wwPDB EM Validation Summary Report (i)

Sep 28, 2024 – 09:19 pm BST

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)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

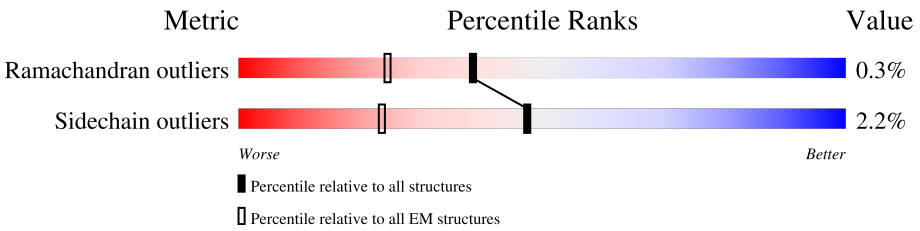
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (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	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	33% 88% 12%
2	I	499	24% 89% 7% •
3	J	119	35% 81% 19%
4	N	205	37% 71% • 27%
5	H	325	39% 96% • •
6	K	100	38% 84% • 15%
7	Y	106	61% 91% • 8%
8	Z	143	53% 98% •
9	V	65	57% 88% 12%

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Mol	Chain	Length	Quality of chain
10	W	65	18% 57% 43%
11	S	131	32% 77% 23%
12	i	81	22% 69% 7% 22%
13	j	83	39% 77% 5% 18%
14	G	394	15% 96%
15	C	748	23% 92% 7%
16	T	402	38% 81% 18%
17	F	190	19% 91% 6%
18	B	255	26% 86% 14%
19	O	154	12% 72% 28%
20	P	110	27% 65% 35%
21	R	169	28% 70% 28%
22	U	159	59% 76% 23%
23	E	218	12% 66% 30%
24	D	222	18% 77% 20%
25	X	133	53% 77% 23%
26	c	106	33% 92% 7%
27	Q	97	38% 94% 5%
28	k	122	61% 64% 36%
29	r	24	58% 100%
30	n	113	12% 21% 76%
31	o	252	39% 80% 20%
32	p	275	48% 78% 19%
32	q	275	51% 81% 17%
33	z	610	80% 77% 5% 18%

2 Entry composition (i)

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
			Total	C	N	O	S		
7	Y	98	774	484	133	145	12	0	0

- Molecule 8 is a protein called B16.6.

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

- Molecule 9 is a protein called MWFE.

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

- Molecule 10 is a protein called B9.

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

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

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

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

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

- Molecule 13 is a protein called 15kDa.

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

- 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
			Total	C	N	O	S		
21	R	121	977	614	165	193	5	0	0

- Molecule 22 is a protein called B17.2.

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

- Molecule 23 is a protein called PSST.

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

- Molecule 24 is a protein called TYKY.

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

- Molecule 25 is a protein called B14.

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

- Molecule 26 is a protein called MNLL.

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

- Molecule 27 is a protein called B8.

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

- Molecule 28 is a protein called ACPM1.

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

- Molecule 29 is a protein called Unk1.

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

- Molecule 30 is a protein called P2.

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

- Molecule 31 is a protein called CAL1.

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

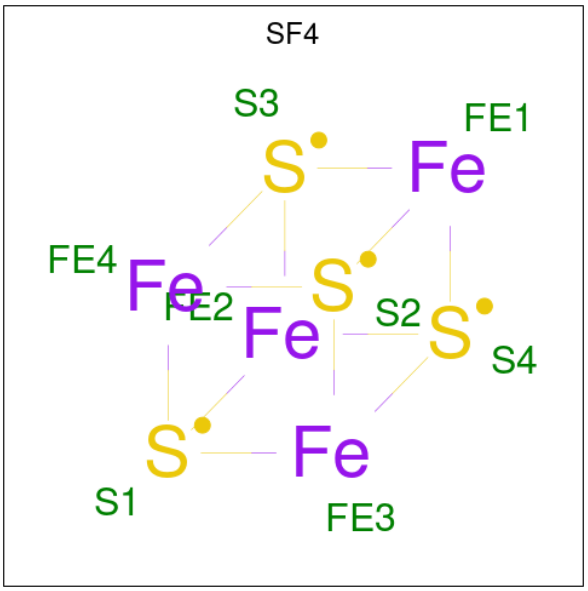
- Molecule 32 is a protein called CA1.

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

- Molecule 33 is a protein called GLDH.

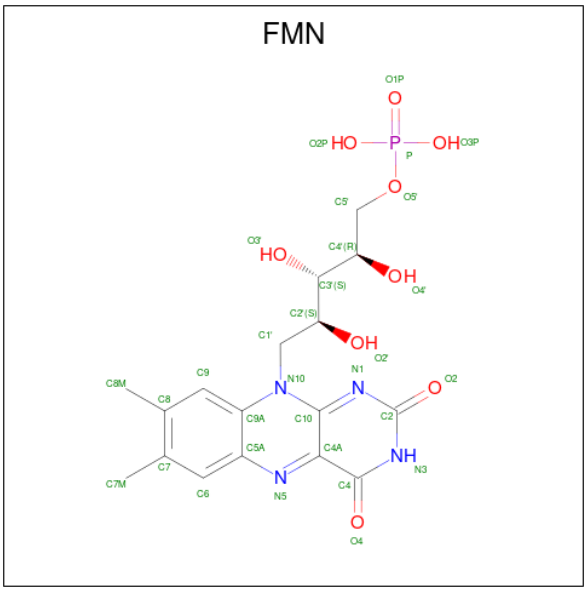
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	z	499	3992	2527	700	754	11	0	0

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



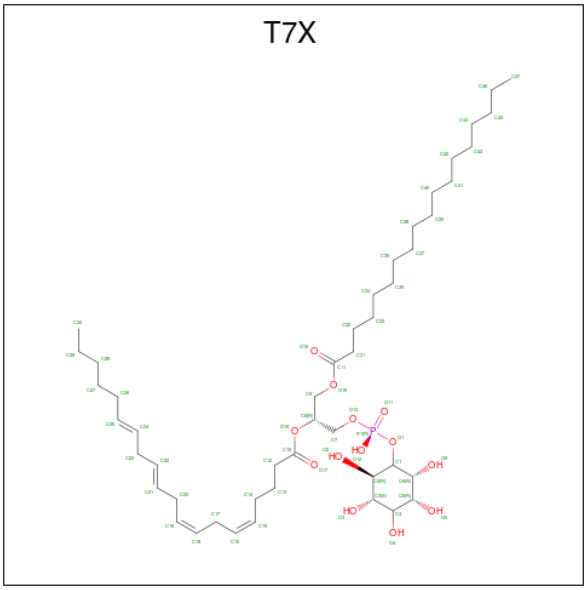
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
34	A	1	8	4	4	0
34	C	1	8	4	4	0
34	C	1	8	4	4	0
34	E	1	8	4	4	0
34	D	1	8	4	4	0
34	D	1	8	4	4	0

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



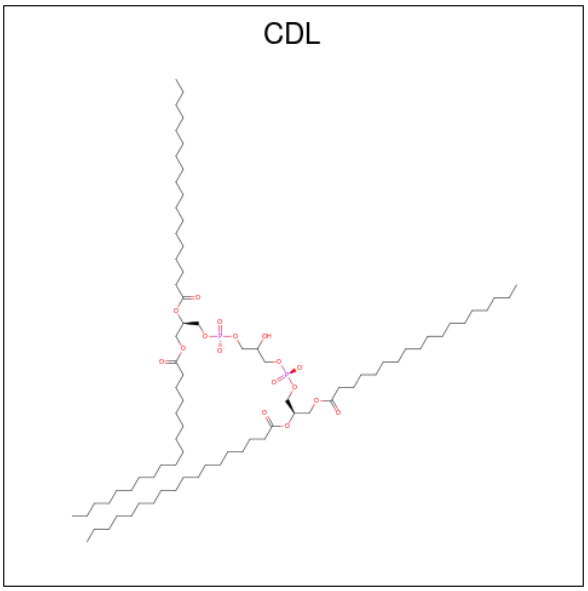
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
35	A	1	31	17	4	9	1	0

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



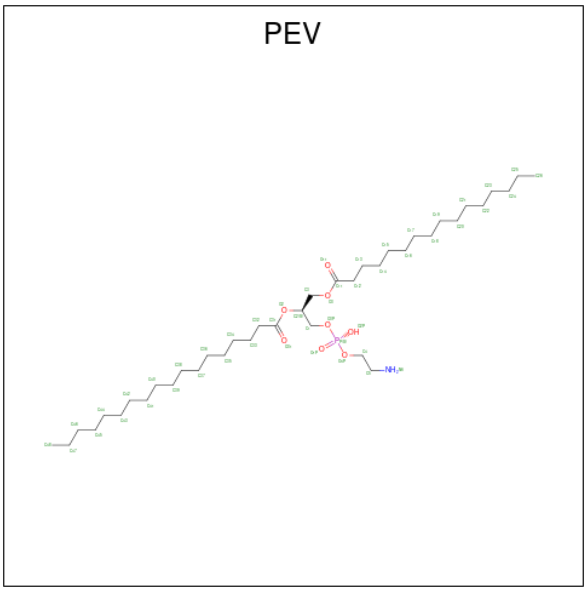
Mol	Chain	Residues	Atoms					AltConf
			Total	C	O	P		
36	I	1	42	28	13	1		0
			Total	C	O	P		
36	c	1	37	23	13	1		0

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



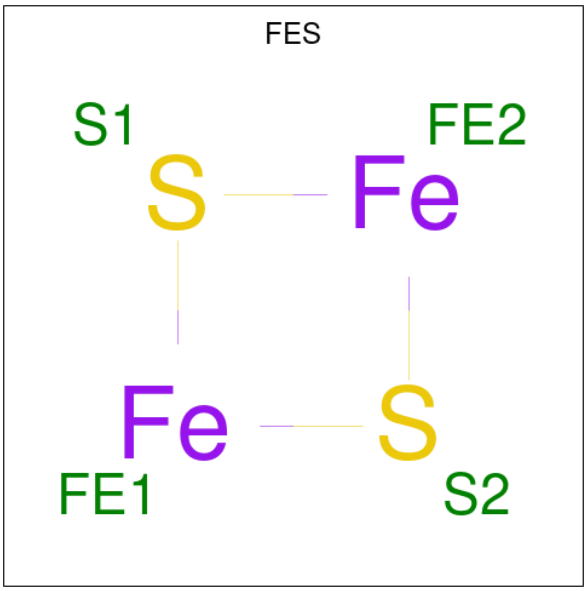
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
37	i	1	90	71	17	2	0

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



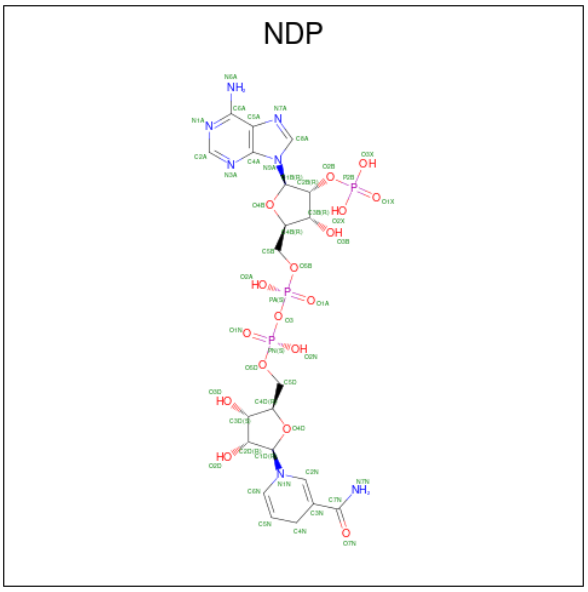
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
38	G	1	28	18	1	8	1	0

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



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

- Molecule 40 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

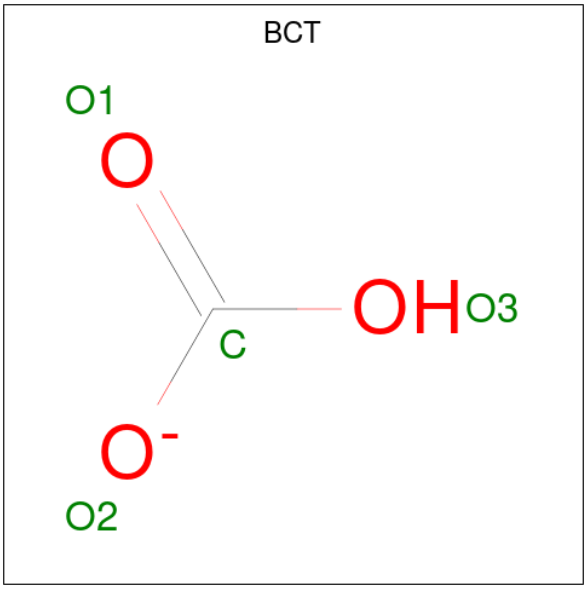


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
40	T	1	48	21	7	17	3	0

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

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

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



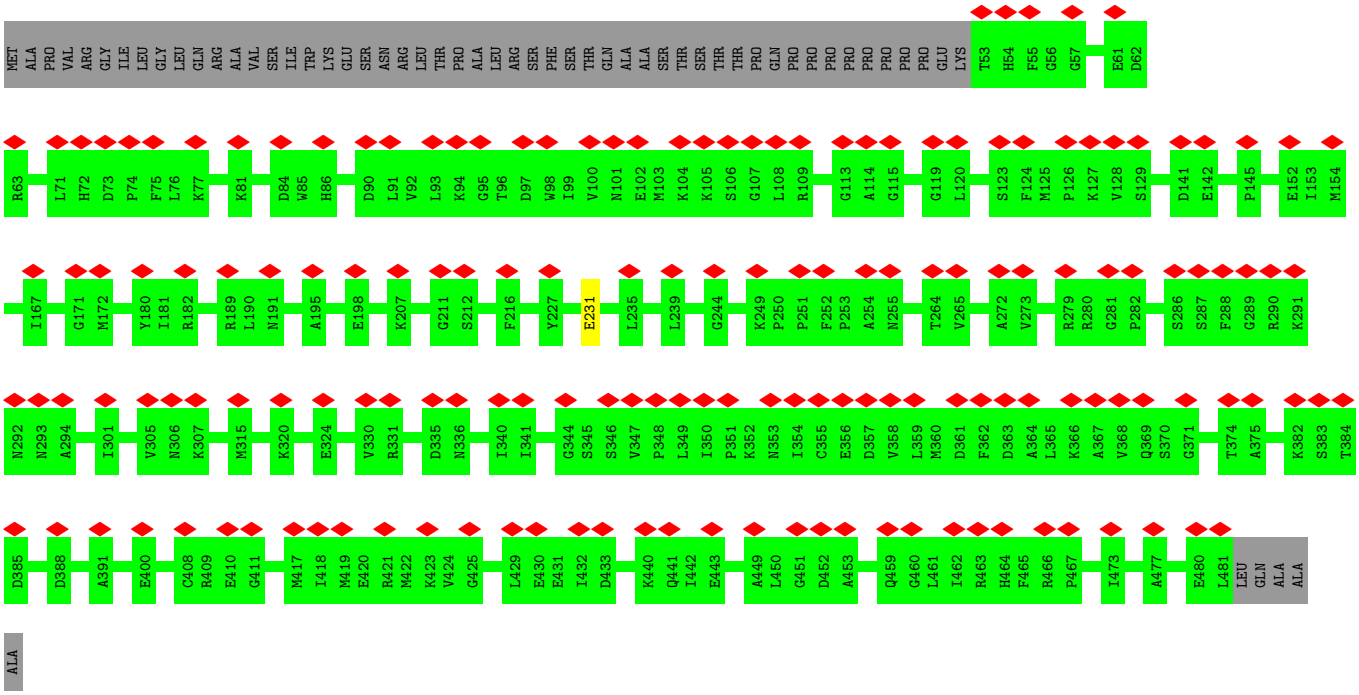
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
42	q	1	4	1	3	0

3 Residue-property plots (i)

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

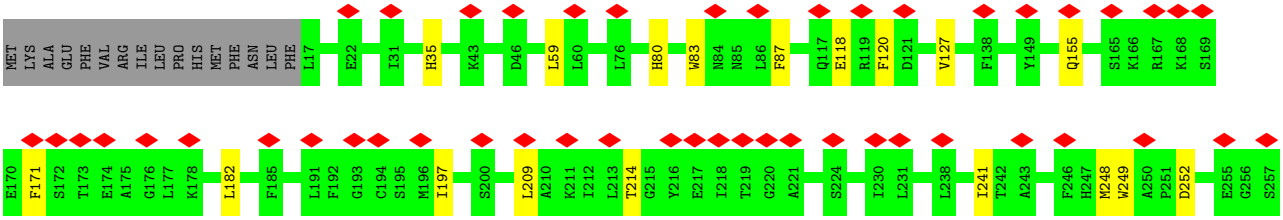
- Molecule 1: 51kDa

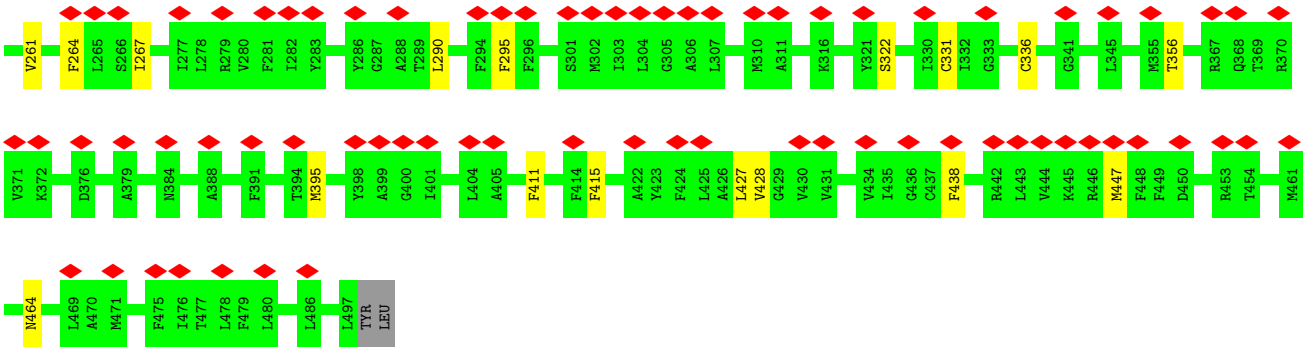
Chain A:



- Molecule 2: Nad2m

Chain I:



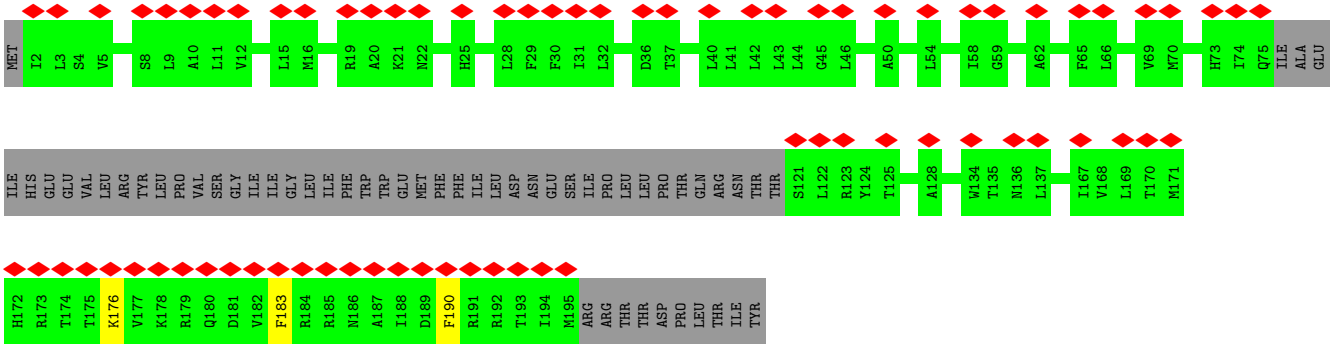


- Molecule 3: Nad3m

Chain J:

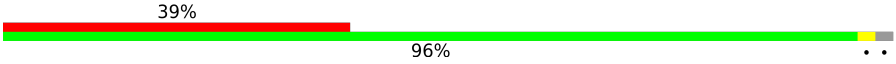
- Molecule 4: Nad6m

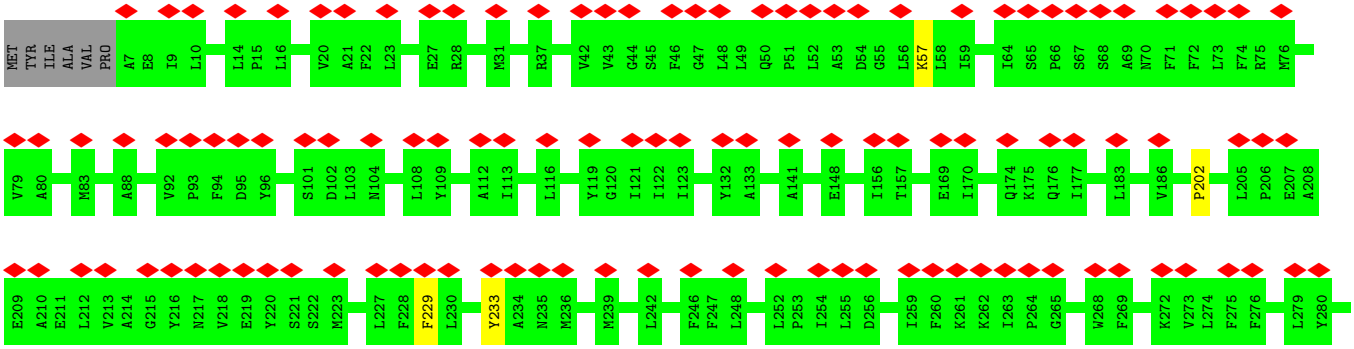
Chain N:

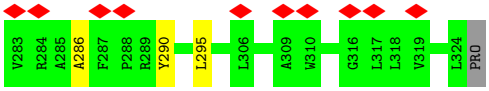


- Molecule 5: Nad1m

Chain H:

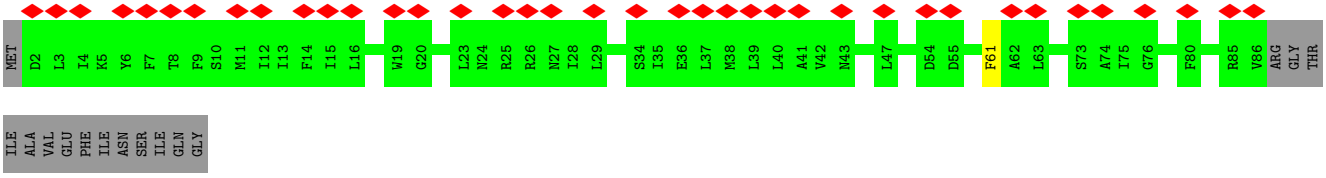






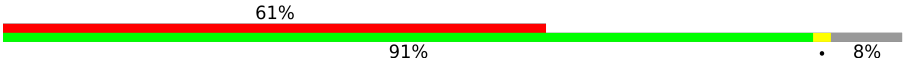
- Molecule 6: Nad4Lm

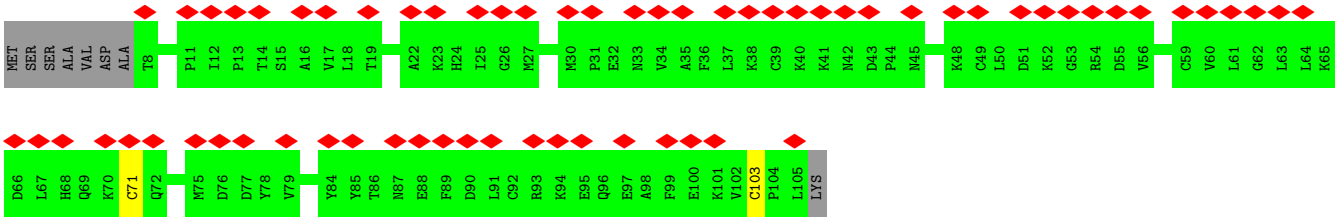
Chain K:



- Molecule 7: PGIV

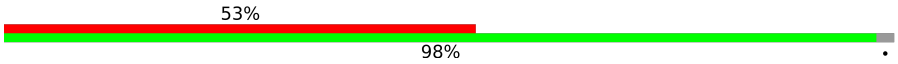
Chain Y:

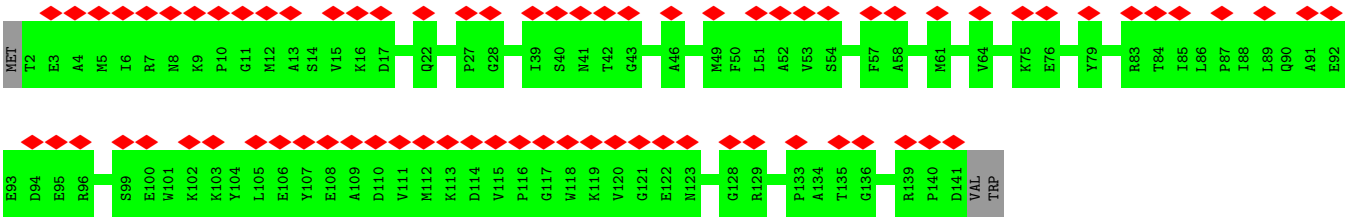




- Molecule 8: B16.6

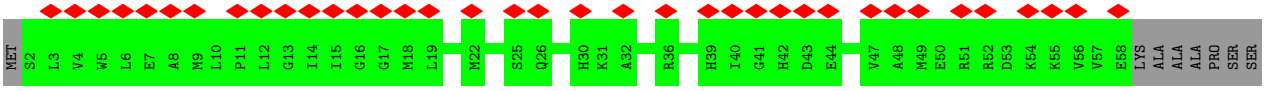
Chain Z:





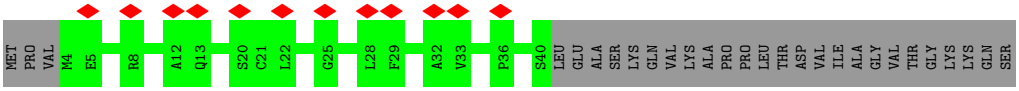
- Molecule 9: MWFE

Chain V:



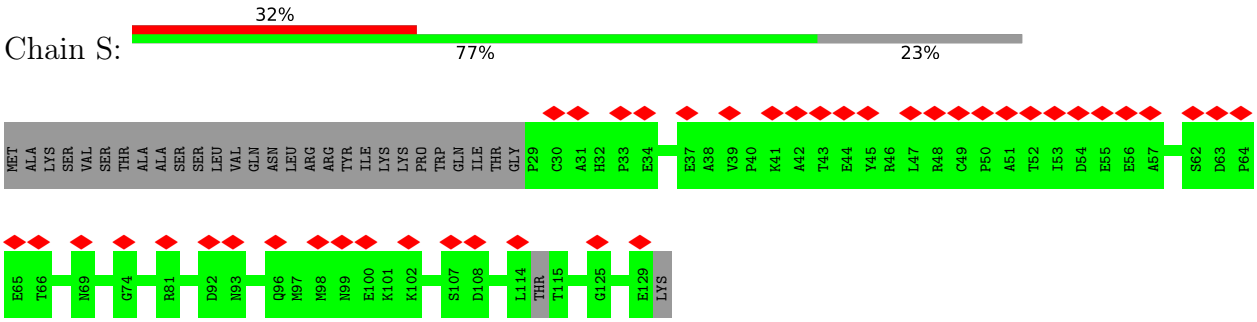
- Molecule 10: B9

Chain W:



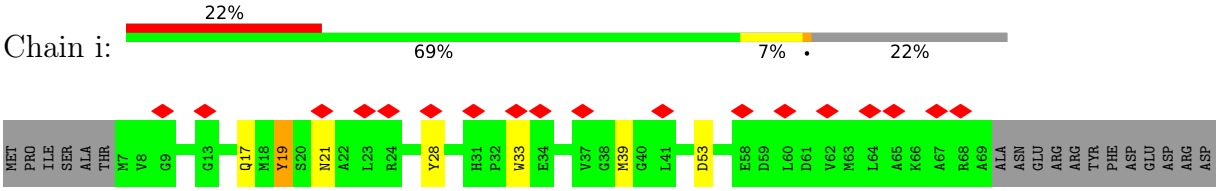
- Molecule 11: B14.5a

Chain S:



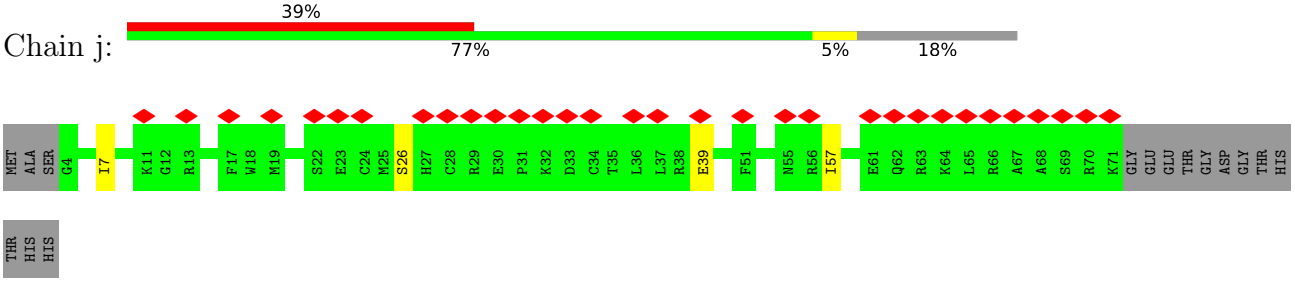
- Molecule 12: B14.5b

Chain i:



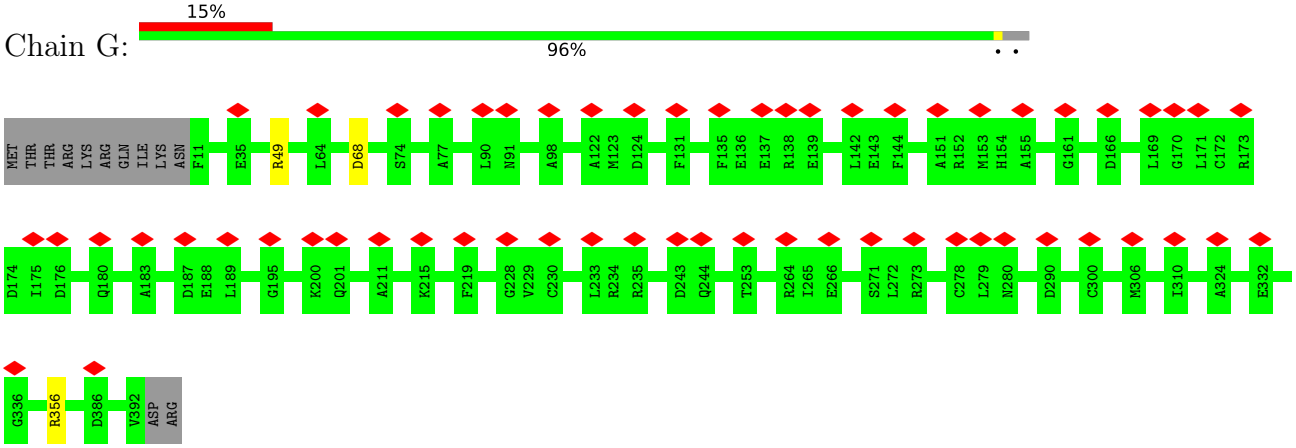
- Molecule 13: 15kDa

Chain j:



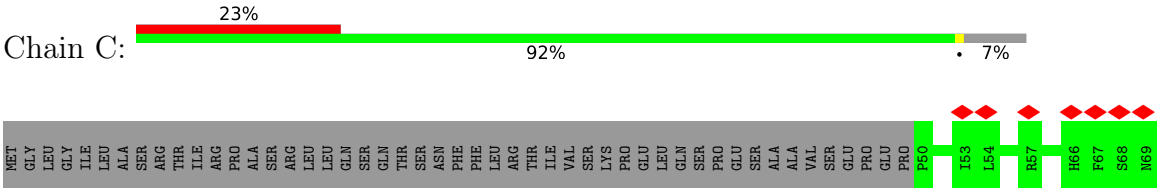
- Molecule 14: Nad7m

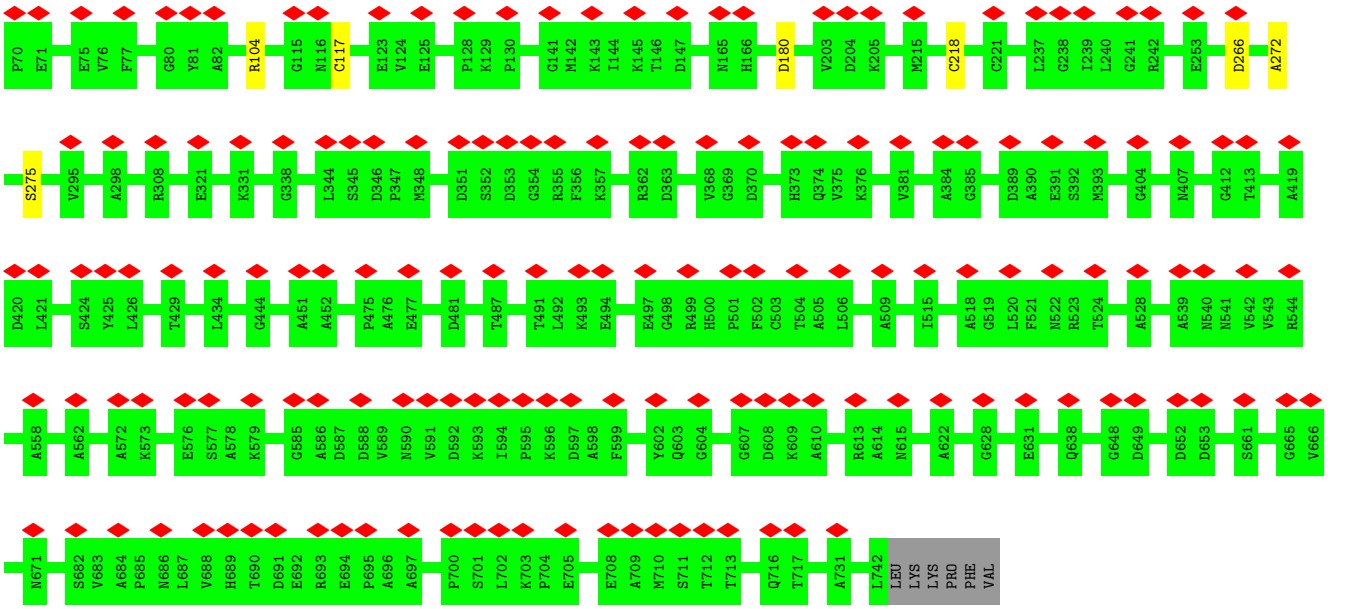
Chain G:



- Molecule 15: 75kDa

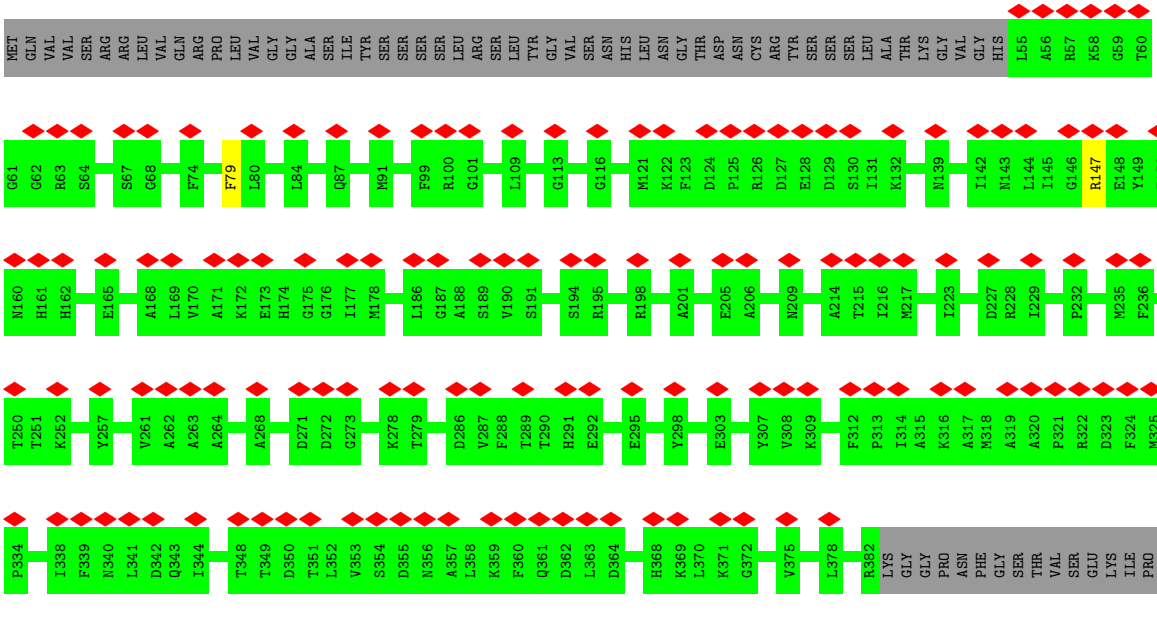
Chain C:





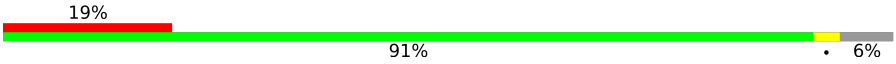
- Molecule 16: 39kDa

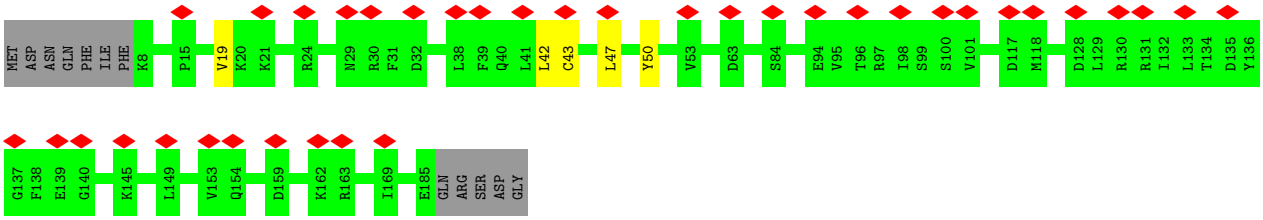
Chain T:



- Molecule 17: Nad9m

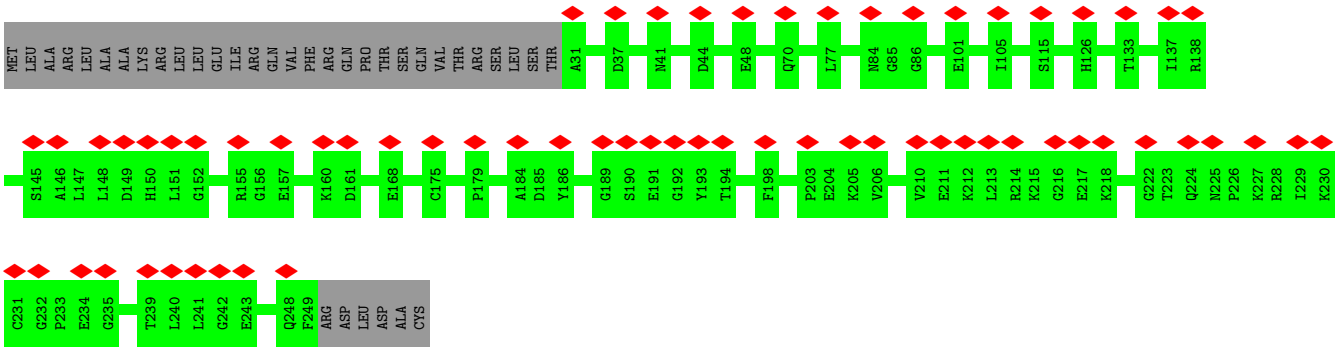
Chain F:





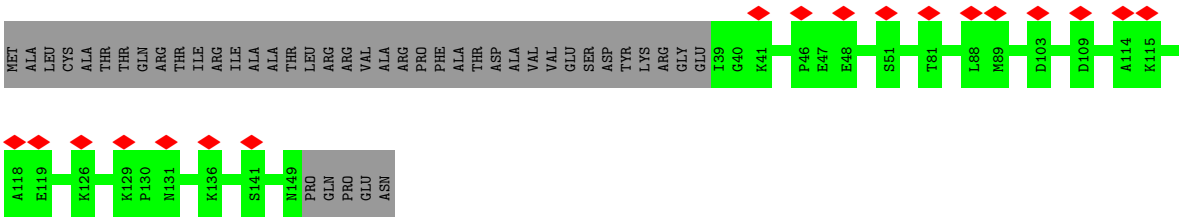
- Molecule 18: 24kDa

Chain B:



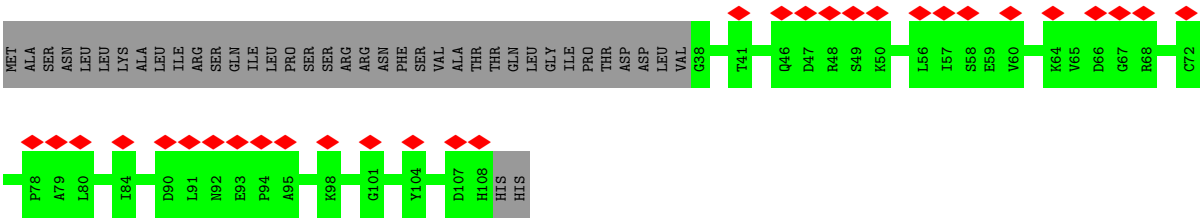
- Molecule 19: 18kDa

Chain O:



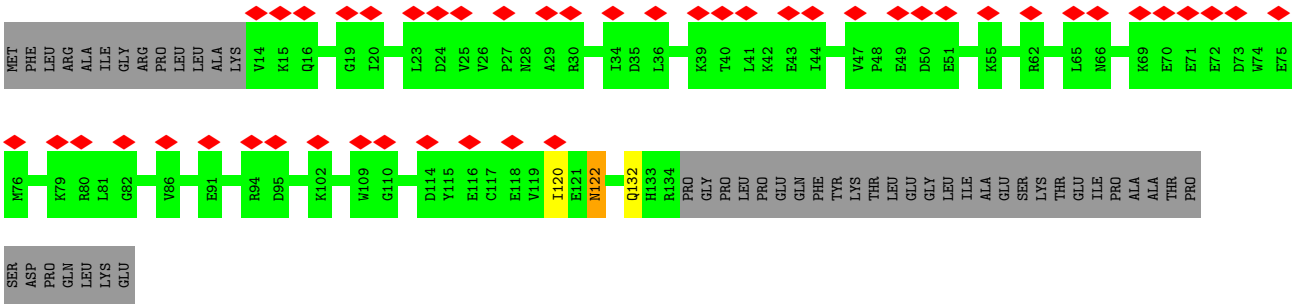
- Molecule 20: 13kDa

Chain P:



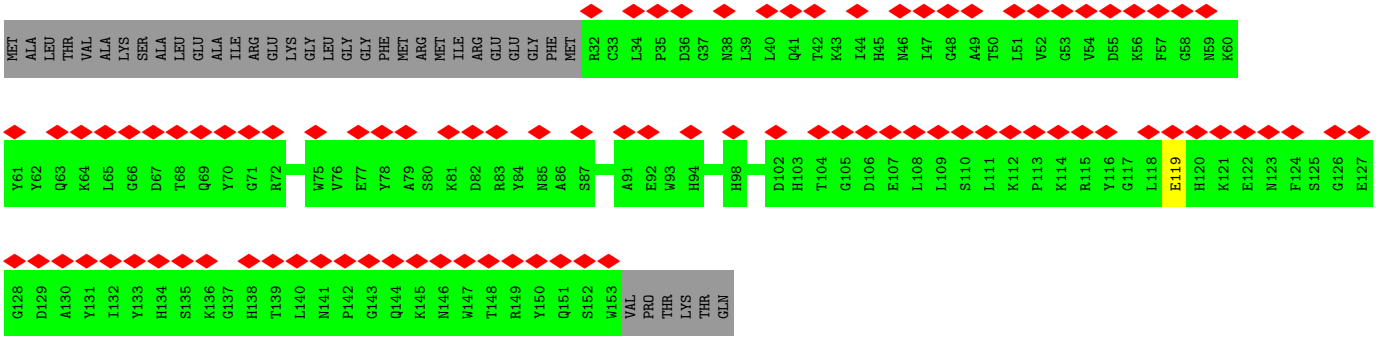
- Molecule 21: B13

Chain R:



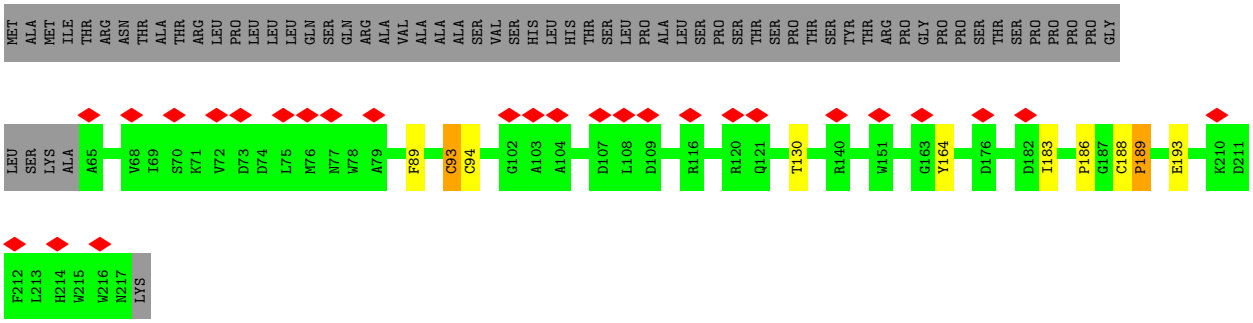
- Molecule 22: B17.2

Chain U:



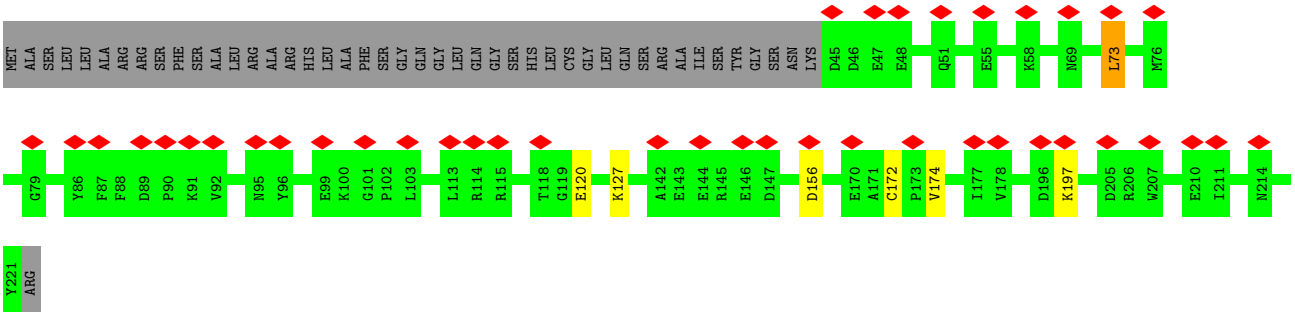
- Molecule 23: PSST

Chain E:



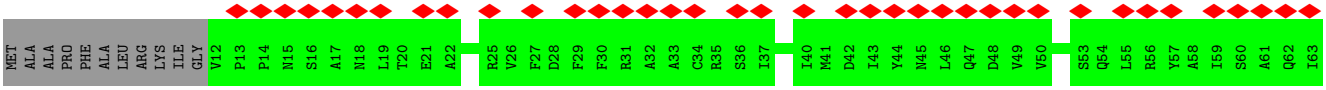
- Molecule 24: TYKY

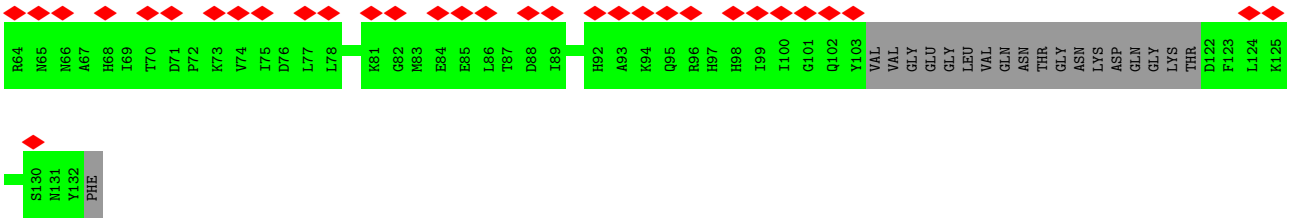
Chain D:



- Molecule 25: B14

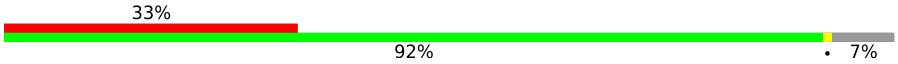
Chain X:

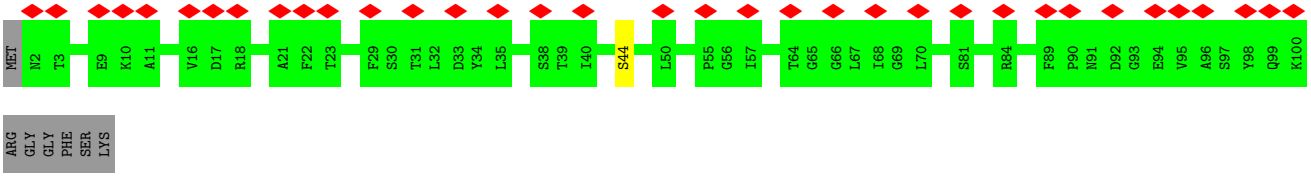




- Molecule 26: MNLL

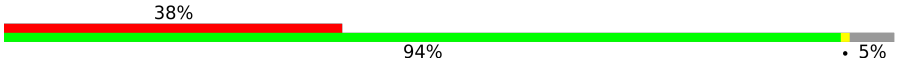
Chain c:

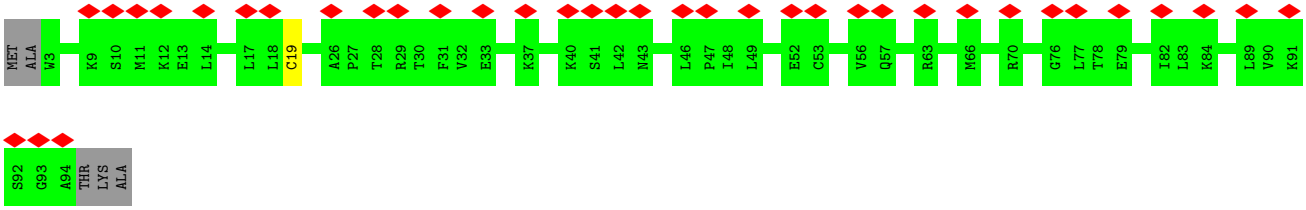




- Molecule 27: B8

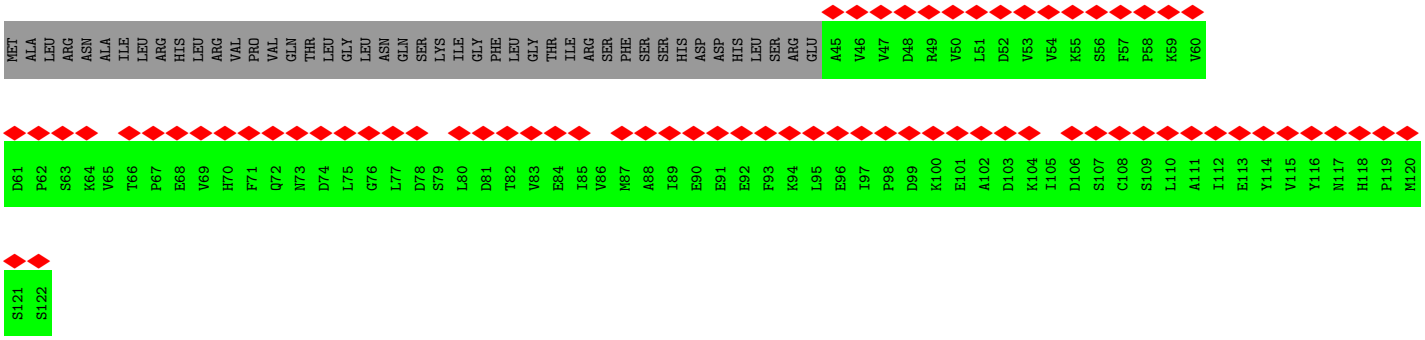
Chain Q:





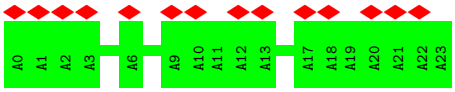
- Molecule 28: ACPM1

Chain k:



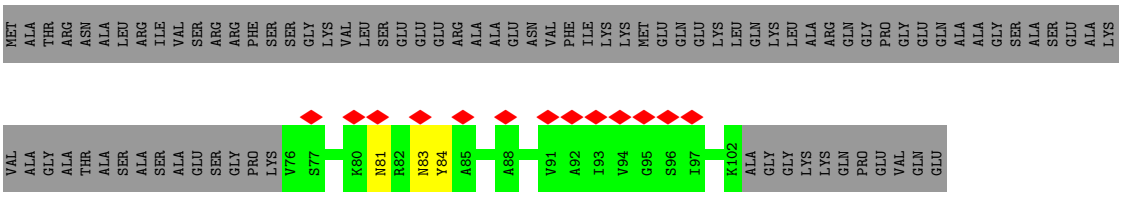
- Molecule 29: Unk1

Chain r:



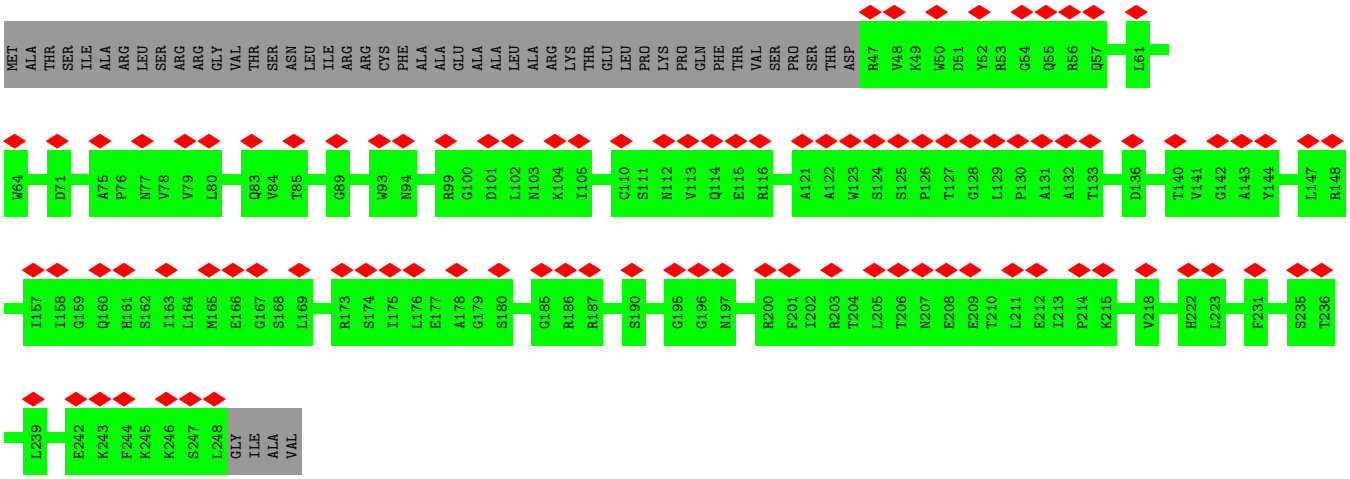
- Molecule 30: P2

Chain n:



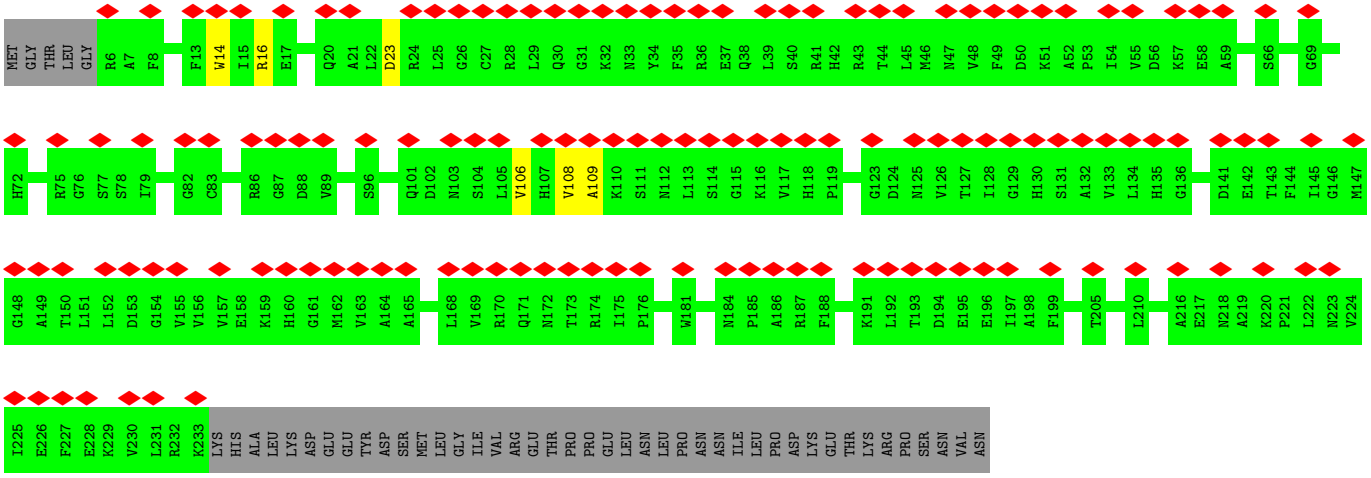
- Molecule 31: CAL1

Chain o:



- Molecule 32: CA1

Chain q:



- Molecule 32: CA1

Chain p:

MET GLY THR LEU GLY R6 A7 F8 F13 R16 E17 T18 G19 Q20 A21 L25 L29 Q30 Y34 F35 R36 E37 Q38 H42 R43 T44 L45 M46 F49 D50 K51 A52 P53 I54 V55 D56 K57 E58 A59 F60 V61 A65 I68 H72 I73 G74 R75 I79 W80

L85 R86 G87 D88 V89 N90 T91 V92 S93 V94 G95 N99 I100 Q101 D102 N103 H107 V108 A109 K110 S111 N112 L113 S114 G115 K116 V117 H118 P119 T120 I121 I122 G123 D124 N125 H130 S131 A132 V133 L134 H135 G136 C137 T138 V139 E140 D141 E142 I145 G146 M147 G148 A149 T150 L151

L152 D153 G154 V155 V156 V157 E158 K159 H160 V163 A164 A165 G166 A167 L168 V169 R170 Q171 N172 T173 R174 I175 P176 S177 G178 E179 V180 W181 G182 G183 N184 P185 F188 L189 R190 K191 L192 T193 D194 E195 E196 I197 A198 F199 I200 S201 Q202 N206 Y207 S208 Q212 A213 H214 A215 A216 E217

N218 A219 K220 P221 L222 F227 E228 K229 VAL LEU ARG LYS LYS HIS ALA LEU LYS ASP GLU GLU TYR ASP SER MET LEU GLY ILE VAL ARG GLU THR PRO PRO GLU LEU ASN LEU PRO ASN ASN ILE LEU PRO ASP LYS GLU THR LYS ARG PRO SER ASN VAL ASN

- Molecule 33: GLDH

Chain z:

MET LEU ARG SER LEU LEU LEU LEU ARG ARG SER VAL GLY HIS SER LEU GLY THR LEU SER PRO SER SER SER THR ILE ARG SER SER PHE SER PRO HIS ARG THR LEU CYS THR THR THR GLY GLN THR LEU THR PRO PRO PRO PRO PRO PRO ARG PRO PRO PRO PRO PRO ALA THR ALA

SER GLU ALA GLN PHE ARG LYS TYR ALA GLY TYR ALA ALA LEU ALA ILE PHE SER GLY VAL ALA THR TYR PHE SER PHE PRO PHE PRO GLU ASN ALA LYS HIS LYS LYS ALA GLN ILE PHE ARG TYR ALA PRO LEU PRO E107 D108 L109 H110 T111 V112 S113 E120 V121 Q122 T123 R124 N125

F126 N127 Q128 P129 E130 N131 L132 A133 D134 L135 E136 A137 L138 V139 K140 E141 S142 H143 E144 K145 K146 L147 R148 I149 R150 P151 V152 G153 S154 G155 L156 S157 P158 N159 G160 I161 G162 L163 S164 R165 S166 G167 M168 V169 N170 L171 A172 L173 M174 D175 K176 V177 L178 E179 V180 D181 K182 E183 K184 K185

R186 V187 T188 V189 Q190 A191 G192 I193 R194 V195 Q196 Q197 L198 V199 D200 A201 I202 K203 D204 Y205 G206 L207 T208 L209 Q210 N211 F212 A213 S214 I215 R216 E217 Q218 Q219 I220 G221 G222 I223 I224 Q225 V226 G227 A228 H229 G230 T231 G232 A233 R234 L235 P236 P237 I238 D239 E240 Q241 V242 I243 S244 M245

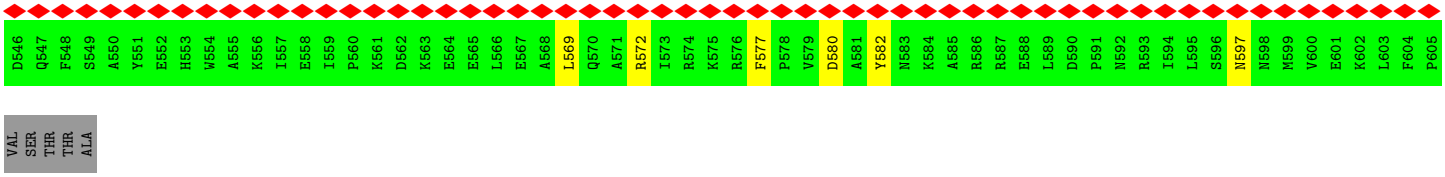
K246 L247 V248 T249 P250 A251 K252 G253 T254 I255 E256 L257 S258 R259 E260 K261 D262 P263 E264 L265 F266 H267 L268 A269 R270 C271 G272 L273 G274 G275 L276 G277 V278 V279 A280 E281 V282 T283 L284 Q285 C286 V287 A288 R289 H290 E291 L292 V293 E294 H295 T296 Y297 V298 S299 N300 L301 Q302 E303 I304 K305

K306 N307 H308 K309 K310 L311 L312 S313 A314 N315 K316 H317 V318 K319 Y320 L321 Y322 I323 P324 Y325 T326 D327 T328 V329 V330 V331 V332 T333 C334 N335 P336 V337 S338 K339 W340 S341 G342 P343 P344 K345 D346 K347 P348 K349 Y350 T351 T352 D353 E354 A355 V356 Q357 H358 V359 R360 D361 L362 Y363 R364 E365

S366 I367 V368 K369 Y370 R371 V372 Q373 D374 S375 G376 K377 K378 S379 P380 D381 S382 S383 E384 P385 D386 I387 Q388 E389 L390 S391 F392 T393 E394 L395 R396 D397 K398 L399 L400 A401 L402 D403 P404 L405 N406 D407 V408 H409 V410 A411 K412 V413 N414 Q415 A416 E417 A418 E419 F420 W421 K422 K423 S424 E425

G426 Y427 R428 V429 G430 W431 S432 D433 E434 I435 L436 G437 F438 D439 C440 G441 G442 Q443 Q444 W445 V446 S447 E448 S449 C450 F451 P452 A453 G454 T455 L456 A457 N458 P459 S460 M461 K462 D463 L464 E465 Y466 I467 E468 E469 L470 K471 K472 L473 I474 E475 K476 E477 A478 I479 P480 A481 P482 A483 P484 I485

E486 Q487 R488 W489 T490 A491 R492 S493 K494 S495 P496 I497 S498 P499 A500 F501 S502 T503 S504 E505 D506 D507 I508 F509 S510 W511 V512 G513 I514 I515 M516 Y517 L518 P519 T520 A521 D522 P523 R524 Q525 R526 K527 D528 I529 T530 D531 E532 F533 F534 H535 Y536 R537 H538 L539 T540 Q541 K542 Q543 L544 W545


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 (i)

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 ($e^-/Å^2$)	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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	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 (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	427/486 (88%)	381 (89%)	46 (11%)	0	100	100
2	I	479/499 (96%)	465 (97%)	13 (3%)	1 (0%)	44	74
3	J	92/119 (77%)	86 (94%)	6 (6%)	0	100	100
4	N	145/205 (71%)	125 (86%)	19 (13%)	1 (1%)	19	52
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%)	13	44
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%)	8	36
13	j	66/83 (80%)	63 (96%)	2 (3%)	1 (2%)	8	37
14	G	380/394 (96%)	348 (92%)	32 (8%)	0	100	100
15	C	691/748 (92%)	617 (89%)	73 (11%)	1 (0%)	48	79
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%)	16	49
22	U	120/159 (76%)	98 (82%)	22 (18%)	0	100	100
23	E	151/218 (69%)	134 (89%)	16 (11%)	1 (1%)	19	52
24	D	175/222 (79%)	159 (91%)	14 (8%)	2 (1%)	12	42
25	X	99/133 (74%)	92 (93%)	7 (7%)	0	100	100

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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%)	2	21
31	o	200/252 (79%)	172 (86%)	28 (14%)	0	100	100
32	p	222/275 (81%)	191 (86%)	28 (13%)	3 (1%)	9	37
32	q	226/275 (82%)	196 (87%)	27 (12%)	3 (1%)	10	39
33	z	495/610 (81%)	476 (96%)	15 (3%)	4 (1%)	16	49
All	All	6177/7436 (83%)	5565 (90%)	591 (10%)	21 (0%)	38	69

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 (i)

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%)	91	92
2	I	399/416 (96%)	365 (92%)	34 (8%)	8	31
3	J	87/106 (82%)	87 (100%)	0	100	100
4	N	133/186 (72%)	131 (98%)	2 (2%)	60	74
5	H	266/272 (98%)	264 (99%)	2 (1%)	79	84
6	K	74/86 (86%)	73 (99%)	1 (1%)	62	75
7	Y	88/94 (94%)	87 (99%)	1 (1%)	70	79

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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	17
13	j	62/73 (85%)	59 (95%)	3 (5%)	21	46
14	G	328/340 (96%)	325 (99%)	3 (1%)	75	82
15	C	576/625 (92%)	571 (99%)	5 (1%)	75	82
16	T	271/334 (81%)	269 (99%)	2 (1%)	81	86
17	F	168/179 (94%)	164 (98%)	4 (2%)	44	62
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%)	52	69
22	U	104/133 (78%)	103 (99%)	1 (1%)	73	80
23	E	129/184 (70%)	122 (95%)	7 (5%)	18	43
24	D	157/191 (82%)	151 (96%)	6 (4%)	28	52
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%)	67	77
28	k	73/112 (65%)	73 (100%)	0	100	100
30	n	21/84 (25%)	19 (90%)	2 (10%)	7	26
31	o	171/211 (81%)	171 (100%)	0	100	100
32	p	181/228 (79%)	176 (97%)	5 (3%)	38	59
32	q	184/228 (81%)	182 (99%)	2 (1%)	70	79
33	z	440/534 (82%)	412 (94%)	28 (6%)	14	39
All	All	5297/6293 (84%)	5178 (98%)	119 (2%)	47	64

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

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

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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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	$\#\|Z\| > 2$
34	SF4	A	501	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
34	SF4	D	302	24	0,12,12	-	-	-		
39	FES	C	803	15	0,4,4	-	-	-		
34	SF4	E	301	23	0,12,12	-	-	-		
39	FES	B	301	-	0,4,4	-	-	-		
36	T7X	I	501	-	42,42,61	0.31	0	52,54,73	0.50	0
35	FMN	A	502	-	33,33,33	0.62	0	48,50,50	0.72	1 (2%)
40	NDP	T	501	-	45,52,52	0.62	0	53,80,80	0.83	2 (3%)
38	PEV	G	601	-	27,27,48	0.35	0	30,32,53	0.37	0
37	CDL	i	201	-	89,89,99	0.28	0	95,101,111	0.57	2 (2%)
42	BCT	q	802	41	2,3,3	0.60	0	2,3,3	0.24	0
34	SF4	D	301	24	0,12,12	-	-	-		
34	SF4	C	802	15	0,12,12	-	-	-		
36	T7X	c	301	-	37,37,61	0.33	0	47,49,73	0.39	0
34	SF4	C	801	15	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
34	SF4	A	501	1	-	-	0/6/5/5
34	SF4	D	302	24	-	-	0/6/5/5
39	FES	C	803	15	-	-	0/1/1/1
34	SF4	E	301	23	-	-	0/6/5/5
39	FES	B	301	-	-	-	0/1/1/1
36	T7X	I	501	-	-	13/37/61/80	0/1/1/1
35	FMN	A	502	-	-	6/18/18/18	0/3/3/3
40	NDP	T	501	-	-	6/30/77/77	0/5/5/5
38	PEV	G	601	-	-	12/30/30/52	-
37	CDL	i	201	-	-	31/100/100/110	-
34	SF4	D	301	24	-	-	0/6/5/5
34	SF4	C	802	15	-	-	0/6/5/5
36	T7X	c	301	-	-	2/32/56/80	0/1/1/1
34	SF4	C	801	15	-	-	0/6/5/5

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:

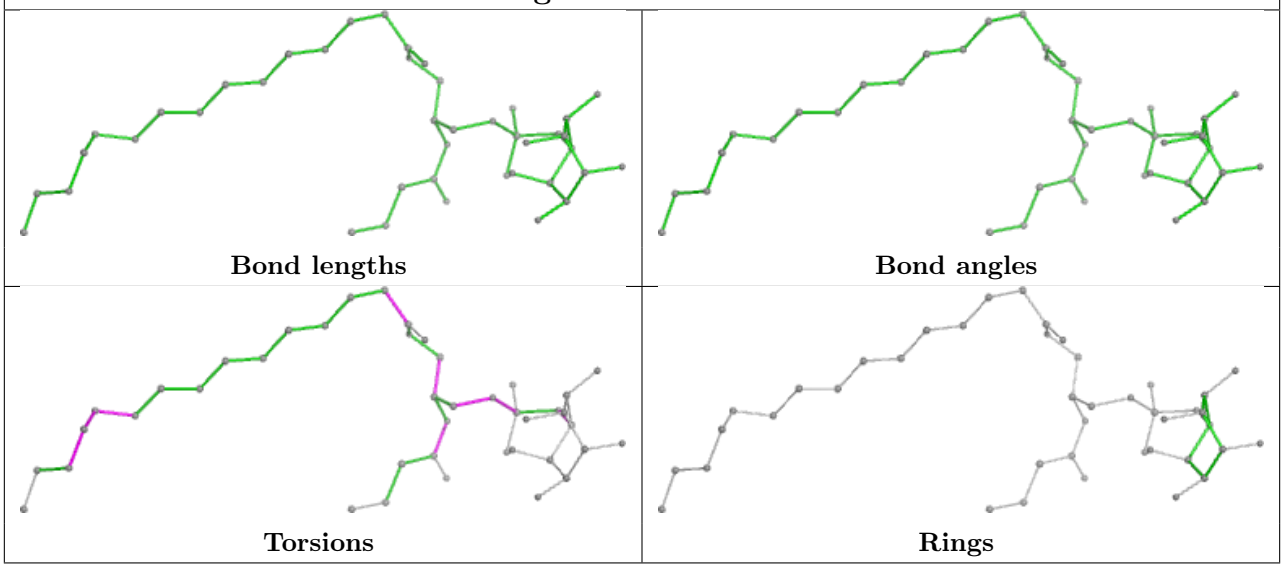
Mol	Chain	Res	Type	Atoms
35	A	502	FMN	N10-C1'-C2'-C3'
35	A	502	FMN	O3'-C3'-C4'-C5'
36	I	501	T7X	C6-C1-O1-P1
36	I	501	T7X	C7-O13-P1-O1
36	I	501	T7X	C8-C7-O13-P1

There are no ring outliers.

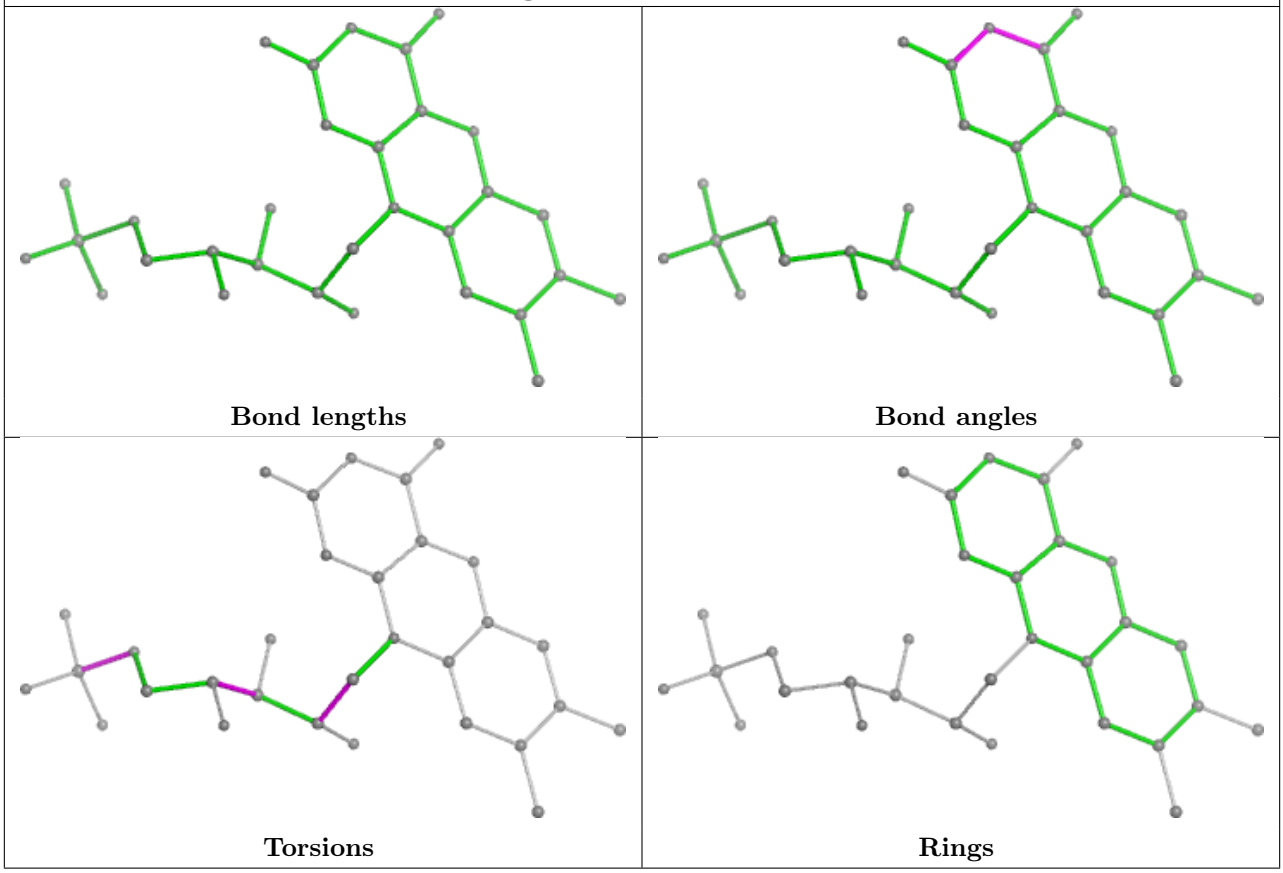
No monomer is involved in short contacts.

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.

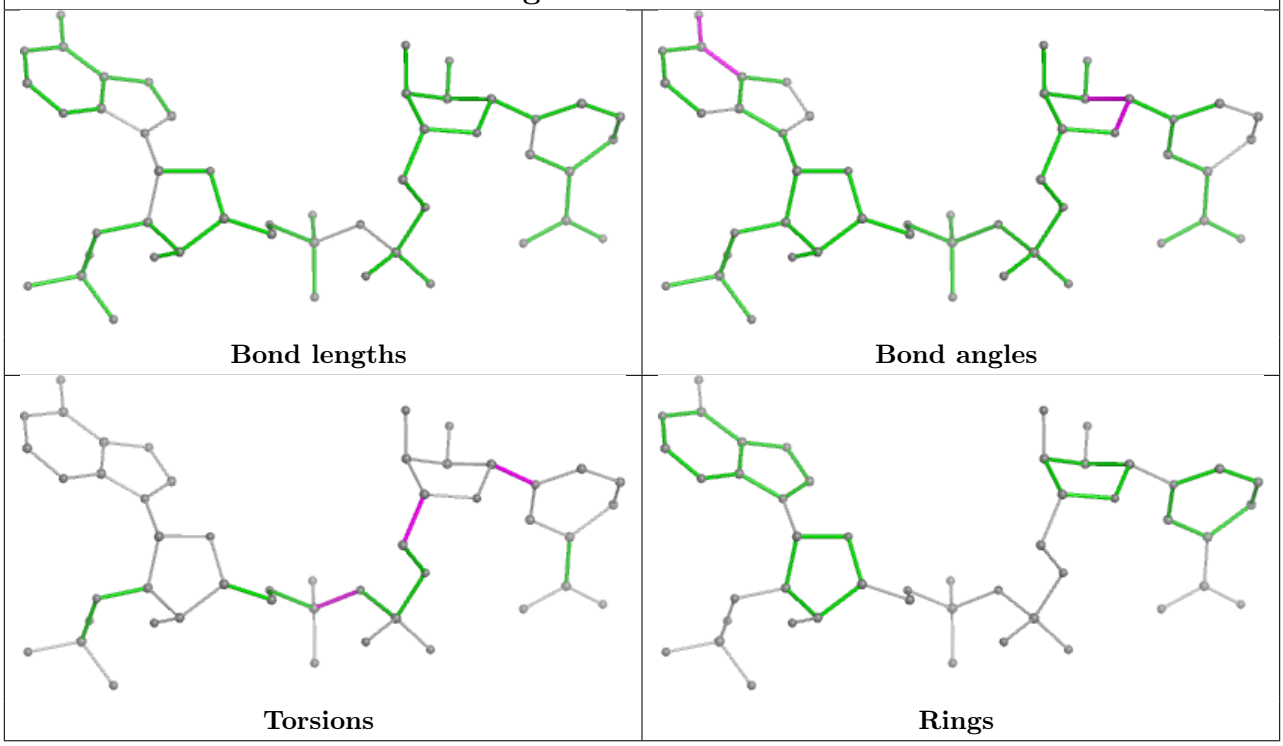
Ligand T7X I 501



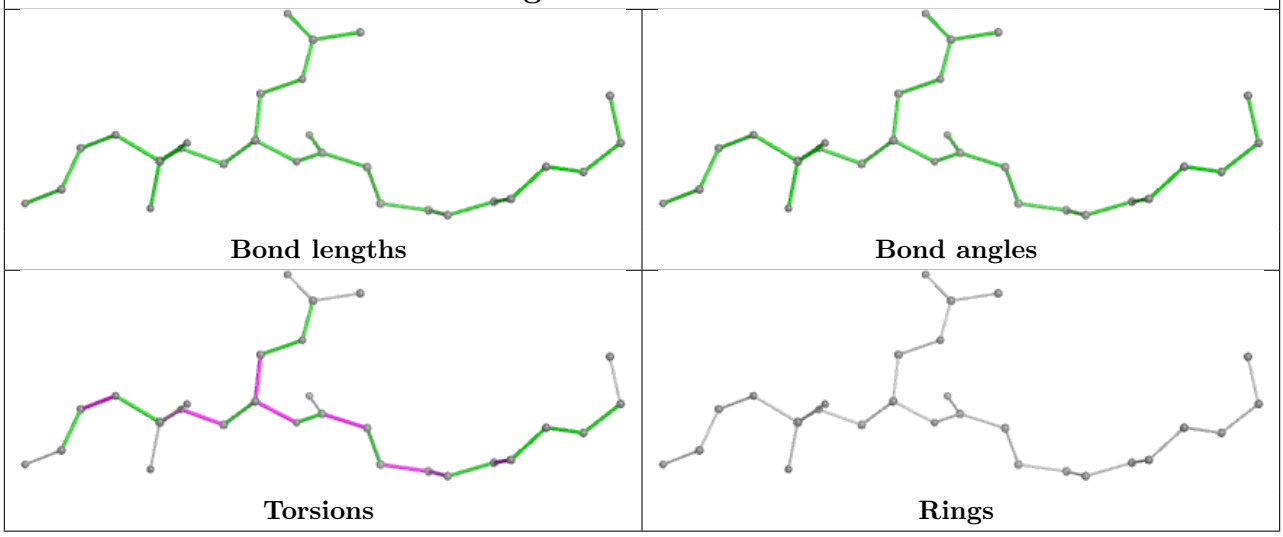
Ligand FMN A 502



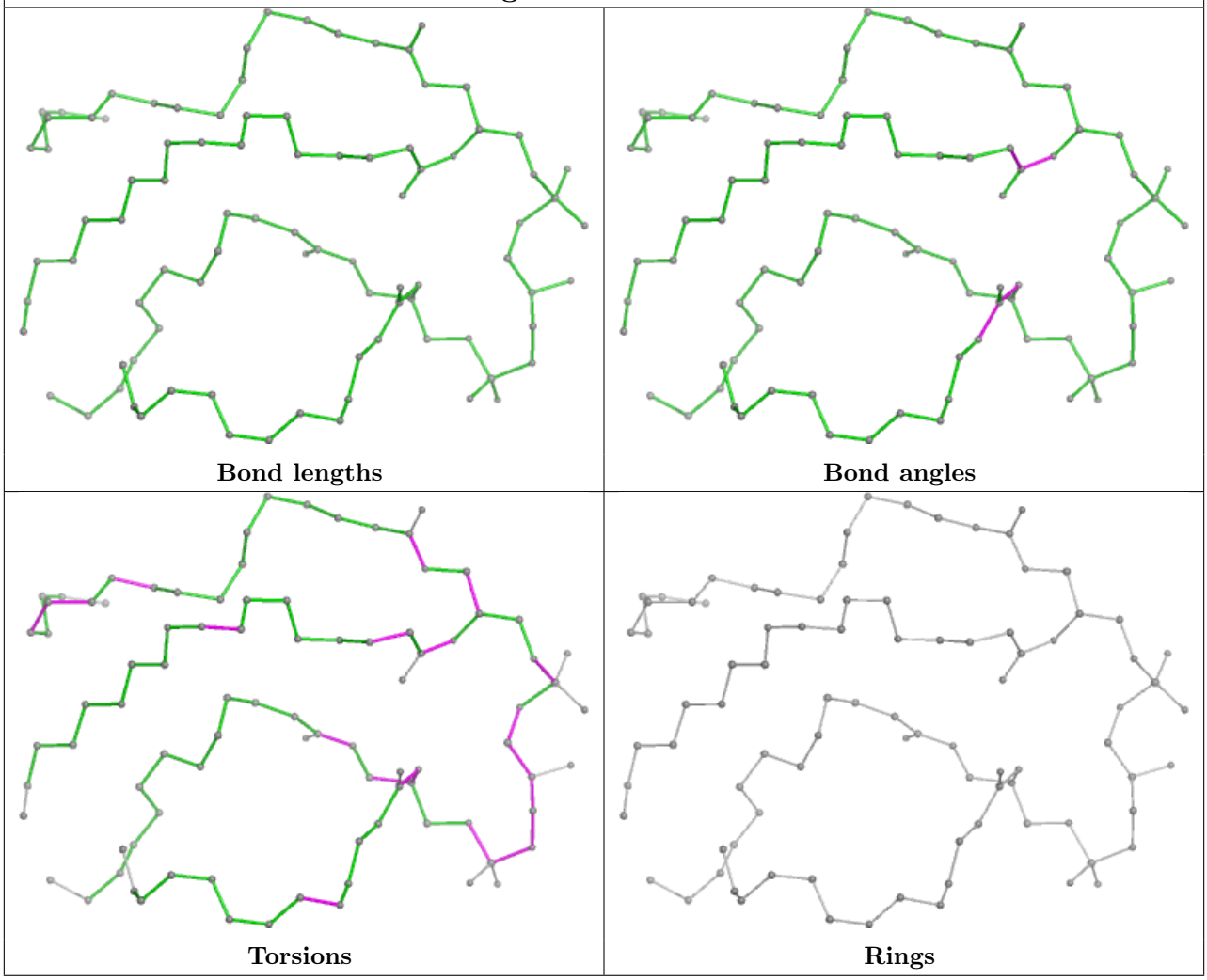
Ligand NDP T 501



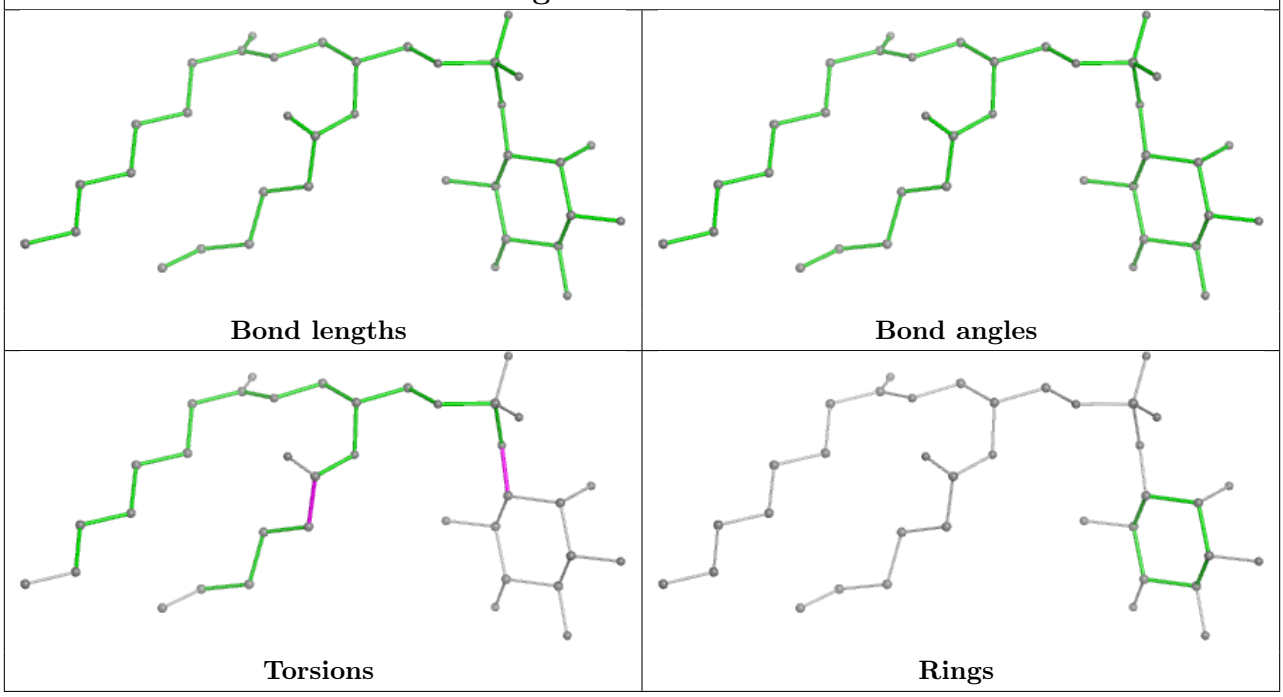
Ligand PEV G 601



Ligand CDL i 201



Ligand T7X c 301



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

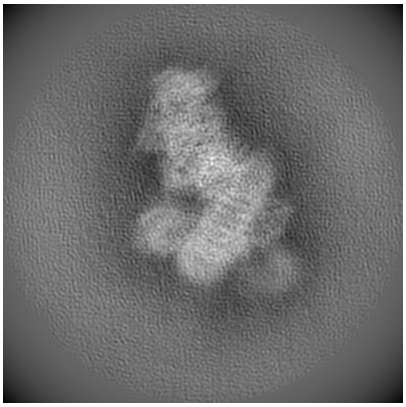
6 Map visualisation (i)

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.

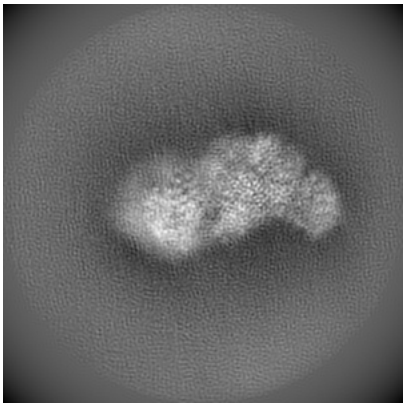
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

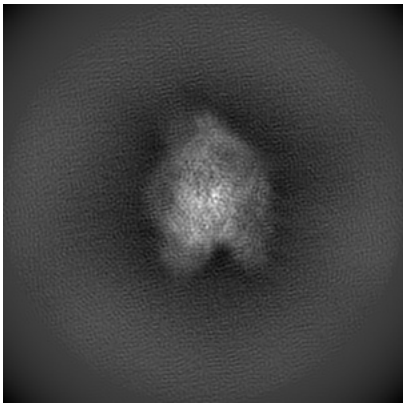
6.1.1 Primary map



X



Y

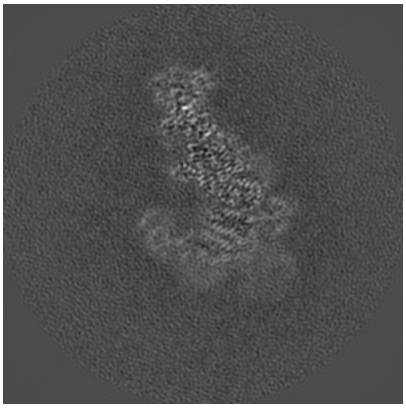


Z

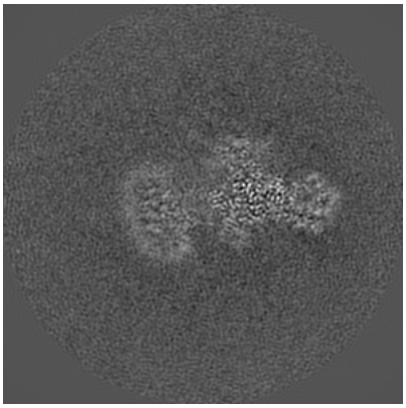
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

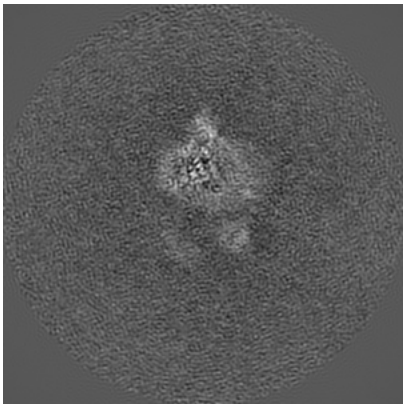
6.2.1 Primary map



X Index: 180



Y Index: 180

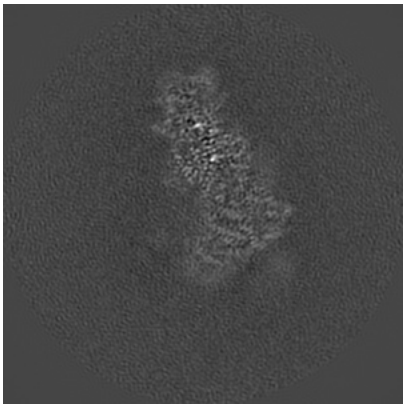


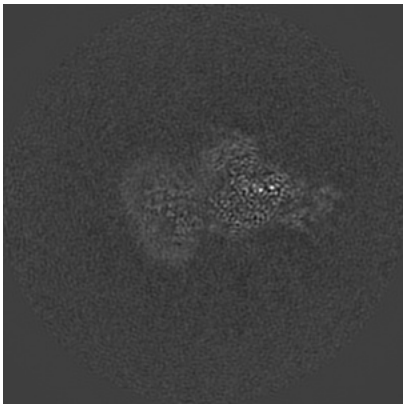
Z Index: 180

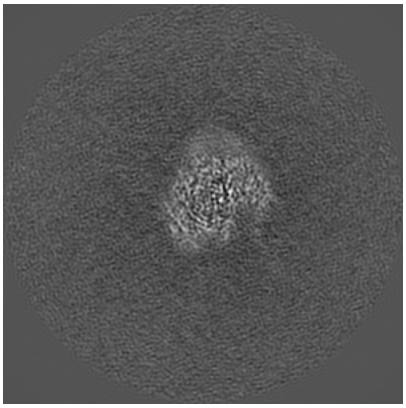
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 190

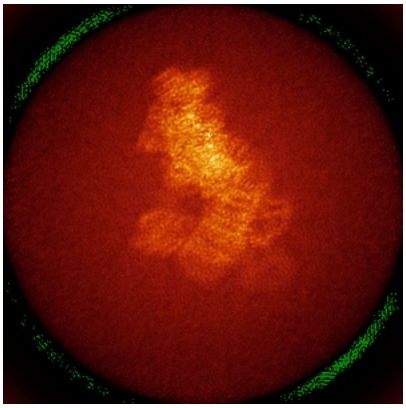

Y Index: 186

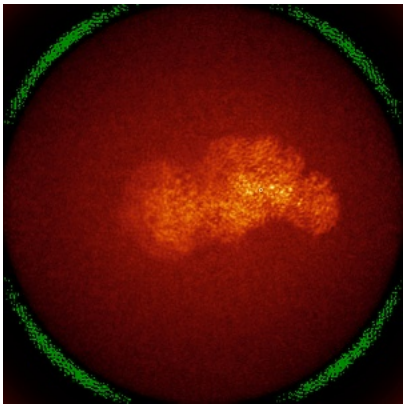

Z Index: 213

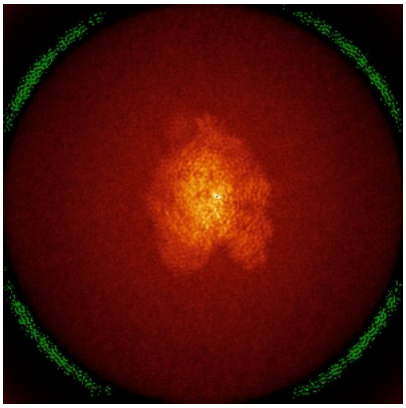
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X

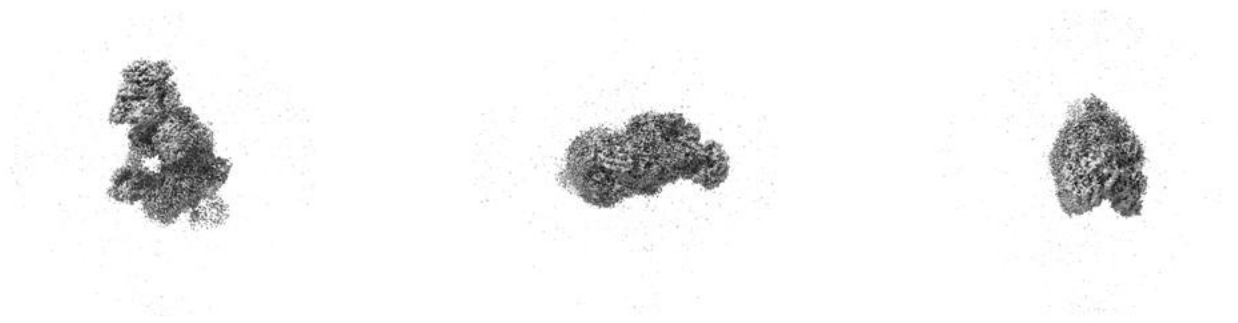

Y


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



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.

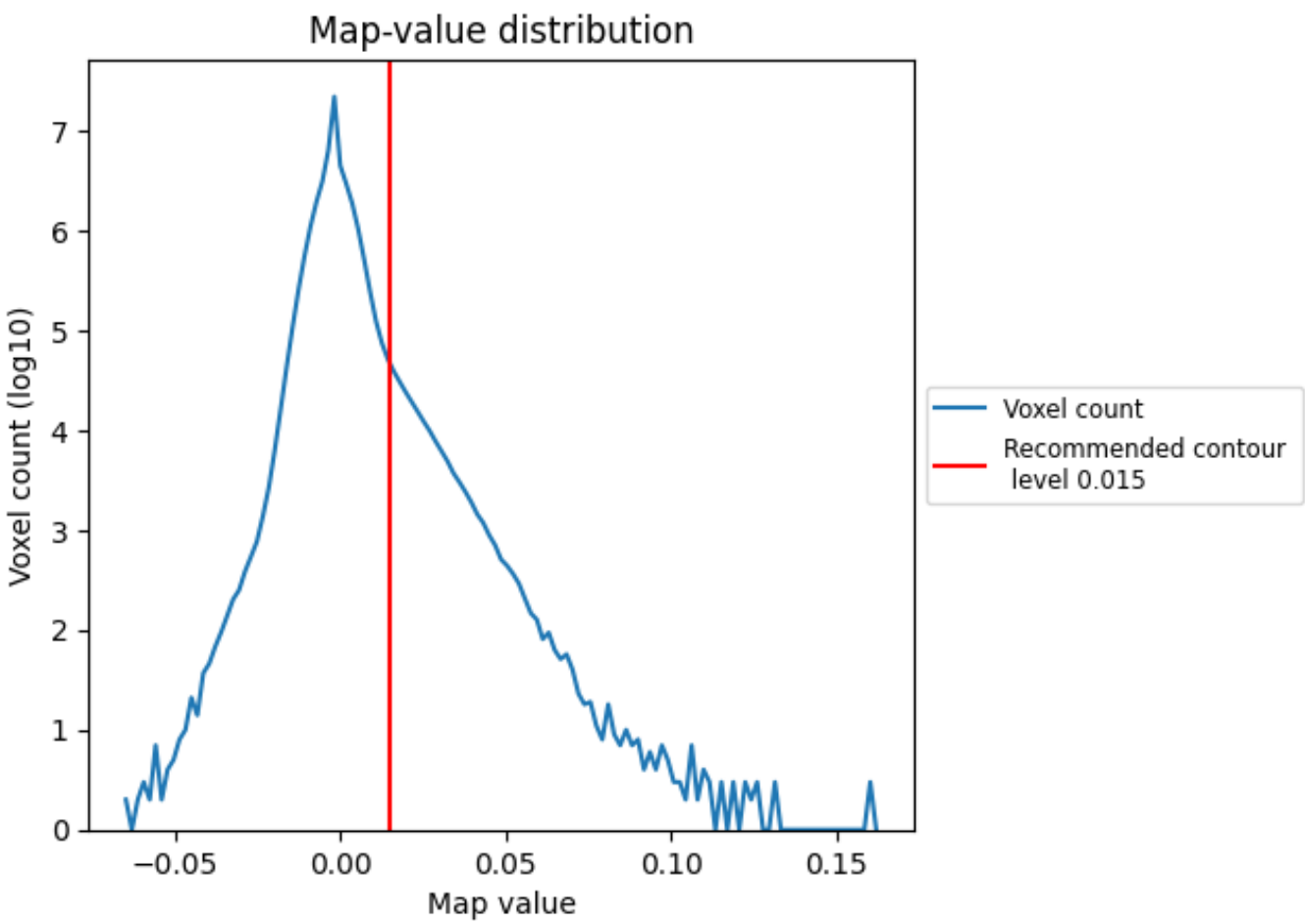
6.6 Mask visualisation (i)

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

7 Map analysis (i)

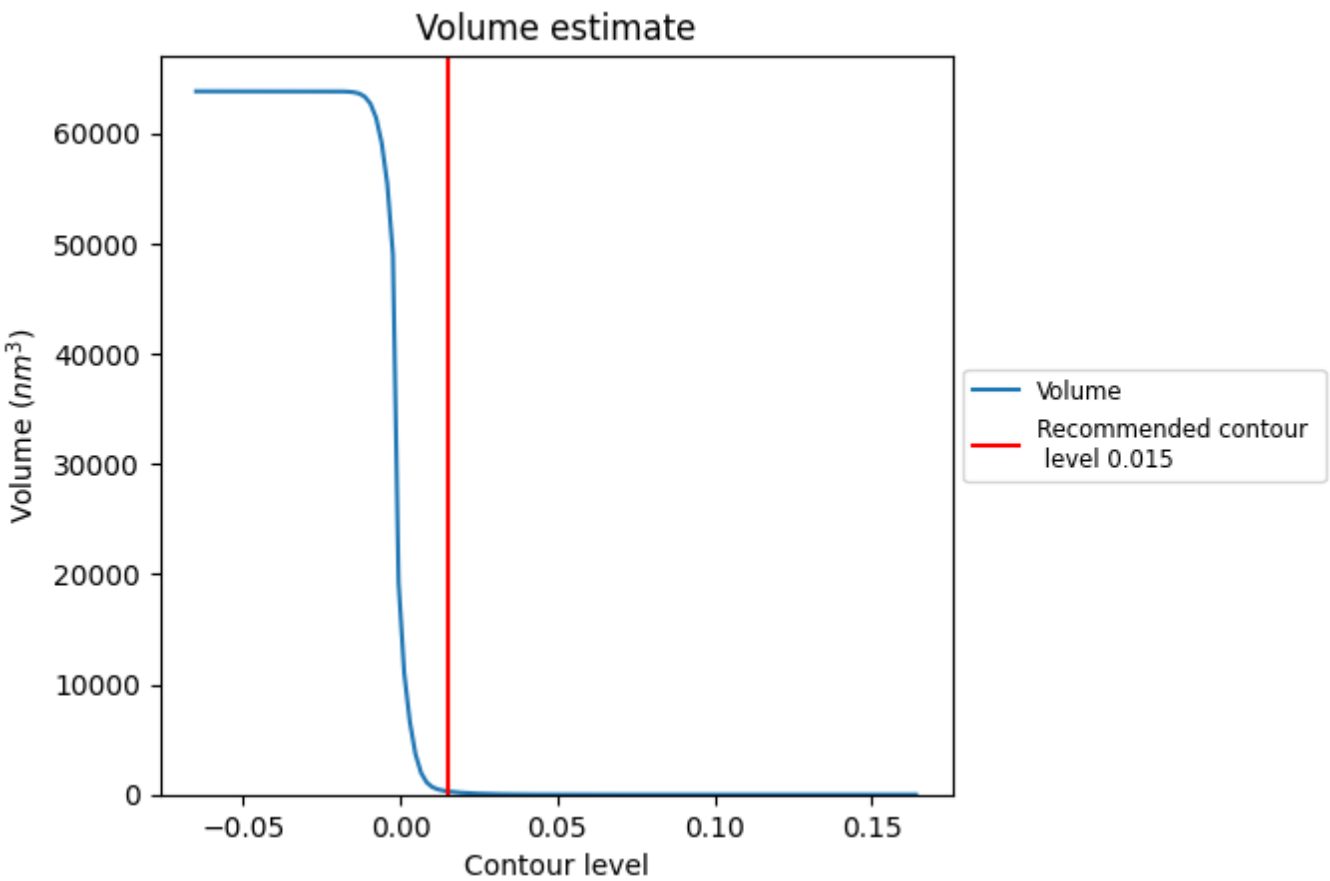
This section contains the results of statistical analysis of the map.

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.

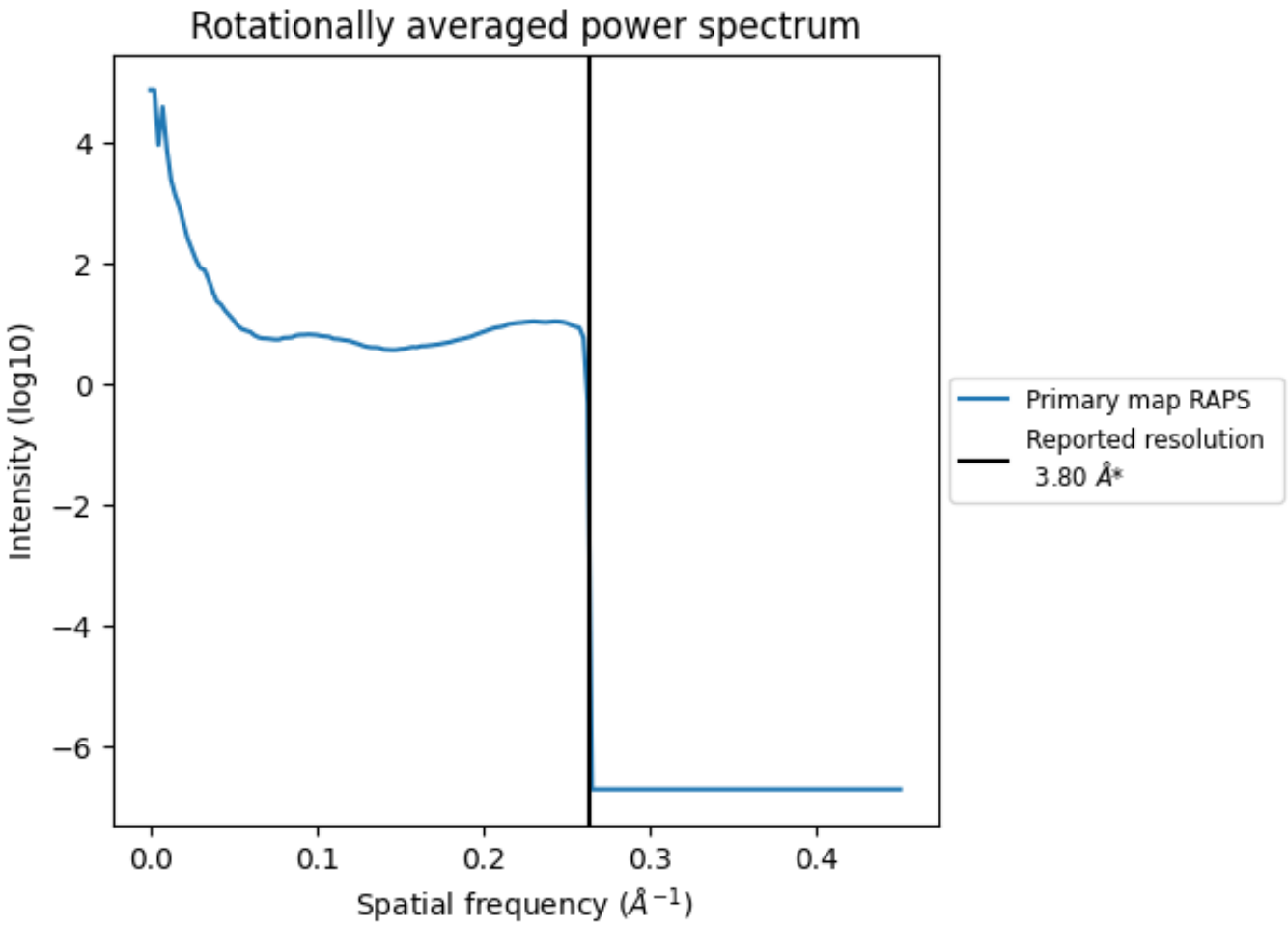
7.2 Volume estimate (i)



The volume at the recommended contour level is 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}

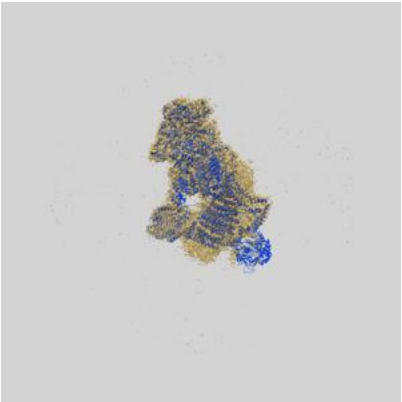
8 Fourier-Shell correlation (i)

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

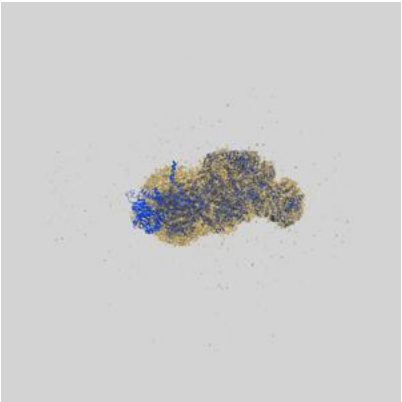
9 Map-model fit (i)

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.

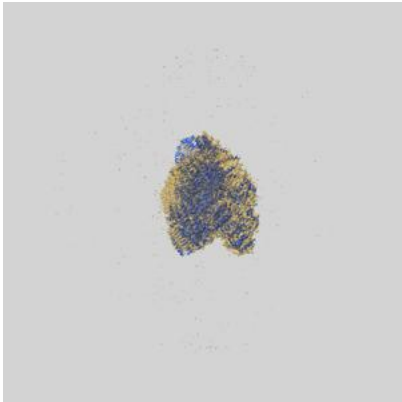
9.1 Map-model overlay (i)



X



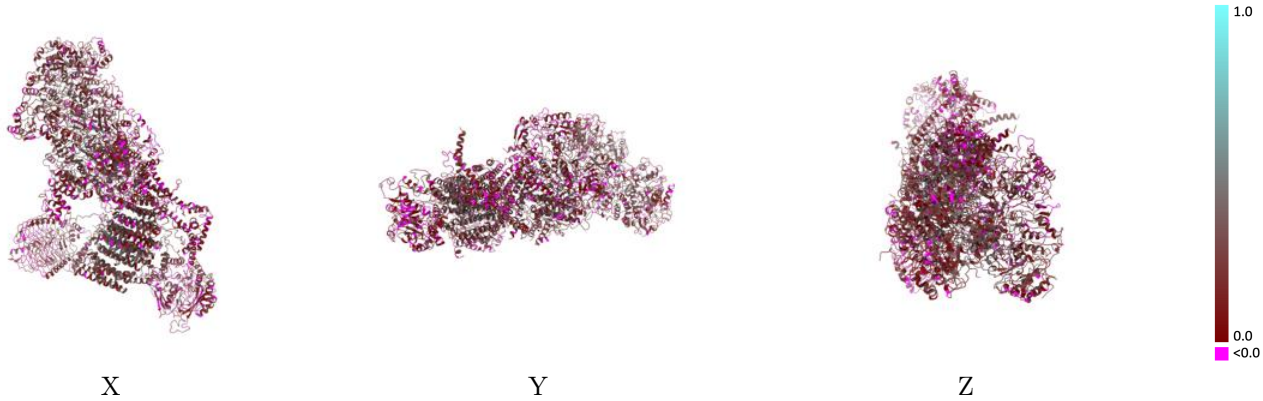
Y



Z

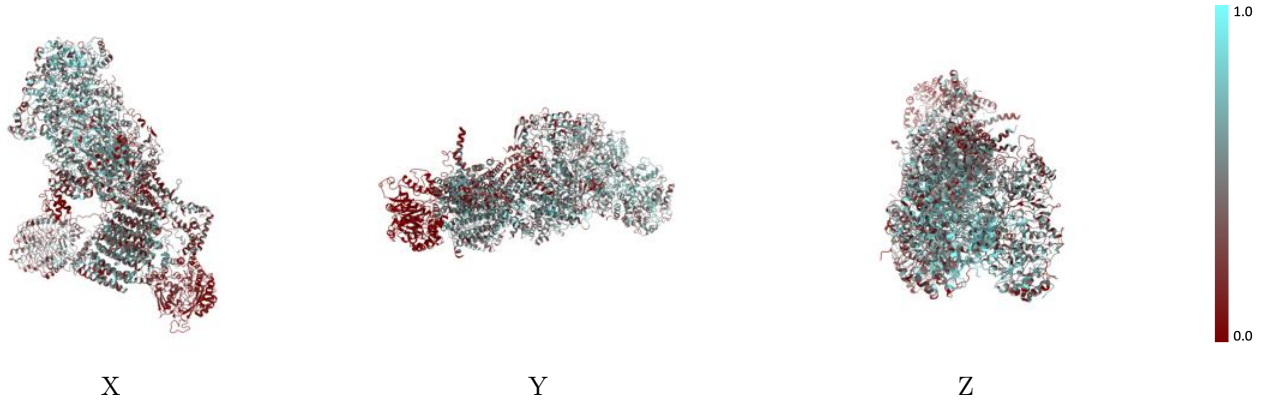
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



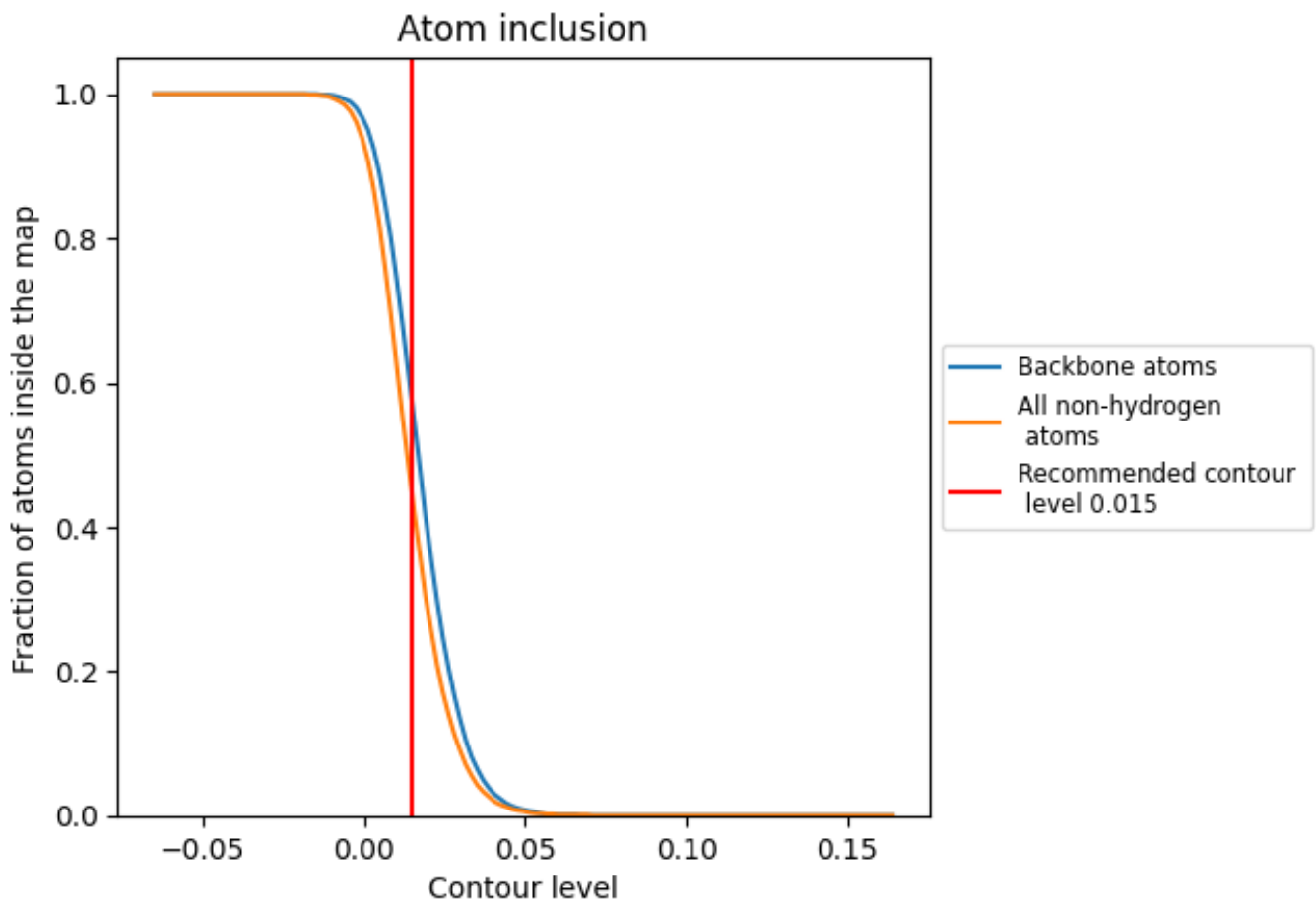
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion (i)



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	0.4440	0.2070
A	0.5070	0.2170
B	0.5480	0.2030
C	0.5700	0.2510
D	0.5610	0.1890
E	0.6000	0.2640
F	0.5930	0.2850
G	0.6280	0.3100
H	0.4640	0.2140
I	0.5300	0.3190
J	0.4150	0.2400
K	0.4550	0.2170
N	0.3870	0.2390
O	0.6150	0.3120
P	0.4510	0.1600
Q	0.4600	0.1990
R	0.4950	0.2050
S	0.4550	0.2110
T	0.4280	0.1380
U	0.2380	0.0680
V	0.3470	0.0900
W	0.5280	0.2830
X	0.3220	0.1470
Y	0.3060	0.0680
Z	0.3940	0.1600
c	0.4890	0.2340
i	0.4740	0.2120
j	0.4560	0.2920
k	0.0980	0.0790
n	0.4250	0.2870
o	0.3980	0.1560
p	0.3520	0.1240
q	0.3380	0.0930
r	0.4500	0.1890
z	0.0330	0.1250