wwPDB EM Validation Summary Report (i)

Aug 26, 2026 – 01:00 pm BST

PDB ID	:	7A24 / pdb_00007a24
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 (i)) were used in the production of this report:

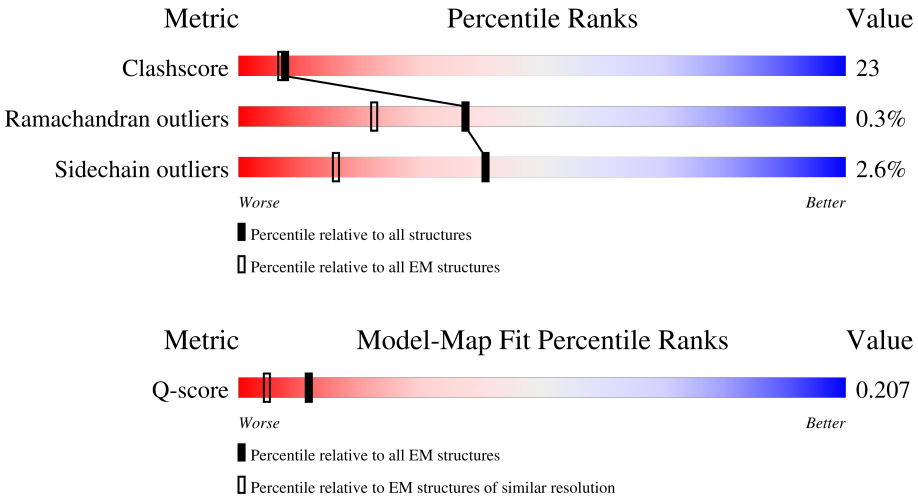
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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% 50% 38% 12%
2	I	499	24% 56% 36% 5% •
3	J	119	35% 50% 31% 19%
4	N	205	37% 43% 29% 27%

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Mol	Chain	Length	Quality of chain
5	H	325	39% 55% 41%
6	K	100	38% 48% 37% 15%
7	Y	106	61% 51% 41% 8%
8	Z	143	53% 64% 34%
9	V	65	57% 57% 31% 12%
10	W	65	18% 32% 22% 43%
11	S	131	32% 56% 21% 23%
12	i	81	22% 41% 26% 10% 22%
13	j	83	39% 52% 28% 18%
14	G	394	15% 49% 47%
15	C	748	23% 50% 42% 7%
16	T	402	38% 48% 34% 18%
17	F	190	19% 38% 54% 6%
18	B	255	26% 56% 29% 14%
19	O	154	12% 54% 18% 28%
20	P	110	27% 50% 15% 35%
21	R	169	28% 40% 29% 28%
22	U	159	59% 50% 27% 23%
23	E	218	12% 38% 28% 30%
24	D	222	18% 40% 37% 20%
25	X	133	53% 54% 23% 23%
26	c	106	33% 67% 26% 7%
27	Q	97	38% 54% 41% 5%
28	k	122	61% 34% 30% 36%
29	r	24	58% 83% 17%

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Mol	Chain	Length	Quality of chain
30	n	113	12% 17% 6% 76%
31	o	252	39% 43% 37% 20%
32	p	275	48% 43% 36% 19%
32	q	275	51% 47% 33% 17%
33	z	610	80% 49% 29% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	SF4	A	501	-	-	X	-
34	SF4	D	301	-	-	X	-
34	SF4	E	301	-	-	X	-
37	CDL	i	201	-	-	X	-
39	FES	B	301	-	-	X	-

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
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
14	G	382	Total	C	N	O	S	0	0
			3049	1939	535	551	24		

- Molecule 15 is a protein called 75kDa.

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

- Molecule 16 is a protein called 39kDa.

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

- Molecule 17 is a protein called Nad9m.

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

- Molecule 18 is a protein called 24kDa.

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

- Molecule 19 is a protein called 18kDa.

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

- Molecule 20 is a protein called 13kDa.

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

- Molecule 21 is a protein called B13.

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

- Molecule 22 is a protein called B17.2.

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

- Molecule 23 is a protein called PSST.

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

- Molecule 24 is a protein called TYKY.

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

- Molecule 25 is a protein called B14.

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

- Molecule 26 is a protein called MNLL.

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

- Molecule 27 is a protein called B8.

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

- Molecule 28 is a protein called ACPM1.

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

- Molecule 29 is a protein called Unk1.

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

- Molecule 30 is a protein called P2.

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

- Molecule 31 is a protein called CAL1.

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

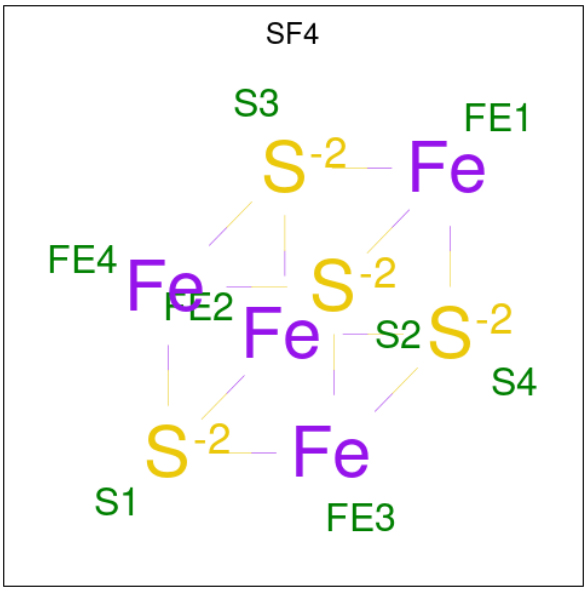
- Molecule 32 is a protein called CA1.

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

- Molecule 33 is a protein called GLDH.

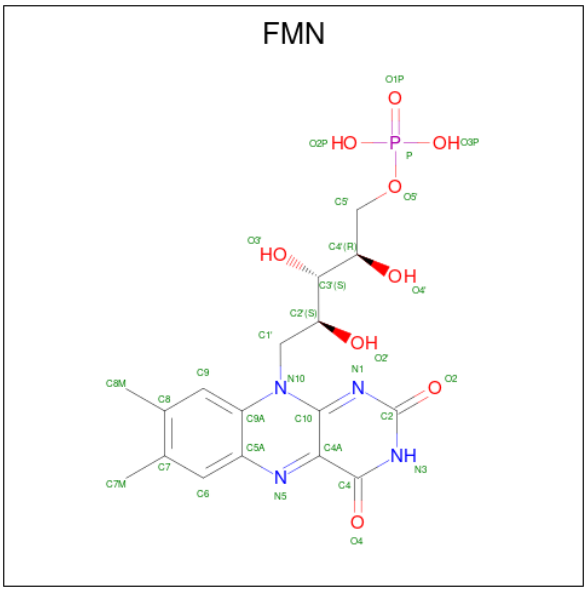
Mol	Chain	Residues	Atoms					AltConf	Trace
33	z	499	Total	C	N	O	S	0	0
			3992	2527	700	754	11		

- Molecule 34 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



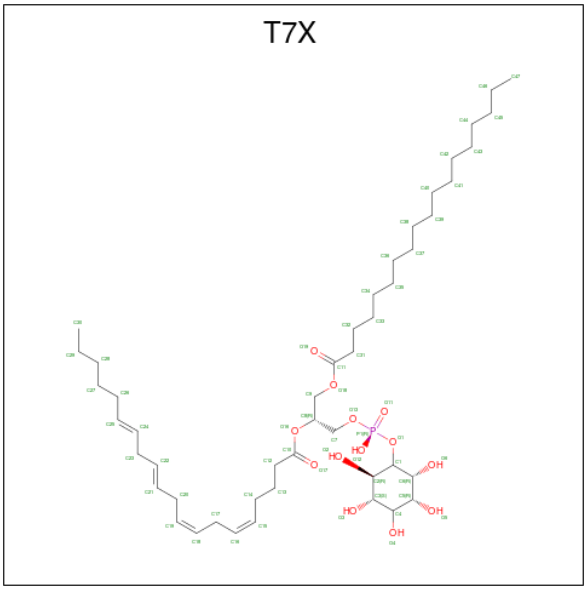
Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	Fe	S	0
			8	4	4	
34	C	1	Total	Fe	S	0
			8	4	4	
34	C	1	Total	Fe	S	0
			8	4	4	
34	E	1	Total	Fe	S	0
			8	4	4	
34	D	1	Total	Fe	S	0
			8	4	4	
34	D	1	Total	Fe	S	0
			8	4	4	

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



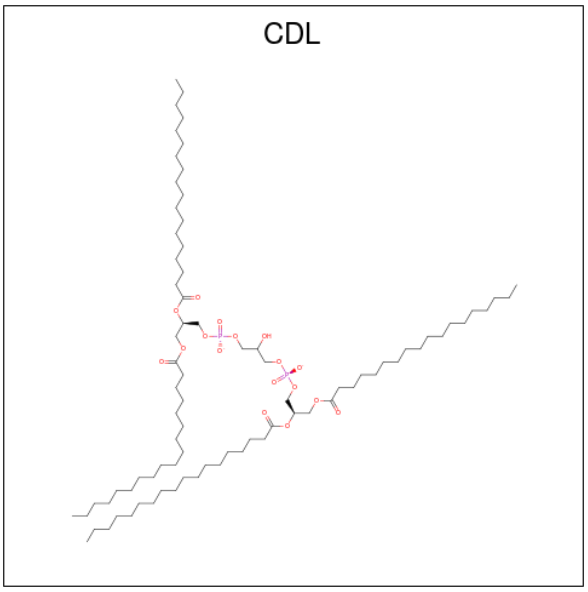
Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

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



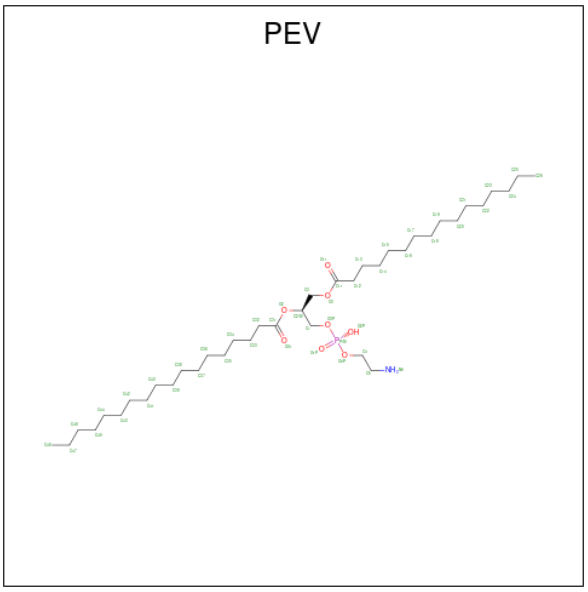
Mol	Chain	Residues	Atoms				AltConf
36	I	1	Total	C	O	P	0
			42	28	13	1	
36	c	1	Total	C	O	P	0
			37	23	13	1	

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



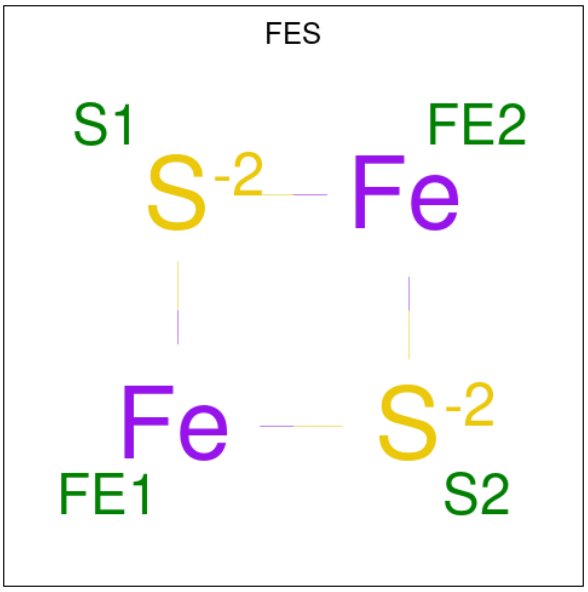
Mol	Chain	Residues	Atoms				AltConf
37	i	1	Total	C	O	P	0
			90	71	17	2	

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



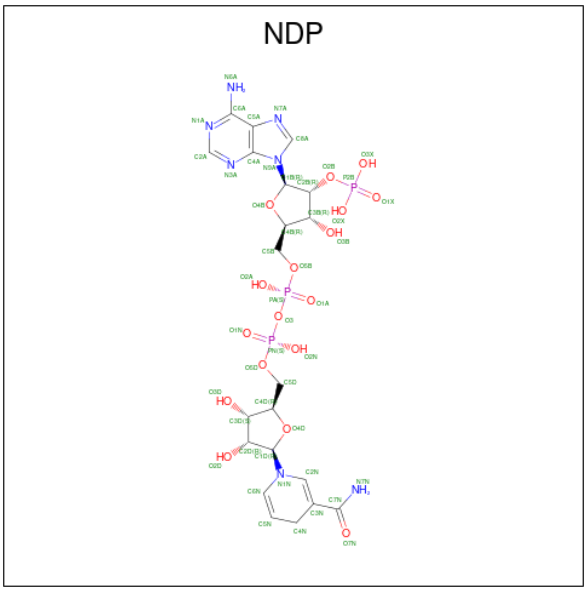
Mol	Chain	Residues	Atoms					AltConf
38	G	1	Total	C	N	O	P	0
			28	18	1	8	1	

- Molecule 39 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

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

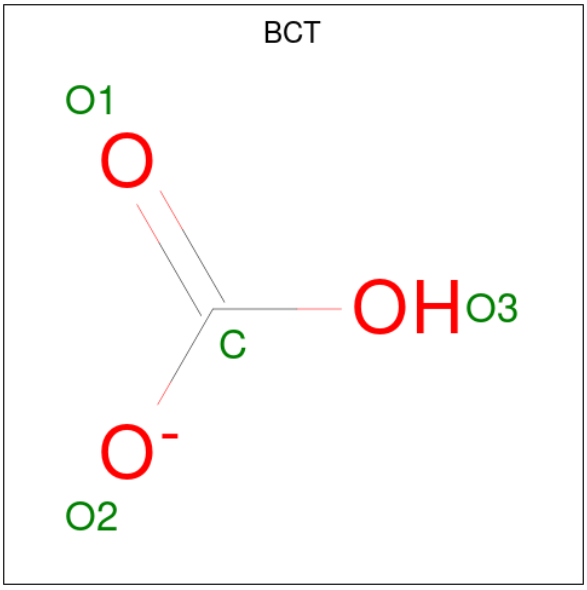


Mol	Chain	Residues	Atoms					AltConf
40	T	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 41 is ZINC ION (CCD ID: 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 (CCD ID: BCT) (formula: CHO_3).



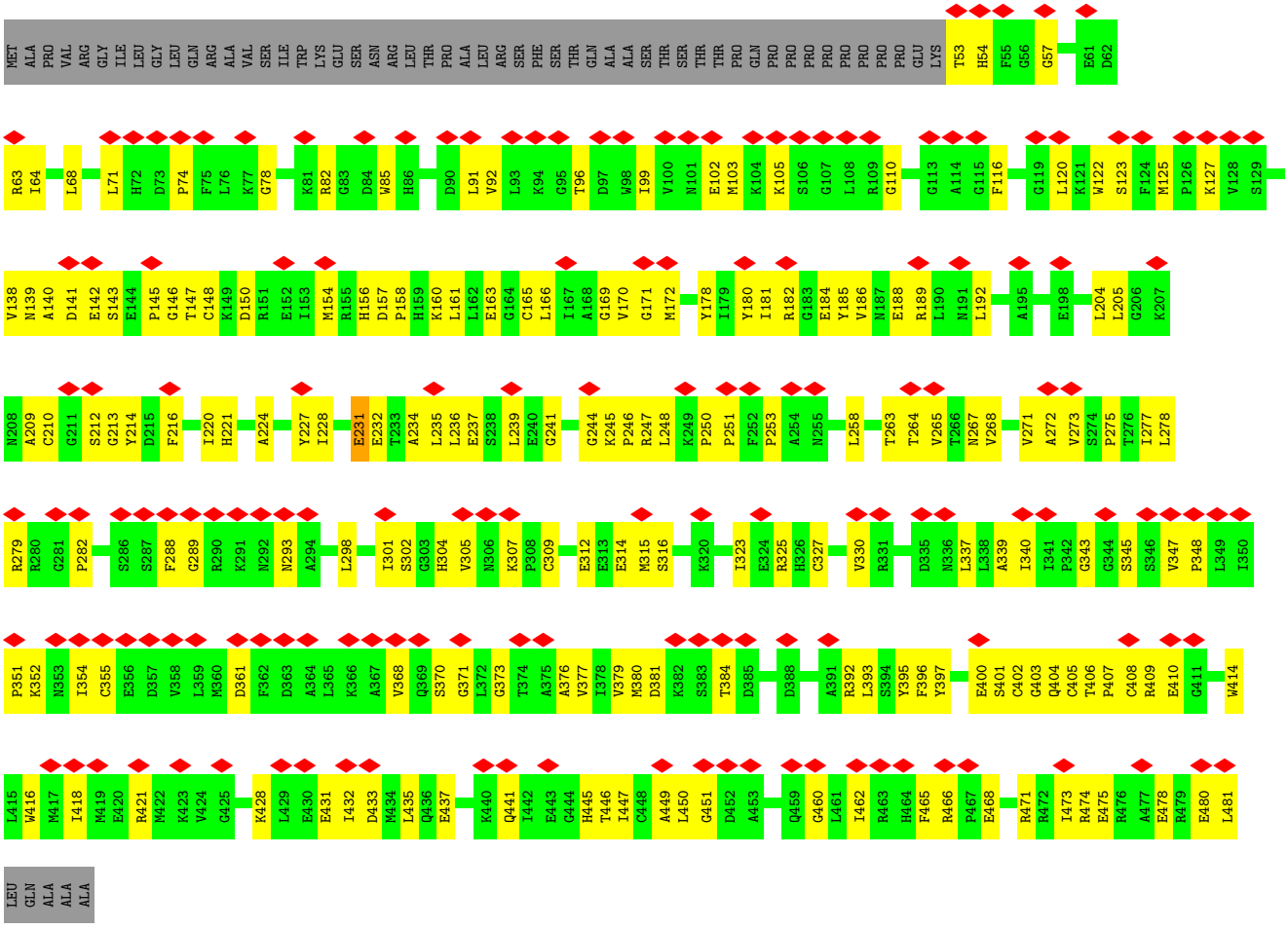
Mol	Chain	Residues	Atoms	AltConf
42	q	1	Total C O 4 1 3	0

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.

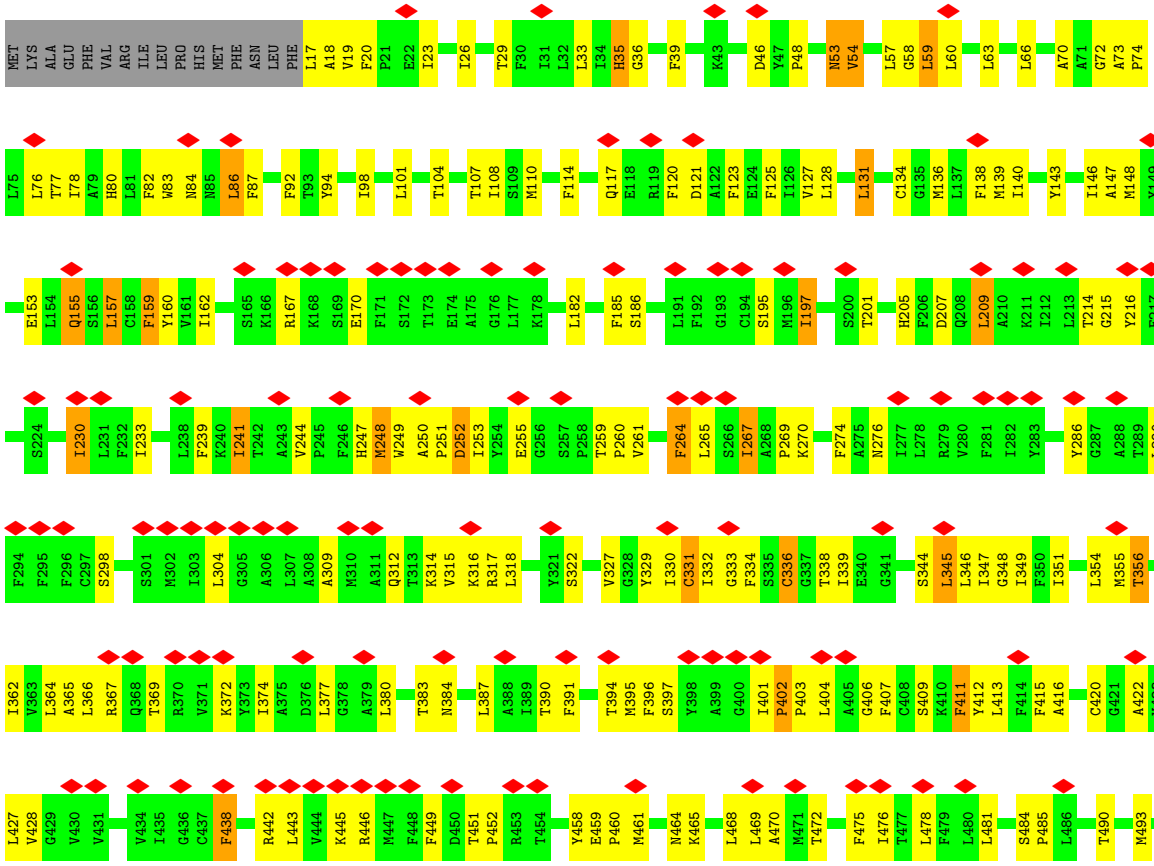
• Molecule 1: 51kDa

Chain A:



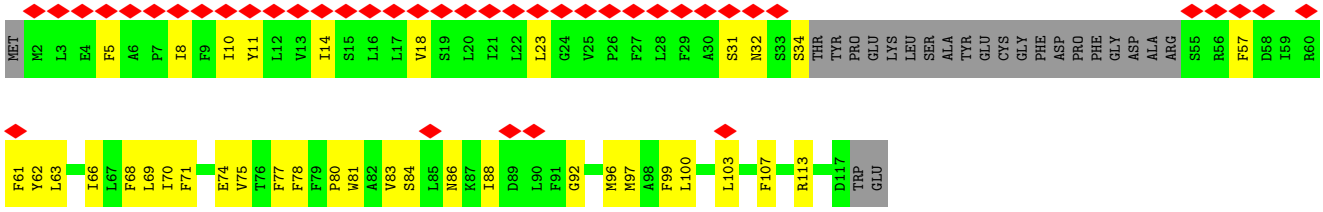
• Molecule 2: Nad2m

Chain I:



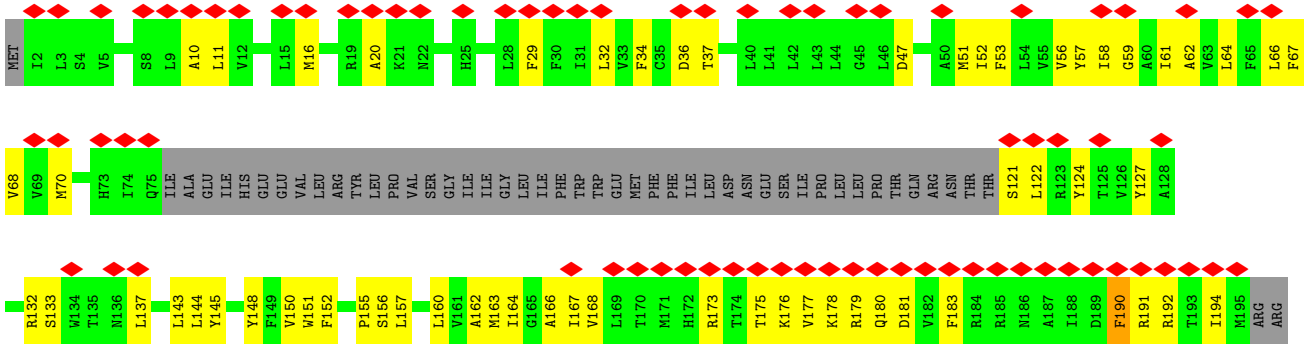
• Molecule 3: Nad3m

Chain J:



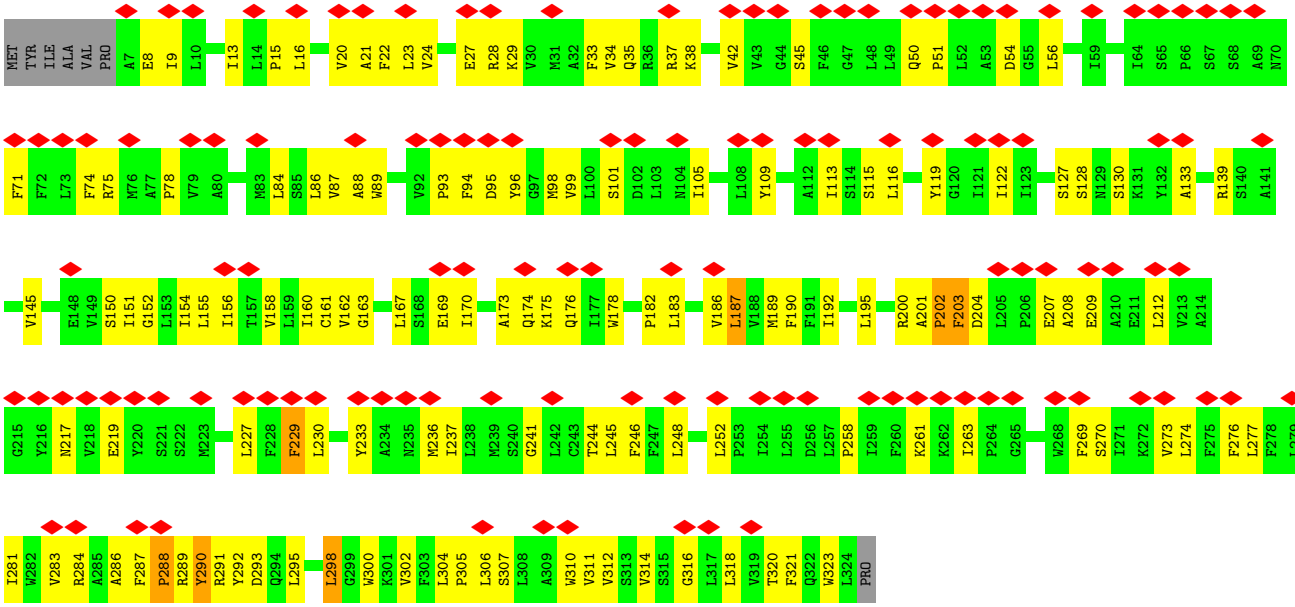
• Molecule 4: Nad6m

Chain N:



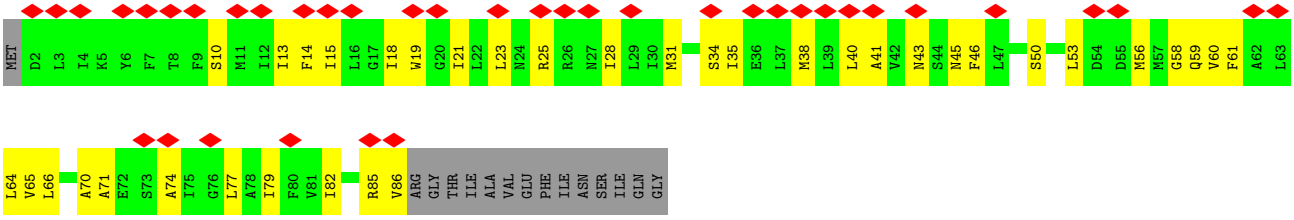
- Molecule 5: Nad1m

Chain H:



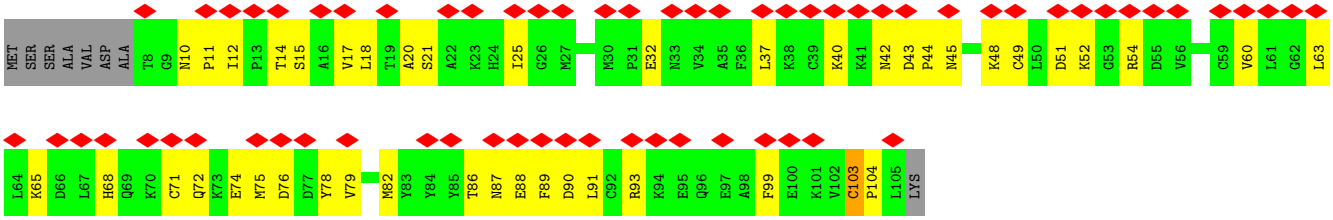
- Molecule 6: Nad4Lm

Chain K:



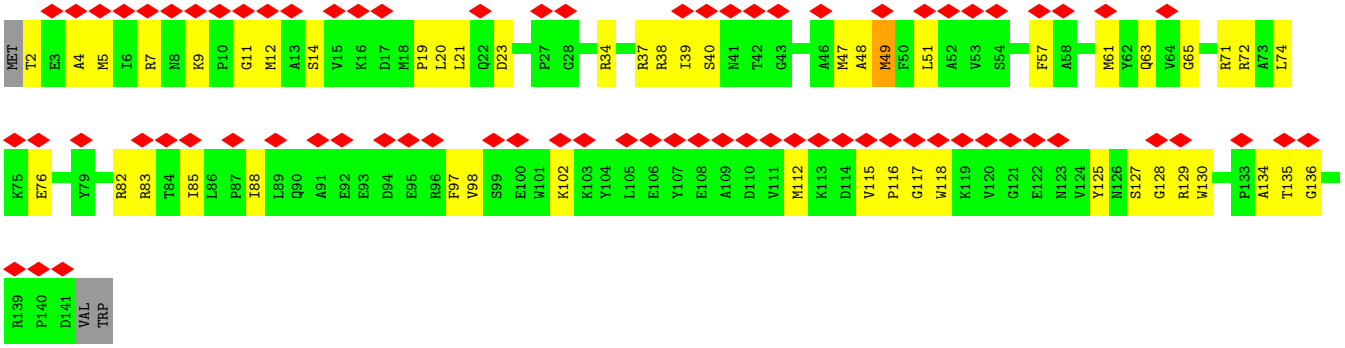
- Molecule 7: PGIV

Chain Y:



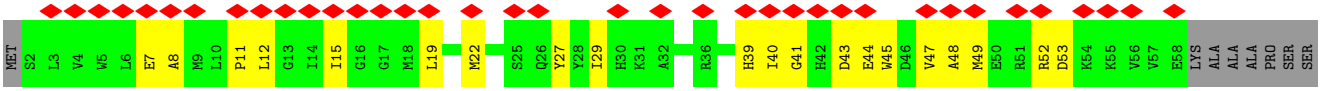
- Molecule 8: B16.6

Chain Z:



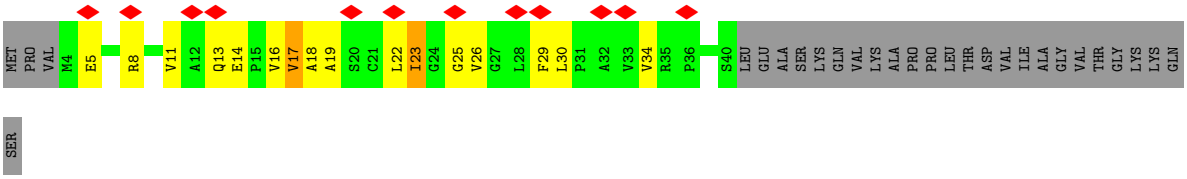
• Molecule 9: MWFE

Chain V:



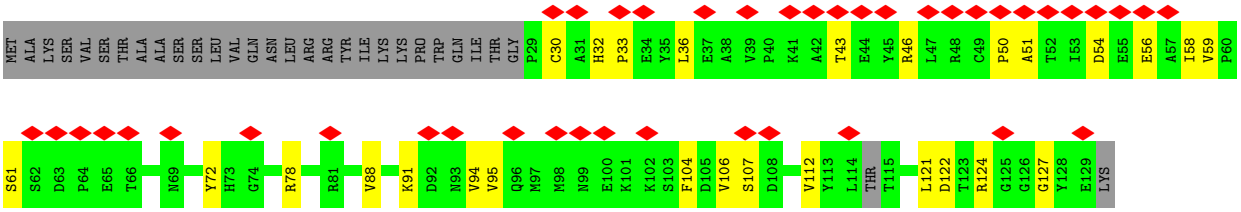
• Molecule 10: B9

Chain W:



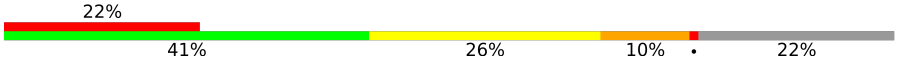
• Molecule 11: B14.5a

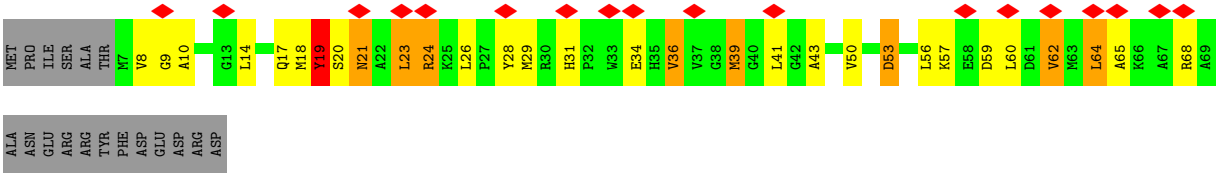
Chain S:



• Molecule 12: B14.5b

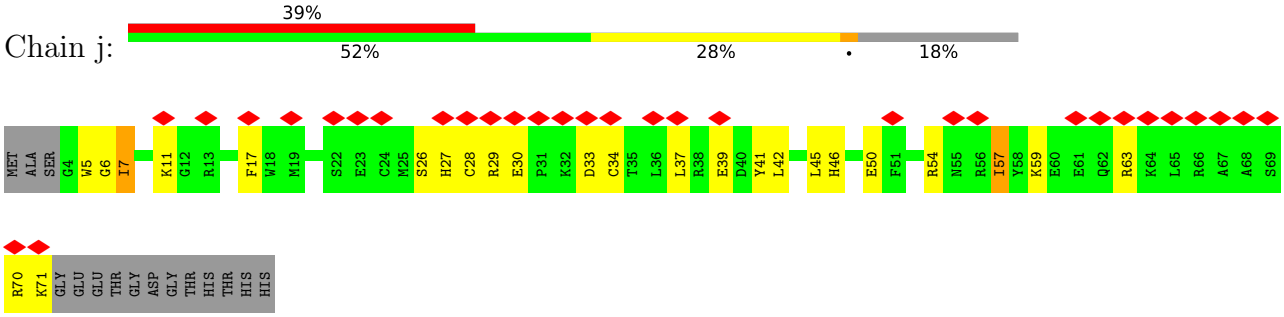
Chain i:





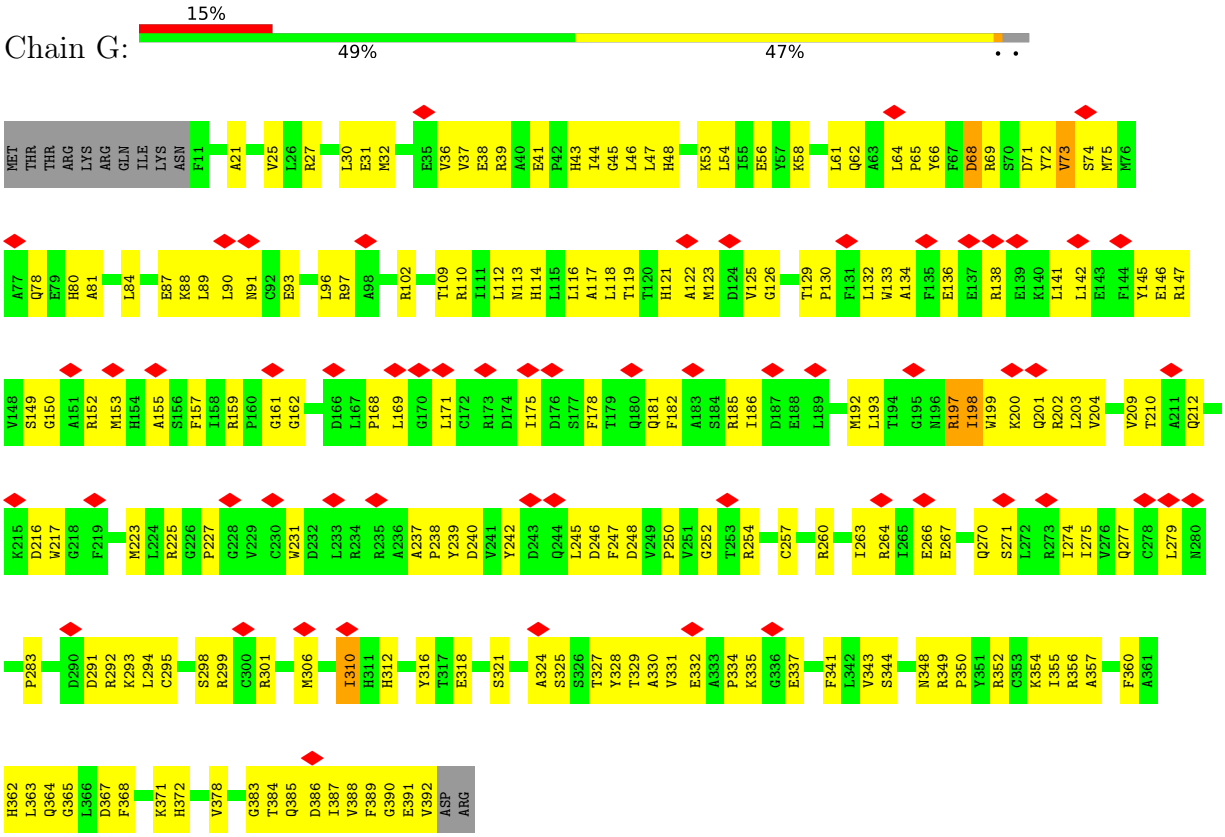
• Molecule 13: 15kDa

Chain j:



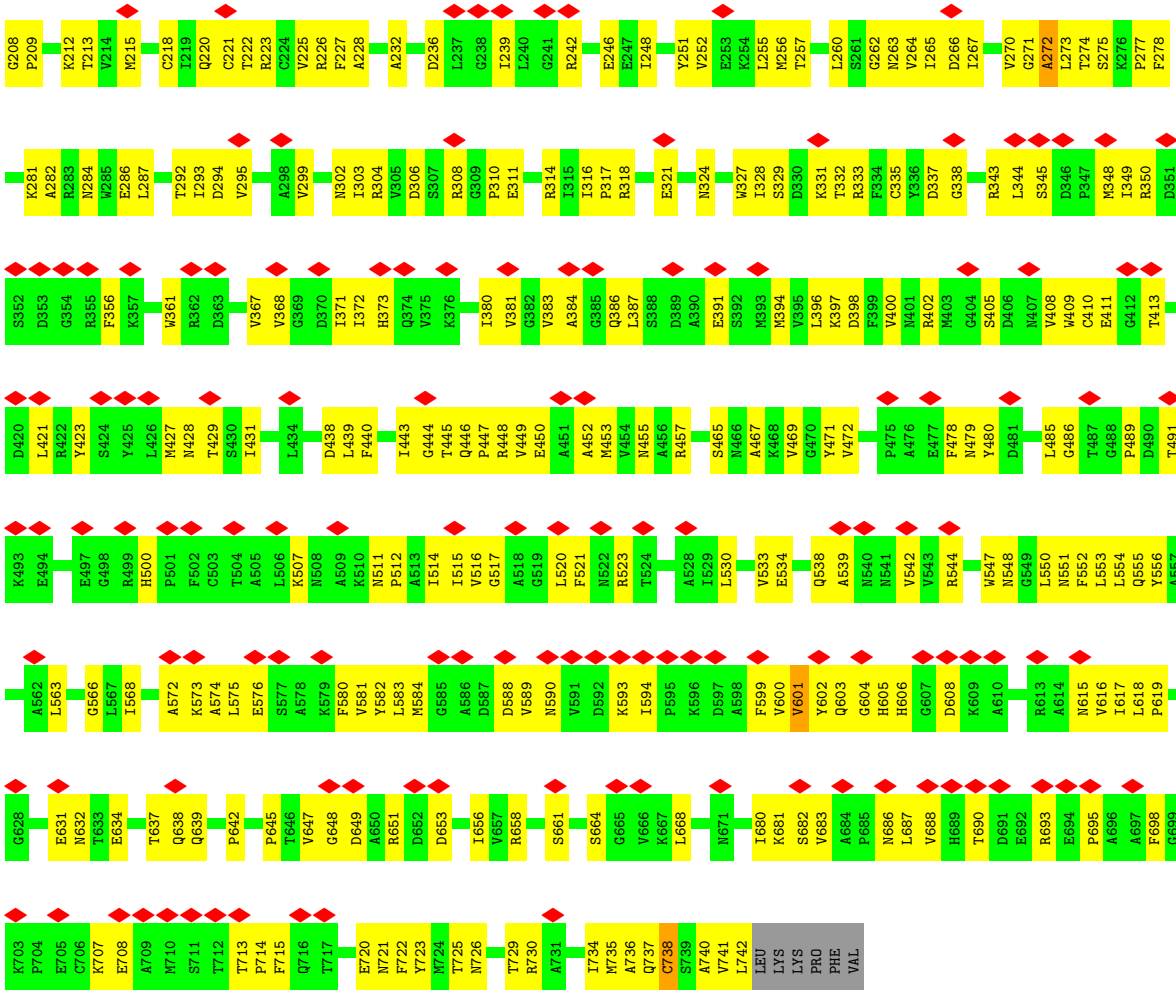
• Molecule 14: Nad7m

Chain G:



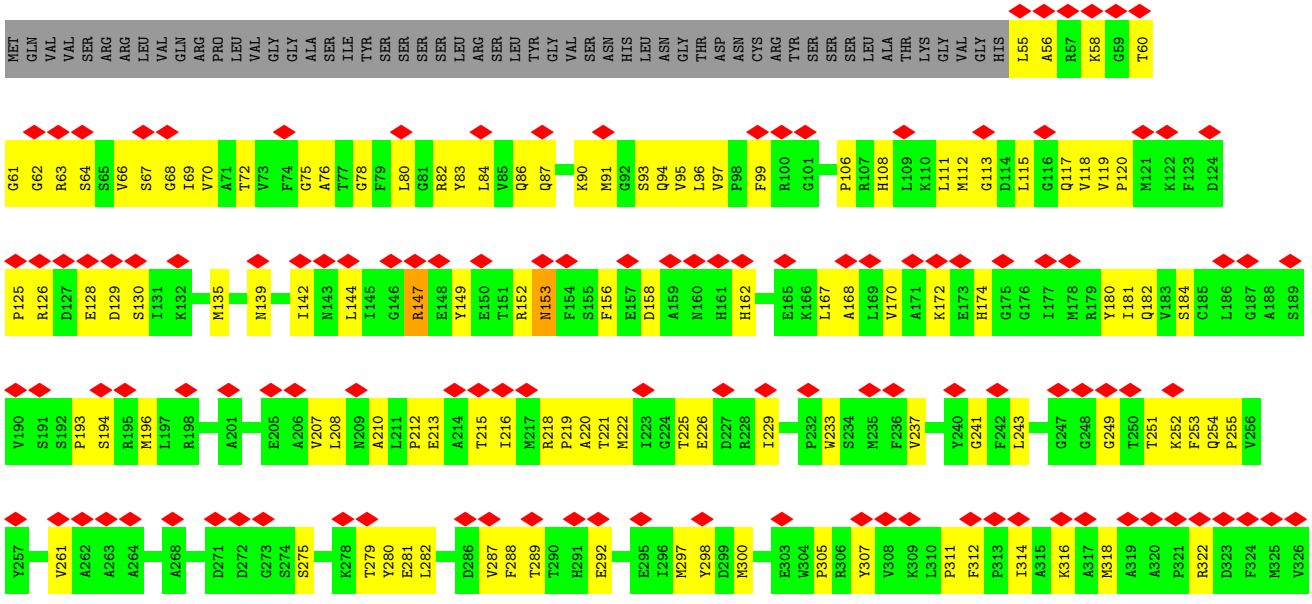
• Molecule 15: 75kDa

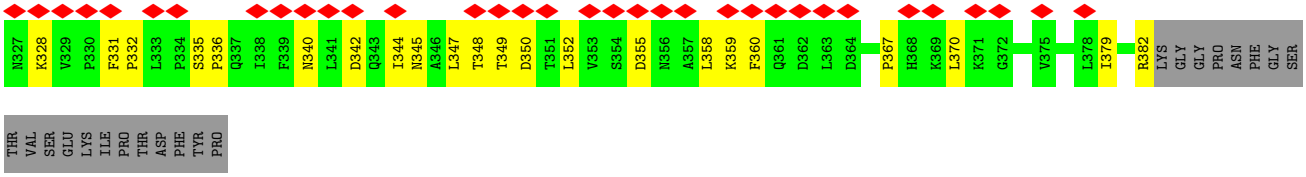
Chain C:



• Molecule 16: 39kDa

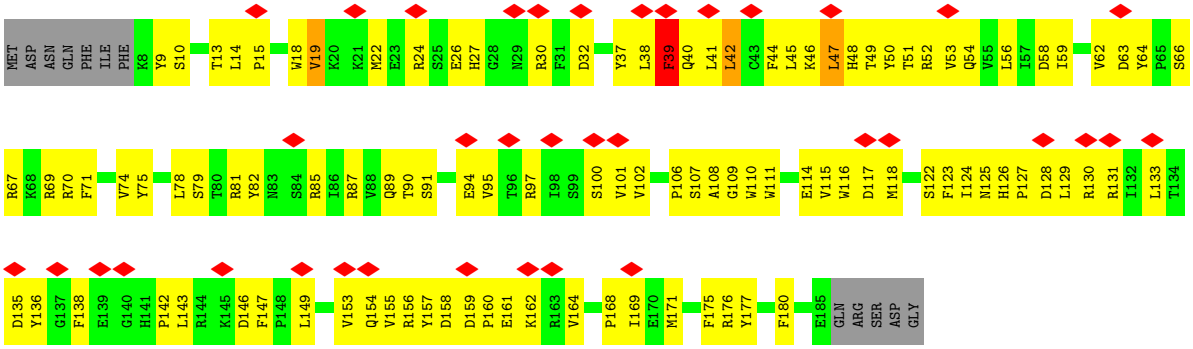
Chain T:





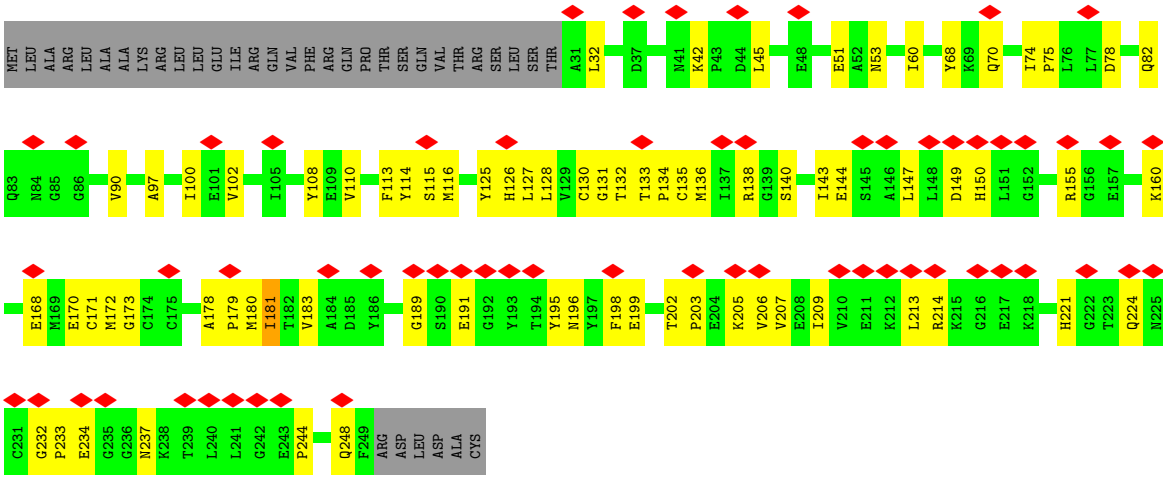
• Molecule 17: Nad9m

Chain F:



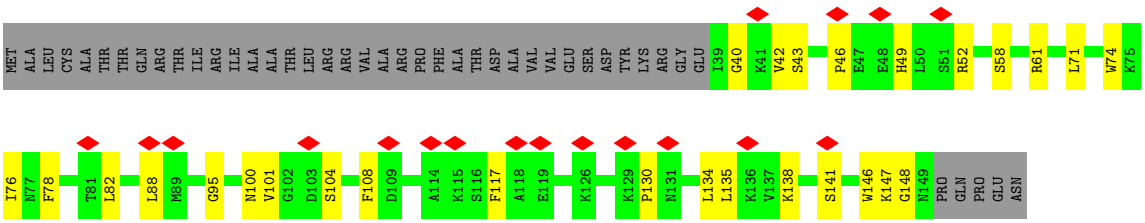
• Molecule 18: 24kDa

Chain B:



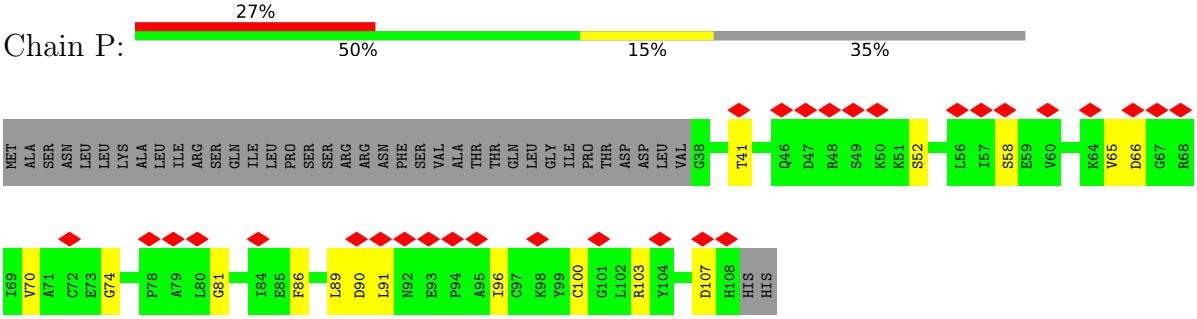
• Molecule 19: 18kDa

Chain O:



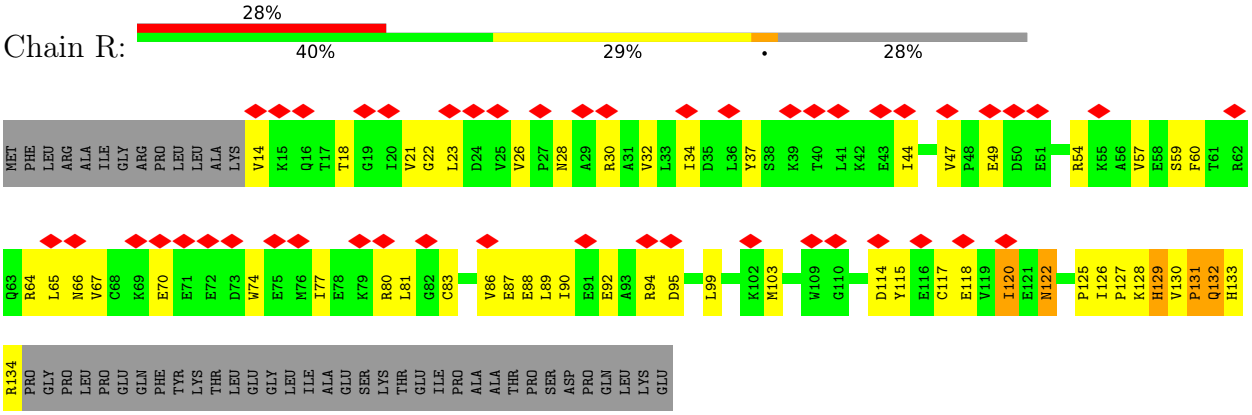
• Molecule 20: 13kDa

Chain P:



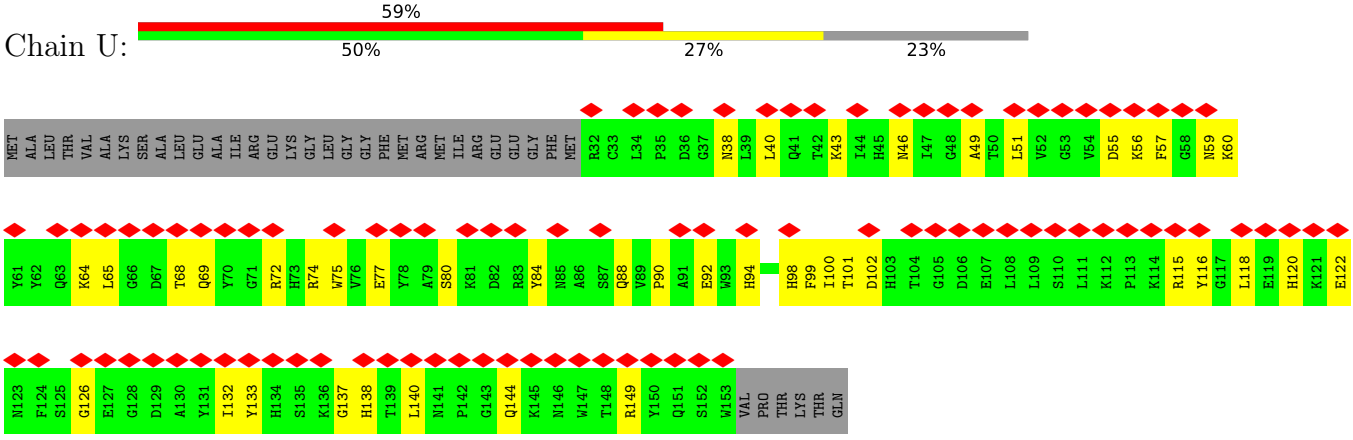
• Molecule 21: B13

Chain R:



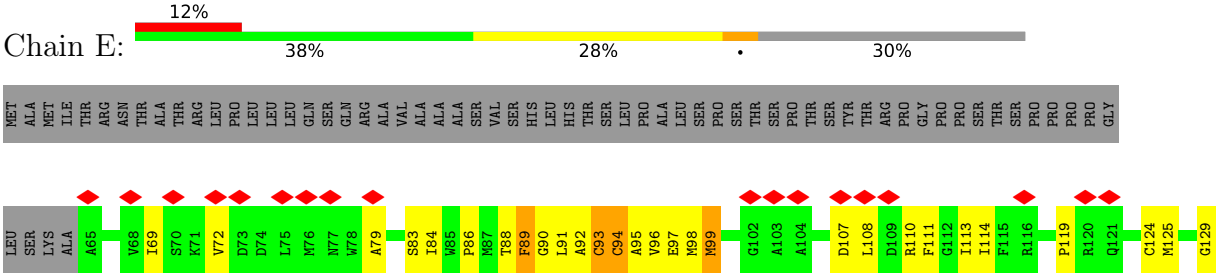
• Molecule 22: B17.2

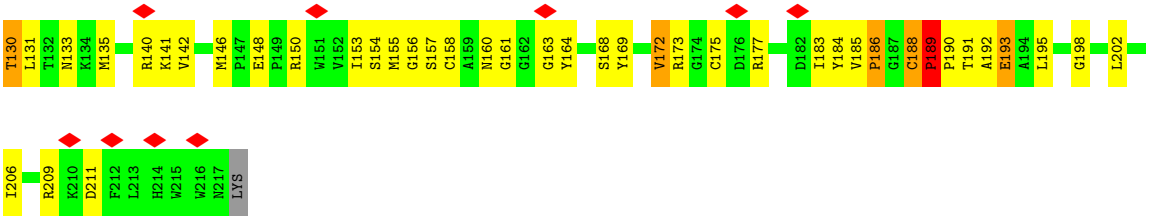
Chain U:



• Molecule 23: PSST

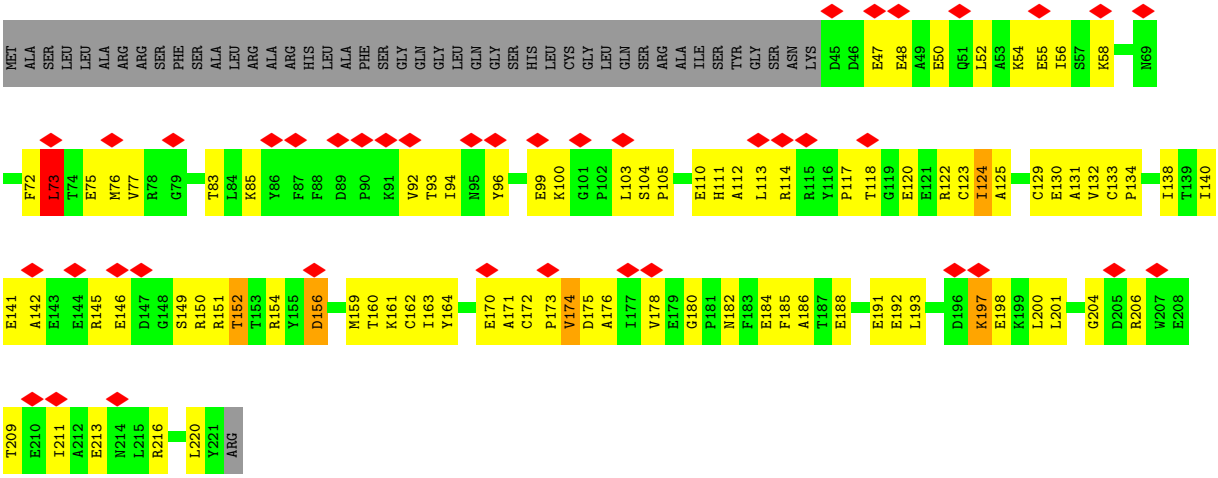
Chain E:





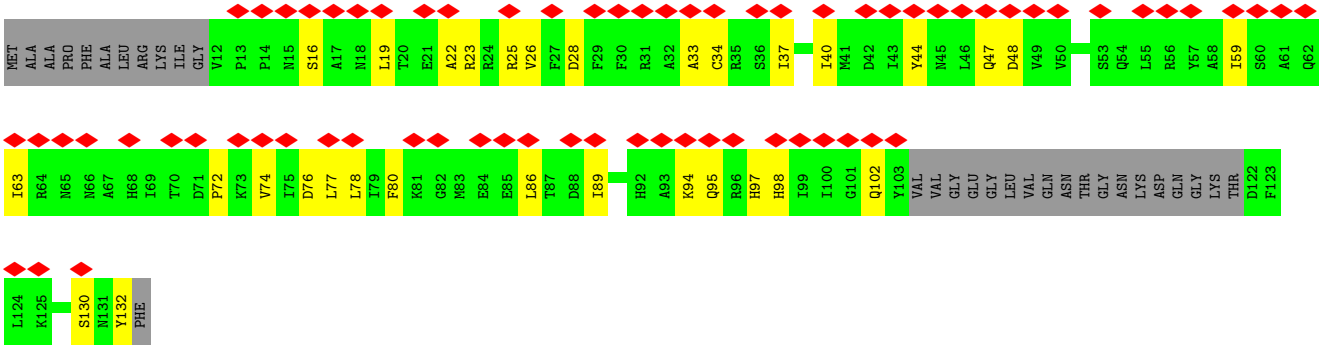
• Molecule 24: TYKY

Chain D:



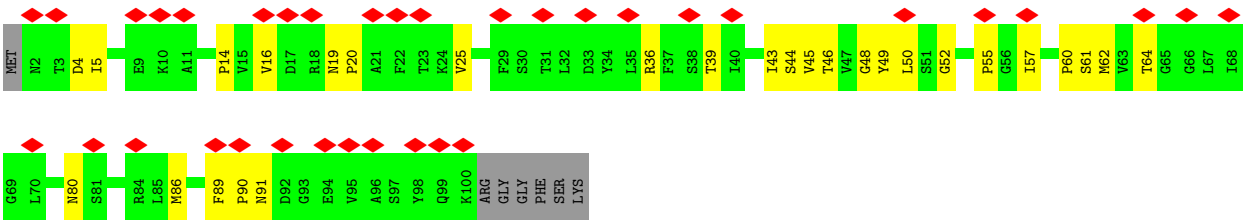
• Molecule 25: B14

Chain X:



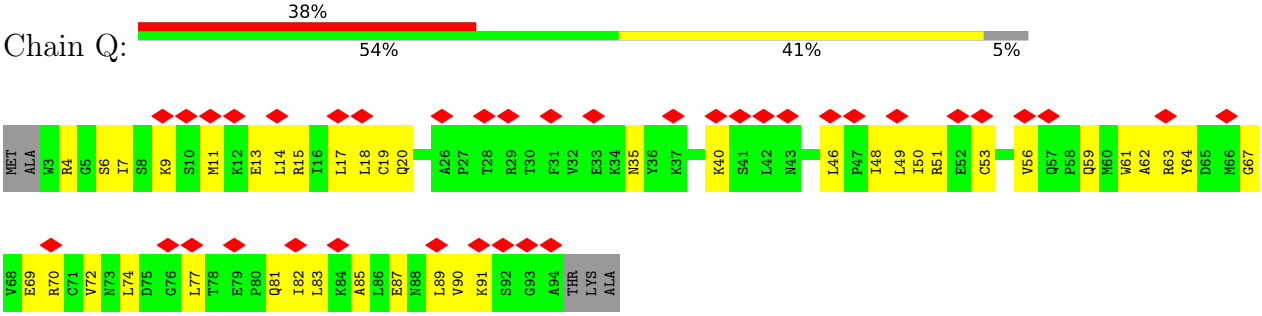
• Molecule 26: MNLL

Chain c:



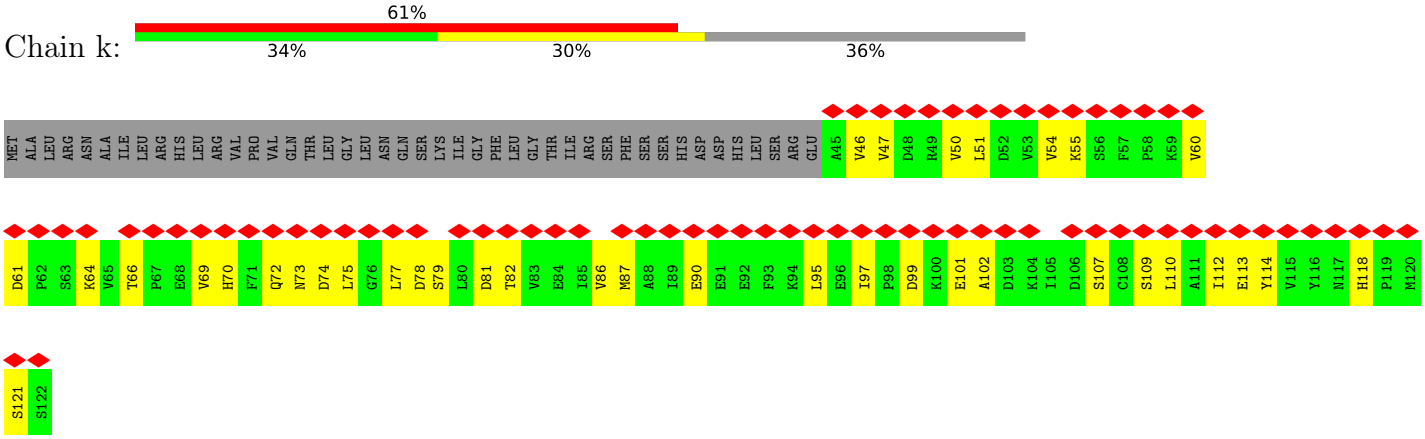
• Molecule 27: B8

Chain Q:



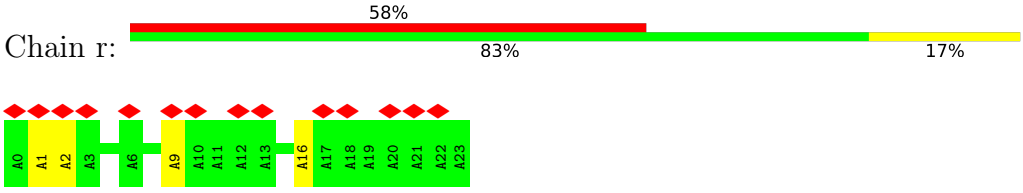
• Molecule 28: ACPM1

Chain k:



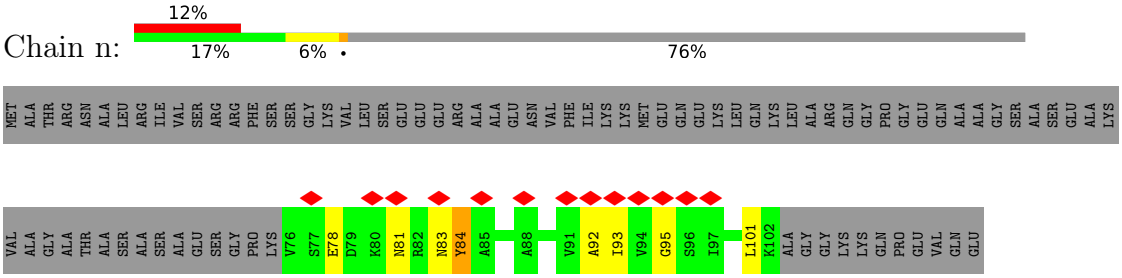
• Molecule 29: Unk1

Chain r:



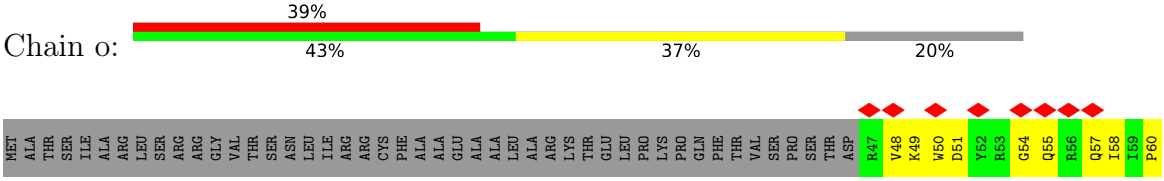
• Molecule 30: P2

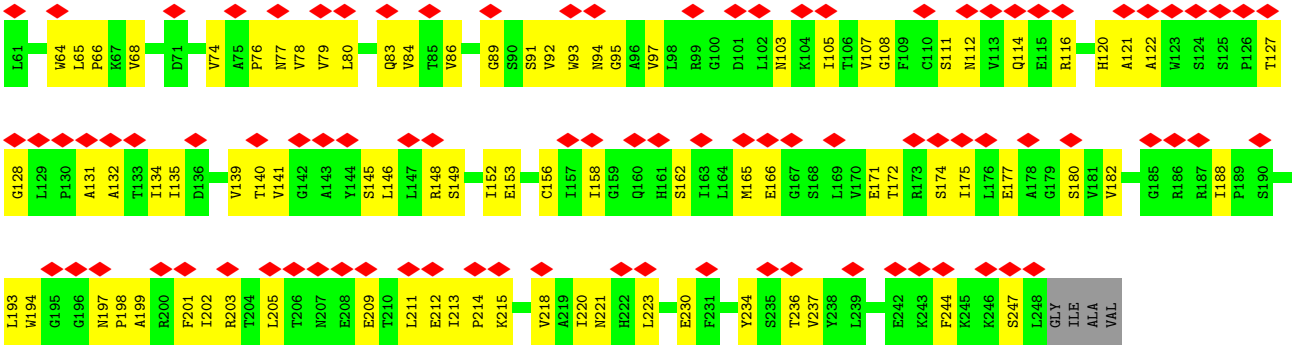
Chain n:



• Molecule 31: CAL1

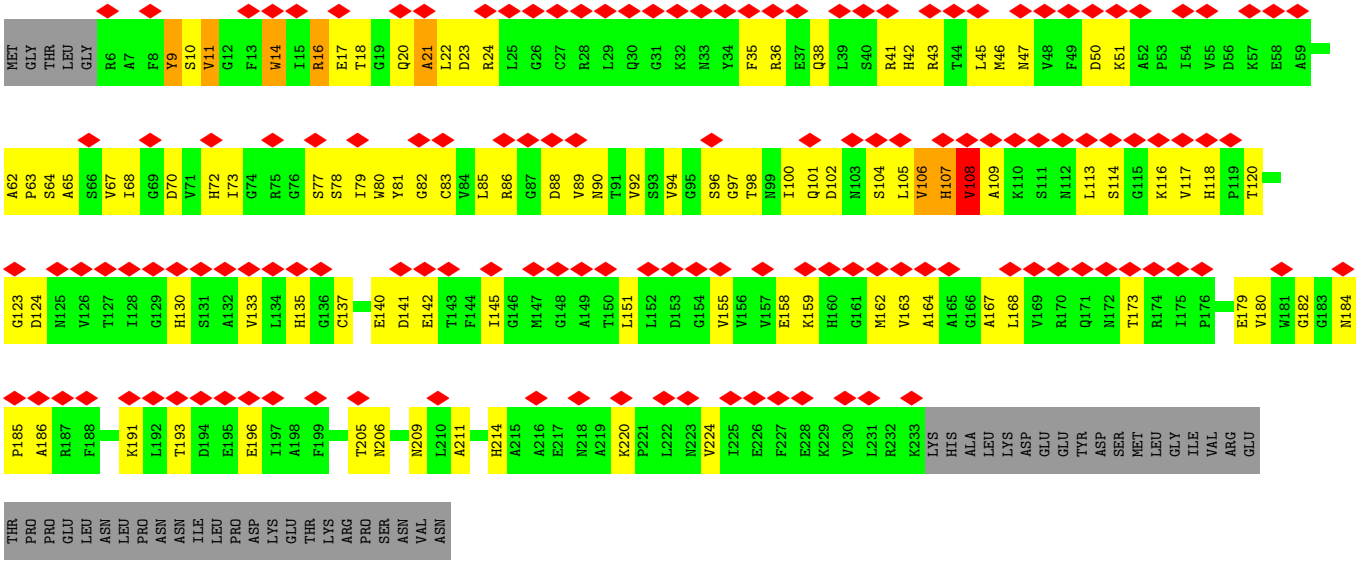
Chain o:





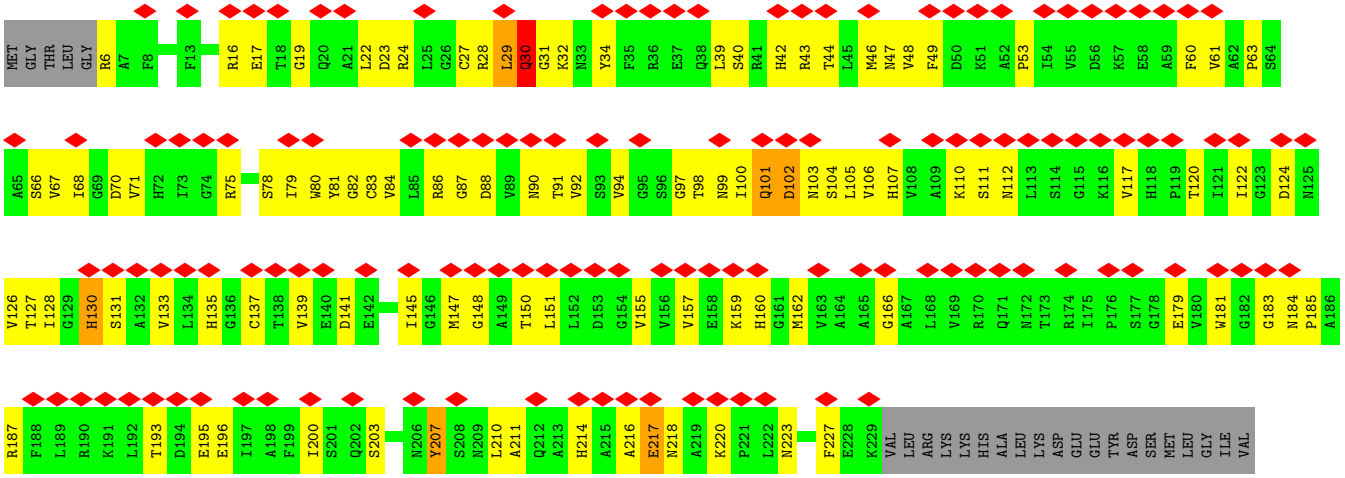
• Molecule 32: CA1

Chain q:



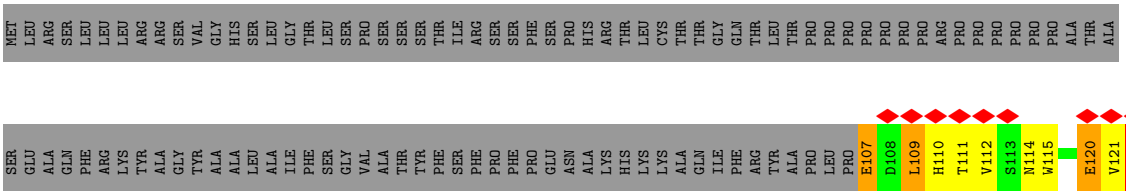
• Molecule 32: CA1

Chain p:



• Molecule 33: GLDH

Chain z:



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

5.1 Standard geometry

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

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	0.40	0/3401	0.59	0/4588
2	I	0.89	0/3855	1.34	8/5234 (0.2%)
3	J	0.31	0/826	0.41	0/1120
4	N	0.41	0/1227	0.58	1/1664 (0.1%)
5	H	0.57	2/2565 (0.1%)	0.81	9/3492 (0.3%)
6	K	0.40	0/677	0.55	0/916
7	Y	0.45	0/788	0.63	0/1059
8	Z	0.38	0/1132	0.65	1/1530 (0.1%)
9	V	0.26	0/473	0.39	0/636
10	W	0.71	0/277	1.00	2/375 (0.5%)
11	S	0.25	0/840	0.47	0/1141
12	i	0.88	0/502	1.41	3/676 (0.4%)
13	j	0.87	0/595	1.27	0/791
14	G	0.52	0/3120	0.69	2/4221 (0.0%)
15	C	0.48	0/5386	0.69	5/7299 (0.1%)
16	T	0.44	0/2591	0.64	0/3509
17	F	0.47	0/1564	0.71	2/2120 (0.1%)
18	B	0.31	0/1743	0.48	0/2364
19	O	0.41	0/899	0.46	0/1215
20	P	0.46	0/567	0.64	0/768
21	R	0.50	0/995	0.82	4/1349 (0.3%)
22	U	0.40	0/1044	0.52	0/1413
23	E	0.67	1/1250 (0.1%)	0.97	4/1697 (0.2%)
24	D	0.70	0/1467	1.04	3/1981 (0.2%)
25	X	0.19	0/861	0.35	0/1166
26	c	0.48	1/760 (0.1%)	0.61	0/1028
27	Q	0.23	0/734	0.37	0/989
28	k	0.13	0/625	0.33	0/848
29	r	0.16	0/119	0.31	0/165
30	n	0.95	0/208	1.32	0/282
31	o	0.25	0/1606	0.46	0/2192
32	p	0.44	0/1737	0.75	4/2353 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	q	0.35	0/1768	0.70	4/2395 (0.2%)
33	z	0.98	0/4078	1.20	2/5520 (0.0%)
All	All	0.57	4/50280 (0.0%)	0.81	54/68096 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
32	q	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	E	186	PRO	N-CD	-10.09	1.33	1.47
5	H	288	PRO	C-O	-6.28	1.16	1.23
26	c	44	SER	CA-CB	-5.83	1.44	1.53
5	H	307	SER	CA-CB	-5.06	1.45	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	202	PRO	N-CA-C	-11.73	98.59	113.84
23	E	189	PRO	N-CA-C	-10.56	97.81	110.70
2	I	53	ASN	N-CA-C	-9.88	100.78	113.12
32	q	9	TYR	N-CA-C	-9.18	102.09	113.38
5	H	229	PHE	CB-CA-C	8.60	125.46	110.85

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)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3328	0	3314	166	0
2	I	3754	0	3862	245	0
3	J	800	0	816	42	0
4	N	1201	0	1284	57	0
5	H	2493	0	2590	146	0
6	K	667	0	719	44	0
7	Y	774	0	767	37	0
8	Z	1103	0	1093	52	0
9	V	461	0	459	22	0
10	W	273	0	294	13	0
11	S	821	0	795	31	0
12	i	492	0	513	23	0
13	j	582	0	556	25	0
14	G	3049	0	3016	193	0
15	C	5288	0	5278	277	0
16	T	2535	0	2583	104	0
17	F	1518	0	1470	103	0
18	B	1702	0	1685	65	0
19	O	874	0	865	28	0
20	P	554	0	544	12	0
21	R	977	0	960	59	0
22	U	1011	0	952	42	0
23	E	1215	0	1195	87	0
24	D	1438	0	1368	97	0
25	X	843	0	834	24	0
26	c	744	0	742	35	0
27	Q	722	0	752	28	0
28	k	614	0	603	30	0
29	r	120	0	122	4	0
30	n	205	0	209	8	0
31	o	1568	0	1579	83	0
32	p	1705	0	1688	101	0
32	q	1736	0	1723	121	0
33	z	3992	0	3996	208	0
34	A	8	0	0	3	0
34	C	16	0	0	1	0
34	D	16	0	0	3	0
34	E	8	0	0	6	0
35	A	31	0	19	3	0
36	I	42	0	0	2	0
36	c	37	0	0	0	0
37	i	90	0	130	34	0
38	G	28	0	29	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	B	4	0	0	2	0
39	C	4	0	0	0	0
40	T	48	0	26	4	0
41	P	1	0	0	0	0
41	q	1	0	0	0	0
42	q	4	0	1	1	0
All	All	49497	0	49431	2258	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

The worst 5 of 2258 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:461:MET:CE	2:I:465:LYS:HE3	1.34	1.55
33:z:122:GLN:CD	33:z:172:ALA:HB1	1.25	1.54
33:z:129:PRO:CB	33:z:170:ASN:HB2	1.04	1.51
33:z:129:PRO:CA	33:z:170:ASN:HB2	1.40	1.47
33:z:129:PRO:HB3	33:z:170:ASN:CB	1.48	1.43

There are no symmetry-related clashes.

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%)	43 73
3	J	92/119 (77%)	86 (94%)	6 (6%)	0	100 100
4	N	145/205 (71%)	125 (86%)	19 (13%)	1 (1%)	18 51
5	H	316/325 (97%)	284 (90%)	32 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	K	83/100 (83%)	81 (98%)	2 (2%)	0	100	100
7	Y	96/106 (91%)	88 (92%)	7 (7%)	1 (1%)	12	43
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%)	7	35
13	j	66/83 (80%)	63 (96%)	2 (3%)	1 (2%)	8	36
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	48
22	U	120/159 (76%)	98 (82%)	22 (18%)	0	100	100
23	E	151/218 (69%)	134 (89%)	16 (11%)	1 (1%)	18	51
24	D	175/222 (79%)	159 (91%)	14 (8%)	2 (1%)	11	41
25	X	99/133 (74%)	92 (93%)	7 (7%)	0	100	100
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	20
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%)	9	38
33	z	495/610 (81%)	476 (96%)	15 (3%)	4 (1%)	16	48
All	All	6177/7436 (83%)	5565 (90%)	591 (10%)	21 (0%)	37	67

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%)	86 84
2	I	399/416 (96%)	365 (92%)	34 (8%)	10 33
3	J	87/106 (82%)	87 (100%)	0	100 100
4	N	133/186 (72%)	132 (99%)	1 (1%)	73 76
5	H	266/272 (98%)	264 (99%)	2 (1%)	73 76
6	K	74/86 (86%)	74 (100%)	0	100 100
7	Y	88/94 (94%)	88 (100%)	0	100 100
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%)	29 (97%)	1 (3%)	33 56
11	S	92/118 (78%)	92 (100%)	0	100 100
12	i	50/66 (76%)	37 (74%)	13 (26%)	0 3
13	j	62/73 (85%)	57 (92%)	5 (8%)	11 35
14	G	328/340 (96%)	325 (99%)	3 (1%)	70 74
15	C	576/625 (92%)	570 (99%)	6 (1%)	68 74
16	T	271/334 (81%)	269 (99%)	2 (1%)	76 77
17	F	168/179 (94%)	163 (97%)	5 (3%)	36 57
18	B	188/220 (86%)	186 (99%)	2 (1%)	65 73
19	O	93/128 (73%)	93 (100%)	0	100 100
20	P	62/97 (64%)	62 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	R	108/148 (73%)	106 (98%)	2 (2%)	50 66
22	U	104/133 (78%)	104 (100%)	0	100 100
23	E	129/184 (70%)	121 (94%)	8 (6%)	16 42
24	D	157/191 (82%)	152 (97%)	5 (3%)	34 56
25	X	92/114 (81%)	92 (100%)	0	100 100
26	c	79/84 (94%)	78 (99%)	1 (1%)	61 71
27	Q	82/85 (96%)	81 (99%)	1 (1%)	63 72
28	k	73/112 (65%)	73 (100%)	0	100 100
30	n	21/84 (25%)	19 (90%)	2 (10%)	8 30
31	o	171/211 (81%)	171 (100%)	0	100 100
32	p	181/228 (79%)	177 (98%)	4 (2%)	45 63
32	q	184/228 (81%)	179 (97%)	5 (3%)	39 59
33	z	440/534 (82%)	404 (92%)	36 (8%)	10 35
All	All	5297/6293 (84%)	5158 (97%)	139 (3%)	41 60

5 of 139 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	z	249	THR
33	z	317	HIS
33	z	510	SER
12	i	53	ASP
12	i	50	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
18	B	118	ASN
33	z	241	GLN
22	U	138	HIS
33	z	218	GLN
32	q	209	ASN

5.3.3 RNA

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	C	802	15	0,12,12	-	-	-		
36	T7X	c	301	-	37,37,61	0.33	0	47,49,73	0.39	0
38	PEV	G	601	-	27,27,48	0.35	0	30,32,53	0.37	0
34	SF4	A	501	1	0,12,12	-	-	-		
35	FMN	A	502	-	33,33,33	0.62	0	48,50,50	0.72	1 (2%)
37	CDL	i	201	-	89,89,99	0.28	0	95,101,111	0.57	2 (2%)
34	SF4	D	301	24	0,12,12	-	-	-		
34	SF4	C	801	15	0,12,12	-	-	-		
40	NDP	T	501	-	49,52,52	0.49	0	66,80,80	0.69	1 (1%)
34	SF4	D	302	24	0,12,12	-	-	-		
36	T7X	I	501	-	42,42,61	0.31	0	52,54,73	0.50	0
39	FES	C	803	15	0,4,4	-	-	-		
39	FES	B	301	-	0,4,4	-	-	-		
34	SF4	E	301	23	0,12,12	-	-	-		
42	BCT	q	802	41	2,3,3	0.60	0	2,3,3	0.24	0

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

There are no bond length outliers.

All (4) 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
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.

11 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	G	601	PEV	6	0
34	A	501	SF4	3	0

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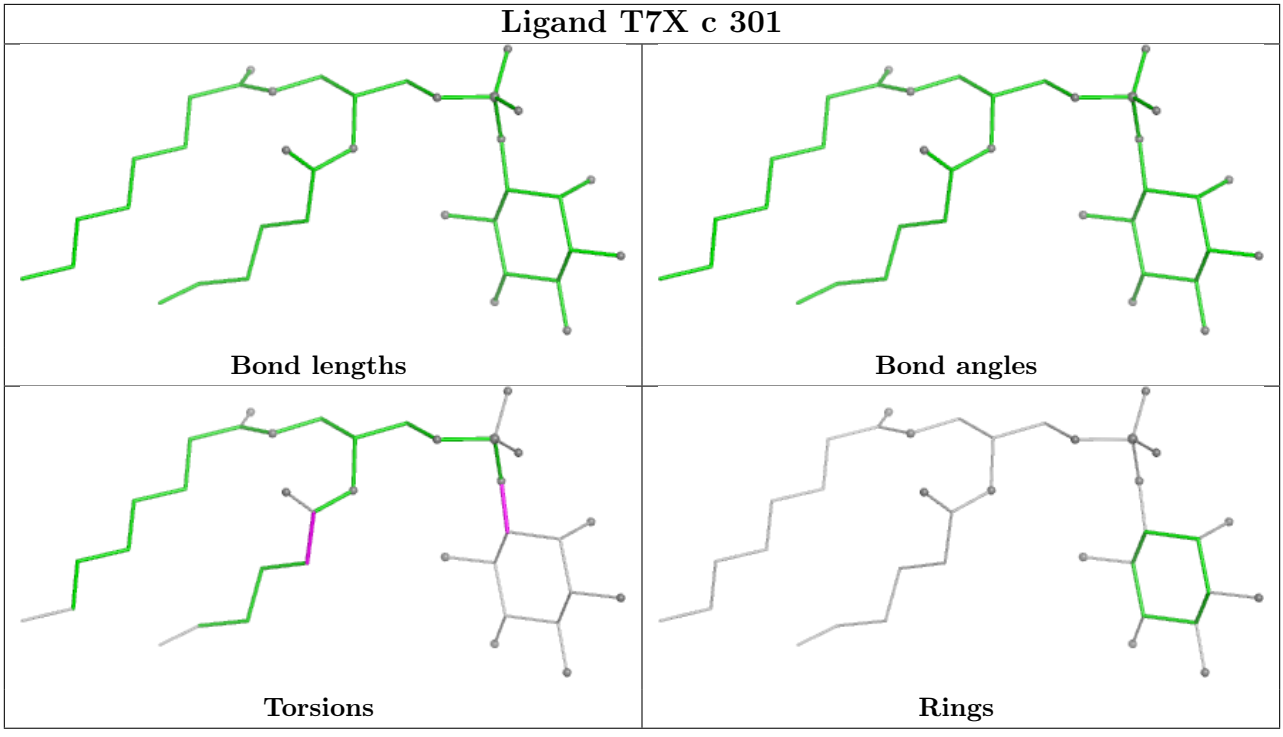
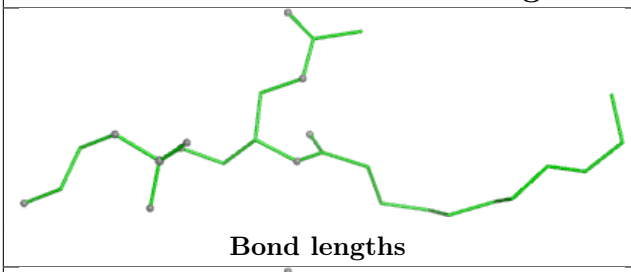
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	A	502	FMN	3	0
37	i	201	CDL	34	0
34	D	301	SF4	3	0
34	C	801	SF4	1	0
40	T	501	NDP	4	0
36	I	501	T7X	2	0
39	B	301	FES	2	0
34	E	301	SF4	6	0
42	q	802	BCT	1	0

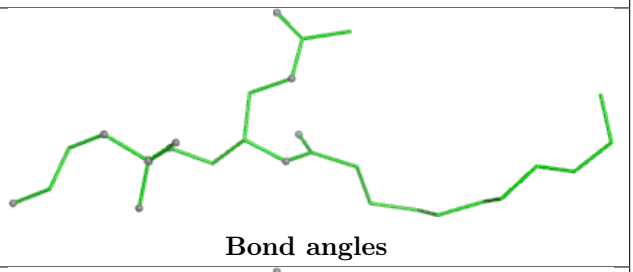
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



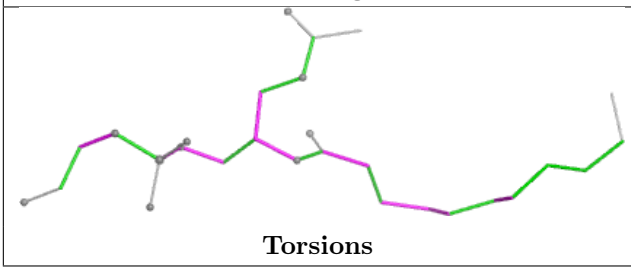
Ligand PEV G 601



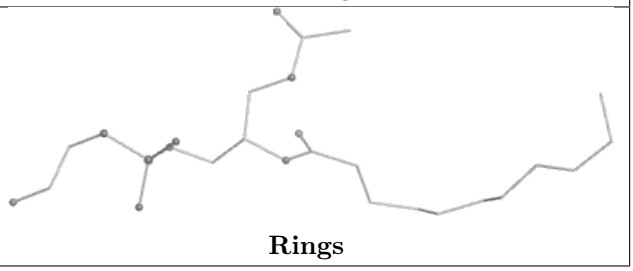
Bond lengths



Bond angles

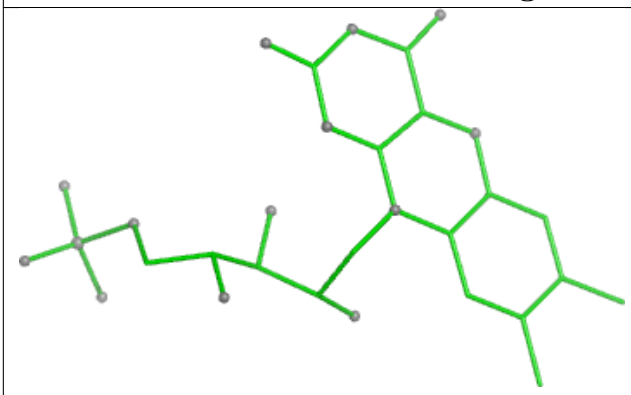


Torsions

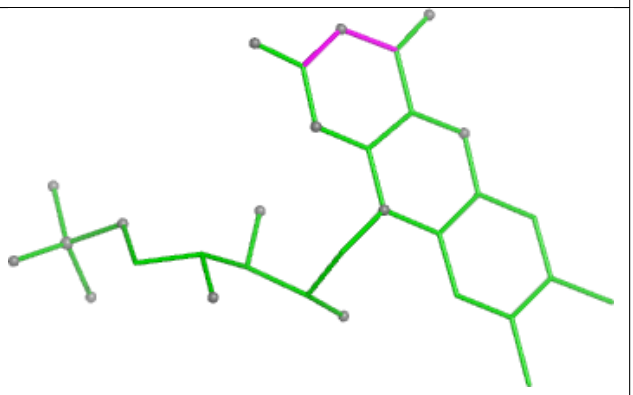


Rings

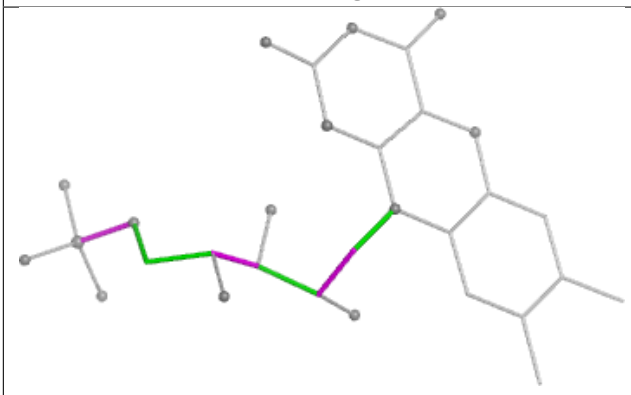
Ligand FMN A 502



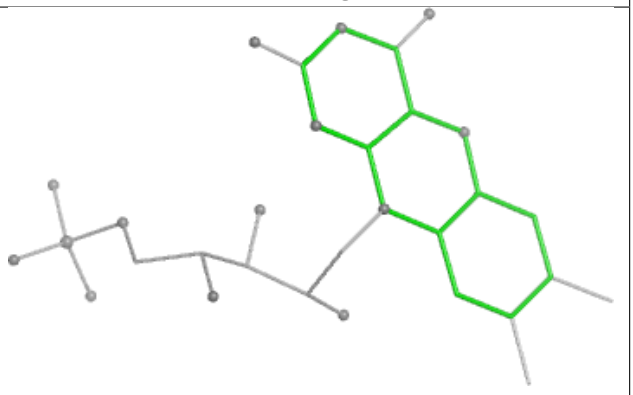
Bond lengths



Bond angles

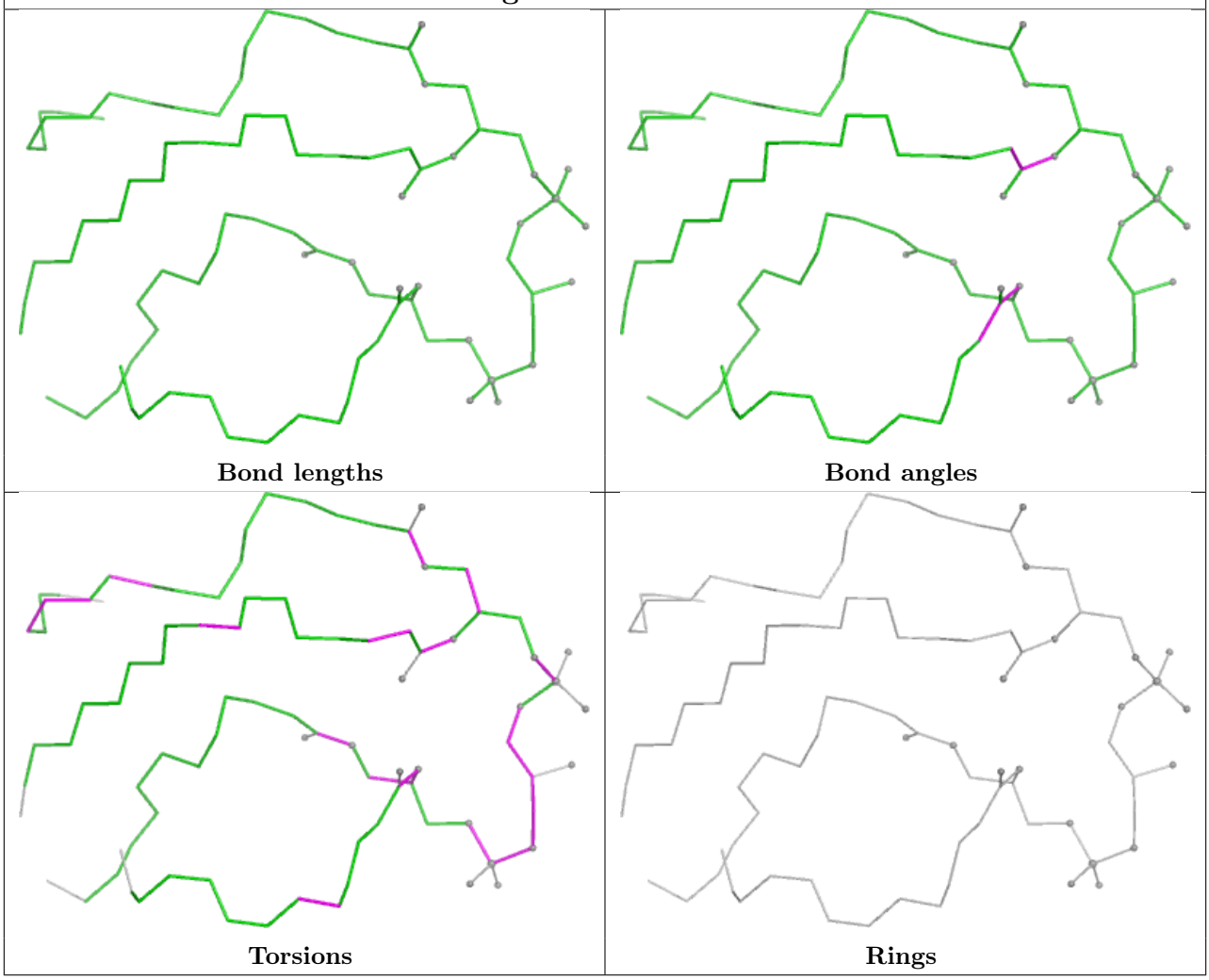


Torsions

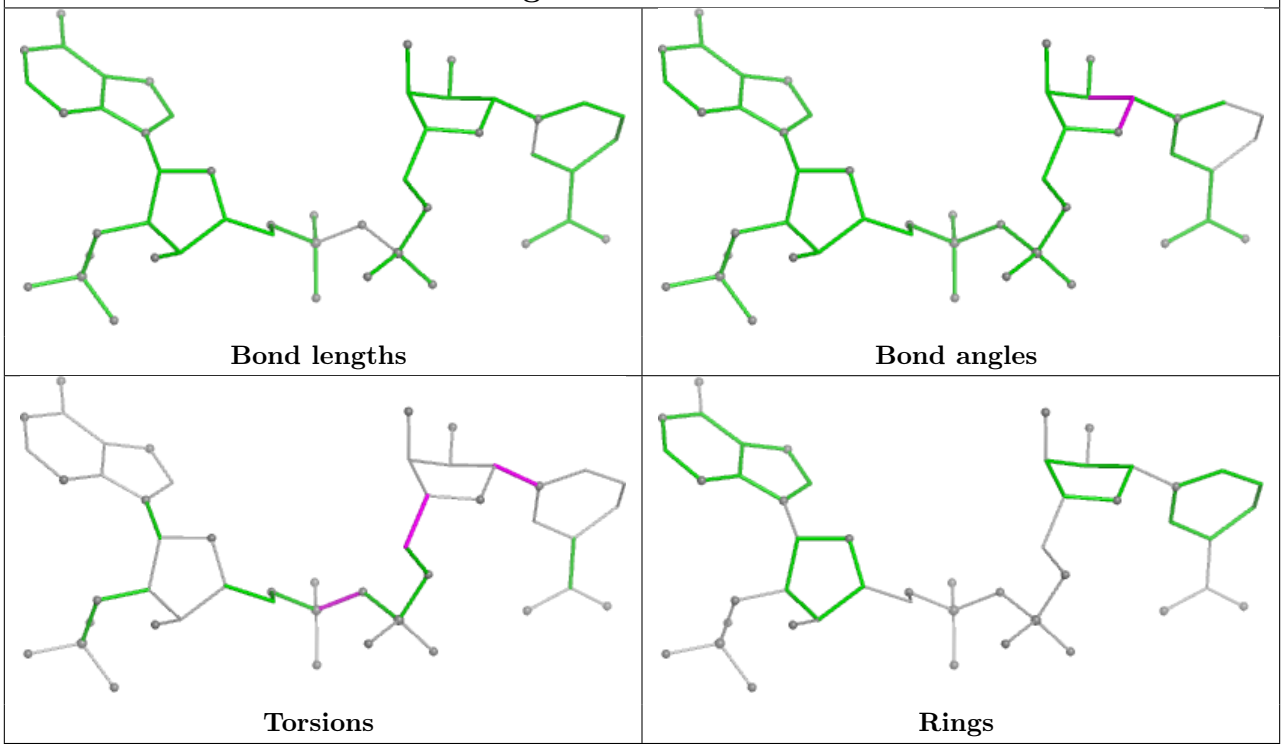


Rings

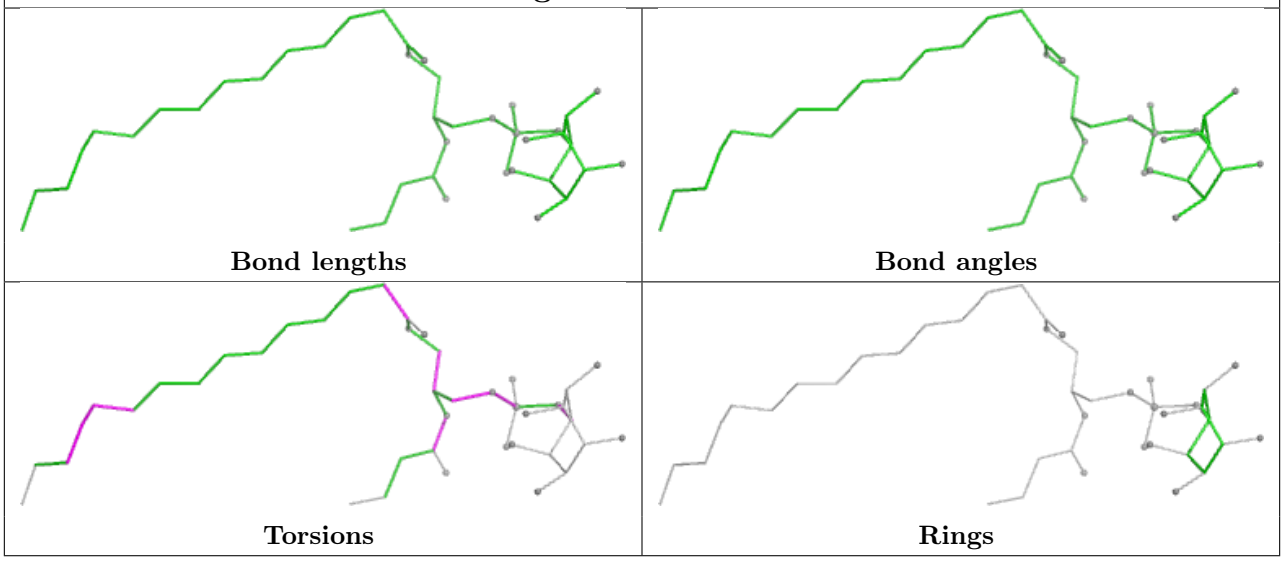
Ligand CDL i 201



Ligand NDP T 501



Ligand T7X I 501



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

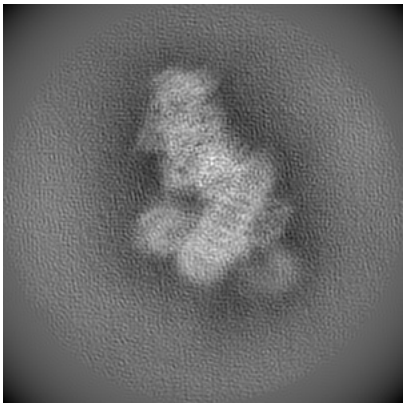
6 Map visualisation

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.

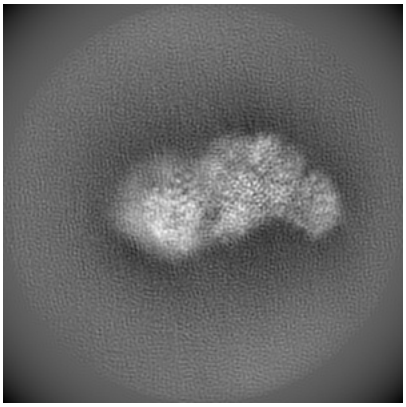
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

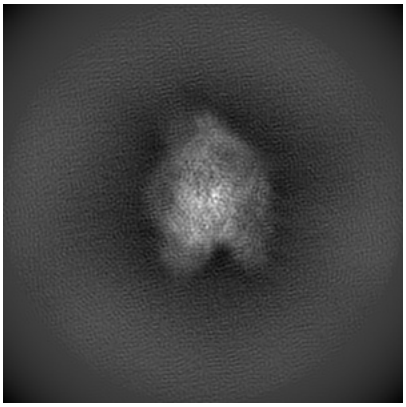
6.1.1 Primary map



X



Y

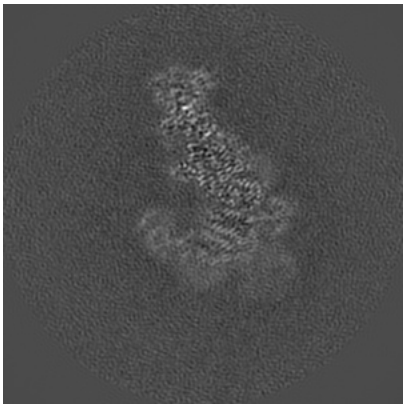


Z

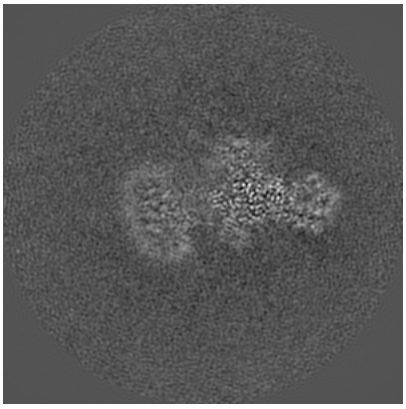
The images above show the map projected in three orthogonal directions.

6.2 Central slices

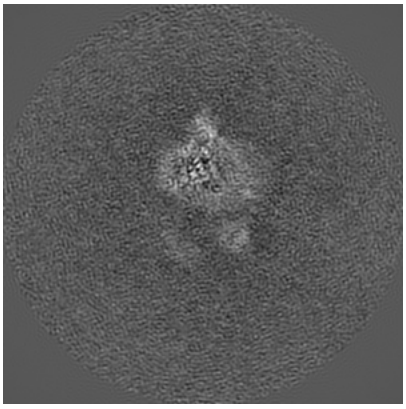
6.2.1 Primary map



X Index: 180



Y Index: 180

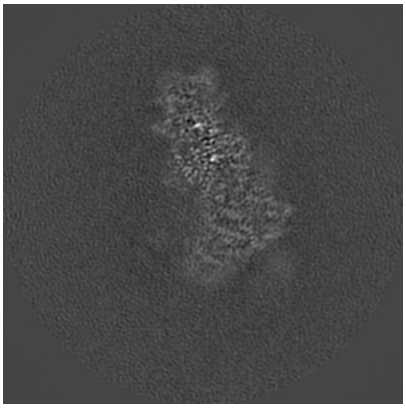


Z Index: 180

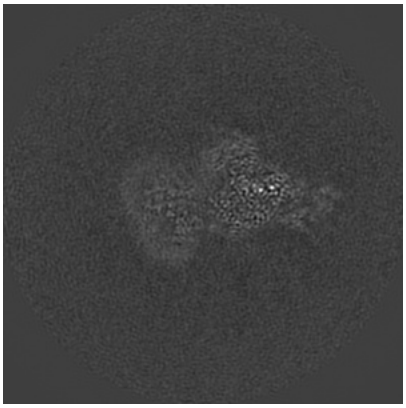
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

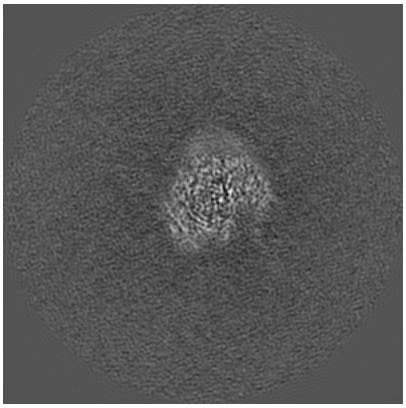
6.3.1 Primary map



X Index: 190



Y Index: 186

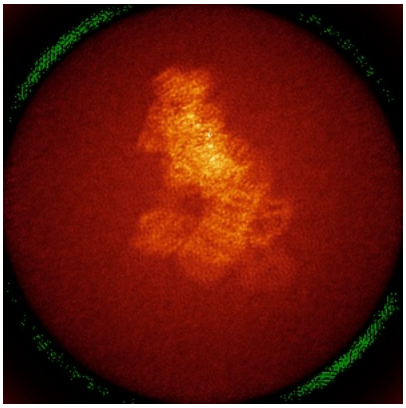


Z Index: 213

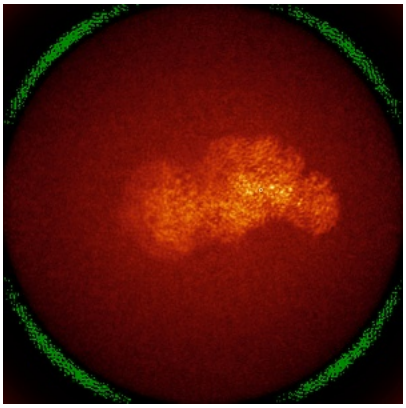
The images above show the largest variance slices of the map in three orthogonal directions.

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

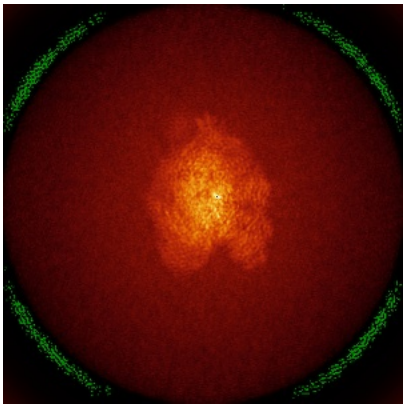
6.4.1 Primary map



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.

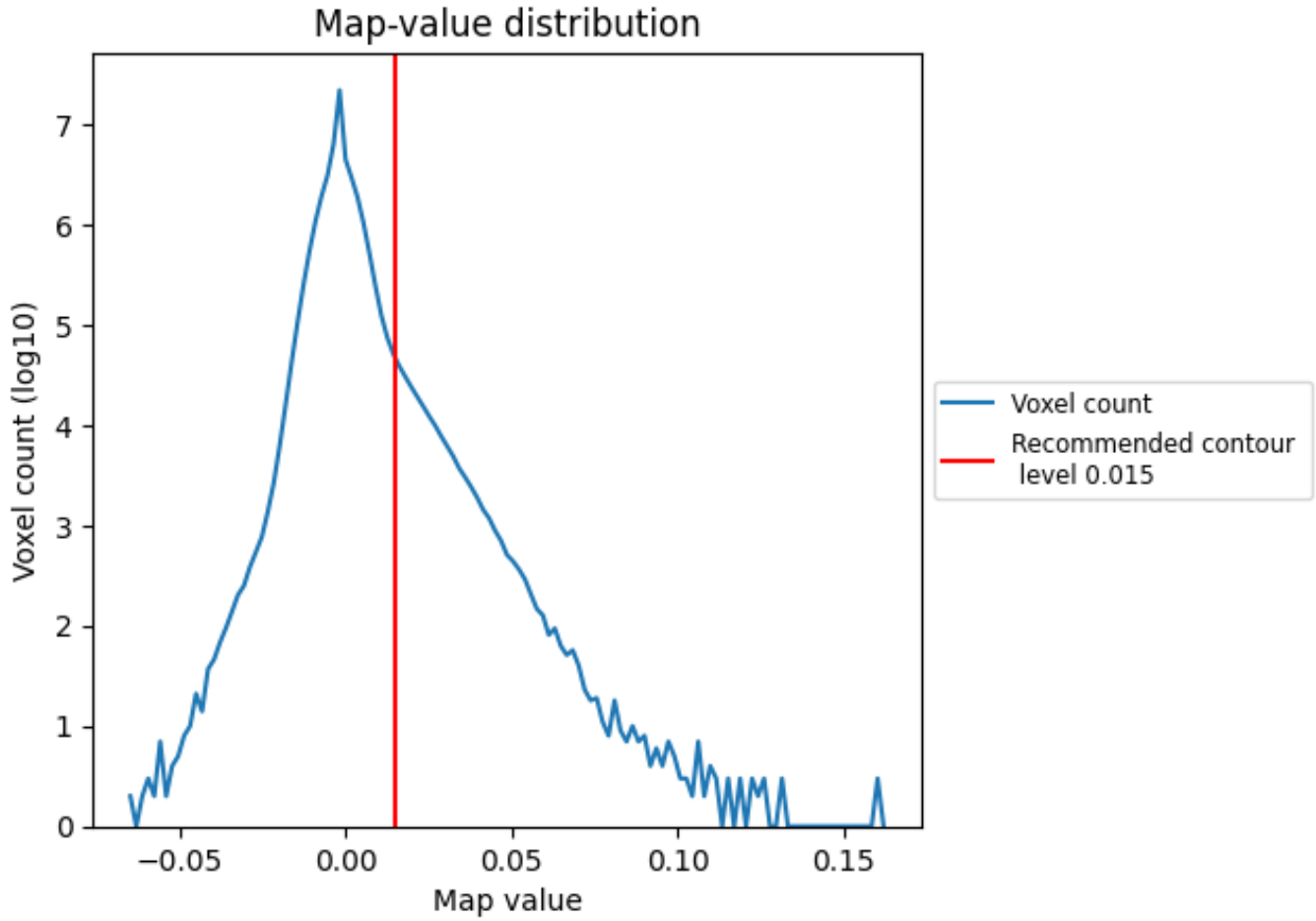
6.6 Mask visualisation (i)

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

7 Map analysis

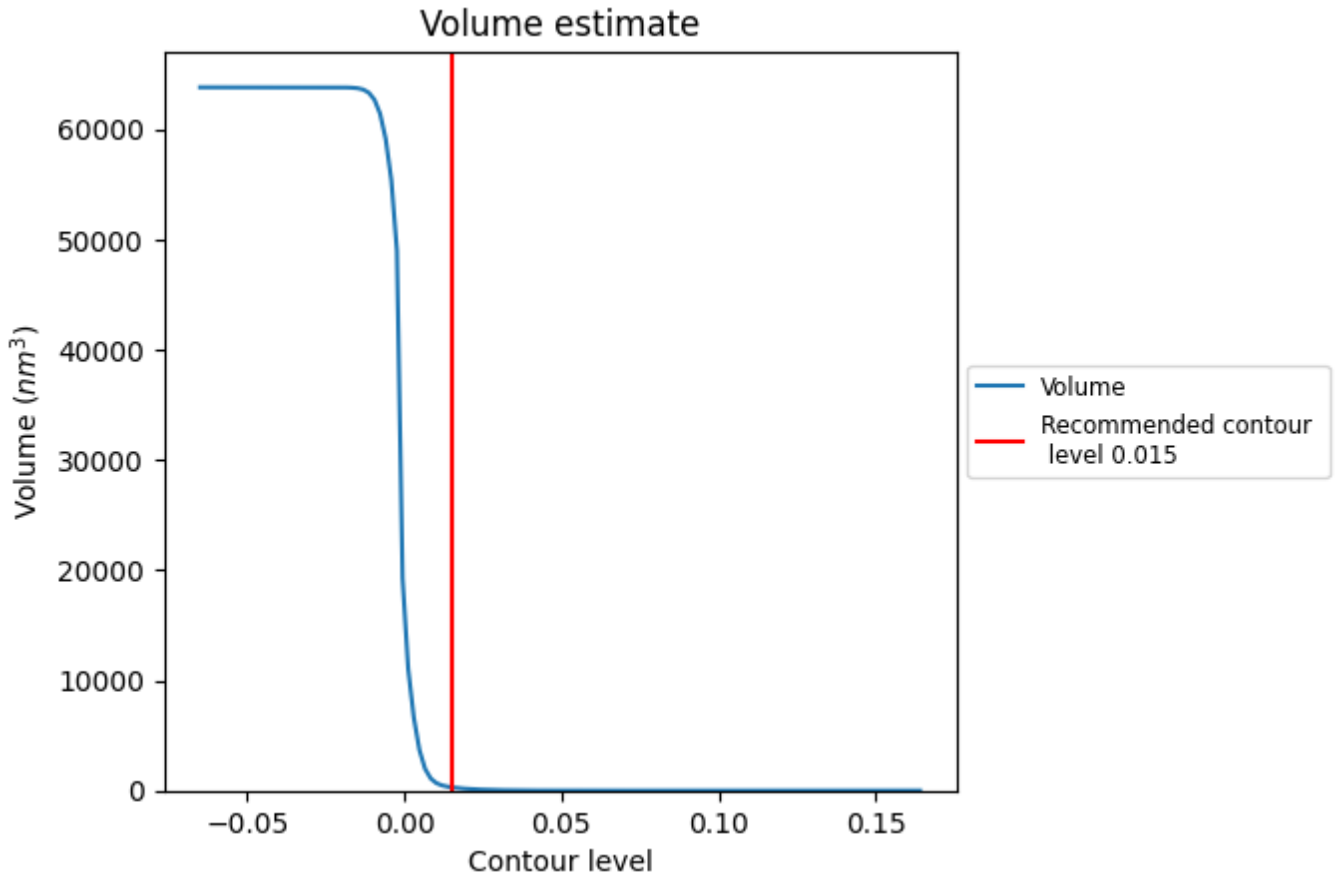
This section contains the results of statistical analysis of the map.

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.

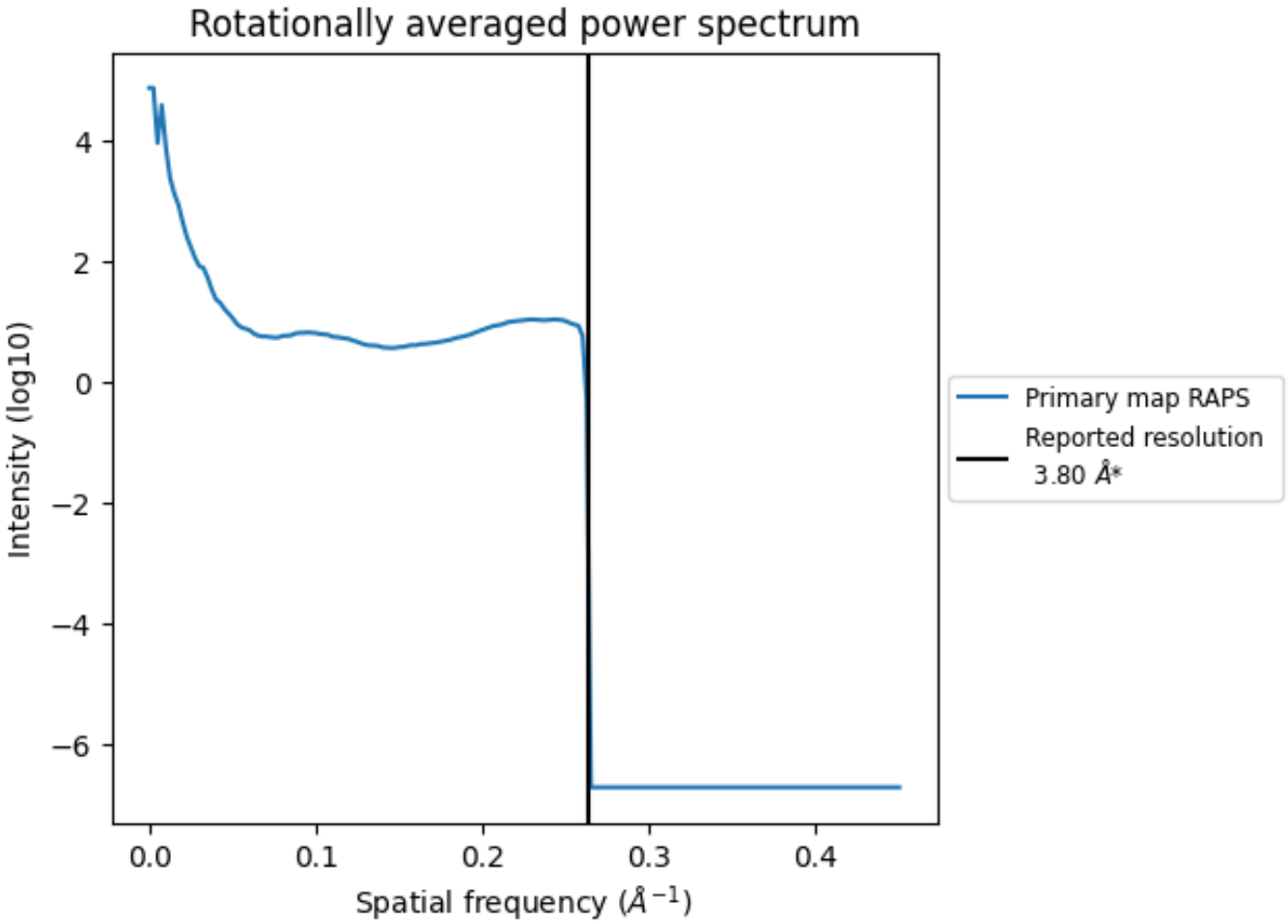
7.2 Volume estimate (i)



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}

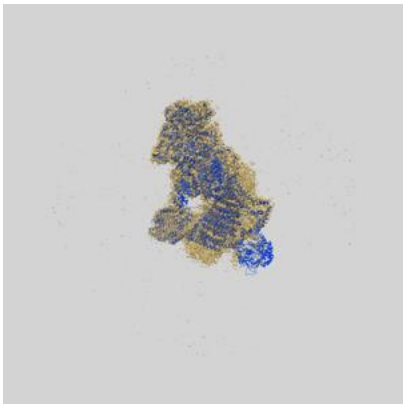
8 Fourier-Shell correlation

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

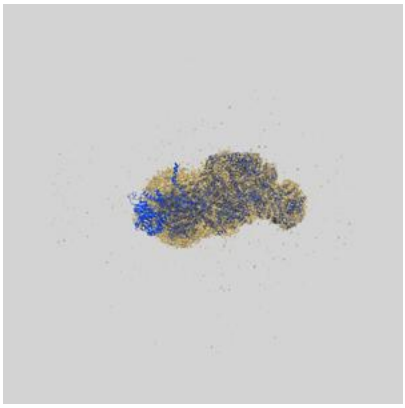
9 Map-model fit

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 15.

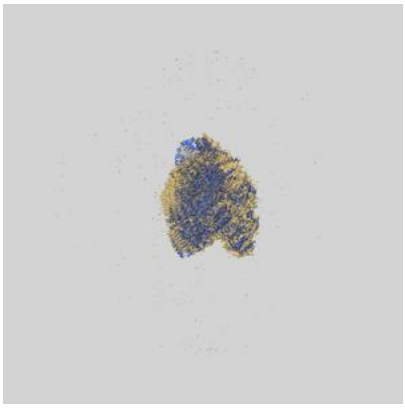
9.1 Map-model overlay



X



Y



Z

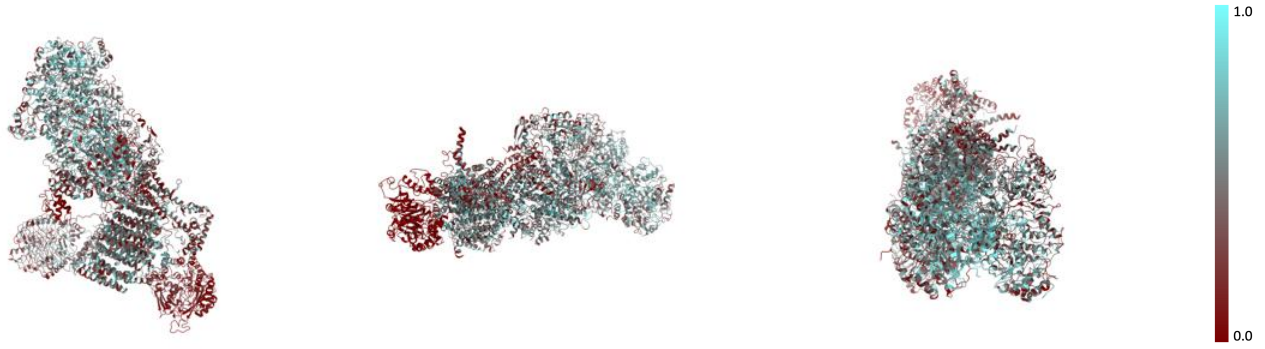
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

X Y Z

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.

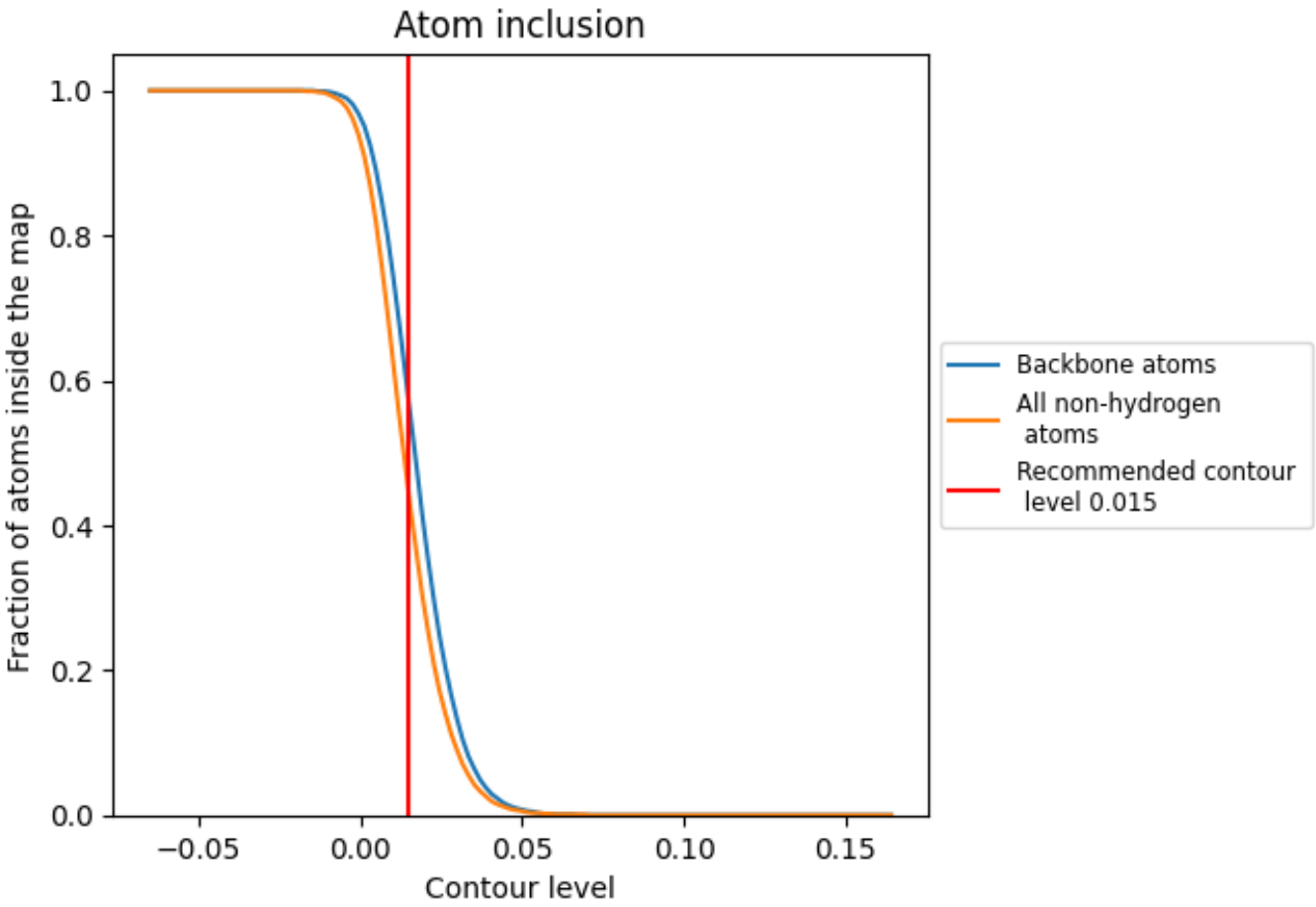
9.3 Atom inclusion mapped to coordinate model



X Y Z

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

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