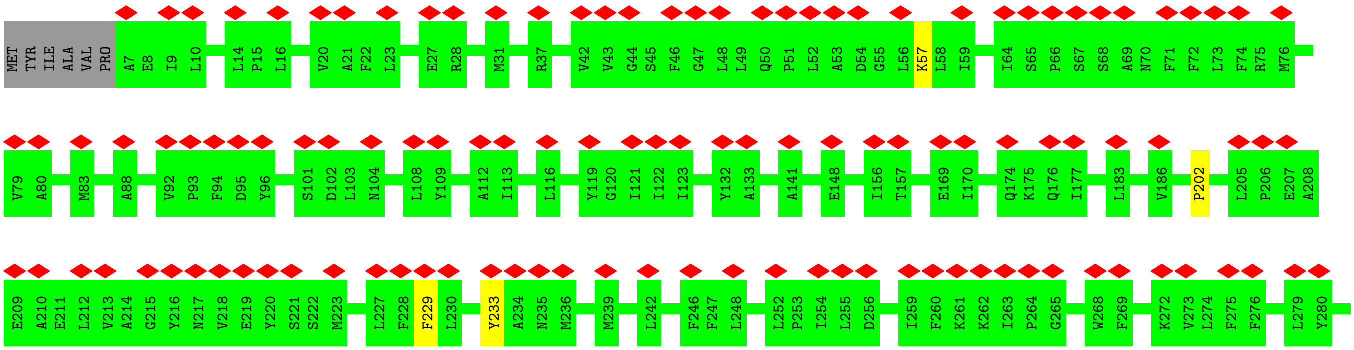
Chain N:

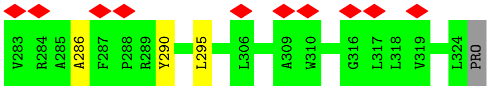


- Molecule 5: Nad1m

Chain H:

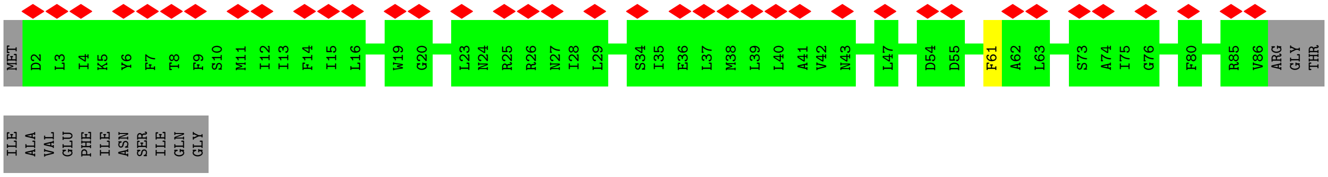






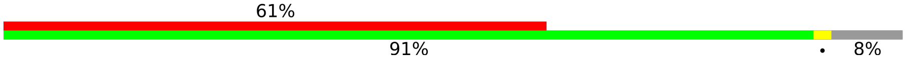
- Molecule 6: Nad4Lm

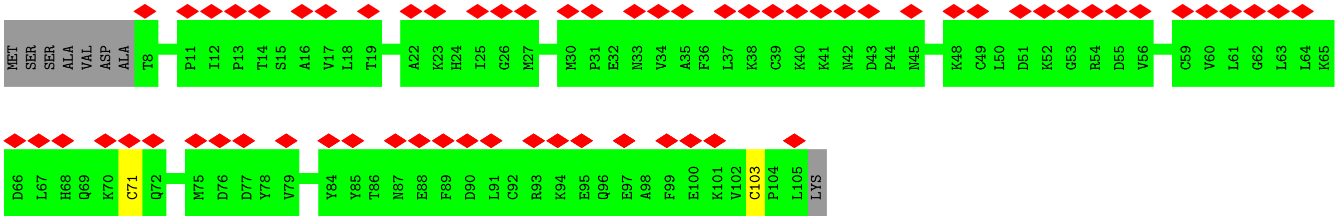
Chain K:



- Molecule 7: PGIV

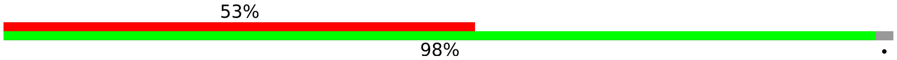
Chain Y:

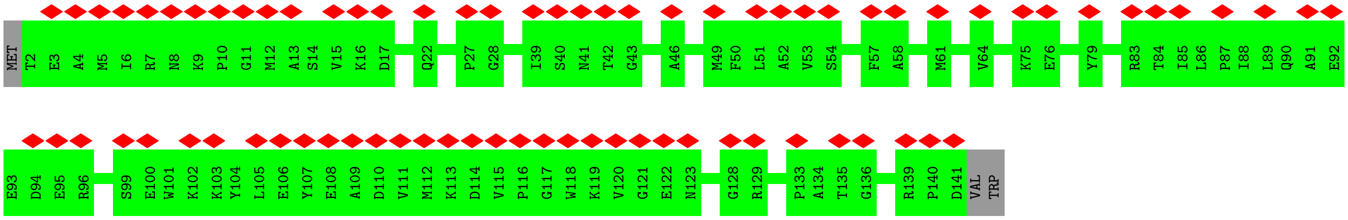




- Molecule 8: B16.6

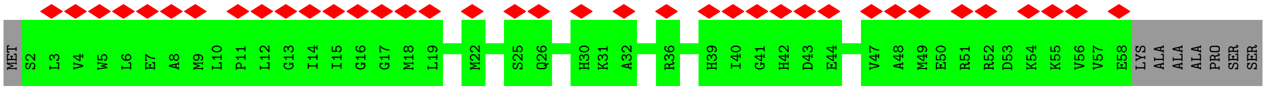
Chain Z:





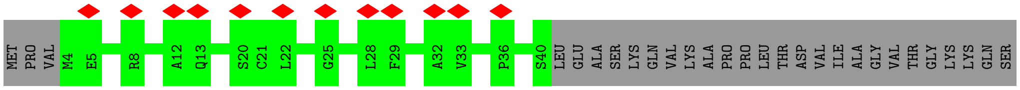
- Molecule 9: MWFE

Chain V:



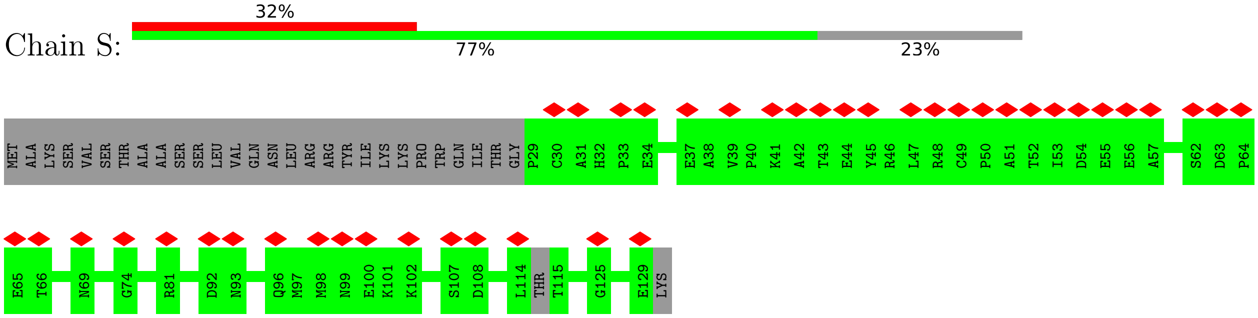
- Molecule 10: B9

Chain W:



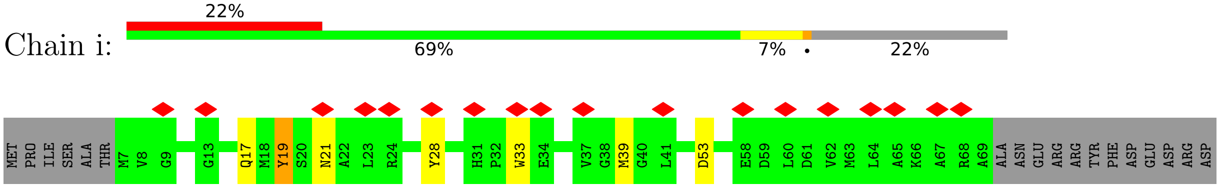
- Molecule 11: B14.5a

Chain S:



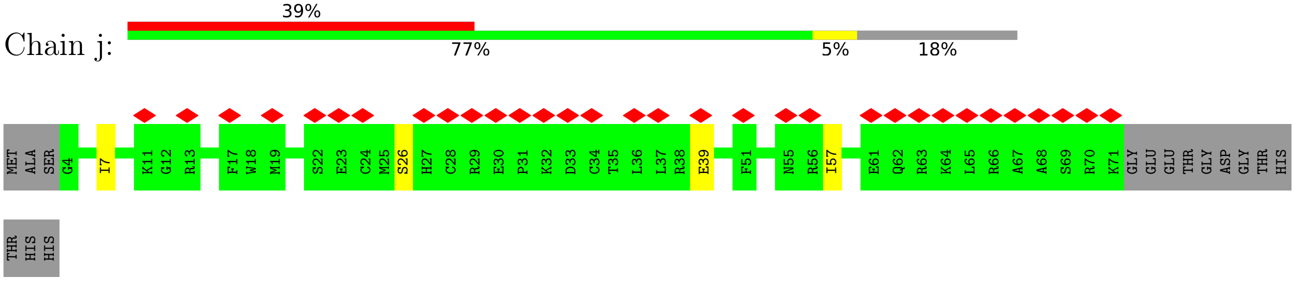
- Molecule 12: B14.5b

Chain i:



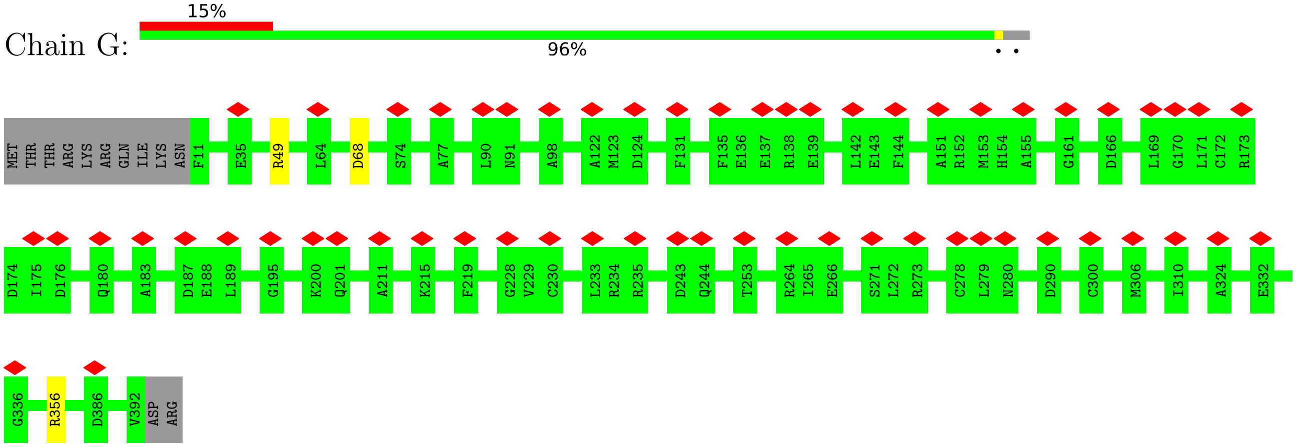
- Molecule 13: 15kDa

Chain j:



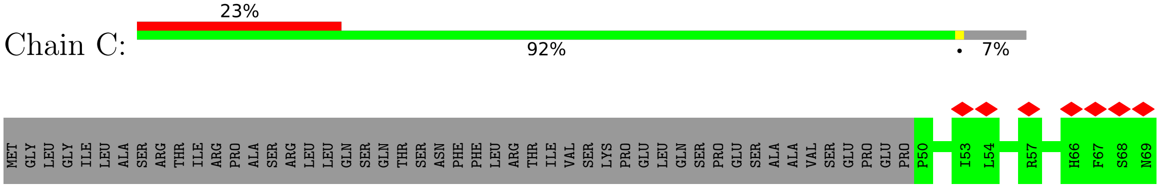
- Molecule 14: Nad7m

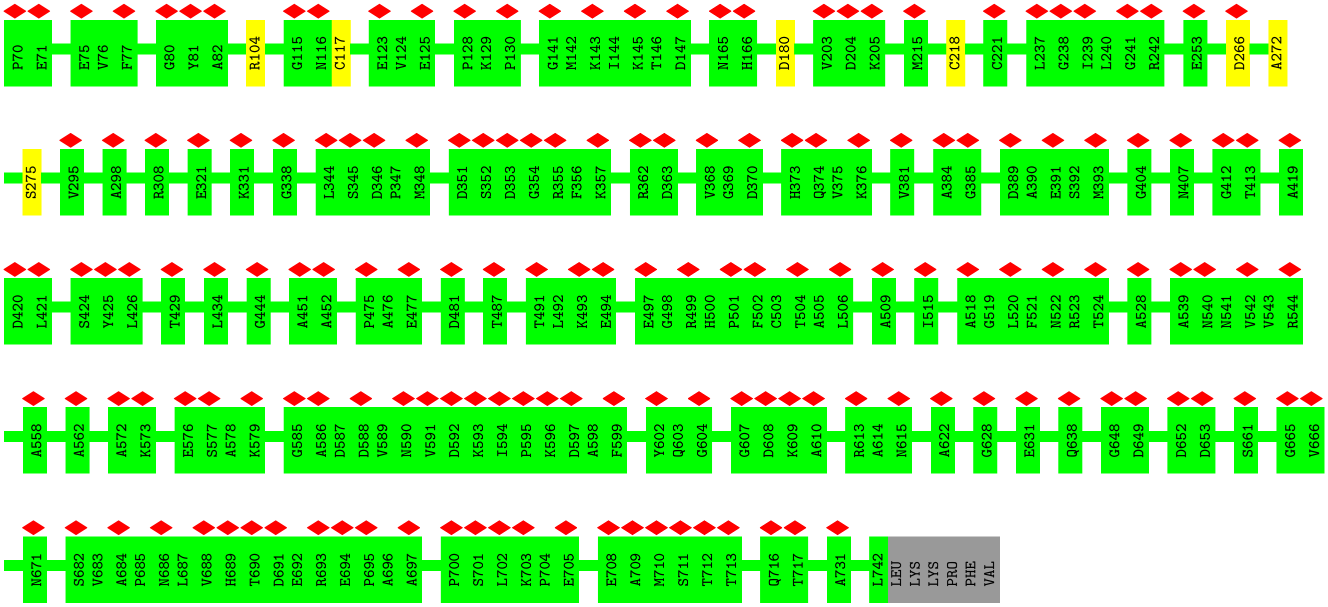
Chain G:



- Molecule 15: 75kDa

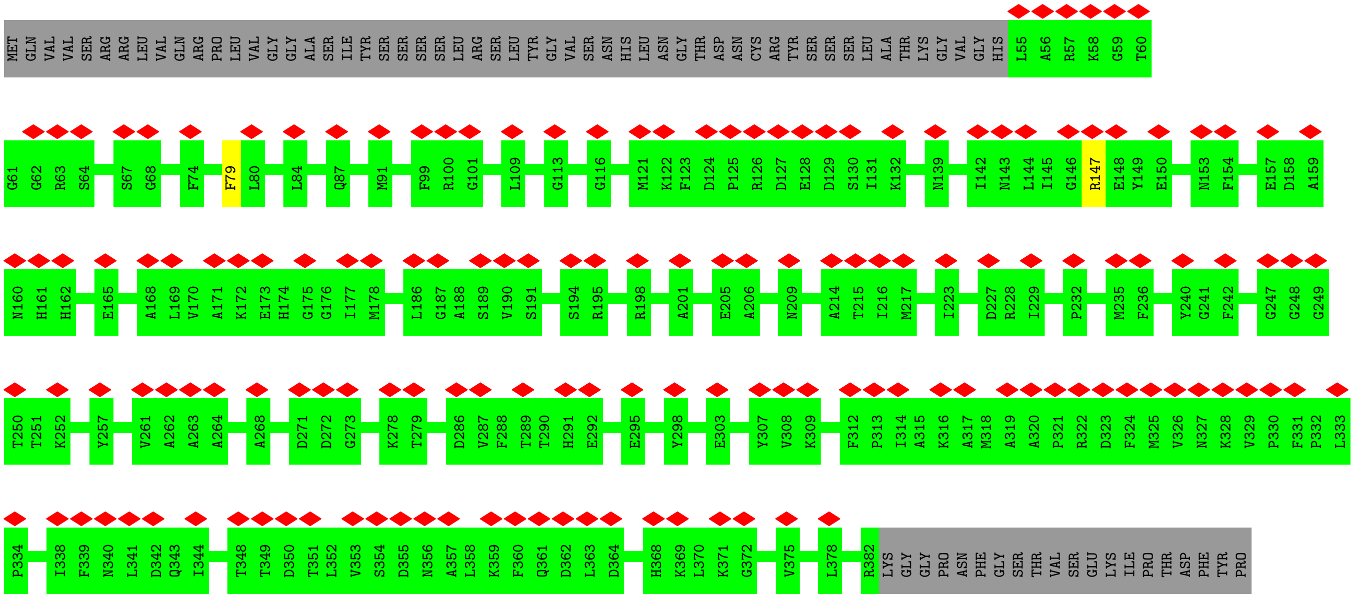
Chain C:





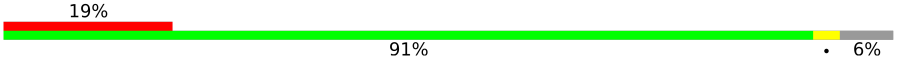
- Molecule 16: 39kDa

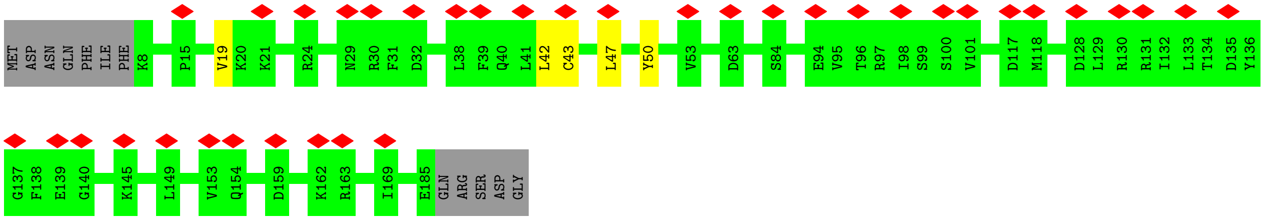
Chain T:



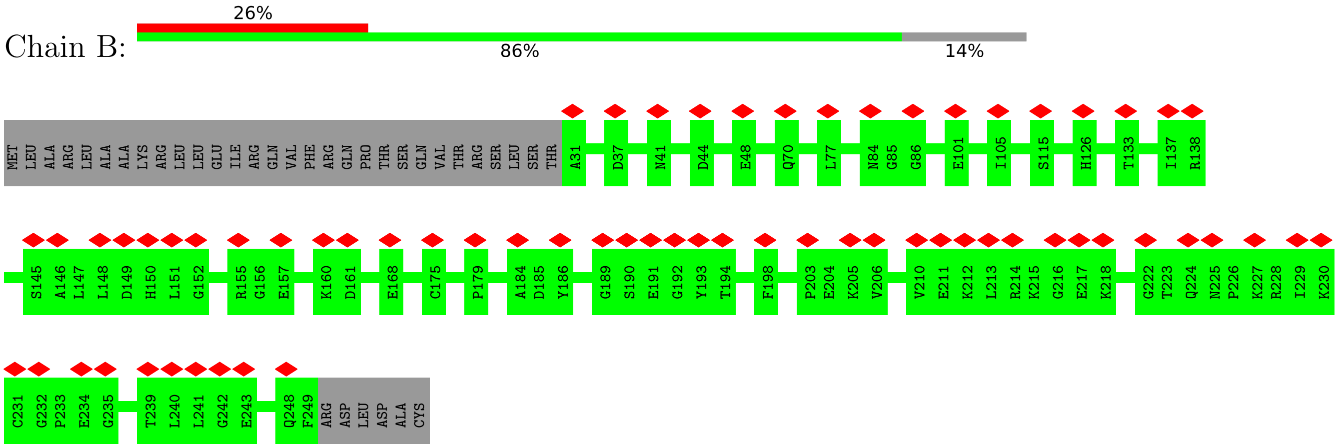
- Molecule 17: Nad9m

Chain F:

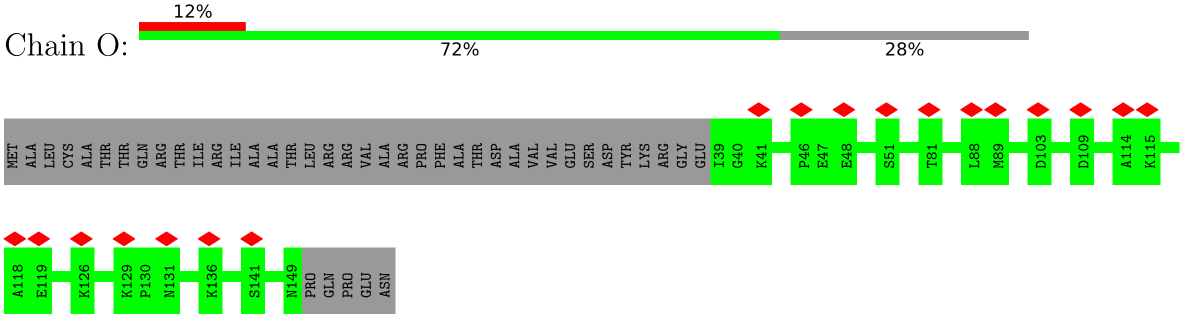




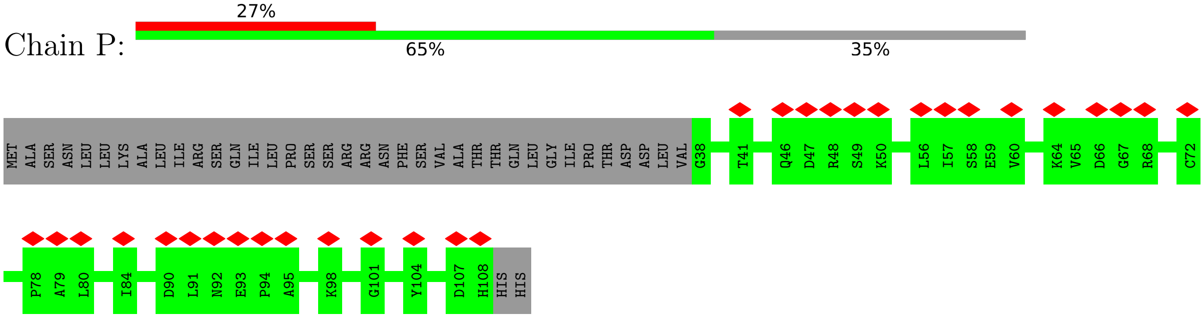
- Molecule 18: 24kDa



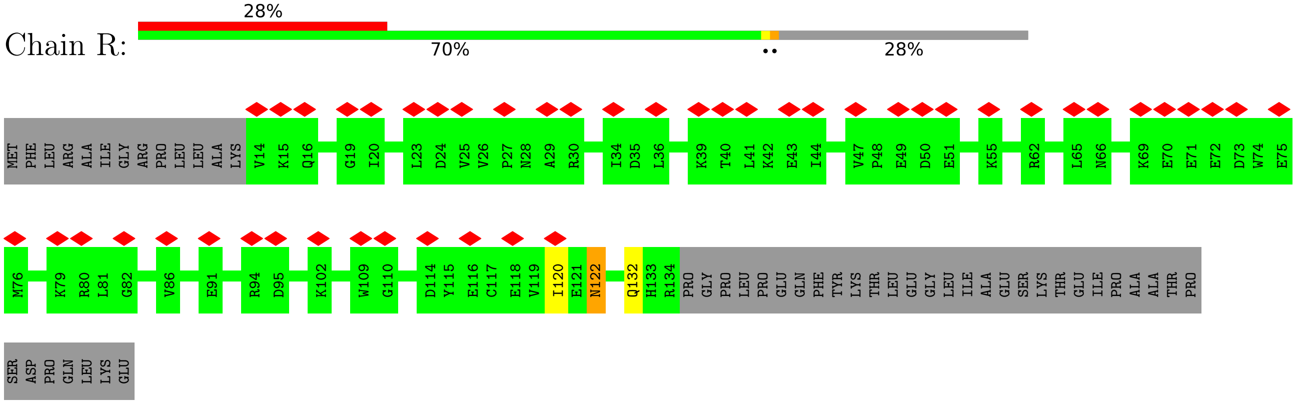
- Molecule 19: 18kDa



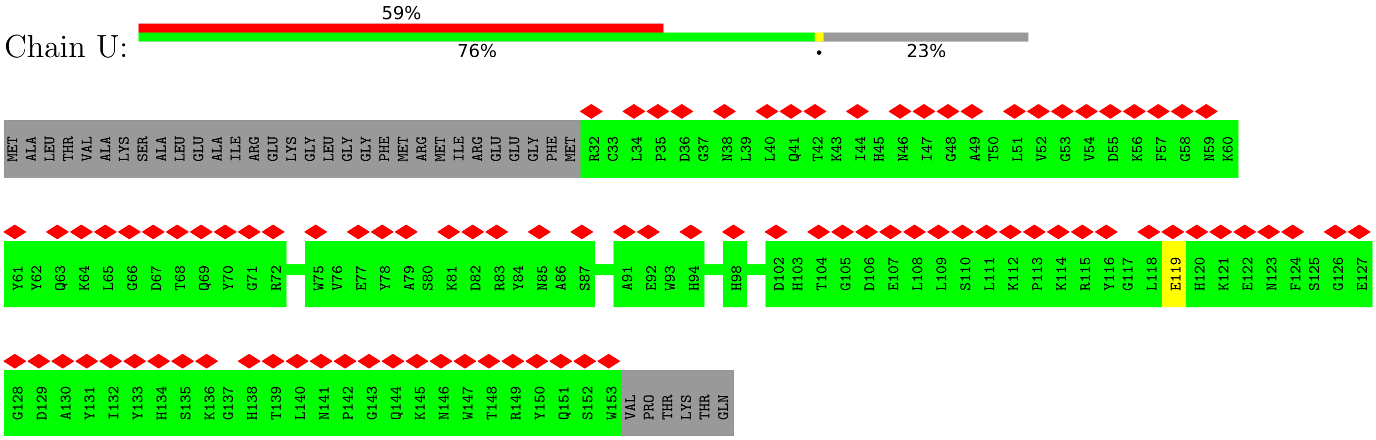
- Molecule 20: 13kDa



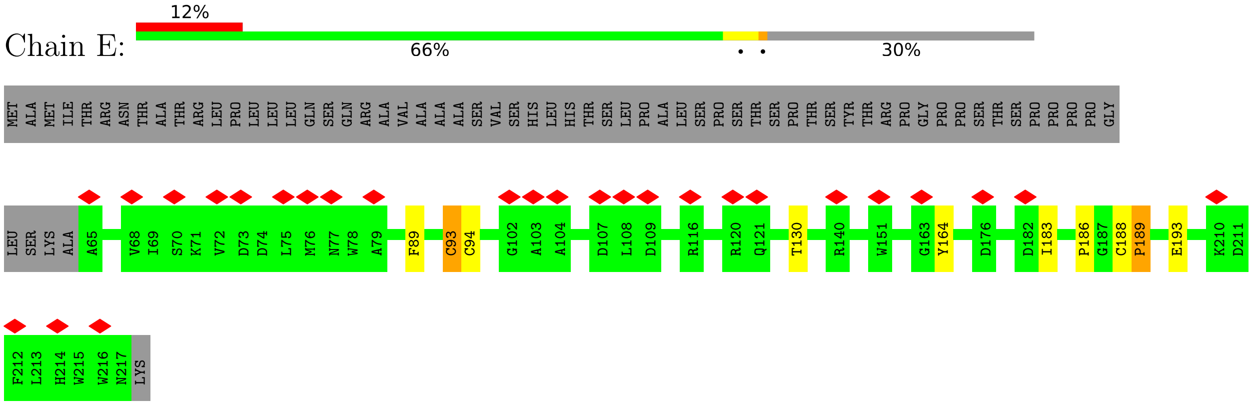
- Molecule 21: B13



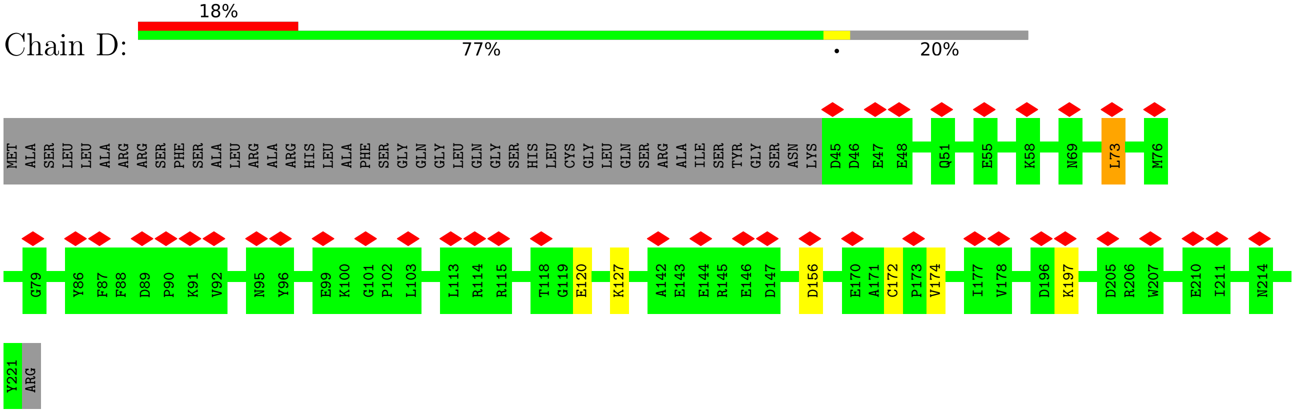
- Molecule 22: B17.2



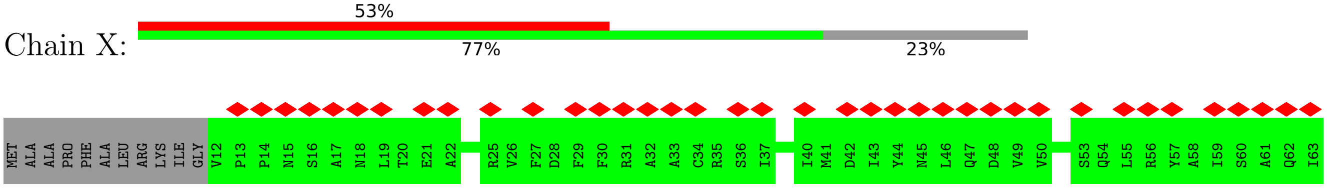
- Molecule 23: PSST

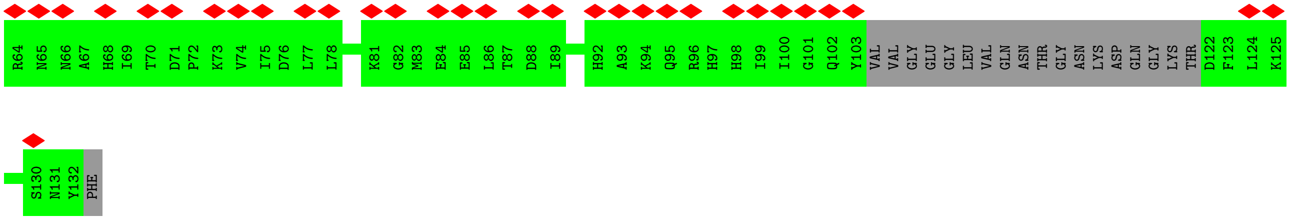


- Molecule 24: TYKY



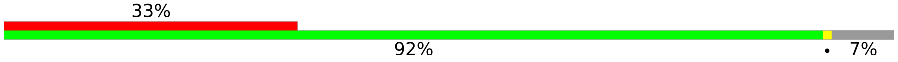
- Molecule 25: B14

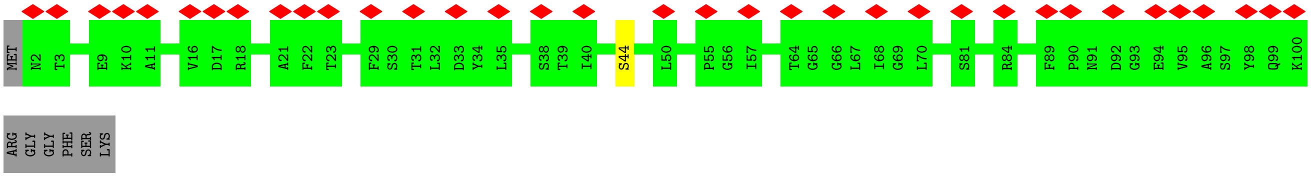




- Molecule 26: MNLL

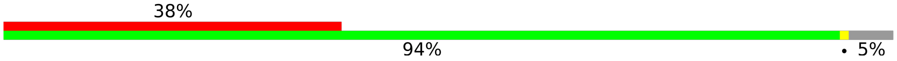
Chain c:

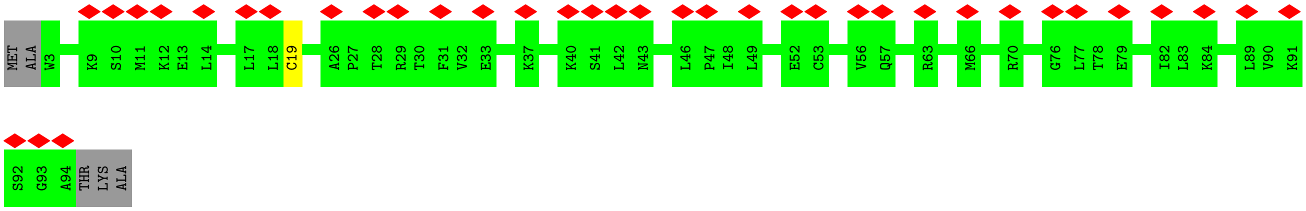




- Molecule 27: B8

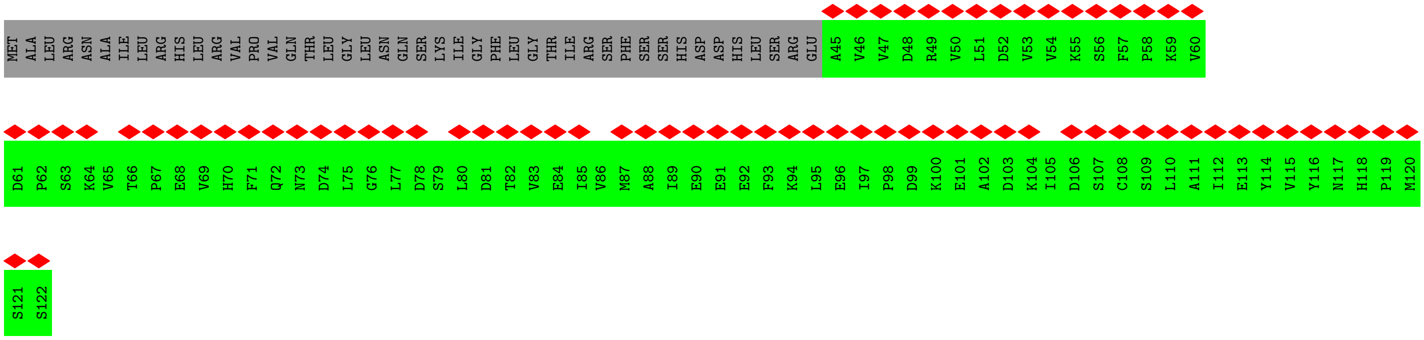
Chain Q:





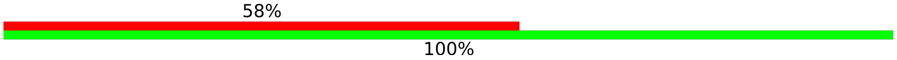
- Molecule 28: ACPM1

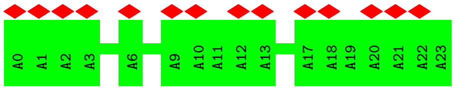
Chain k:



- Molecule 29: Unk1

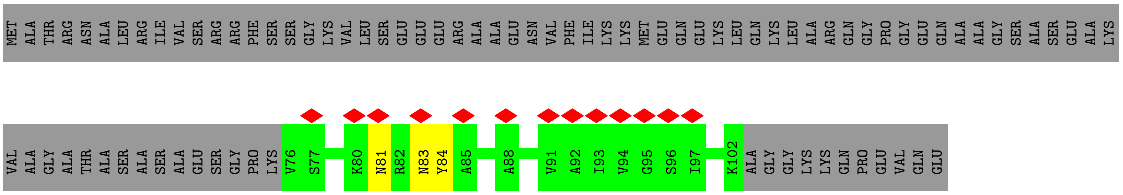
Chain r:





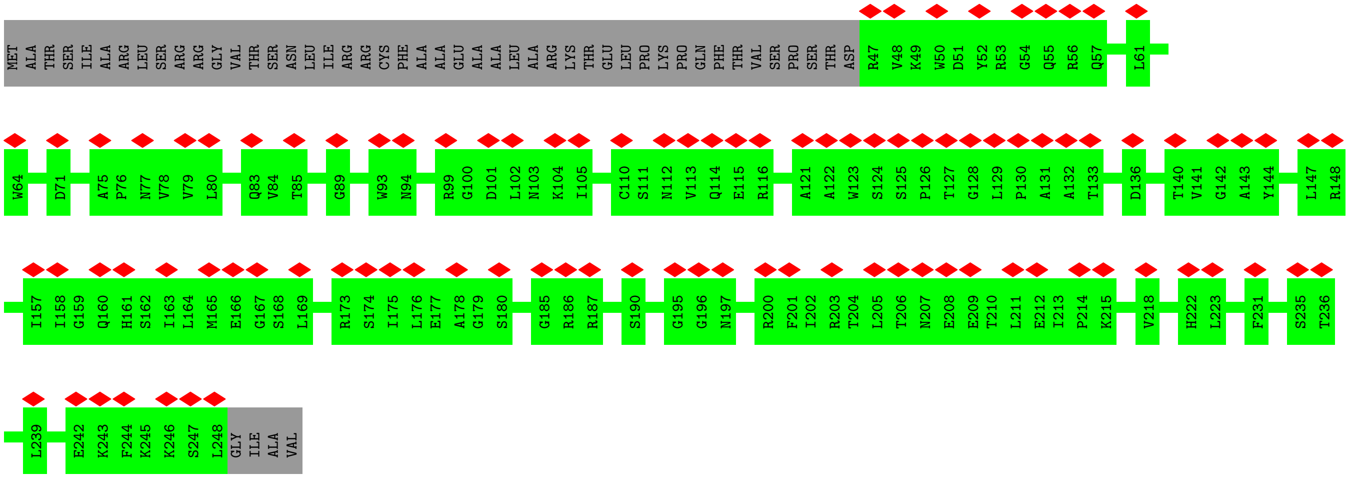
- Molecule 30: P2

Chain n:



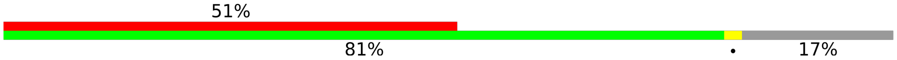
- Molecule 31: CAL1

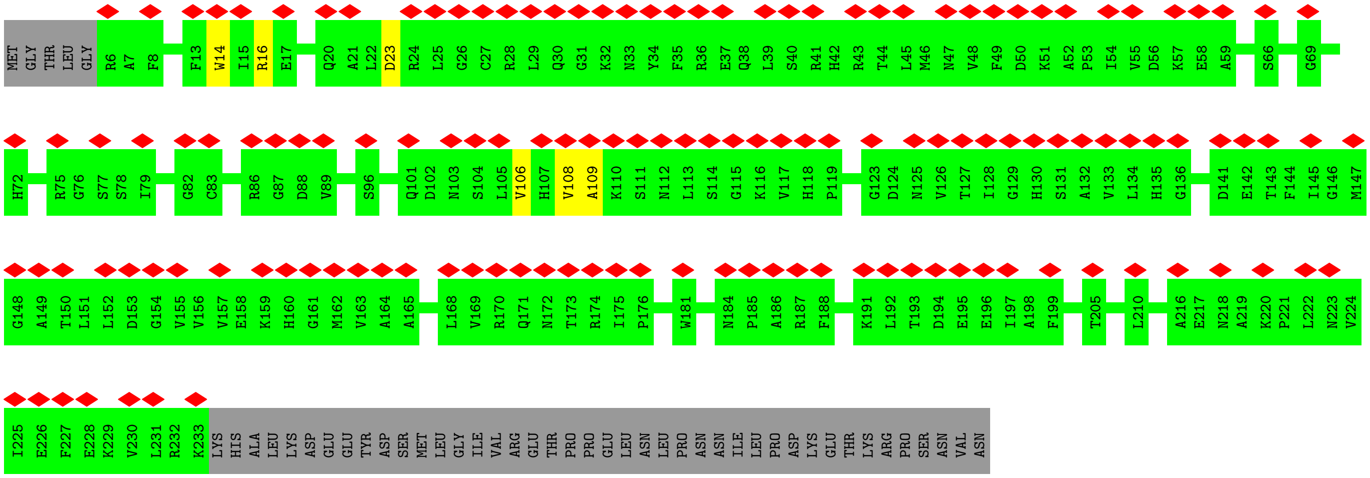
Chain o:



- Molecule 32: CA1

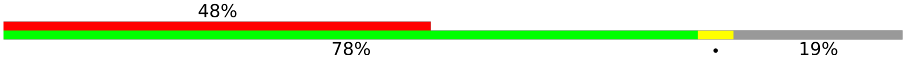
Chain q:

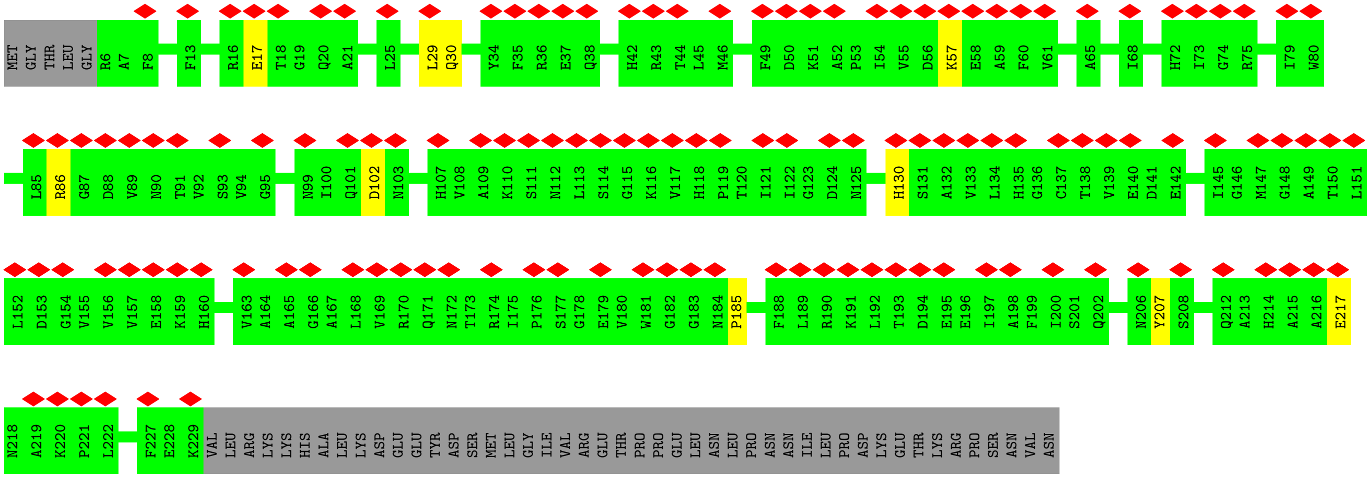




- Molecule 32: CA1

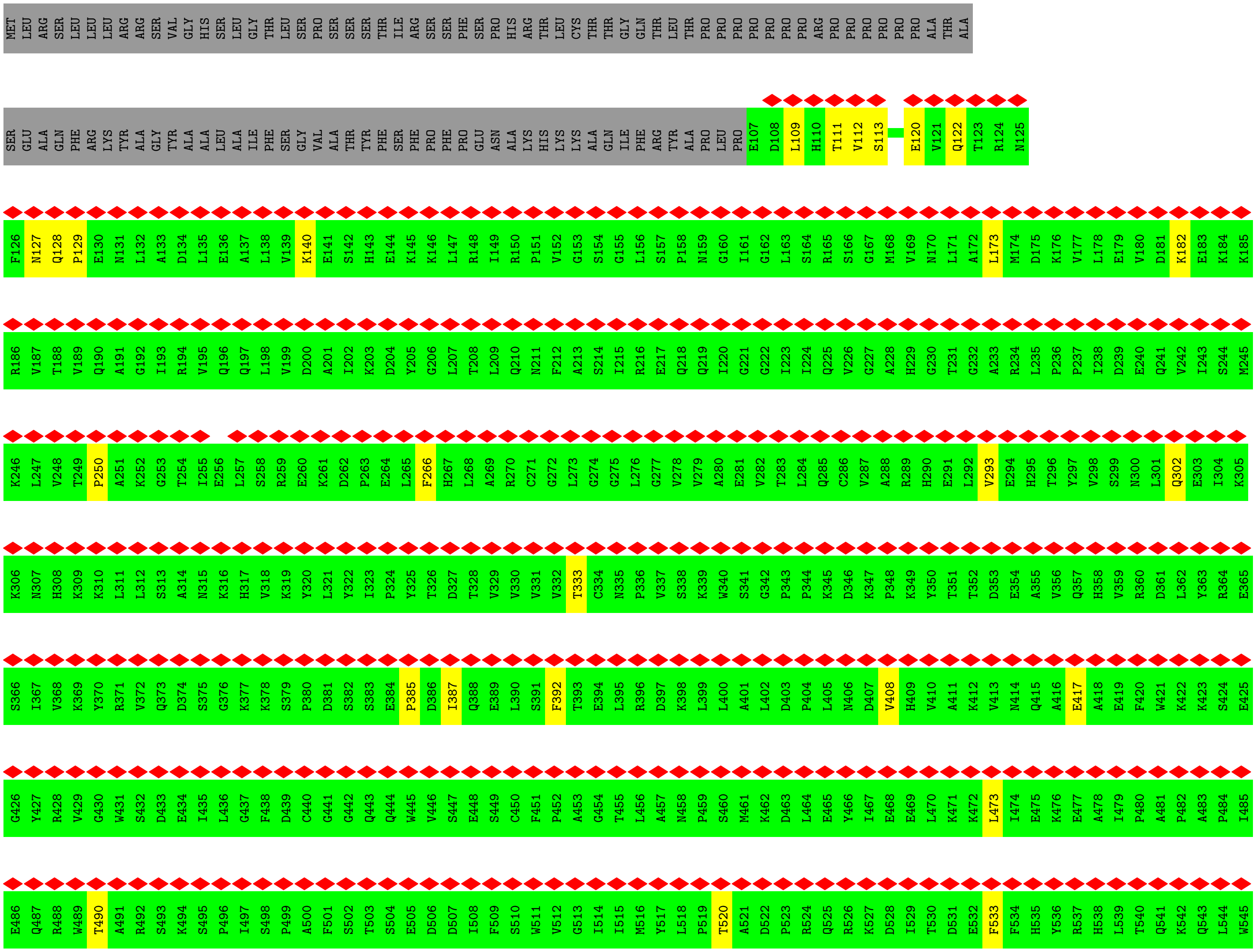
Chain p:

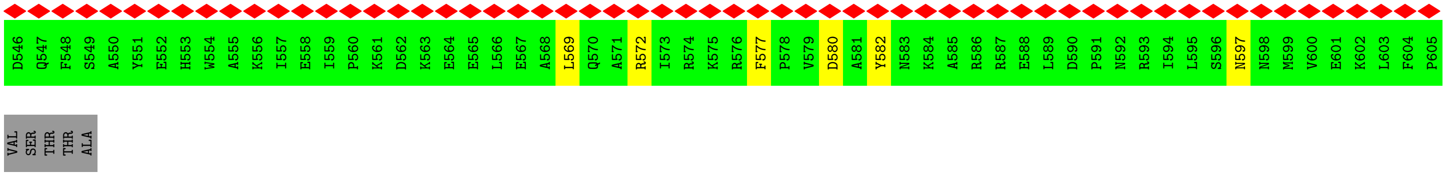




- Molecule 33: GLDH

Chain z:




D546
Q547
F548
S549
A550
Y551
E552
H553
W554
A555
K556
I557
E558
I559
P560
K561
D562
K563
E564
E565
L566
E567
A568
L569
Q570
A571
R572
I573
R574
K575
R576
F577
P578
V579
D580
A581
Y582
N583
K584
A585
R586
R587
E588
L589
D590
P591
N592
R593
I594
L595
S596
N597
N598
M599
V600
E601
K602
L603
F604
P605
VAL
SER
THR
THR
ALA

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36513	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.164	Depositor
Minimum map value	-0.065	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	399.6, 399.6, 399.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, FMN, FES, SF4, PEV, BCT, NDP, ZN, T7X

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	0.41	0/3401	0.51	0/4588
2	I	0.60	0/3855	0.72	0/5234
3	J	0.42	0/826	0.49	0/1120
4	N	0.43	0/1227	0.53	0/1664
5	H	0.50	0/2565	0.64	5/3492 (0.1%)
6	K	0.37	0/677	0.47	0/916
7	Y	0.41	0/788	0.49	0/1059
8	Z	0.37	0/1132	0.55	0/1530
9	V	0.33	0/473	0.43	0/636
10	W	0.50	0/277	0.63	0/375
11	S	0.36	0/840	0.49	0/1141
12	i	0.59	0/502	0.78	0/676
13	j	0.58	0/595	0.68	0/791
14	G	0.51	0/3120	0.56	0/4221
15	C	0.43	0/5386	0.55	1/7299 (0.0%)
16	T	0.40	0/2591	0.52	0/3509
17	F	0.47	0/1564	0.57	1/2120 (0.0%)
18	B	0.38	0/1743	0.49	0/2364
19	O	0.45	0/899	0.48	0/1215
20	P	0.41	0/567	0.52	0/768
21	R	0.42	0/995	0.63	1/1349 (0.1%)
22	U	0.42	0/1044	0.50	0/1413
23	E	0.58	1/1250 (0.1%)	0.68	3/1697 (0.2%)
24	D	0.53	0/1467	0.64	0/1981
25	X	0.29	0/861	0.40	0/1166
26	c	0.44	1/760 (0.1%)	0.50	0/1028
27	Q	0.32	0/734	0.46	0/989
28	k	0.24	0/625	0.43	0/848
29	r	0.25	0/119	0.46	0/165
30	n	0.66	0/208	0.70	0/282
31	o	0.32	0/1606	0.48	0/2192
32	p	0.38	0/1737	0.59	2/2353 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	q	0.34	0/1768	0.56	0/2395
33	z	0.63	0/4078	0.65	0/5520
All	All	0.47	2/50280 (0.0%)	0.57	13/68096 (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
32	q	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	E	186	PRO	N-CD	-10.16	1.33	1.47
26	c	44	SER	CA-CB	-5.44	1.44	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	229	PHE	CB-CA-C	7.53	125.46	110.40
21	R	122	ASN	CB-CA-C	-7.14	96.11	110.40
23	E	94	CYS	CB-CA-C	6.70	123.80	110.40
23	E	189	PRO	N-CA-C	-5.50	97.81	112.10
23	E	93	CYS	CA-CB-SG	-5.36	104.35	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	q	109	ALA	Peptide

5.2 Too-close contacts ⓘ

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	
1	A	427/486 (88%)	381 (89%)	46 (11%)	0	100	100
2	I	479/499 (96%)	465 (97%)	13 (3%)	1 (0%)	47	79
3	J	92/119 (77%)	86 (94%)	6 (6%)	0	100	100
4	N	145/205 (71%)	125 (86%)	19 (13%)	1 (1%)	22	60
5	H	316/325 (97%)	284 (90%)	32 (10%)	0	100	100
6	K	83/100 (83%)	81 (98%)	2 (2%)	0	100	100
7	Y	96/106 (91%)	88 (92%)	7 (7%)	1 (1%)	15	52
8	Z	138/143 (96%)	110 (80%)	28 (20%)	0	100	100
9	V	55/65 (85%)	52 (94%)	3 (6%)	0	100	100
10	W	35/65 (54%)	31 (89%)	4 (11%)	0	100	100
11	S	99/131 (76%)	86 (87%)	13 (13%)	0	100	100
12	i	61/81 (75%)	57 (93%)	3 (5%)	1 (2%)	9	44
13	j	66/83 (80%)	63 (96%)	2 (3%)	1 (2%)	10	46
14	G	380/394 (96%)	348 (92%)	32 (8%)	0	100	100
15	C	691/748 (92%)	617 (89%)	73 (11%)	1 (0%)	51	83
16	T	326/402 (81%)	280 (86%)	46 (14%)	0	100	100
17	F	176/190 (93%)	151 (86%)	25 (14%)	0	100	100
18	B	217/255 (85%)	184 (85%)	33 (15%)	0	100	100
19	O	109/154 (71%)	102 (94%)	7 (6%)	0	100	100
20	P	69/110 (63%)	64 (93%)	5 (7%)	0	100	100
21	R	119/169 (70%)	104 (87%)	14 (12%)	1 (1%)	19	57
22	U	120/159 (76%)	98 (82%)	22 (18%)	0	100	100
23	E	151/218 (69%)	134 (89%)	16 (11%)	1 (1%)	22	60
24	D	175/222 (79%)	159 (91%)	14 (8%)	2 (1%)	14	51
25	X	99/133 (74%)	92 (93%)	7 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	c	97/106 (92%)	91 (94%)	6 (6%)	0	100	100
27	Q	90/97 (93%)	81 (90%)	9 (10%)	0	100	100
28	k	76/122 (62%)	74 (97%)	2 (3%)	0	100	100
29	r	22/24 (92%)	18 (82%)	4 (18%)	0	100	100
30	n	25/113 (22%)	24 (96%)	0	1 (4%)	3	28
31	o	200/252 (79%)	172 (86%)	28 (14%)	0	100	100
32	p	222/275 (81%)	191 (86%)	28 (13%)	3 (1%)	11	46
32	q	226/275 (82%)	196 (87%)	27 (12%)	3 (1%)	12	48
33	z	495/610 (81%)	476 (96%)	15 (3%)	4 (1%)	19	57
All	All	6177/7436 (83%)	5565 (90%)	591 (10%)	21 (0%)	44	74

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	q	108	VAL
2	I	59	LEU
13	j	26	SER
15	C	272	ALA
24	D	120	GLU

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	349/396 (88%)	348 (100%)	1 (0%)	92	96
2	I	399/416 (96%)	365 (92%)	34 (8%)	10	40
3	J	87/106 (82%)	87 (100%)	0	100	100
4	N	133/186 (72%)	131 (98%)	2 (2%)	65	81
5	H	266/272 (98%)	264 (99%)	2 (1%)	81	89
6	K	74/86 (86%)	73 (99%)	1 (1%)	67	81
7	Y	88/94 (94%)	87 (99%)	1 (1%)	73	85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	Z	112/115 (97%)	112 (100%)	0	100	100
9	V	48/53 (91%)	48 (100%)	0	100	100
10	W	30/53 (57%)	30 (100%)	0	100	100
11	S	92/118 (78%)	92 (100%)	0	100	100
12	i	50/66 (76%)	43 (86%)	7 (14%)	3	21
13	j	62/73 (85%)	59 (95%)	3 (5%)	25	56
14	G	328/340 (96%)	325 (99%)	3 (1%)	78	88
15	C	576/625 (92%)	571 (99%)	5 (1%)	78	88
16	T	271/334 (81%)	269 (99%)	2 (1%)	84	91
17	F	168/179 (94%)	164 (98%)	4 (2%)	49	71
18	B	188/220 (86%)	188 (100%)	0	100	100
19	O	93/128 (73%)	93 (100%)	0	100	100
20	P	62/97 (64%)	62 (100%)	0	100	100
21	R	108/148 (73%)	106 (98%)	2 (2%)	57	76
22	U	104/133 (78%)	103 (99%)	1 (1%)	76	86
23	E	129/184 (70%)	122 (95%)	7 (5%)	22	53
24	D	157/191 (82%)	151 (96%)	6 (4%)	33	61
25	X	92/114 (81%)	92 (100%)	0	100	100
26	c	79/84 (94%)	79 (100%)	0	100	100
27	Q	82/85 (96%)	81 (99%)	1 (1%)	71	84
28	k	73/112 (65%)	73 (100%)	0	100	100
30	n	21/84 (25%)	19 (90%)	2 (10%)	8	34
31	o	171/211 (81%)	171 (100%)	0	100	100
32	p	181/228 (79%)	176 (97%)	5 (3%)	43	68
32	q	184/228 (81%)	182 (99%)	2 (1%)	73	85
33	z	440/534 (82%)	412 (94%)	28 (6%)	17	48
All	All	5297/6293 (84%)	5178 (98%)	119 (2%)	54	72

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	C	266	ASP
33	z	490	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	E	164	TYR
33	z	473	LEU
33	z	597	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
22	U	46	ASN
31	o	114	GLN
22	U	134	HIS
25	X	15	ASN
32	q	72	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 2 are 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	$\#\|Z\| > 2$
38	PEV	G	601	-	27,27,48	0.35	0	30,32,53	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\lvert Z\rvert > 2$	Counts	RMSZ	#$\lvert Z\rvert > 2$
39	FES	C	803	15	0,4,4	-	-	-		
42	BCT	q	802	41	2,3,3	0.60	0	2,3,3	0.24	0
34	SF4	C	801	15	0,12,12	-	-	-		
34	SF4	E	301	23	0,12,12	-	-	-		
34	SF4	C	802	15	0,12,12	-	-	-		
40	NDP	T	501	-	45,52,52	0.62	0	53,80,80	0.83	2 (3%)
37	CDL	i	201	-	89,89,99	0.28	0	95,101,111	0.57	2 (2%)
36	T7X	c	301	-	37,37,61	0.33	0	47,49,73	0.39	0
36	T7X	I	501	-	42,42,61	0.31	0	52,54,73	0.50	0
39	FES	B	301	-	0,4,4	-	-	-		
34	SF4	A	501	1	0,12,12	-	-	-		
34	SF4	D	302	24	0,12,12	-	-	-		
34	SF4	D	301	24	0,12,12	-	-	-		
35	FMN	A	502	-	33,33,33	0.62	0	48,50,50	0.72	1 (2%)

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
38	PEV	G	601	-	-	12/30/30/52	-
39	FES	C	803	15	-	-	0/1/1/1
40	NDP	T	501	-	-	6/30/77/77	0/5/5/5
34	SF4	C	801	15	-	-	0/6/5/5
34	SF4	C	802	15	-	-	0/6/5/5
35	FMN	A	502	-	-	6/18/18/18	0/3/3/3
34	SF4	E	301	23	-	-	0/6/5/5
36	T7X	c	301	-	-	2/32/56/80	0/1/1/1
36	T7X	I	501	-	-	13/37/61/80	0/1/1/1
39	FES	B	301	-	-	-	0/1/1/1
34	SF4	A	501	1	-	-	0/6/5/5
34	SF4	D	302	24	-	-	0/6/5/5
34	SF4	D	301	24	-	-	0/6/5/5
37	CDL	i	201	-	-	31/100/100/110	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	i	201	CDL	OB6-CB5-C51	2.63	117.16	111.50
40	T	501	NDP	O4D-C1D-C2D	-2.40	101.42	106.64
40	T	501	NDP	C5A-C6A-N6A	2.33	123.90	120.35
35	A	502	FMN	C4-N3-C2	-2.08	121.79	125.64
37	i	201	CDL	OA6-CA5-C11	2.01	115.82	111.50

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

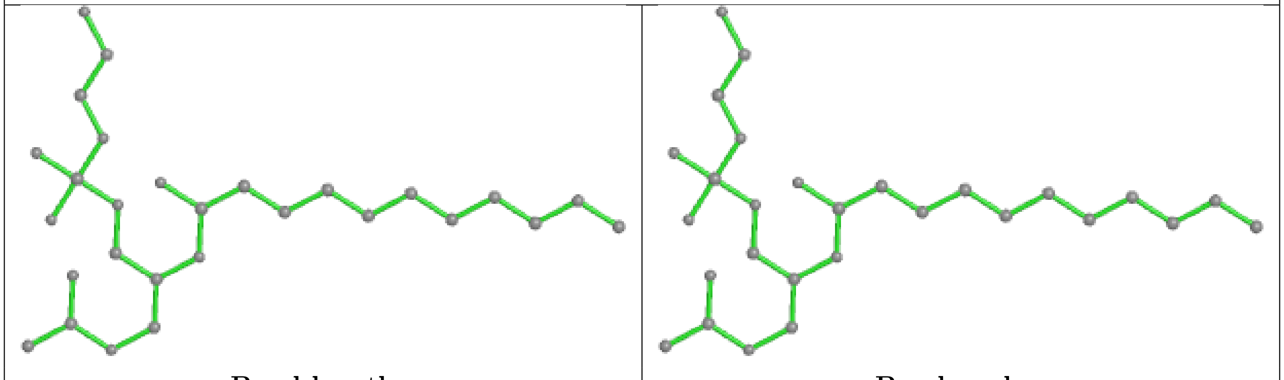
Mol	Chain	Res	Type	Atoms
35	A	502	FMN	N10-C1'-C2'-C3'
35	A	502	FMN	O3'-C3'-C4'-C5'
36	I	501	T7X	C6-C1-O1-P1
36	I	501	T7X	C7-O13-P1-O1
36	I	501	T7X	C8-C7-O13-P1

There are no ring outliers.

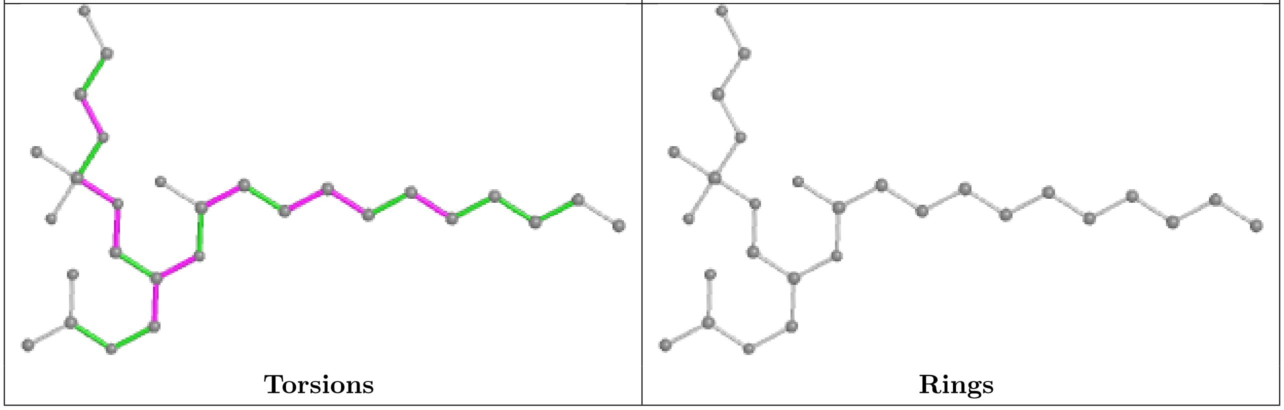
No monomer is involved in short contacts.

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 then 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.

Ligand PEV G 601

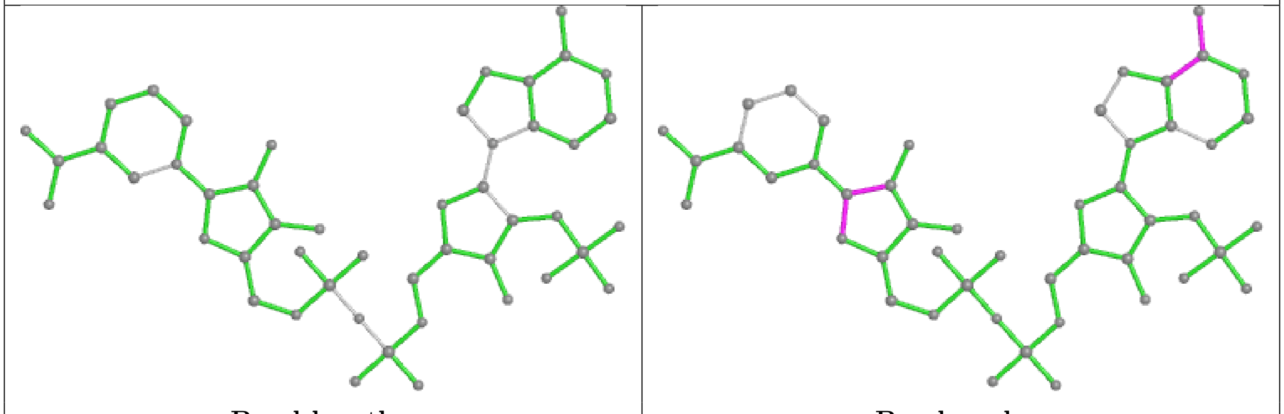


Bond lengths **Bond angles**

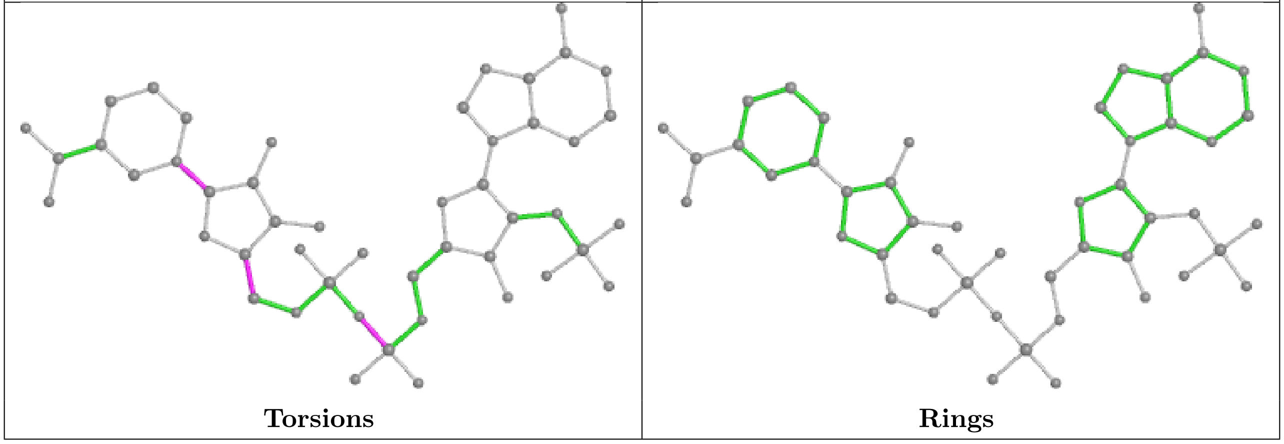


Torsions **Rings**

Ligand NDP T 501

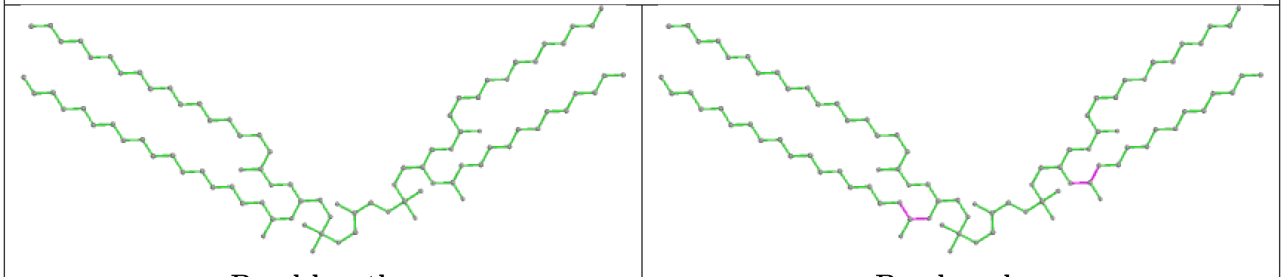


Bond lengths **Bond angles**

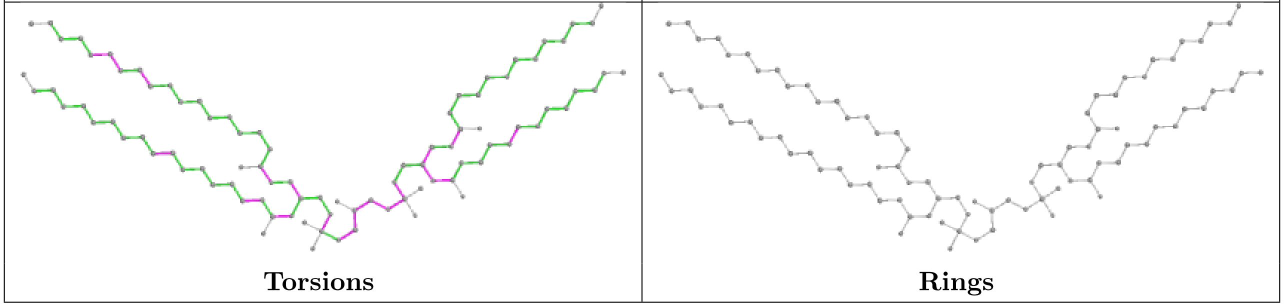


Torsions **Rings**

Ligand CDL i 201

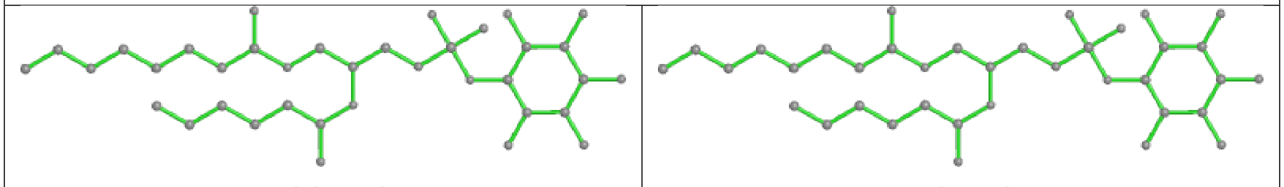


Bond lengths | Bond angles

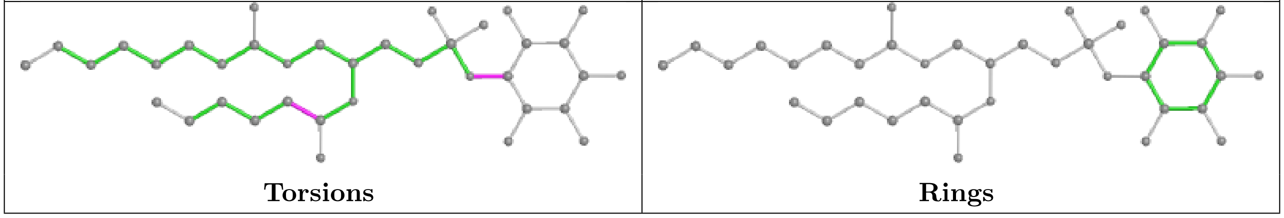


Torsions | Rings

Ligand T7X c 301

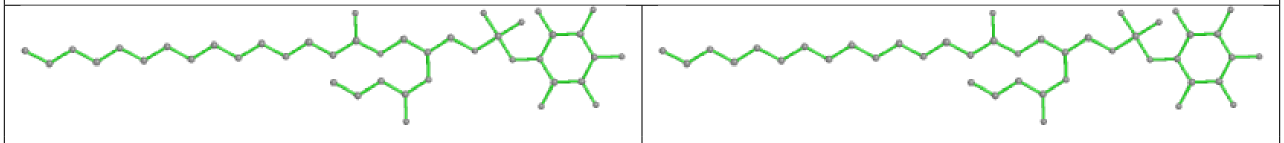


Bond lengths | Bond angles

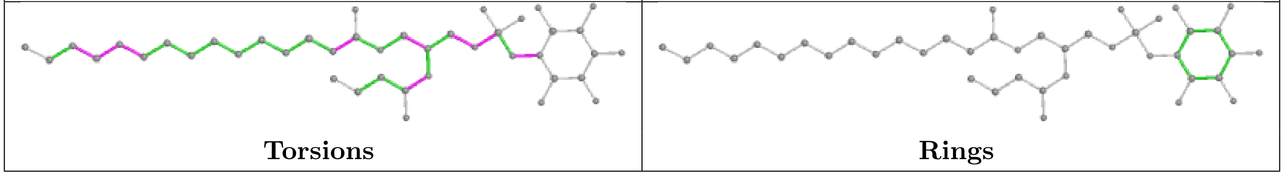


Torsions | Rings

Ligand T7X I 501

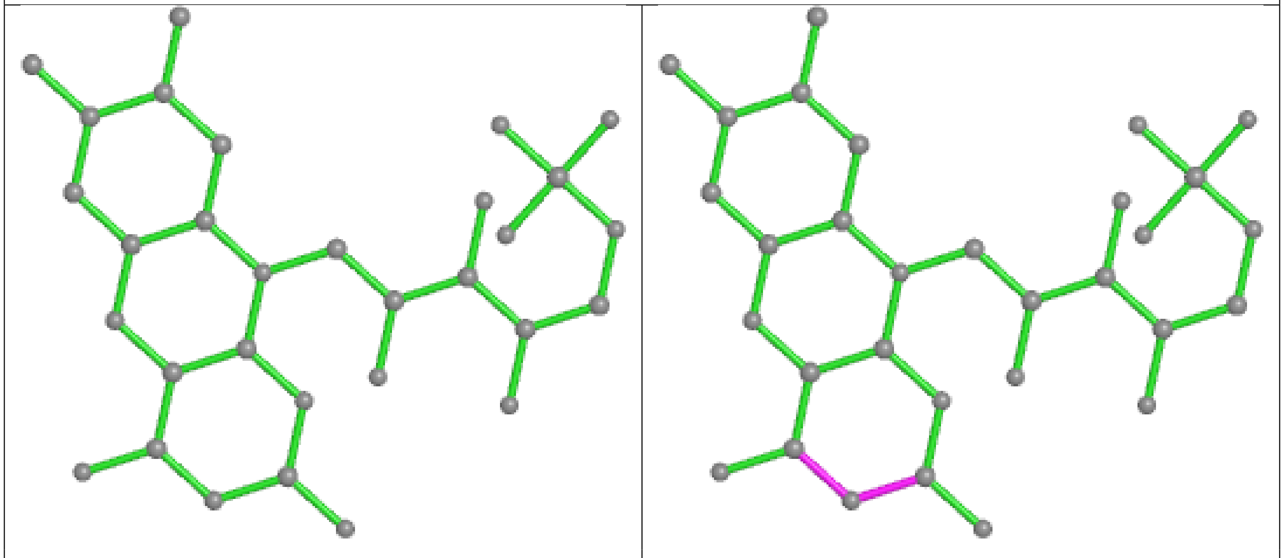


Bond lengths | Bond angles

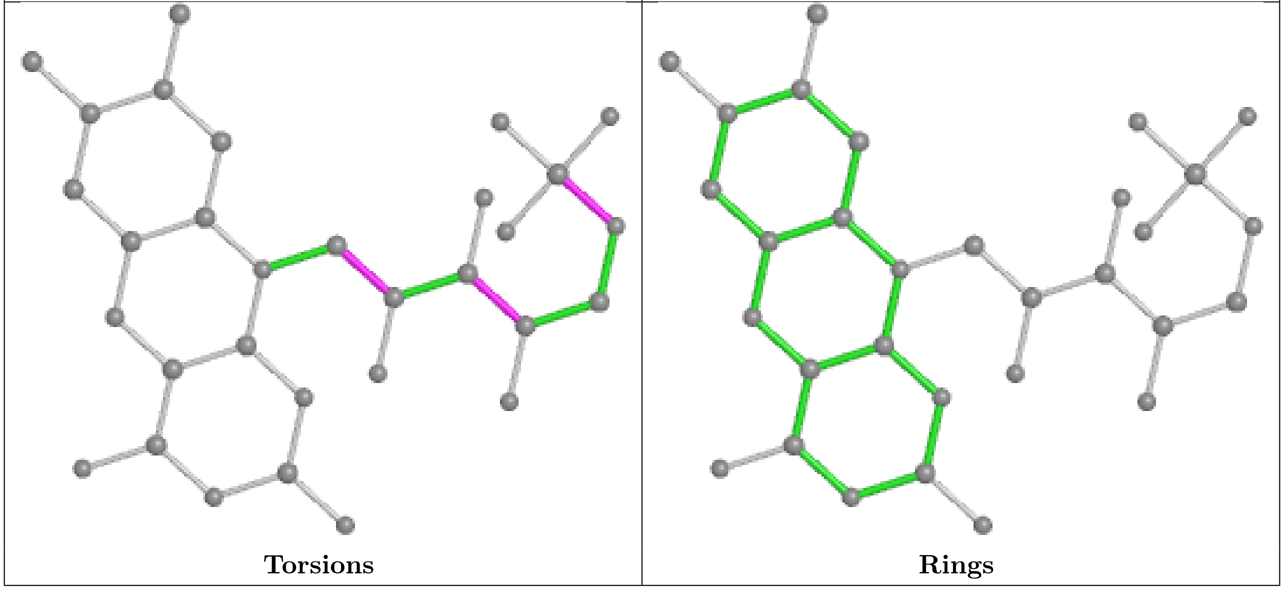


Torsions | Rings

Ligand FMN A 502



Bond lengths **Bond angles**



Torsions **Rings**

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
33	z	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	z	144:GLU	C	145:LYS	N	3.49

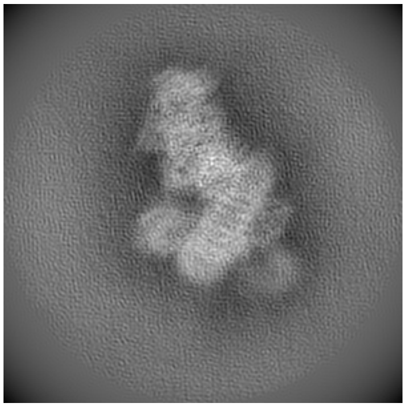
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11615. These allow visual inspection of the internal detail of the map and identification of artifacts.

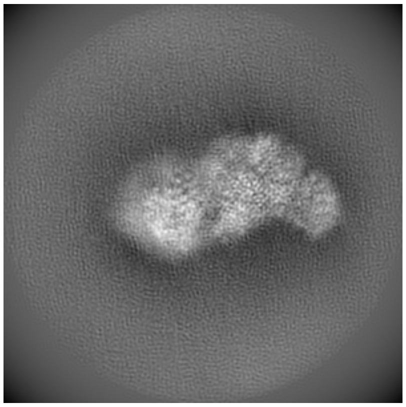
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

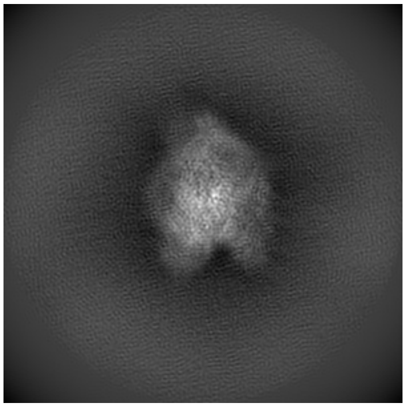
6.1.1 Primary map



X



Y

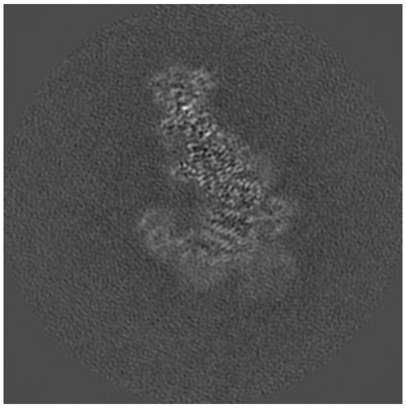


Z

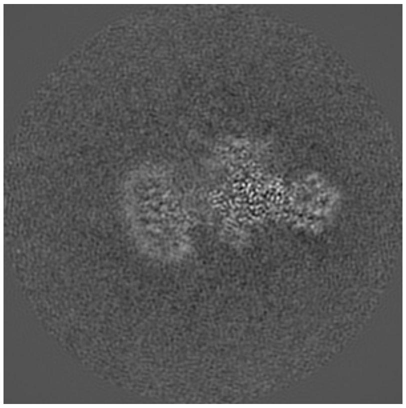
The images above show the map projected in three orthogonal directions.

6.2 Central slices

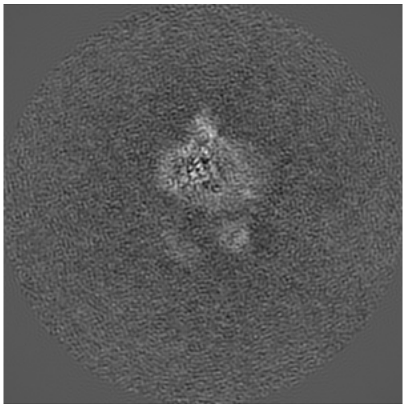
6.2.1 Primary map



X Index: 180



Y Index: 180

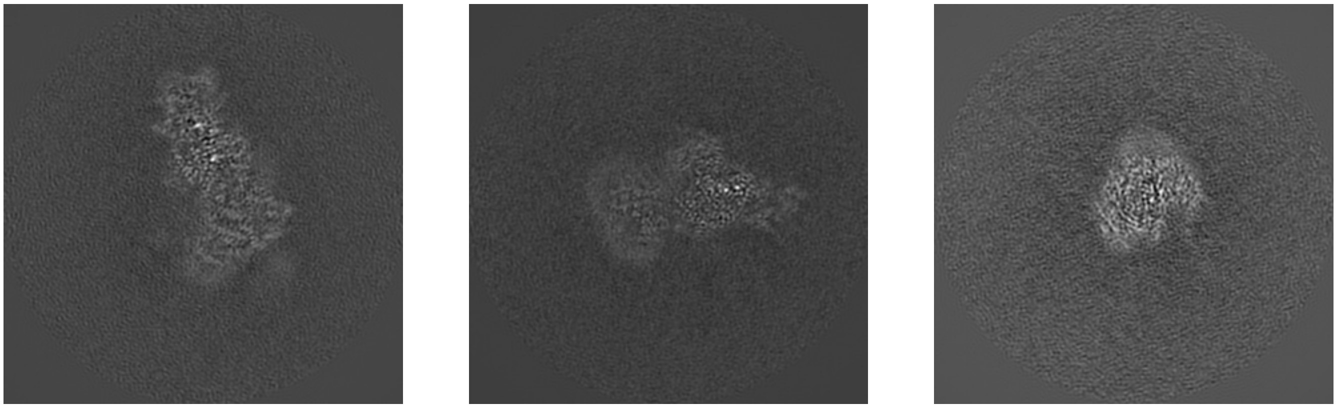


Z Index: 180

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

6.3 Largest variance slices

6.3.1 Primary map

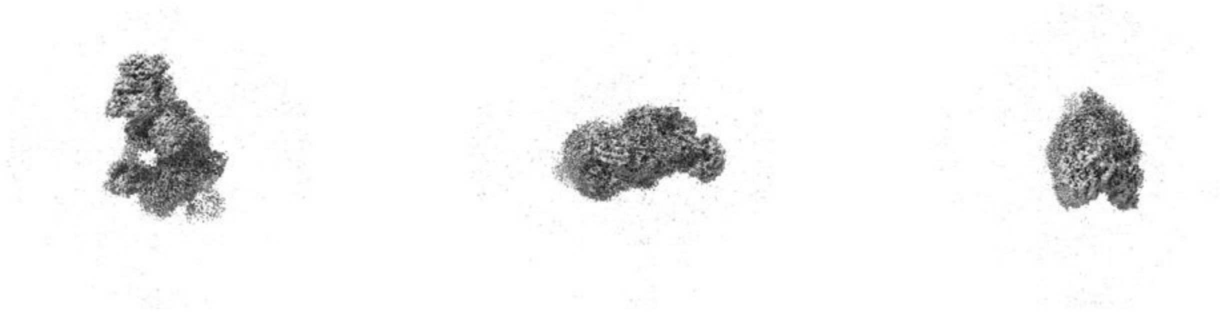


X Index: 190 Y Index: 186 Z Index: 213

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

6.4 Orthogonal surface views

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

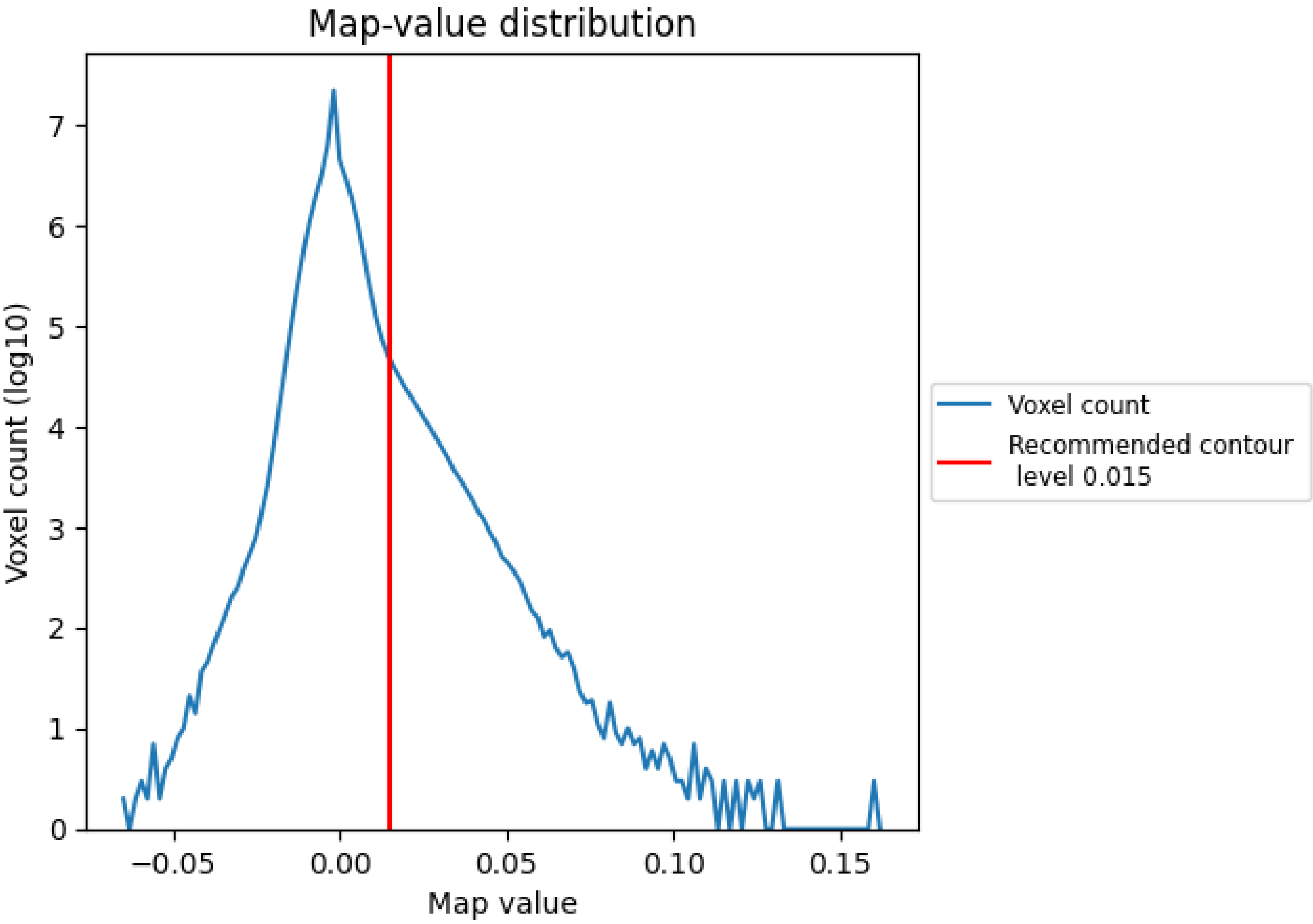
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

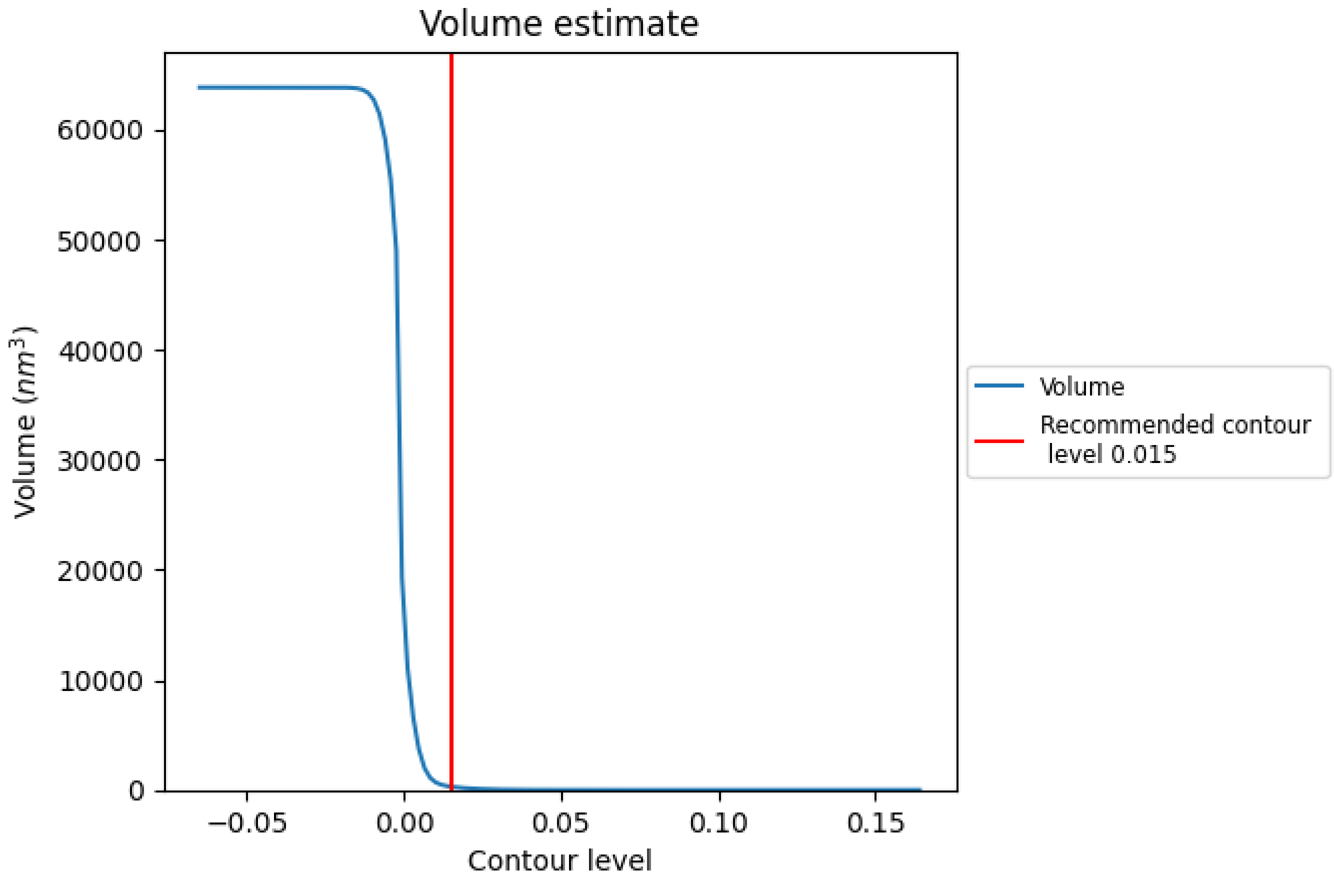
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

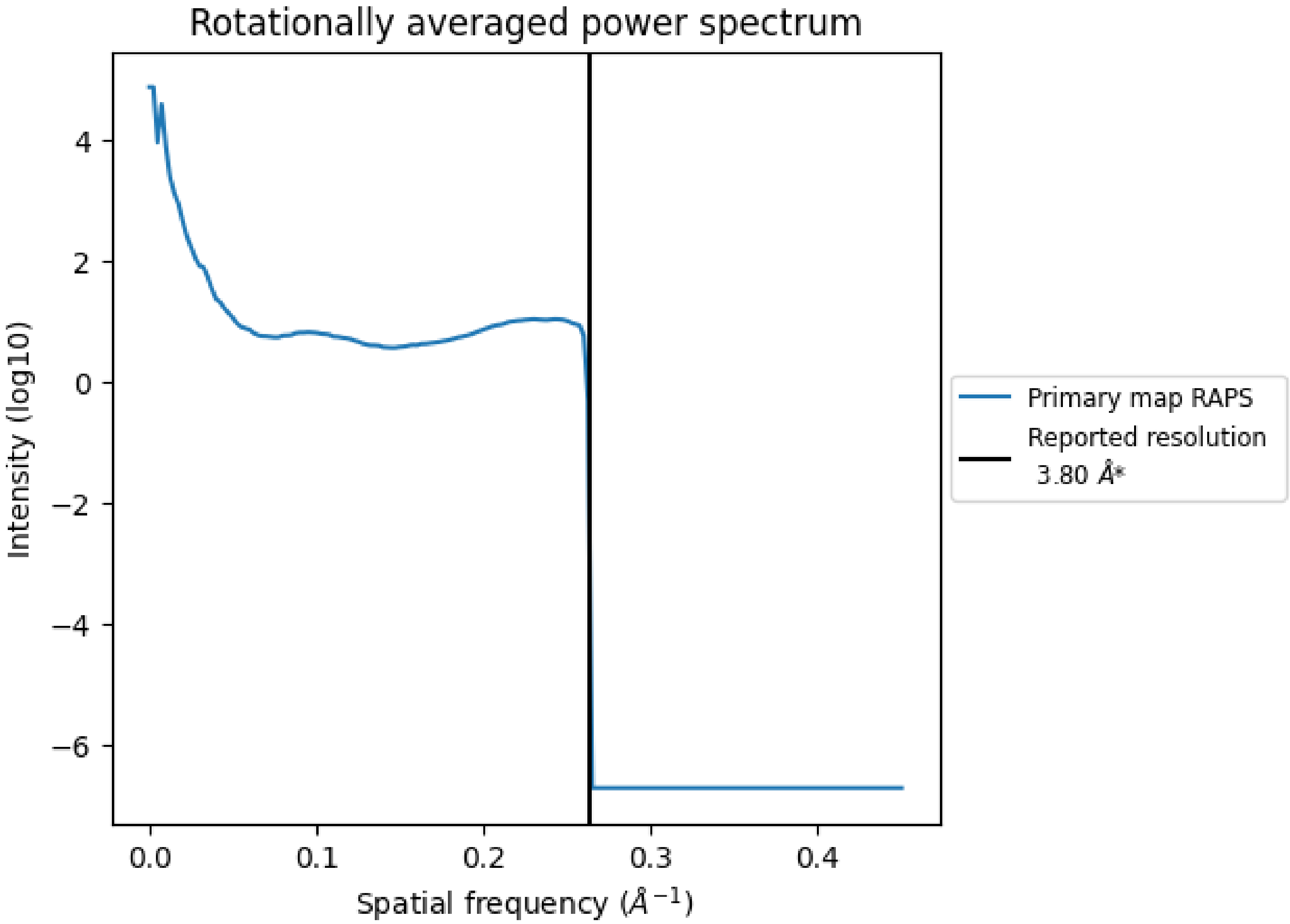
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 304 nm^3; this corresponds to an approximate mass of 274 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 0.263 Å^{-1}

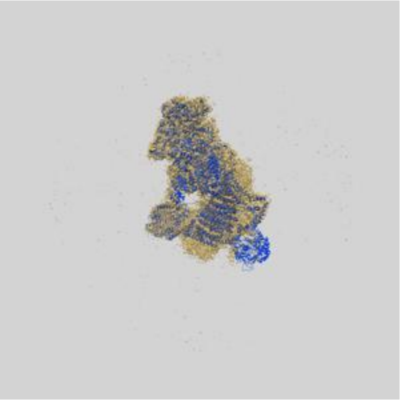
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

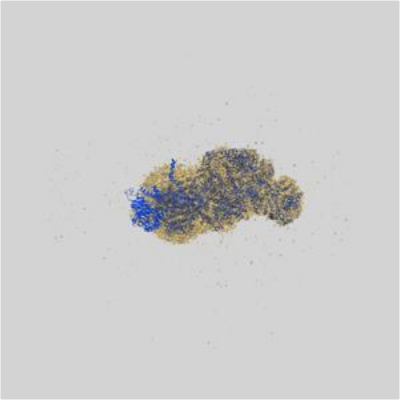
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-11615 and PDB model 7A24. Per-residue inclusion information can be found in section 3 on page 14.

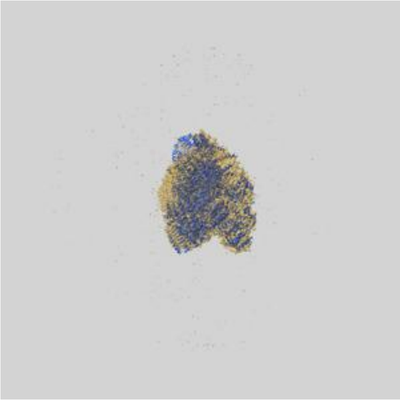
9.1 Map-model overlay ⓘ



X



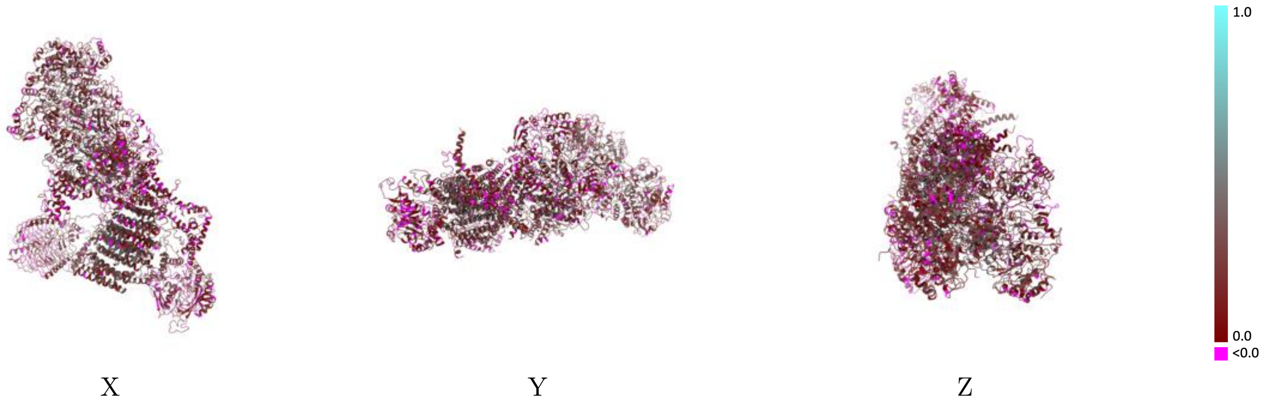
Y



Z

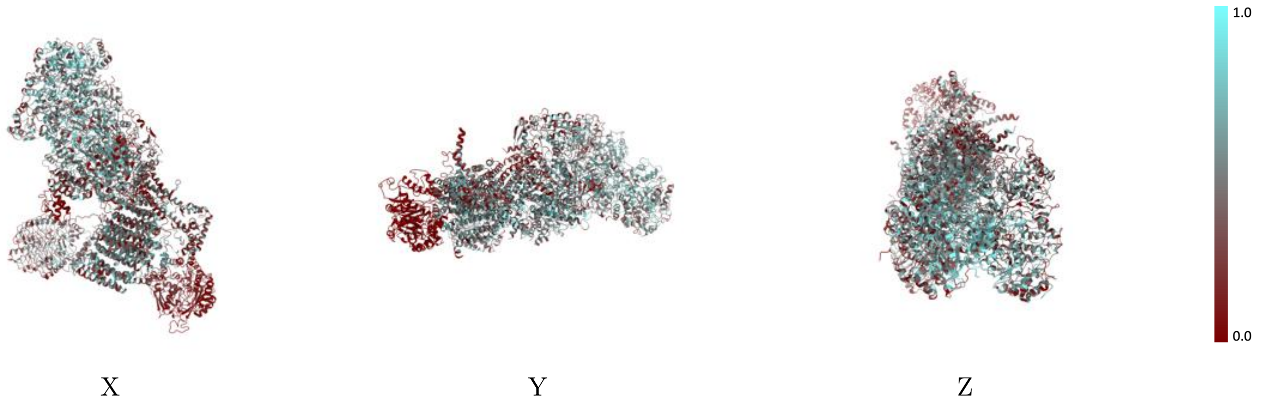
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



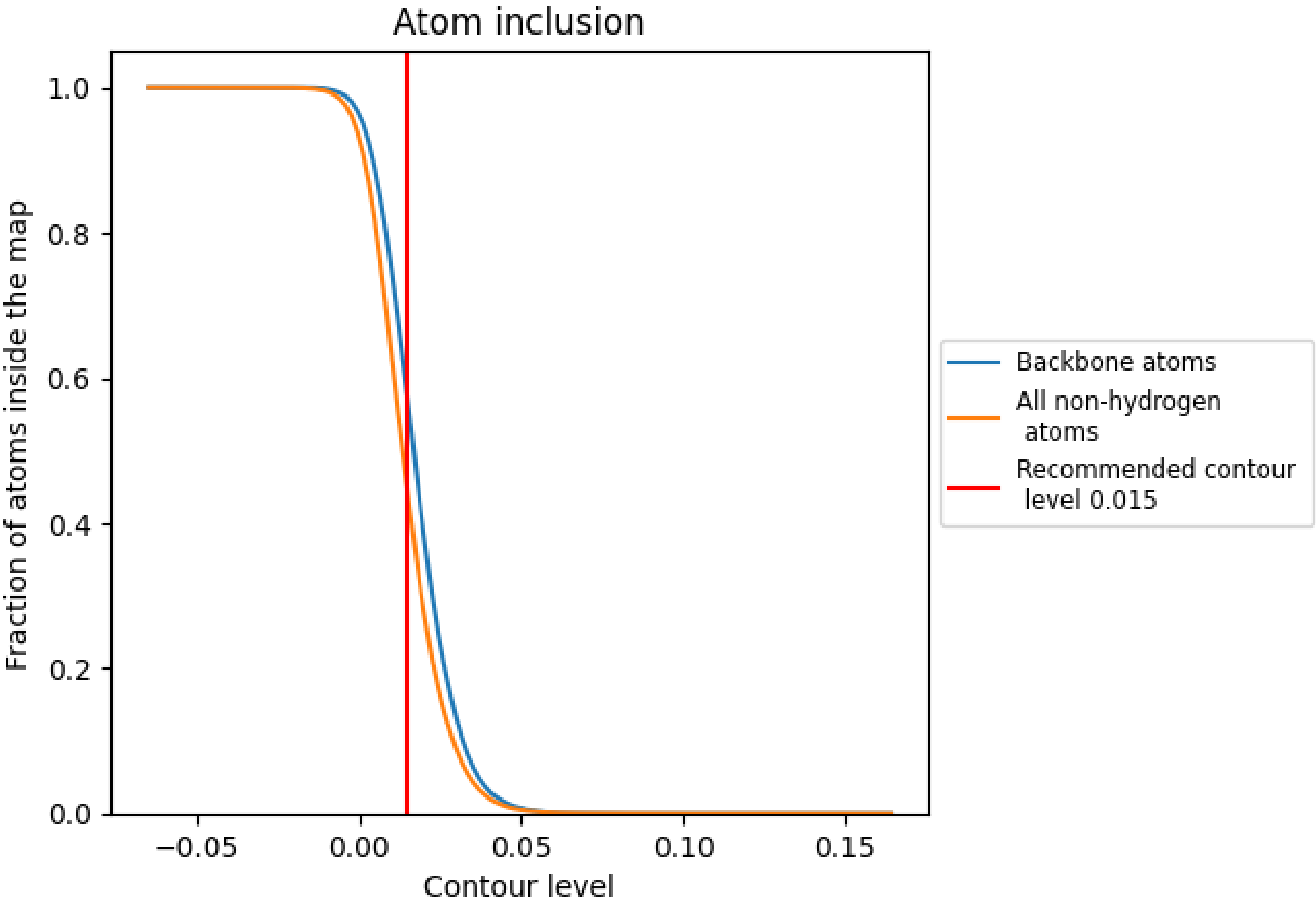
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.015).

9.4 Atom inclusion ⓘ



At the recommended contour level, 57% of all backbone atoms, 44% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4435	0.2070
A	0.5068	0.2170
B	0.5485	0.2030
C	0.5702	0.2510
D	0.5610	0.1890
E	0.6002	0.2640
F	0.5926	0.2850
G	0.6281	0.3100
H	0.4644	0.2140
I	0.5301	0.3190
J	0.4150	0.2400
K	0.4552	0.2170
N	0.3872	0.2390
O	0.6147	0.3120
P	0.4505	0.1600
Q	0.4603	0.1990
R	0.4953	0.2050
S	0.4548	0.2110
T	0.4277	0.1380
U	0.2376	0.0680
V	0.3467	0.0900
W	0.5279	0.2830
X	0.3224	0.1470
Y	0.3058	0.0680
Z	0.3940	0.1590
c	0.4889	0.2340
i	0.4738	0.2120
j	0.4562	0.2920
k	0.0984	0.0790
n	0.4250	0.2870
o	0.3978	0.1560
p	0.3523	0.1240
q	0.3382	0.0930
r	0.4500	0.1890
z	0.0332	0.1250