



Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 03:42 am GMT

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

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

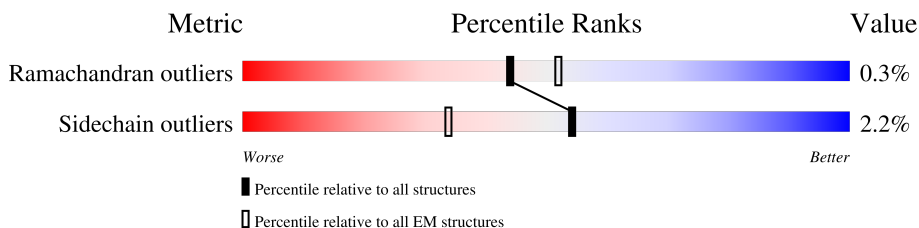
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	486	
2	I	499	
3	J	119	
4	N	205	
5	H	325	
6	K	100	
7	Y	106	
8	Z	143	
9	V	65	

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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
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		

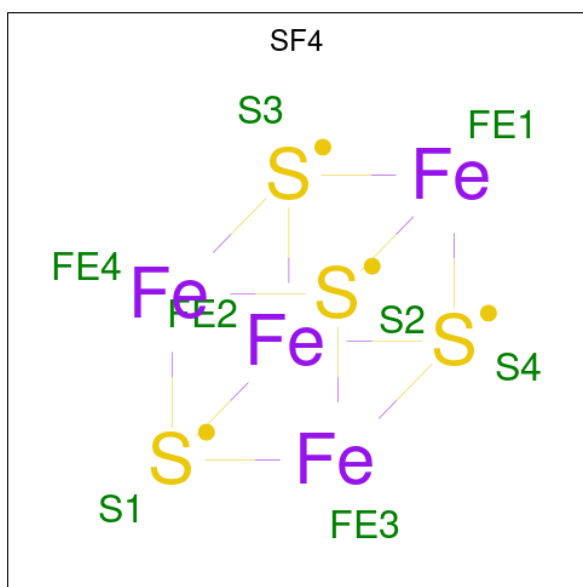
- Molecule 32 is a protein called CA1.

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.

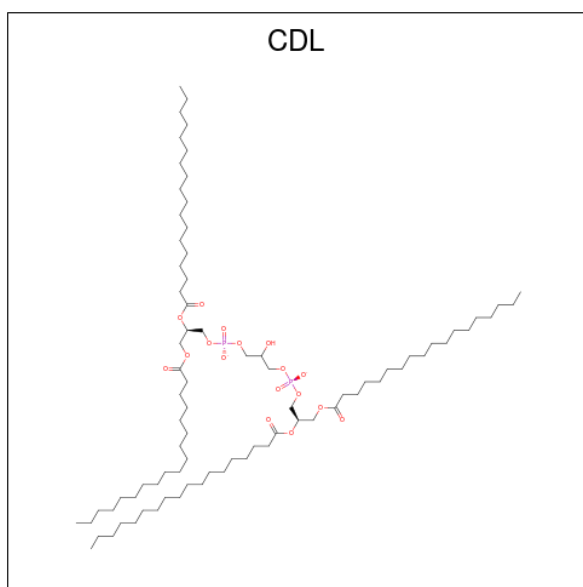
Mol	Chain	Residues	Atoms					AltConf	Trace
33	z	499	Total	C	N	O	S	0	0
			3992	2527	700	754	11		

- Molecule 34 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



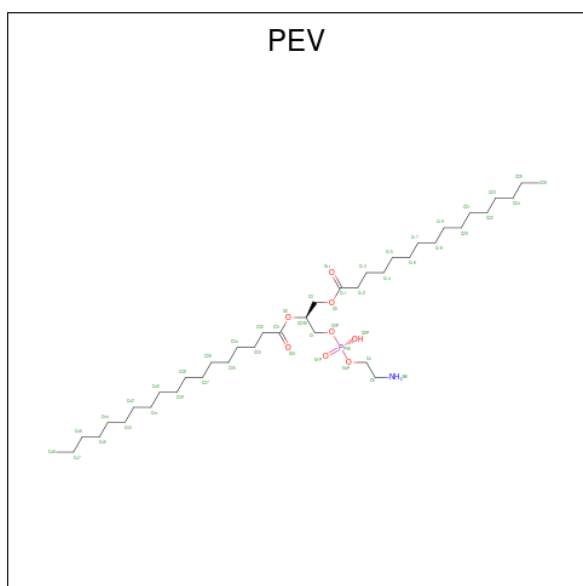
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
34	A	1	8	4	4	0
34	C	1	16	8	8	0
34	C	1	16	8	8	0
34	E	1	8	4	4	0
34	D	1	16	8	8	0
34	D	1	16	8	8	0

- Molecule 35 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



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: C₃₉H₇₈NO₈P).



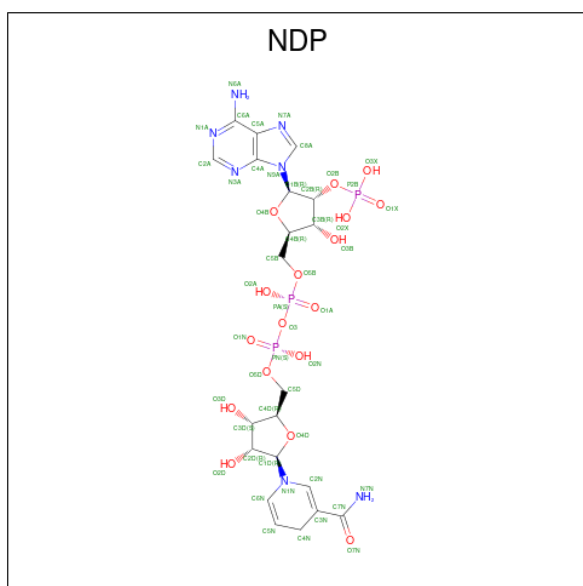
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
38	G	1	28	18	1	8	1	0

- Molecule 39 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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 (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

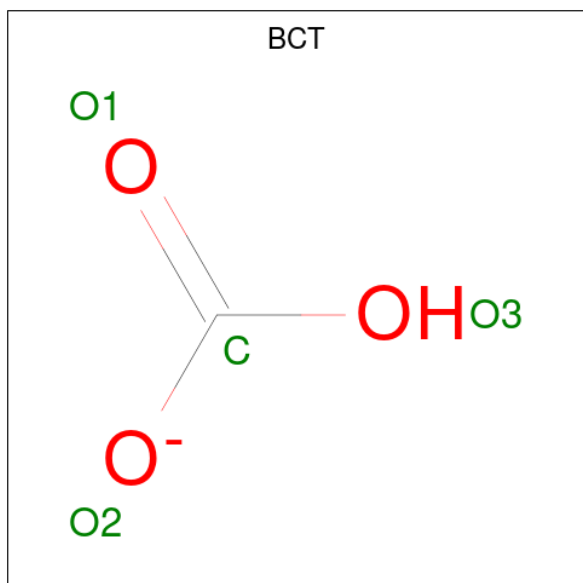


Mol	Chain	Residues	Atoms					AltConf
40	T	1	Total	C	N	O	P	0
			48	21	7	17	3	

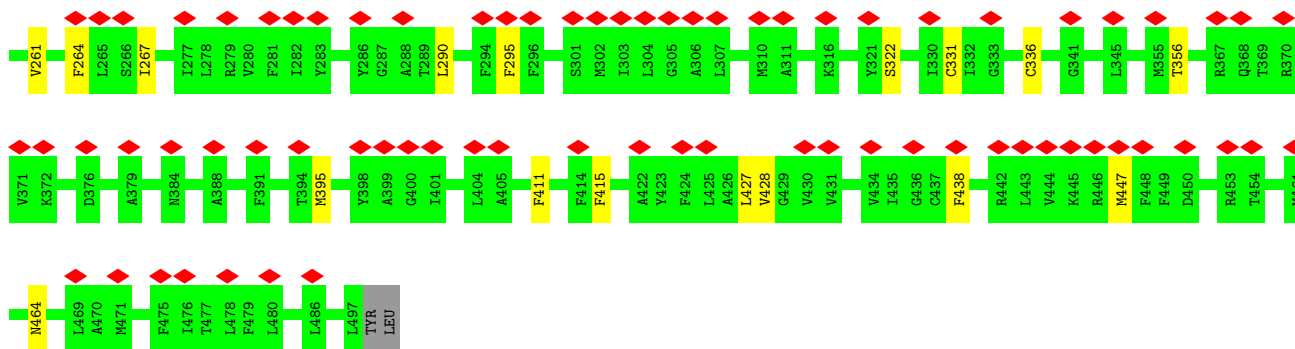
- Molecule 41 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

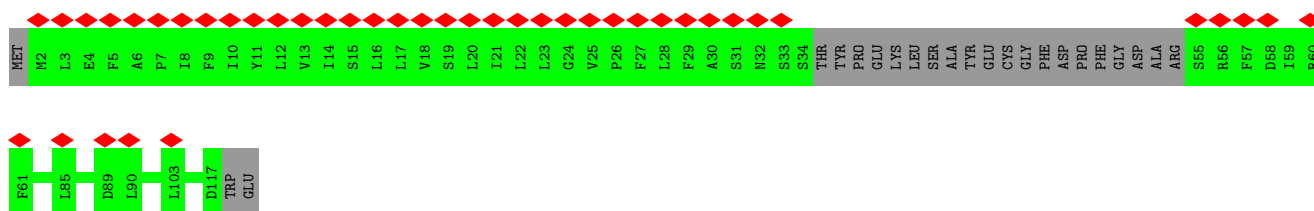
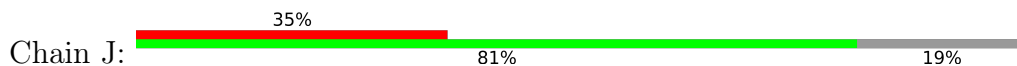
- Molecule 42 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



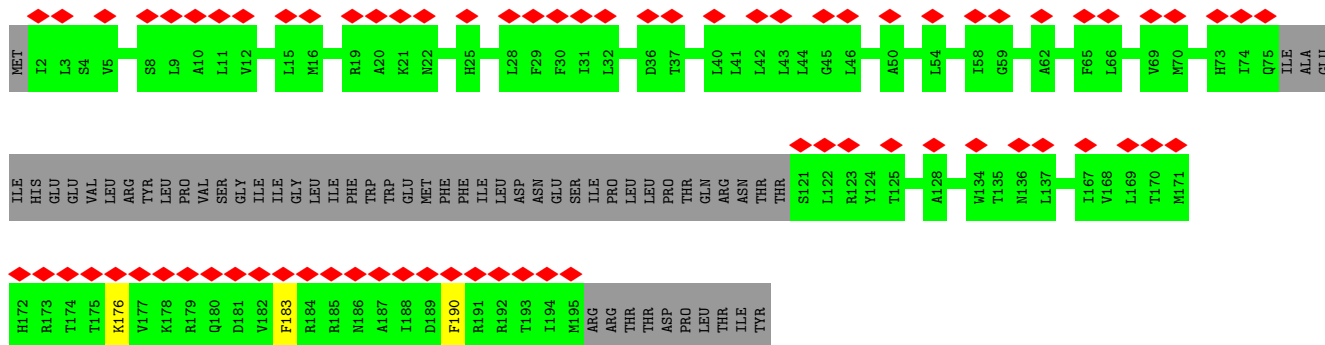
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
42	q	1	4	1	3	0



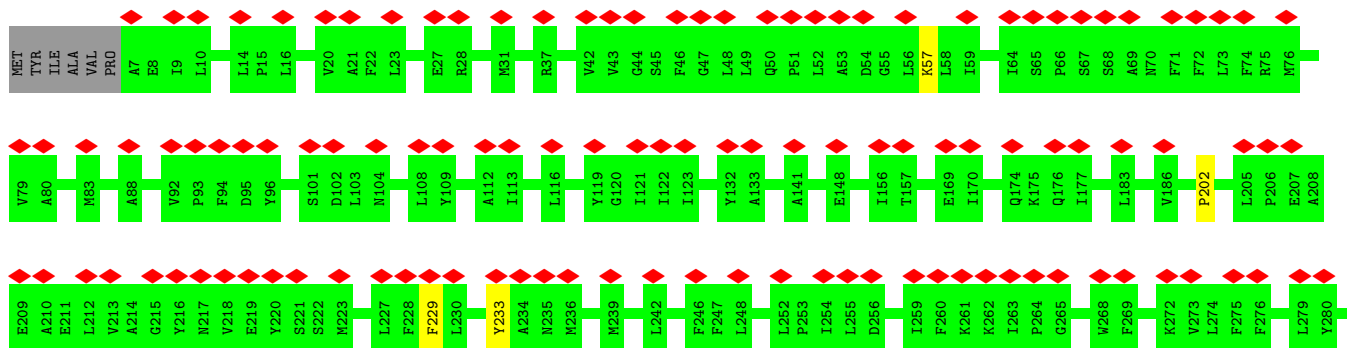
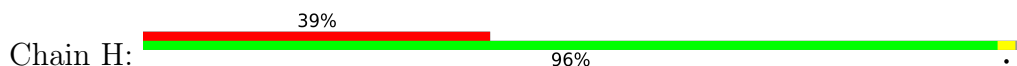
• Molecule 3: Nad3m

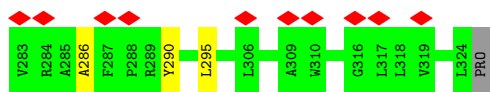


• Molecule 4: Nad6m

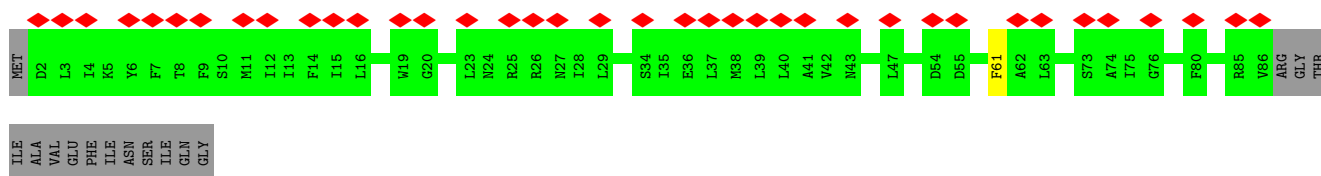
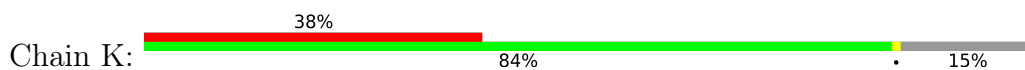


• Molecule 5: Nad1m

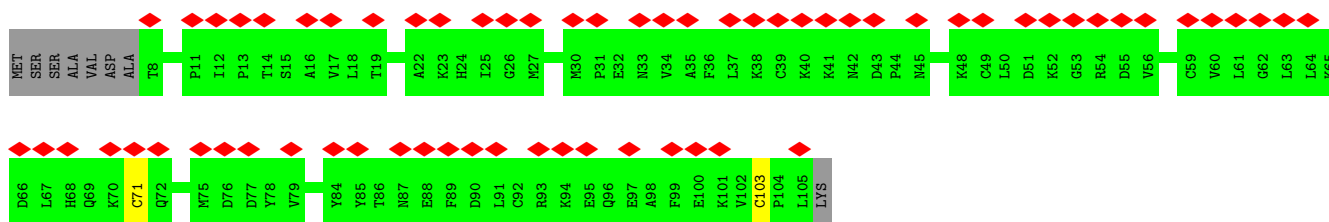




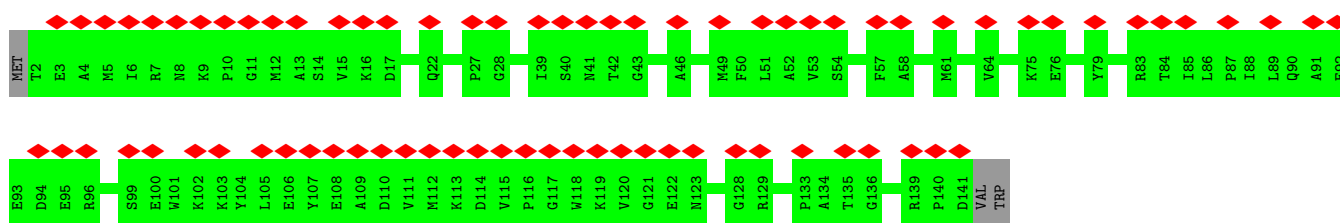
• Molecule 6: Nad4Lm



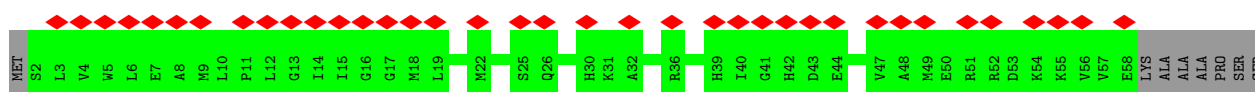
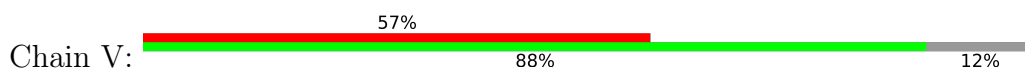
• Molecule 7: PGIV



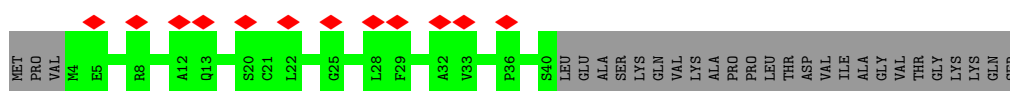
• Molecule 8: B16.6



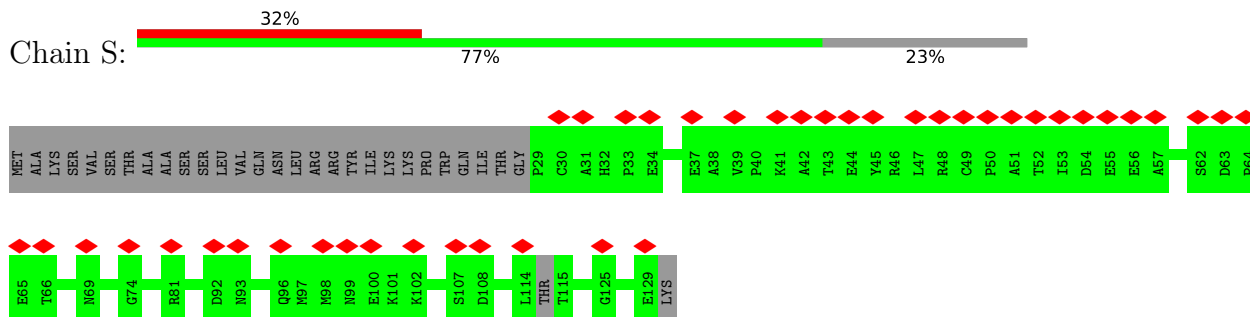
• Molecule 9: MWFE



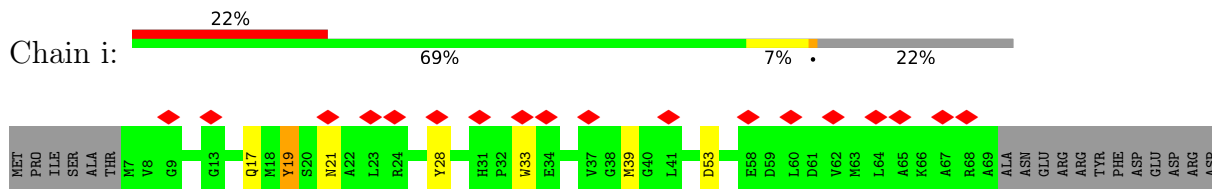
• Molecule 10: B9



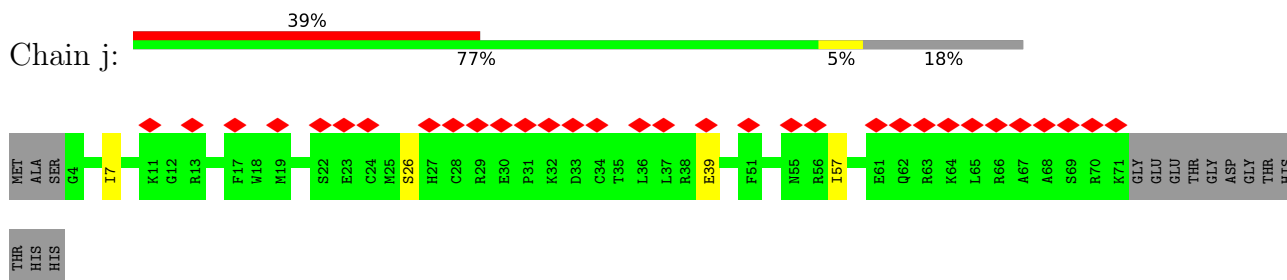
• Molecule 11: B14.5a



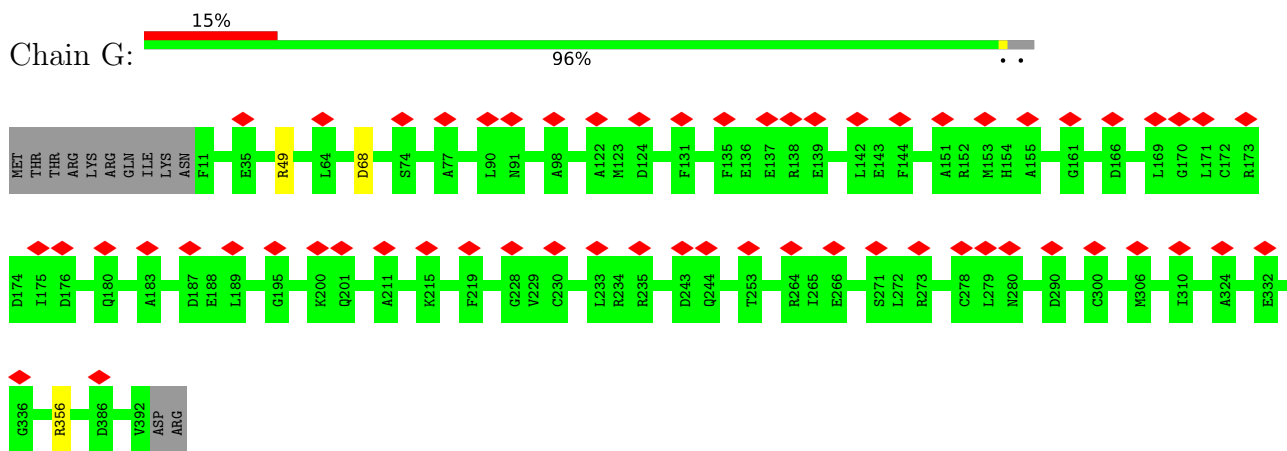
• Molecule 12: B14.5b



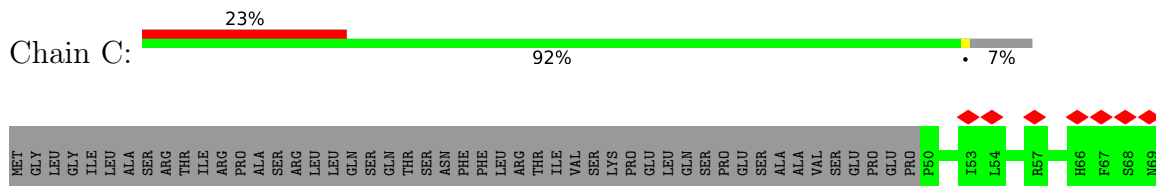
• Molecule 13: 15kDa

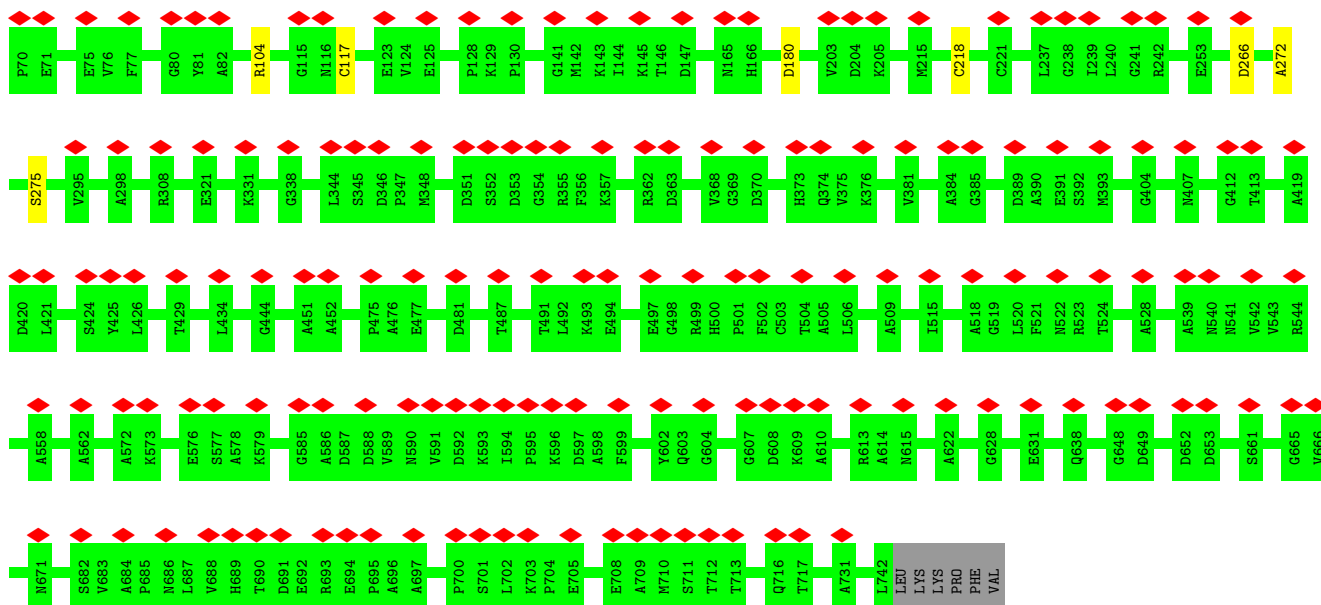


• Molecule 14: Nad7m

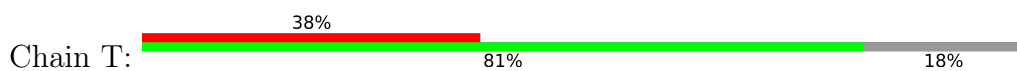


• Molecule 15: 75kDa

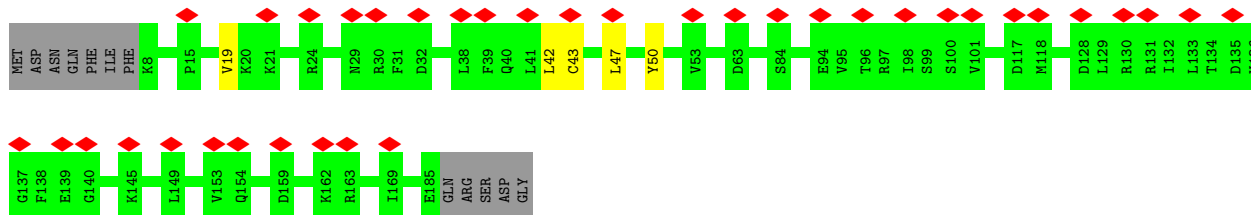
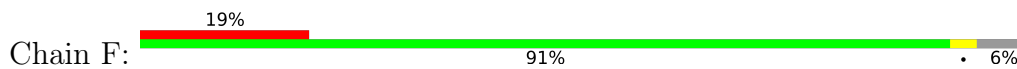




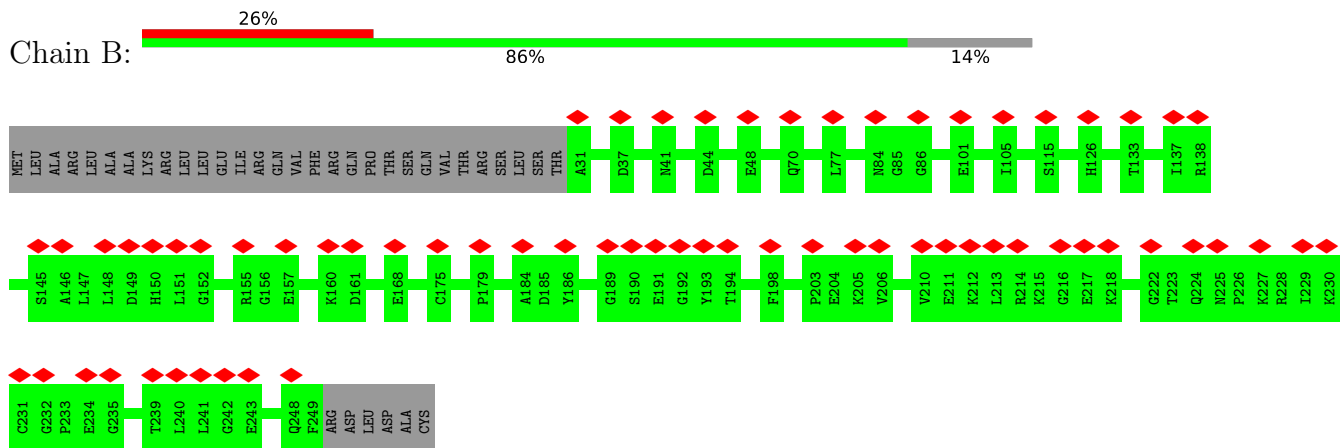
• Molecule 16: 39kDa



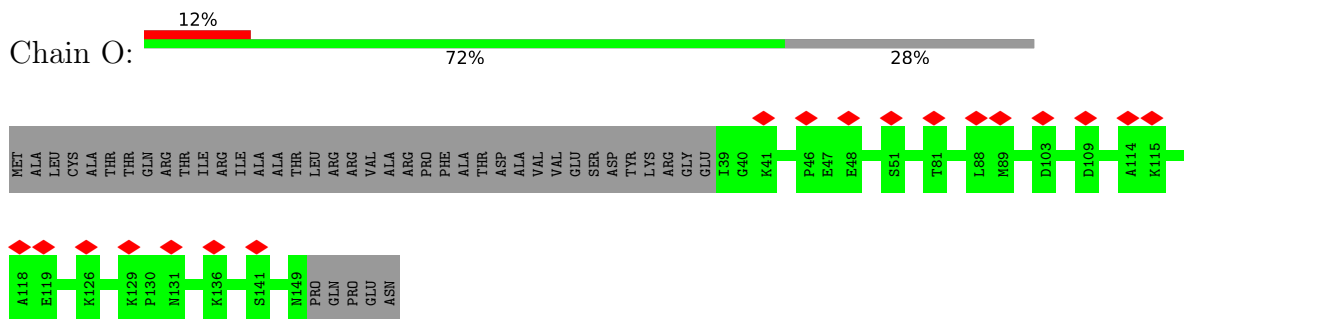
• Molecule 17: Nad9m



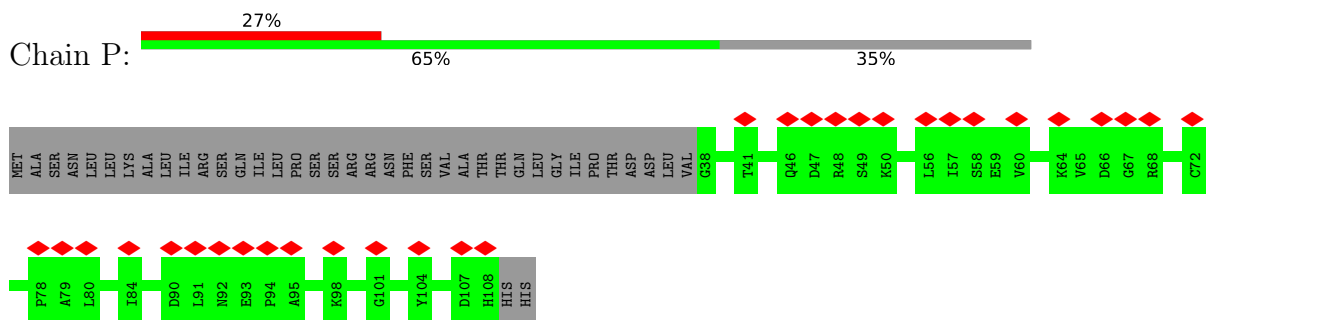
• Molecule 18: 24kDa



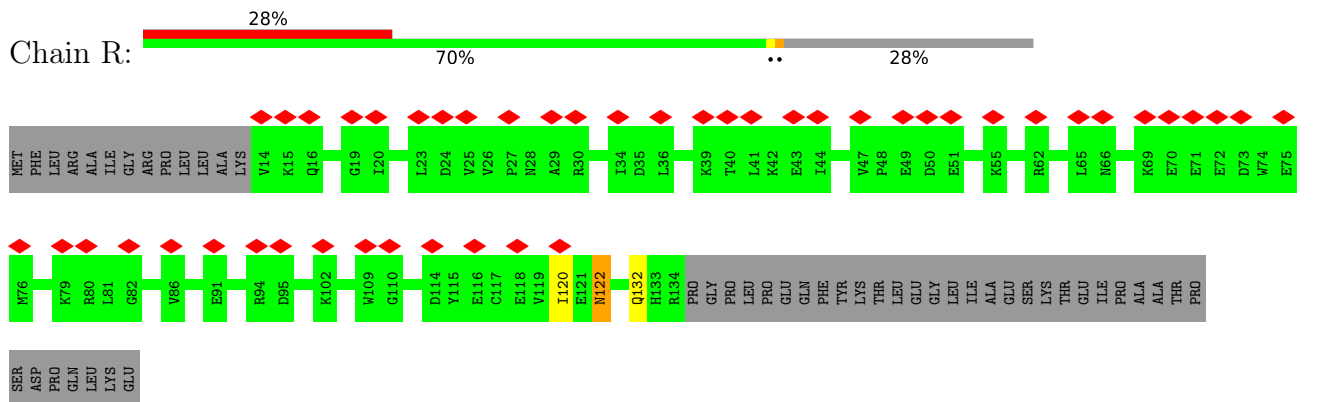
• Molecule 19: 18kDa



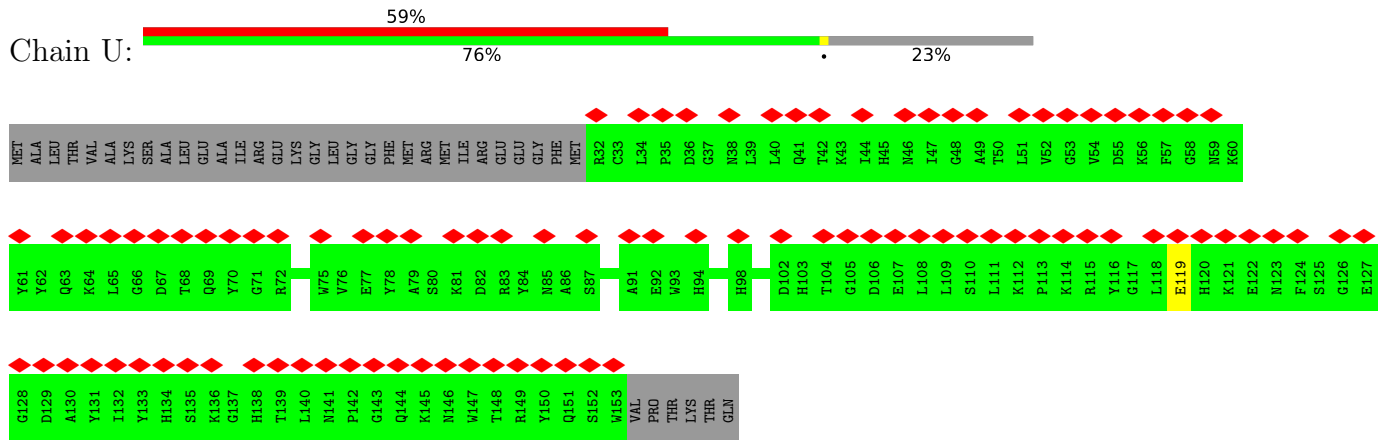
• Molecule 20: 13kDa



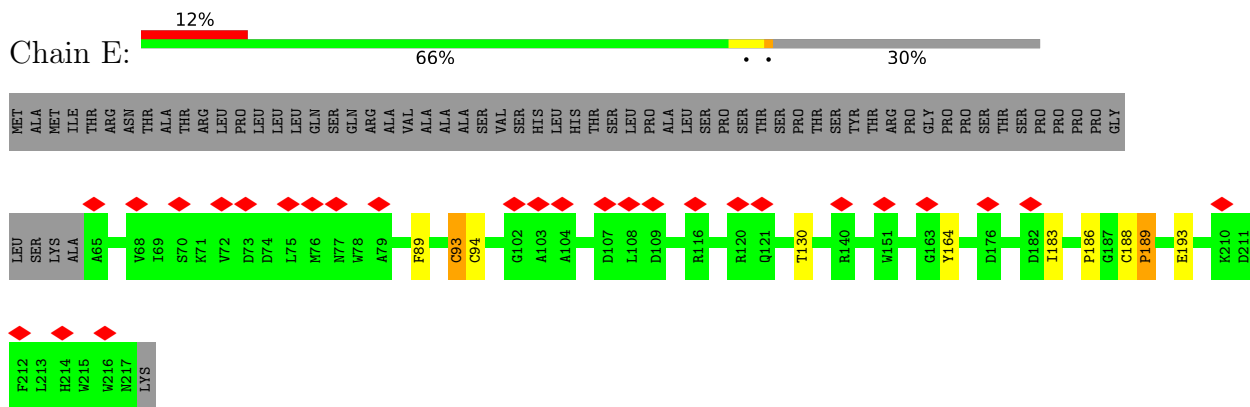
• Molecule 21: B13



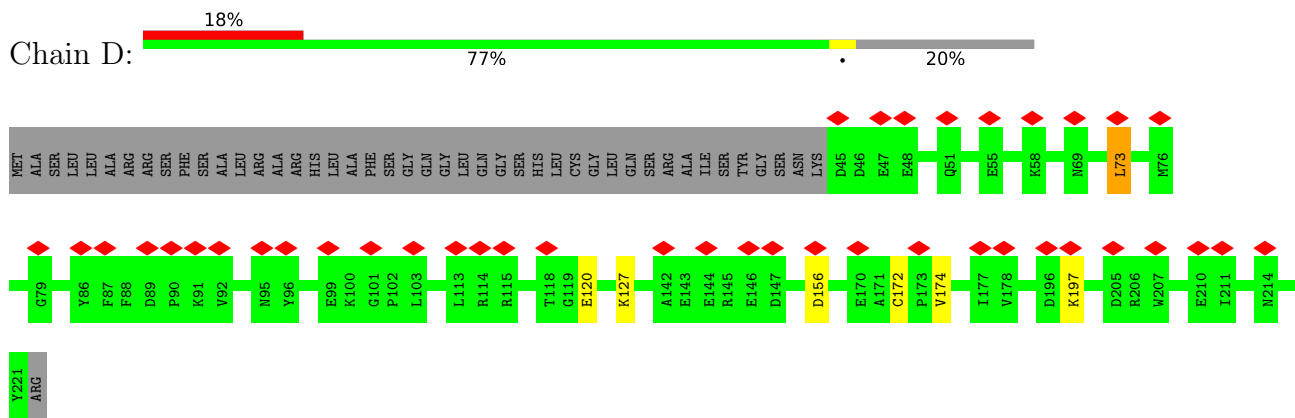
• Molecule 22: B17.2



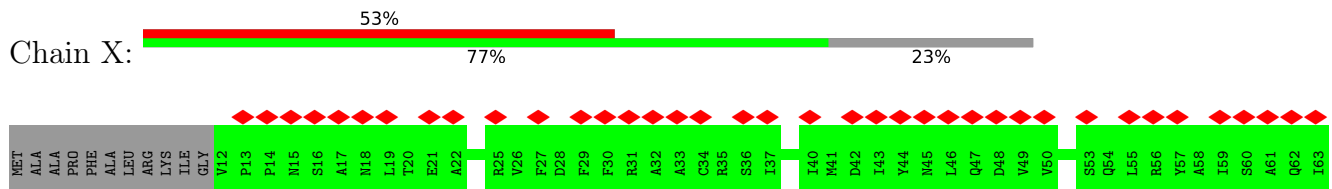
• Molecule 23: PSST

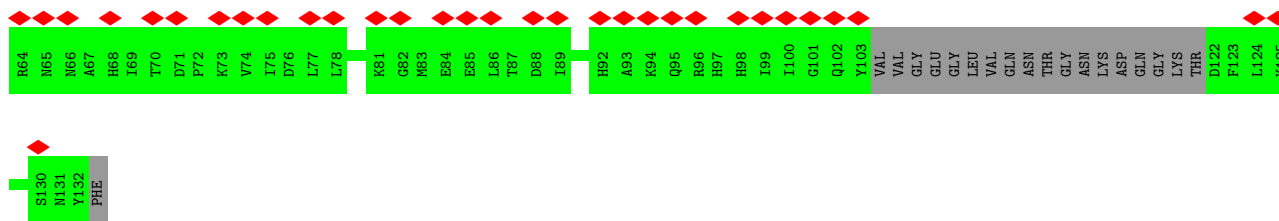


• Molecule 24: TYKY

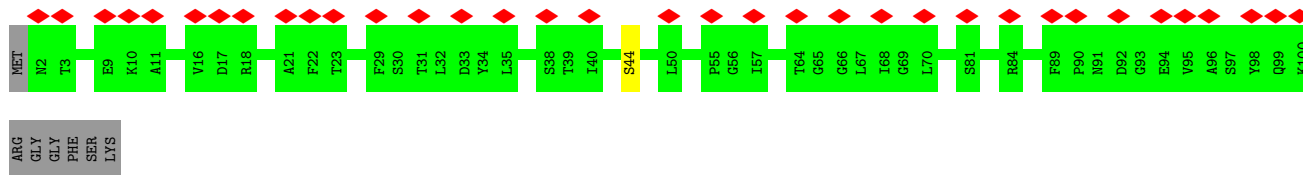
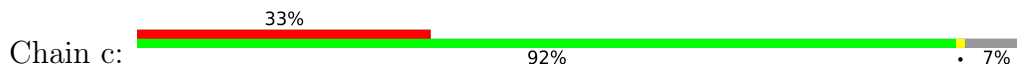


• Molecule 25: B14

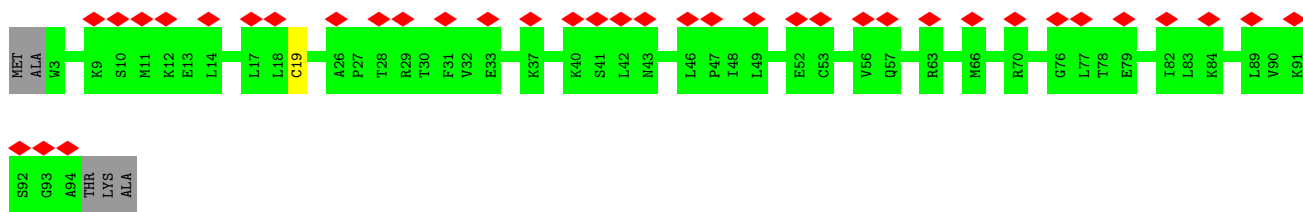
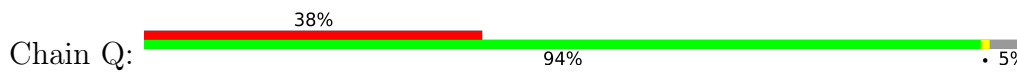




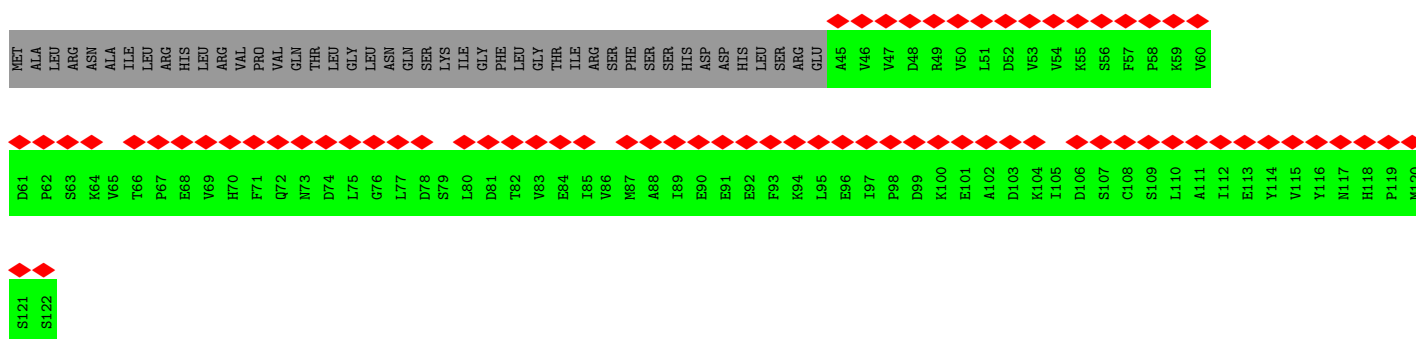
• Molecule 26: MNLL



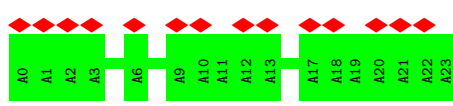
• Molecule 27: B8



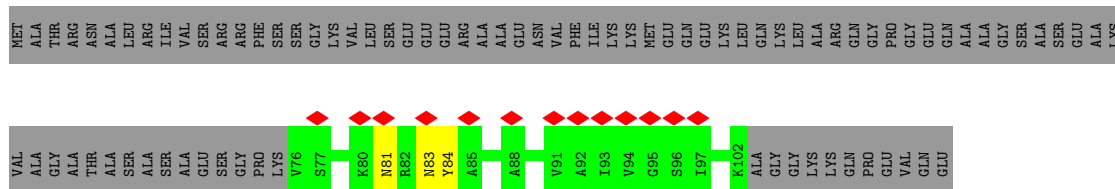
• Molecule 28: ACPM1



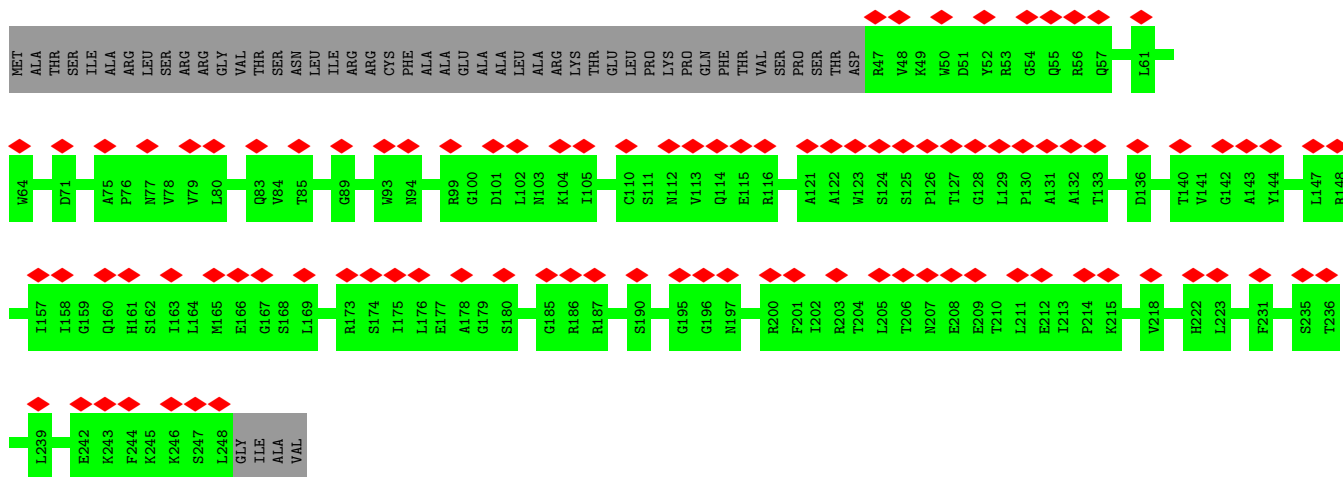
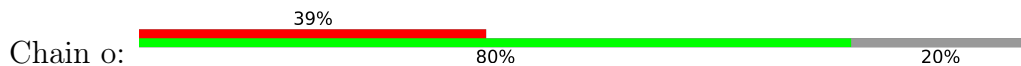
• Molecule 29: Unk1



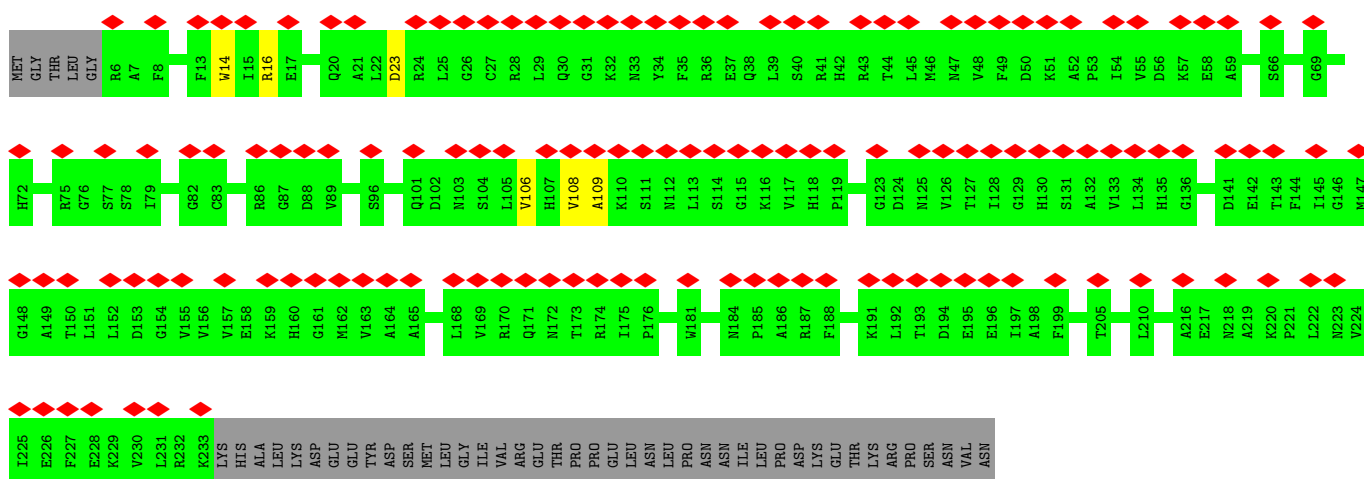
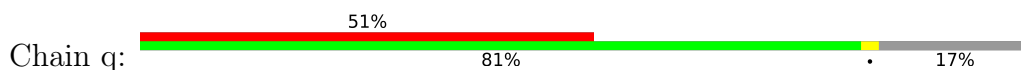
• Molecule 30: P2



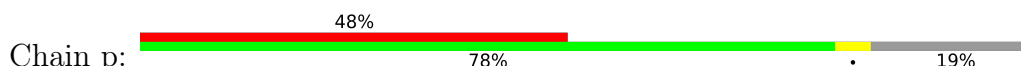
• Molecule 31: CAL1



• Molecule 32: CA1



• Molecule 32: CA1



DS46	Q647	FS48	S649	A650	Y651	E652	H653	W654	A655	K656	I657	E658	I659	P660	K661	D662	K663	E664	E665	L666	E667	A668	L669	Q670	A671	R672	I673	R674	K675	R676	F677	P678	V679	D680	A681	Y682	N683	K684	A685	R686	R687	E688	L689	D690	P691	N692	R693	I694	L695	S696	N697	N698	M699	V600	E601	K602	L603	F604	P605
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VAL
SER
THR
ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36513	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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 (\AA)	399.6, 399.6, 399.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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: CDL, FMN, FES, SF4, PEV, BCT, NDP, ZN, T7X

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

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

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

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

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

All (2) bond length outliers are listed below:

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

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
5	H	286	ALA	N-CA-CB	-5.28	102.71	110.10
32	p	185	PRO	N-CA-C	-5.25	98.45	112.10
5	H	295	LEU	CA-CB-CG	5.25	127.36	115.30
5	H	202	PRO	N-CA-C	-5.20	98.59	112.10
17	F	50	TYR	CB-CA-C	5.18	120.77	110.40
32	p	130	HIS	CB-CA-C	-5.18	100.03	110.40
15	C	117	CYS	CA-CB-SG	-5.13	104.77	114.00
5	H	233	TYR	CB-CA-C	5.08	120.56	110.40

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	U	120/159 (76%)	98 (82%)	22 (18%)	0	100	100
23	E	151/218 (69%)	134 (89%)	16 (11%)	1 (1%)	22	60
24	D	175/222 (79%)	159 (91%)	14 (8%)	2 (1%)	14	51
25	X	99/133 (74%)	92 (93%)	7 (7%)	0	100	100
26	c	97/106 (92%)	91 (94%)	6 (6%)	0	100	100
27	Q	90/97 (93%)	81 (90%)	9 (10%)	0	100	100
28	k	76/122 (62%)	74 (97%)	2 (3%)	0	100	100
29	r	22/24 (92%)	18 (82%)	4 (18%)	0	100	100
30	n	25/113 (22%)	24 (96%)	0	1 (4%)	3	28
31	o	200/252 (79%)	172 (86%)	28 (14%)	0	100	100
32	p	222/275 (81%)	191 (86%)	28 (13%)	3 (1%)	11	46
32	q	226/275 (82%)	196 (87%)	27 (12%)	3 (1%)	12	48
33	z	495/610 (81%)	476 (96%)	15 (3%)	4 (1%)	19	57
All	All	6177/7436 (83%)	5565 (90%)	591 (10%)	21 (0%)	44	74

All (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
30	n	81	ASN
32	q	23	ASP
32	q	106	VAL
32	p	30	GLN
32	p	102	ASP
32	p	217	GLU
7	Y	103	CYS
33	z	128	GLN
12	i	19	TYR
23	E	189	PRO
24	D	73	LEU
4	N	183	PHE
33	z	385	PRO
33	z	250	PRO

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Mol	Chain	Res	Type
33	z	129	PRO
21	R	120	ILE

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%)	92	96
2	I	399/416 (96%)	365 (92%)	34 (8%)	10	40
3	J	87/106 (82%)	87 (100%)	0	100	100
4	N	133/186 (72%)	131 (98%)	2 (2%)	65	81
5	H	266/272 (98%)	264 (99%)	2 (1%)	81	89
6	K	74/86 (86%)	73 (99%)	1 (1%)	67	81
7	Y	88/94 (94%)	87 (99%)	1 (1%)	73	85
8	Z	112/115 (97%)	112 (100%)	0	100	100
9	V	48/53 (91%)	48 (100%)	0	100	100
10	W	30/53 (57%)	30 (100%)	0	100	100
11	S	92/118 (78%)	92 (100%)	0	100	100
12	i	50/66 (76%)	43 (86%)	7 (14%)	3	21
13	j	62/73 (85%)	59 (95%)	3 (5%)	25	56
14	G	328/340 (96%)	325 (99%)	3 (1%)	78	88
15	C	576/625 (92%)	571 (99%)	5 (1%)	78	88
16	T	271/334 (81%)	269 (99%)	2 (1%)	84	91
17	F	168/179 (94%)	164 (98%)	4 (2%)	49	71
18	B	188/220 (86%)	188 (100%)	0	100	100
19	O	93/128 (73%)	93 (100%)	0	100	100
20	P	62/97 (64%)	62 (100%)	0	100	100
21	R	108/148 (73%)	106 (98%)	2 (2%)	57	76
22	U	104/133 (78%)	103 (99%)	1 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	E	129/184 (70%)	122 (95%)	7 (5%)	22	53
24	D	157/191 (82%)	151 (96%)	6 (4%)	33	61
25	X	92/114 (81%)	92 (100%)	0	100	100
26	c	79/84 (94%)	79 (100%)	0	100	100
27	Q	82/85 (96%)	81 (99%)	1 (1%)	71	84
28	k	73/112 (65%)	73 (100%)	0	100	100
30	n	21/84 (25%)	19 (90%)	2 (10%)	8	34
31	o	171/211 (81%)	171 (100%)	0	100	100
32	p	181/228 (79%)	176 (97%)	5 (3%)	43	68
32	q	184/228 (81%)	182 (99%)	2 (1%)	73	85
33	z	440/534 (82%)	412 (94%)	28 (6%)	17	48
All	All	5297/6293 (84%)	5178 (98%)	119 (2%)	54	72

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	GLU
2	I	35	HIS
2	I	80	HIS
2	I	83	TRP
2	I	87	PHE
2	I	118	GLU
2	I	120	PHE
2	I	127	VAL
2	I	155	GLN
2	I	171	PHE
2	I	182	LEU
2	I	197	ILE
2	I	209	LEU
2	I	214	THR
2	I	241	ILE
2	I	248	MET
2	I	249	TRP
2	I	252	ASP
2	I	261	VAL
2	I	264	PHE
2	I	267	ILE
2	I	290	LEU

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Mol	Chain	Res	Type
2	I	295	PHE
2	I	322	SER
2	I	331	CYS
2	I	336	CYS
2	I	356	THR
2	I	395	MET
2	I	411	PHE
2	I	415	PHE
2	I	427	LEU
2	I	428	VAL
2	I	438	PHE
2	I	447	MET
2	I	464	ASN
4	N	176	LYS
4	N	190	PHE
5	H	57	LYS
5	H	290	TYR
6	K	61	PHE
7	Y	71	CYS
12	i	17	GLN
12	i	19	TYR
12	i	21	ASN
12	i	28	TYR
12	i	33	TRP
12	i	39	MET
12	i	53	ASP
13	j	7	ILE
13	j	39	GLU
13	j	57	ILE
14	G	49	ARG
14	G	68	ASP
14	G	356	ARG
15	C	104	ARG
15	C	180	ASP
15	C	218	CYS
15	C	266	ASP
15	C	275	SER
16	T	79	PHE
16	T	147	ARG
17	F	19	VAL
17	F	42	LEU
17	F	43	CYS

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Mol	Chain	Res	Type
17	F	47	LEU
21	R	122	ASN
21	R	132	GLN
22	U	119	GLU
23	E	89	PHE
23	E	93	CYS
23	E	130	THR
23	E	164	TYR
23	E	183	ILE
23	E	188	CYS
23	E	193	GLU
24	D	73	LEU
24	D	127	LYS
24	D	156	ASP
24	D	172	CYS
24	D	174	VAL
24	D	197	LYS
27	Q	19	CYS
30	n	83	ASN
30	n	84	TYR
32	q	14	TRP
32	q	16	ARG
32	p	17	GLU
32	p	29	LEU
32	p	57	LYS
32	p	86	ARG
32	p	207	TYR
33	z	109	LEU
33	z	111	THR
33	z	112	VAL
33	z	113	SER
33	z	120	GLU
33	z	122	GLN
33	z	127	ASN
33	z	140	LYS
33	z	173	LEU
33	z	182	LYS
33	z	266	PHE
33	z	293	VAL
33	z	302	GLN
33	z	333	THR
33	z	387	ILE

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Mol	Chain	Res	Type
33	z	392	PHE
33	z	408	VAL
33	z	417	GLU
33	z	473	LEU
33	z	490	THR
33	z	520	THR
33	z	533	PHE
33	z	569	LEU
33	z	572	ARG
33	z	577	PHE
33	z	580	ASP
33	z	582	TYR
33	z	597	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	426	ASN
1	A	441	GLN
2	I	53	ASN
2	I	80	HIS
2	I	117	GLN
2	I	247	HIS
2	I	276	ASN
2	I	291	GLN
2	I	292	GLN
2	I	312	GLN
2	I	368	GLN
4	N	25	HIS
4	N	73	HIS
5	H	322	GLN
6	K	27	ASN
6	K	43	ASN
7	Y	45	ASN
7	Y	87	ASN
8	Z	63	GLN
9	V	30	HIS
9	V	34	HIS
9	V	39	HIS
9	V	42	HIS
12	i	21	ASN
13	j	27	HIS

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Mol	Chain	Res	Type
14	G	23	HIS
14	G	113	ASN
14	G	212	GLN
14	G	277	GLN
15	C	116	ASN
15	C	165	ASN
15	C	182	GLN
15	C	184	GLN
15	C	284	ASN
15	C	428	ASN
15	C	522	ASN
15	C	538	GLN
15	C	569	GLN
15	C	605	HIS
15	C	606	HIS
15	C	716	GLN
16	T	117	GLN
16	T	153	ASN
16	T	182	GLN
16	T	209	ASN
16	T	291	HIS
16	T	340	ASN
17	F	54	GLN
17	F	125	ASN
18	B	33	ASN
18	B	84	ASN
18	B	126	HIS
18	B	196	ASN
19	O	49	HIS
19	O	77	ASN
20	P	92	ASN
22	U	41	GLN
22	U	46	ASN
22	U	69	GLN
22	U	134	HIS
22	U	138	HIS
22	U	141	ASN
23	E	100	HIS
24	D	111	HIS
24	D	190	HIS
25	X	15	ASN
25	X	98	HIS

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Mol	Chain	Res	Type
25	X	131	ASN
27	Q	35	ASN
30	n	81	ASN
31	o	77	ASN
31	o	114	GLN
31	o	120	HIS
32	q	33	ASN
32	q	47	ASN
32	q	72	HIS
32	q	90	ASN
32	q	130	HIS
32	q	184	ASN
32	q	206	ASN
32	q	209	ASN
32	q	218	ASN
32	q	223	ASN
32	p	99	ASN
32	p	130	HIS
32	p	160	HIS
32	p	214	HIS
32	p	223	ASN
33	z	127	ASN
33	z	170	ASN
33	z	302	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	PEV	G	601	-	-	12/30/30/52	-
39	FES	C	803	15	-	-	0/1/1/1
40	NDP	T	501	-	-	6/30/77/77	0/5/5/5
34	SF4	C	801	15	-	-	0/6/5/5
34	SF4	C	802	15	-	-	0/6/5/5
35	FMN	A	502	-	-	6/18/18/18	0/3/3/3
34	SF4	E	301	23	-	-	0/6/5/5
36	T7X	c	301	-	-	2/32/56/80	0/1/1/1
36	T7X	I	501	-	-	13/37/61/80	0/1/1/1
39	FES	B	301	-	-	-	0/1/1/1
34	SF4	A	501	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	SF4	D	302	24	-	-	0/6/5/5
34	SF4	D	301	24	-	-	0/6/5/5
37	CDL	i	201	-	-	31/100/100/110	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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.

All (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
36	I	501	T7X	C12-C10-O16-C8
36	I	501	T7X	O17-C10-O16-C8
37	i	201	CDL	CA3-OA5-PA1-OA4
37	i	201	CDL	OA7-CA5-OA6-CA4
37	i	201	CDL	C11-CA5-OA6-CA4
37	i	201	CDL	CB2-OB2-PB2-OB3
37	i	201	CDL	OB7-CB5-OB6-CB4
37	i	201	CDL	C51-CB5-OB6-CB4
38	G	601	PEV	C2-C1-O3P-P
37	i	201	CDL	O1-C1-CB2-OB2
35	A	502	FMN	C2'-C3'-C4'-C5'
37	i	201	CDL	CA2-C1-CB2-OB2
37	i	201	CDL	O1-C1-CA2-OA2
35	A	502	FMN	O3'-C3'-C4'-O4'
35	A	502	FMN	C2'-C3'-C4'-O4'
37	i	201	CDL	CB2-OB2-PB2-OB5
40	T	501	NDP	C2D-C1D-N1N-C6N
37	i	201	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
37	i	201	CDL	OA6-CA4-CA6-OA8
40	T	501	NDP	C2D-C1D-N1N-C2N
37	i	201	CDL	C38-C39-C40-C41
37	i	201	CDL	CA3-CA4-CA6-OA8
36	I	501	T7X	C39-C40-C41-C42
37	i	201	CDL	OB6-CB4-CB6-OB8
37	i	201	CDL	C31-CA7-OA8-CA6
37	i	201	CDL	C1-CA2-OA2-PA1
38	G	601	PEV	O2-C2-C3-O3
37	i	201	CDL	C53-C54-C55-C56
36	I	501	T7X	O16-C8-C9-O18
37	i	201	CDL	C40-C41-C42-C43
36	I	501	T7X	C7-O13-P1-O12
37	i	201	CDL	CB2-OB2-PB2-OB4
37	i	201	CDL	C71-CB7-OB8-CB6
38	G	601	PEV	C5-C4-O4P-P
37	i	201	CDL	CA5-C11-C12-C13
37	i	201	CDL	OA9-CA7-OA8-CA6
40	T	501	NDP	O4D-C1D-N1N-C6N
36	I	501	T7X	C7-C8-C9-O18
38	G	601	PEV	C3-C2-O2-C31
35	A	502	FMN	C5 ² -O5 ² -P-O1P
37	i	201	CDL	CB3-OB5-PB2-OB2
38	G	601	PEV	C1-O3P-P-O4P
38	G	601	PEV	C1-C2-C3-O3
38	G	601	PEV	C35-C36-C37-C38
36	I	501	T7X	C38-C39-C40-C41
37	i	201	CDL	CB3-CB4-CB6-OB8
37	i	201	CDL	C41-C42-C43-C44
37	i	201	CDL	CB6-CB4-OB6-CB5
40	T	501	NDP	O4D-C1D-N1N-C2N
37	i	201	CDL	OB9-CB7-OB8-CB6
38	G	601	PEV	C33-C34-C35-C36
37	i	201	CDL	CB2-C1-CA2-OA2
40	T	501	NDP	PN-O3-PA-O1A
37	i	201	CDL	C16-C17-C18-C19
40	T	501	NDP	O4D-C4D-C5D-O5D
36	c	301	T7X	C6-C1-O1-P1
38	G	601	PEV	C32-C33-C34-C35
37	i	201	CDL	CA3-OA5-PA1-OA3
38	G	601	PEV	C1-O3P-P-O1P
36	c	301	T7X	O16-C10-C12-C13

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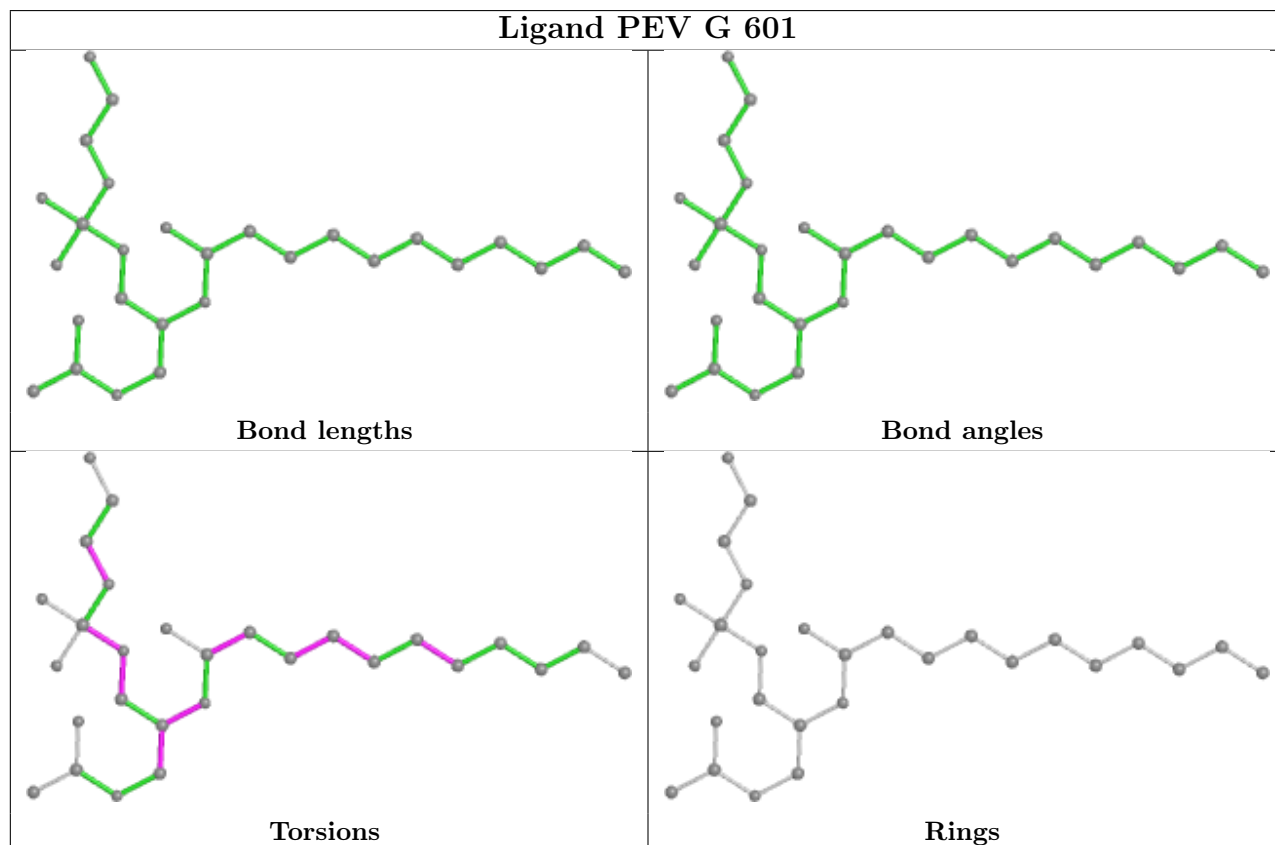
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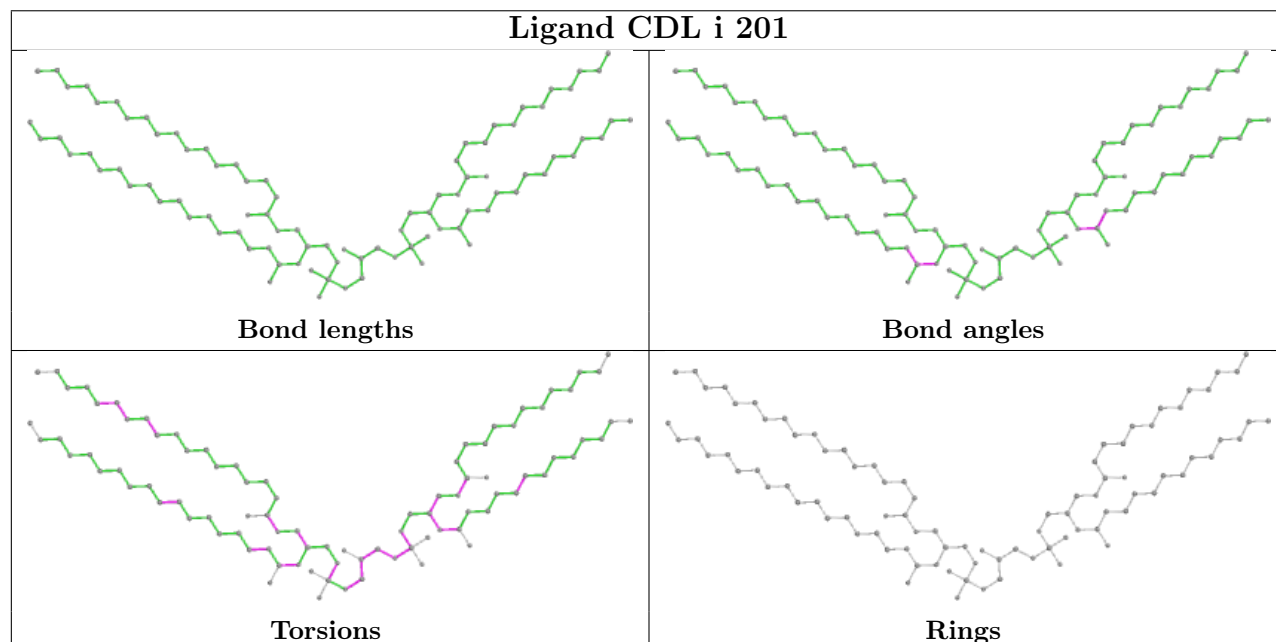
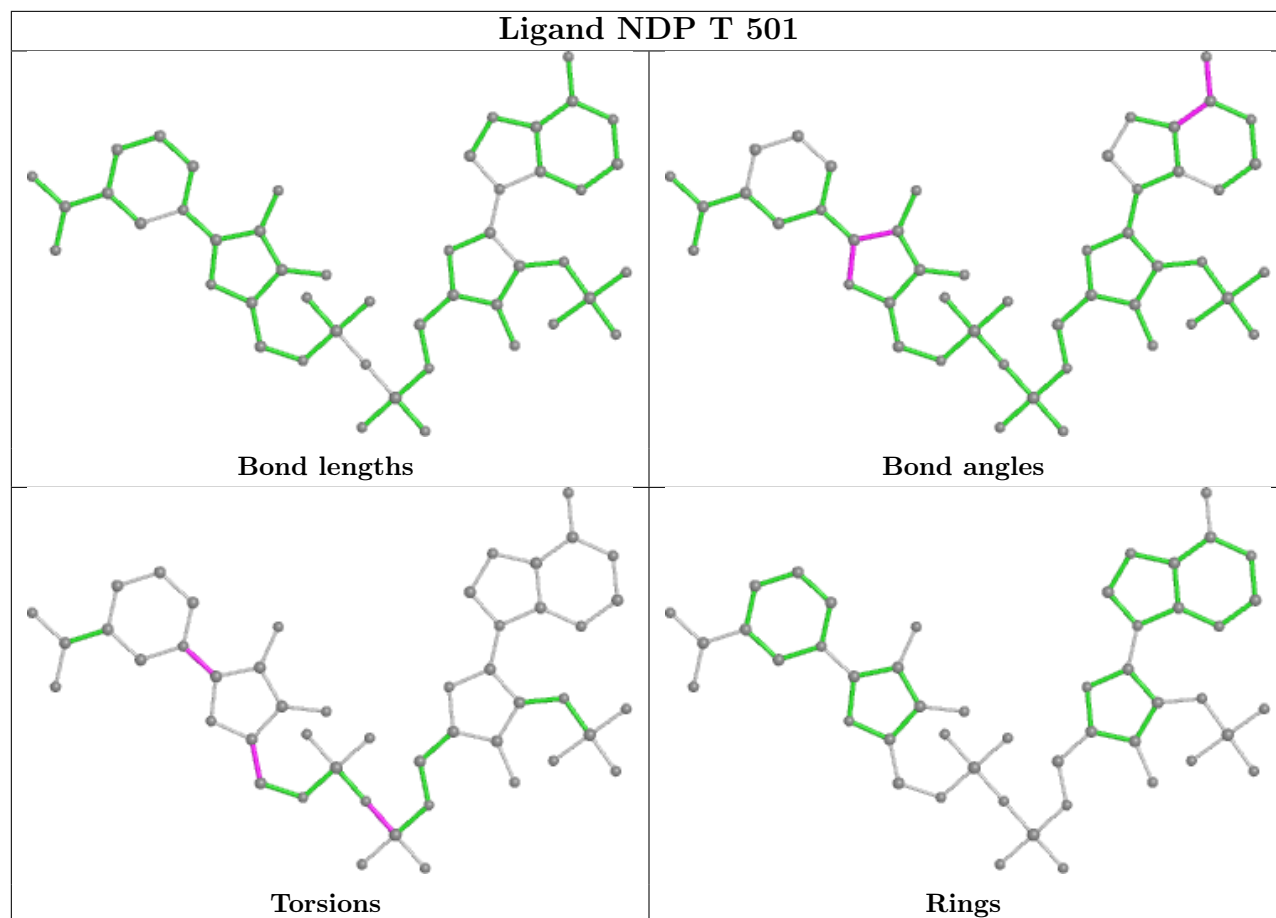
Mol	Chain	Res	Type	Atoms
36	I	501	T7X	O18-C11-C31-C32
38	G	601	PEV	O2-C31-C32-C33
36	I	501	T7X	O19-C11-C31-C32
38	G	601	PEV	O31-C31-C32-C33
36	I	501	T7X	C40-C41-C42-C43

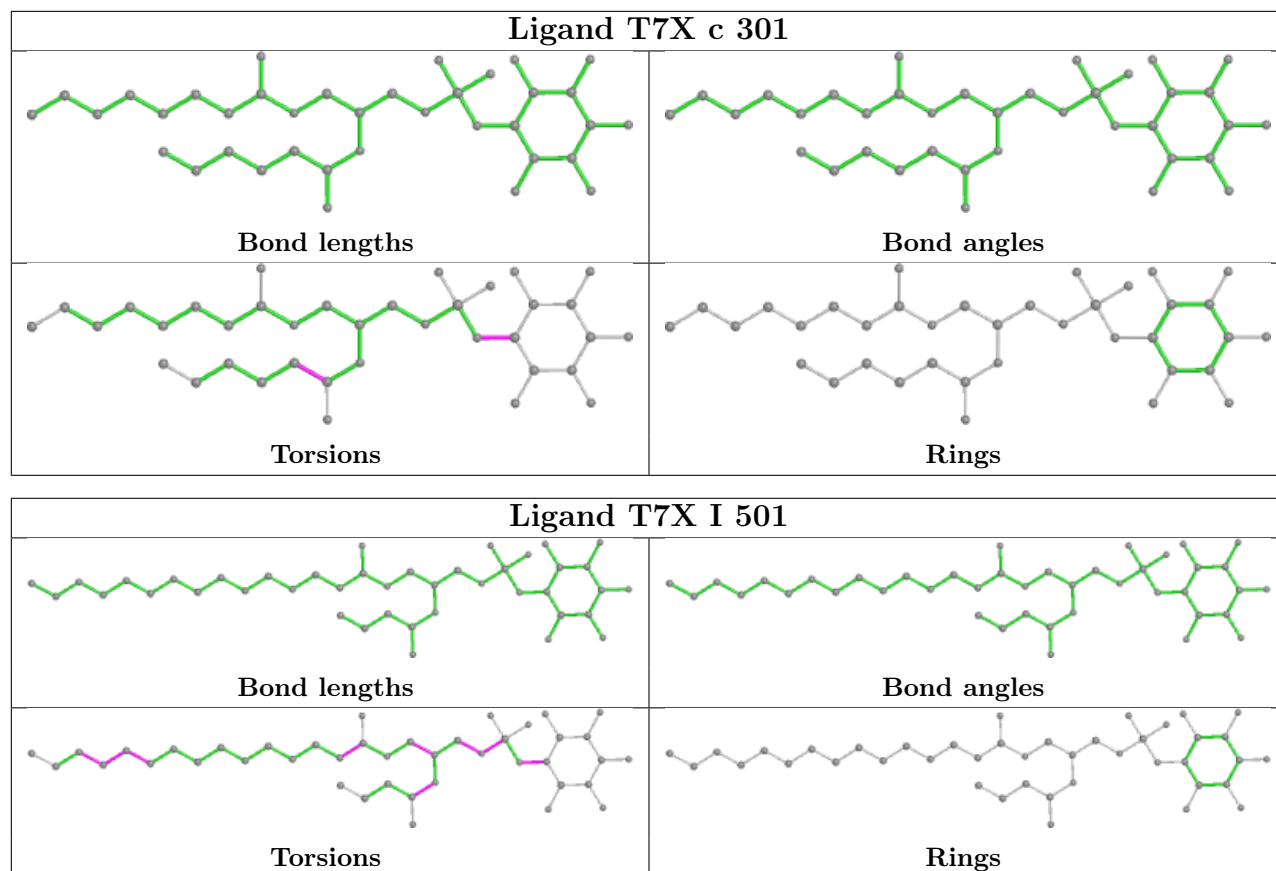
There are no ring outliers.

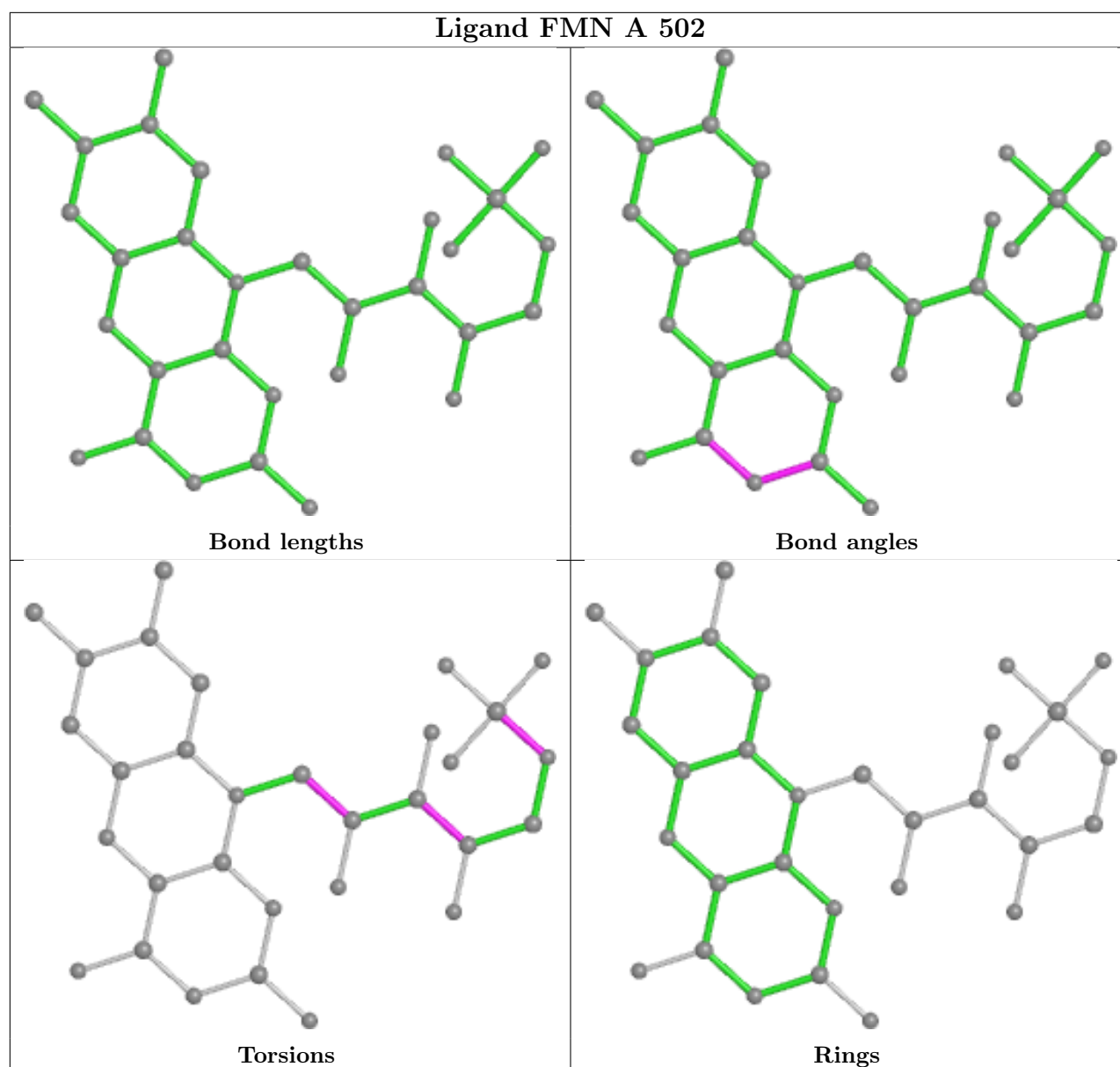
No monomer is involved in short contacts.

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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

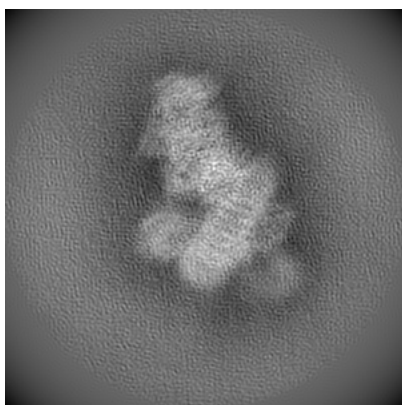
6 Map visualisation [i](#)

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.

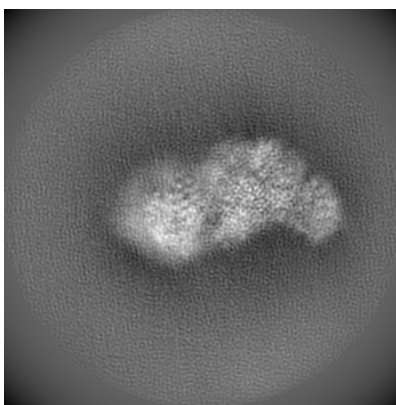
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

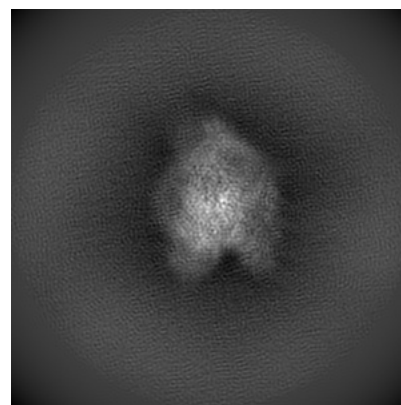
6.1.1 Primary map



X



Y

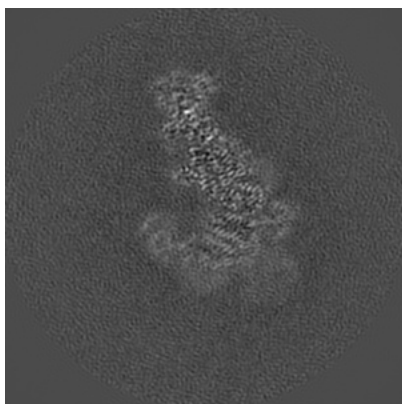


Z

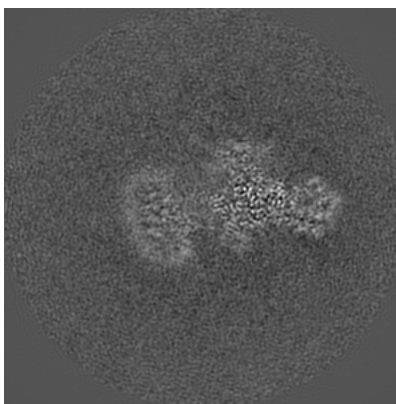
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

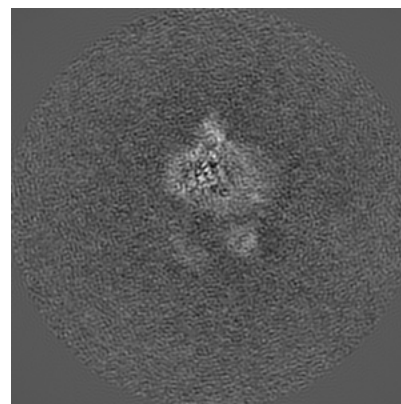
6.2.1 Primary map



X Index: 180



Y Index: 180

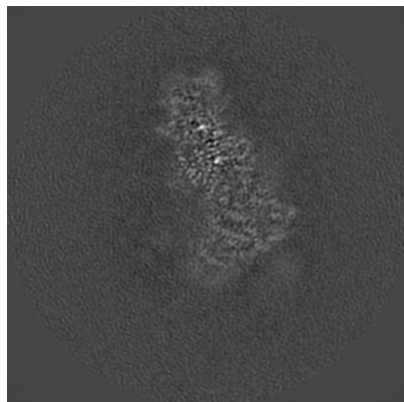


Z Index: 180

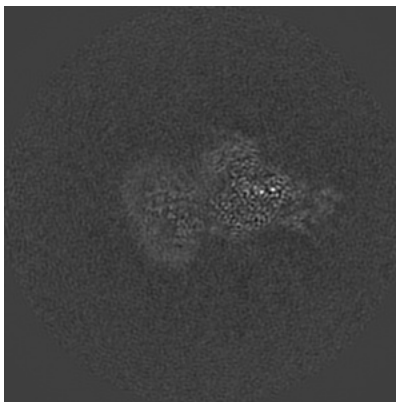
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

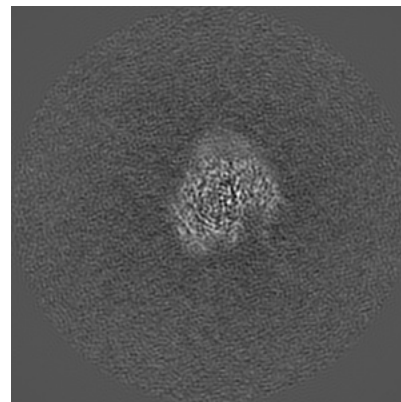
6.3.1 Primary map



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 surface views [i](#)

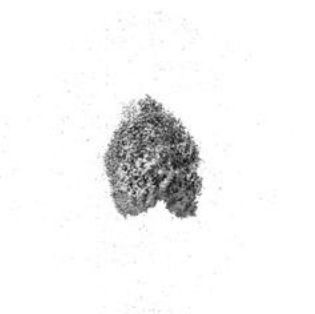
6.4.1 Primary map



X



Y



Z

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

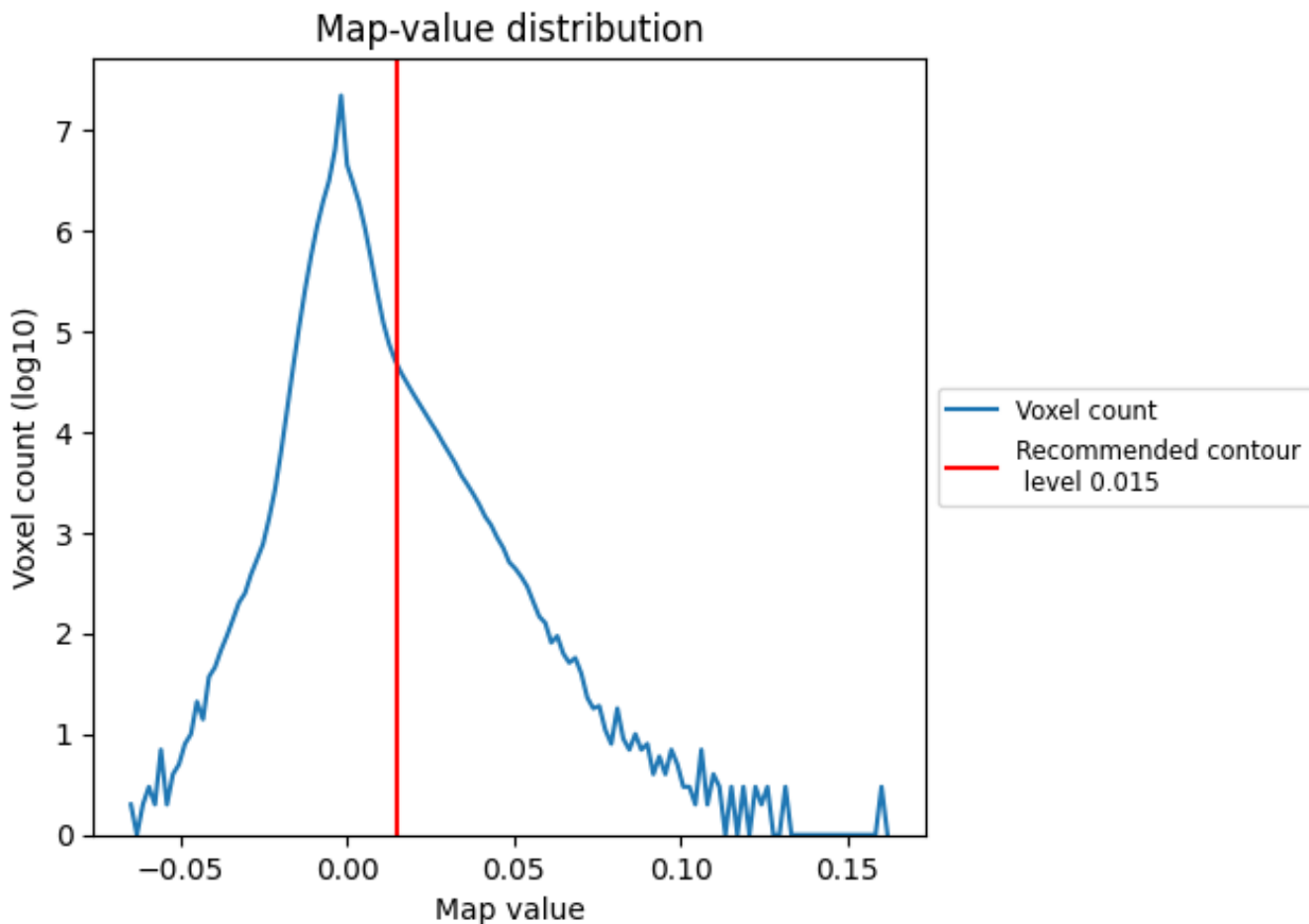
6.5 Mask visualisation

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

7 Map analysis [i](#)

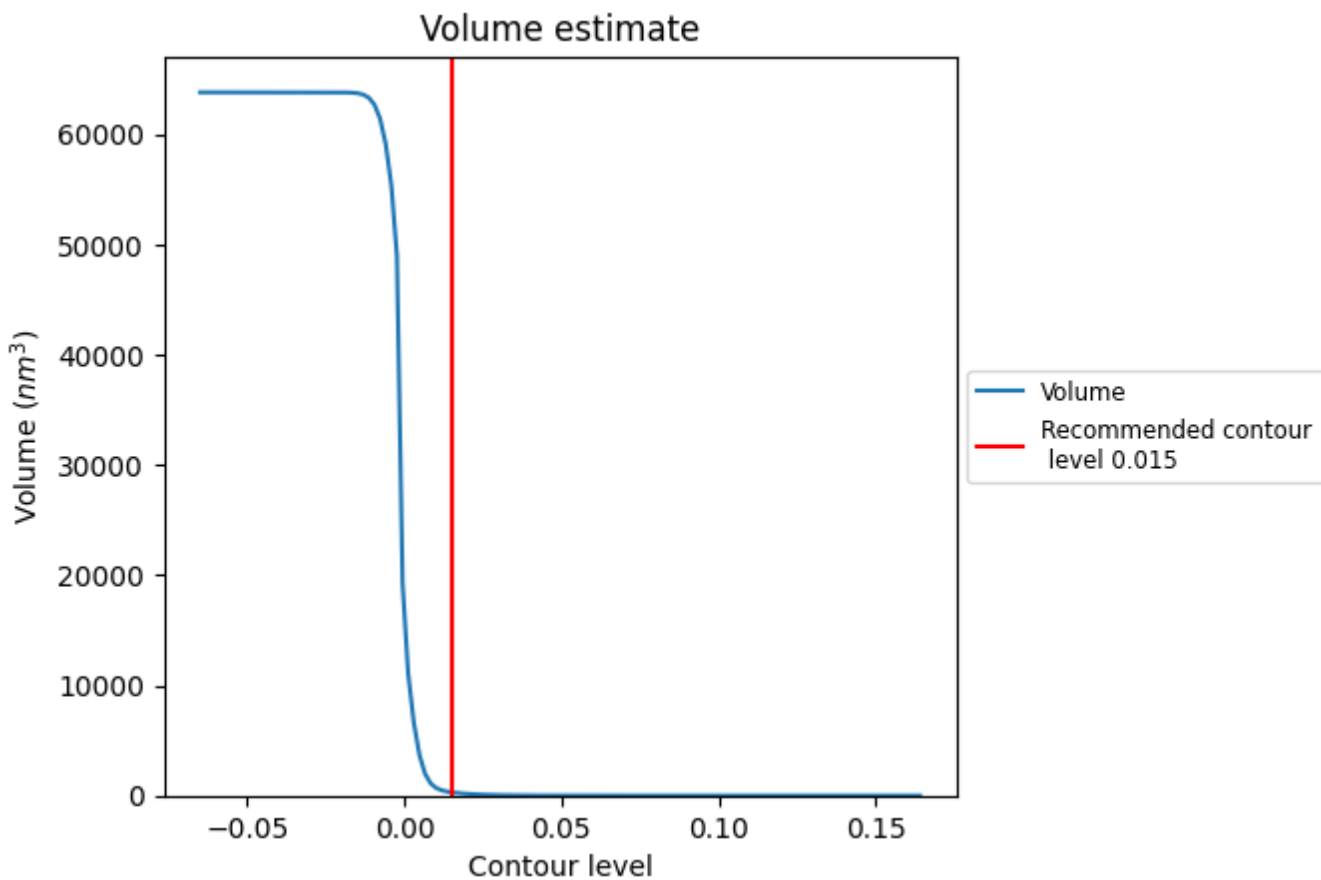
This section contains the results of statistical analysis of the map.

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.

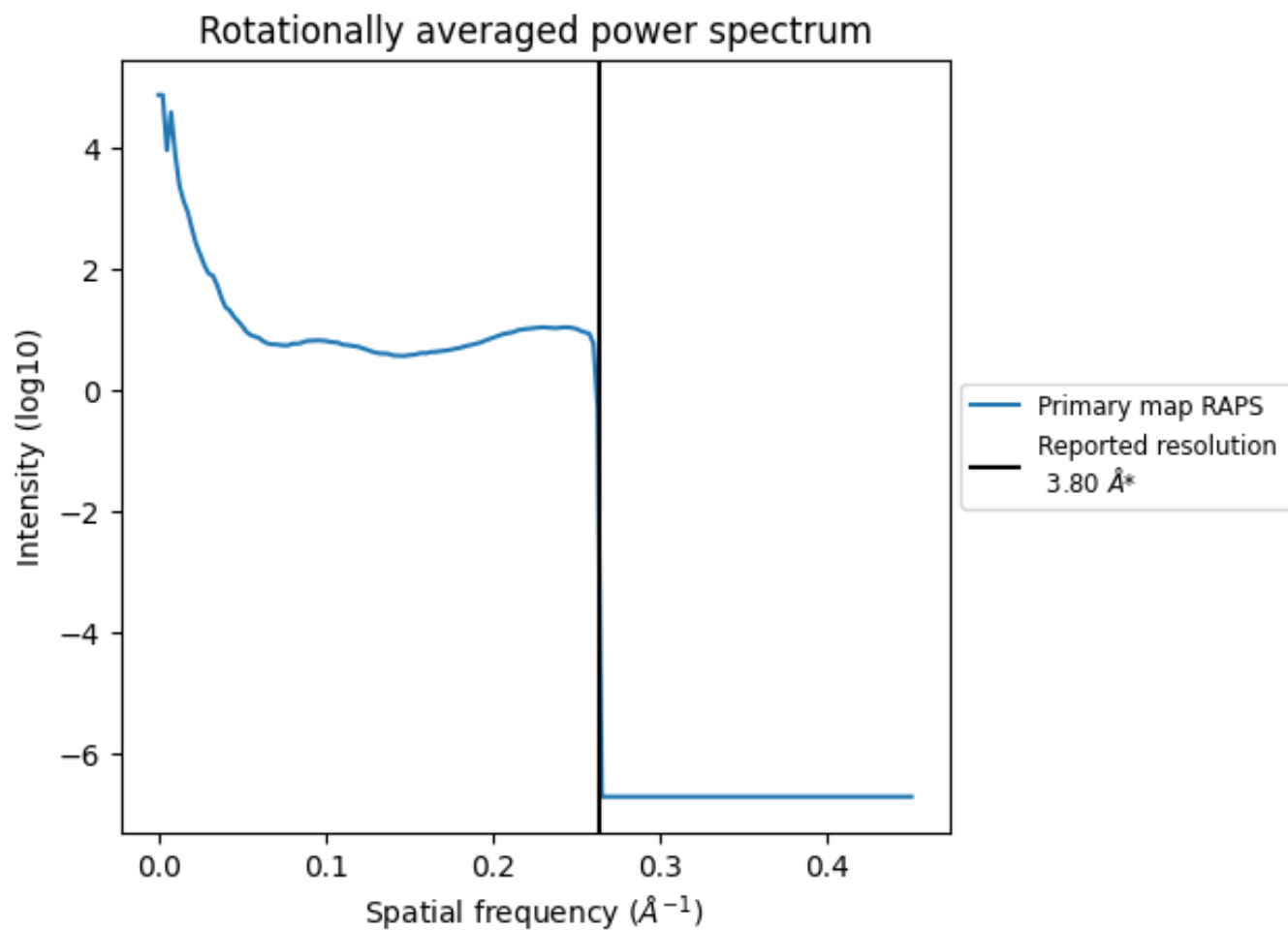
7.2 Volume estimate [i](#)



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

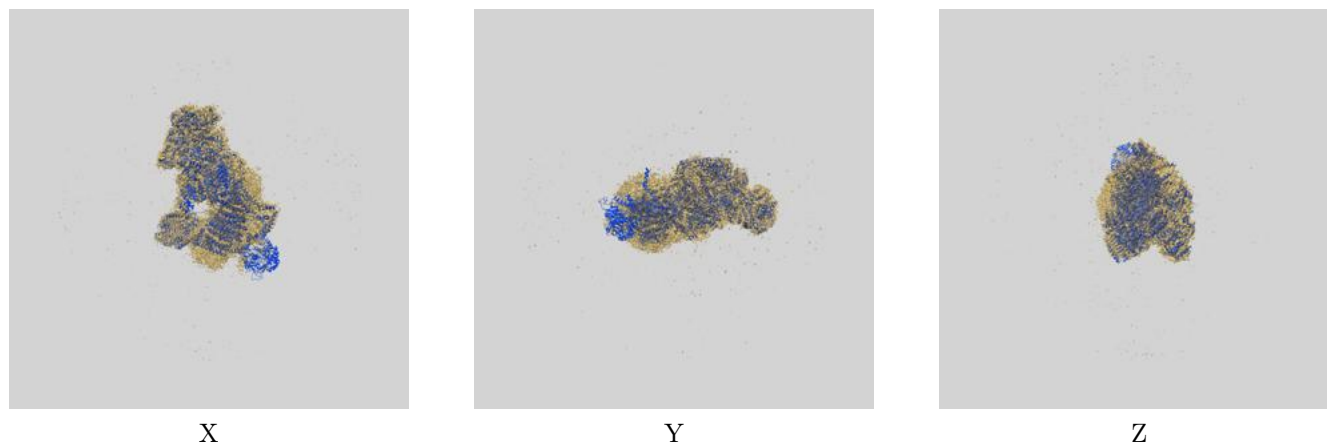
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

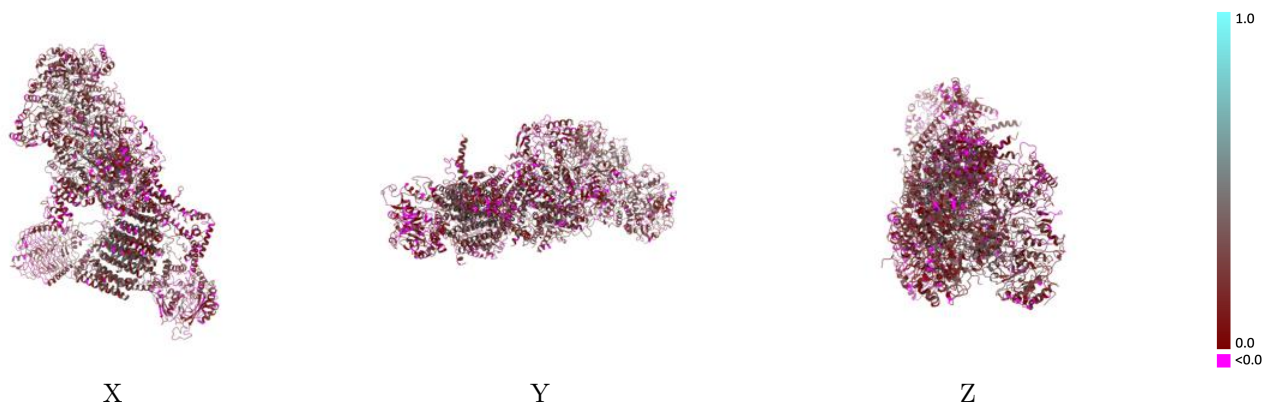
This section contains information regarding the fit between EMDB map EMD-11615 and PDB model 7A24. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



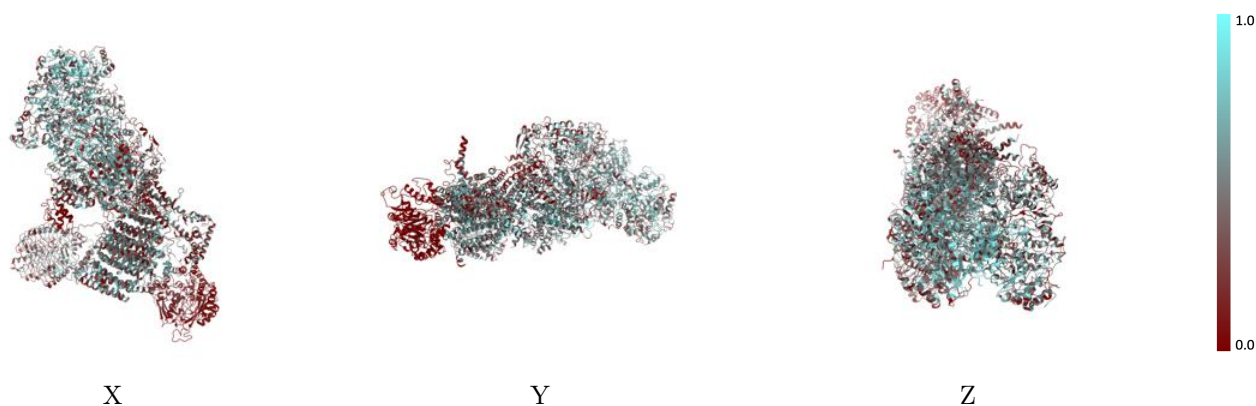
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



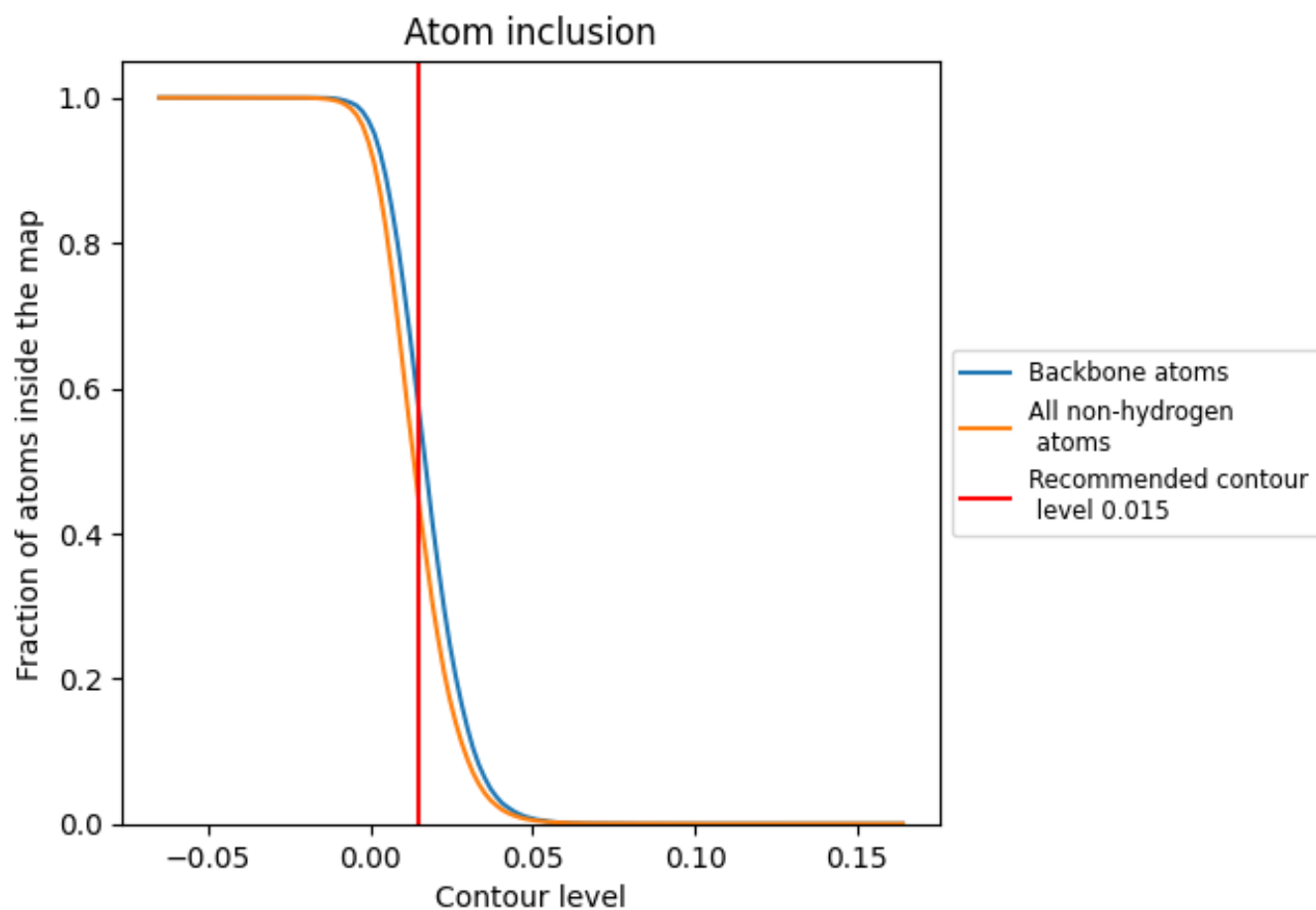
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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







































































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

