Full wwPDB EM Validation Report (i)

Dec 18, 2022 – 12:29 pm GMT

PDB ID	:	7AJD
EMDB ID	:	EMD-11430
Title	:	bovine ATP synthase dimer state1:state3
Authors	:	Spikes, T.E.; Montgomery, M.G.; Walker, J.E.
Deposited on	:	2020-09-29
Resolution	:	9.00 Å(reported)
Based on initial models	:	6ZQN, 6ZPO

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:

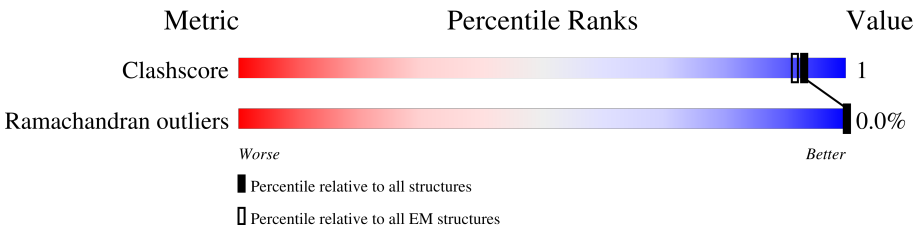
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 9.00 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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	8	66	• 62% 38%
1	A8	66	6% 62% 38%
2	A	510	10% 98% •
2	AA	510	16% 96% • •
2	AB	510	26% 97% • •
2	AC	510	15% 93% • 5%
2	B	510	5% 93% • 6%
2	C	510	5% 96% • •
3	AD	482	13% 96% • •

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Mol	Chain	Length	Quality of chain
3	AE	482	16% 96%
3	AF	482	14% 96%
3	D	482	97%
3	E	482	5% 96%
3	F	482	96%
4	AG	273	8% 100%
4	G	273	98%
5	AH	146	8% 90% 10%
5	H	146	90% 10%
6	AI	50	16% 94% 6%
6	I	50	6% 94% 6%
7	AJ	66	15% 71% 29%
7	J	66	6% 71% 29%
8	AK	75	23% 88% 11%
8	AL	75	23% 95%
8	AM	75	23% 96%
8	AN	75	37% 96%
8	AO	75	35% 95% 5%
8	AP	75	29% 87% 11%
8	AQ	75	35% 96%
8	AR	75	21% 97%
8	K	75	16% 89% 9%
8	L	75	20% 92% 7%
8	M	75	17% 95% 5%
8	N	75	9% 100%

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Mol	Chain	Length	Quality of chain
8	O	75	16% 100%
8	P	75	5% 99%
8	Q	75	16% 97%
8	R	75	7% 92% 8%
9	AS	190	14% 96%
9	S	190	6% 99%
10	Aa	226	15% 100%
10	a	226	12% 100%
11	Ab	214	15% 98%
11	b	214	6% 98%
12	Ad	160	21% 97%
12	d	160	9% 98%
13	Ae	70	17% 80% 20%
13	e	70	80% 20%
14	Af	87	20% 95% 5%
14	f	87	15% 95% 5%
15	Ag	102	8% 77% 23%
15	g	102	7% 77% 23%
16	Ah	76	28% 82% 18%
16	h	76	9% 82% 18%
17	Aj	60	20% 80% 20%
17	j	60	8% 80% 20%
18	Ak	57	19% 63% 37%
18	k	57	18% 63% 37%

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 51424 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 ATP synthase protein 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	8	41	205	123	41	41	0	0
1	A8	41	205	123	41	41	0	0

- Molecule 2 is a protein called ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	A	508	2491	1475	508	508	0	0
2	B	477	2339	1385	477	477	0	0
2	C	498	2443	1447	498	498	0	0
2	AA	501	2457	1455	501	501	0	0
2	AB	502	2462	1458	502	502	0	0
2	AC	483	2369	1403	483	483	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	GLN	variant	UNP P19483
A	481	GLY	SER	microheterogeneity	UNP P19483
B	1	GLU	GLN	variant	UNP P19483
B	481	GLY	SER	microheterogeneity	UNP P19483
C	1	GLU	GLN	variant	UNP P19483
C	481	GLY	SER	microheterogeneity	UNP P19483
AA	1	GLU	GLN	variant	UNP P19483
AA	481	GLY	SER	microheterogeneity	UNP P19483
AB	1	GLU	GLN	variant	UNP P19483

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Chain	Residue	Modelled	Actual	Comment	Reference
AB	481	GLY	SER	microheterogeneity	UNP P19483
AC	1	GLU	GLN	variant	UNP P19483
AC	481	GLY	SER	microheterogeneity	UNP P19483

- Molecule 3 is a protein called ATP synthase subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	D	469	2300	1362	469	469	0	0
3	E	467	2290	1356	467	467	0	0
3	F	467	2290	1356	467	467	0	0
3	AD	469	2300	1362	469	469	0	0
3	AE	467	2290	1356	467	467	0	0
3	AF	467	2290	1356	467	467	0	0

- Molecule 4 is a protein called ATP synthase subunit gamma, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	G	272	1347	803	272	272	0	0
4	AG	272	1347	803	272	272	0	0

- Molecule 5 is a protein called ATP synthase subunit delta, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	H	132	653	389	132	132	0	0
5	AH	131	648	386	131	131	0	0

- Molecule 6 is a protein called ATP synthase subunit epsilon, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	I	47	233	139	47	47	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	AI	47	233	139	47	47	0	0

- Molecule 7 is a protein called ATPase inhibitor, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	J	47	231	137	47	47	0	0
7	AJ	47	231	137	47	47	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	61	HIS	-	expression tag	UNP P01096
J	62	HIS	-	expression tag	UNP P01096
J	63	HIS	-	expression tag	UNP P01096
J	64	HIS	-	expression tag	UNP P01096
J	65	HIS	-	expression tag	UNP P01096
J	66	HIS	-	expression tag	UNP P01096
AJ	61	HIS	-	expression tag	UNP P01096
AJ	62	HIS	-	expression tag	UNP P01096
AJ	63	HIS	-	expression tag	UNP P01096
AJ	64	HIS	-	expression tag	UNP P01096
AJ	65	HIS	-	expression tag	UNP P01096
AJ	66	HIS	-	expression tag	UNP P01096

- Molecule 8 is a protein called ATP synthase F(0) complex subunit C2, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	K	74	359	211	74	74	0	0
8	L	74	359	211	74	74	0	0
8	M	75	364	214	75	75	0	0
8	N	75	364	214	75	75	0	0
8	O	75	364	214	75	75	0	0
8	P	74	359	211	74	74	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	Q	75	364	214	75	75	0	0
8	R	75	364	214	75	75	0	0
8	AK	74	359	211	74	74	0	0
8	AL	74	359	211	74	74	0	0
8	AM	75	364	214	75	75	0	0
8	AN	75	364	214	75	75	0	0
8	AO	75	364	214	75	75	0	0
8	AP	74	359	211	74	74	0	0
8	AQ	75	364	214	75	75	0	0
8	AR	75	364	214	75	75	0	0

- Molecule 9 is a protein called ATP synthase subunit O, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	S	188	931	555	188	188	0	0
9	AS	187	926	552	187	187	0	0

- Molecule 10 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	a	226	1119	667	226	226	0	0
10	Aa	226	1119	667	226	226	0	0

- Molecule 11 is a protein called ATP synthase F(0) complex subunit B1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	b	209	1035	617	209	209	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	Ab	209	1035	617	209	209	0	0

- Molecule 12 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	d	156	778	466	156	156	0	0
12	Ad	155	773	463	155	155	0	0

- Molecule 13 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	e	56	277	165	56	56	0	0
13	Ae	56	277	165	56	56	0	0

- Molecule 14 is a protein called ATP synthase subunit f, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	f	83	409	243	83	83	0	0
14	Af	83	409	243	83	83	0	0

- Molecule 15 is a protein called ATP synthase subunit g, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	g	79	390	232	79	79	0	0
15	Ag	79	390	232	79	79	0	0

- Molecule 16 is a protein called ATP synthase-coupling factor 6, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	h	62	306	182	62	62	0	0
16	Ah	62	306	182	62	62	0	0

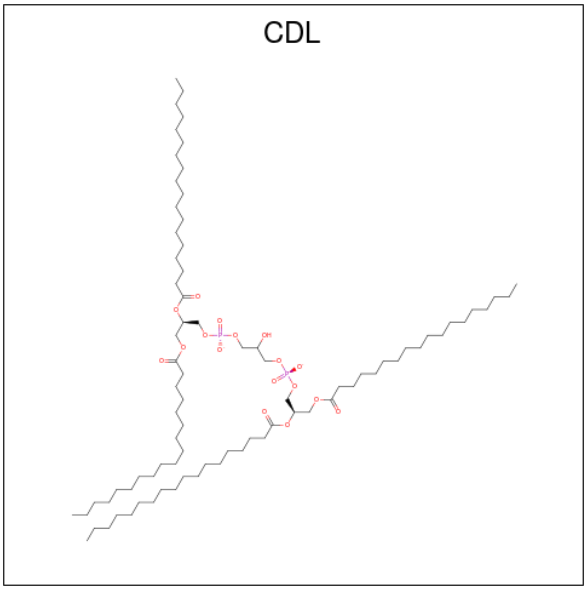
- Molecule 17 is a protein called ATP synthase subunit ATP5MPL, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	j	48	238	142	48	48	0	0
17	Aj	48	238	142	48	48	0	0

- Molecule 18 is a protein called ATP synthase membrane subunit DAPIT, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	k	36	177	105	36	36	0	0
18	Ak	36	177	105	36	36	0	0

- Molecule 19 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
19	a	1	84	65	17	2	0
19	b	1	83	64	17	2	0
19	f	1	78	59	17	2	0
19	Aa	1	84	65	17	2	0
19	Ab	1	83	64	17	2	0

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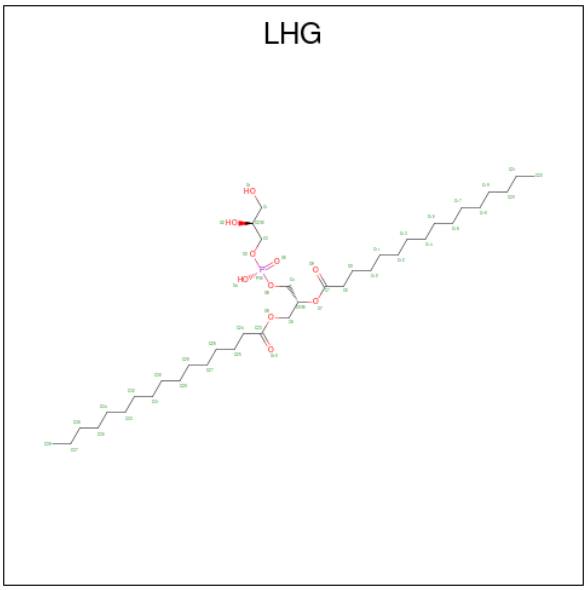
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
19	Af	1	78	59	17	2	0

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



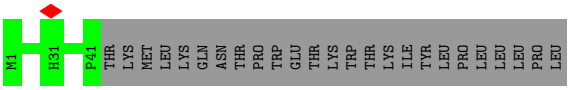
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
20	f	1	88	66	20	2	0
			Total	C	O	P	
20	f	1	88	66	20	2	0
			Total	C	O	P	
20	Af	1	88	66	20	2	0
			Total	C	O	P	
20	Af	1	88	66	20	2	0

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.

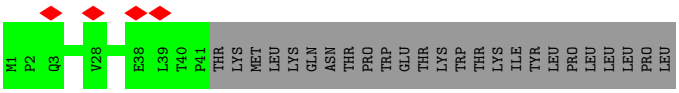
• Molecule 1: ATP synthase protein 8

Chain 8:



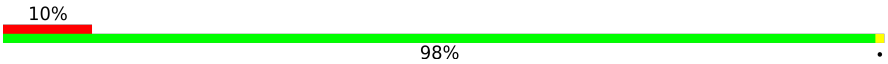
• Molecule 1: ATP synthase protein 8

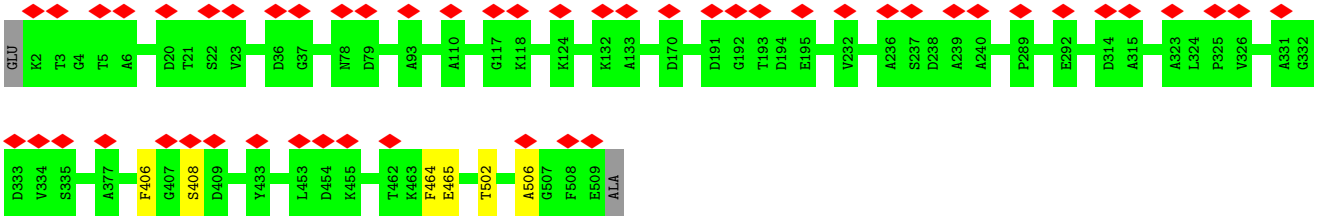
Chain A8:



• Molecule 2: ATP synthase subunit alpha, mitochondrial

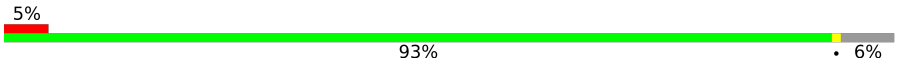
Chain A:

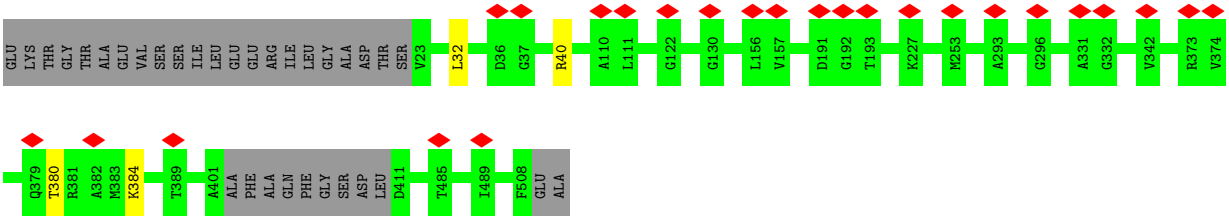




• Molecule 2: ATP synthase subunit alpha, mitochondrial

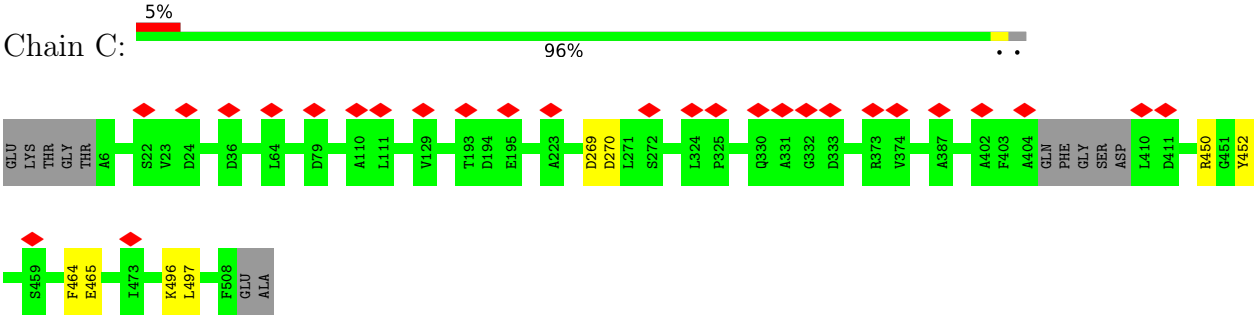
Chain B:





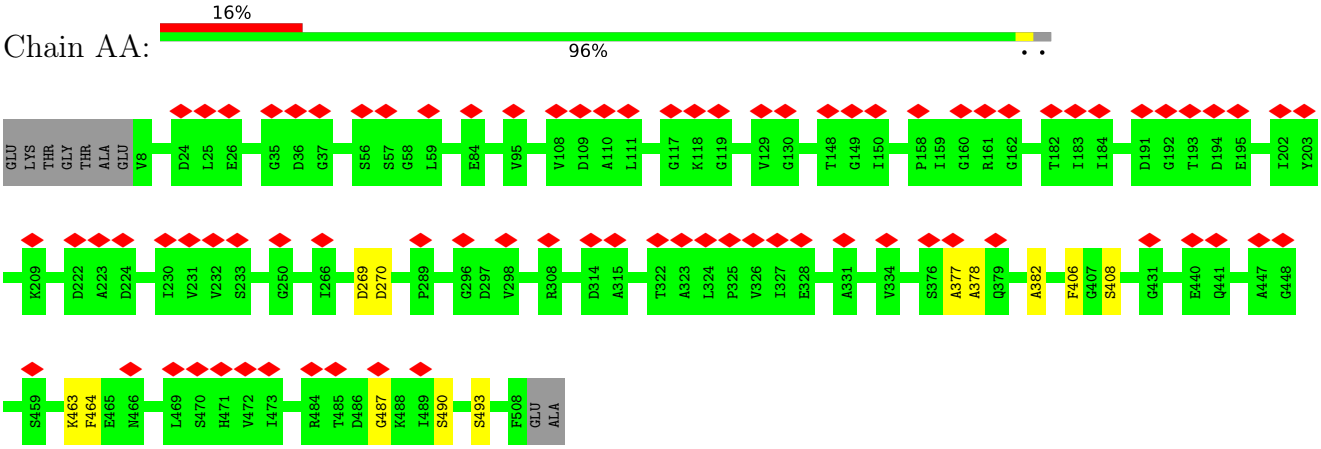
• Molecule 2: ATP synthase subunit alpha, mitochondrial

Chain C:



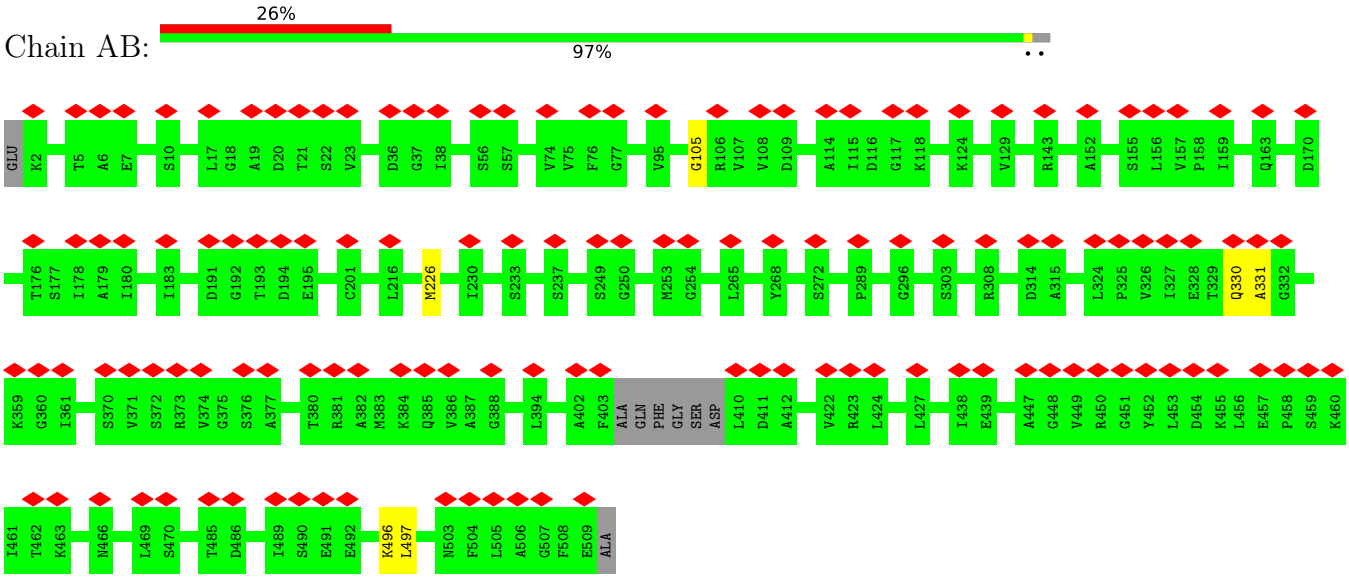
• Molecule 2: ATP synthase subunit alpha, mitochondrial

Chain AA:



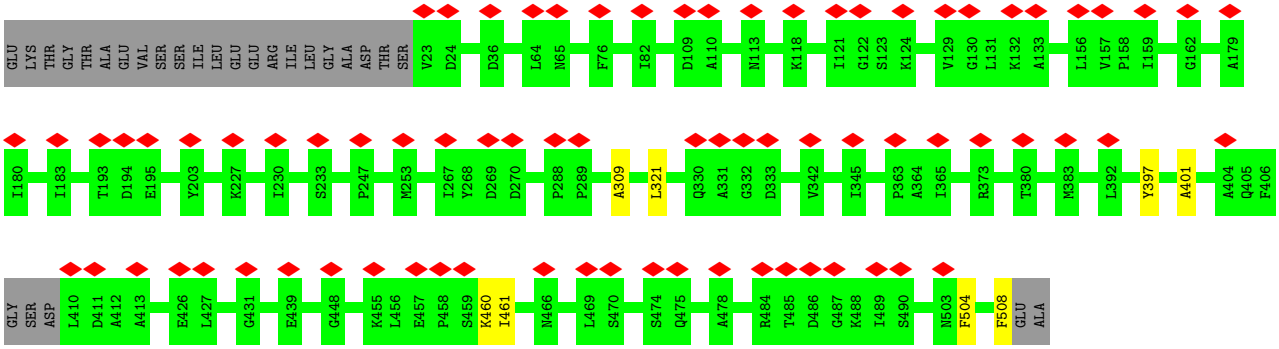
• Molecule 2: ATP synthase subunit alpha, mitochondrial

Chain AB:



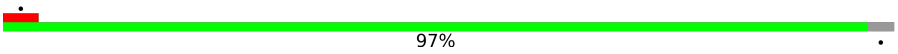
• Molecule 2: ATP synthase subunit alpha, mitochondrial

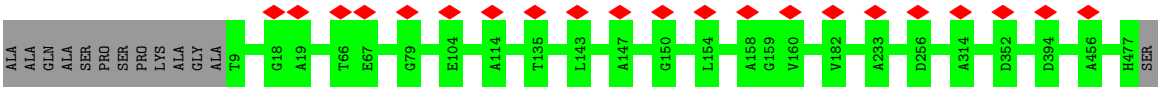
Chain AC:



• Molecule 3: ATP synthase subunit beta, mitochondrial

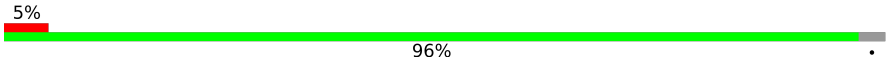
Chain D:

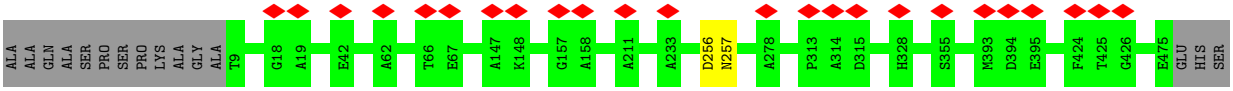




• Molecule 3: ATP synthase subunit beta, mitochondrial

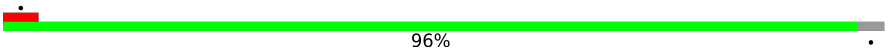
Chain E:

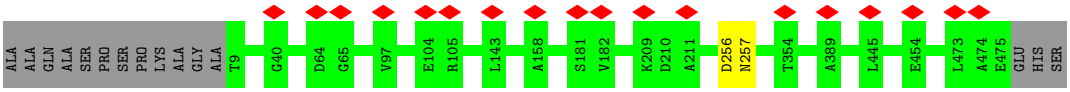




• Molecule 3: ATP synthase subunit beta, mitochondrial

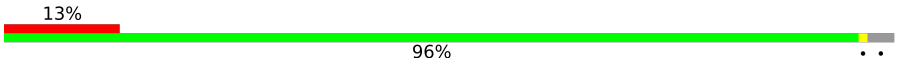
Chain F:

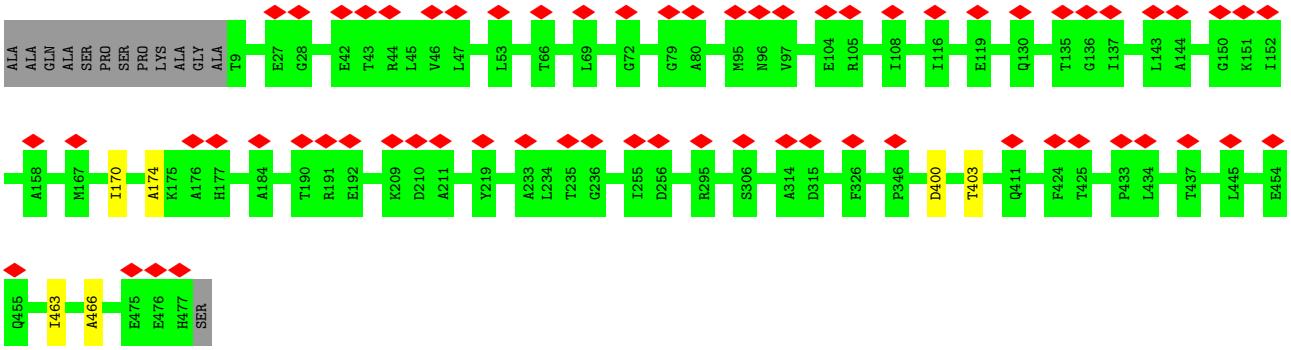




• Molecule 3: ATP synthase subunit beta, mitochondrial

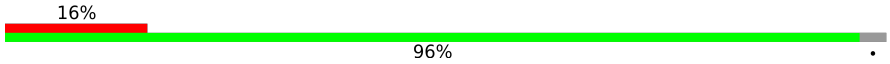
Chain AD:

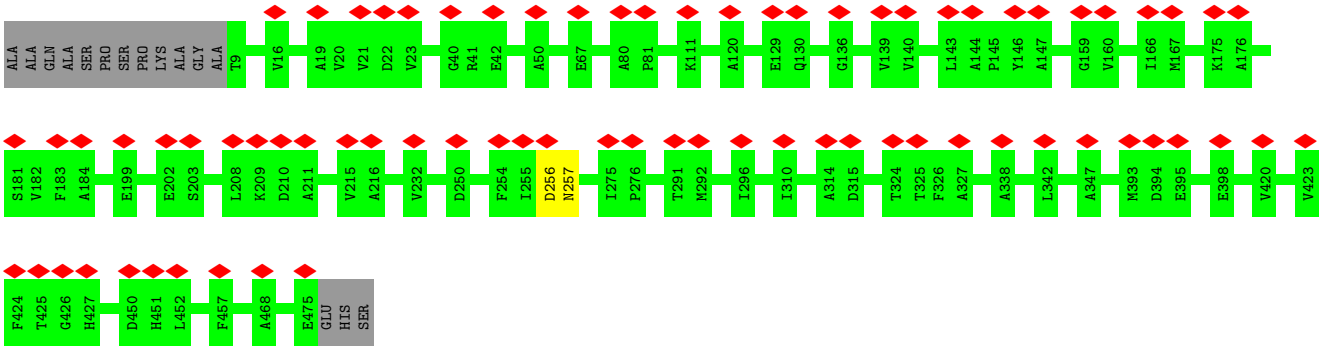




• Molecule 3: ATP synthase subunit beta, mitochondrial

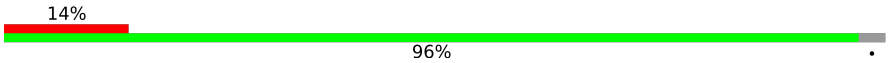
Chain AE:

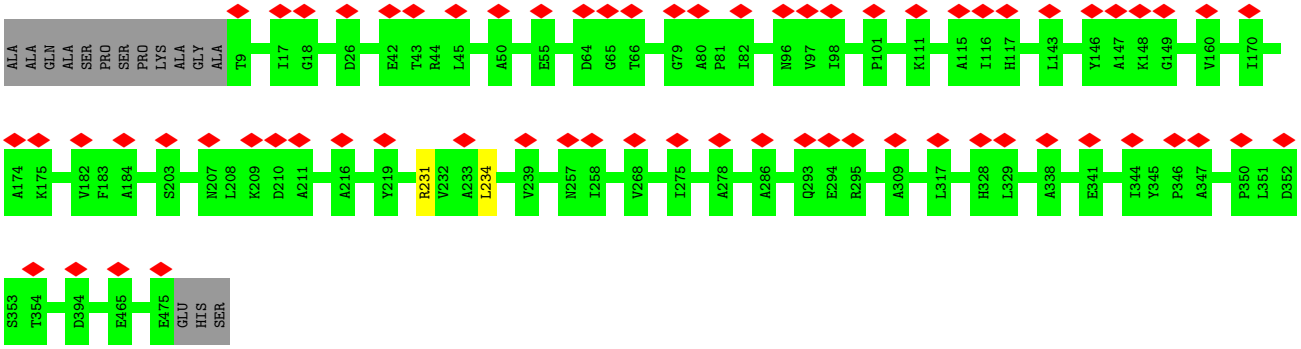




- Molecule 3: ATP synthase subunit beta, mitochondrial

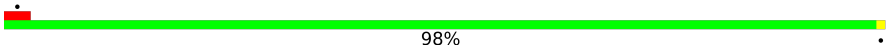
Chain AF:

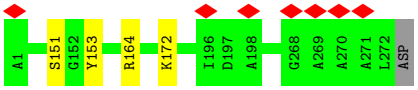




- Molecule 4: ATP synthase subunit gamma, mitochondrial

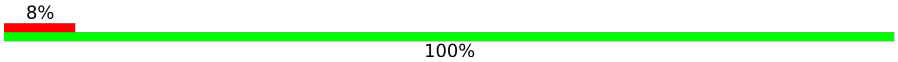
Chain G:

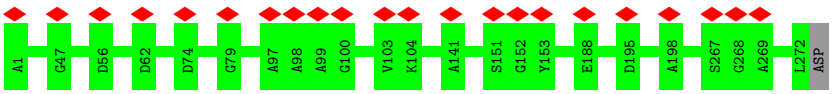




- Molecule 4: ATP synthase subunit gamma, mitochondrial

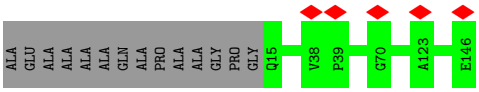
Chain AG:





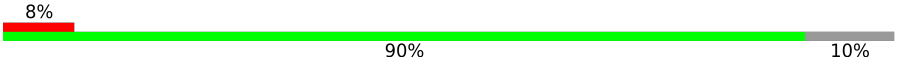
- Molecule 5: ATP synthase subunit delta, mitochondrial

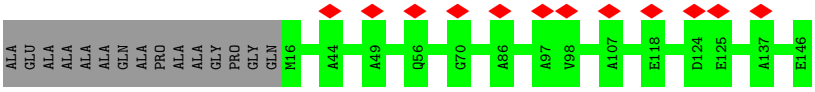
Chain H:



• Molecule 5: ATP synthase subunit delta, mitochondrial

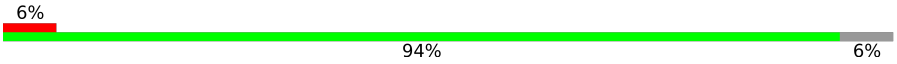
Chain AH:

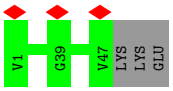




• Molecule 6: ATP synthase subunit epsilon, mitochondrial

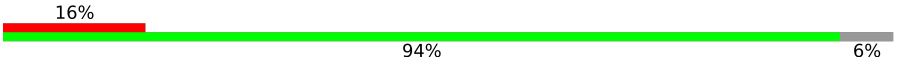
Chain I:

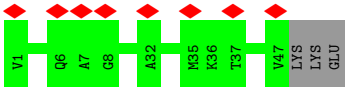




• Molecule 6: ATP synthase subunit epsilon, mitochondrial

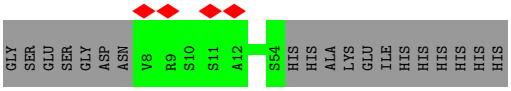
Chain AI:





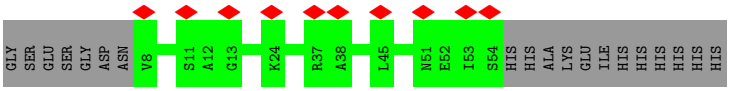
• Molecule 7: ATPase inhibitor, mitochondrial

Chain J:



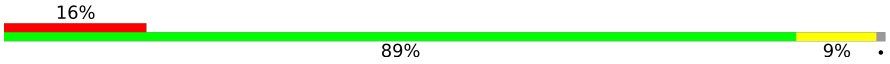
• Molecule 7: ATPase inhibitor, mitochondrial

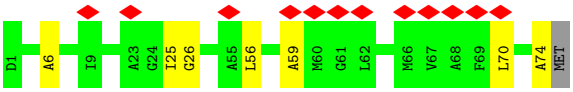
Chain AJ:



• Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

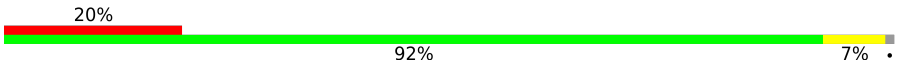
Chain K:

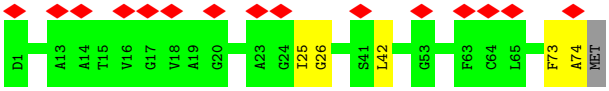




• Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

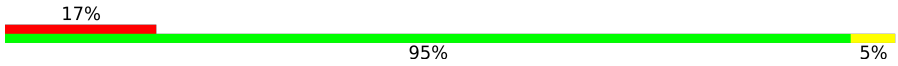
Chain L:

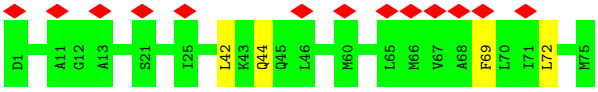




• Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

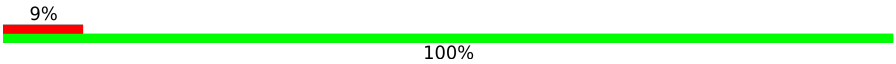
Chain M:

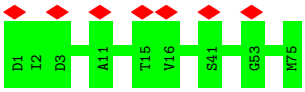




• Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

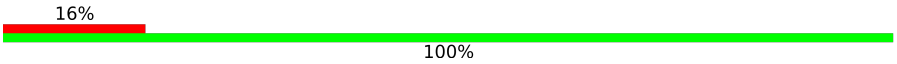
Chain N:

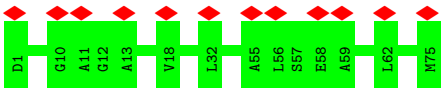




• Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

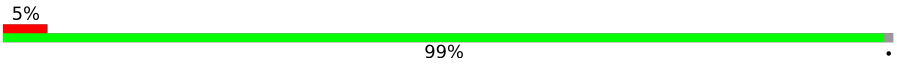
Chain O:

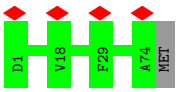




• Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

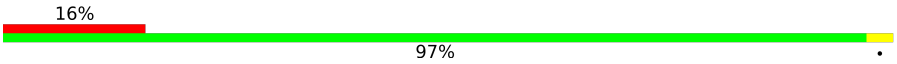
Chain P:

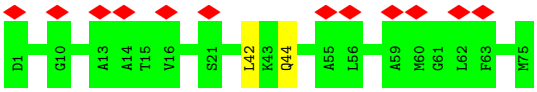




• Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

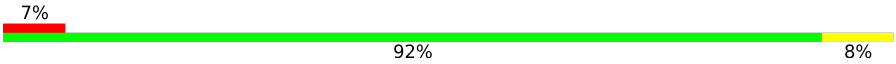
Chain Q:

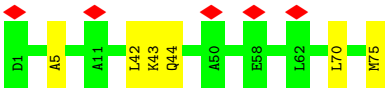




• Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

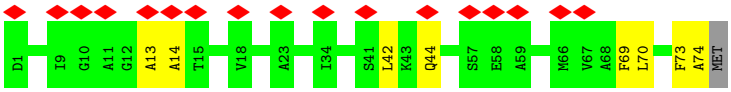
Chain R:





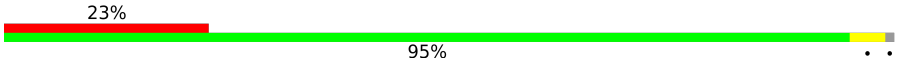
• Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

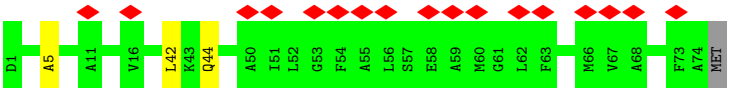
Chain AK:



• Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

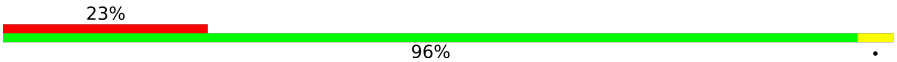
Chain AL:

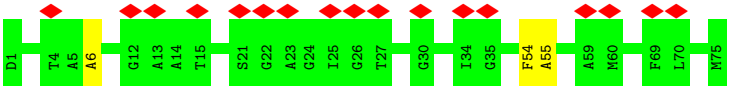




• Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

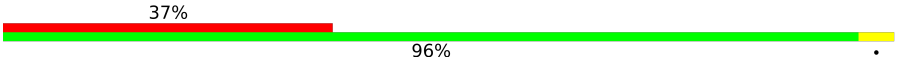
Chain AM:

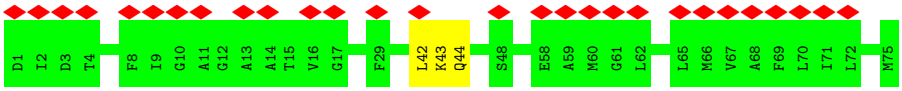




• Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

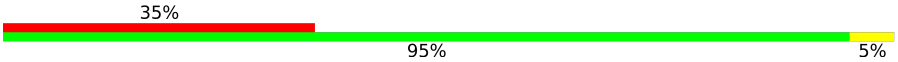
Chain AN:

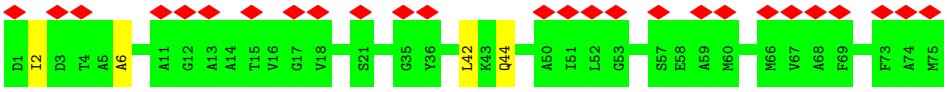




• Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

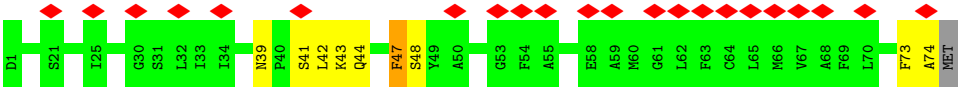
Chain AO:





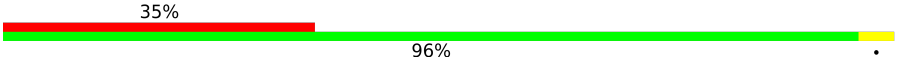
• Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

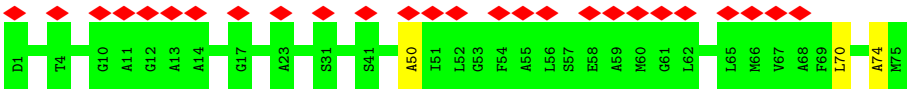
Chain AP:



• Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

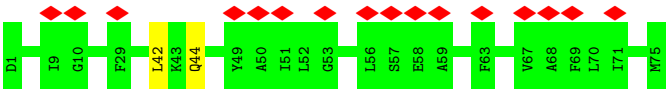
Chain AQ:





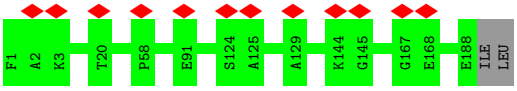
• Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

Chain AR: 21% 97%



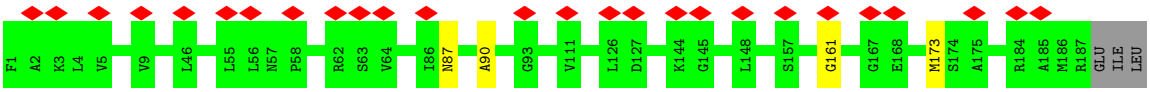
• Molecule 9: ATP synthase subunit O, mitochondrial

Chain S: 6% 99%



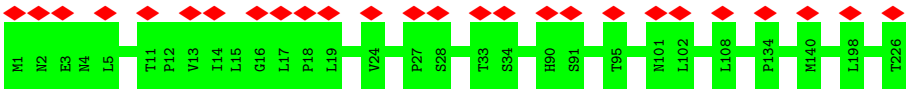
• Molecule 9: ATP synthase subunit O, mitochondrial

Chain AS: 14% 96%



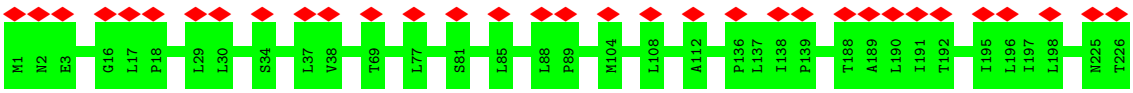
• Molecule 10: ATP synthase subunit a

Chain a: 12% 100%



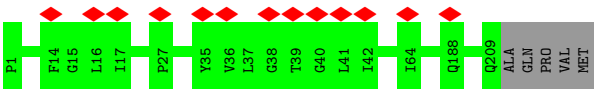
• Molecule 10: ATP synthase subunit a

Chain Aa: 15% 100%



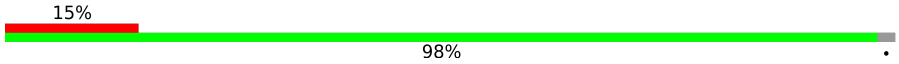
• Molecule 11: ATP synthase F(0) complex subunit B1, mitochondrial

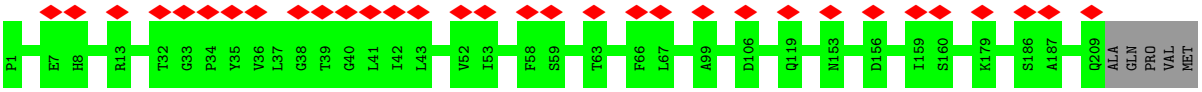
Chain b: 6% 98%



• Molecule 11: ATP synthase F(0) complex subunit B1, mitochondrial

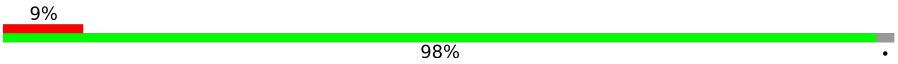
Chain Ab:

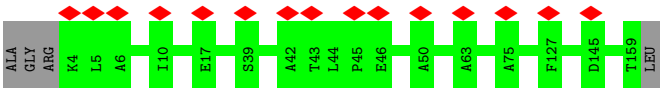




• Molecule 12: ATP synthase subunit d, mitochondrial

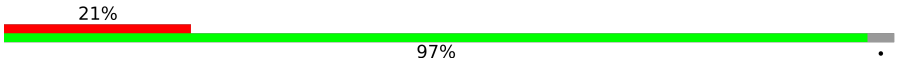
Chain d:

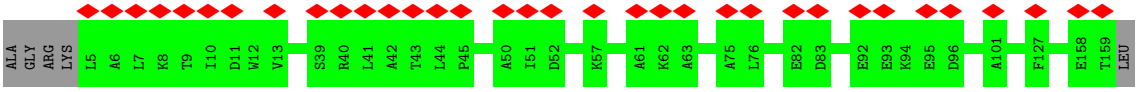




• Molecule 12: ATP synthase subunit d, mitochondrial

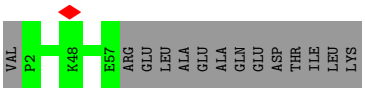
Chain Ad:





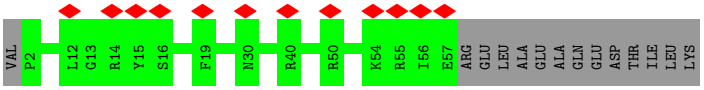
• Molecule 13: ATP synthase subunit e, mitochondrial

Chain e:



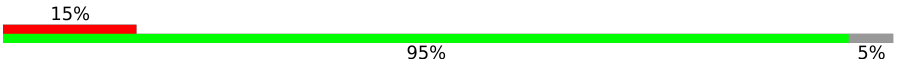
• Molecule 13: ATP synthase subunit e, mitochondrial

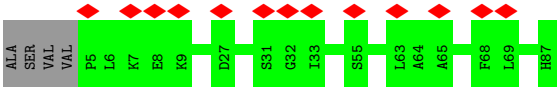
Chain Ae:



• Molecule 14: ATP synthase subunit f, mitochondrial

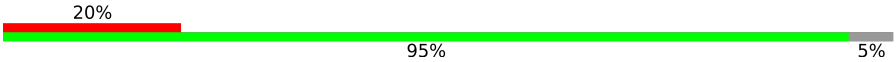
Chain f:

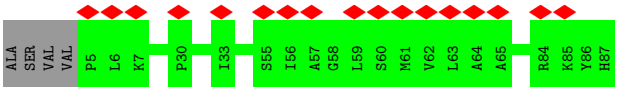




• Molecule 14: ATP synthase subunit f, mitochondrial

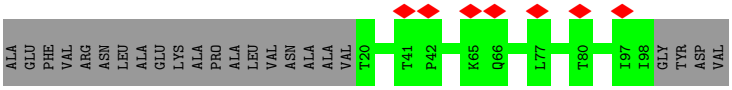
Chain Af:





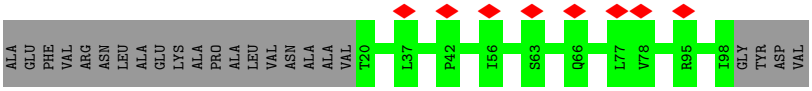
• Molecule 15: ATP synthase subunit g, mitochondrial

Chain g:



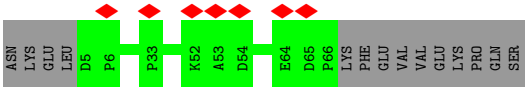
• Molecule 15: ATP synthase subunit g, mitochondrial

Chain Ag:



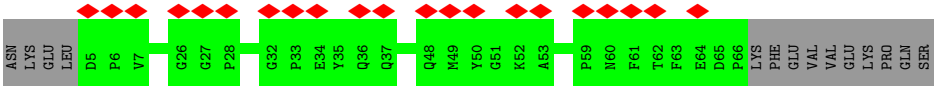
• Molecule 16: ATP synthase-coupling factor 6, mitochondrial

Chain h:



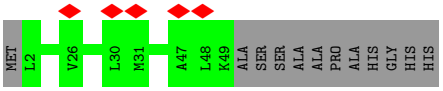
• Molecule 16: ATP synthase-coupling factor 6, mitochondrial

Chain Ah:



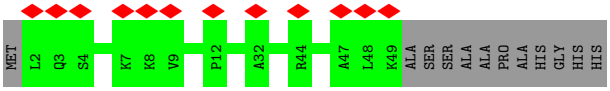
• Molecule 17: ATP synthase subunit ATP5MPL, mitochondrial

Chain j:



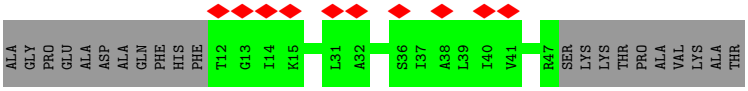
• Molecule 17: ATP synthase subunit ATP5MPL, mitochondrial

Chain Aj:



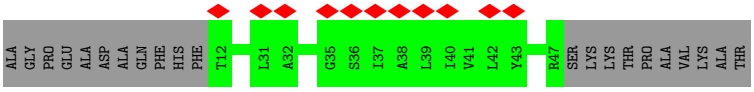
• Molecule 18: ATP synthase membrane subunit DAPIT, mitochondrial

Chain k:



• Molecule 18: ATP synthase membrane subunit DAPIT, mitochondrial

Chain Ak:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12721	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 ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0129	Depositor
Map size (Å)	524.0, 524.0, 524.0	wwPDB
Map dimensions	500, 500, 500	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: CDL, LHG, M3L

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	8	0.32	0/204	0.48	0/284
1	A8	0.54	0/204	0.60	0/284
2	A	0.28	0/2490	0.47	0/3455
2	AA	0.31	0/2456	0.48	0/3408
2	AB	0.31	0/2460	0.48	0/3412
2	AC	0.31	0/2367	0.48	0/3283
2	B	0.28	0/2337	0.47	0/3241
2	C	0.28	0/2441	0.47	0/3386
3	AD	0.32	0/2299	0.49	0/3190
3	AE	0.31	0/2289	0.48	0/3176
3	AF	0.31	0/2289	0.49	0/3176
3	D	0.28	0/2299	0.47	0/3190
3	E	0.28	0/2289	0.47	0/3176
3	F	0.28	0/2289	0.46	0/3176
4	AG	0.29	0/1346	0.46	0/1875
4	G	0.28	0/1346	0.45	0/1875
5	AH	0.32	0/647	0.51	0/900
5	H	0.30	0/652	0.51	0/907
6	AI	0.30	0/232	0.46	0/322
6	I	0.28	0/232	0.44	0/322
7	AJ	0.29	0/230	0.47	0/318
7	J	0.27	0/230	0.42	0/318
8	AK	0.31	0/353	0.49	0/486
8	AL	0.30	0/353	0.51	0/486
8	AM	0.32	0/358	0.53	0/493
8	AN	0.29	0/358	0.52	0/493
8	AO	0.33	0/358	0.63	0/493
8	AP	0.64	1/353 (0.3%)	0.61	0/486
8	AQ	0.29	0/358	0.73	1/493 (0.2%)
8	AR	0.31	0/358	0.51	0/493
8	K	0.29	0/353	0.48	0/486
8	L	0.30	0/353	0.48	0/486

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	M	0.28	0/358	0.48	0/493
8	N	0.28	0/358	0.50	0/493
8	O	0.29	0/358	0.47	0/493
8	P	0.27	0/353	0.47	0/486
8	Q	0.28	0/358	0.51	0/493
8	R	0.28	0/358	0.48	0/493
9	AS	0.28	0/925	0.45	0/1288
9	S	0.26	0/930	0.43	0/1295
10	Aa	0.34	0/1118	0.48	0/1557
10	a	0.29	0/1118	0.47	0/1557
11	Ab	0.29	0/1034	0.44	0/1440
11	b	0.28	0/1034	0.45	0/1440
12	Ad	0.27	0/772	0.43	0/1078
12	d	0.26	0/777	0.44	0/1085
13	Ae	0.29	0/276	0.51	0/383
13	e	0.27	0/276	0.44	0/383
14	Af	0.29	0/408	0.44	0/566
14	f	0.27	0/408	0.48	0/566
15	Ag	0.27	0/389	0.49	0/540
15	g	0.29	0/389	0.48	0/540
16	Ah	0.27	0/305	0.48	0/423
16	h	0.24	0/305	0.44	0/423
17	Aj	0.27	0/237	0.44	0/329
17	j	0.24	0/237	0.43	0/329
18	Ak	0.24	0/176	0.40	0/243
18	k	0.24	0/176	0.39	0/243
All	All	0.30	1/50616 (0.0%)	0.48	1/70228 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	AP	47	PHE	C-O	-8.81	1.06	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	AQ	50	ALA	N-CA-CB	5.74	118.13	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	8	205	0	81	0	0
1	A8	205	0	81	0	0
2	A	2491	0	1191	3	0
2	AA	2457	0	1173	6	0
2	AB	2462	0	1174	3	0
2	AC	2369	0	1131	4	0
2	B	2339	0	1113	2	0
2	C	2443	0	1168	4	0
3	AD	2300	0	1094	3	0
3	AE	2290	0	1090	1	0
3	AF	2290	0	1090	1	0
3	D	2300	0	1094	0	0
3	E	2290	0	1090	1	0
3	F	2290	0	1090	1	0
4	AG	1347	0	641	0	0
4	G	1347	0	641	2	0
5	AH	648	0	324	0	0
5	H	653	0	326	0	0
6	AI	233	0	119	0	0
6	I	233	0	119	0	0
7	AJ	231	0	124	0	0
7	J	231	0	124	0	0
8	AK	359	0	198	4	0
8	AL	359	0	198	3	0
8	AM	364	0	201	3	0
8	AN	364	0	201	2	0
8	AO	364	0	201	2	0
8	AP	359	0	198	4	0
8	AQ	364	0	201	1	0
8	AR	364	0	201	1	0
8	K	359	0	199	4	0
8	L	359	0	198	2	0
8	M	364	0	200	3	0
8	N	364	0	201	0	0
8	O	364	0	201	0	0
8	P	359	0	199	0	0
8	Q	364	0	201	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	R	364	0	200	4	0
9	AS	926	0	425	2	0
9	S	931	0	427	0	0
10	Aa	1119	0	498	0	0
10	a	1119	0	498	0	0
11	Ab	1035	0	459	0	0
11	b	1035	0	459	0	0
12	Ad	773	0	342	0	0
12	d	778	0	344	0	0
13	Ae	277	0	129	0	0
13	e	277	0	129	0	0
14	Af	409	0	184	0	0
14	f	409	0	184	0	0
15	Ag	390	0	178	0	0
15	g	390	0	178	0	0
16	Ah	306	0	128	0	0
16	h	306	0	128	0	0
17	Aj	238	0	107	0	0
17	j	238	0	107	0	0
18	Ak	177	0	80	0	0
18	k	177	0	80	0	0
19	Aa	84	0	115	0	0
19	Ab	83	0	113	0	0
19	Af	78	0	103	0	0
19	a	84	0	115	0	0
19	b	83	0	113	0	0
19	f	78	0	103	0	0
20	Af	88	0	122	0	0
20	f	88	0	122	0	0
All	All	51424	0	25246	64	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (64) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:42:LEU:O	8:M:44:GLN:N	2.13	0.82
8:R:42:LEU:O	8:R:44:GLN:N	2.17	0.78
8:AO:42:LEU:O	8:AO:44:GLN:N	2.17	0.77
8:AK:42:LEU:O	8:AK:44:GLN:N	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AP:47:PHE:O	8:AP:48:SER:C	2.25	0.68
8:AL:42:LEU:O	8:AL:44:GLN:N	2.29	0.66
8:Q:42:LEU:O	8:Q:44:GLN:N	2.27	0.65
8:AK:69:PHE:O	8:AK:73:PHE:N	2.32	0.63
3:AF:231:ARG:O	3:AF:234:LEU:N	2.33	0.61
8:AR:42:LEU:O	8:AR:44:GLN:N	2.33	0.58
4:G:164:ARG:N	4:G:172:LYS:O	2.40	0.55
8:AK:70:LEU:O	8:AK:74:ALA:N	2.41	0.54
2:AA:406:PHE:O	2:AA:408:SER:N	2.42	0.53
9:AS:161:GLY:HA3	9:AS:173:MET:O	2.11	0.51
3:AD:170:ILE:O	3:AD:174:ALA:HB3	2.12	0.50
2:AA:490:SER:O	2:AA:493:SER:N	2.44	0.50
8:AO:2:ILE:O	8:AO:6:ALA:N	2.37	0.50
2:B:32:LEU:N	2:B:40:ARG:O	2.43	0.50
2:B:380:THR:O	2:B:384:LYS:N	2.44	0.49
3:AD:400:ASP:O	3:AD:403:THR:N	2.46	0.48
2:A:406:PHE:O	2:A:408:SER:N	2.46	0.48
8:L:73:PHE:O	8:L:74:ALA:HB2	2.14	0.48
8:AN:42:LEU:O	8:AN:44:GLN:N	2.47	0.47
8:AM:54:PHE:O	8:AM:55:ALA:C	2.52	0.47
8:AP:42:LEU:O	8:AP:43:M3L:C	2.62	0.47
2:AC:397:TYR:O	2:AC:401:ALA:N	2.48	0.46
2:AA:377:ALA:O	2:AA:378:ALA:HB3	2.16	0.46
8:AL:5:ALA:HB1	8:AM:6:ALA:HB2	1.97	0.46
2:AB:330:GLN:O	2:AB:331:ALA:C	2.54	0.45
8:K:56:LEU:O	8:K:59:ALA:HB3	2.16	0.45
2:C:464:PHE:O	2:C:465:GLU:C	2.56	0.44
9:AS:87:ASN:O	9:AS:90:ALA:N	2.50	0.44
2:AC:504:PHE:O	2:AC:508:PHE:N	2.50	0.44
8:AL:5:ALA:HB1	8:AM:6:ALA:CB	2.47	0.44
3:AD:463:ILE:O	3:AD:466:ALA:HB3	2.17	0.43
8:M:42:LEU:C	8:M:44:GLN:H	2.19	0.43
3:AE:256:ASP:HA	3:AE:257:ASN:HA	1.80	0.43
2:A:464:PHE:O	2:A:465:GLU:C	2.57	0.43
8:R:42:LEU:O	8:R:43:M3L:C	2.67	0.43
8:AK:13:ALA:O	8:AK:14:ALA:C	2.58	0.42
2:AA:269:ASP:HA	2:AA:270:ASP:HA	1.86	0.42
8:L:25:ILE:O	8:L:26:GLY:C	2.57	0.42
2:AB:496:LYS:O	2:AB:497:LEU:C	2.57	0.42
8:AP:73:PHE:O	8:AP:74:ALA:HB2	2.20	0.42
2:A:502:THR:O	2:A:506:ALA:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:496:LYS:O	2:C:497:LEU:C	2.58	0.41
2:C:269:ASP:HA	2:C:270:ASP:HA	1.87	0.41
2:AC:460:LYS:O	2:AC:461:ILE:C	2.58	0.41
2:AA:463:LYS:O	2:AA:464:PHE:C	2.59	0.41
8:AP:39:ASN:O	8:AP:41:SER:N	2.54	0.41
2:AC:309:ALA:HB1	2:AC:321:LEU:O	2.19	0.41
8:K:6:ALA:HB2	8:R:5:ALA:HB1	2.03	0.41
8:AN:42:LEU:O	8:AN:43:M3L:C	2.69	0.41
3:E:256:ASP:HA	3:E:257:ASN:HA	1.90	0.41
3:F:256:ASP:HA	3:F:257:ASN:HA	1.89	0.41
8:R:70:LEU:O	8:R:75:MET:N	2.54	0.40
4:G:151:SER:O	4:G:153:TYR:N	2.47	0.40
2:AB:105:GLY:HA2	2:AB:226:MET:O	2.21	0.40
8:AQ:70:LEU:O	8:AQ:74:ALA:O	2.40	0.40
8:K:25:ILE:O	8:K:26:GLY:C	2.60	0.40
8:K:70:LEU:O	8:K:74:ALA:N	2.54	0.40
8:M:69:PHE:O	8:M:72:LEU:N	2.53	0.40
2:AA:382:ALA:N	2:AA:487:GLY:O	2.51	0.40
2:C:450:ARG:O	2:C:452:TYR:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8	39/66 (59%)	29 (74%)	10 (26%)	0	100	100
1	A8	39/66 (59%)	33 (85%)	6 (15%)	0	100	100
2	A	506/510 (99%)	475 (94%)	31 (6%)	0	100	100
2	AA	499/510 (98%)	450 (90%)	49 (10%)	0	100	100
2	AB	498/510 (98%)	453 (91%)	45 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AC	479/510 (94%)	423 (88%)	56 (12%)	0	100	100
2	B	473/510 (93%)	449 (95%)	24 (5%)	0	100	100
2	C	494/510 (97%)	461 (93%)	33 (7%)	0	100	100
3	AD	467/482 (97%)	430 (92%)	37 (8%)	0	100	100
3	AE	465/482 (96%)	423 (91%)	42 (9%)	0	100	100
3	AF	465/482 (96%)	421 (90%)	44 (10%)	0	100	100
3	D	467/482 (97%)	440 (94%)	27 (6%)	0	100	100
3	E	465/482 (96%)	434 (93%)	31 (7%)	0	100	100
3	F	465/482 (96%)	431 (93%)	34 (7%)	0	100	100
4	AG	270/273 (99%)	255 (94%)	15 (6%)	0	100	100
4	G	270/273 (99%)	259 (96%)	11 (4%)	0	100	100
5	AH	129/146 (88%)	115 (89%)	14 (11%)	0	100	100
5	H	130/146 (89%)	119 (92%)	11 (8%)	0	100	100
6	AI	45/50 (90%)	45 (100%)	0	0	100	100
6	I	45/50 (90%)	43 (96%)	2 (4%)	0	100	100
7	AJ	45/66 (68%)	41 (91%)	4 (9%)	0	100	100
7	J	45/66 (68%)	44 (98%)	1 (2%)	0	100	100
8	AK	71/75 (95%)	66 (93%)	5 (7%)	0	100	100
8	AL	71/75 (95%)	70 (99%)	1 (1%)	0	100	100
8	AM	72/75 (96%)	66 (92%)	6 (8%)	0	100	100
8	AN	72/75 (96%)	67 (93%)	5 (7%)	0	100	100
8	AO	72/75 (96%)	70 (97%)	2 (3%)	0	100	100
8	AP	71/75 (95%)	67 (94%)	3 (4%)	1 (1%)	11	46
8	AQ	72/75 (96%)	69 (96%)	3 (4%)	0	100	100
8	AR	72/75 (96%)	66 (92%)	6 (8%)	0	100	100
8	K	71/75 (95%)	69 (97%)	2 (3%)	0	100	100
8	L	71/75 (95%)	66 (93%)	4 (6%)	1 (1%)	11	46
8	M	72/75 (96%)	71 (99%)	1 (1%)	0	100	100
8	N	72/75 (96%)	71 (99%)	1 (1%)	0	100	100
8	O	72/75 (96%)	70 (97%)	2 (3%)	0	100	100
8	P	71/75 (95%)	70 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	Q	72/75 (96%)	69 (96%)	3 (4%)	0	100	100
8	R	72/75 (96%)	67 (93%)	5 (7%)	0	100	100
9	AS	185/190 (97%)	173 (94%)	12 (6%)	0	100	100
9	S	186/190 (98%)	177 (95%)	9 (5%)	0	100	100
10	Aa	224/226 (99%)	195 (87%)	29 (13%)	0	100	100
10	a	224/226 (99%)	207 (92%)	17 (8%)	0	100	100
11	Ab	207/214 (97%)	197 (95%)	10 (5%)	0	100	100
11	b	207/214 (97%)	201 (97%)	6 (3%)	0	100	100
12	Ad	153/160 (96%)	136 (89%)	17 (11%)	0	100	100
12	d	154/160 (96%)	142 (92%)	12 (8%)	0	100	100
13	Ae	54/70 (77%)	53 (98%)	1 (2%)	0	100	100
13	e	54/70 (77%)	53 (98%)	1 (2%)	0	100	100
14	Af	81/87 (93%)	71 (88%)	10 (12%)	0	100	100
14	f	81/87 (93%)	79 (98%)	2 (2%)	0	100	100
15	Ag	77/102 (76%)	70 (91%)	7 (9%)	0	100	100
15	g	77/102 (76%)	70 (91%)	7 (9%)	0	100	100
16	Ah	60/76 (79%)	53 (88%)	7 (12%)	0	100	100
16	h	60/76 (79%)	48 (80%)	12 (20%)	0	100	100
17	Aj	46/60 (77%)	44 (96%)	2 (4%)	0	100	100
17	j	46/60 (77%)	44 (96%)	2 (4%)	0	100	100
18	Ak	34/57 (60%)	34 (100%)	0	0	100	100
18	k	34/57 (60%)	32 (94%)	2 (6%)	0	100	100
All	All	10190/10838 (94%)	9446 (93%)	742 (7%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	AP	44	GLN
8	L	42	LEU

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

16 non-standard protein/DNA/RNA residues are 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	$\#\|Z\| > 2$
8	M3L	R	43	8	3,4,12	0.71	0	2,4,16	0.26	0
8	M3L	AM	43	8	3,4,12	0.97	0	2,4,16	0.27	0
8	M3L	M	43	8	3,4,12	0.73	0	2,4,16	0.60	0
8	M3L	AN	43	8	3,4,12	0.69	0	2,4,16	0.16	0
8	M3L	AQ	43	8	3,4,12	0.88	0	2,4,16	0.25	0
8	M3L	AR	43	8	3,4,12	0.87	0	2,4,16	0.42	0
8	M3L	Q	43	8	3,4,12	0.75	0	2,4,16	0.85	0
8	M3L	K	43	8	3,4,12	1.02	0	2,4,16	0.14	0
8	M3L	AK	43	8	3,4,12	0.86	0	2,4,16	0.24	0
8	M3L	AP	43	8	3,4,12	0.79	0	2,4,16	0.40	0
8	M3L	AL	43	8	3,4,12	0.78	0	2,4,16	0.78	0
8	M3L	AO	43	8	3,4,12	0.65	0	2,4,16	0.74	0
8	M3L	O	43	8	3,4,12	0.85	0	2,4,16	0.23	0
8	M3L	L	43	8	3,4,12	0.88	0	2,4,16	0.52	0
8	M3L	P	43	8	3,4,12	0.88	0	2,4,16	0.74	0
8	M3L	N	43	8	3,4,12	0.87	0	2,4,16	0.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	M3L	R	43	8	-	0/0/2/12	-
8	M3L	AM	43	8	-	0/0/2/12	-
8	M3L	M	43	8	-	0/0/2/12	-
8	M3L	AN	43	8	-	0/0/2/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	M3L	AQ	43	8	-	0/0/2/12	-
8	M3L	AR	43	8	-	0/0/2/12	-
8	M3L	Q	43	8	-	0/0/2/12	-
8	M3L	K	43	8	-	0/0/2/12	-
8	M3L	AK	43	8	-	0/0/2/12	-
8	M3L	AP	43	8	-	0/0/2/12	-
8	M3L	AL	43	8	-	0/0/2/12	-
8	M3L	AO	43	8	-	0/0/2/12	-
8	M3L	O	43	8	-	0/0/2/12	-
8	M3L	L	43	8	-	0/0/2/12	-
8	M3L	P	43	8	-	0/0/2/12	-
8	M3L	N	43	8	-	0/0/2/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	R	43	M3L	1	0
8	AN	43	M3L	1	0
8	AP	43	M3L	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands are 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	$\#\|Z\| > 2$
19	CDL	b	301	-	82,82,99	0.98	6 (7%)	88,94,111	1.12	4 (4%)
19	CDL	f	101	-	77,77,99	1.00	6 (7%)	83,89,111	1.10	5 (6%)
19	CDL	Aa	301	-	83,83,99	0.98	7 (8%)	89,95,111	1.11	4 (4%)
20	LHG	Af	102	-	38,38,48	0.70	1 (2%)	41,44,54	1.32	5 (12%)
20	LHG	f	103	-	48,48,48	0.61	0	51,54,54	1.22	4 (7%)
20	LHG	Af	103	-	48,48,48	0.62	1 (2%)	51,54,54	1.22	4 (7%)
20	LHG	f	102	-	38,38,48	0.52	0	41,44,54	0.58	1 (2%)
19	CDL	a	301	-	83,83,99	0.98	7 (8%)	89,95,111	1.10	4 (4%)
19	CDL	Af	101	-	77,77,99	1.00	6 (7%)	83,89,111	1.12	4 (4%)
19	CDL	Ab	301	-	82,82,99	0.98	6 (7%)	88,94,111	1.16	5 (5%)

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
19	CDL	b	301	-	-	32/93/93/110	-
19	CDL	f	101	-	-	29/88/88/110	-
19	CDL	Aa	301	-	-	41/94/94/110	-
20	LHG	Af	102	-	-	14/43/43/53	-
20	LHG	f	103	-	-	12/53/53/53	-
20	LHG	Af	103	-	-	17/53/53/53	-
20	LHG	f	102	-	-	17/43/43/53	-
19	CDL	a	301	-	-	28/94/94/110	-
19	CDL	Af	101	-	-	42/88/88/110	-
19	CDL	Ab	301	-	-	34/93/93/110	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	f	101	CDL	OA6-CA4	-2.77	1.39	1.46
19	Af	101	CDL	OA6-CA4	-2.77	1.39	1.46
19	b	301	CDL	OA6-CA4	-2.74	1.39	1.46
19	Ab	301	CDL	OA6-CA4	-2.74	1.39	1.46
19	a	301	CDL	OB8-CB7	2.71	1.41	1.33
19	Aa	301	CDL	OB8-CB7	2.69	1.41	1.33
19	f	101	CDL	OB8-CB7	2.68	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Aa	301	CDL	OA6-CA4	-2.66	1.39	1.46
19	Aa	301	CDL	OB6-CB4	-2.64	1.40	1.46
19	Af	101	CDL	OB8-CB7	2.64	1.41	1.33
19	Ab	301	CDL	OB8-CB7	2.62	1.41	1.33
19	b	301	CDL	OB8-CB7	2.60	1.40	1.33
19	Ab	301	CDL	OB6-CB4	-2.55	1.40	1.46
19	a	301	CDL	OB6-CB4	-2.53	1.40	1.46
19	a	301	CDL	OA6-CA4	-2.51	1.40	1.46
19	Af	101	CDL	OB6-CB4	-2.47	1.40	1.46
19	f	101	CDL	OB6-CB5	2.47	1.41	1.34
19	f	101	CDL	OB6-CB4	-2.45	1.40	1.46
19	Af	101	CDL	OB6-CB5	2.43	1.41	1.34
19	a	301	CDL	OB6-CB5	2.42	1.41	1.34
19	b	301	CDL	OB6-CB5	2.41	1.41	1.34
19	b	301	CDL	OB6-CB4	-2.38	1.40	1.46
19	Ab	301	CDL	OA8-CA7	2.37	1.40	1.33
19	Ab	301	CDL	OB6-CB5	2.36	1.41	1.34
19	b	301	CDL	OA8-CA7	2.34	1.40	1.33
20	Af	102	LHG	O7-C5	-2.32	1.40	1.46
19	Aa	301	CDL	OB6-CB5	2.31	1.40	1.34
19	Aa	301	CDL	OA8-CA7	2.29	1.40	1.33
19	a	301	CDL	OA8-CA6	-2.27	1.40	1.45
19	Aa	301	CDL	OA8-CA6	-2.26	1.40	1.45
19	a	301	CDL	OA8-CA7	2.25	1.39	1.33
19	Af	101	CDL	OA8-CA6	-2.24	1.40	1.45
19	f	101	CDL	OA8-CA7	2.24	1.39	1.33
20	Af	103	LHG	O7-C5	-2.23	1.41	1.46
19	Af	101	CDL	OA8-CA7	2.19	1.39	1.33
19	f	101	CDL	OA8-CA6	-2.17	1.40	1.45
19	a	301	CDL	OA6-CA5	2.15	1.40	1.34
19	b	301	CDL	OA8-CA6	-2.15	1.40	1.45
19	Ab	301	CDL	OA8-CA6	-2.08	1.40	1.45
19	Aa	301	CDL	OA6-CA5	2.07	1.40	1.34

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	b	301	CDL	OA6-CA5-C11	4.57	121.35	111.50
20	Af	102	LHG	O4-P-O5	4.32	133.58	112.24
20	Af	103	LHG	O4-P-O5	4.22	133.12	112.24
19	Ab	301	CDL	OA6-CA5-C11	4.20	120.55	111.50
20	f	103	LHG	O4-P-O5	4.19	132.94	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	b	301	CDL	OB6-CB5-C51	4.10	120.33	111.50
19	Ab	301	CDL	OB6-CB5-C51	4.09	120.32	111.50
19	a	301	CDL	OA6-CA5-C11	4.08	120.30	111.50
19	Af	101	CDL	OB6-CB5-C51	4.00	120.13	111.50
19	f	101	CDL	OA6-CA5-C11	4.00	120.11	111.50
19	Aa	301	CDL	OA6-CA5-C11	3.99	120.10	111.50
19	Aa	301	CDL	OB6-CB5-C51	3.93	119.98	111.50
19	Af	101	CDL	OA6-CA5-C11	3.90	119.90	111.50
19	a	301	CDL	OB6-CB5-C51	3.87	119.83	111.50
19	f	101	CDL	OB6-CB5-C51	3.80	119.68	111.50
19	b	301	CDL	OA8-CA7-C31	2.76	120.56	111.91
20	f	103	LHG	O8-C23-C24	2.75	120.53	111.91
19	Ab	301	CDL	OA8-CA7-C31	2.74	120.52	111.91
19	Ab	301	CDL	OB8-CB7-C71	2.68	120.32	111.91
19	f	101	CDL	OA8-CA7-C31	2.67	120.30	111.91
20	Af	103	LHG	O8-C23-C24	2.67	120.28	111.91
19	Aa	301	CDL	OA8-CA7-C31	2.61	120.09	111.91
20	Af	102	LHG	O8-C23-C24	2.58	120.00	111.91
19	Af	101	CDL	OA8-CA7-C31	2.57	119.97	111.91
20	Af	102	LHG	C11-C10-C9	-2.52	101.66	114.42
19	a	301	CDL	OA8-CA7-C31	2.45	119.59	111.91
19	Aa	301	CDL	OB8-CB7-C71	2.44	119.56	111.91
19	Af	101	CDL	OB8-CB7-C71	2.39	119.42	111.91
19	a	301	CDL	OB8-CB7-C71	2.38	119.38	111.91
20	f	103	LHG	C11-C10-C9	-2.31	102.70	114.42
20	Af	103	LHG	C11-C10-C9	-2.31	102.71	114.42
19	b	301	CDL	OB8-CB7-C71	2.30	119.13	111.91
19	Ab	301	CDL	CA4-OA6-CA5	-2.20	112.36	117.79
19	f	101	CDL	OB8-CB7-C71	2.20	118.80	111.91
20	Af	102	LHG	C27-C26-C25	-2.16	103.47	114.42
20	f	103	LHG	C20-C19-C18	-2.15	103.49	114.42
20	Af	102	LHG	C18-C17-C16	-2.10	103.77	114.42
20	f	102	LHG	O4-P-O6	-2.04	98.27	107.75
19	f	101	CDL	CA4-OA6-CA5	-2.04	112.78	117.79
20	Af	103	LHG	C20-C19-C18	-2.03	104.12	114.42

There are no chirality outliers.

All (266) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	a	301	CDL	CB2-OB2-PB2-OB3
19	b	301	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
19	b	301	CDL	CA2-OA2-PA1-OA3
19	b	301	CDL	CA2-OA2-PA1-OA4
19	b	301	CDL	CA2-OA2-PA1-OA5
19	b	301	CDL	CB2-OB2-PB2-OB3
19	b	301	CDL	CB2-OB2-PB2-OB4
19	f	101	CDL	O1-C1-CA2-OA2
19	f	101	CDL	CA2-C1-CB2-OB2
19	f	101	CDL	C11-CA5-OA6-CA4
19	f	101	CDL	OB5-CB3-CB4-OB6
19	Aa	301	CDL	CB2-OB2-PB2-OB3
19	Ab	301	CDL	C1-CA2-OA2-PA1
19	Ab	301	CDL	CA2-OA2-PA1-OA3
19	Ab	301	CDL	CA2-OA2-PA1-OA4
19	Ab	301	CDL	CB2-OB2-PB2-OB3
19	Ab	301	CDL	CB2-OB2-PB2-OB4
19	Ab	301	CDL	CB3-OB5-PB2-OB2
19	Ab	301	CDL	CB3-OB5-PB2-OB3
19	Ab	301	CDL	CB3-OB5-PB2-OB4
19	Af	101	CDL	C11-CA5-OA6-CA4
19	Af	101	CDL	CB2-OB2-PB2-OB3
19	Af	101	CDL	CB2-OB2-PB2-OB4
19	Af	101	CDL	CB3-OB5-PB2-OB3
19	Af	101	CDL	OB5-CB3-CB4-OB6
19	Af	101	CDL	C51-CB5-OB6-CB4
20	f	103	LHG	C1-C2-C3-O3
20	Af	102	LHG	C3-O3-P-O4
20	Af	103	LHG	C1-C2-C3-O3
19	f	101	CDL	OA7-CA5-OA6-CA4
19	Af	101	CDL	OA7-CA5-OA6-CA4
19	Af	101	CDL	OB7-CB5-OB6-CB4
19	a	301	CDL	C31-CA7-OA8-CA6
19	Aa	301	CDL	C31-CA7-OA8-CA6
19	a	301	CDL	OA9-CA7-OA8-CA6
19	f	101	CDL	O1-C1-CB2-OB2
19	Af	101	CDL	O1-C1-CA2-OA2
20	f	103	LHG	O2-C2-C3-O3
20	Af	103	LHG	O2-C2-C3-O3
19	Aa	301	CDL	C1-CB2-OB2-PB2
19	Aa	301	CDL	OA9-CA7-OA8-CA6
19	f	101	CDL	CB2-C1-CA2-OA2
20	f	102	LHG	O2-C2-C3-O3
19	b	301	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	f	101	CDL	CB5-C51-C52-C53
19	b	301	CDL	C71-C72-C73-C74
19	a	301	CDL	CA5-C11-C12-C13
19	a	301	CDL	CA7-C31-C32-C33
19	Ab	301	CDL	CA5-C11-C12-C13
20	f	102	LHG	C23-C24-C25-C26
20	f	103	LHG	C7-C8-C9-C10
20	Af	103	LHG	C7-C8-C9-C10
19	Af	101	CDL	C1-CA2-OA2-PA1
19	Af	101	CDL	CB5-C51-C52-C53
19	a	301	CDL	CB5-C51-C52-C53
19	Aa	301	CDL	CA5-C11-C12-C13
19	Aa	301	CDL	CB5-C51-C52-C53
19	b	301	CDL	CB2-OB2-PB2-OB5
19	Ab	301	CDL	CA2-OA2-PA1-OA5
19	Ab	301	CDL	CB2-OB2-PB2-OB5
19	Af	101	CDL	CA2-OA2-PA1-OA5
19	Af	101	CDL	CB2-OB2-PB2-OB5
19	Af	101	CDL	CB3-OB5-PB2-OB2
20	Af	102	LHG	C3-O3-P-O6
19	Af	101	CDL	CB2-C1-CA2-OA2
19	Af	101	CDL	C19-C20-C21-C22
20	f	103	LHG	C28-C29-C30-C31
19	Af	101	CDL	C21-C22-C23-C24
20	f	102	LHG	C13-C14-C15-C16
19	Aa	301	CDL	C75-C76-C77-C78
20	Af	103	LHG	C28-C29-C30-C31
19	b	301	CDL	CB4-CB3-OB5-PB2
19	Ab	301	CDL	CB4-CB3-OB5-PB2
20	f	103	LHG	C5-C4-O6-P
20	Af	102	LHG	C7-C8-C9-C10
19	f	101	CDL	C21-C22-C23-C24
19	f	101	CDL	C40-C41-C42-C43
19	Af	101	CDL	C40-C41-C42-C43
20	f	103	LHG	C15-C16-C17-C18
20	Af	102	LHG	O1-C1-C2-C3
20	Af	103	LHG	O1-C1-C2-C3
19	Ab	301	CDL	C11-CA5-OA6-CA4
19	b	301	CDL	C13-C14-C15-C16
19	Aa	301	CDL	C71-C72-C73-C74
19	f	101	CDL	C19-C20-C21-C22
19	b	301	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
19	Ab	301	CDL	C60-C61-C62-C63
19	Af	101	CDL	C37-C38-C39-C40
19	Ab	301	CDL	C13-C14-C15-C16
19	Aa	301	CDL	C73-C74-C75-C76
19	a	301	CDL	C11-CA5-OA6-CA4
19	b	301	CDL	C60-C61-C62-C63
19	Ab	301	CDL	OA7-CA5-OA6-CA4
19	Ab	301	CDL	C73-C74-C75-C76
19	b	301	CDL	C73-C74-C75-C76
19	a	301	CDL	OA7-CA5-OA6-CA4
19	f	101	CDL	OB7-CB5-OB6-CB4
19	Ab	301	CDL	C54-C55-C56-C57
19	b	301	CDL	C53-C54-C55-C56
20	f	102	LHG	C11-C10-C9-C8
19	b	301	CDL	C11-CA5-OA6-CA4
19	f	101	CDL	C51-CB5-OB6-CB4
19	b	301	CDL	OA7-CA5-OA6-CA4
19	b	301	CDL	OB6-CB4-CB6-OB8
20	Af	102	LHG	C13-C14-C15-C16
20	Af	103	LHG	C31-C32-C33-C34
19	a	301	CDL	C1-CB2-OB2-PB2
20	Af	103	LHG	C5-C4-O6-P
19	Aa	301	CDL	C54-C55-C56-C57
19	a	301	CDL	OB5-CB3-CB4-CB6
19	f	101	CDL	OB5-CB3-CB4-CB6
19	Aa	301	CDL	OB5-CB3-CB4-CB6
20	f	103	LHG	O6-C4-C5-C6
19	b	301	CDL	C54-C55-C56-C57
19	Af	101	CDL	C71-C72-C73-C74
19	f	101	CDL	C37-C38-C39-C40
19	Ab	301	CDL	C71-C72-C73-C74
20	f	102	LHG	C4-C5-C6-O8
19	Aa	301	CDL	C12-C13-C14-C15
19	Aa	301	CDL	CA7-C31-C32-C33
20	f	103	LHG	C11-C12-C13-C14
19	a	301	CDL	C13-C14-C15-C16
20	Af	102	LHG	C27-C28-C29-C30
19	f	101	CDL	OA5-CA3-CA4-OA6
19	Af	101	CDL	C17-C18-C19-C20
19	Ab	301	CDL	OB6-CB4-CB6-OB8
20	f	103	LHG	C29-C30-C31-C32
19	b	301	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
19	Aa	301	CDL	C71-CB7-OB8-CB6
19	a	301	CDL	C54-C55-C56-C57
19	Af	101	CDL	OB5-CB3-CB4-CB6
20	f	102	LHG	C26-C27-C28-C29
20	Af	103	LHG	C14-C15-C16-C17
19	f	101	CDL	C17-C18-C19-C20
19	f	101	CDL	C74-C75-C76-C77
19	Ab	301	CDL	C11-C12-C13-C14
19	a	301	CDL	C71-CB7-OB8-CB6
19	b	301	CDL	CB3-CB4-CB6-OB8
20	Af	102	LHG	C4-C5-C6-O8
19	f	101	CDL	C13-C14-C15-C16
19	Aa	301	CDL	C13-C14-C15-C16
20	f	102	LHG	C27-C28-C29-C30
19	Ab	301	CDL	C16-C17-C18-C19
20	f	102	LHG	O7-C5-C6-O8
19	a	301	CDL	C12-C13-C14-C15
19	Aa	301	CDL	C74-C75-C76-C77
19	Ab	301	CDL	C53-C54-C55-C56
19	Aa	301	CDL	OB9-CB7-OB8-CB6
19	f	101	CDL	OA5-CA3-CA4-CA6
20	Af	103	LHG	O6-C4-C5-C6
19	a	301	CDL	C74-C75-C76-C77
20	Af	103	LHG	C15-C16-C17-C18
20	Af	103	LHG	C13-C14-C15-C16
19	f	101	CDL	C31-CA7-OA8-CA6
19	a	301	CDL	OB9-CB7-OB8-CB6
19	a	301	CDL	OB5-CB3-CB4-OB6
20	f	103	LHG	O6-C4-C5-O7
20	Af	103	LHG	O6-C4-C5-O7
19	Aa	301	CDL	C52-C53-C54-C55
19	b	301	CDL	C71-CB7-OB8-CB6
20	f	103	LHG	C31-C32-C33-C34
19	Aa	301	CDL	OB7-CB5-OB6-CB4
19	f	101	CDL	C32-C33-C34-C35
19	b	301	CDL	C16-C17-C18-C19
19	b	301	CDL	CA3-OA5-PA1-OA2
19	Aa	301	CDL	CA2-OA2-PA1-OA5
19	Ab	301	CDL	C51-C52-C53-C54
20	Af	102	LHG	C2-C3-O3-P
19	Aa	301	CDL	CA3-OA5-PA1-OA3
19	Af	101	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
19	Af	101	CDL	CA2-OA2-PA1-OA4
19	Af	101	CDL	CA3-OA5-PA1-OA4
19	Aa	301	CDL	C56-C57-C58-C59
19	f	101	CDL	OA9-CA7-OA8-CA6
20	f	103	LHG	C14-C15-C16-C17
19	Aa	301	CDL	C77-C78-C79-C80
19	Aa	301	CDL	OB5-CB3-CB4-OB6
19	Ab	301	CDL	OB5-CB3-CB4-OB6
19	a	301	CDL	C52-C53-C54-C55
19	Aa	301	CDL	C51-CB5-OB6-CB4
19	b	301	CDL	OB9-CB7-OB8-CB6
19	a	301	CDL	C60-C61-C62-C63
20	Af	102	LHG	O7-C5-C6-O8
20	f	102	LHG	C2-C3-O3-P
19	a	301	CDL	C73-C74-C75-C76
20	Af	102	LHG	O1-C1-C2-O2
19	a	301	CDL	C56-C57-C58-C59
19	Af	101	CDL	C73-C74-C75-C76
19	a	301	CDL	C53-C54-C55-C56
20	Af	103	LHG	C32-C33-C34-C35
20	Af	103	LHG	O10-C23-O8-C6
20	f	102	LHG	C16-C17-C18-C19
19	b	301	CDL	C12-C11-CA5-OA6
20	Af	103	LHG	C11-C12-C13-C14
19	Af	101	CDL	C13-C14-C15-C16
19	a	301	CDL	CA2-OA2-PA1-OA5
19	a	301	CDL	CB3-OB5-PB2-OB2
19	Aa	301	CDL	CB3-OB5-PB2-OB2
19	Ab	301	CDL	CA3-OA5-PA1-OA2
20	f	102	LHG	C3-O3-P-O6
19	Af	101	CDL	C72-C73-C74-C75
19	Ab	301	CDL	CB3-CB4-CB6-OB8
19	Af	101	CDL	CA3-CA4-CA6-OA8
19	Af	101	CDL	C52-C53-C54-C55
19	Aa	301	CDL	CA4-CA3-OA5-PA1
19	Af	101	CDL	C1-CB2-OB2-PB2
19	Af	101	CDL	CA5-C11-C12-C13
19	Aa	301	CDL	C1-CA2-OA2-PA1
19	f	101	CDL	C42-C43-C44-C45
19	Aa	301	CDL	C39-C40-C41-C42
19	f	101	CDL	CA3-CA4-CA6-OA8
20	f	102	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
19	b	301	CDL	C58-C59-C60-C61
19	Aa	301	CDL	CA4-CA6-OA8-CA7
19	a	301	CDL	C14-C15-C16-C17
20	Af	103	LHG	C34-C35-C36-C37
19	a	301	CDL	C1-CA2-OA2-PA1
19	Af	101	CDL	C31-CA7-OA8-CA6
19	f	101	CDL	C36-C37-C38-C39
19	Aa	301	CDL	C14-C15-C16-C17
19	Aa	301	CDL	C53-C54-C55-C56
19	b	301	CDL	CA4-CA3-OA5-PA1
19	Aa	301	CDL	C31-C32-C33-C34
19	Af	101	CDL	CB3-CB4-CB6-OB8
19	Af	101	CDL	OA9-CA7-OA8-CA6
19	Aa	301	CDL	C76-C77-C78-C79
19	Aa	301	CDL	C60-C61-C62-C63
19	Ab	301	CDL	C12-C11-CA5-OA6
20	Af	102	LHG	C16-C17-C18-C19
19	Ab	301	CDL	OB5-CB3-CB4-CB6
19	Ab	301	CDL	C59-C60-C61-C62
20	f	102	LHG	C24-C23-O8-C6
19	Aa	301	CDL	CB2-OB2-PB2-OB5
19	a	301	CDL	C33-C34-C35-C36
19	Af	101	CDL	C31-C32-C33-C34
19	Aa	301	CDL	OA7-CA5-OA6-CA4
19	f	101	CDL	C52-C53-C54-C55
19	Aa	301	CDL	C16-C17-C18-C19
20	Af	102	LHG	C10-C11-C12-C13
20	f	102	LHG	O7-C7-C8-C9
19	Aa	301	CDL	C11-C12-C13-C14
19	Af	101	CDL	CA2-C1-CB2-OB2
20	Af	102	LHG	C1-C2-C3-O3
19	Af	101	CDL	C53-C54-C55-C56
19	Ab	301	CDL	C33-C34-C35-C36
20	Af	102	LHG	C24-C25-C26-C27
19	b	301	CDL	C57-C58-C59-C60
19	a	301	CDL	CA4-CA3-OA5-PA1
19	Af	101	CDL	CA4-CA3-OA5-PA1
19	b	301	CDL	CB3-OB5-PB2-OB3
19	f	101	CDL	CB3-OB5-PB2-OB3
19	Af	101	CDL	CB3-OB5-PB2-OB4
20	f	102	LHG	C3-O3-P-O5
20	Af	103	LHG	C29-C30-C31-C32

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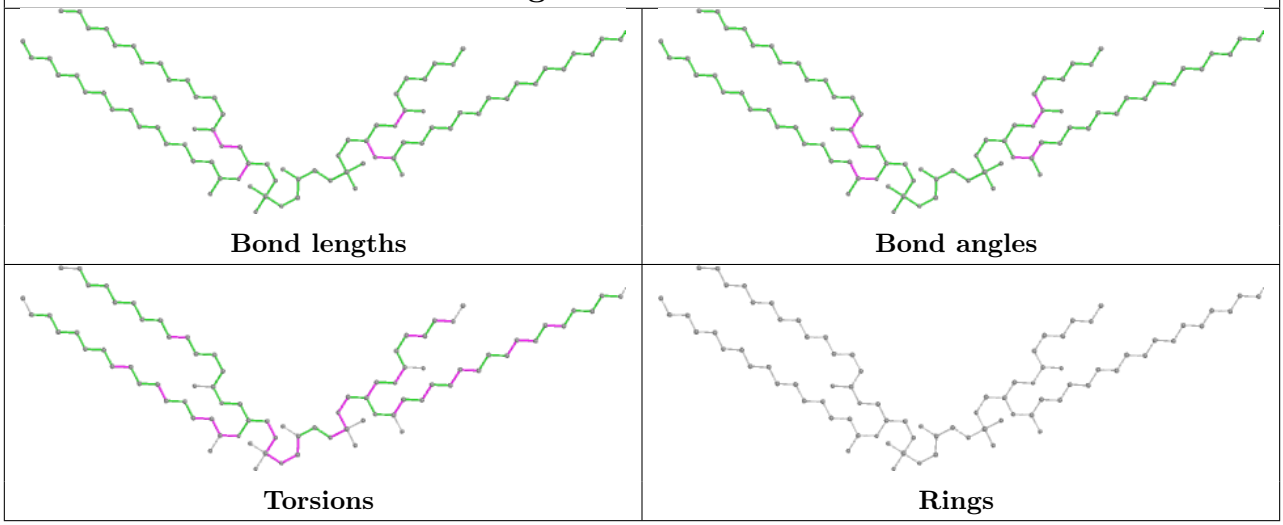
Mol	Chain	Res	Type	Atoms
19	Af	101	CDL	CB4-CB6-OB8-CB7
19	Ab	301	CDL	CB6-CB4-OB6-CB5
19	Aa	301	CDL	C12-C11-CA5-OA6
20	f	102	LHG	O10-C23-O8-C6
19	b	301	CDL	CB2-C1-CA2-OA2
19	Aa	301	CDL	C12-C11-CA5-OA7
19	Ab	301	CDL	C72-C71-CB7-OB8
19	Af	101	CDL	C35-C36-C37-C38
19	b	301	CDL	C52-C51-CB5-OB6
20	f	102	LHG	O9-C7-C8-C9
19	f	101	CDL	C32-C31-CA7-OA8
19	Ab	301	CDL	C52-C51-CB5-OB6

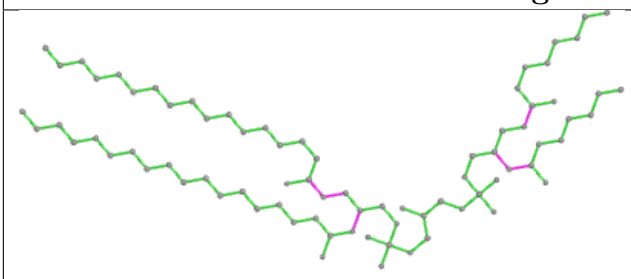
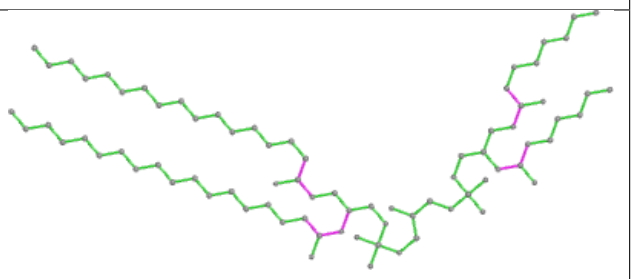
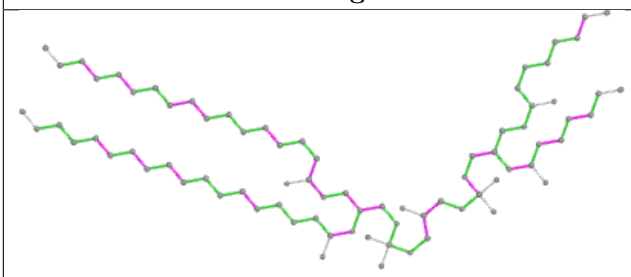
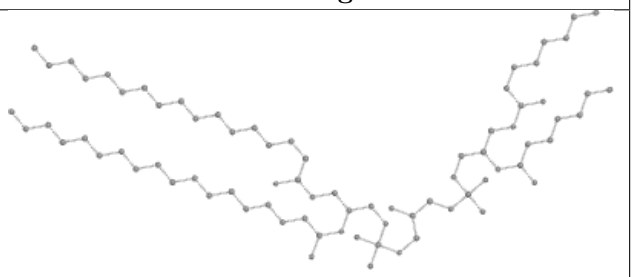
There are no ring outliers.

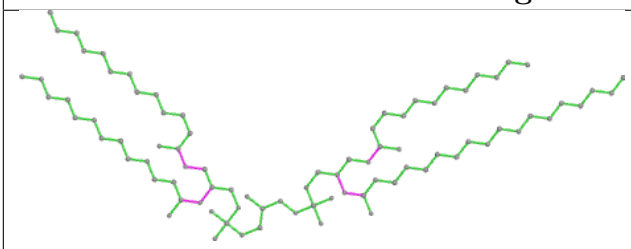
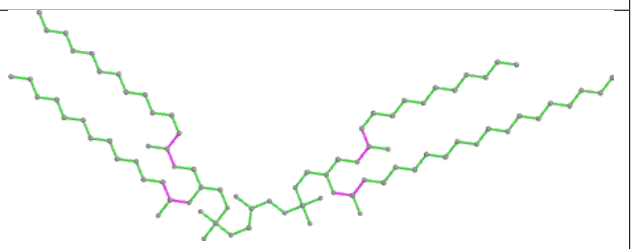
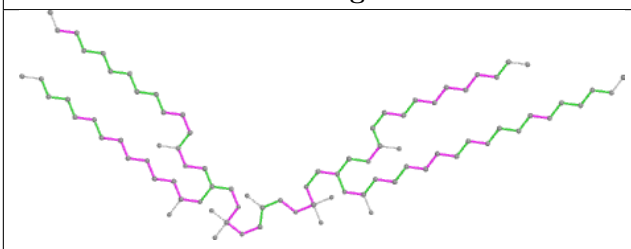
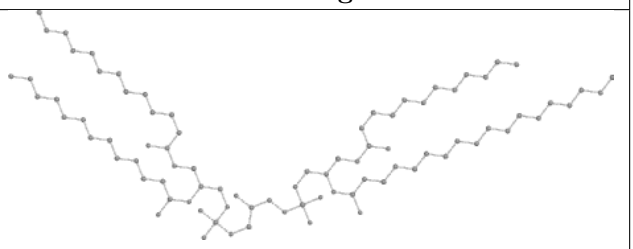
No monomer is involved in short contacts.

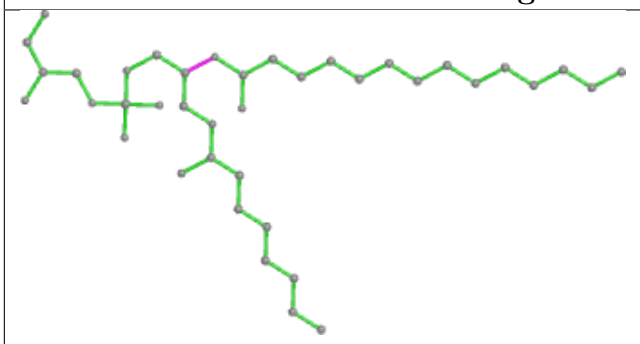
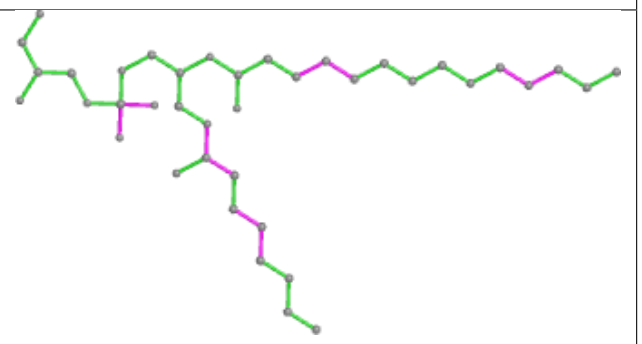
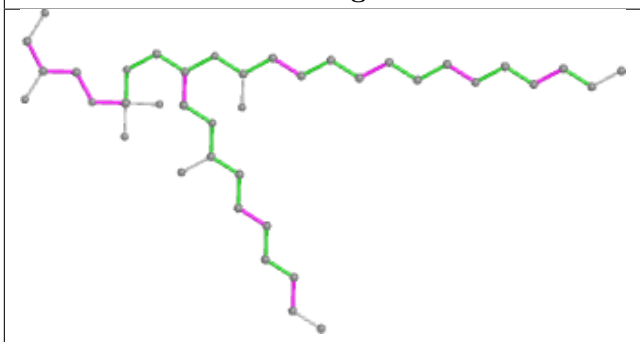
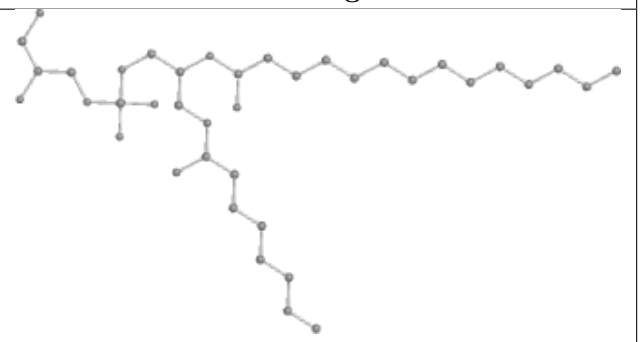
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 b 301

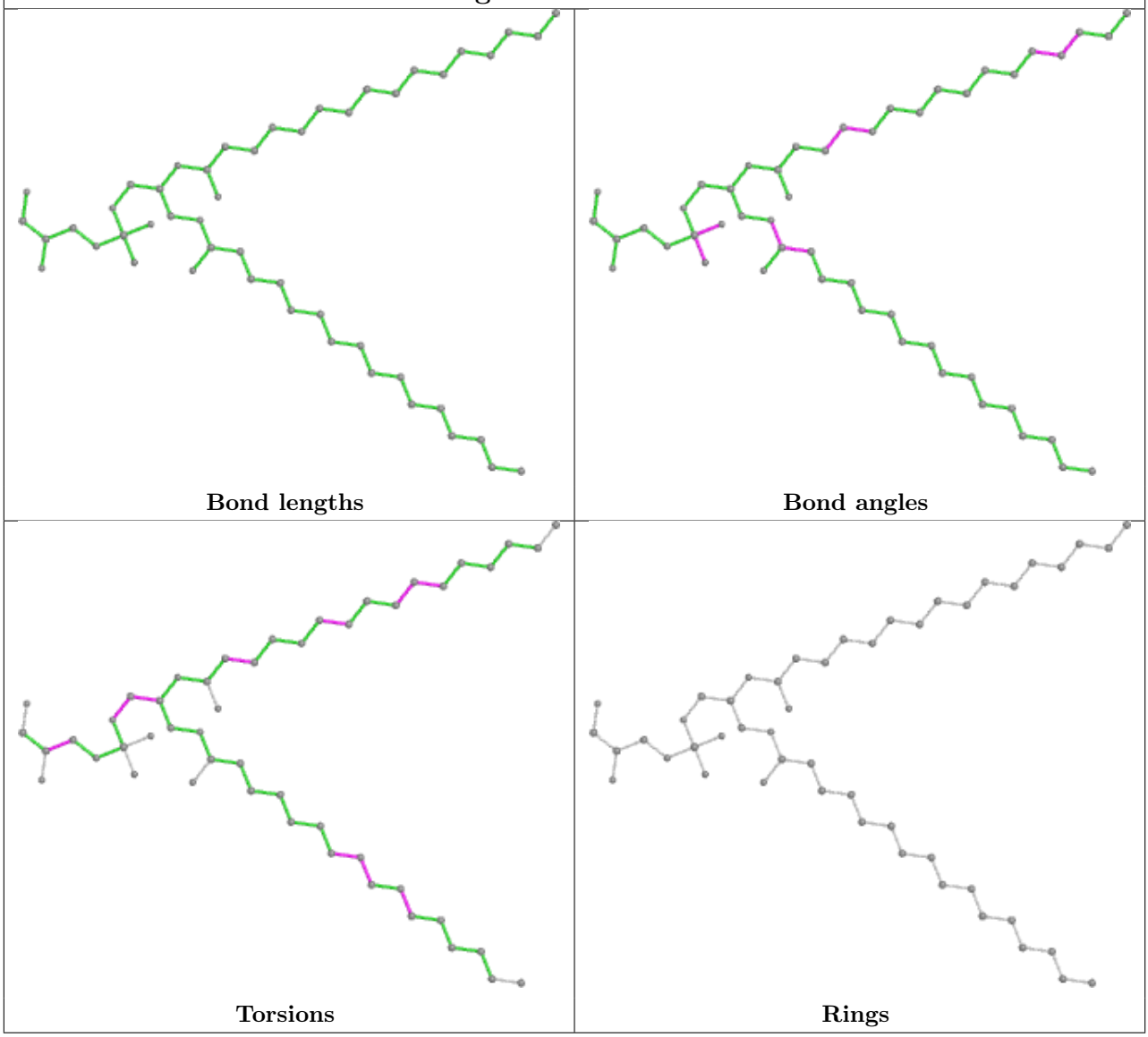


Ligand CDL f 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

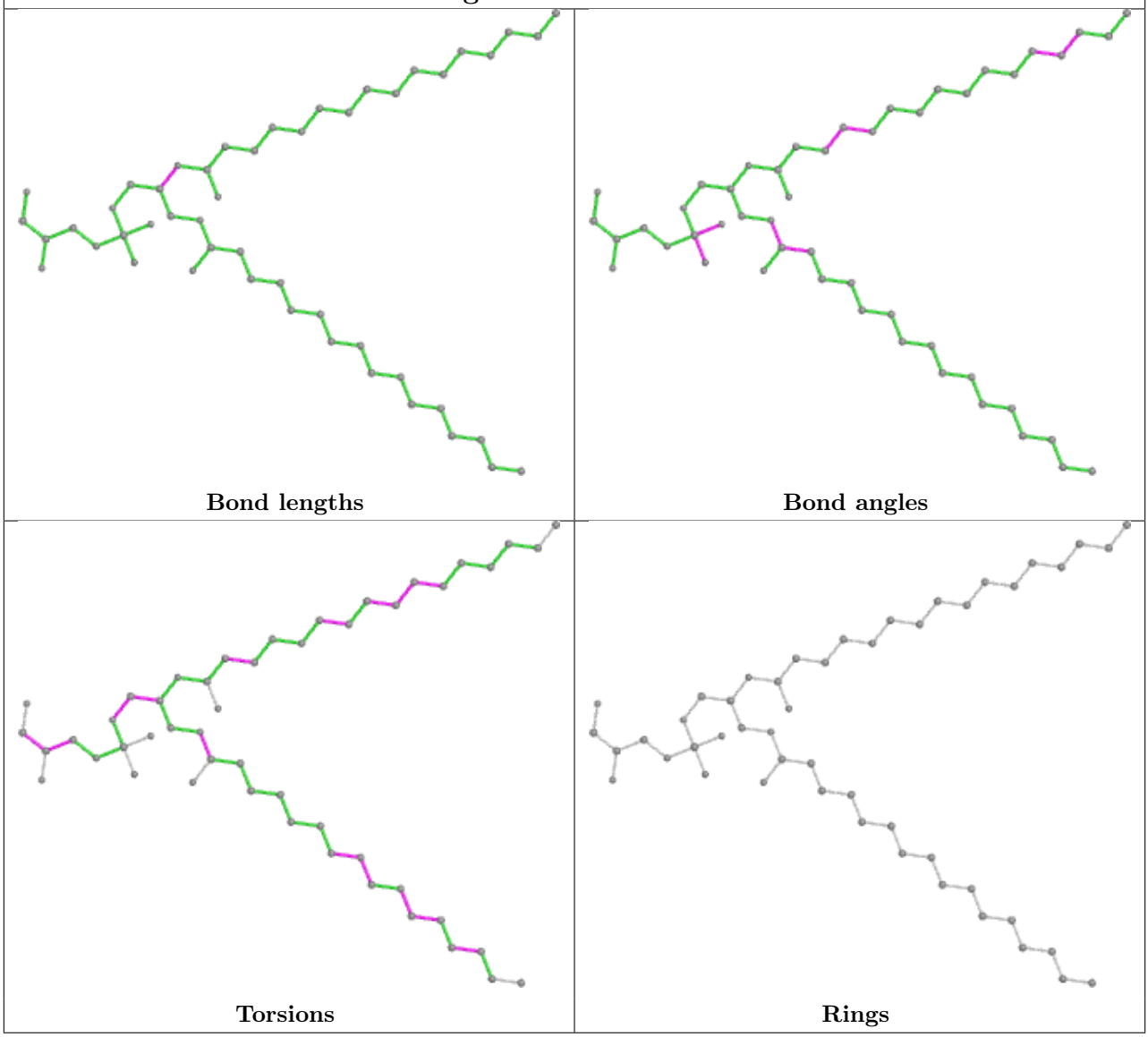
Ligand CDL Aa 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG Af 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

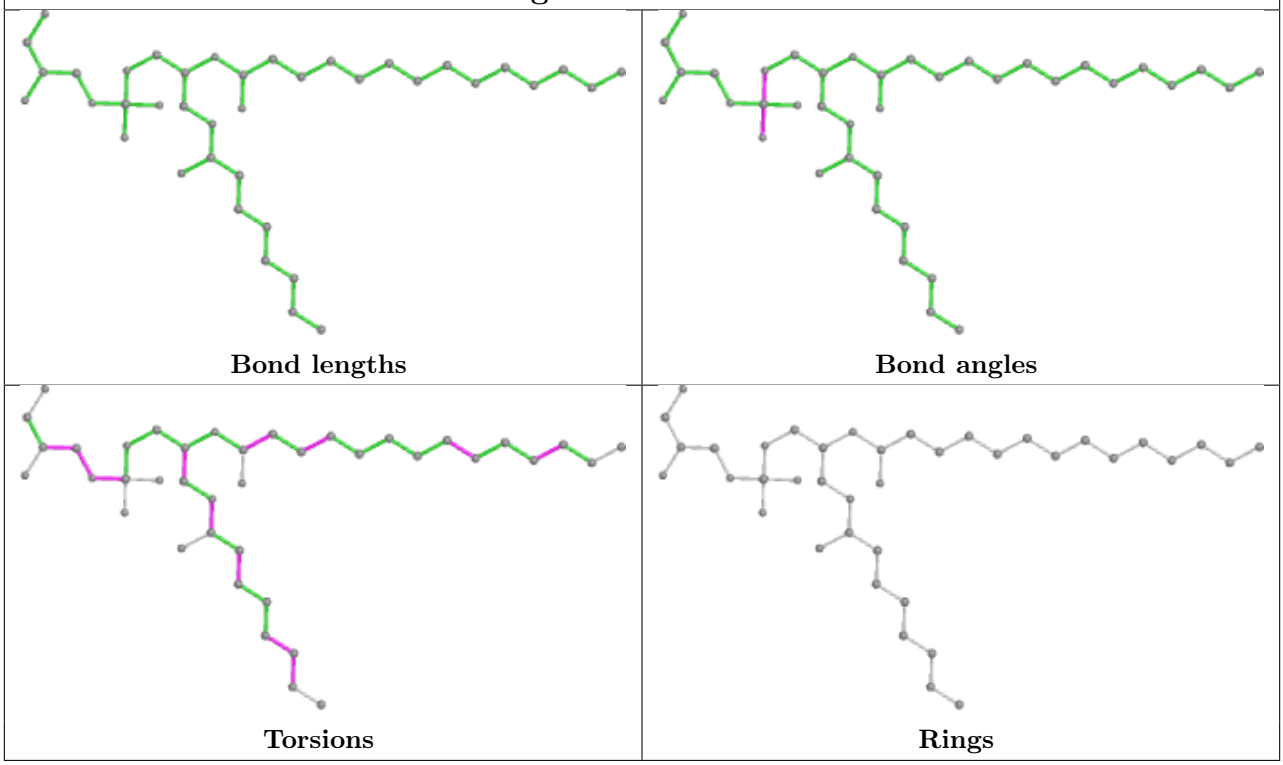
Ligand LHG f 103



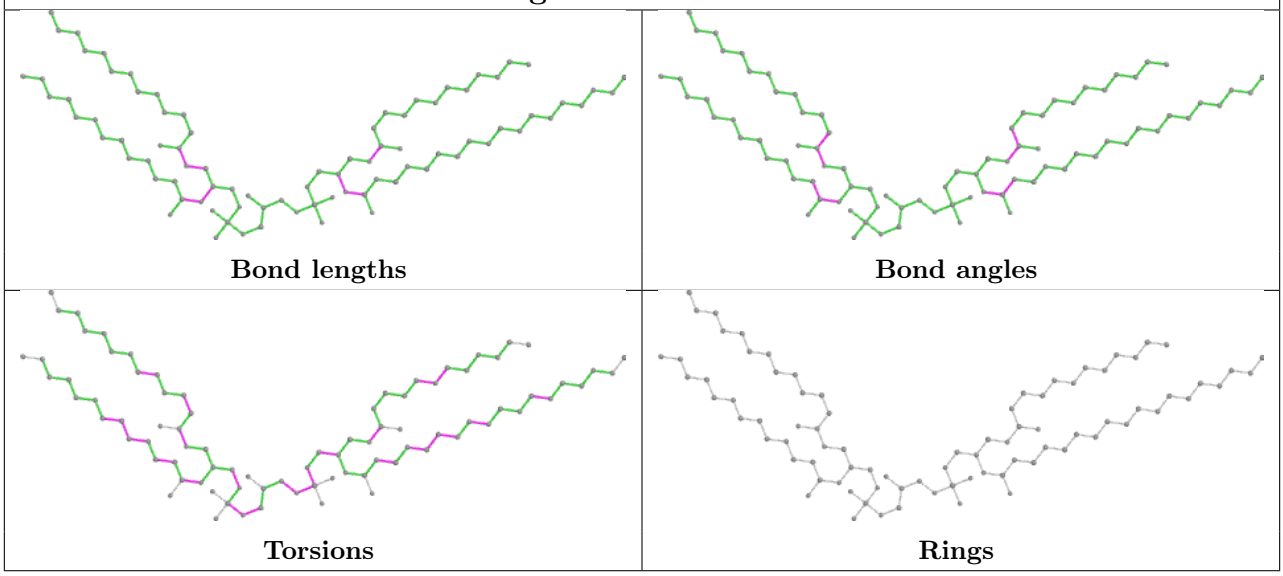
Ligand LHG Af 103



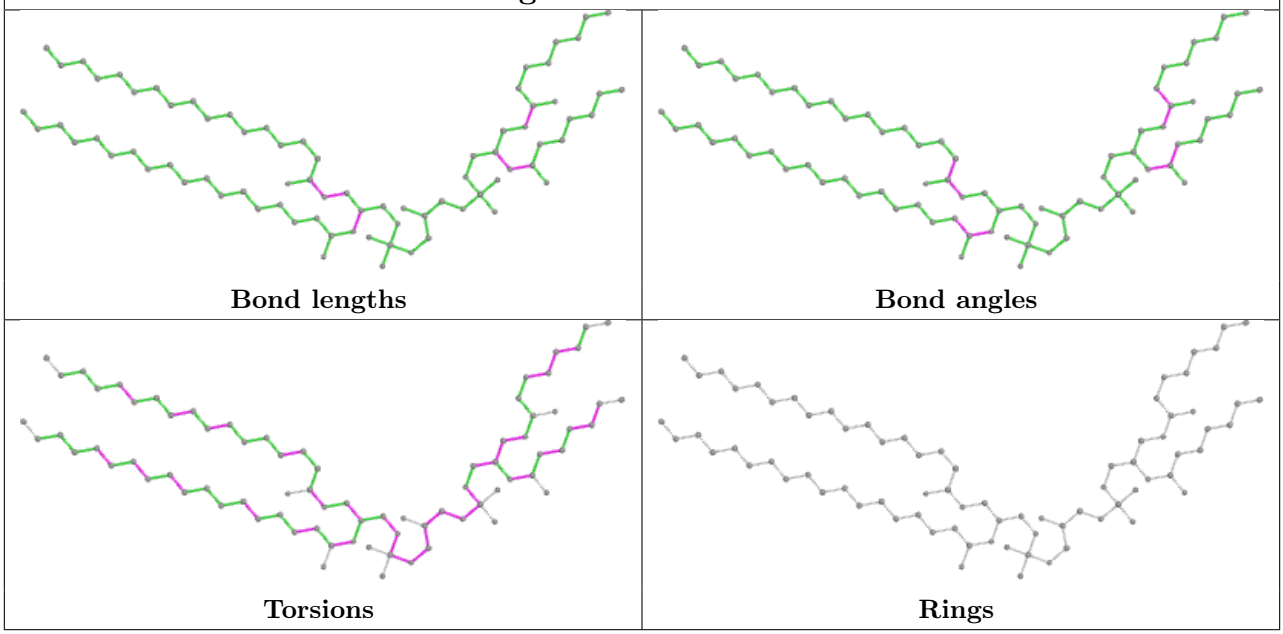
Ligand LHG f 102



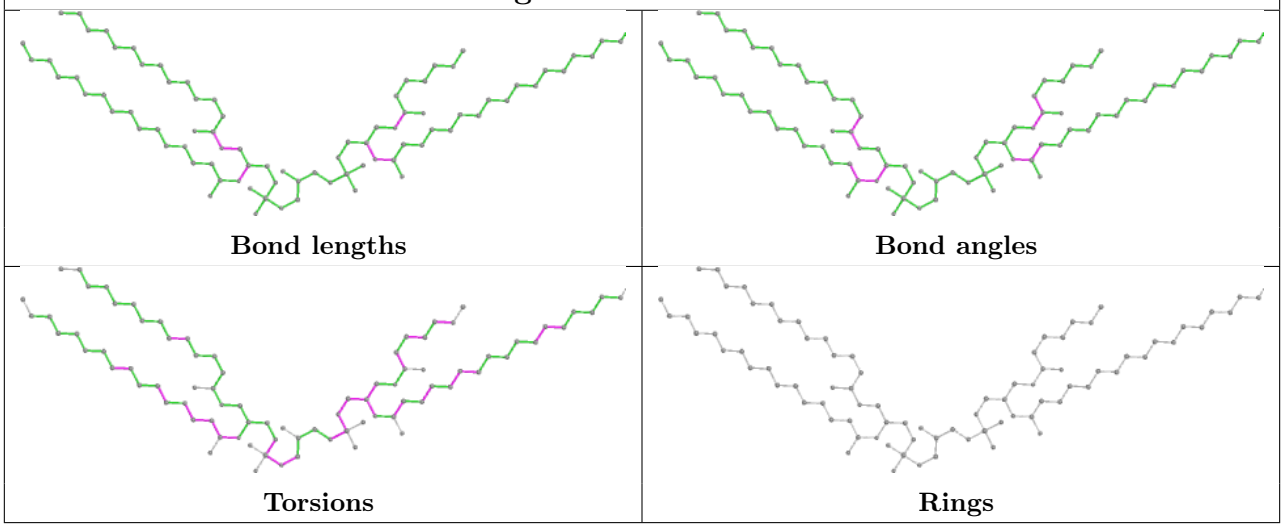
Ligand CDL a 301



Ligand CDL Af 101



Ligand CDL Ab 301



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.

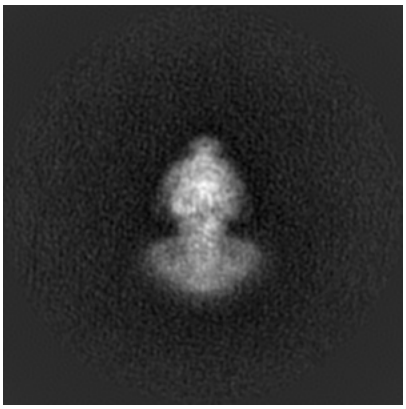
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11430. These allow visual inspection of the internal detail of the map and identification of artifacts.

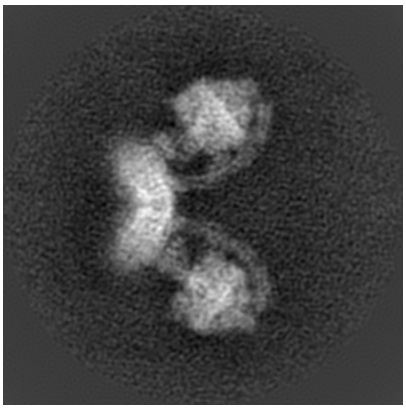
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

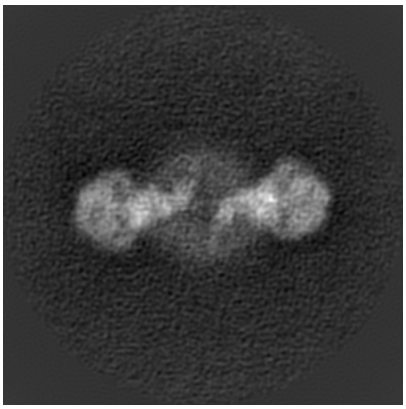
6.1.1 Primary map



X

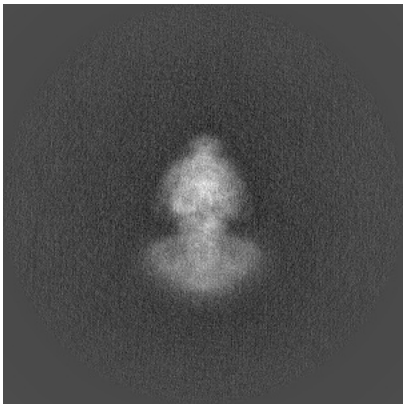


Y

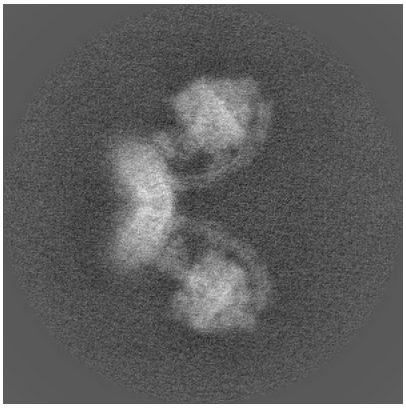


Z

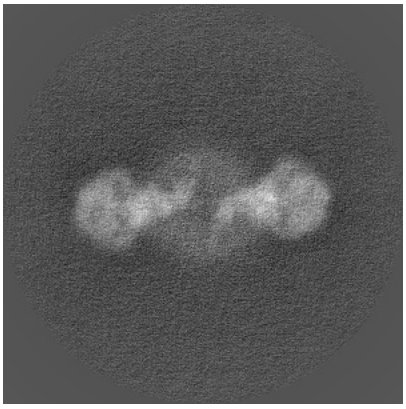
6.1.2 Raw map



X



Y

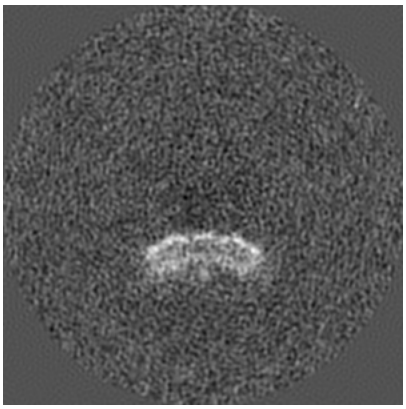


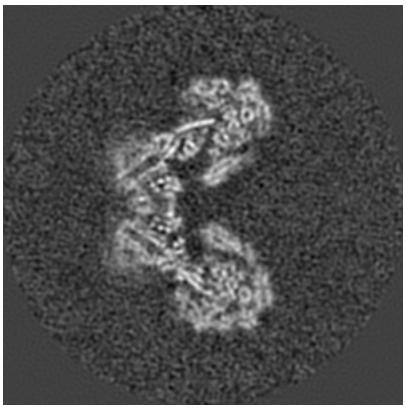
Z

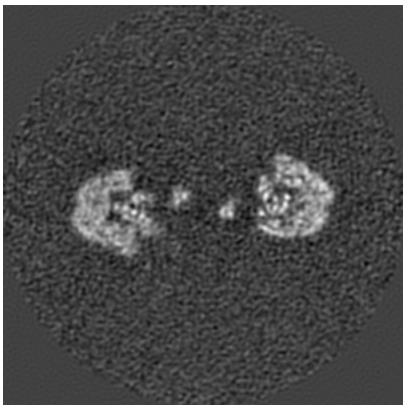
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

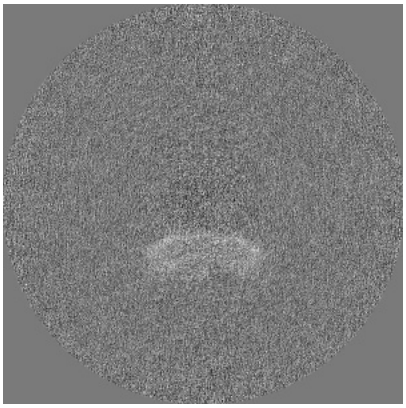
6.2.1 Primary map

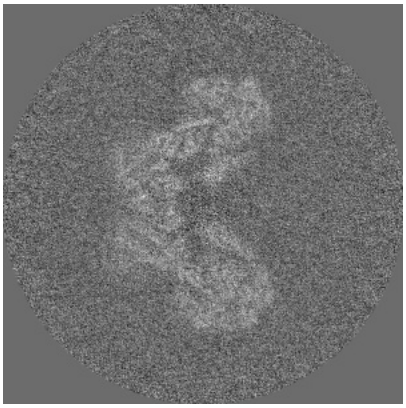

X Index: 250

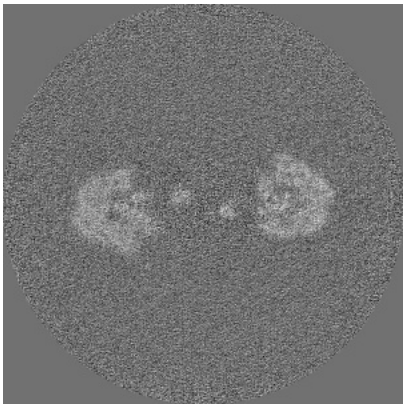

Y Index: 250


Z Index: 250

6.2.2 Raw map


X Index: 250

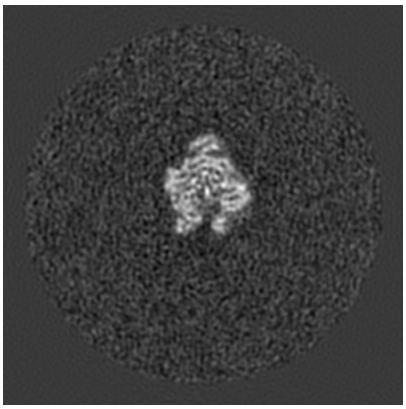

Y Index: 250

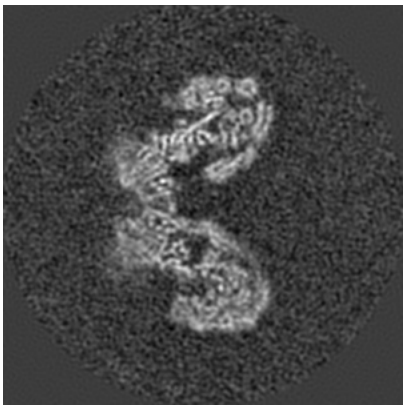

Z Index: 250

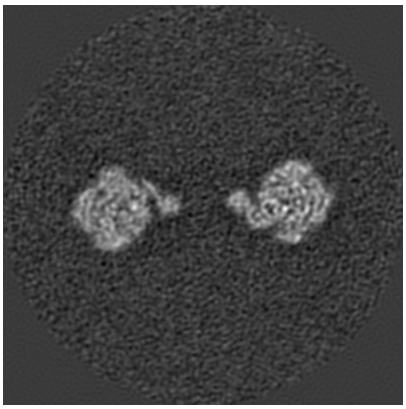
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

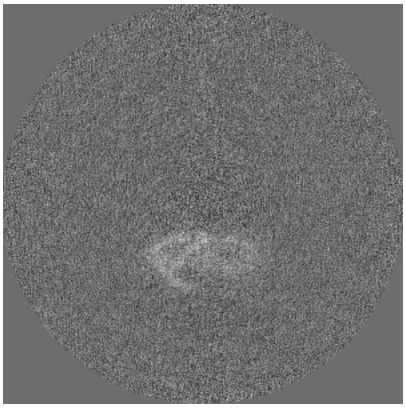
6.3.1 Primary map

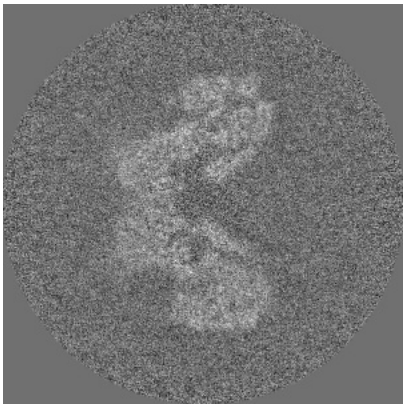

X Index: 365

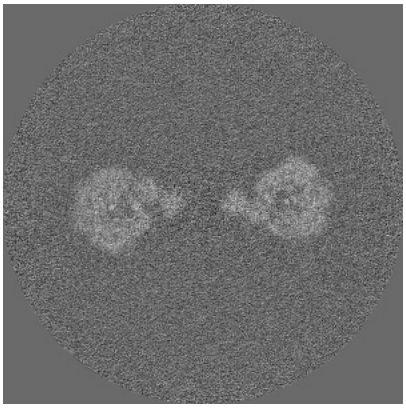

Y Index: 257


Z Index: 275

6.3.2 Raw map


X Index: 262


Y Index: 255


Z Index: 263

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

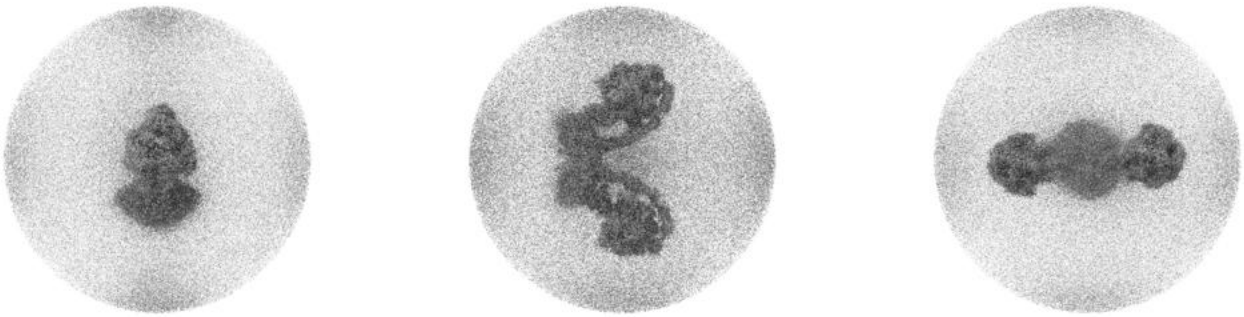
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0129. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

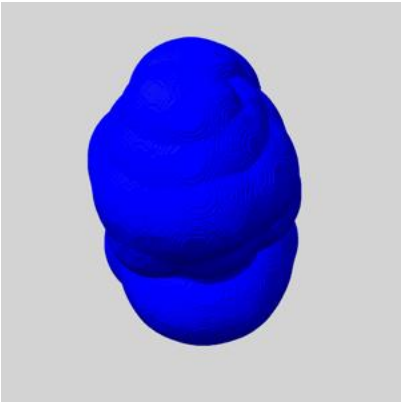
6.5 Mask visualisation (i)

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

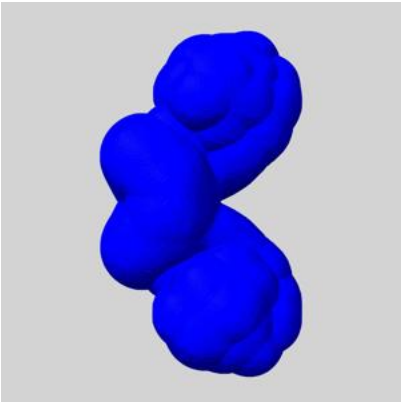
A mask typically either:

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

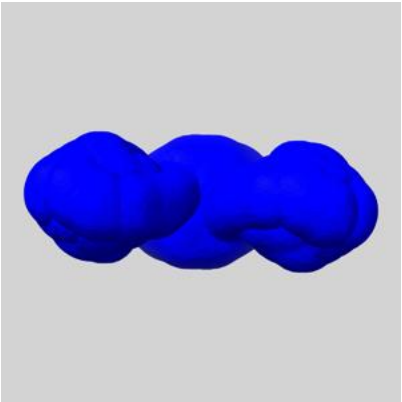
6.5.1 emd_11430_msk_1.map (i)



X



Y

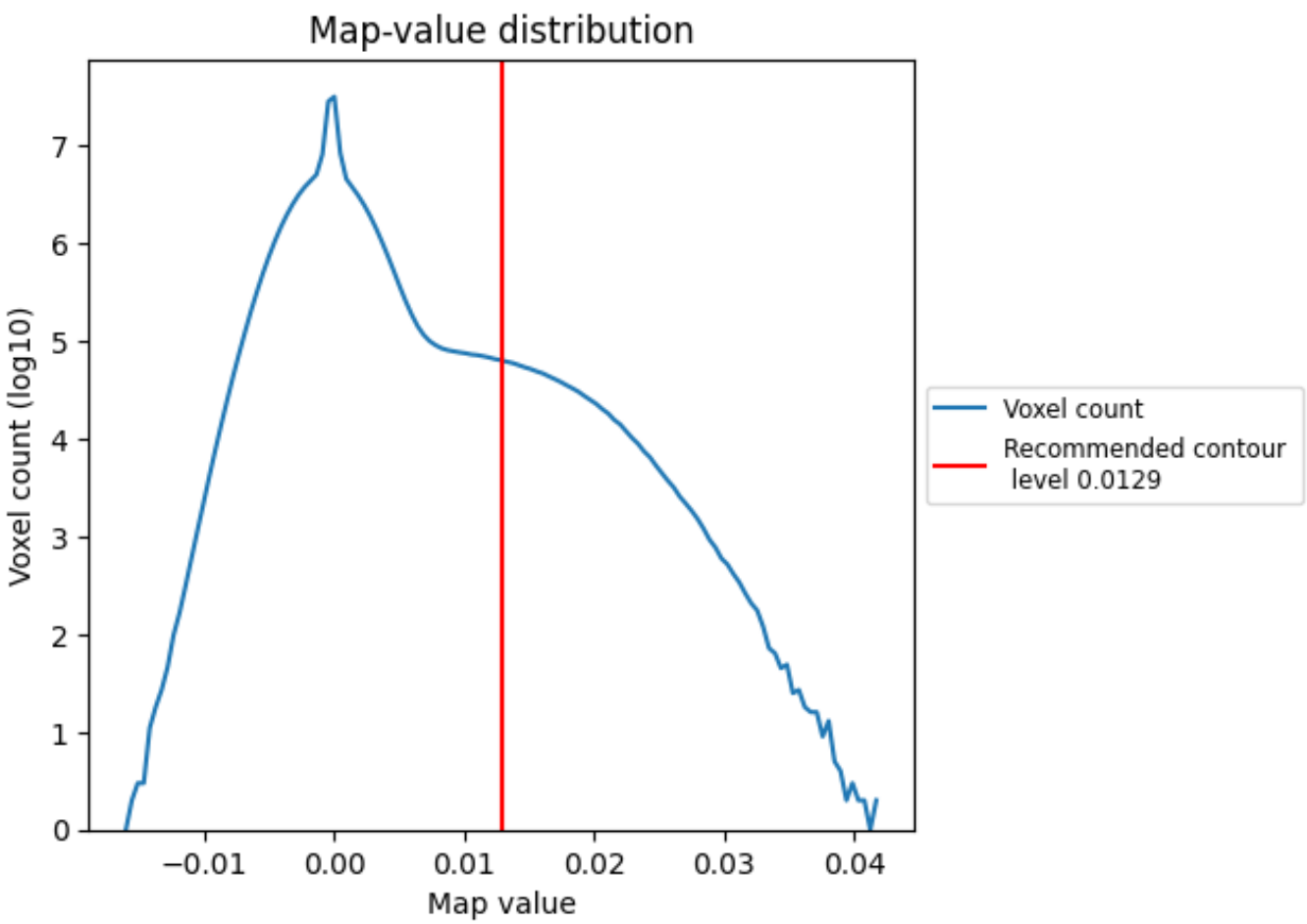


Z

7 Map analysis (i)

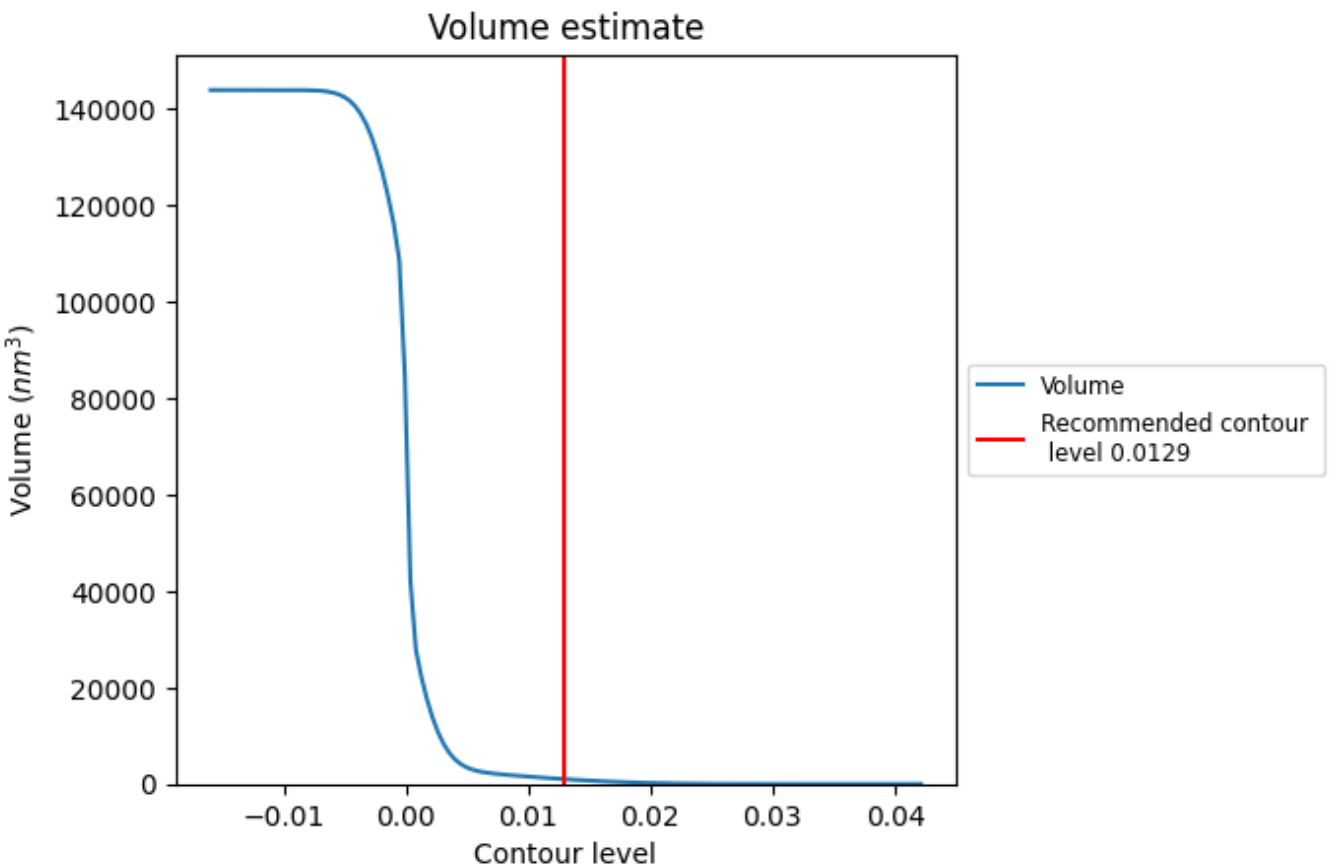
This section contains the results of statistical analysis of the map.

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.

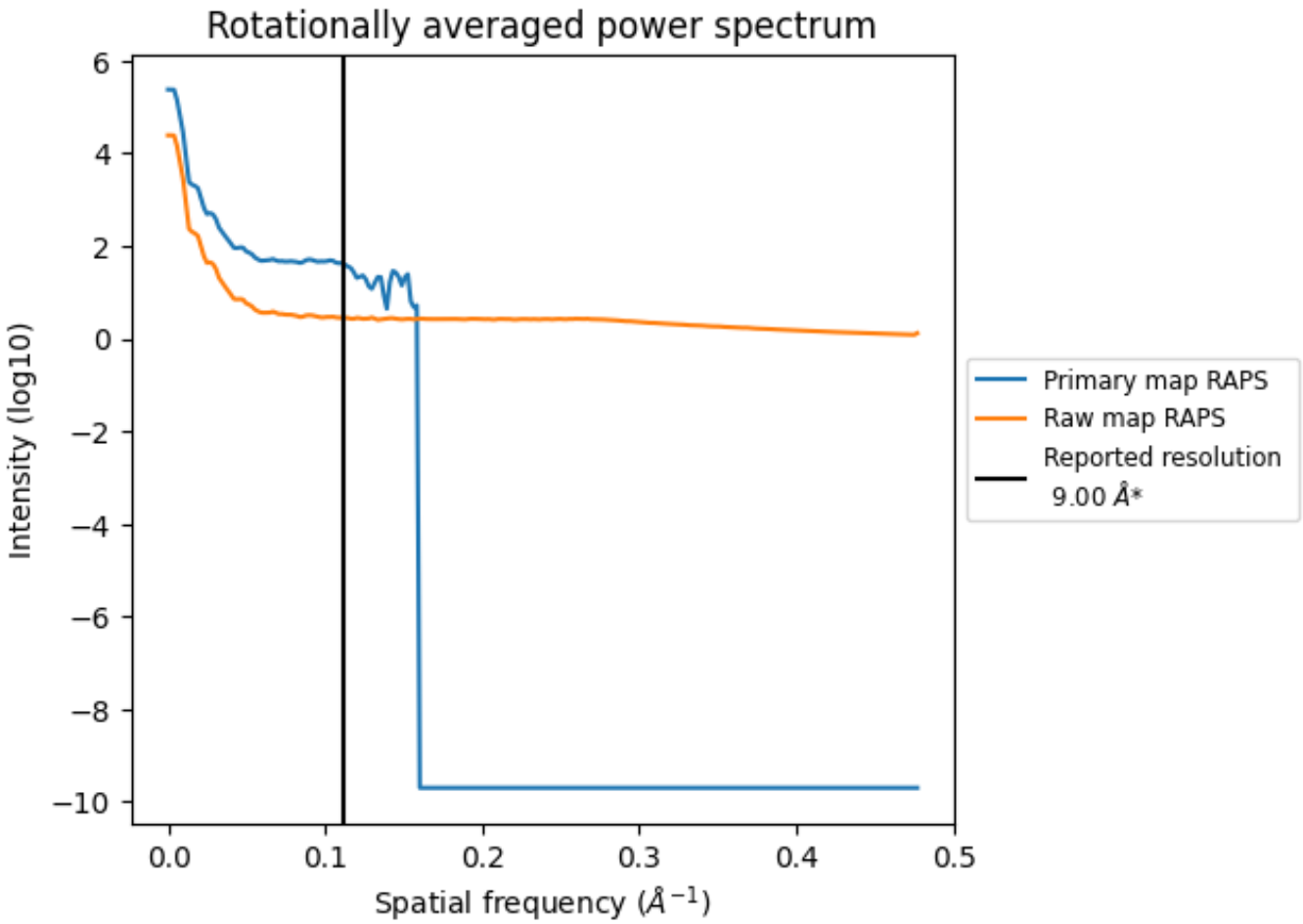
7.2 Volume estimate (i)



The volume at the recommended contour level is 1011 nm^3; this corresponds to an approximate mass of 914 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)

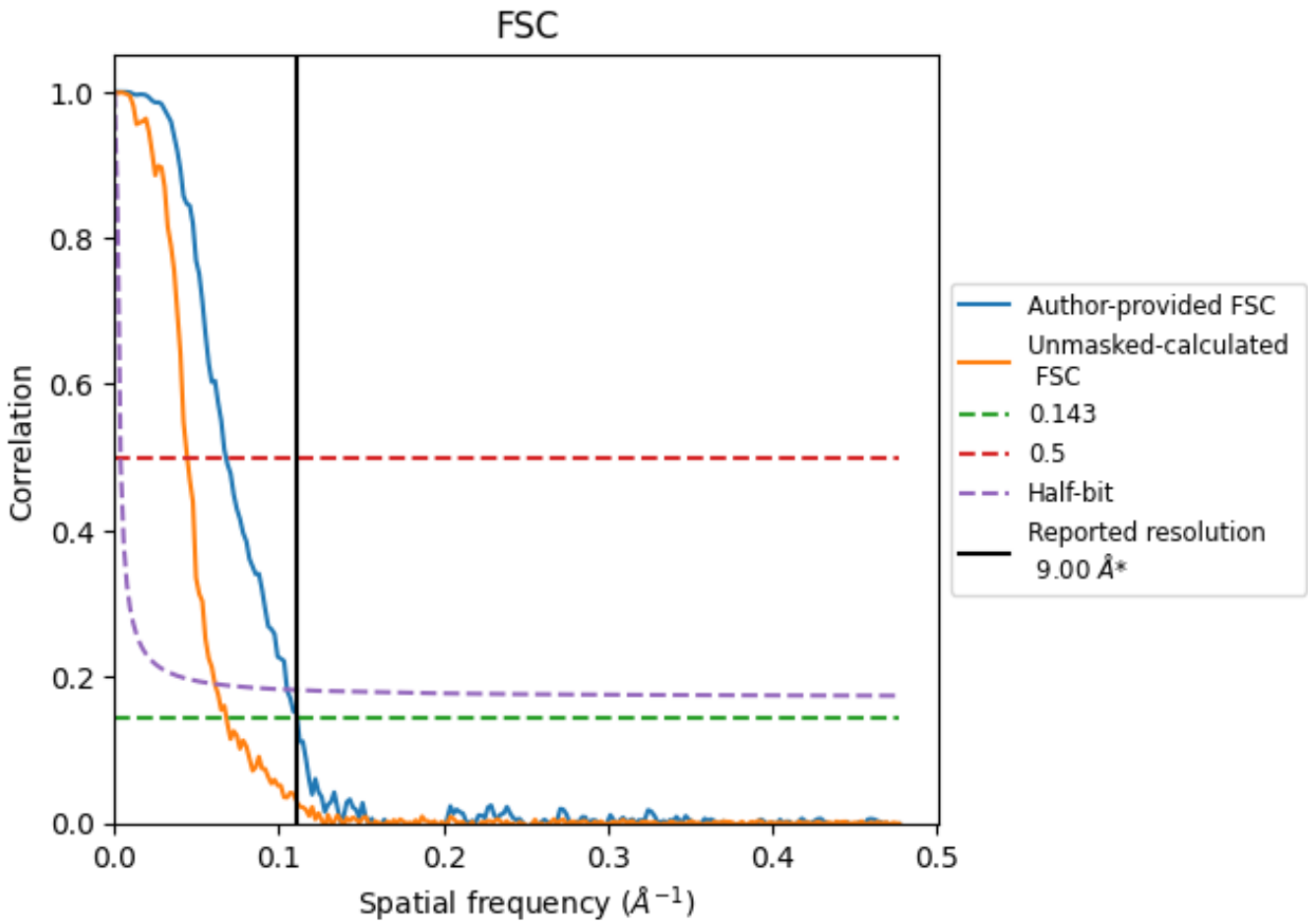


*Reported resolution corresponds to spatial frequency of 0.111 Å^{-1}

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 0.111 Å^{-1}

8.2 Resolution estimates (i)

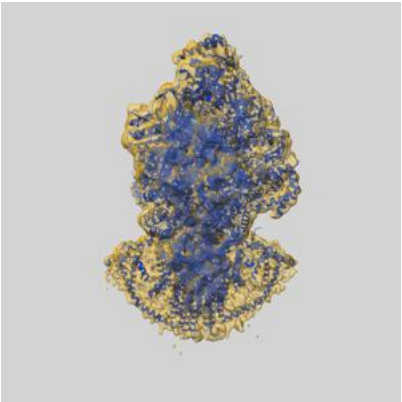
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.00	-	-
Author-provided FSC curve	9.00	14.75	9.53
Unmasked-calculated*	14.68	22.62	16.39

*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 14.68 differs from the reported value 9.0 by more than 10 %

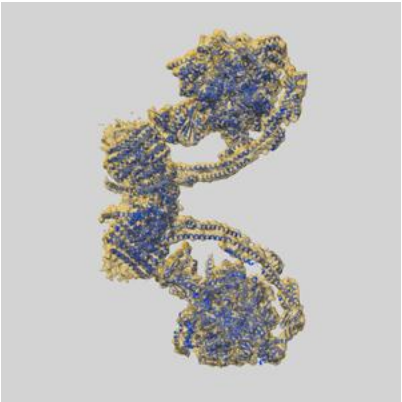
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11430 and PDB model 7AJD. Per-residue inclusion information can be found in section 3 on page 12.

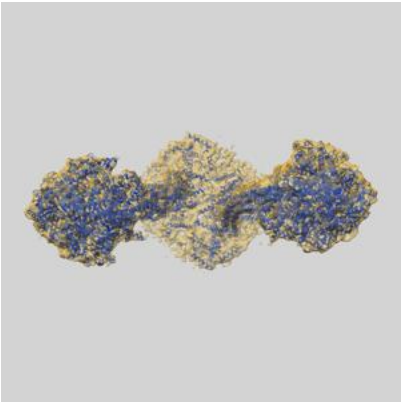
9.1 Map-model overlay (i)



X



Y



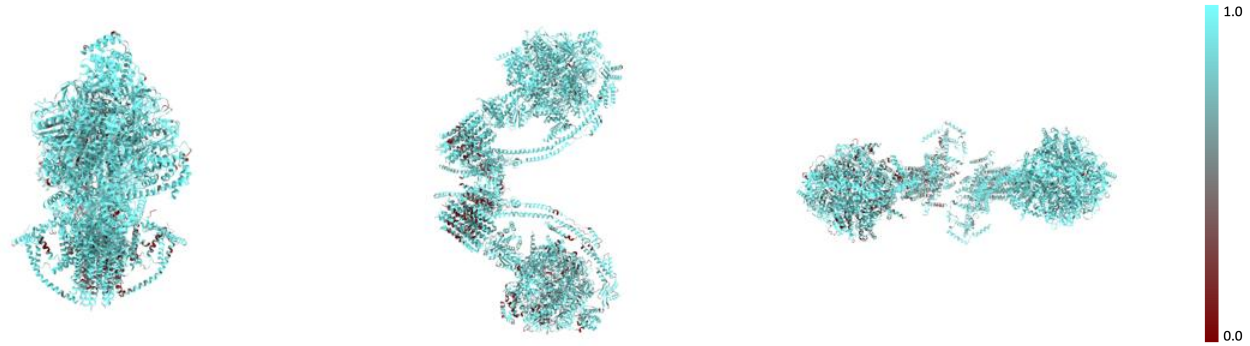
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0129 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)

This section was not generated.

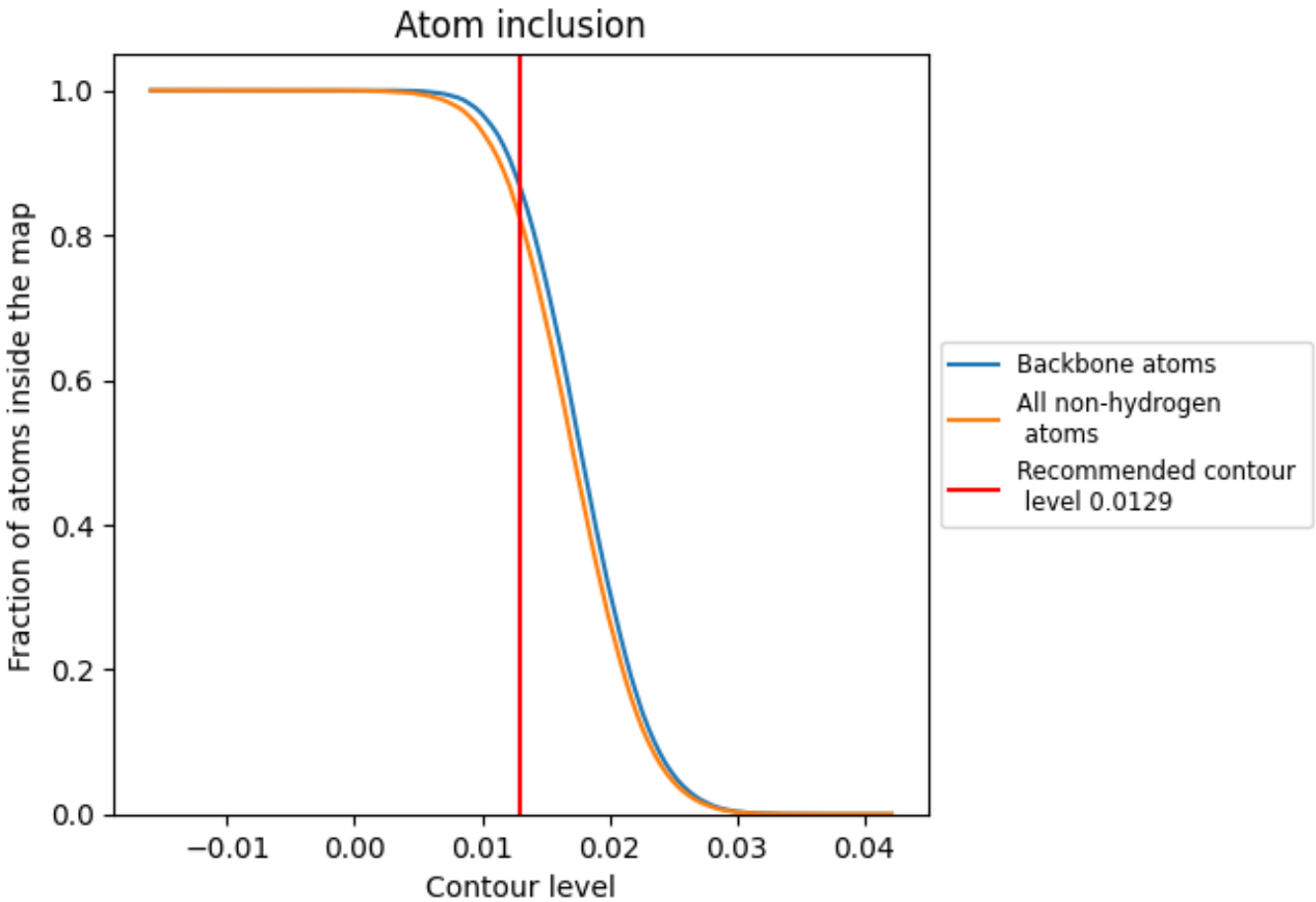
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0129).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 83% 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 (0.0129) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.8283
8	0.9073
A	0.8627
A8	0.8439
AA	0.7880
AB	0.7108
AC	0.8033
AD	0.8043
AE	0.8017
AF	0.8092
AG	0.8768
AH	0.8657
AI	0.8283
AJ	0.7576
AK	0.7465
AL	0.7521
AM	0.7473
AN	0.6429
AO	0.6731
AP	0.6574
AQ	0.6264
AR	0.7473
AS	0.8294
Aa	0.7506
Ab	0.7665
Ad	0.7633
Ae	0.7617
Af	0.6174
Ag	0.8513
Ah	0.6667
Aj	0.7605
Ak	0.7288
B	0.9047
C	0.8993
D	0.9057

Continued on next page...

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Chain	Atom inclusion
E	0.9162
F	0.9079
G	0.9369
H	0.9142
I	0.8927
J	0.8442
K	0.7911
L	0.7521
M	0.8049
N	0.8297
O	0.7967
P	0.8969
Q	0.8104
R	0.8709
S	0.9184
a	0.7930
b	0.8730
d	0.8792
e	0.9458
f	0.6991
g	0.8974
h	0.8889
j	0.8487
k	0.7288