Full wwPDB EM Validation Report (i)

Sep 28, 2024 – 06:13 pm BST

PDB ID	:	8BA0
EMDB ID	:	EMD-15937
Title	:	Drosophila melanogaster complex I in the Twisted state (Dm2)
Authors	:	Agip, A.N.A.; Chung, I.; Sanchez-Martinez, A.; Whitworth, A.J.; Hirst, J.
Deposited on	:	2022-10-10
Resolution	:	3.68 Å(reported)
Based on initial model	:	6ZR2

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 (i) symbol.

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

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

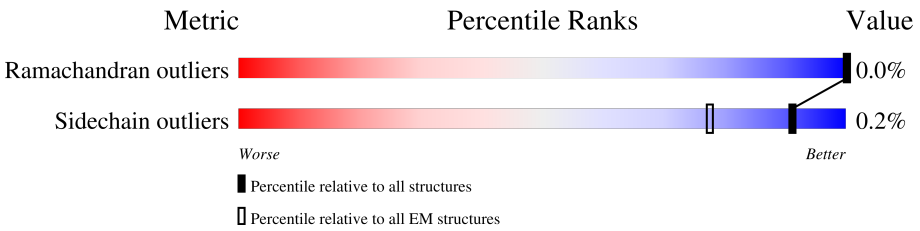
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.68 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	117	19% 99% •
2	B	182	7% 99% ••
3	C	209	9% 100%
4	D	428	14% 99% •
5	E	214	10% 100%
6	F	439	6% 100%
7	G	731	8% 92% 7%
8	H	315	8% 100%
9	I	186	5% 99% •

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Mol	Chain	Length	Quality of chain
10	J	167	16% 98%
11	K	93	32% 100%
12	L	577	29% 100%
13	M	446	23% 100%
14	N	341	22% 100%
15	O	368	30% 99%
16	P	377	12% 100%
17	Q	130	12% 100%
18	R	89	7% 100%
19	T	152	25% 51% 49%
19	U	152	30% 54% 44%
20	V	118	8% 100%
21	W	114	9% 100%
22	X	174	18% 99%
23	Y	167	60% 100%
24	Z	146	10% 100%
25	a	73	16% 100%
26	b	66	21% 100%
27	d	115	25% 100%
28	e	100	14% 100%
29	f	56	48% 100%
30	g	106	39% 99%
31	h	145	17% 100%
32	i	161	42% 99%
33	j	59	49% 98%

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Mol	Chain	Length	Quality of chain
34	k	84	52% 99%
35	l	144	38% 100%
36	m	108	31% 100%
37	n	134	38% 100%
38	o	112	30% 99%
39	p	151	16% 99%
40	q	135	21% 100%
41	r	103	23% 86% 14%
42	s	62	35% 100%

2 Entry composition (i)

There are 51 unique types of molecules in this entry. The entry contains 65912 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 NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	117	956	652	141	156	7	0	0

- Molecule 2 is a protein called LD31474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	182	1435	920	251	250	14	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	209	1726	1103	303	315	5	0	0

- Molecule 4 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	428	3424	2196	577	628	23	0	0

- Molecule 5 is a protein called NADH dehydrogenase (Ubiquinone) 24 kDa subunit, isoform A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	214	1679	1062	285	320	12	0	0

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	439	3367	2129	599	613	26	0	0

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	677	5146	3225	912	980	29	0	0

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	315	2571	1764	367	418	22	0	0

- Molecule 9 is a protein called NADH dehydrogenase (ubiquinone) 23 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	186	1485	935	251	287	12	0	0

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	167	1351	917	192	227	15	0	0

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	93	771	526	110	123	12	0	0

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	577	4606	3092	680	774	60	0	0

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	446	3617	2459	533	583	42	0	0

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	341	2796	1893	411	458	34	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	368	3007	1927	504	560	16	0	0

- Molecule 16 is a protein called NADH dehydrogenase (Ubiquinone) 39 kDa subunit, isoform A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	377	3032	1934	546	542	10	0	0

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	130	1054	659	198	193	4	0	0

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	89	716	453	130	129	4	0	0

- Molecule 19 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	T	77	615	398	94	121	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	U	85	684	442	103	137	2	0	0

- Molecule 20 is a protein called NADH dehydrogenase (Ubiquinone) 13 kDa B subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	V	118	922	588	162	168	4	0	0

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W	114	968	620	172	170	6	0	0

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	X	174	1383	867	240	266	10	0	0

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Y	167	1277	829	212	230	6	0	0

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Z	146	1201	787	203	209	2	0	0

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	a	73	601	386	101	108	6	0	0

- Molecule 26 is a protein called RH45008p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	b	66	519	327	95	96	1	0	0

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	d	115	907	590	159	157	1	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	e	100	828	523	145	149	11	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	f	56	437	283	77	74	3	0	0

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	g	106	870	560	140	169	1	0	0

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	h	145	1234	795	213	223	3	0	0

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	i	161	1302	829	242	226	5	0	0

- Molecule 33 is a protein called GEO11417p1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	j	59	489	319	88	81	1	0	0

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	k	84	671	437	117	116	1	0	0

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	l	144	1201	783	191	223	4	0	0

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	m	108	892	571	163	157	1	0	0

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	n	134	1152	735	218	196	3	0	0

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	o	112	937	596	163	169	9	0	0

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	p	151	1266	795	233	228	10	0	0

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	q	135	1130	735	189	201	5	0	0

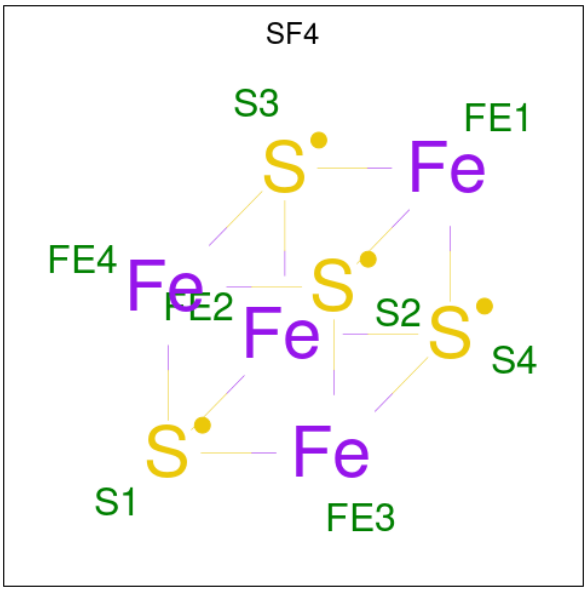
- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	r	89	724	457	136	130	1	0	0

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

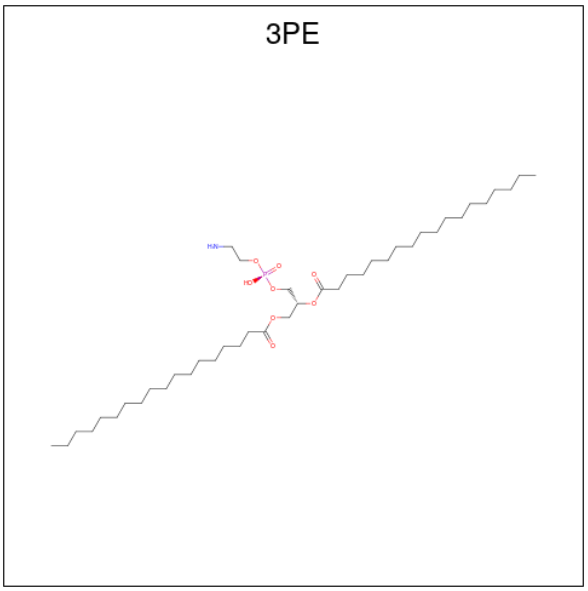
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	s	62	456	288	75	90	3	0	0

- Molecule 43 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



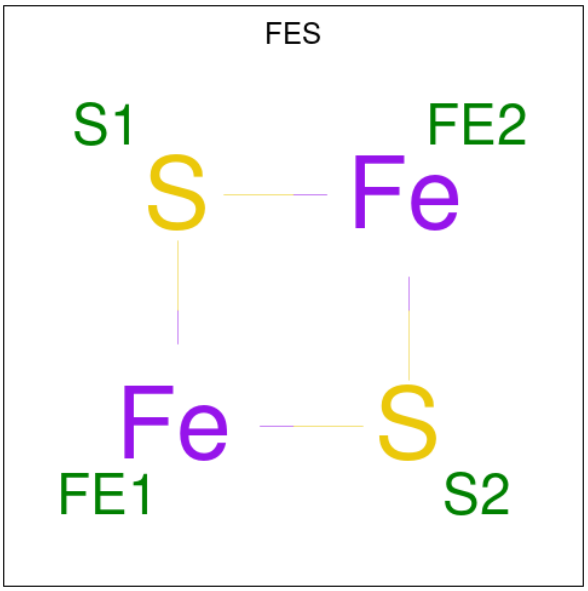
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
43	B	1	8	4	4	0
43	F	1	8	4	4	0
43	G	1	8	4	4	0
43	G	1	8	4	4	0
43	I	1	8	4	4	0
43	I	1	8	4	4	0

- Molecule 44 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



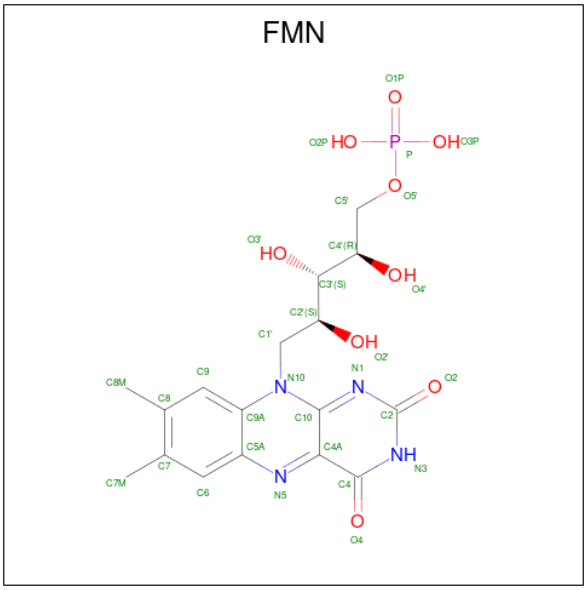
Mol	Chain	Residues	Atoms					AltConf
44	B	1	Total	C	N	O	P	0
			42	32	1	8	1	
44	B	1	Total	C	N	O	P	0
			26	16	1	8	1	
44	L	1	Total	C	N	O	P	0
			35	25	1	8	1	
44	Y	1	Total	C	N	O	P	0
			20	10	1	8	1	
44	Y	1	Total	C	N	O	P	0
			22	12	1	8	1	
44	Y	1	Total	C	N	O	P	0
			25	15	1	8	1	

- Molecule 45 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



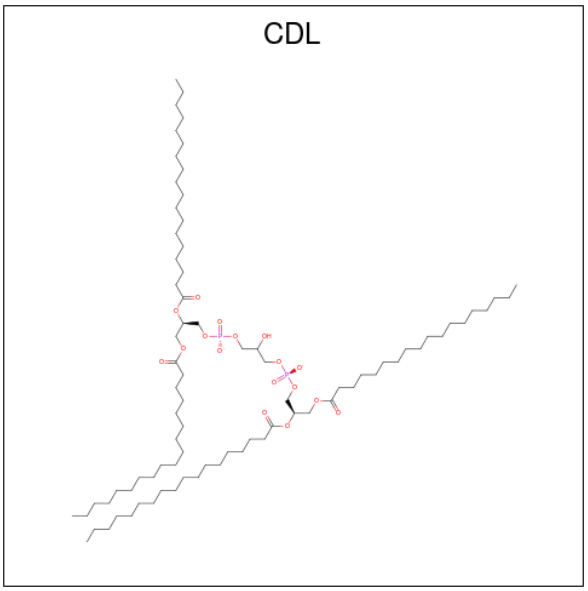
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	E	1	4	2	2	0
45	G	1	4	2	2	0

- Molecule 46 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



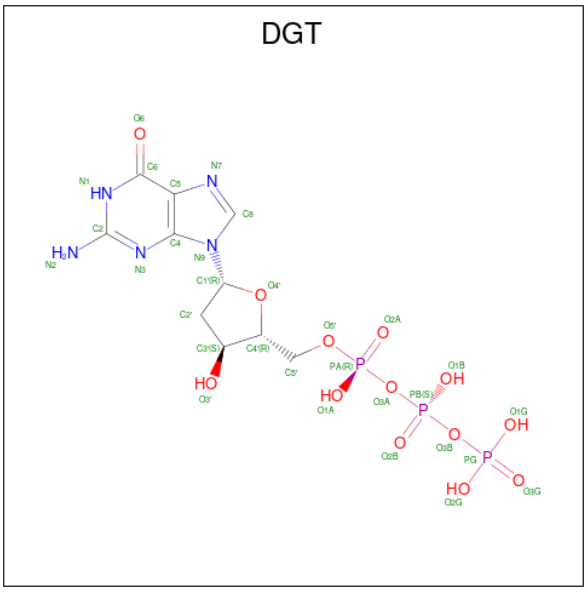
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	F	1	31	17	4	9	1	0

- Molecule 47 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



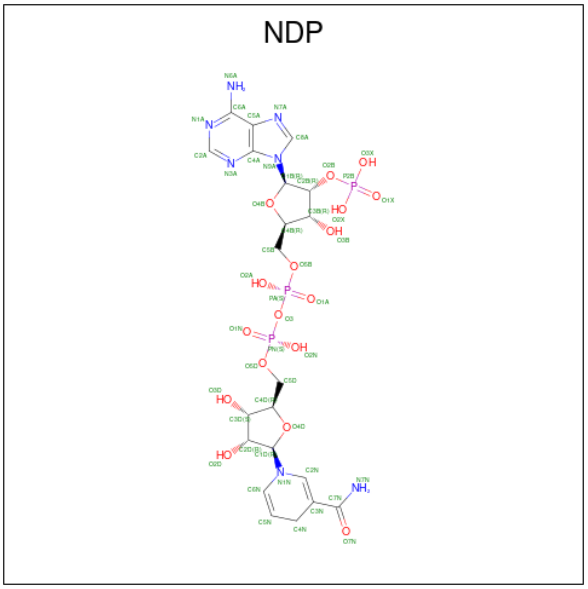
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
47	M	1	55	36	17	2	0
			Total	C	O	P	
47	P	1	41	22	17	2	0

- Molecule 48 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	O	1	31	10	5	13	3	0

- Molecule 49 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

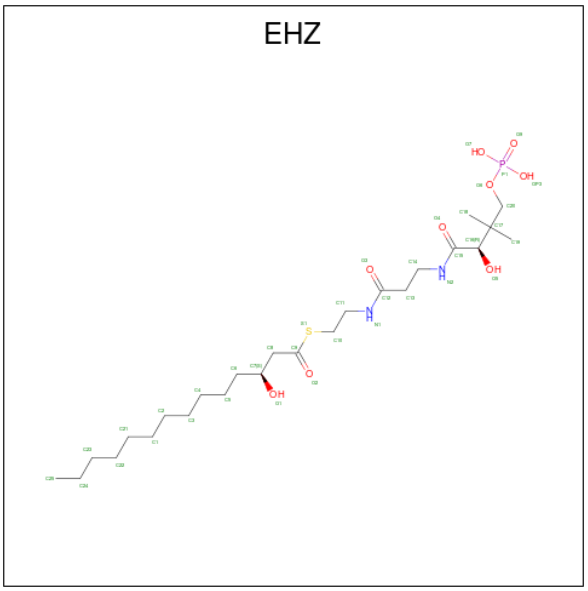


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	P	1	48	21	7	17	3	0

- Molecule 50 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
50	R	1	1	1	0

- Molecule 51 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



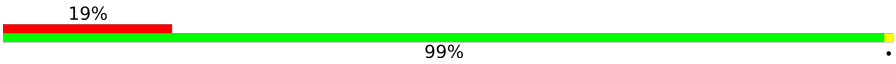
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
51	T	1	37	25	2	8	1	1	0
			Total	C	N	O	P	S	
51	U	1	37	25	2	8	1	1	0

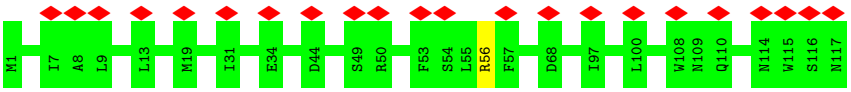
3 Residue-property plots (i)

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: NADH-ubiquinone oxidoreductase chain 3

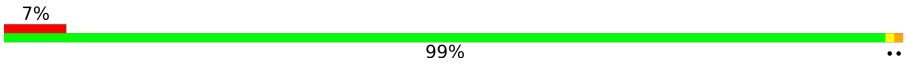
Chain A:

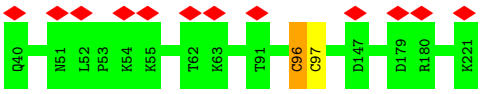




• Molecule 2: LD31474p

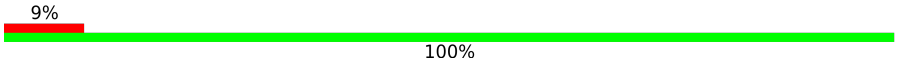
Chain B:

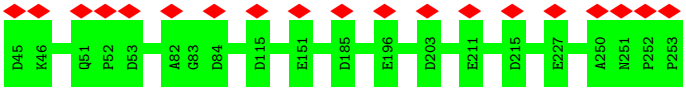




• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

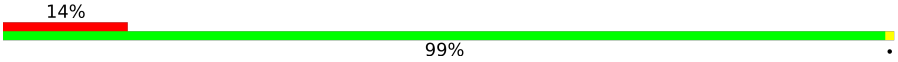
Chain C:

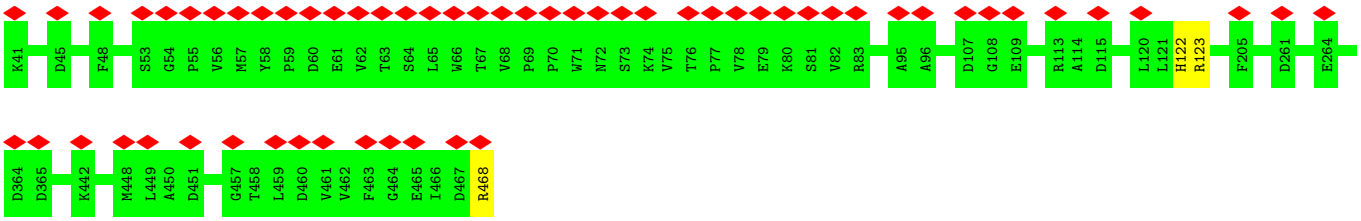




• Molecule 4: Complex I-49kD

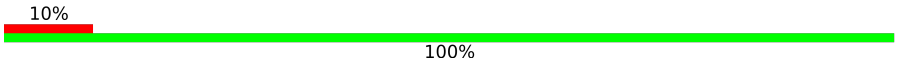
Chain D:

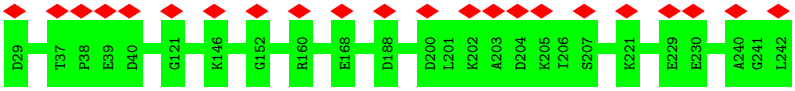




• Molecule 5: NADH dehydrogenase (Ubiquinone) 24 kDa subunit, isoform A

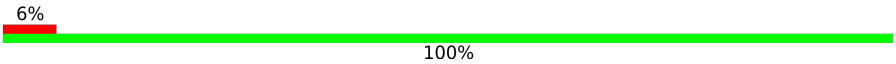
Chain E:

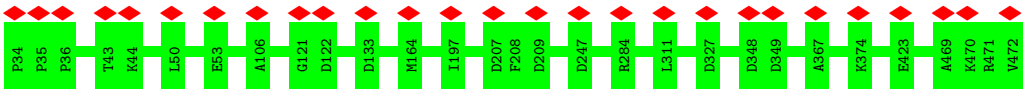




• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

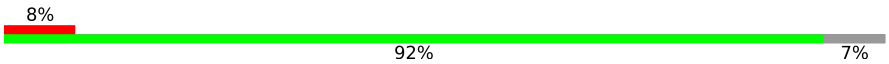
Chain F:

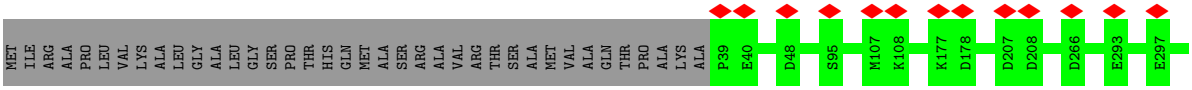


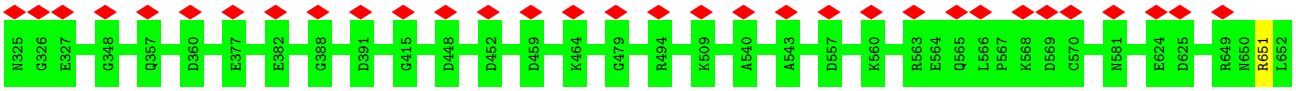


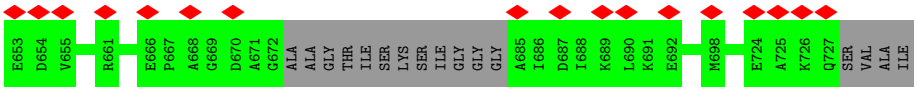
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:



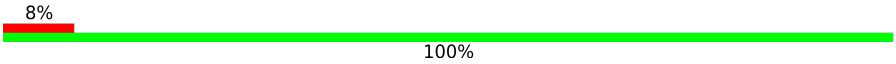


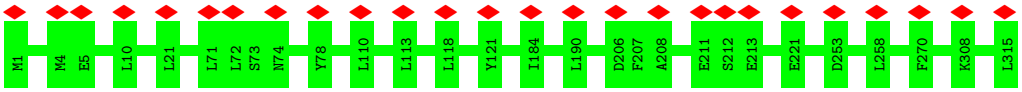




• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

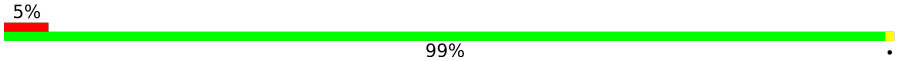
Chain H:

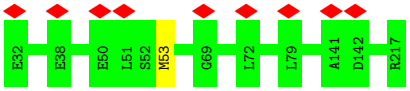




• Molecule 9: NADH dehydrogenase (ubiquinone) 23 kDa subunit

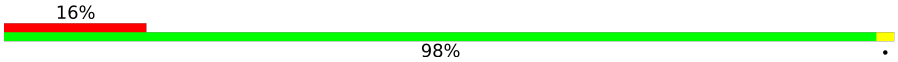
Chain I:

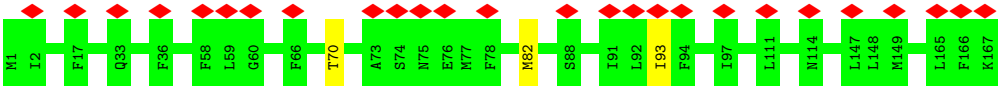




• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

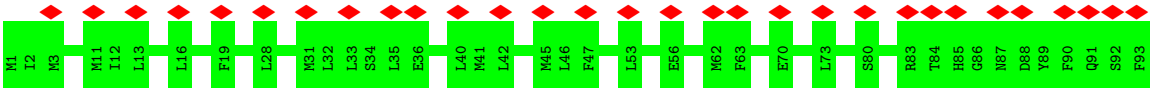
Chain J:





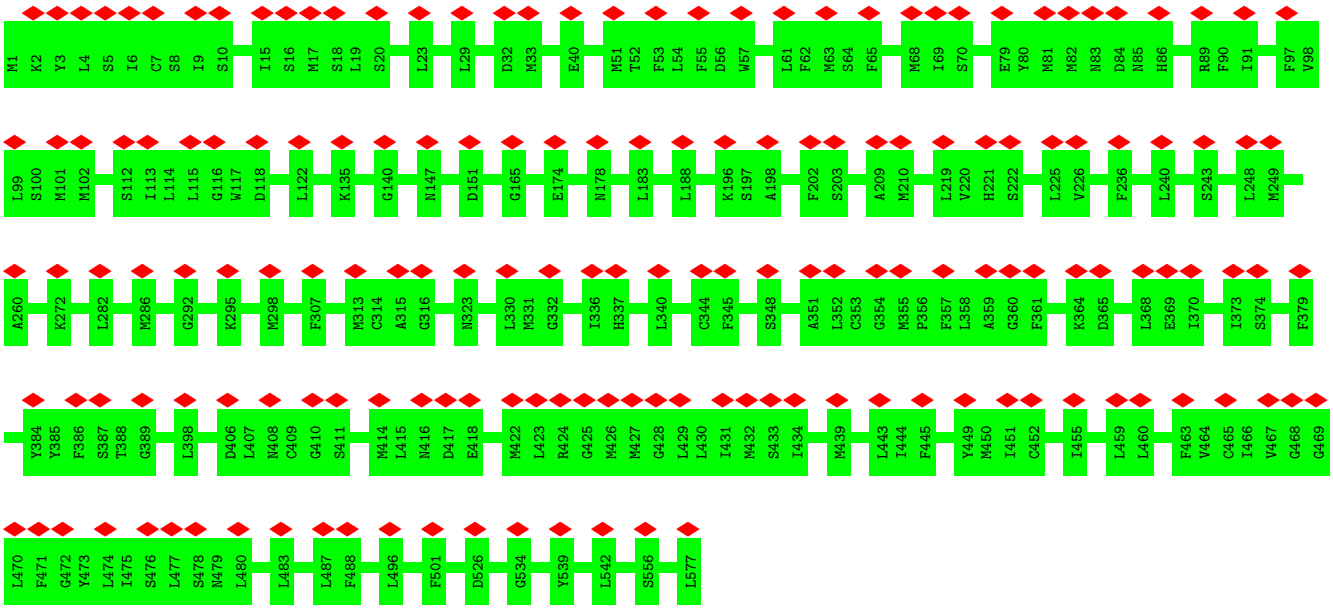
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K: 32% 100%



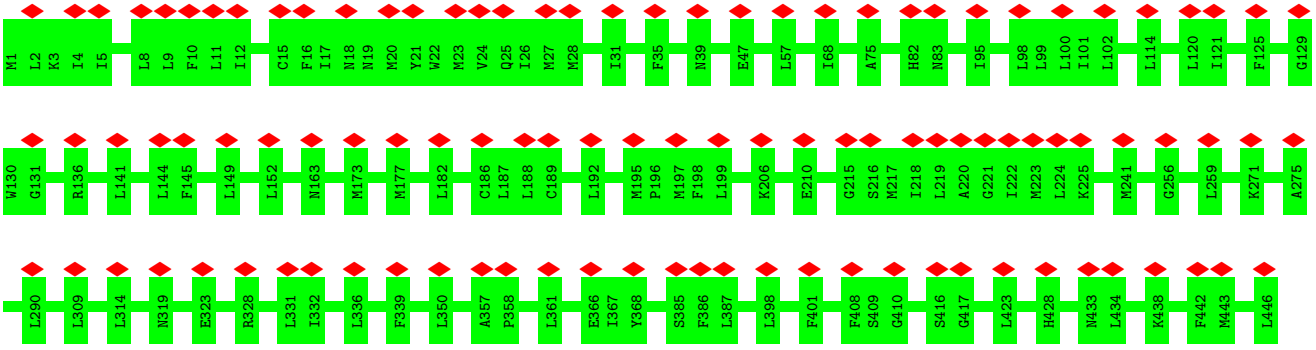
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L: 29% 100%



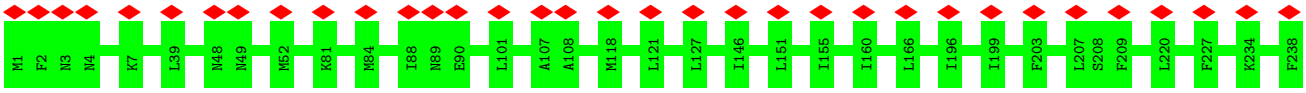
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

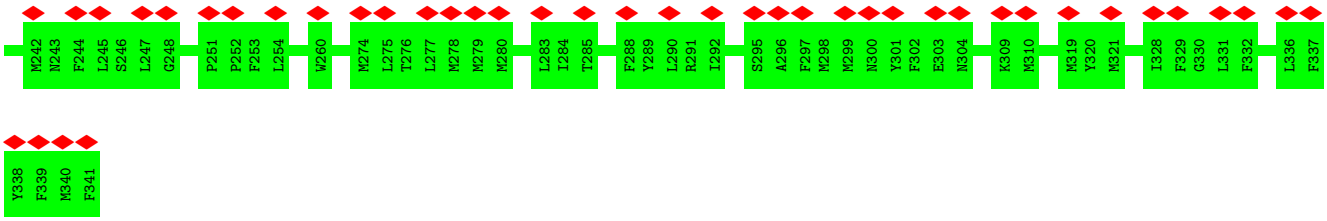
Chain M: 23% 100%



• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

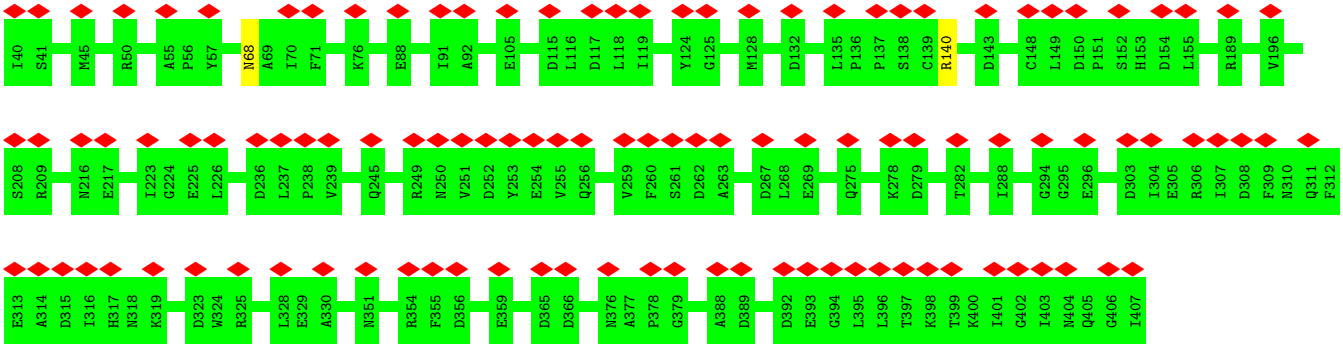
Chain N: 22% 100%





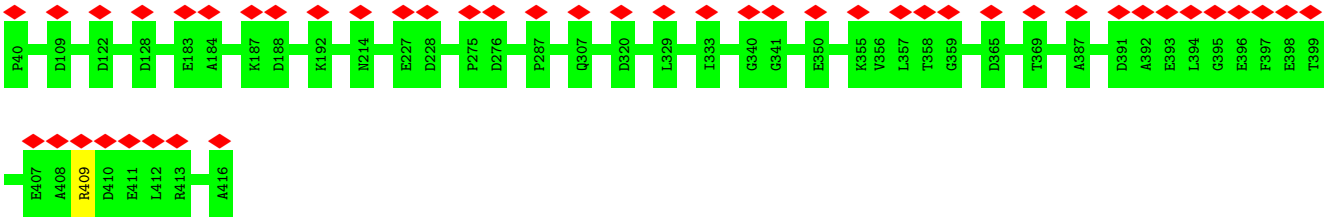
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O: 30% 99%



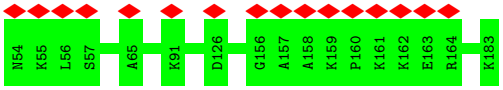
• Molecule 16: NADH dehydrogenase (Ubiquinone) 39 kDa subunit, isoform A

Chain P: 12% 100%



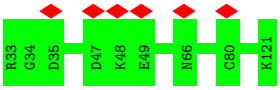
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q: 12% 100%



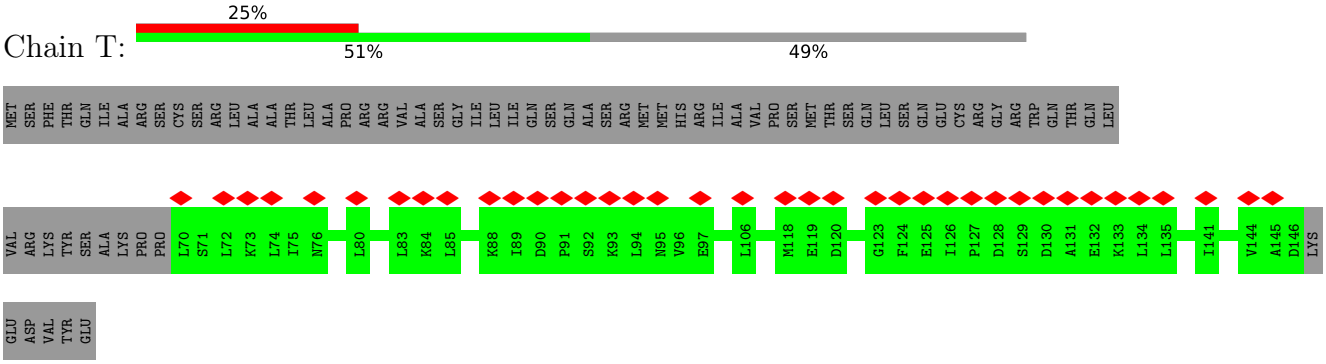
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R: 7% 100%



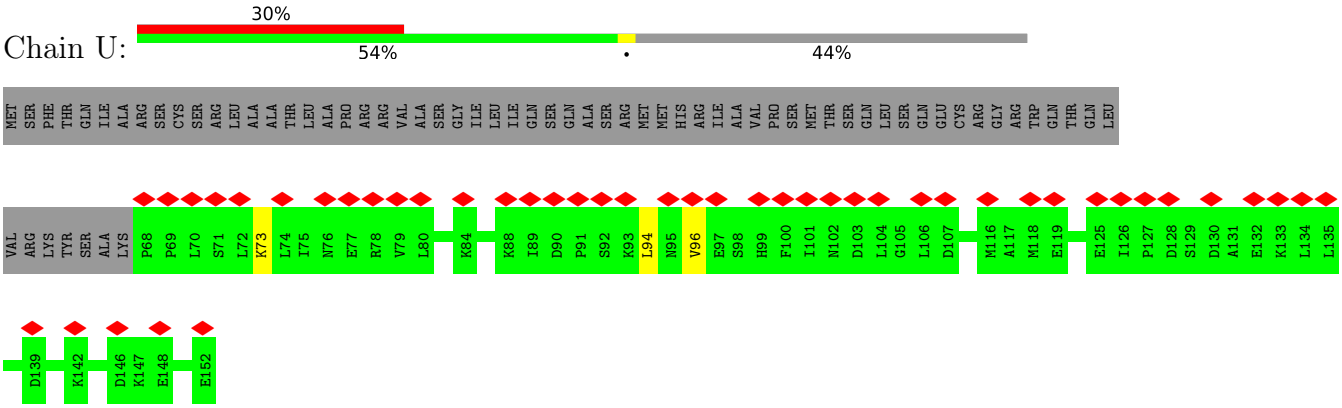
• Molecule 19: Acyl carrier protein, mitochondrial

Chain T:



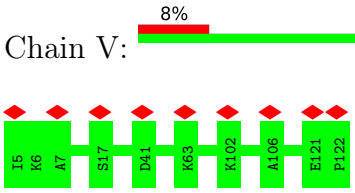
- Molecule 19: Acyl carrier protein, mitochondrial

Chain U:



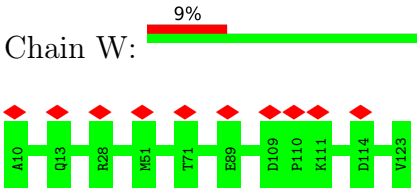
- Molecule 20: NADH dehydrogenase (Ubiquinone) 13 kDa B subunit

Chain V:



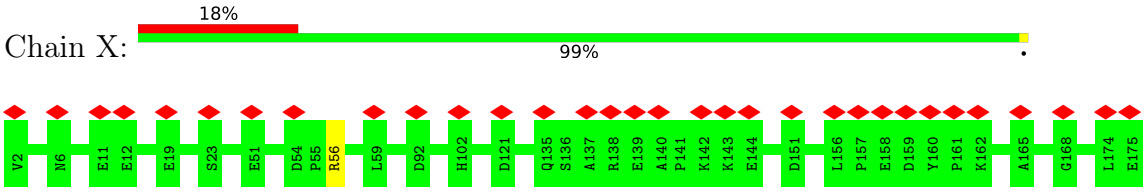
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:



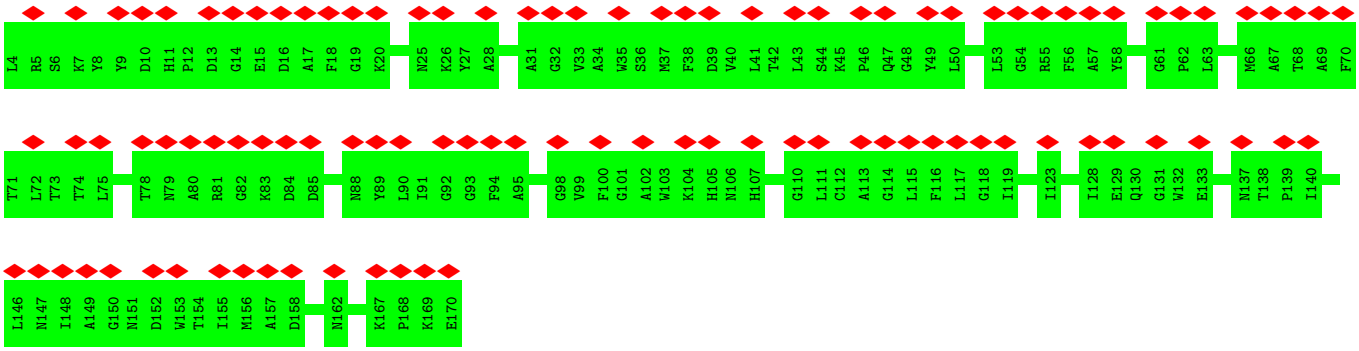
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:



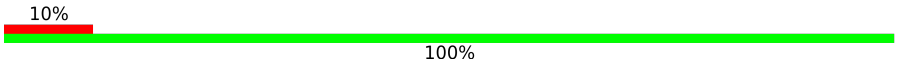
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

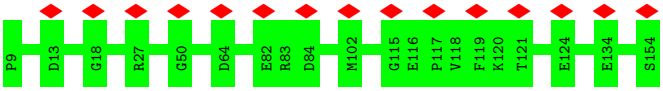
Chain Y:



• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

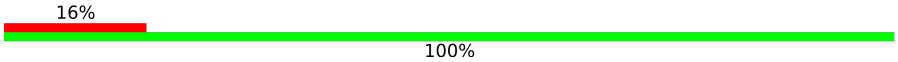
Chain Z:

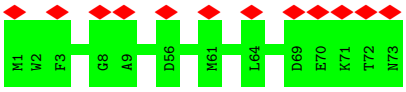




• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

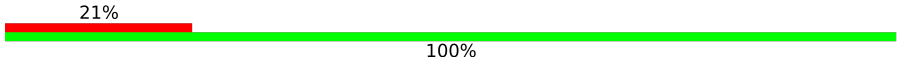
Chain a:

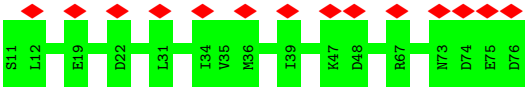




• Molecule 26: RH45008p

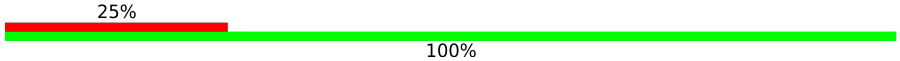
Chain b:

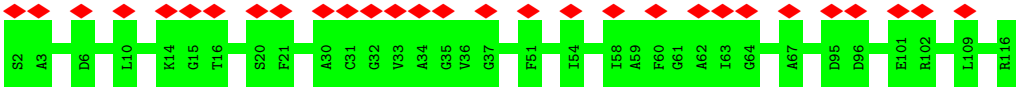




• Molecule 27: NADH dehydrogenase [ubiquinone] 1 subunit C2

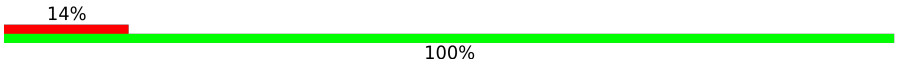
Chain d:

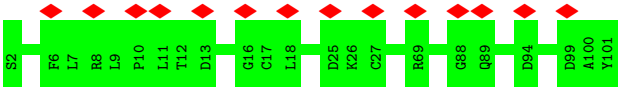




• Molecule 28: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

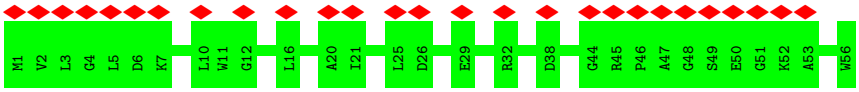
Chain e:





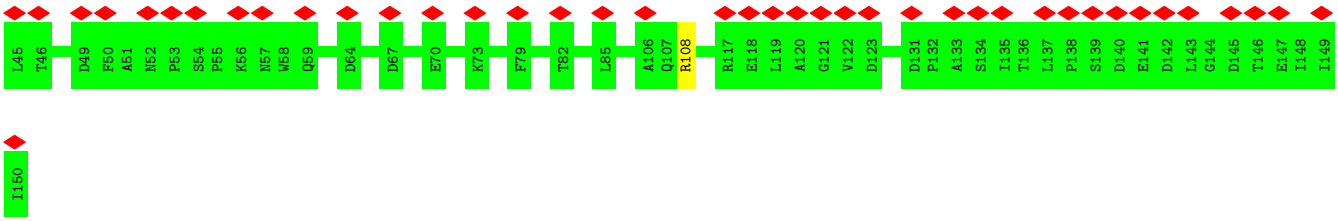
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f: 48% 100%



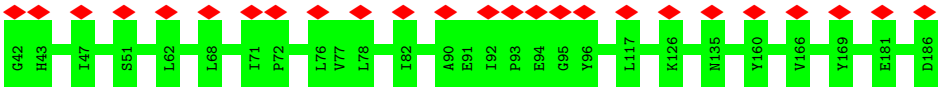
• Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g: 39% 99%



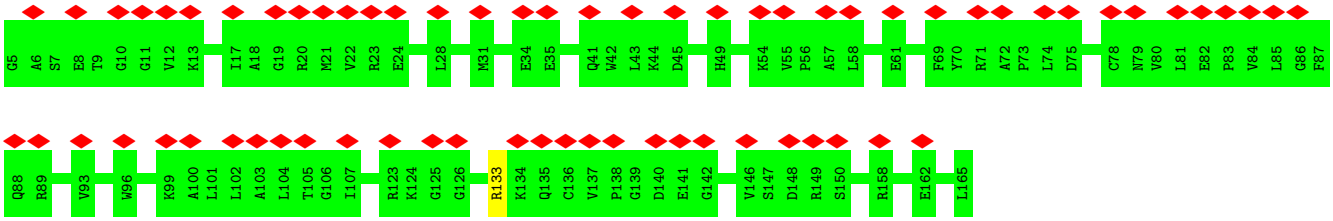
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h: 17% 100%



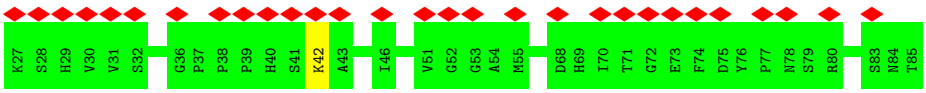
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i: 42% 99%



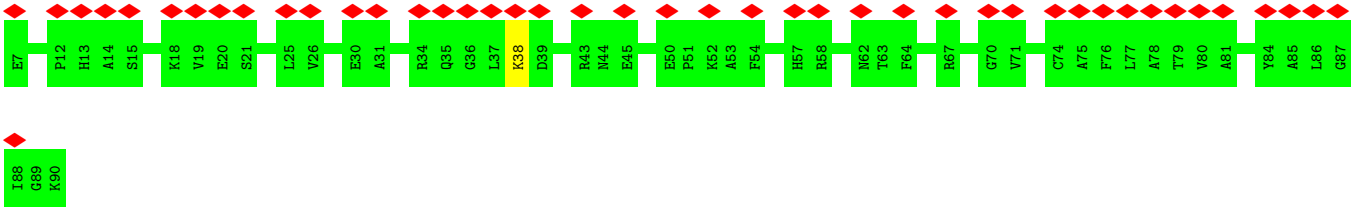
• Molecule 33: GEO11417p1

Chain j: 49% 98%



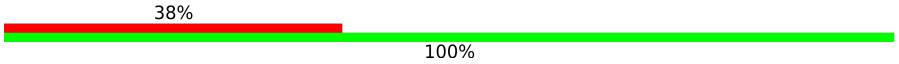
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

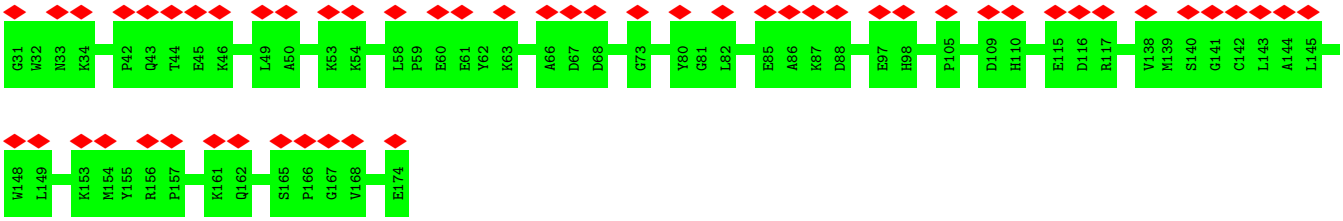
Chain k: 52% 99%



• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

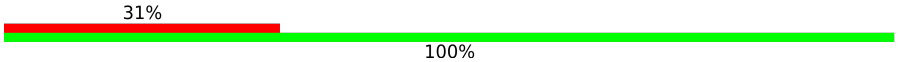
Chain l:

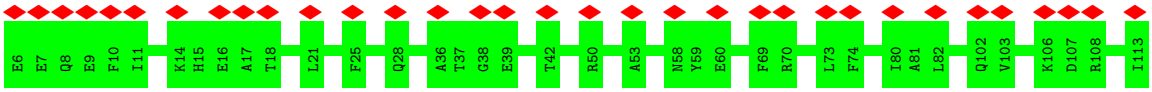




• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

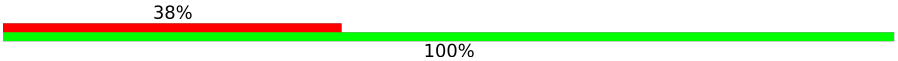
Chain m:

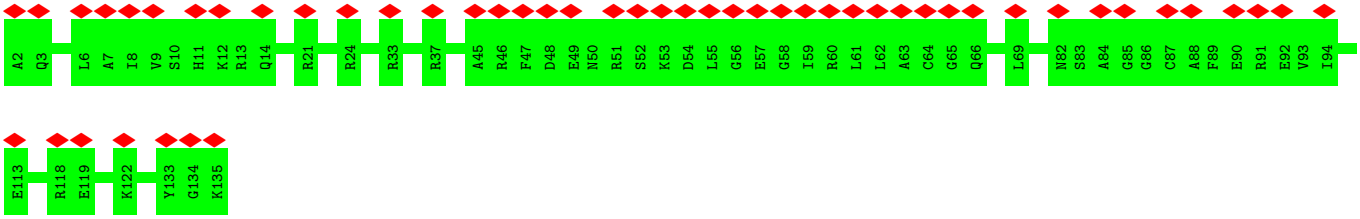




• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

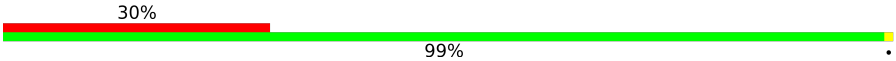
Chain n:

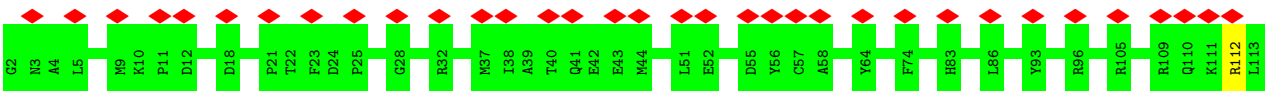




• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

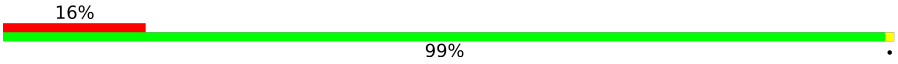
Chain o:

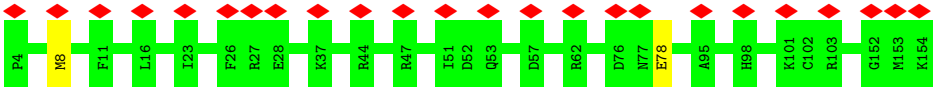




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

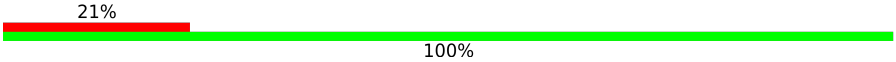
Chain p:

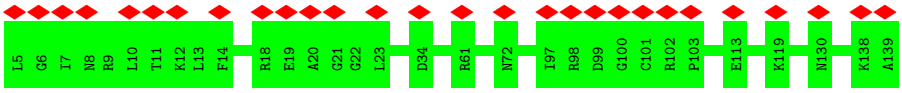




• Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

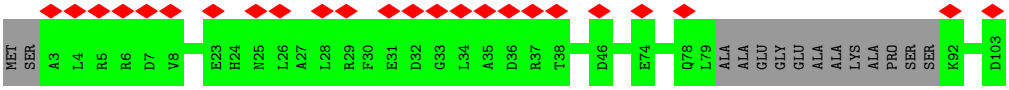
Chain q:





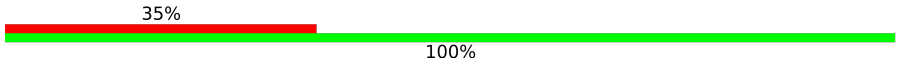
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

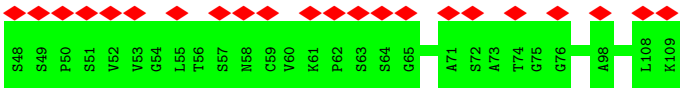
Chain r:



• Molecule 42: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12343	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	41.88	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.016	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	471.59998, 471.59998, 471.59998	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, ZN, DGT, CDL, 3PE, NDP, FES, EHZ, SF4, 2MR

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	0.34	0/979	0.51	0/1325
2	B	0.54	1/1473 (0.1%)	0.56	1/1997 (0.1%)
3	C	0.40	0/1774	0.51	0/2412
4	D	0.41	0/3495	0.50	0/4737
5	E	0.37	0/1718	0.47	0/2328
6	F	0.38	0/3447	0.52	0/4659
7	G	0.36	0/5229	0.49	0/7088
8	H	0.40	0/2651	0.49	0/3593
9	I	0.47	0/1518	0.53	0/2050
10	J	0.35	0/1377	0.57	2/1863 (0.1%)
11	K	0.40	0/792	0.55	0/1066
12	L	0.35	0/4726	0.49	0/6396
13	M	0.37	0/3723	0.47	0/5045
14	N	0.37	0/2875	0.51	0/3890
15	O	0.34	0/3082	0.49	0/4168
16	P	0.36	0/3108	0.50	0/4205
17	Q	0.37	0/1082	0.48	0/1465
18	R	0.44	0/733	0.47	0/987
19	T	0.29	0/624	0.50	0/843
19	U	0.33	0/696	0.62	3/940 (0.3%)
20	V	0.32	0/942	0.45	0/1278
21	W	0.37	0/988	0.49	0/1329
22	X	0.33	0/1416	0.47	0/1911
23	Y	0.29	0/1314	0.44	0/1784
24	Z	0.36	0/1239	0.47	0/1682
25	a	0.38	0/614	0.52	0/827
26	b	0.34	0/528	0.52	0/714
27	d	0.33	0/935	0.48	0/1271
28	e	0.36	0/846	0.52	0/1128
29	f	0.33	0/448	0.59	0/600
30	g	0.36	0/895	0.55	1/1222 (0.1%)
31	h	0.37	0/1269	0.47	0/1714

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	i	0.34	0/1338	0.53	0/1808
33	j	0.31	0/513	0.44	0/704
34	k	0.34	0/690	0.54	0/936
35	l	0.37	0/1250	0.46	0/1701
36	m	0.34	0/913	0.50	0/1222
37	n	0.34	0/1185	0.48	0/1597
38	o	0.30	0/960	0.49	0/1290
39	p	0.43	2/1299 (0.2%)	0.52	0/1752
40	q	0.41	0/1169	0.46	0/1585
41	r	0.35	0/740	0.50	0/1003
42	s	0.38	0/469	0.48	0/637
All	All	0.37	3/67062 (0.0%)	0.50	7/90752 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	96	CYS	CB-SG	-9.70	1.65	1.82
39	p	78	GLU	CG-CD	-5.41	1.43	1.51
39	p	78	GLU	CB-CG	-5.18	1.42	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	U	96	VAL	CG1-CB-CG2	6.80	121.77	110.90
10	J	93	ILE	CG1-CB-CG2	6.21	125.05	111.40
2	B	97	CYS	CA-CB-SG	5.99	124.77	114.00
19	U	94	LEU	CB-CG-CD2	5.72	120.72	111.00
19	U	94	LEU	CB-CG-CD1	5.51	120.37	111.00
30	g	108	ARG	NE-CZ-NH1	-5.22	117.69	120.30
10	J	70	THR	CA-CB-CG2	5.03	119.44	112.40

There are no chirality outliers.

There are no planarity outliers.

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	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
2	B	180/182 (99%)	167 (93%)	12 (7%)	1 (1%)	22	54
3	C	207/209 (99%)	185 (89%)	22 (11%)	0	100	100
4	D	425/428 (99%)	397 (93%)	27 (6%)	1 (0%)	44	72
5	E	212/214 (99%)	195 (92%)	17 (8%)	0	100	100
6	F	437/439 (100%)	405 (93%)	32 (7%)	0	100	100
7	G	673/731 (92%)	622 (92%)	51 (8%)	0	100	100
8	H	313/315 (99%)	282 (90%)	31 (10%)	0	100	100
9	I	184/186 (99%)	174 (95%)	10 (5%)	0	100	100
10	J	165/167 (99%)	150 (91%)	15 (9%)	0	100	100
11	K	91/93 (98%)	84 (92%)	7 (8%)	0	100	100
12	L	575/577 (100%)	535 (93%)	40 (7%)	0	100	100
13	M	444/446 (100%)	412 (93%)	32 (7%)	0	100	100
14	N	339/341 (99%)	317 (94%)	22 (6%)	0	100	100
15	O	366/368 (100%)	328 (90%)	38 (10%)	0	100	100
16	P	375/377 (100%)	345 (92%)	30 (8%)	0	100	100
17	Q	128/130 (98%)	111 (87%)	17 (13%)	0	100	100
18	R	87/89 (98%)	80 (92%)	7 (8%)	0	100	100
19	T	75/152 (49%)	70 (93%)	5 (7%)	0	100	100
19	U	83/152 (55%)	69 (83%)	14 (17%)	0	100	100
20	V	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
21	W	112/114 (98%)	105 (94%)	7 (6%)	0	100	100
22	X	172/174 (99%)	157 (91%)	15 (9%)	0	100	100
23	Y	165/167 (99%)	157 (95%)	8 (5%)	0	100	100
24	Z	144/146 (99%)	138 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	a	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
26	b	64/66 (97%)	58 (91%)	6 (9%)	0	100	100
27	d	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
28	e	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
29	f	54/56 (96%)	42 (78%)	12 (22%)	0	100	100
30	g	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
31	h	143/145 (99%)	132 (92%)	11 (8%)	0	100	100
32	i	159/161 (99%)	147 (92%)	12 (8%)	0	100	100
33	j	57/59 (97%)	53 (93%)	4 (7%)	0	100	100
34	k	82/84 (98%)	64 (78%)	17 (21%)	1 (1%)	11	41
35	l	142/144 (99%)	125 (88%)	17 (12%)	0	100	100
36	m	106/108 (98%)	93 (88%)	13 (12%)	0	100	100
37	n	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
38	o	110/112 (98%)	99 (90%)	11 (10%)	0	100	100
39	p	149/151 (99%)	136 (91%)	13 (9%)	0	100	100
40	q	133/135 (98%)	123 (92%)	10 (8%)	0	100	100
41	r	85/103 (82%)	81 (95%)	4 (5%)	0	100	100
42	s	60/62 (97%)	51 (85%)	9 (15%)	0	100	100
All	All	8045/8346 (96%)	7397 (92%)	645 (8%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	96	CYS
34	k	38	LYS
4	D	122	HIS

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	110/110 (100%)	109 (99%)	1 (1%)	75	84
2	B	152/152 (100%)	152 (100%)	0	100	100
3	C	187/187 (100%)	187 (100%)	0	100	100
4	D	367/367 (100%)	366 (100%)	1 (0%)	91	94
5	E	185/185 (100%)	185 (100%)	0	100	100
6	F	351/351 (100%)	351 (100%)	0	100	100
7	G	546/582 (94%)	545 (100%)	1 (0%)	92	95
8	H	282/282 (100%)	282 (100%)	0	100	100
9	I	159/159 (100%)	158 (99%)	1 (1%)	84	90
10	J	161/161 (100%)	160 (99%)	1 (1%)	84	90
11	K	88/88 (100%)	88 (100%)	0	100	100
12	L	518/518 (100%)	518 (100%)	0	100	100
13	M	404/404 (100%)	404 (100%)	0	100	100
14	N	317/317 (100%)	317 (100%)	0	100	100
15	O	324/324 (100%)	322 (99%)	2 (1%)	84	90
16	P	319/319 (100%)	318 (100%)	1 (0%)	91	94
17	Q	114/114 (100%)	114 (100%)	0	100	100
18	R	77/77 (100%)	77 (100%)	0	100	100
19	T	71/136 (52%)	71 (100%)	0	100	100
19	U	79/136 (58%)	78 (99%)	1 (1%)	65	77
20	V	97/97 (100%)	97 (100%)	0	100	100
21	W	107/107 (100%)	107 (100%)	0	100	100
22	X	150/150 (100%)	149 (99%)	1 (1%)	81	88
23	Y	128/128 (100%)	128 (100%)	0	100	100
24	Z	128/128 (100%)	128 (100%)	0	100	100
25	a	65/65 (100%)	65 (100%)	0	100	100
26	b	52/52 (100%)	52 (100%)	0	100	100
27	d	93/93 (100%)	93 (100%)	0	100	100
28	e	88/88 (100%)	88 (100%)	0	100	100
29	f	43/43 (100%)	43 (100%)	0	100	100
30	g	95/95 (100%)	95 (100%)	0	100	100
31	h	130/130 (100%)	130 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	i	133/133 (100%)	132 (99%)	1 (1%)	79	85
33	j	51/51 (100%)	50 (98%)	1 (2%)	50	68
34	k	69/69 (100%)	69 (100%)	0	100	100
35	l	121/121 (100%)	121 (100%)	0	100	100
36	m	89/89 (100%)	89 (100%)	0	100	100
37	n	117/117 (100%)	117 (100%)	0	100	100
38	o	101/101 (100%)	100 (99%)	1 (1%)	73	82
39	p	135/135 (100%)	134 (99%)	1 (1%)	81	88
40	q	116/116 (100%)	116 (100%)	0	100	100
41	r	78/86 (91%)	78 (100%)	0	100	100
42	s	50/50 (100%)	50 (100%)	0	100	100
All	All	7047/7213 (98%)	7033 (100%)	14 (0%)	91	95

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ARG
4	D	468	ARG
7	G	651	ARG
9	I	53	MET
10	J	82	MET
15	O	68	ASN
15	O	140	ARG
16	P	409	ARG
19	U	73	LYS
22	X	56	ARG
32	i	133	ARG
33	j	42	LYS
38	o	112	ARG
39	p	8	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	41	GLN
4	D	152	ASN
5	E	52	ASN

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Mol	Chain	Res	Type
5	E	82	GLN
5	E	195	GLN
6	F	437	HIS
7	G	296	ASN
7	G	644	ASN
14	N	182	HIS
19	T	111	HIS
21	W	39	GLN
22	X	172	HIS
31	h	63	HIS
35	l	98	HIS
39	p	43	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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\#\|Z\| > 2$
4	2MR	D	123	4	10,12,13	2.34	2 (20%)	5,13,15	4.11	2 (40%)

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
4	2MR	D	123	4	-	1/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	123	2MR	CZ-NH2	5.13	1.44	1.33
4	D	123	2MR	CZ-NE	4.97	1.44	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	123	2MR	NE-CZ-NH2	-8.69	111.51	119.48
4	D	123	2MR	CG-CD-NE	-2.24	105.80	112.21

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	123	2MR	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
43	SF4	F	502	6	0,12,12	-	-	-		
43	SF4	I	302	9	0,12,12	-	-	-		
47	CDL	P	502	-	40,40,99	1.25	5 (12%)	46,52,111	1.16	4 (8%)
48	DGT	O	501	-	26,33,33	3.28	12 (46%)	32,52,52	1.65	8 (25%)
43	SF4	I	301	9	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
45	FES	E	301	5	0,4,4	-	-	-		
44	3PE	Y	303	-	24,24,50	1.22	3 (12%)	27,29,55	1.11	2 (7%)
44	3PE	Y	302	-	21,21,50	1.28	4 (19%)	24,26,55	1.34	2 (8%)
51	EHZ	U	201	19	29,36,37	1.75	6 (20%)	35,44,47	1.61	6 (17%)
43	SF4	G	802	7	0,12,12	-	-	-		
44	3PE	Y	301	-	19,19,50	1.27	3 (15%)	22,24,55	1.04	1 (4%)
47	CDL	M	501	-	54,54,99	1.14	6 (11%)	60,66,111	1.17	3 (5%)
49	NDP	P	501	-	45,52,52	4.17	22 (48%)	53,80,80	2.23	7 (13%)
44	3PE	L	601	-	34,34,50	1.03	4 (11%)	37,39,55	1.22	2 (5%)
43	SF4	B	301	2	0,12,12	-	-	-		
44	3PE	B	303	-	25,25,50	1.20	4 (16%)	28,30,55	1.35	2 (7%)
43	SF4	G	801	7	0,12,12	-	-	-		
46	FMN	F	501	-	33,33,33	2.60	10 (30%)	48,50,50	1.71	13 (27%)
51	EHZ	T	201	19	29,36,37	1.67	5 (17%)	35,44,47	1.63	3 (8%)
44	3PE	B	302	-	41,41,50	0.96	4 (9%)	44,46,55	0.98	2 (4%)
45	FES	G	803	7	0,4,4	-	-	-		

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
47	CDL	P	502	-	-	19/49/49/110	-
43	SF4	F	502	6	-	-	0/6/5/5
43	SF4	I	302	9	-	-	0/6/5/5
48	DGT	O	501	-	-	8/18/34/34	0/3/3/3
43	SF4	I	301	9	-	-	0/6/5/5
45	FES	E	301	5	-	-	0/1/1/1
44	3PE	Y	303	-	-	15/28/28/54	-
44	3PE	Y	302	-	-	11/25/25/54	-
51	EHZ	U	201	19	-	9/42/44/45	-
43	SF4	G	802	7	-	-	0/6/5/5
44	3PE	Y	301	-	-	14/22/22/54	-
47	CDL	M	501	-	-	35/64/64/110	-
49	NDP	P	501	-	-	11/30/77/77	0/5/5/5
44	3PE	L	601	-	-	15/38/38/54	-
43	SF4	B	301	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	3PE	B	303	-	-	10/29/29/54	-
43	SF4	G	801	7	-	-	0/6/5/5
46	FMN	F	501	-	-	11/18/18/18	0/3/3/3
51	EHZ	T	201	19	-	10/42/44/45	-
44	3PE	B	302	-	-	18/45/45/54	-
45	FES	G	803	7	-	-	0/1/1/1

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	P	501	NDP	O4B-C1B	14.04	1.60	1.41
49	P	501	NDP	C6N-C5N	11.97	1.54	1.33
49	P	501	NDP	C7N-N7N	8.30	1.55	1.33
48	O	501	DGT	C3'-C4'	-7.97	1.31	1.53
48	O	501	DGT	O4'-C4'	7.85	1.62	1.45
49	P	501	NDP	O4D-C1D	7.81	1.60	1.42
49	P	501	NDP	C2D-C1D	-7.22	1.30	1.53
49	P	501	NDP	O4D-C4D	-6.80	1.29	1.45
46	F	501	FMN	C4A-N5	6.58	1.43	1.30
46	F	501	FMN	C10-N1	6.02	1.45	1.33
48	O	501	DGT	C2-N3	5.56	1.46	1.33
51	U	201	EHZ	C12-N1	5.48	1.45	1.33
51	T	201	EHZ	C15-N2	5.41	1.45	1.33
49	P	501	NDP	O4B-C4B	-5.28	1.33	1.45
51	U	201	EHZ	C15-N2	5.27	1.45	1.33
49	P	501	NDP	P2B-O2B	5.25	1.69	1.59
51	T	201	EHZ	C12-N1	5.12	1.45	1.33
48	O	501	DGT	O4'-C1'	-5.01	1.31	1.42
48	O	501	DGT	C4-N3	4.84	1.49	1.37
46	F	501	FMN	C9A-N10	4.71	1.49	1.41
46	F	501	FMN	C5A-N5	4.63	1.48	1.39
48	O	501	DGT	C2-N2	4.58	1.45	1.34
46	F	501	FMN	C2-N1	4.40	1.47	1.36
49	P	501	NDP	C2N-C3N	4.31	1.47	1.34
49	P	501	NDP	O7N-C7N	-4.12	1.14	1.24
46	F	501	FMN	C2-N3	4.04	1.48	1.39
49	P	501	NDP	C6A-N6A	3.80	1.47	1.34
49	P	501	NDP	C5A-C4A	-3.80	1.30	1.40
49	P	501	NDP	O2D-C2D	3.79	1.51	1.43
46	F	501	FMN	C4-N3	3.59	1.45	1.38
46	F	501	FMN	O2-C2	-3.47	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	F	501	FMN	C10-N10	3.31	1.44	1.37
48	O	501	DGT	C6-N1	3.18	1.42	1.37
49	P	501	NDP	C4N-C3N	3.10	1.56	1.49
51	U	201	EHZ	O6-C20	-2.86	1.37	1.44
48	O	501	DGT	C5-C6	2.85	1.53	1.47
48	O	501	DGT	O3'-C3'	2.82	1.49	1.43
44	Y	303	3PE	O21-C2	-2.78	1.39	1.46
49	P	501	NDP	C4N-C5N	2.77	1.56	1.48
44	B	302	3PE	O21-C2	-2.69	1.39	1.46
47	P	502	CDL	OA6-CA4	-2.65	1.40	1.46
46	F	501	FMN	O4-C4	-2.64	1.18	1.23
47	M	501	CDL	OA6-CA4	-2.61	1.40	1.46
49	P	501	NDP	O3B-C3B	-2.60	1.36	1.43
48	O	501	DGT	C5-C4	-2.59	1.36	1.43
48	O	501	DGT	C2-N1	2.59	1.44	1.37
47	M	501	CDL	OB6-CB4	-2.57	1.40	1.46
49	P	501	NDP	O3D-C3D	-2.57	1.36	1.43
44	L	601	3PE	O21-C2	-2.54	1.40	1.46
49	P	501	NDP	C2A-N3A	2.49	1.36	1.32
44	Y	301	3PE	O21-C2	-2.48	1.40	1.46
44	Y	303	3PE	O31-C31	2.46	1.40	1.33
47	M	501	CDL	OB6-CB5	2.44	1.41	1.34
51	U	201	EHZ	C9-S1	2.44	1.82	1.76
44	Y	302	3PE	O31-C31	2.42	1.40	1.33
44	B	303	3PE	O31-C3	-2.39	1.39	1.45
44	B	303	3PE	O21-C2	-2.39	1.40	1.46
48	O	501	DGT	O6-C6	-2.39	1.18	1.23
47	M	501	CDL	OA8-CA7	2.38	1.40	1.33
47	P	502	CDL	OB6-CB5	2.37	1.41	1.34
51	U	201	EHZ	O4-C15	-2.36	1.18	1.23
44	B	302	3PE	O31-C3	-2.36	1.39	1.45
49	P	501	NDP	C6N-N1N	2.29	1.43	1.37
44	B	302	3PE	O31-C31	2.29	1.40	1.33
51	U	201	EHZ	O3-C12	-2.28	1.18	1.23
51	T	201	EHZ	O4-C15	-2.26	1.18	1.23
44	Y	302	3PE	O21-C21	2.26	1.40	1.34
51	T	201	EHZ	O3-C12	-2.25	1.18	1.23
44	B	303	3PE	O21-C21	2.25	1.40	1.34
44	B	303	3PE	O31-C31	2.24	1.39	1.33
44	Y	301	3PE	O31-C3	-2.23	1.40	1.45
44	Y	302	3PE	O31-C3	-2.20	1.40	1.45
44	Y	301	3PE	O21-C21	2.20	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	L	601	3PE	O31-C31	2.18	1.39	1.33
51	T	201	EHZ	C9-S1	2.17	1.81	1.76
44	L	601	3PE	O31-C3	-2.16	1.40	1.45
49	P	501	NDP	C7N-C3N	2.14	1.53	1.48
44	L	601	3PE	O21-C21	2.14	1.40	1.34
49	P	501	NDP	P2B-O1X	2.13	1.57	1.50
44	Y	302	3PE	O21-C2	-2.13	1.41	1.46
47	M	501	CDL	OA8-CA6	-2.11	1.40	1.45
47	P	502	CDL	OA8-CA6	-2.11	1.40	1.45
47	P	502	CDL	OA6-CA5	2.08	1.40	1.34
44	B	302	3PE	O21-C21	2.08	1.40	1.34
49	P	501	NDP	PA-O5B	2.08	1.67	1.59
47	M	501	CDL	OA6-CA5	2.05	1.40	1.34
44	Y	303	3PE	O21-C21	2.02	1.40	1.34
47	P	502	CDL	OB6-CB4	-2.02	1.41	1.46

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	P	501	NDP	C5A-C6A-N6A	8.81	133.74	120.35
49	P	501	NDP	C1B-N9A-C4A	-7.73	113.06	126.64
51	T	201	EHZ	C8-C9-S1	6.55	121.73	113.63
49	P	501	NDP	N6A-C6A-N1A	-6.24	105.62	118.57
49	P	501	NDP	N3A-C2A-N1A	-5.45	120.16	128.68
44	B	303	3PE	O21-C21-C22	4.71	121.66	111.50
46	F	501	FMN	C9-C8-C7	4.56	126.20	119.67
44	L	601	3PE	O21-C21-C22	4.43	121.05	111.50
44	Y	302	3PE	O21-C21-C22	4.36	120.89	111.50
47	M	501	CDL	OA6-CA5-C11	4.31	120.78	111.50
51	U	201	EHZ	C8-C9-S1	4.00	118.57	113.63
51	U	201	EHZ	C10-S1-C9	3.88	113.97	101.87
44	Y	303	3PE	O21-C21-C22	3.85	119.80	111.50
47	M	501	CDL	OB6-CB5-C51	3.73	119.55	111.50
49	P	501	NDP	PN-O3-PA	-3.73	120.02	132.83
46	F	501	FMN	C7M-C7-C6	3.66	126.26	119.49
46	F	501	FMN	C4-N3-C2	-3.60	118.99	125.64
47	P	502	CDL	OB6-CB5-C51	3.57	119.20	111.50
48	O	501	DGT	PA-O3A-PB	-3.53	120.70	132.83
44	B	302	3PE	O21-C21-C22	3.50	119.05	111.50
48	O	501	DGT	C5-C6-N1	3.49	120.12	113.95
51	U	201	EHZ	C13-C14-N2	-3.44	104.96	111.90
47	P	502	CDL	OA6-CA5-C11	3.44	120.38	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	O	501	DGT	PB-O3B-PG	-3.35	121.33	132.83
44	Y	302	3PE	O31-C31-C32	3.29	120.01	111.38
49	P	501	NDP	C3N-C2N-N1N	-3.28	118.42	123.10
44	Y	301	3PE	O21-C21-C22	3.19	119.70	110.80
51	T	201	EHZ	O2-C9-S1	-3.16	118.51	122.61
48	O	501	DGT	C2-N1-C6	-3.16	119.28	125.10
46	F	501	FMN	C4A-C10-N10	3.10	121.02	116.48
44	L	601	3PE	O31-C31-C32	2.95	121.16	111.91
46	F	501	FMN	C8M-C8-C7	-2.91	114.77	120.74
44	B	303	3PE	O31-C31-C32	2.75	120.54	111.91
51	U	201	EHZ	C18-C17-C16	2.71	113.51	108.82
51	U	201	EHZ	C18-C17-C20	-2.70	103.82	108.23
48	O	501	DGT	C2'-C3'-C4'	2.69	108.36	102.76
46	F	501	FMN	C6-C7-C8	-2.65	115.88	119.67
51	U	201	EHZ	C14-C13-C12	-2.60	108.03	112.36
48	O	501	DGT	C8-N7-C5	2.59	107.92	102.99
46	F	501	FMN	C6-C5A-C9A	2.55	122.55	118.94
46	F	501	FMN	C4-C4A-C10	2.55	121.08	116.79
48	O	501	DGT	C2'-C1'-N9	-2.53	108.44	114.27
46	F	501	FMN	O4-C4-C4A	-2.52	119.91	126.60
49	P	501	NDP	C3D-C2D-C1D	2.48	106.14	101.43
44	B	302	3PE	O31-C31-C32	2.46	119.61	111.91
48	O	501	DGT	O6-C6-C5	-2.42	119.65	124.37
46	F	501	FMN	C4A-C4-N3	2.37	119.20	113.19
46	F	501	FMN	C5'-C4'-C3'	-2.32	107.73	112.20
47	M	501	CDL	OA8-CA7-C31	2.25	118.98	111.91
44	Y	303	3PE	O31-C31-C32	2.23	118.91	111.91
47	P	502	CDL	OB6-CB4-CB3	2.16	116.20	108.40
46	F	501	FMN	C10-C4A-N5	-2.15	120.28	124.86
51	T	201	EHZ	C10-C11-N1	-2.11	107.98	112.42
47	P	502	CDL	CB6-CB4-CB3	-2.05	106.93	111.79
46	F	501	FMN	C4A-C10-N1	-2.04	120.00	124.73

There are no chirality outliers.

All (186) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	B	303	3PE	O13-C11-C12-N
44	L	601	3PE	C1-O11-P-O12
44	L	601	3PE	C1-O11-P-O13
44	L	601	3PE	C1-O11-P-O14
44	Y	301	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
44	Y	301	3PE	C1-O11-P-O14
44	Y	301	3PE	C11-O13-P-O14
44	Y	301	3PE	O13-C11-C12-N
44	Y	302	3PE	C22-C21-O21-C2
44	Y	303	3PE	C1-O11-P-O14
44	Y	303	3PE	C12-C11-O13-P
44	Y	303	3PE	O11-C1-C2-O21
44	Y	303	3PE	O22-C21-O21-C2
44	Y	303	3PE	C22-C21-O21-C2
46	F	501	FMN	C1'-C2'-C3'-C4'
46	F	501	FMN	O4'-C4'-C5'-O5'
46	F	501	FMN	C5'-O5'-P-O1P
46	F	501	FMN	C5'-O5'-P-O2P
46	F	501	FMN	C5'-O5'-P-O3P
47	M	501	CDL	O1-C1-CB2-OB2
47	M	501	CDL	CA2-OA2-PA1-OA3
47	M	501	CDL	CA2-OA2-PA1-OA5
47	M	501	CDL	OA7-CA5-OA6-CA4
47	M	501	CDL	CB3-OB5-PB2-OB3
47	M	501	CDL	CB3-OB5-PB2-OB4
47	P	502	CDL	C11-CA5-OA6-CA4
47	P	502	CDL	CB3-OB5-PB2-OB4
48	O	501	DGT	PB-O3B-PG-O2G
48	O	501	DGT	C5'-O5'-PA-O1A
48	O	501	DGT	C5'-O5'-PA-O2A
49	P	501	NDP	C5B-O5B-PA-O1A
49	P	501	NDP	O4B-C4B-C5B-O5B
49	P	501	NDP	C2N-C3N-C7N-O7N
49	P	501	NDP	C2N-C3N-C7N-N7N
51	T	201	EHZ	C7-C8-C9-S1
51	U	201	EHZ	S1-C10-C11-N1
51	U	201	EHZ	C11-C10-S1-C9
44	Y	302	3PE	O22-C21-O21-C2
47	P	502	CDL	OA7-CA5-OA6-CA4
47	M	501	CDL	C11-CA5-OA6-CA4
44	Y	301	3PE	C32-C31-O31-C3
47	P	502	CDL	C51-CB5-OB6-CB4
49	P	501	NDP	C3B-C4B-C5B-O5B
44	Y	301	3PE	C2-C1-O11-P
47	P	502	CDL	CB4-CB3-OB5-PB2
44	L	601	3PE	C32-C31-O31-C3
44	Y	301	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
47	M	501	CDL	CA7-C31-C32-C33
51	U	201	EHZ	C5-C6-C7-O1
47	P	502	CDL	OB7-CB5-OB6-CB4
44	B	302	3PE	C1-O11-P-O13
44	B	303	3PE	C1-O11-P-O13
44	Y	301	3PE	C1-O11-P-O13
44	Y	302	3PE	C1-O11-P-O13
44	Y	303	3PE	C1-O11-P-O13
47	M	501	CDL	CB3-OB5-PB2-OB2
47	P	502	CDL	CB2-OB2-PB2-OB5
47	P	502	CDL	CB3-OB5-PB2-OB2
47	M	501	CDL	CA2-C1-CB2-OB2
49	P	501	NDP	O4D-C1D-N1N-C6N
47	M	501	CDL	C51-CB5-OB6-CB4
47	P	502	CDL	CB3-CB4-OB6-CB5
47	M	501	CDL	OB7-CB5-OB6-CB4
44	L	601	3PE	C22-C23-C24-C25
47	M	501	CDL	OB6-CB4-CB6-OB8
44	L	601	3PE	O32-C31-O31-C3
44	B	302	3PE	C22-C21-O21-C2
47	P	502	CDL	C51-C52-C53-C54
47	M	501	CDL	C51-C52-C53-C54
44	Y	303	3PE	C22-C23-C24-C25
44	B	302	3PE	C28-C29-C2A-C2B
44	B	302	3PE	O22-C21-O21-C2
46	F	501	FMN	O2'-C2'-C3'-C4'
47	P	502	CDL	C71-CB7-OB8-CB6
47	M	501	CDL	C11-C12-C13-C14
47	M	501	CDL	C13-C14-C15-C16
44	L	601	3PE	C22-C21-O21-C2
47	P	502	CDL	O1-C1-CB2-OB2
47	M	501	CDL	C53-C54-C55-C56
51	U	201	EHZ	C1-C21-C22-C23
44	L	601	3PE	O22-C21-O21-C2
44	Y	301	3PE	C11-O13-P-O11
47	P	502	CDL	C1-CB2-OB2-PB2
46	F	501	FMN	C3'-C4'-C5'-O5'
44	L	601	3PE	C2-C3-O31-C31
44	L	601	3PE	C1-C2-C3-O31
44	B	302	3PE	C24-C25-C26-C27
51	T	201	EHZ	O4-C15-C16-O5
51	T	201	EHZ	C21-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
44	B	302	3PE	C3B-C3C-C3D-C3E
46	F	501	FMN	O2'-C2'-C3'-O3'
44	Y	303	3PE	O11-C1-C2-C3
51	U	201	EHZ	C1-C2-C3-C4
47	M	501	CDL	C1-CB2-OB2-PB2
47	M	501	CDL	CB4-CB3-OB5-PB2
51	T	201	EHZ	S1-C10-C11-N1
47	M	501	CDL	C54-C55-C56-C57
44	B	302	3PE	C1-C2-C3-O31
47	M	501	CDL	CB3-CB4-CB6-OB8
47	P	502	CDL	OB9-CB7-OB8-CB6
51	T	201	EHZ	N2-C15-C16-C17
47	P	502	CDL	C31-CA7-OA8-CA6
44	Y	302	3PE	O11-C1-C2-O21
44	B	302	3PE	C29-C2A-C2B-C2C
44	L	601	3PE	C32-C33-C34-C35
44	B	302	3PE	O21-C2-C3-O31
51	U	201	EHZ	O2-C9-S1-C10
44	L	601	3PE	C28-C29-C2A-C2B
44	Y	302	3PE	O11-C1-C2-C3
51	U	201	EHZ	C8-C9-S1-C10
44	B	302	3PE	C26-C27-C28-C29
44	Y	301	3PE	C1-C2-C3-O31
44	B	303	3PE	O11-C1-C2-O21
51	U	201	EHZ	O1-C7-C8-C9
49	P	501	NDP	C5B-O5B-PA-O3
48	O	501	DGT	PA-O3A-PB-O2B
47	M	501	CDL	CB2-OB2-PB2-OB5
44	B	302	3PE	C1-O11-P-O12
44	B	302	3PE	C1-O11-P-O14
44	B	303	3PE	C1-O11-P-O12
44	B	303	3PE	C1-O11-P-O14
44	B	303	3PE	C11-O13-P-O12
44	Y	302	3PE	C1-O11-P-O12
44	Y	302	3PE	C1-O11-P-O14
44	Y	302	3PE	C11-O13-P-O12
44	Y	303	3PE	C1-O11-P-O12
44	Y	303	3PE	C11-O13-P-O12
47	P	502	CDL	CB2-OB2-PB2-OB3
49	P	501	NDP	C5B-O5B-PA-O2A
44	B	303	3PE	O11-C1-C2-C3
44	B	303	3PE	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
44	L	601	3PE	C12-C11-O13-P
44	Y	301	3PE	C12-C11-O13-P
44	Y	301	3PE	O21-C21-C22-C23
44	L	601	3PE	C34-C35-C36-C37
47	M	501	CDL	CA3-CA4-CA6-OA8
44	L	601	3PE	O21-C2-C3-O31
44	Y	301	3PE	O21-C2-C3-O31
47	M	501	CDL	OA6-CA4-CA6-OA8
47	M	501	CDL	C15-C16-C17-C18
44	B	302	3PE	C34-C35-C36-C37
47	M	501	CDL	C52-C51-CB5-OB6
44	Y	301	3PE	O22-C21-C22-C23
47	M	501	CDL	CA3-CA4-OA6-CA5
47	M	501	CDL	OA5-CA3-CA4-OA6
44	Y	302	3PE	C11-O13-P-O11
44	B	302	3PE	C25-C26-C27-C28
46	F	501	FMN	C2'-C3'-C4'-O4'
51	U	201	EHZ	C2-C3-C4-C5
47	P	502	CDL	CA2-C1-CB2-OB2
44	Y	303	3PE	C31-C32-C33-C34
51	T	201	EHZ	O4-C15-C16-C17
51	T	201	EHZ	C7-C8-C9-O2
44	Y	302	3PE	C3-C2-O21-C21
47	M	501	CDL	C71-CB7-OB8-CB6
44	Y	303	3PE	C11-O13-P-O11
47	P	502	CDL	OA9-CA7-OA8-CA6
44	B	302	3PE	C37-C38-C39-C3A
51	T	201	EHZ	C11-C10-S1-C9
47	M	501	CDL	C17-C18-C19-C20
44	B	302	3PE	C23-C24-C25-C26
47	M	501	CDL	CA4-CA6-OA8-CA7
49	P	501	NDP	C3B-C2B-O2B-P2B
44	Y	302	3PE	C1-C2-O21-C21
51	T	201	EHZ	C12-C13-C14-N2
44	Y	303	3PE	O31-C31-C32-C33
47	M	501	CDL	C52-C53-C54-C55
47	M	501	CDL	OA5-CA3-CA4-CA6
44	B	303	3PE	O31-C31-C32-C33
48	O	501	DGT	C5'-O5'-PA-O3A
49	P	501	NDP	C2B-O2B-P2B-O3X
47	M	501	CDL	C12-C11-CA5-OA6
44	B	302	3PE	O31-C31-C32-C33

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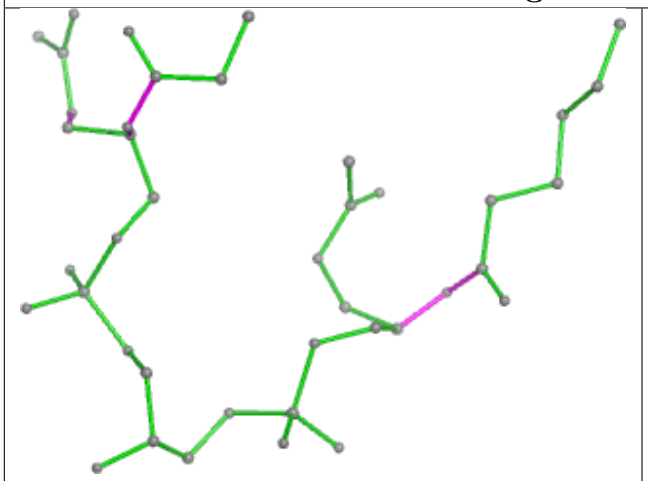
Mol	Chain	Res	Type	Atoms
48	O	501	DGT	PA-O3A-PB-O1B
44	Y	303	3PE	O32-C31-C32-C33
44	B	302	3PE	O32-C31-C32-C33
47	P	502	CDL	CA3-OA5-PA1-OA3
49	P	501	NDP	C5D-O5D-PN-O1N
48	O	501	DGT	O4'-C4'-C5'-O5'
44	Y	303	3PE	O13-C11-C12-N
48	O	501	DGT	PB-O3B-PG-O3G
46	F	501	FMN	C1'-C2'-C3'-O3'
46	F	501	FMN	O3'-C3'-C4'-O4'
44	B	303	3PE	O32-C31-C32-C33
47	M	501	CDL	C12-C11-CA5-OA7
51	T	201	EHZ	C5-C6-C7-O1

There are no ring outliers.

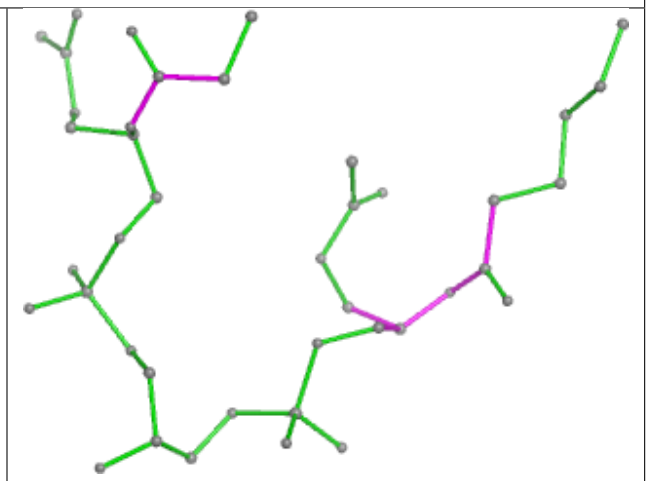
No monomer is involved in short contacts.

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

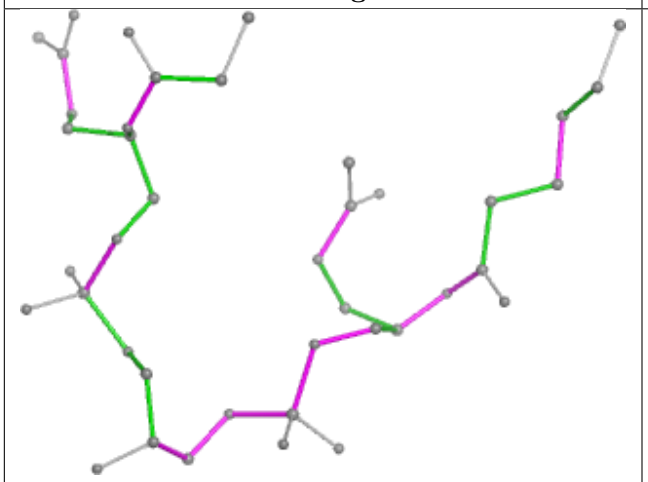
Ligand CDL P 502



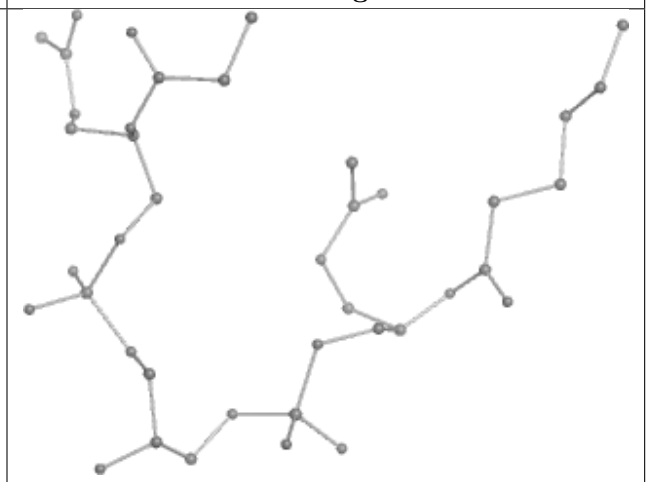
Bond lengths



Bond angles

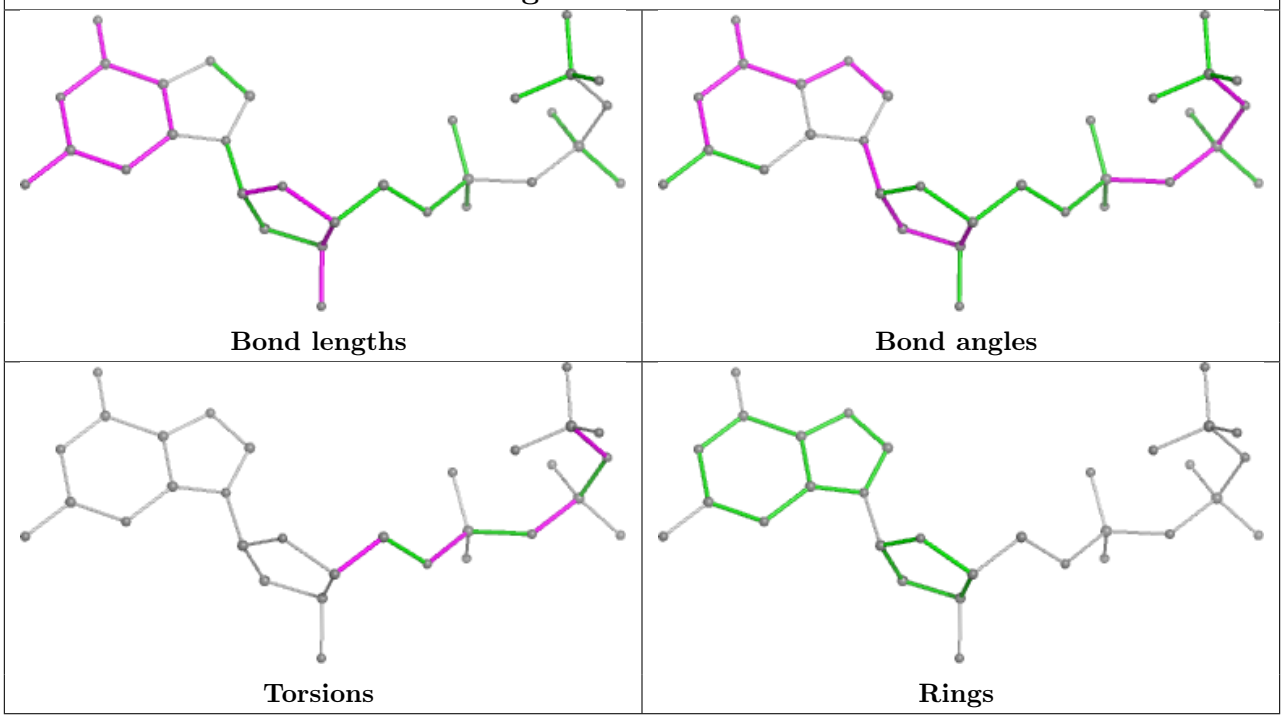


Torsions

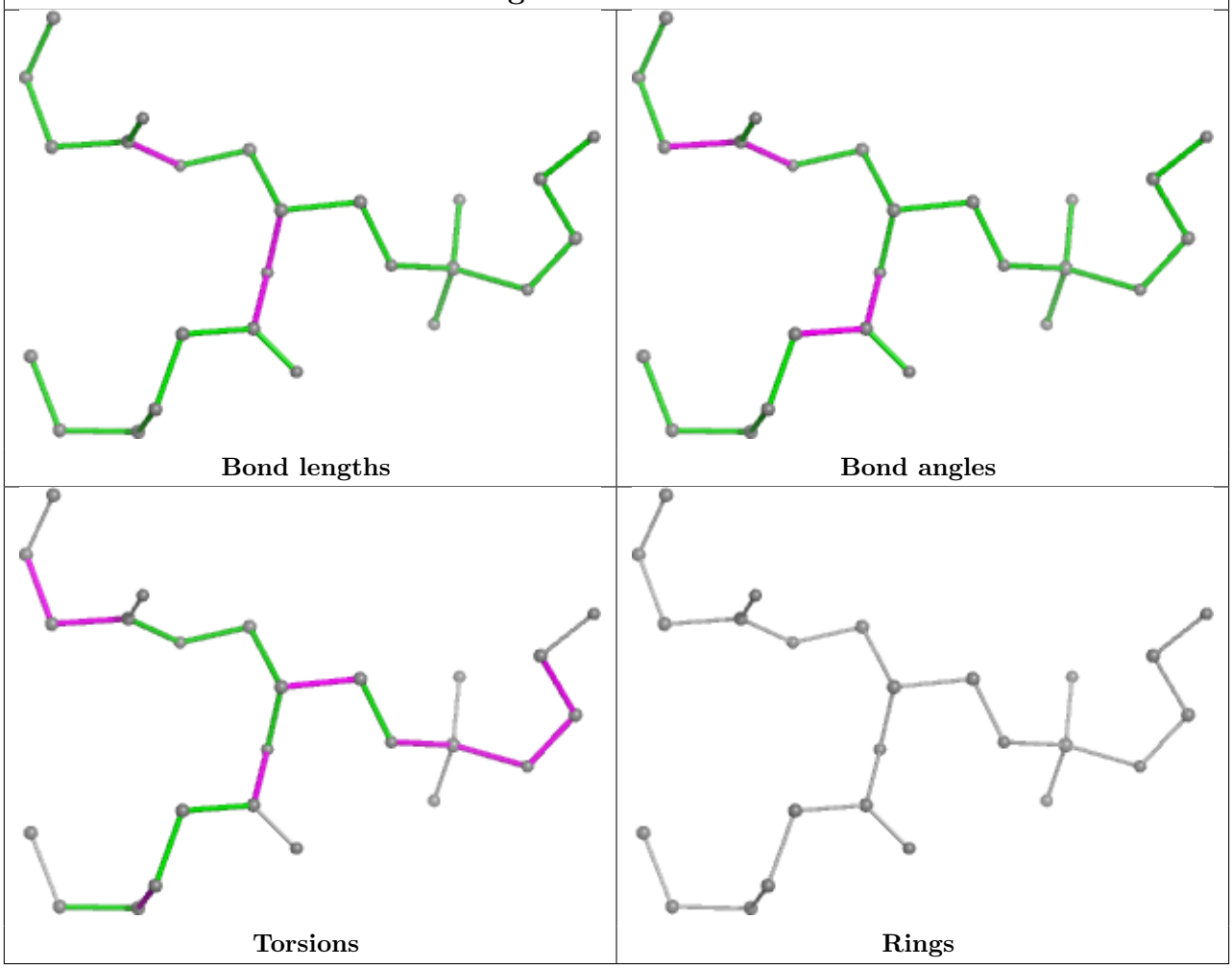


Rings

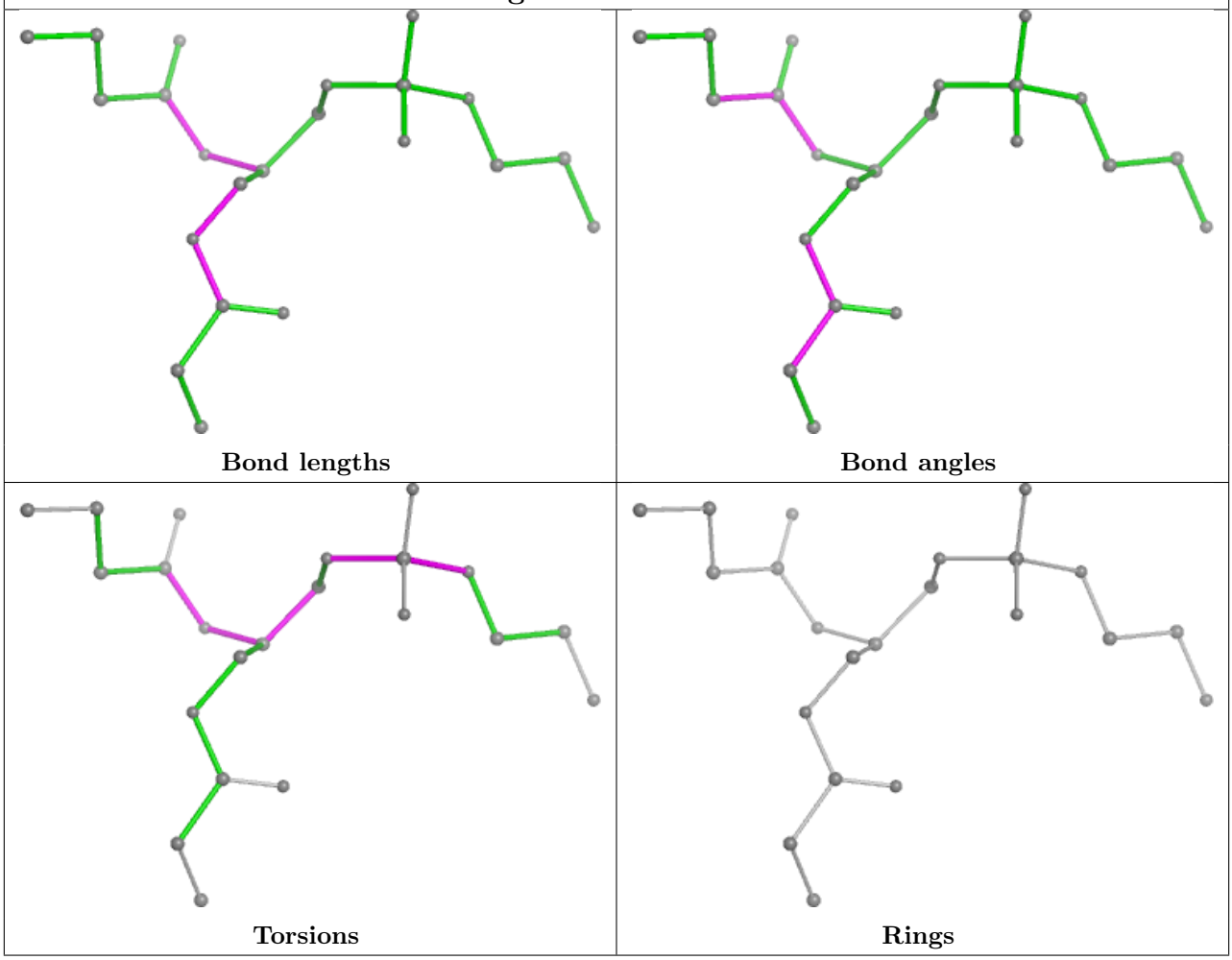
Ligand DGT O 501



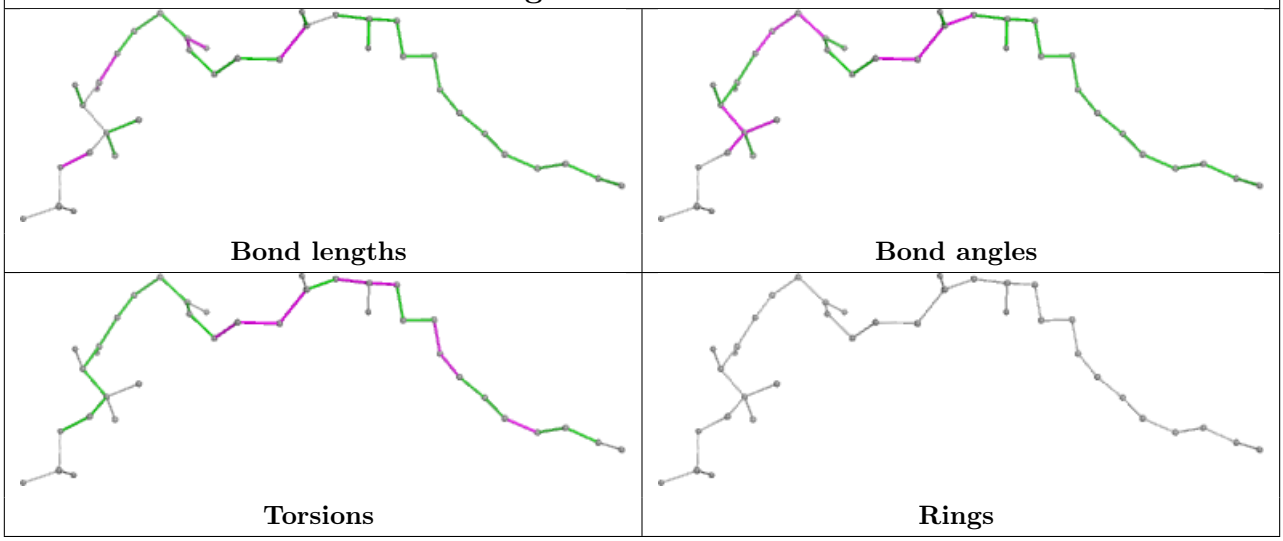
Ligand 3PE Y 303



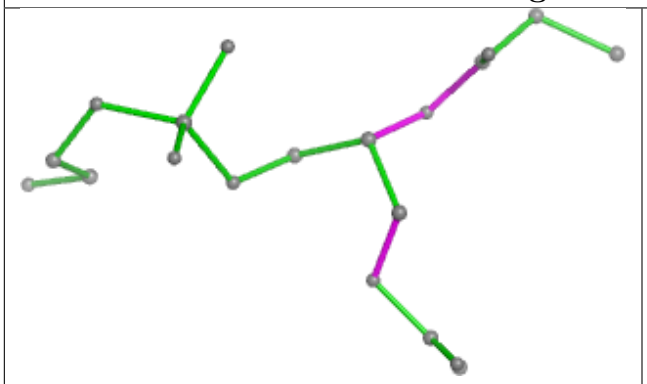
Ligand 3PE Y 302



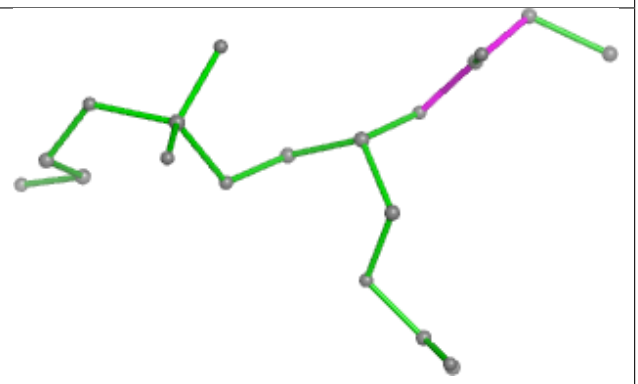
Ligand EHZ U 201



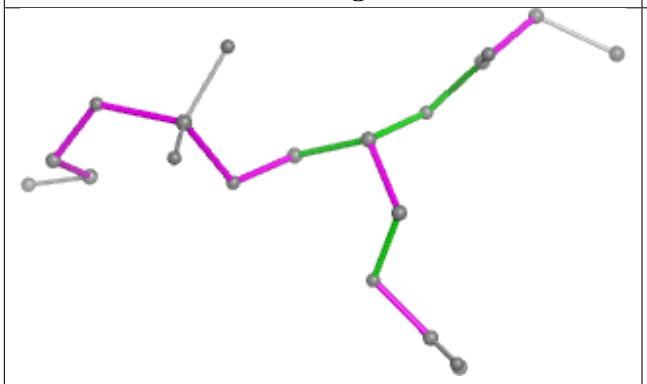
Ligand 3PE Y 301



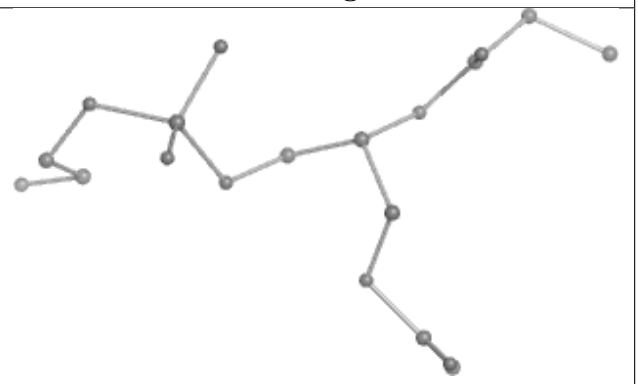
Bond lengths



Bond angles

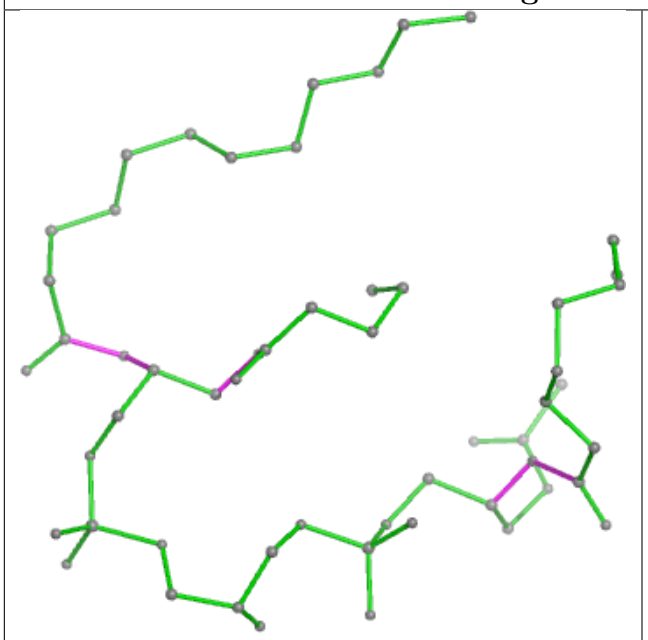


Torsions

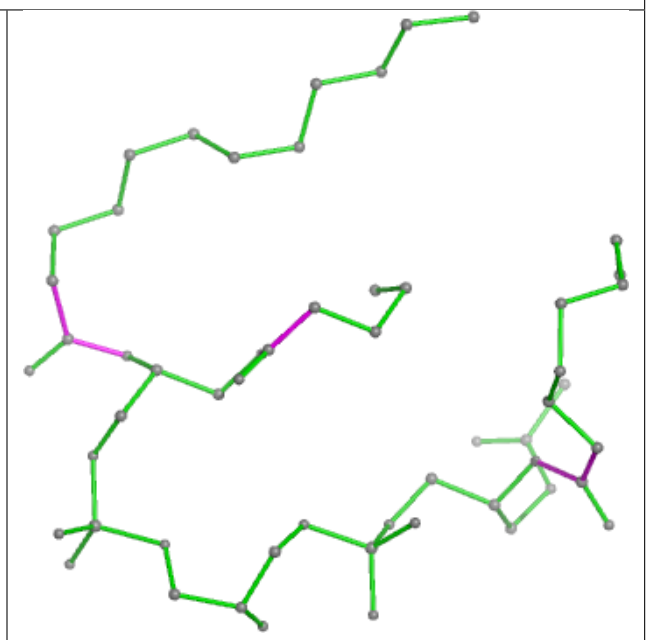


Rings

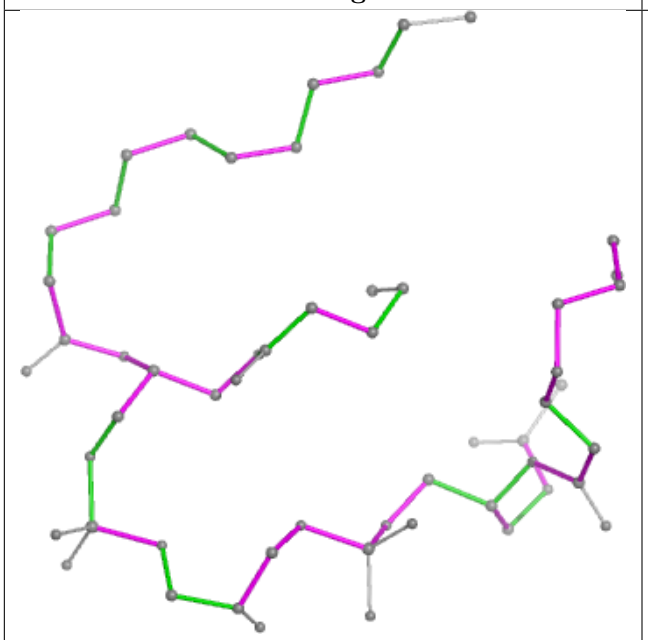
Ligand CDL M 501



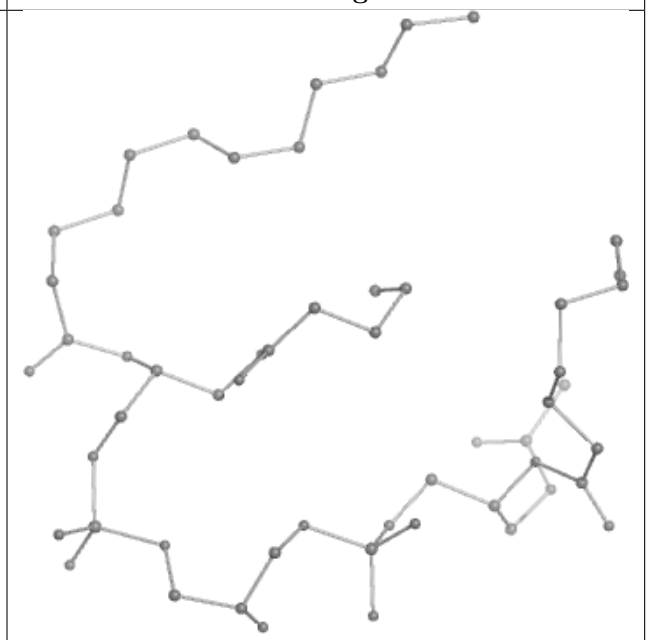
Bond lengths



Bond angles

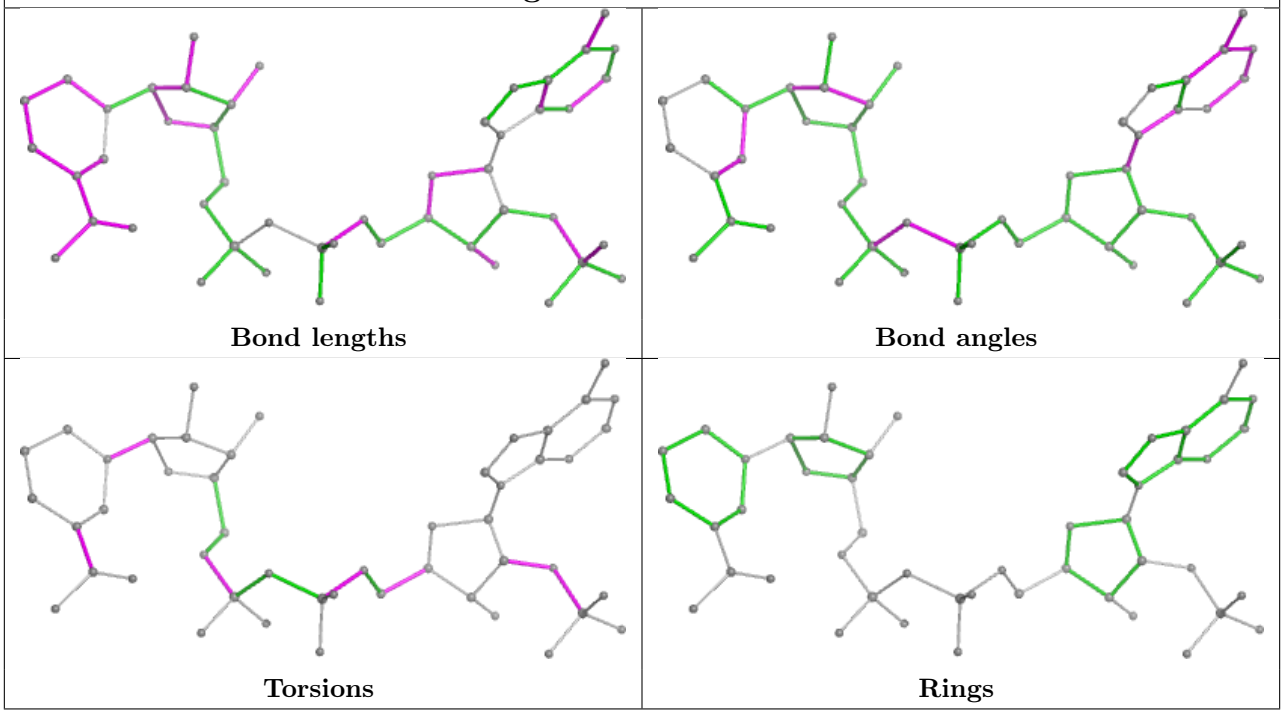


Torsions

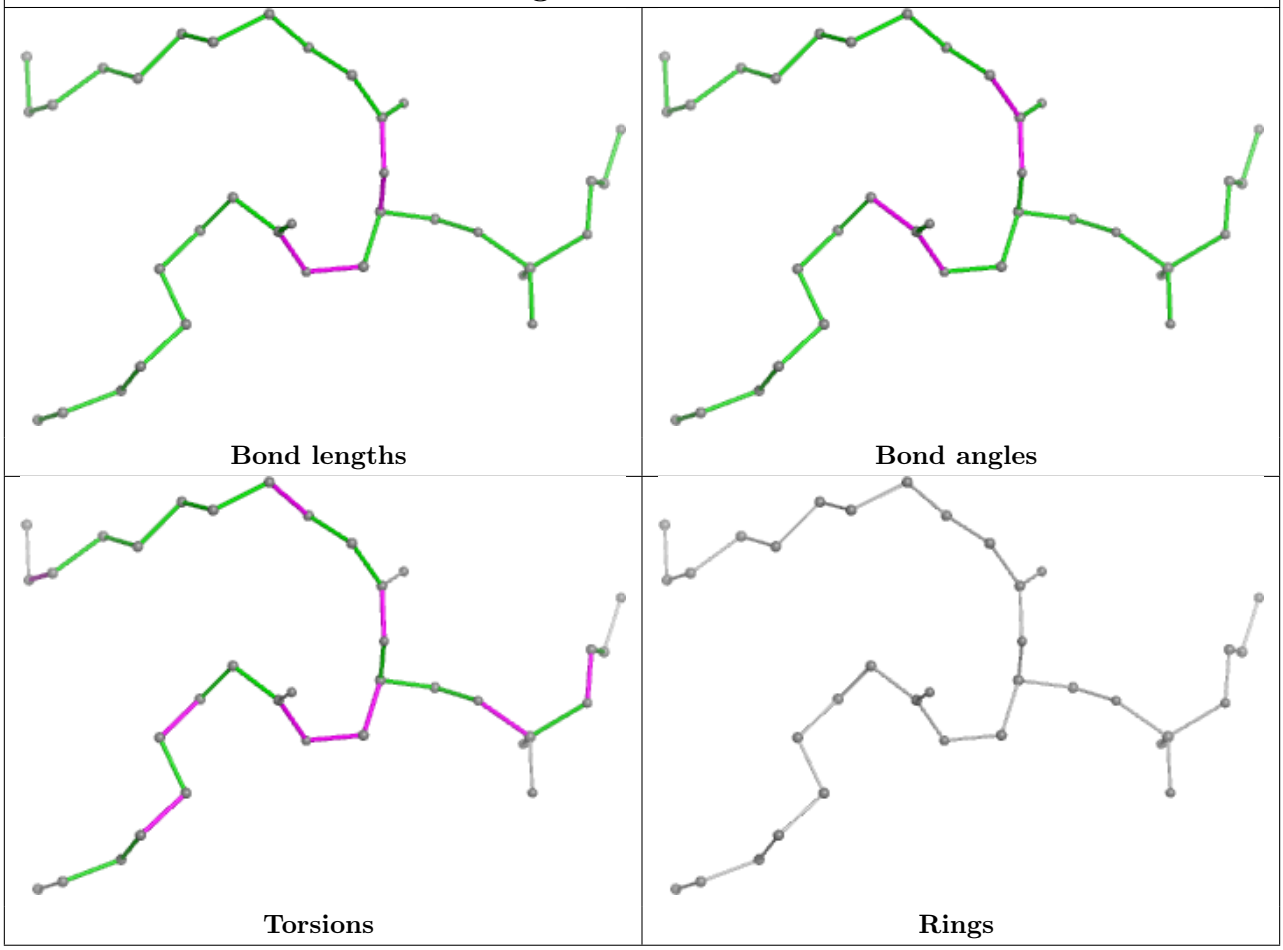


Rings

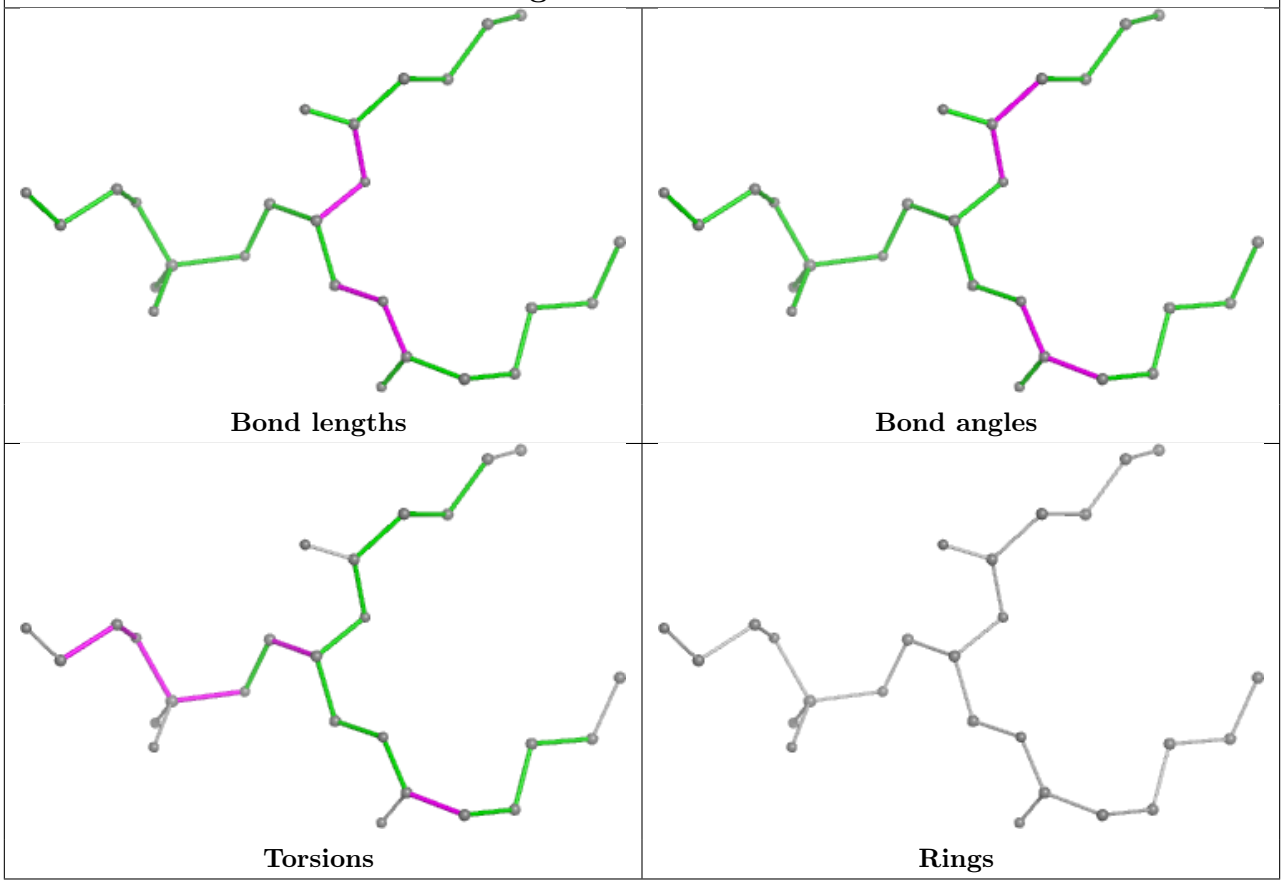
Ligand NDP P 501



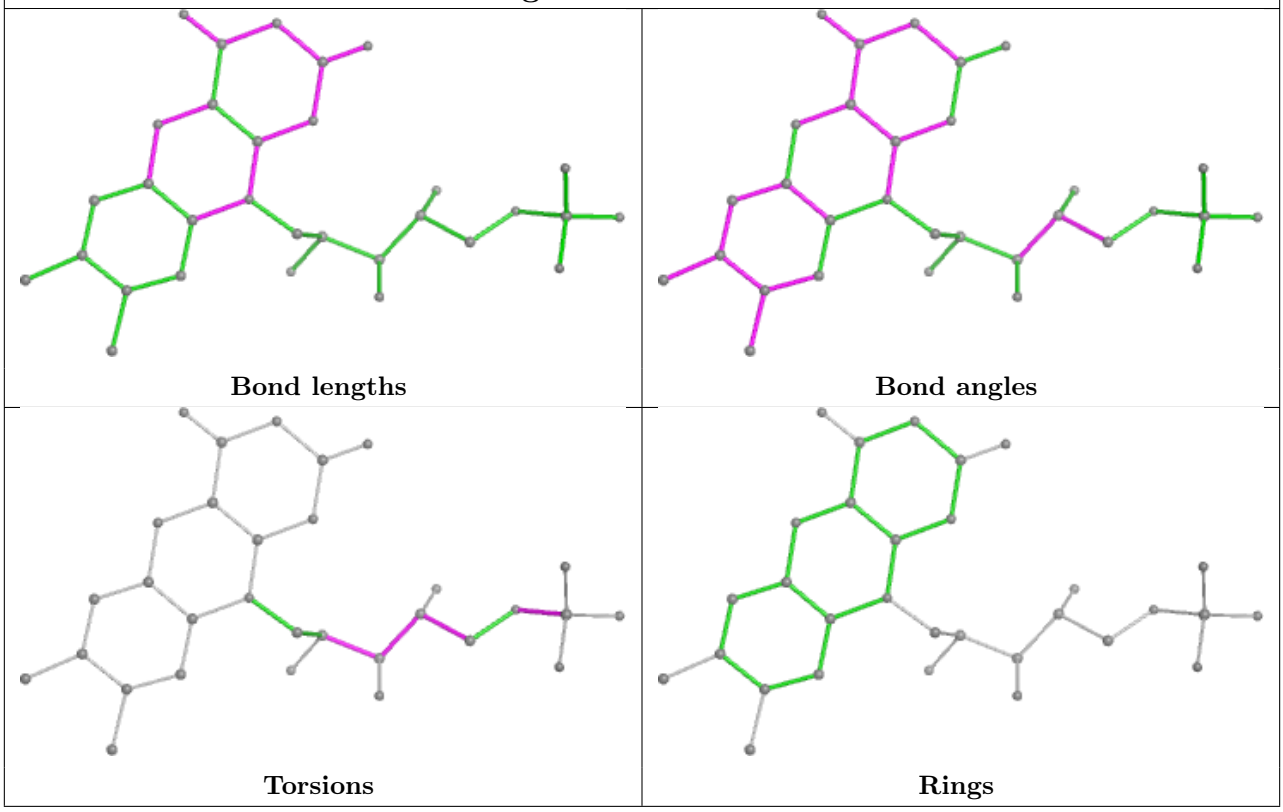
Ligand 3PE L 601

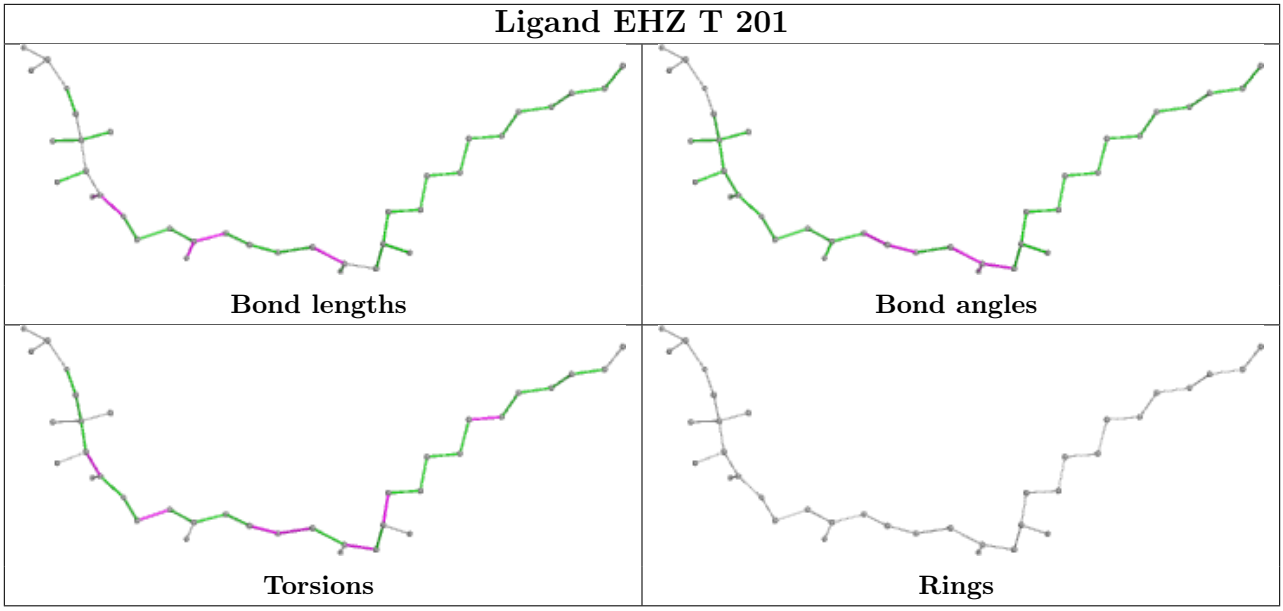


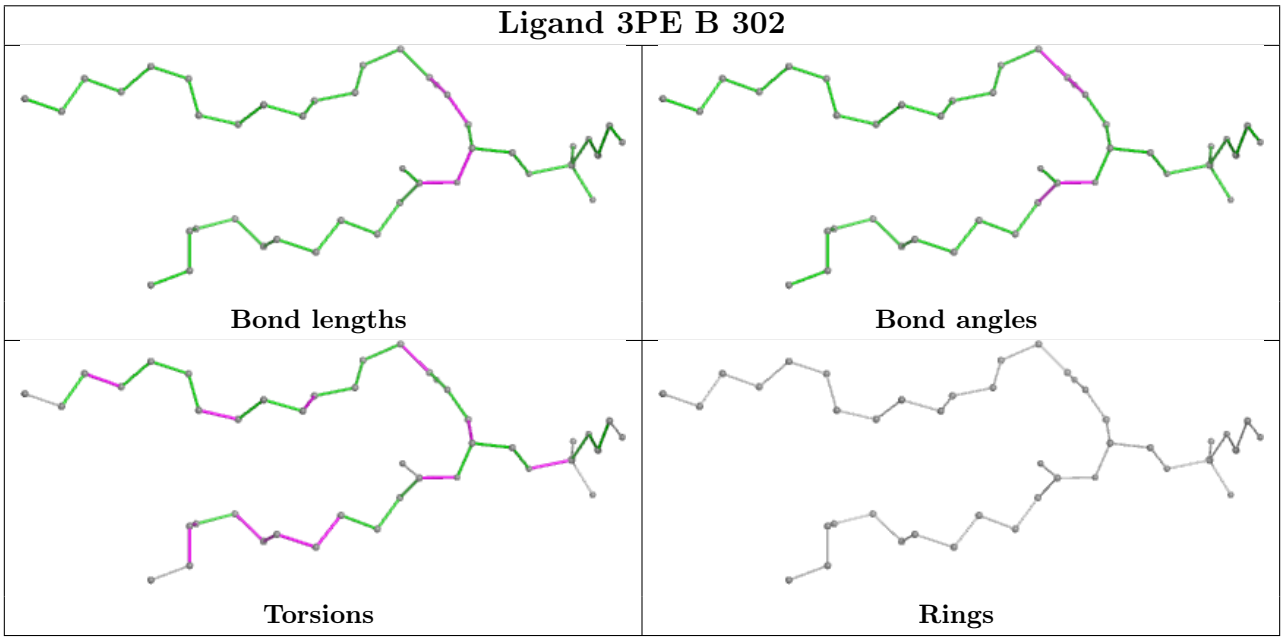
Ligand 3PE B 303



Ligand FMN F 501







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

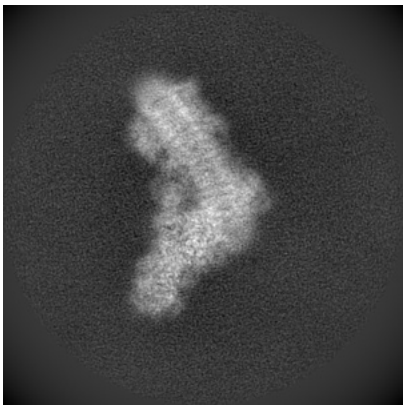
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-15937. These allow visual inspection of the internal detail of the map and identification of artifacts.

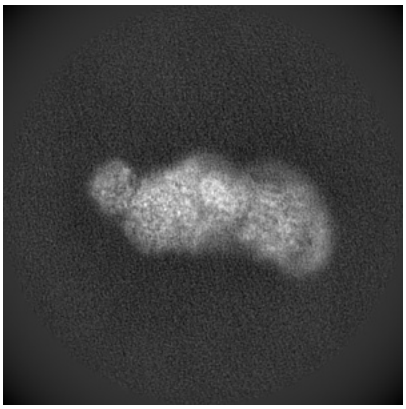
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

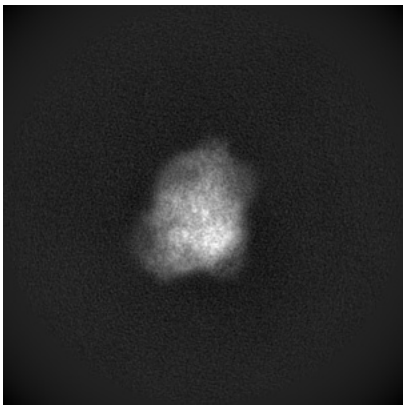
6.1.1 Primary map



X

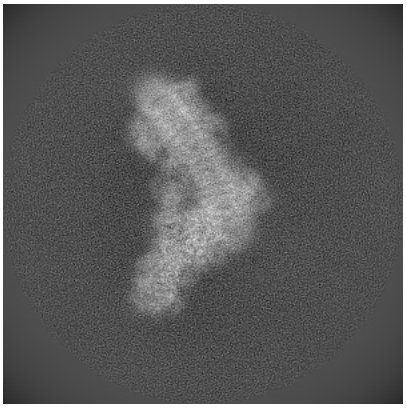


Y

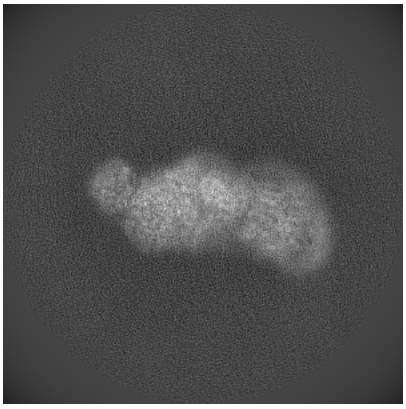


Z

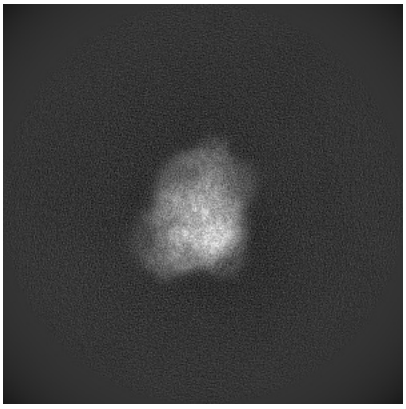
6.1.2 Raw map



X



Y

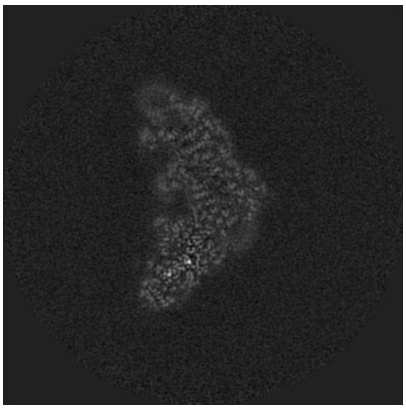


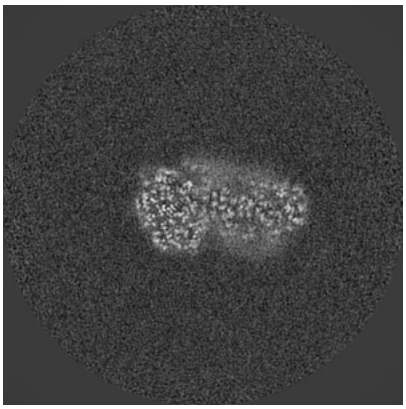
Z

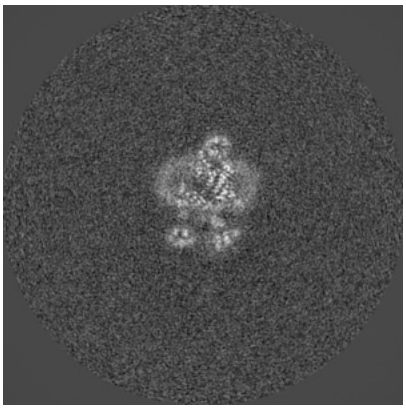
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

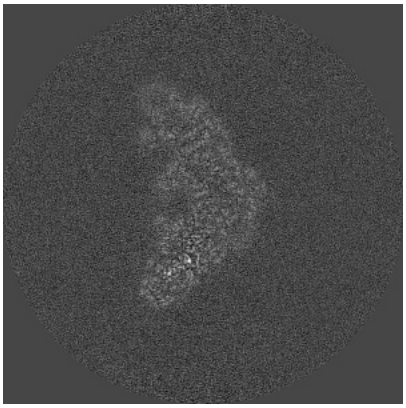
6.2.1 Primary map

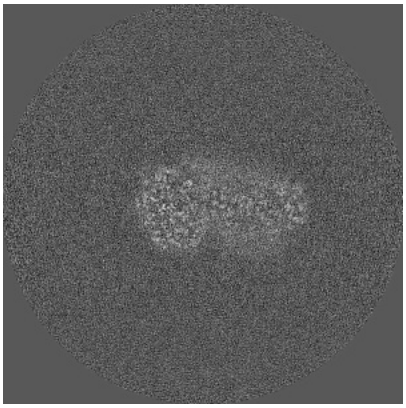

X Index: 225

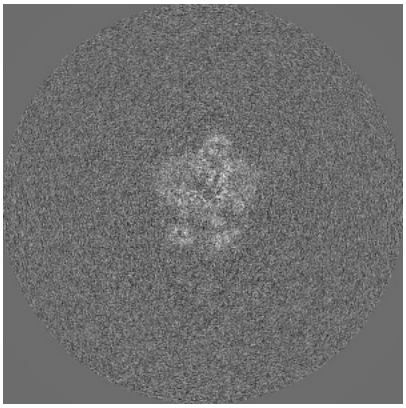

Y Index: 225


Z Index: 225

6.2.2 Raw map


X Index: 225

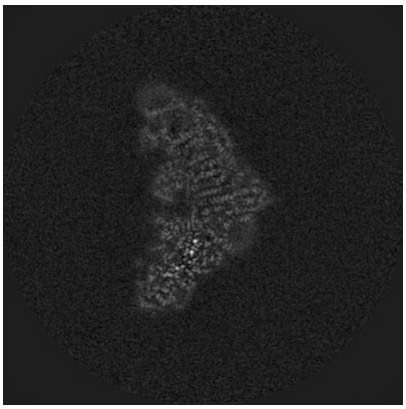

Y Index: 225

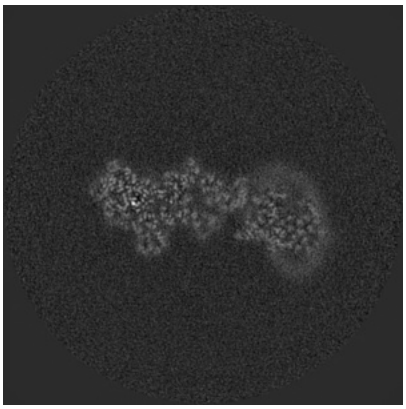

Z Index: 225

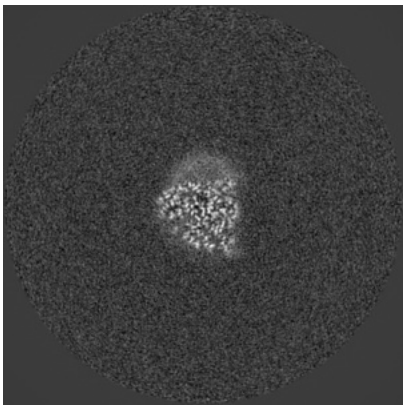
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

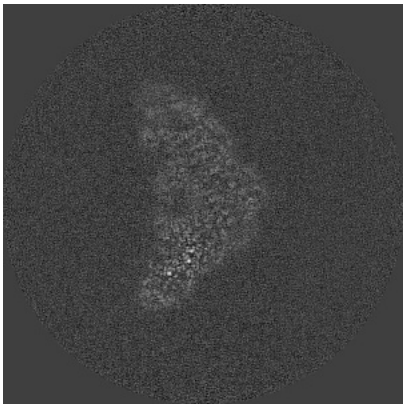
6.3.1 Primary map

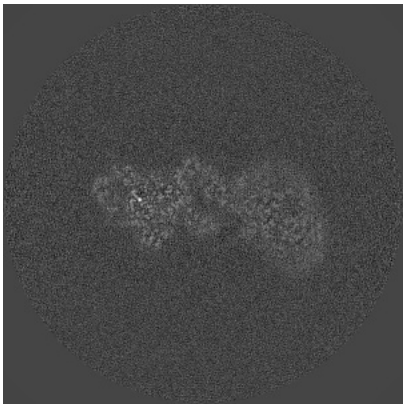

X Index: 228

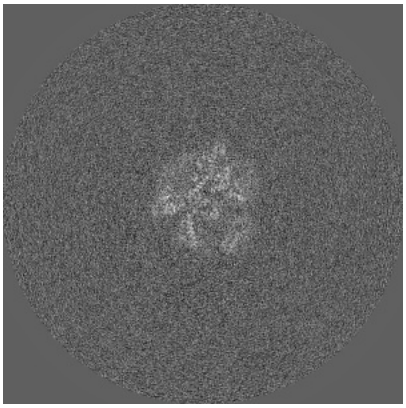

Y Index: 188


Z Index: 188

6.3.2 Raw map


X Index: 226

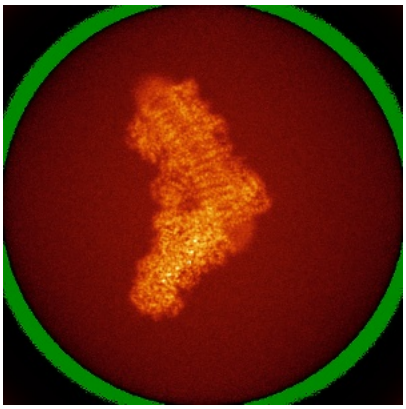

Y Index: 195

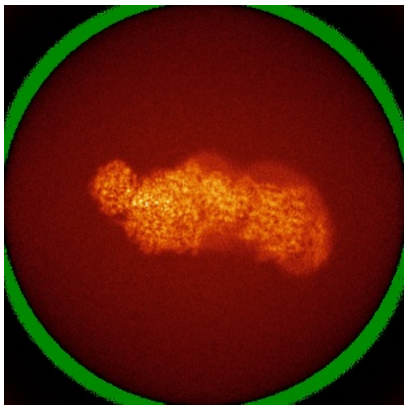

Z Index: 215

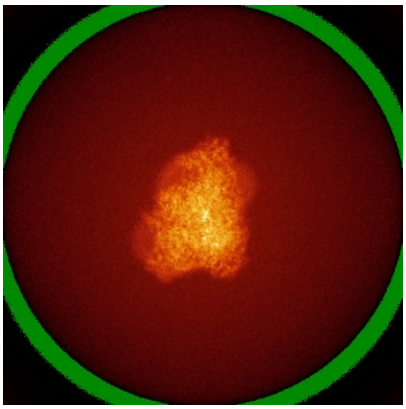
The images above show the largest variance slices of the map in three orthogonal directions.

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

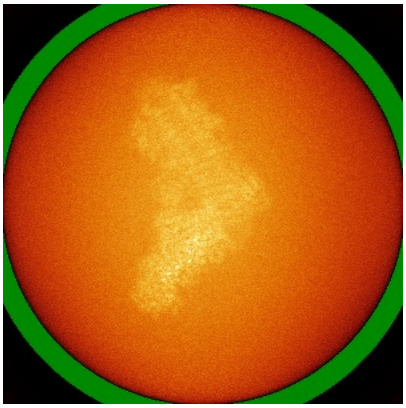
6.4.1 Primary map

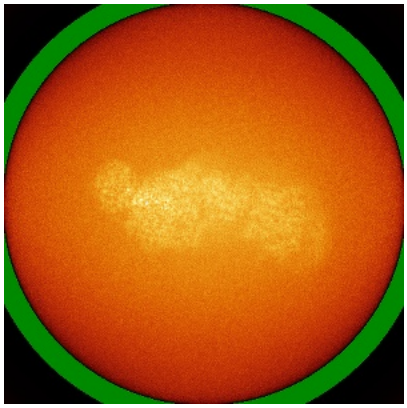

X

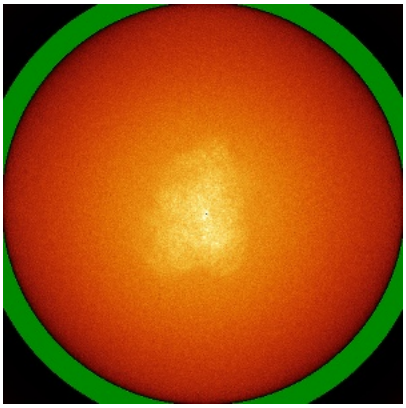

Y


Z

6.4.2 Raw 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.

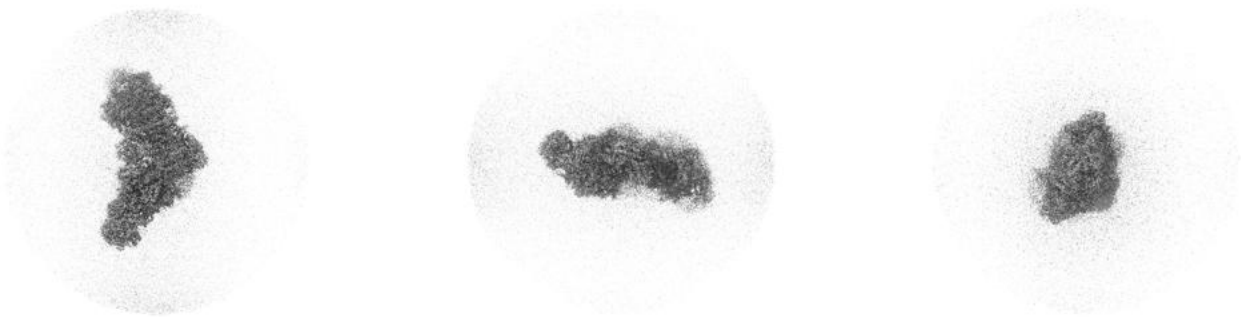
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

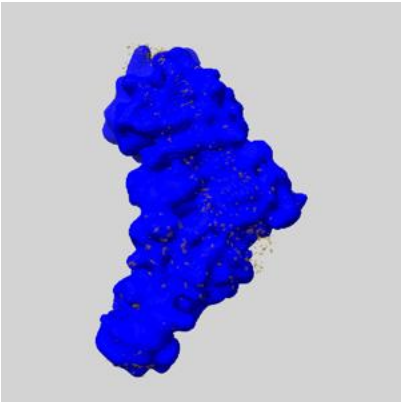
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

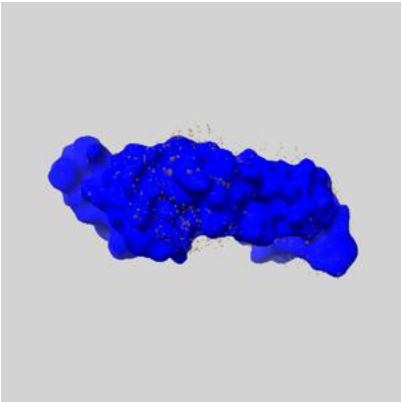
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

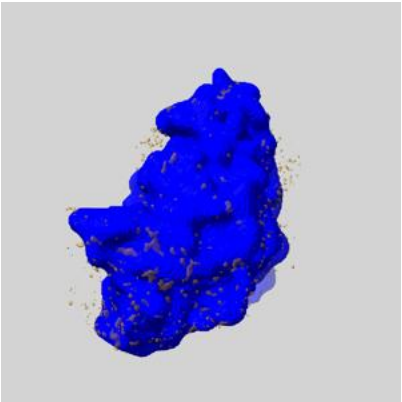
6.6.1 emd_15937_msk_1.map (i)



X



Y

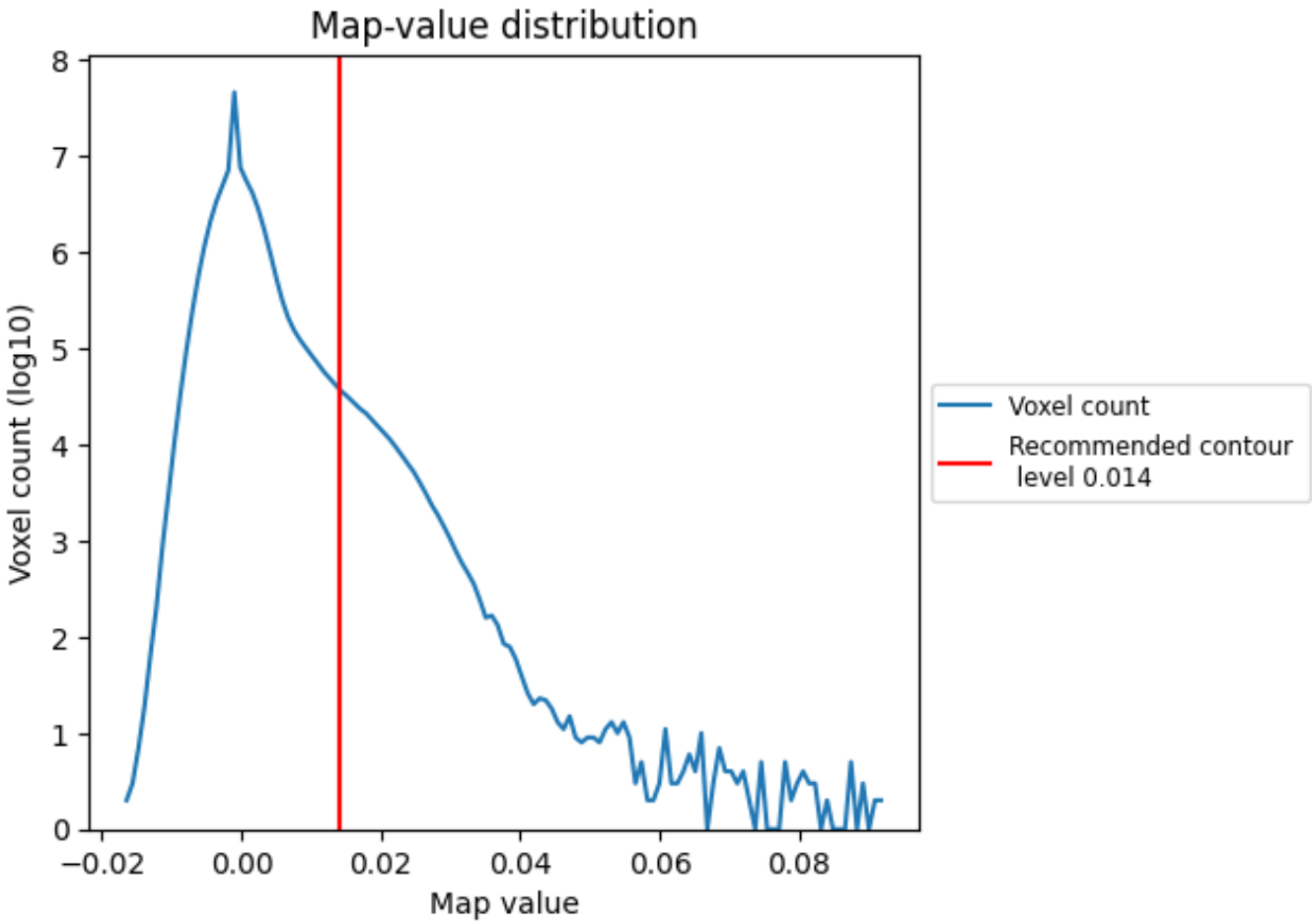


Z

7 Map analysis (i)

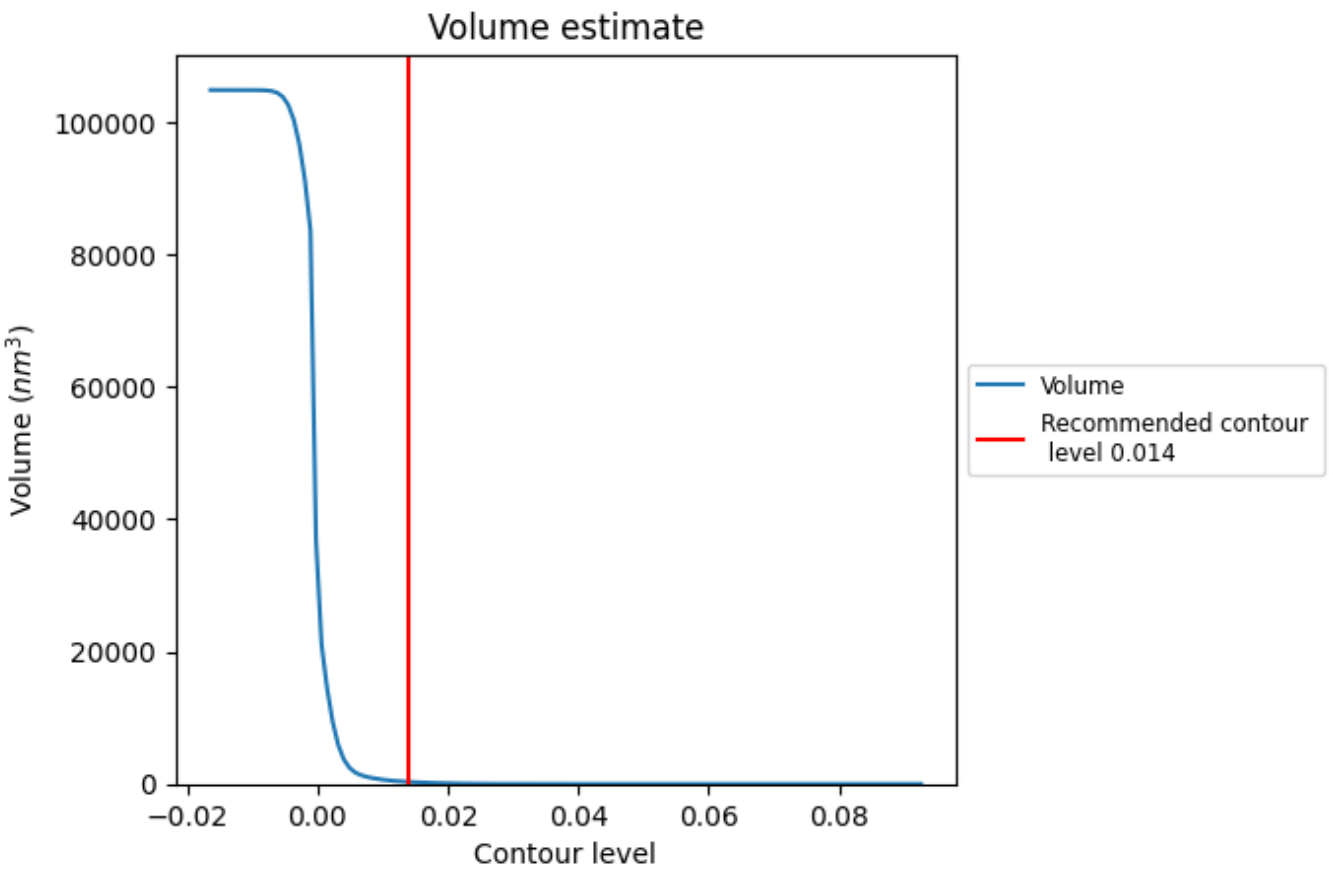
This section contains the results of statistical analysis of the map.

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.

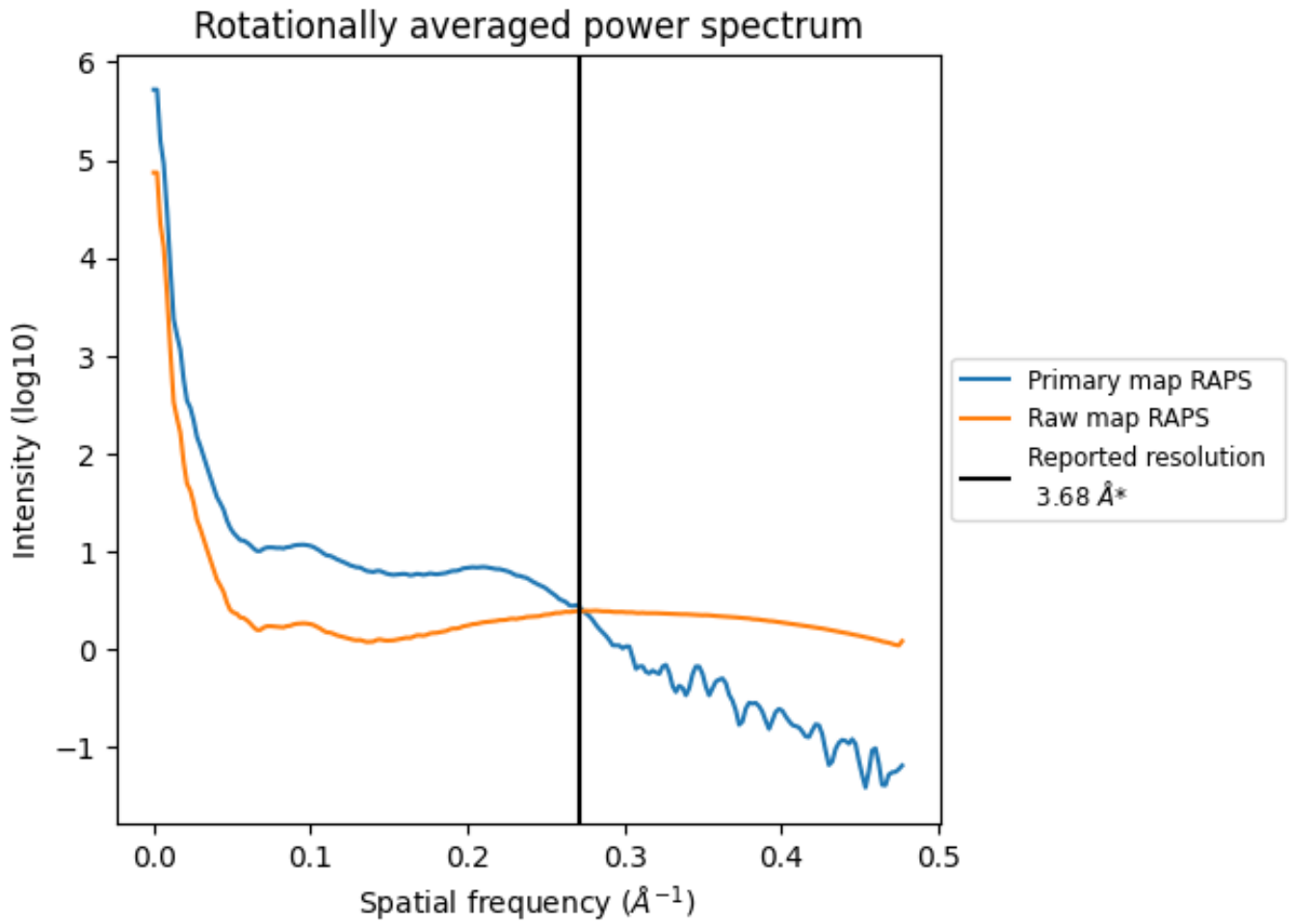
7.2 Volume estimate (i)



The volume at the recommended contour level is 306 nm^3; this corresponds to an approximate mass of 277 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)

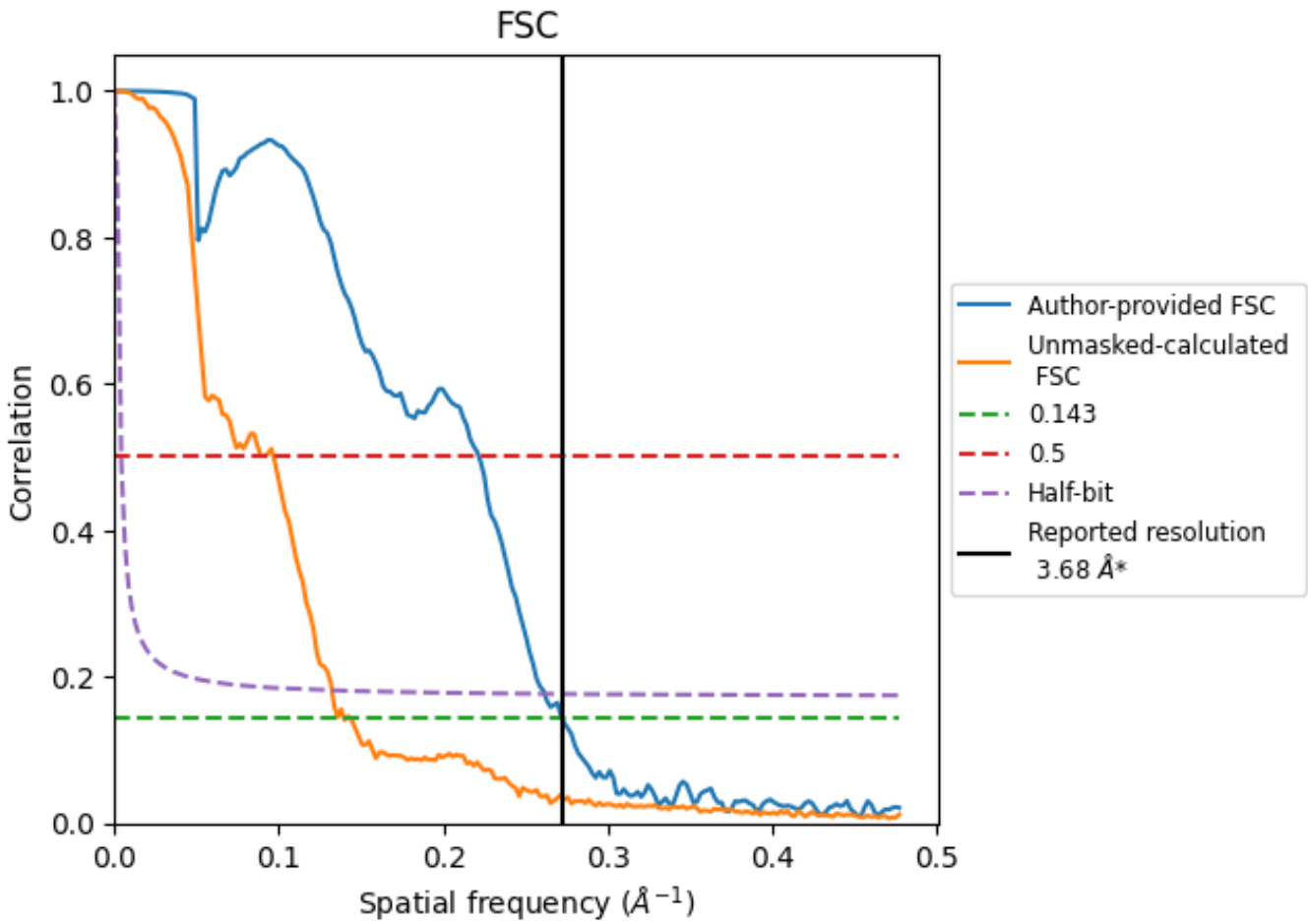


*Reported resolution corresponds to spatial frequency of 0.272 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.272 Å^{-1}

8.2 Resolution estimates (i)

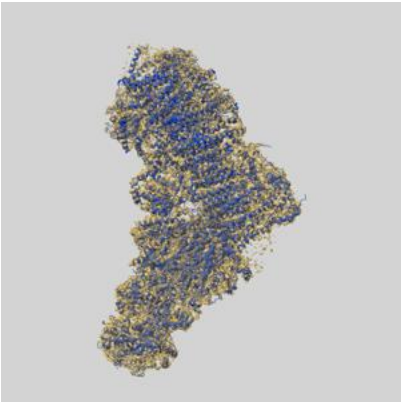
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.68	-	-
Author-provided FSC curve	3.68	4.51	3.82
Unmasked-calculated*	7.16	10.34	7.56

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.16 differs from the reported value 3.68 by more than 10 %

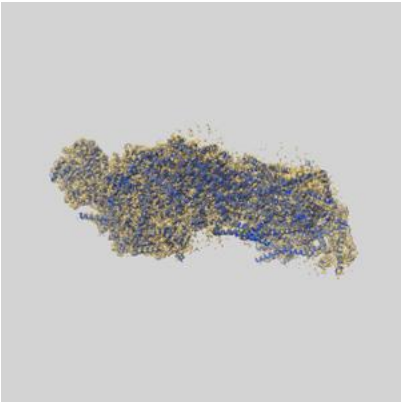
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-15937 and PDB model 8BA0. Per-residue inclusion information can be found in section 3 on page 18.

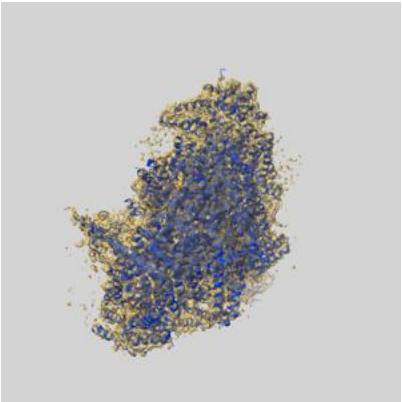
9.1 Map-model overlay (i)



X



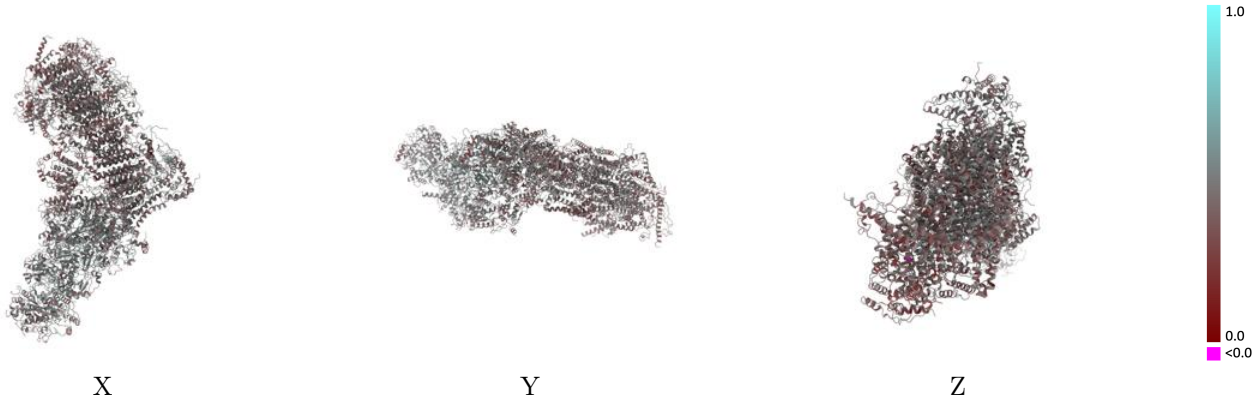
Y



Z

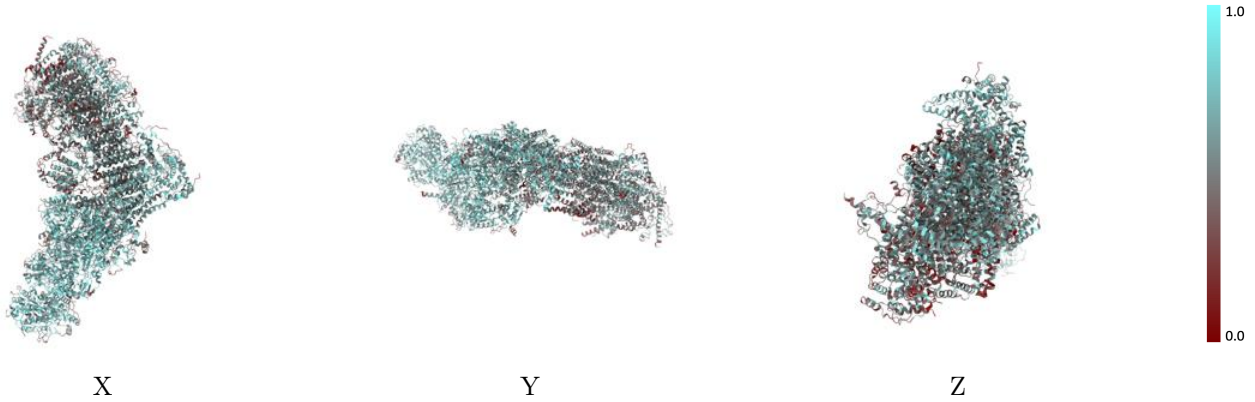
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



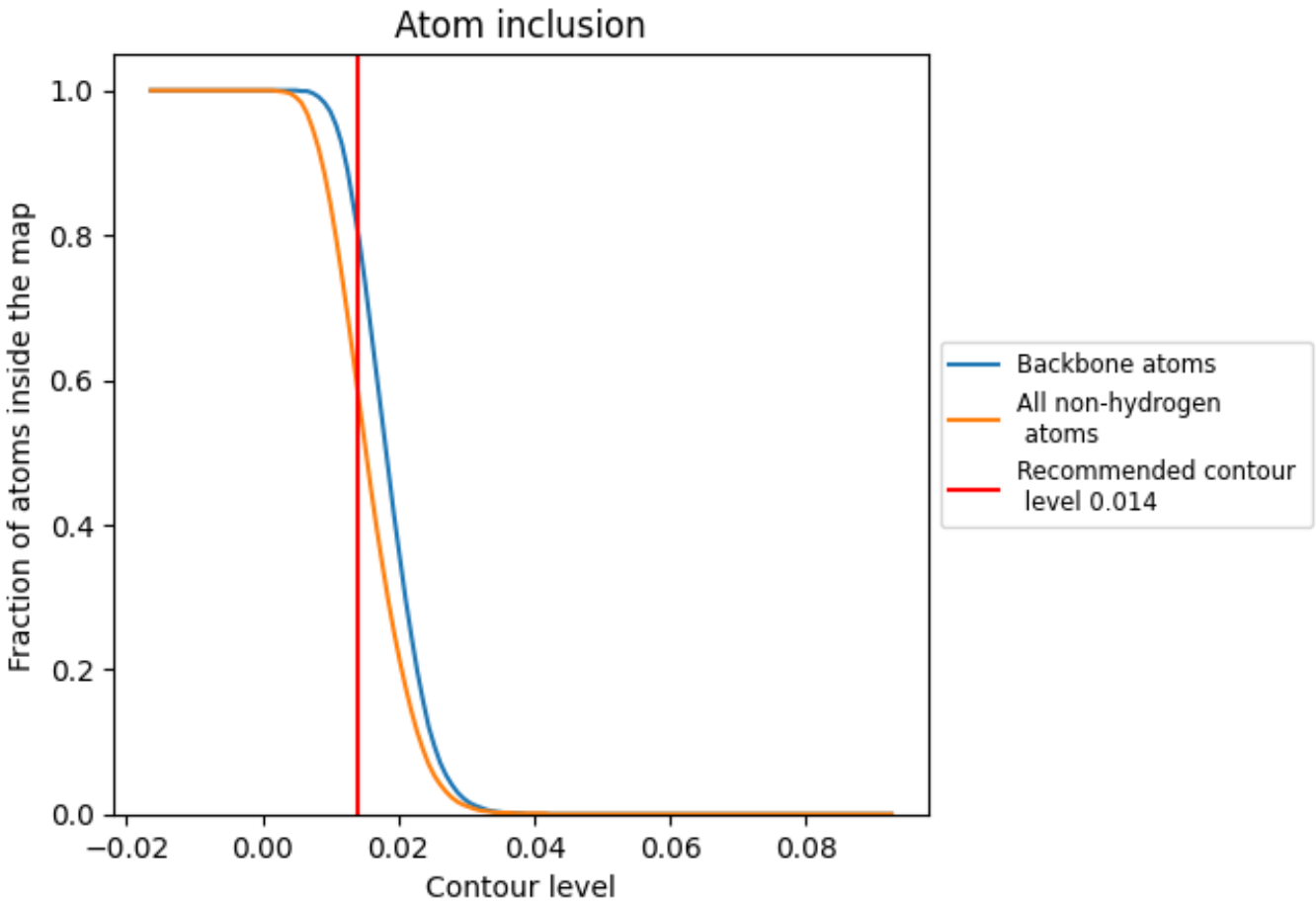
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5860	0.4350
A	0.5360	0.4170
B	0.6870	0.4910
C	0.6970	0.4850
D	0.6480	0.4690
E	0.6550	0.4450
F	0.6990	0.4630
G	0.6740	0.4700
H	0.6250	0.4540
I	0.7260	0.4840
J	0.5520	0.4190
K	0.5080	0.3880
L	0.5020	0.4150
M	0.5280	0.4370
N	0.5530	0.4160
O	0.5270	0.3950
P	0.6500	0.4570
Q	0.6790	0.4770
R	0.7190	0.4840
T	0.3900	0.3360
U	0.3560	0.3490
V	0.6260	0.4280
W	0.6280	0.4340
X	0.5960	0.4400
Y	0.3630	0.3980
Z	0.6770	0.4570
a	0.6050	0.4390
b	0.6110	0.4360
d	0.5470	0.4220
e	0.6250	0.4280
f	0.4200	0.4020
g	0.4780	0.4170
h	0.5780	0.4270
i	0.4700	0.3860
j	0.4530	0.3710

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Chain	Atom inclusion	Q-score
k	0.4210	0.3490
l	0.4920	0.4160
m	0.5080	0.4120
n	0.4850	0.3810
o	0.5100	0.3770
p	0.6110	0.4220
q	0.6420	0.4640
r	0.5670	0.4520
s	0.5100	0.4130