



# Full wwPDB EM Validation Report ⓘ

Apr 9, 2024 – 06:24 PM JST

PDB ID : 8IOG  
EMDB ID : EMD-35618  
Title : Cryo-EM structure of porcine bc1 complex in isolated state  
Authors : Wang, Y.X.; Dong, J.Q.; Yang, G.F.  
Deposited on : 2023-03-11  
Resolution : 2.88 Å (reported)  
Based on initial model : 5GUP

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

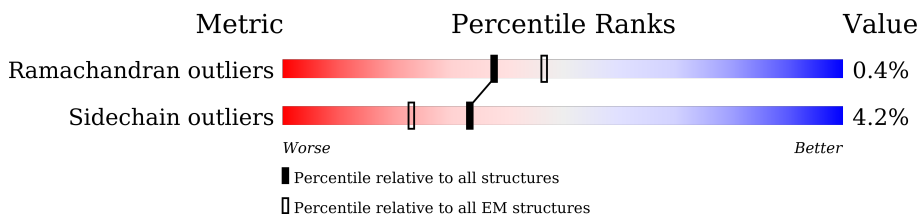
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.88 Å.

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






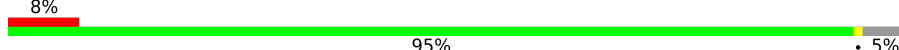
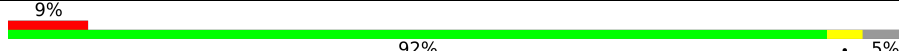
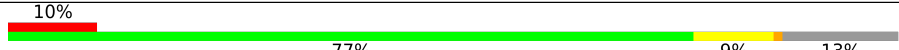
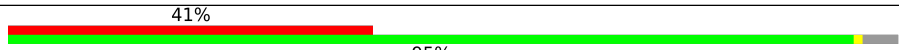
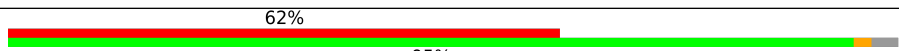


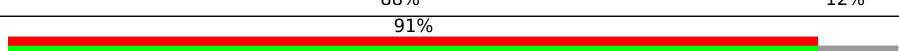

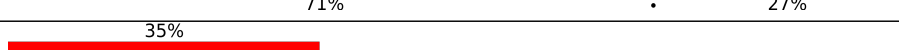
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	379	85% 13% .
1	a	379	87% 11% ..
2	B	326	65% 9% 26%
2	b	326	71% 27% .
3	C	196	97% ..
3	c	196	96% .
4	D	480	89% . 7%
4	d	480	90% . 7%
5	E	453	88% . 8%

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Mol	Chain	Length	Quality of chain
5	e	453	 89% .. 8%
6	F	91	 36% 70% 30%
6	f	91	 54% 70% 30%
7	G	111	 8% 95% . 5%
7	g	111	 9% 92% . 5%
8	H	82	 10% 77% 9% . 13%
8	h	82	 41% 95% ..
9	I	64	 62% 95% ..
9	i	64	 73% 86% 11% .
10	J	56	 88% 88% 12%
10	j	56	 91% 91% 9%
11	K	78	 33% 71% . 27%
11	k	78	 35% 72% . 27%

## 2 Entry composition i

There are 16 unique types of molecules in this entry. The entry contains 33413 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 Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	378	Total 3017	C 2026	N 470	O 501	S 20	0	0
1	a	378	Total 3017	C 2026	N 470	O 501	S 20	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	314	SER	GLY	variant	UNP P24964
a	314	SER	GLY	variant	UNP P24964

- Molecule 2 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	241	Total 1920	C 1225	N 330	O 349	S 16	0	0
2	b	239	Total 1904	C 1214	N 327	O 347	S 16	0	0

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	194	Total 1502	C 946	N 261	O 288	S 7	0	0
3	c	196	Total 1517	C 954	N 265	O 291	S 7	0	0

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	445	Total 3452	C 2157	N 604	O 672	S 19	0	0

*Continued on next page...*

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	446	Total	C	N	O	S	0	0
			3459	2161	605	674	19		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	418	Total	C	N	O	S	0	0
			3134	1962	556	607	9		
5	e	418	Total	C	N	O	S	0	0
			3134	1962	556	607	9		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	64	Total	C	N	O	S	0	0
			528	320	97	106	5		
6	f	64	Total	C	N	O	S	0	0
			528	320	97	106	5		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	106	Total	C	N	O	S	0	0
			921	589	162	168	2		
7	g	106	Total	C	N	O	S	0	0
			921	589	162	168	2		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	71	Total	C	N	O	S	0	0
			608	399	112	95	2		
8	h	79	Total	C	N	O	S	0	0
			666	434	122	108	2		

- Molecule 9 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	62	Total	C	N	O	0	0
			507	331	90	86		
9	i	62	Total	C	N	O	0	0
			507	331	90	86		

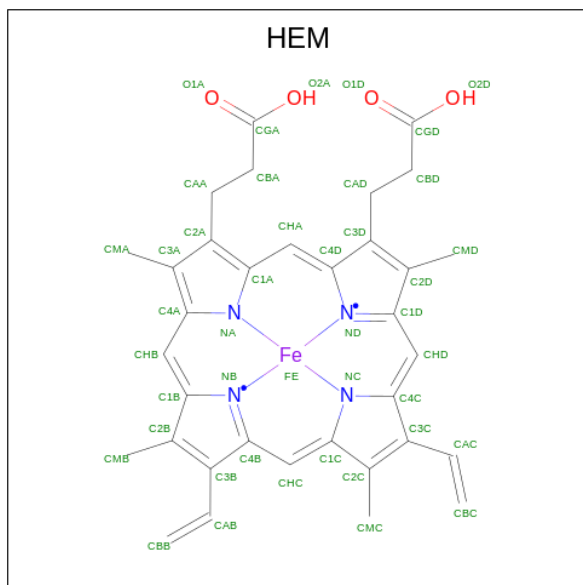
- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	49	Total 405	C 269	N 71	O 63	S 2	0	0
10	j	51	Total 421	C 281	N 74	O 65	S 1	0	0

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

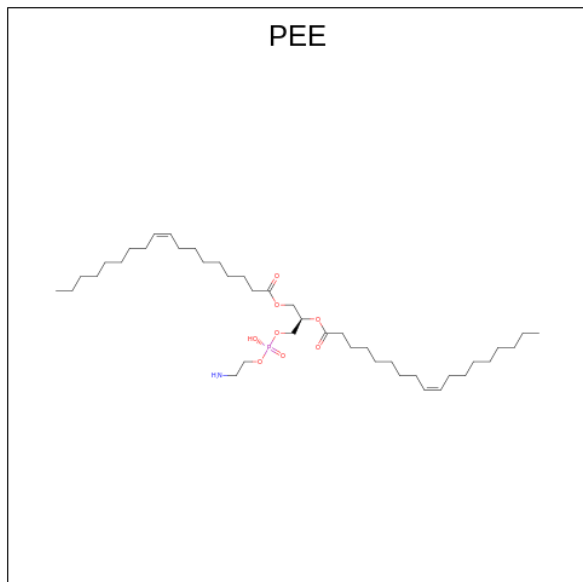
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	57	Total 404	C 252	N 74	O 76	S 2	0	0
11	k	57	Total 404	C 252	N 74	O 76	S 2	0	0

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



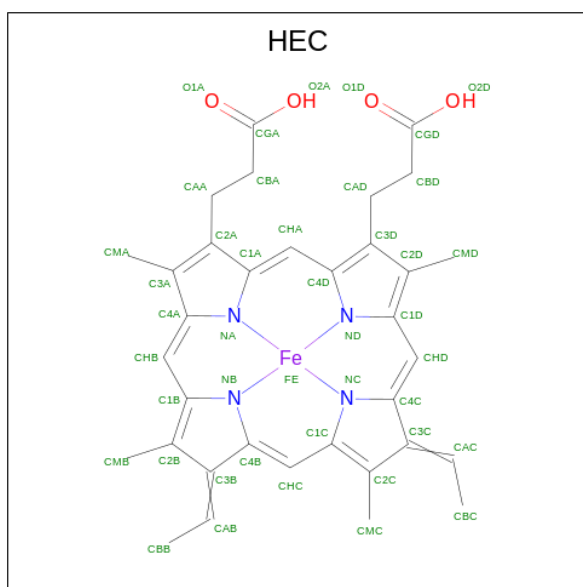
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
12	A	1	Total 43	C 34	Fe 1	N 4	O 4	0
12	A	1	Total 43	C 34	Fe 1	N 4	O 4	0
12	a	1	Total 43	C 34	Fe 1	N 4	O 4	0
12	a	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 13 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula:  $C_{41}H_{78}NO_8P$ ).



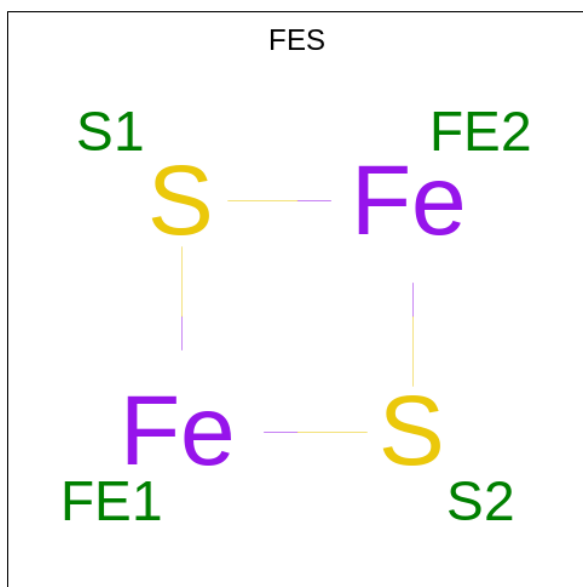
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		
13	A	1	Total	45	35	1	8	1	0
13	D	1	Total	49	39	1	8	1	0
13	a	1	Total	49	39	1	8	1	0

- Molecule 14 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms				AltConf	
14	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

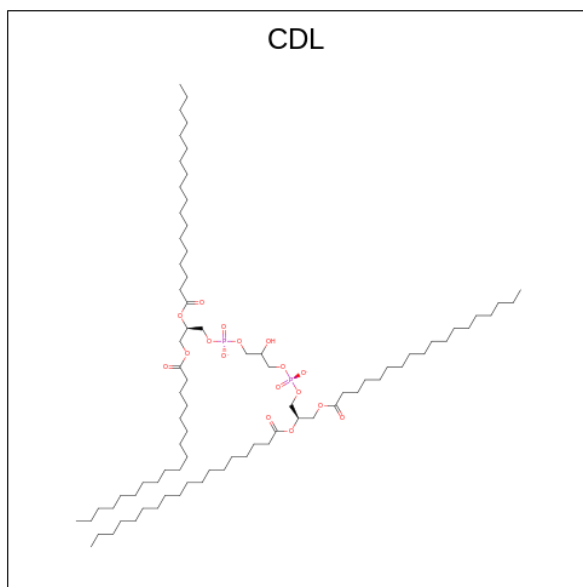
- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
15	C	1	Total	Fe	S	0
			4	2	2	
15	c	1	Total	Fe	S	0
			4	2	2	

- Molecule 16 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



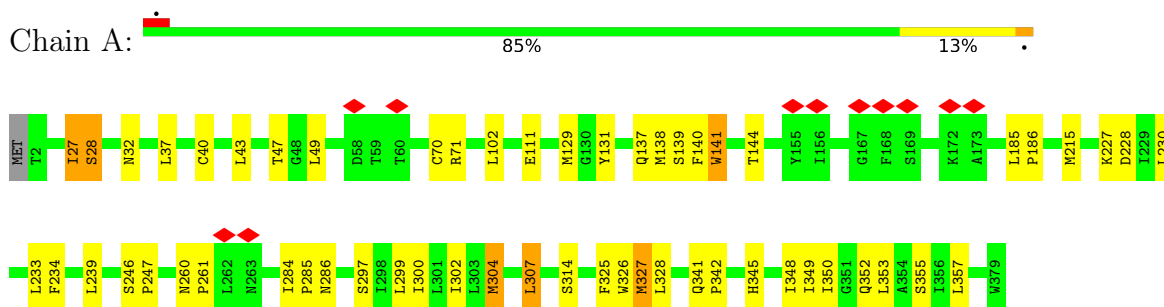


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
16	D	1	64	45	17	2	0
16	a	1	64	45	17	2	0

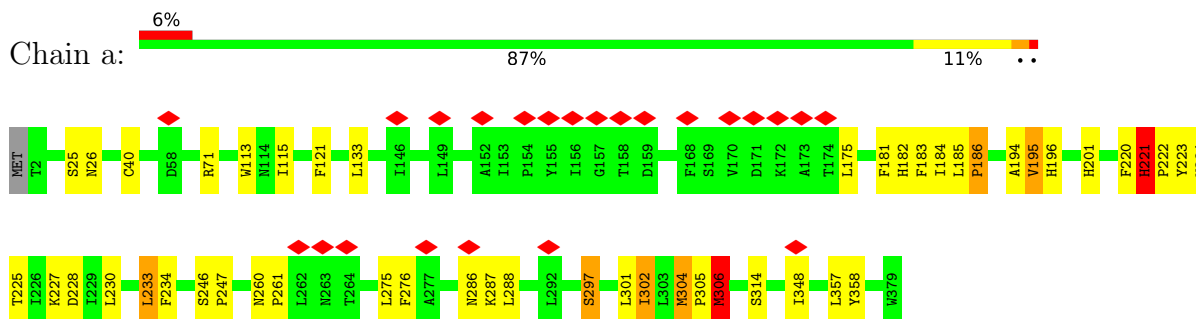
### 3 Residue-property plots [i](#)

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.

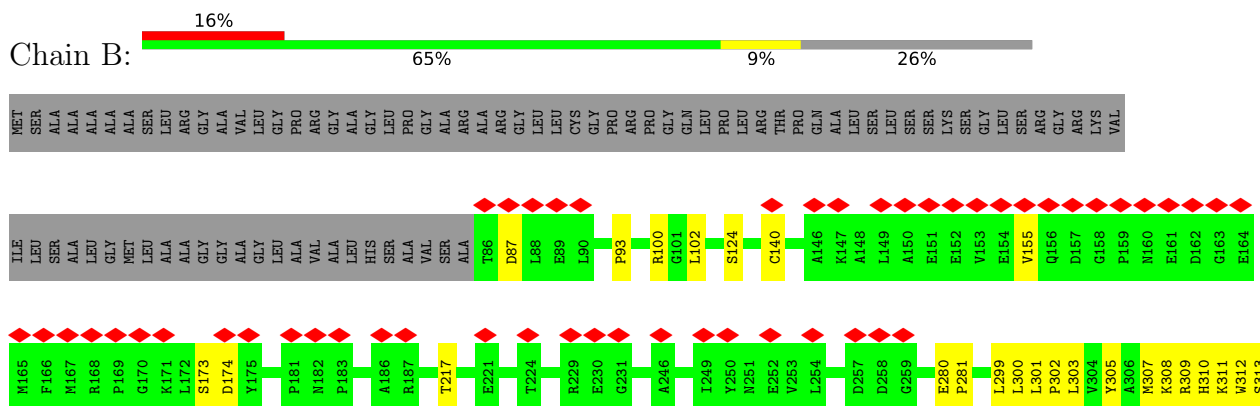
- Molecule 1: Cytochrome b



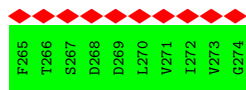
- Molecule 1: Cytochrome b



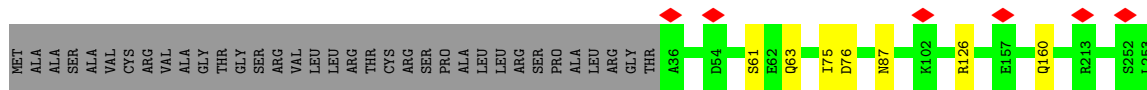
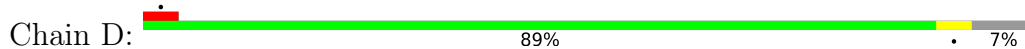
- Molecule 2: Cytochrome c1, heme protein, mitochondrial



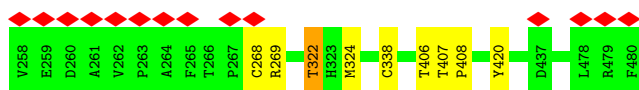
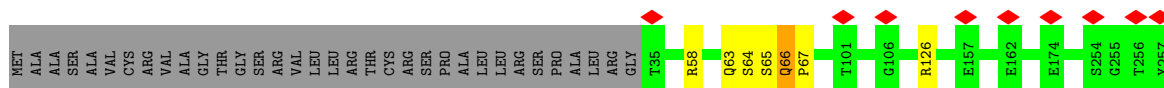
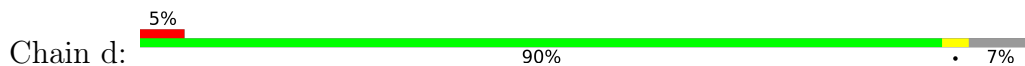




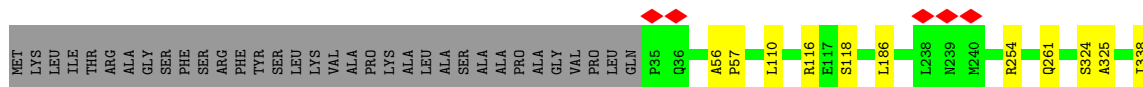
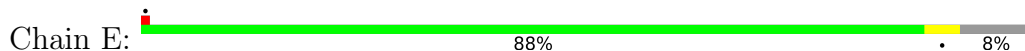
• Molecule 4: Cytochrome b-c1 complex subunit 1, mitochondrial



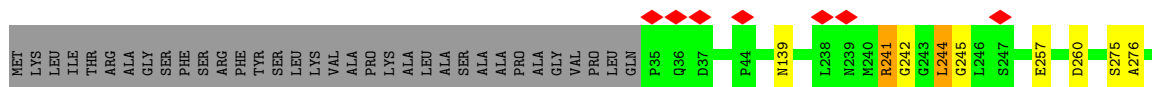
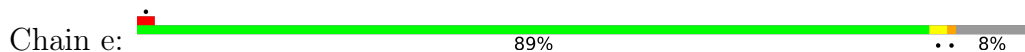
• Molecule 4: Cytochrome b-c1 complex subunit 1, mitochondrial



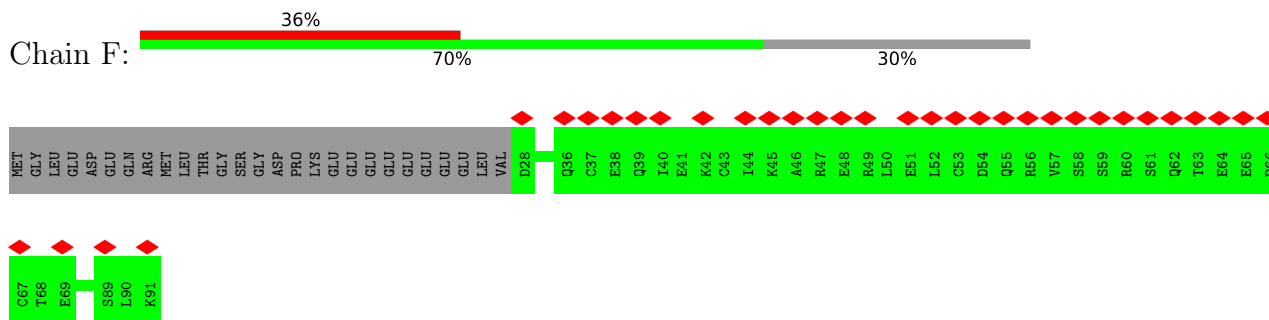
• Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial



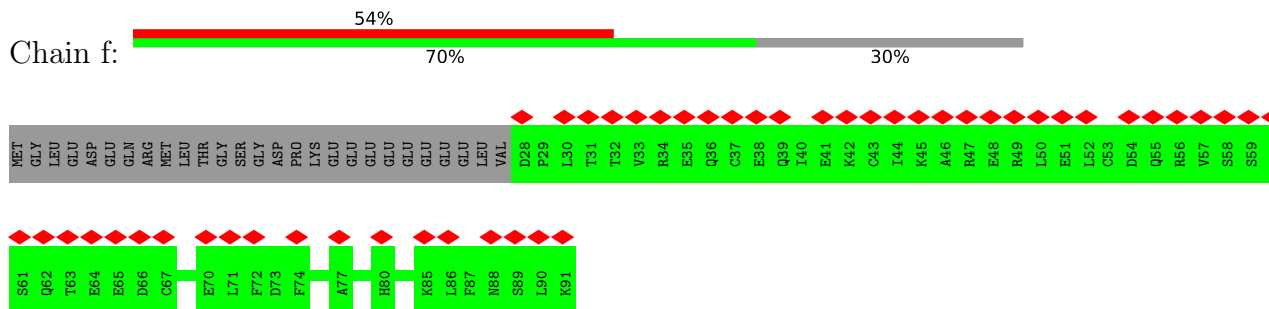
• Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial



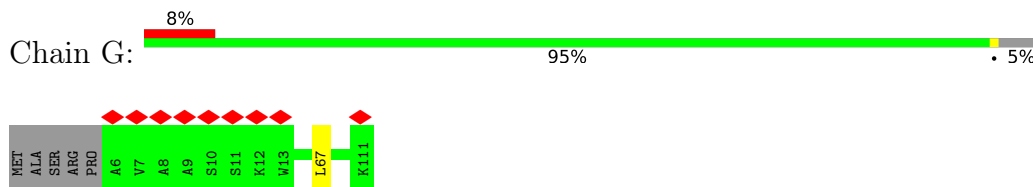
• Molecule 6: Cytochrome b-c1 complex subunit 6



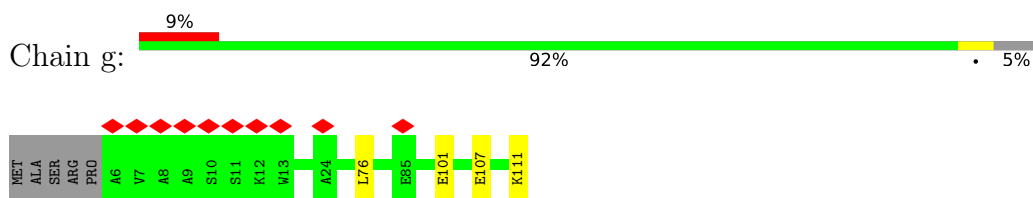
• Molecule 6: Cytochrome b-c1 complex subunit 6



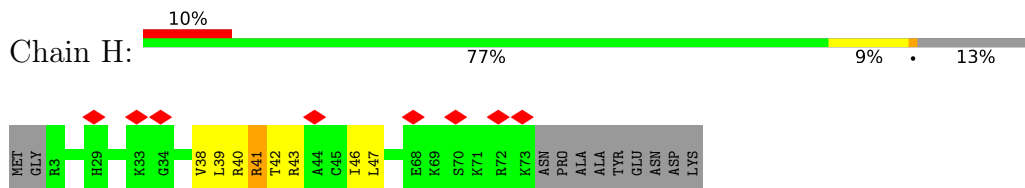
• Molecule 7: Cytochrome b-c1 complex subunit 7



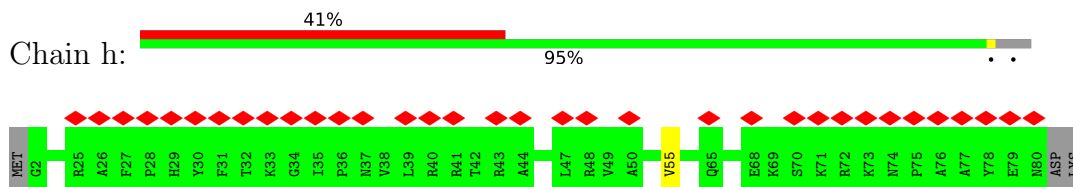
• Molecule 7: Cytochrome b-c1 complex subunit 7



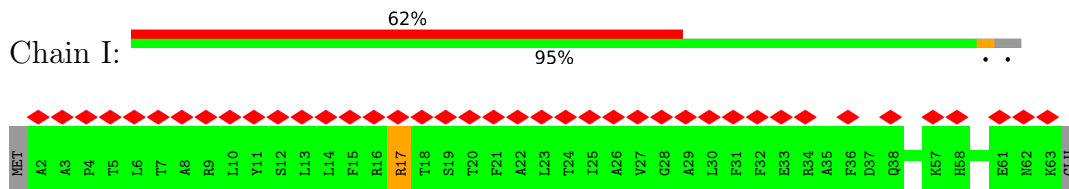
• Molecule 8: Cytochrome b-c1 complex subunit 8



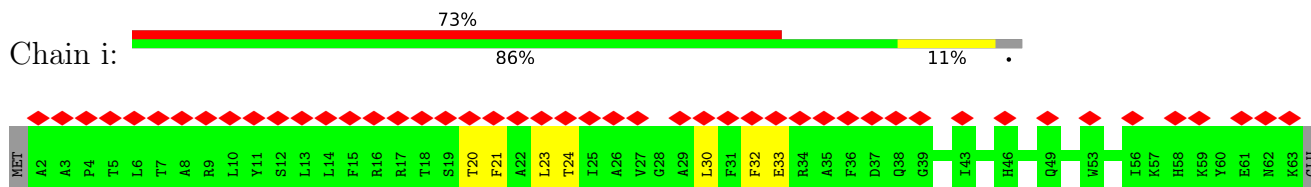
• Molecule 8: Cytochrome b-c1 complex subunit 8



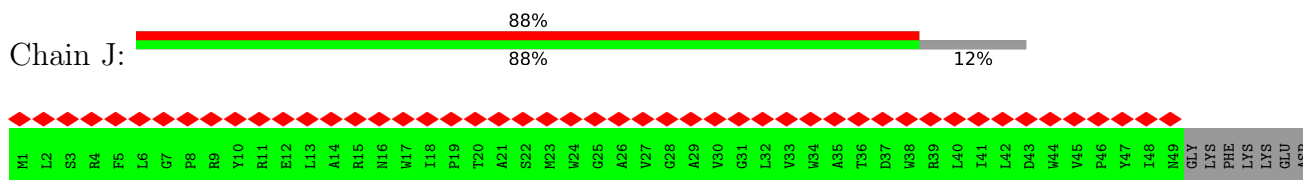
- Molecule 9: Complex III subunit 9



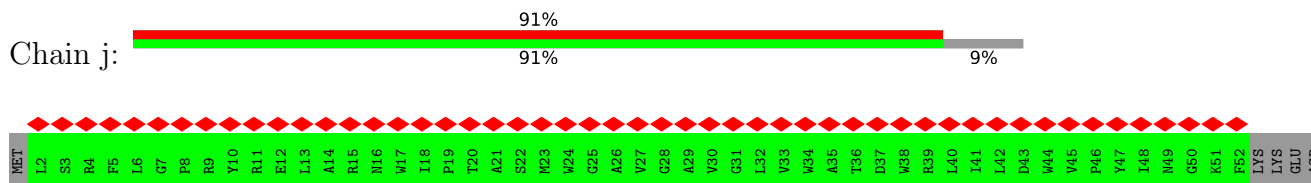
- Molecule 9: Complex III subunit 9



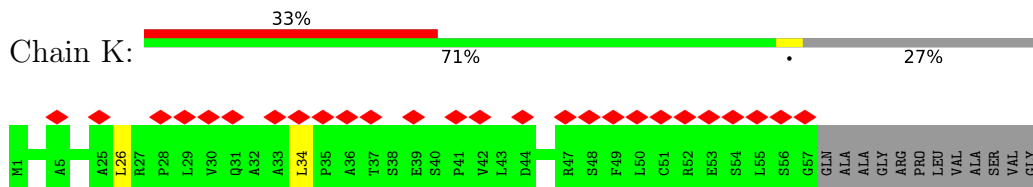
- Molecule 10: Cytochrome b-c1 complex subunit 10



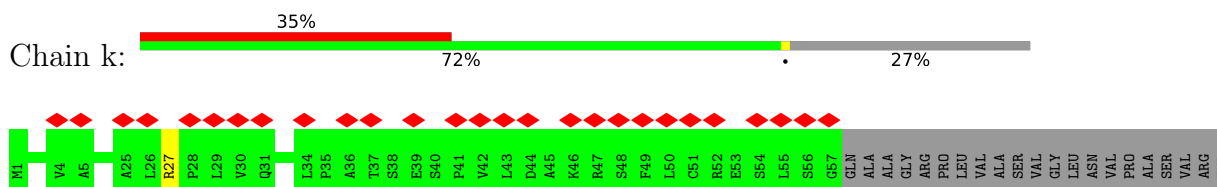
- Molecule 10: Cytochrome b-c1 complex subunit 10



- Molecule 11: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 11: Cytochrome b-c1 complex subunit Rieske, mitochondrial



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98300	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 ( $e^-/\text{\AA}^2$ )	49.21	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.627	Depositor
Minimum map value	-2.368	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.113	Depositor
Recommended contour level	0.3	Depositor
Map size ( $\text{\AA}$ )	240.8, 240.8, 240.8	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.86, 0.86, 0.86	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: PEE, CDL, HEC, FES, HEM

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	0.86	14/3115 (0.4%)	0.91	17/4259 (0.4%)
1	a	0.84	18/3115 (0.6%)	0.88	17/4259 (0.4%)
2	B	0.78	10/1978 (0.5%)	0.80	9/2684 (0.3%)
2	b	0.55	2/1961 (0.1%)	0.59	1/2661 (0.0%)
3	C	0.27	0/1534	0.49	0/2075
3	c	0.28	0/1549	0.50	0/2095
4	D	0.57	3/3524 (0.1%)	0.65	2/4783 (0.0%)
4	d	0.50	0/3531	0.66	3/4793 (0.1%)
5	E	0.65	3/3187 (0.1%)	0.73	4/4314 (0.1%)
5	e	0.51	2/3187 (0.1%)	0.71	7/4314 (0.2%)
6	F	0.25	0/534	0.44	0/714
6	f	0.26	0/534	0.51	0/714
7	G	0.44	0/941	0.59	1/1262 (0.1%)
7	g	0.59	0/941	0.70	2/1262 (0.2%)
8	H	0.51	0/628	0.76	1/848 (0.1%)
8	h	0.33	0/688	0.61	0/931
9	I	0.28	0/520	0.49	0/701
9	i	0.38	0/520	0.62	0/701
10	J	0.25	0/420	0.43	0/576
10	j	0.25	0/437	0.46	0/598
11	K	0.33	0/410	0.79	0/556
11	k	0.29	0/410	0.74	1/556 (0.2%)
All	All	0.59	52/33664 (0.2%)	0.70	65/45656 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	3
4	D	0	2
4	d	0	3
8	h	0	1
9	I	0	1
11	K	0	2
All	All	0	14

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	312	TRP	CB-CG	-10.85	1.30	1.50
2	B	311	LYS	C-O	-9.29	1.05	1.23
1	a	113	TRP	CB-CG	-8.51	1.34	1.50
2	B	93	PRO	CG-CD	-8.21	1.23	1.50
2	B	308	LYS	C-O	-8.17	1.07	1.23
1	A	326	TRP	CE3-CZ3	-7.72	1.25	1.38
1	a	196	HIS	C-O	-6.94	1.10	1.23
1	A	326	TRP	CE2-CZ2	-6.55	1.28	1.39
1	a	224	TYR	CE1-CZ	-6.49	1.30	1.38
5	e	437	SER	CA-CB	-6.42	1.43	1.52
1	a	224	TYR	CG-CD1	-6.29	1.30	1.39
1	a	113	TRP	CG-CD1	-6.19	1.28	1.36
1	A	234	PHE	CB-CG	-6.14	1.41	1.51
5	E	339	TYR	CE1-CZ	-6.14	1.30	1.38
2	B	305	TYR	CE1-CZ	-6.02	1.30	1.38
1	a	115	ILE	C-O	-6.00	1.11	1.23
1	a	195	VAL	C-O	-5.91	1.12	1.23
1	A	325	PHE	CG-CD1	-5.89	1.29	1.38
2	B	305	TYR	CG-CD1	-5.86	1.31	1.39
1	A	327	MET	CA-CB	-5.76	1.41	1.53
1	a	113	TRP	CD2-CE2	-5.76	1.34	1.41
4	D	348	TYR	CE1-CZ	-5.71	1.31	1.38
5	e	438	MET	CA-C	5.69	1.67	1.52
1	a	222	PRO	N-CD	5.62	1.55	1.47
1	a	225	THR	CB-CG2	-5.56	1.34	1.52
1	a	221	HIS	C-O	-5.53	1.12	1.23
1	a	220	PHE	C-O	-5.53	1.12	1.23
4	D	348	TYR	CE2-CZ	-5.49	1.31	1.38
1	A	342	PRO	N-CD	5.48	1.55	1.47
2	B	312	TRP	CE2-CZ2	-5.46	1.30	1.39
1	a	194	ALA	C-O	-5.36	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	325	PHE	CG-CD2	-5.35	1.30	1.38
2	B	312	TRP	CE3-CZ3	-5.34	1.29	1.38
1	a	261	PRO	N-CD	5.34	1.55	1.47
5	E	57	PRO	N-CD	5.32	1.55	1.47
1	a	247	PRO	N-CD	5.29	1.55	1.47
1	A	247	PRO	N-CD	5.28	1.55	1.47
1	A	285	PRO	N-CD	5.27	1.55	1.47
1	A	28	SER	CB-OG	-5.27	1.35	1.42
2	B	315	LEU	C-O	-5.25	1.13	1.23
1	A	186	PRO	N-CD	5.25	1.55	1.47
5	E	437	SER	CA-CB	-5.21	1.45	1.52
1	a	223	TYR	CE1-CZ	-5.21	1.31	1.38
2	b	305	TYR	CB-CG	-5.17	1.43	1.51
1	A	228	ASP	CB-CG	5.14	1.62	1.51
2	B	281	PRO	N-CD	5.12	1.55	1.47
4	D	348	TYR	CG-CD1	-5.08	1.32	1.39
1	a	305	PRO	N-CD	5.07	1.54	1.47
1	A	261	PRO	N-CD	5.04	1.54	1.47
1	a	358	TYR	CE1-CZ	-5.03	1.32	1.38
1	A	325	PHE	CB-CG	-5.02	1.42	1.51
2	B	305	TYR	CG-CD2	-5.00	1.32	1.39

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	93	PRO	N-CD-CG	-11.70	85.65	103.20
1	A	27	ILE	CG1-CB-CG2	-10.94	87.33	111.40
2	B	307	MET	CB-CG-SD	-9.80	83.00	112.40
5	e	440	ALA	N-CA-C	-8.98	86.76	111.00
1	a	233	LEU	CA-CB-CG	8.60	135.07	115.30
1	a	301	LEU	CA-CB-CG	8.24	134.25	115.30
4	d	66	GLN	C-N-CD	-7.92	103.18	120.60
1	A	43	LEU	CA-CB-CG	7.86	133.37	115.30
1	A	327	MET	CB-CG-SD	-7.81	88.97	112.40
1	a	230	LEU	CB-CG-CD1	-7.51	98.23	111.00
1	A	228	ASP	CB-CG-OD1	7.47	125.02	118.30
5	e	439	ALA	N-CA-C	-7.40	91.03	111.00
1	A	304	MET	N-CA-C	7.28	130.66	111.00
1	a	196	HIS	CB-CA-C	-6.95	96.50	110.40
1	a	184	ILE	CB-CA-C	6.84	125.28	111.60
1	A	239	LEU	CB-CG-CD1	-6.81	99.42	111.00
5	e	242	GLY	N-CA-C	6.61	129.62	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	93	PRO	CA-CB-CG	-6.50	91.66	104.00
5	e	245	GLY	N-CA-C	6.37	129.01	113.10
4	d	407	THR	C-N-CD	6.28	141.58	128.40
2	B	315	LEU	CB-CG-CD1	6.26	121.65	111.00
1	A	345	HIS	C-N-CD	6.08	141.18	128.40
2	B	280	GLU	C-N-CD	5.93	140.85	128.40
5	E	325	ALA	N-CA-C	-5.85	95.20	111.00
4	D	407	THR	C-N-CD	5.83	140.65	128.40
1	a	297	SER	N-CA-C	5.82	126.70	111.00
1	A	260	ASN	C-N-CD	5.80	140.58	128.40
1	A	233	LEU	CB-CG-CD1	-5.79	101.16	111.00
1	a	221	HIS	C-N-CD	5.75	140.47	128.40
5	e	437	SER	N-CA-C	-5.72	95.55	111.00
1	A	185	LEU	C-N-CD	5.68	140.32	128.40
1	a	260	ASN	C-N-CD	5.67	140.30	128.40
5	E	56	ALA	C-N-CD	5.63	140.22	128.40
2	B	300	LEU	CB-CG-CD1	-5.60	101.48	111.00
7	G	67	LEU	CA-CB-CG	5.60	128.17	115.30
1	a	246	SER	C-N-CD	5.59	140.14	128.40
1	A	246	SER	C-N-CD	5.57	140.11	128.40
1	A	284	ILE	C-N-CD	5.57	140.09	128.40
1	a	225	THR	N-CA-CB	5.52	120.80	110.30
2	B	320	LEU	C-N-CA	5.44	135.30	121.70
1	A	307	LEU	CA-CB-CG	5.42	127.77	115.30
1	a	196	HIS	C-N-CA	5.40	135.21	121.70
5	e	244	LEU	N-CA-C	5.40	125.57	111.00
5	E	438	MET	CB-CG-SD	-5.40	96.21	112.40
4	d	408	PRO	CA-N-CD	-5.36	103.99	111.50
4	D	315	ASP	CB-CG-OD1	5.36	123.12	118.30
1	a	306	MET	C-N-CA	5.34	135.05	121.70
1	A	341	GLN	C-N-CD	5.33	139.59	128.40
1	a	224	TYR	CB-CA-C	5.31	121.02	110.40
1	A	37	LEU	CB-CG-CD2	-5.27	102.05	111.00
5	E	420	ALA	N-CA-C	-5.25	96.81	111.00
2	B	303	LEU	CB-CG-CD1	5.25	119.93	111.00
1	a	186	PRO	CA-N-CD	-5.23	104.17	111.50
1	a	185	LEU	C-N-CD	5.22	139.36	128.40
7	g	101	GLU	O-C-N	-5.22	114.35	122.70
2	b	307	MET	CB-CG-SD	-5.18	96.87	112.40
11	k	27	ARG	N-CA-C	-5.14	97.11	111.00
7	g	76	LEU	CA-CB-CG	5.13	127.11	115.30
2	B	315	LEU	CB-CG-CD2	-5.11	102.31	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	LEU	CB-CG-CD1	-5.11	102.32	111.00
1	A	299	LEU	CB-CA-C	5.08	119.85	110.20
5	e	276	ALA	N-CA-C	5.06	124.67	111.00
1	a	223	TYR	N-CA-C	5.06	124.66	111.00
1	a	302	ILE	CB-CA-C	-5.06	101.48	111.60
8	H	47	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	GLN	Peptide
1	A	141	TRP	Peptide
4	D	160	GLN	Peptide
4	D	420	TYR	Peptide
9	I	17	ARG	Peptide
11	K	26	LEU	Peptide
11	K	34	LEU	Peptide
1	a	133	LEU	Peptide
1	a	221	HIS	Peptide
1	a	306	MET	Peptide
4	d	322	THR	Peptide
4	d	338	CYS	Peptide
4	d	420	TYR	Peptide
8	h	55	VAL	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	376/379 (99%)	352 (94%)	22 (6%)	2 (0%)	29	59
1	a	376/379 (99%)	340 (90%)	32 (8%)	4 (1%)	14	40
2	B	239/326 (73%)	215 (90%)	20 (8%)	4 (2%)	9	28
2	b	237/326 (73%)	217 (92%)	20 (8%)	0	100	100
3	C	192/196 (98%)	188 (98%)	4 (2%)	0	100	100
3	c	194/196 (99%)	177 (91%)	16 (8%)	1 (0%)	29	59
4	D	443/480 (92%)	424 (96%)	19 (4%)	0	100	100
4	d	444/480 (92%)	400 (90%)	42 (10%)	2 (0%)	29	59
5	E	416/453 (92%)	387 (93%)	28 (7%)	1 (0%)	47	76
5	e	416/453 (92%)	375 (90%)	40 (10%)	1 (0%)	47	76
6	F	62/91 (68%)	59 (95%)	3 (5%)	0	100	100
6	f	62/91 (68%)	59 (95%)	3 (5%)	0	100	100
7	G	104/111 (94%)	95 (91%)	9 (9%)	0	100	100
7	g	104/111 (94%)	90 (86%)	14 (14%)	0	100	100
8	H	69/82 (84%)	56 (81%)	11 (16%)	2 (3%)	4	16
8	h	77/82 (94%)	64 (83%)	13 (17%)	0	100	100
9	I	60/64 (94%)	49 (82%)	11 (18%)	0	100	100
9	i	60/64 (94%)	57 (95%)	3 (5%)	0	100	100
10	J	47/56 (84%)	47 (100%)	0	0	100	100
10	j	49/56 (88%)	45 (92%)	4 (8%)	0	100	100
11	K	55/78 (70%)	33 (60%)	22 (40%)	0	100	100
11	k	55/78 (70%)	34 (62%)	21 (38%)	0	100	100
All	All	4137/4632 (89%)	3763 (91%)	357 (9%)	17 (0%)	38	64

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	302	PRO
1	a	221	HIS
3	c	83	ILE
4	d	66	GLN
4	d	67	PRO
2	B	322	TYR
8	H	41	ARG
1	a	286	ASN

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Mol	Chain	Res	Type
5	e	241	ARG
1	A	286	ASN
2	B	124	SER
5	E	439	ALA
8	H	46	ILE
1	A	314	SER
1	a	314	SER
1	a	304	MET
2	B	301	LEU

### 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	331/332 (100%)	298 (90%)	33 (10%)	7	21
1	a	331/332 (100%)	305 (92%)	26 (8%)	12	32
2	B	206/259 (80%)	193 (94%)	13 (6%)	18	44
2	b	204/259 (79%)	200 (98%)	4 (2%)	55	81
3	C	164/166 (99%)	161 (98%)	3 (2%)	59	83
3	c	165/166 (99%)	159 (96%)	6 (4%)	35	67
4	D	371/397 (94%)	356 (96%)	15 (4%)	31	63
4	d	372/397 (94%)	362 (97%)	10 (3%)	44	75
5	E	327/354 (92%)	314 (96%)	13 (4%)	31	63
5	e	327/354 (92%)	319 (98%)	8 (2%)	49	78
6	F	61/85 (72%)	61 (100%)	0	100	100
6	f	61/85 (72%)	61 (100%)	0	100	100
7	G	95/99 (96%)	95 (100%)	0	100	100
7	g	95/99 (96%)	93 (98%)	2 (2%)	53	80
8	H	65/73 (89%)	59 (91%)	6 (9%)	9	25
8	h	70/73 (96%)	70 (100%)	0	100	100
9	I	50/52 (96%)	49 (98%)	1 (2%)	55	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	i	50/52 (96%)	43 (86%)	7 (14%)	3	9
10	J	40/46 (87%)	40 (100%)	0	100	100
10	j	41/46 (89%)	41 (100%)	0	100	100
11	K	44/59 (75%)	44 (100%)	0	100	100
11	k	44/59 (75%)	44 (100%)	0	100	100
All	All	3514/3844 (91%)	3367 (96%)	147 (4%)	33	61

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ILE
1	A	28	SER
1	A	32	ASN
1	A	40	CYS
1	A	47	THR
1	A	49	LEU
1	A	70	CYS
1	A	71	ARG
1	A	102	LEU
1	A	111	GLU
1	A	129	MET
1	A	131	TYR
1	A	138	MET
1	A	139	SER
1	A	140	PHE
1	A	141	TRP
1	A	144	THR
1	A	215	MET
1	A	227	LYS
1	A	230	LEU
1	A	297	SER
1	A	300	ILE
1	A	302	ILE
1	A	304	MET
1	A	307	LEU
1	A	327	MET
1	A	348	ILE
1	A	349	ILE
1	A	350	ILE
1	A	352	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	353	LEU
1	A	355	SER
1	A	357	LEU
2	B	87	ASP
2	B	100	ARG
2	B	102	LEU
2	B	140	CYS
2	B	155	VAL
2	B	173	SER
2	B	174	ASP
2	B	217	THR
2	B	299	LEU
2	B	309	ARG
2	B	310	HIS
2	B	313	SER
2	B	316	LYS
3	C	89	SER
3	C	96	VAL
3	C	97	LEU
4	D	61	SER
4	D	63	GLN
4	D	75	ILE
4	D	76	ASP
4	D	87	ASN
4	D	126	ARG
4	D	278	ARG
4	D	279	ASP
4	D	325	SER
4	D	328	LEU
4	D	336	LYS
4	D	350	GLU
4	D	351	THR
4	D	407	THR
4	D	416	SER
5	E	110	LEU
5	E	116	ARG
5	E	118	SER
5	E	186	LEU
5	E	254	ARG
5	E	261	GLN
5	E	324	SER
5	E	338	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	E	339	TYR
5	E	387	GLU
5	E	388	SER
5	E	423	ASP
5	E	438	MET
8	H	38	VAL
8	H	39	LEU
8	H	40	ARG
8	H	41	ARG
8	H	42	THR
8	H	43	ARG
9	I	17	ARG
1	a	25	SER
1	a	26	ASN
1	a	40	CYS
1	a	71	ARG
1	a	121	PHE
1	a	175	LEU
1	a	181	PHE
1	a	182	HIS
1	a	183	PHE
1	a	186	PRO
1	a	195	VAL
1	a	201	HIS
1	a	227	LYS
1	a	228	ASP
1	a	233	LEU
1	a	234	PHE
1	a	275	LEU
1	a	276	PHE
1	a	287	LYS
1	a	288	LEU
1	a	297	SER
1	a	302	ILE
1	a	304	MET
1	a	306	MET
1	a	348	ILE
1	a	357	LEU
2	b	296	MET
2	b	297	MET
2	b	307	MET
2	b	309	ARG

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Mol	Chain	Res	Type
3	c	81	THR
3	c	82	ASP
3	c	122	THR
3	c	147	LEU
3	c	156	LEU
3	c	157	SER
4	d	58	ARG
4	d	63	GLN
4	d	64	SER
4	d	65	SER
4	d	126	ARG
4	d	268	CYS
4	d	269	ARG
4	d	322	THR
4	d	324	MET
4	d	406	THR
5	e	139	ASN
5	e	241	ARG
5	e	244	LEU
5	e	257	GLU
5	e	260	ASP
5	e	275	SER
5	e	438	MET
5	e	441	SER
7	g	107	GLU
7	g	111	LYS
9	i	20	THR
9	i	21	PHE
9	i	23	LEU
9	i	24	THR
9	i	30	LEU
9	i	32	PHE
9	i	33	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	137	GLN
1	A	341	GLN
2	B	116	GLN
2	B	182	ASN

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Mol	Chain	Res	Type
2	B	266	GLN
4	D	95	HIS
4	D	308	ASN
4	D	345	ASN
1	a	201	HIS
2	b	116	GLN
3	c	200	HIS
3	c	239	HIS
4	d	469	ASN
6	f	76	HIS
9	i	38	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

13 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
12	HEM	a	402	1	41,50,50	1.56	5 (12%)	45,82,82	1.51	9 (20%)
16	CDL	a	404	-	63,63,99	1.10	8 (12%)	69,75,111	1.12	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	HEM	A	401	1	41,50,50	1.58	4 (9%)	45,82,82	1.85	14 (31%)
13	PEE	A	403	-	44,44,50	1.56	7 (15%)	46,49,55	1.25	3 (6%)
14	HEC	b	401	2	32,50,50	2.23	3 (9%)	24,82,82	1.45	6 (25%)
15	FES	C	301	3	0,4,4	-	-	-	-	-
14	HEC	B	401	2	32,50,50	2.18	3 (9%)	24,82,82	1.77	7 (29%)
16	CDL	D	501	-	63,63,99	1.08	8 (12%)	69,75,111	1.20	4 (5%)
15	FES	c	301	-	0,4,4	-	-	-	-	-
13	PEE	a	403	-	48,48,50	1.53	5 (10%)	51,53,55	1.16	3 (5%)
13	PEE	D	502	-	48,48,50	1.58	8 (16%)	51,53,55	1.20	3 (5%)
12	HEM	A	402	1	41,50,50	1.60	4 (9%)	45,82,82	1.90	14 (31%)
12	HEM	a	401	1	41,50,50	1.50	5 (12%)	45,82,82	1.38	6 (13%)

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
12	HEM	a	402	1	-	4/12/54/54	-
16	CDL	a	404	-	-	38/74/74/110	-
12	HEM	A	401	1	-	7/12/54/54	-
13	PEE	A	403	-	-	24/48/48/54	-
14	HEC	b	401	2	-	3/10/54/54	-
15	FES	C	301	3	-	-	0/1/1/1
14	HEC	B	401	2	-	2/10/54/54	-
16	CDL	D	501	-	-	36/74/74/110	-
15	FES	c	301	-	-	-	0/1/1/1
13	PEE	a	403	-	-	23/52/52/54	-
13	PEE	D	502	-	-	17/52/52/54	-
12	HEM	A	402	1	-	8/12/54/54	-
12	HEM	a	401	1	-	4/12/54/54	-

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	401	HEC	C2B-C3B	-6.75	1.33	1.40
14	b	401	HEC	C3C-C2C	-6.52	1.33	1.40
14	B	401	HEC	C2B-C3B	-6.43	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	401	HEC	C3C-C2C	-6.03	1.34	1.40
12	A	401	HEM	C3C-C2C	-5.96	1.32	1.40
12	A	402	HEM	C3C-C2C	-5.77	1.32	1.40
12	a	402	HEM	C3C-C2C	-5.74	1.32	1.40
14	B	401	HEC	C3D-C2D	5.70	1.54	1.37
14	b	401	HEC	C3D-C2D	5.21	1.53	1.37
12	a	401	HEM	C3C-C2C	-4.84	1.33	1.40
13	a	403	PEE	C18-C19	4.47	1.57	1.31
13	D	502	PEE	C18-C19	4.43	1.57	1.31
13	A	403	PEE	C18-C19	4.42	1.57	1.31
13	D	502	PEE	C39-C38	4.09	1.55	1.31
13	a	403	PEE	C39-C38	4.05	1.55	1.31
13	A	403	PEE	C39-C38	4.01	1.55	1.31
13	D	502	PEE	O3-C30	3.73	1.44	1.33
13	a	403	PEE	O3-C30	3.60	1.43	1.33
13	A	403	PEE	O3-C30	3.41	1.43	1.33
12	A	402	HEM	C3C-CAC	3.35	1.54	1.47
13	D	502	PEE	O2-C10	3.33	1.43	1.34
12	a	401	HEM	C3C-CAC	3.19	1.54	1.47
13	A	403	PEE	O2-C10	3.18	1.43	1.34
13	a	403	PEE	O2-C10	3.06	1.42	1.34
12	A	401	HEM	CAB-C3B	2.95	1.55	1.47
12	A	402	HEM	CAB-C3B	2.89	1.55	1.47
12	a	402	HEM	CAB-C3B	2.87	1.55	1.47
12	a	401	HEM	CAB-C3B	2.85	1.55	1.47
16	D	501	CDL	OA6-CA4	-2.70	1.39	1.46
12	A	401	HEM	C3C-CAC	2.67	1.53	1.47
16	a	404	CDL	OB6-CB4	-2.53	1.40	1.46
13	A	403	PEE	O2-C2	-2.48	1.40	1.46
12	a	402	HEM	C3C-CAC	2.47	1.52	1.47
16	D	501	CDL	OB6-CB4	-2.47	1.40	1.46
13	a	403	PEE	O2-C2	-2.40	1.40	1.46
13	D	502	PEE	C11-C10	2.38	1.57	1.50
16	D	501	CDL	OB8-CB7	2.37	1.40	1.33
16	D	501	CDL	OA8-CA7	2.36	1.40	1.33
12	a	402	HEM	CAA-C2A	2.36	1.55	1.52
16	a	404	CDL	OA6-CA4	-2.35	1.40	1.46
16	a	404	CDL	OB6-CB5	2.34	1.40	1.34
16	a	404	CDL	OA6-CA5	2.32	1.40	1.34
16	a	404	CDL	OB8-CB7	2.29	1.40	1.33
16	a	404	CDL	OA8-CA7	2.29	1.40	1.33
16	a	404	CDL	OB8-CB6	-2.29	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	502	PEE	O2-C2	-2.26	1.41	1.46
13	D	502	PEE	P-O3P	2.23	1.68	1.59
12	a	402	HEM	C3D-C2D	-2.21	1.32	1.36
16	D	501	CDL	OB6-CB5	2.17	1.40	1.34
12	a	401	HEM	FE-NB	2.16	2.07	1.96
12	A	401	HEM	FE-ND	2.16	2.07	1.96
16	D	501	CDL	OA6-CA5	2.12	1.40	1.34
16	a	404	CDL	OA8-CA6	-2.12	1.40	1.45
16	D	501	CDL	OB8-CB6	-2.12	1.40	1.45
13	D	502	PEE	P-O4P	2.11	1.67	1.59
16	D	501	CDL	OA8-CA6	-2.11	1.40	1.45
12	A	402	HEM	CAA-C2A	2.07	1.55	1.52
13	A	403	PEE	P-O3P	2.06	1.67	1.59
12	a	401	HEM	CAA-C2A	2.03	1.55	1.52
13	A	403	PEE	C11-C10	2.01	1.56	1.50

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	402	HEM	CAD-C3D-C4D	5.12	133.60	124.66
12	A	402	HEM	CAD-C3D-C2D	-4.73	119.07	127.88
12	A	401	HEM	C4D-ND-C1D	4.33	109.55	105.07
13	D	502	PEE	O2-C10-C11	4.27	120.70	111.50
16	D	501	CDL	OB6-CB5-C51	4.18	120.52	111.50
16	D	501	CDL	OA6-CA5-C11	4.18	120.52	111.50
16	a	404	CDL	OA6-CA5-C11	4.08	120.30	111.50
12	A	401	HEM	C4C-CHD-C1D	3.86	127.65	122.56
14	B	401	HEC	CMB-C2B-C1B	-3.72	122.75	128.46
13	a	403	PEE	O2-C10-C11	3.67	119.40	111.50
16	a	404	CDL	OB6-CB5-C51	3.66	119.39	111.50
12	A	401	HEM	CAD-C3D-C2D	-3.57	121.23	127.88
12	A	402	HEM	C4C-CHD-C1D	3.52	127.21	122.56
13	A	403	PEE	O2-C10-C11	3.49	119.02	111.50
12	A	401	HEM	C3D-C4D-ND	-3.46	106.31	110.17
12	A	402	HEM	CAD-CBD-CGD	-3.32	106.45	113.60
12	A	401	HEM	CAD-C3D-C4D	3.31	130.44	124.66
12	a	402	HEM	C4C-CHD-C1D	3.22	126.81	122.56
12	A	402	HEM	C4D-ND-C1D	3.13	108.31	105.07
13	A	403	PEE	O3-C30-C31	3.05	121.49	111.91
14	B	401	HEC	CMB-C2B-C3B	3.04	129.40	125.82
16	D	501	CDL	OA8-CA7-C31	2.99	121.30	111.91
13	a	403	PEE	O3-C30-C31	2.97	121.24	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	401	HEM	C2D-C1D-ND	-2.96	106.33	109.88
16	a	404	CDL	OB8-CB7-C71	2.93	121.11	111.91
12	a	402	HEM	C4D-ND-C1D	2.92	108.09	105.07
12	A	401	HEM	C4A-C3A-C2A	2.92	109.03	107.00
12	a	401	HEM	CMC-C2C-C3C	2.89	130.09	124.68
12	A	402	HEM	CHD-C1D-ND	2.86	127.54	124.43
12	a	402	HEM	C2D-C1D-ND	-2.80	106.53	109.88
14	B	401	HEC	C1D-C2D-C3D	-2.78	105.06	107.00
12	a	401	HEM	C4D-ND-C1D	2.69	107.85	105.07
16	D	501	CDL	OB8-CB7-C71	2.68	120.33	111.91
12	A	401	HEM	CHD-C1D-ND	2.66	127.32	124.43
13	D	502	PEE	O3-C30-C31	2.61	120.09	111.91
12	A	402	HEM	C1B-NB-C4B	2.60	107.75	105.07
12	A	401	HEM	CAA-C2A-C3A	-2.59	119.79	127.25
12	a	402	HEM	C2C-C3C-C4C	2.56	108.69	106.90
16	a	404	CDL	OA8-CA7-C31	2.54	119.87	111.91
14	b	401	HEC	CMB-C2B-C1B	-2.50	124.61	128.46
12	a	402	HEM	C3C-C4C-NC	-2.48	106.25	110.94
12	A	401	HEM	C1D-C2D-C3D	2.40	109.48	106.96
14	b	401	HEC	CMC-C2C-C1C	-2.39	124.80	128.46
12	a	401	HEM	C4A-C3A-C2A	2.37	108.65	107.00
12	a	401	HEM	C4B-CHC-C1C	2.34	125.65	122.56
12	A	401	HEM	O2D-CGD-CBD	2.33	121.51	114.03
12	A	402	HEM	C3D-C4D-ND	-2.33	107.58	110.17
12	A	402	HEM	C4A-C3A-C2A	2.32	108.61	107.00
12	a	402	HEM	C1D-C2D-C3D	2.30	109.38	106.96
12	A	401	HEM	C3C-C4C-NC	-2.29	106.62	110.94
14	b	401	HEC	C1D-C2D-C3D	-2.26	105.42	107.00
12	A	402	HEM	C1D-C2D-C3D	2.25	109.33	106.96
12	a	402	HEM	CMB-C2B-C1B	-2.25	121.61	125.04
14	B	401	HEC	CMD-C2D-C3D	2.23	129.14	124.94
12	A	402	HEM	CMA-C3A-C4A	-2.20	125.09	128.46
14	B	401	HEC	CBA-CAA-C2A	-2.15	108.98	112.60
14	B	401	HEC	CAD-CBD-CGD	-2.14	107.77	113.76
12	A	401	HEM	C2C-C3C-C4C	2.12	108.38	106.90
12	a	402	HEM	CHD-C1D-C2D	2.12	128.29	124.98
14	b	401	HEC	CBD-CAD-C3D	-2.10	109.03	112.62
14	b	401	HEC	CAA-CBA-CGA	-2.10	107.87	113.76
12	A	401	HEM	O1D-CGD-CBD	-2.10	116.34	123.08
12	a	401	HEM	C3B-C2B-C1B	2.10	108.04	106.49
12	A	402	HEM	CHA-C4D-C3D	2.09	129.25	125.33
12	a	401	HEM	CMA-C3A-C4A	-2.09	125.25	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	402	HEM	C3B-C2B-C1B	2.06	108.02	106.49
13	D	502	PEE	C17-C18-C19	-2.06	108.93	124.73
13	A	403	PEE	C3-C2-C1	-2.05	106.93	111.79
14	b	401	HEC	CAD-CBD-CGD	-2.03	108.06	113.76
12	A	402	HEM	C2D-C1D-ND	-2.03	107.45	109.88
12	a	402	HEM	CMD-C2D-C1D	2.02	128.11	125.04
13	a	403	PEE	C17-C18-C19	-2.01	109.34	124.73
14	B	401	HEC	CAA-CBA-CGA	-2.00	108.15	113.76

There are no chirality outliers.

All (166) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	401	HEM	C1A-C2A-CAA-CBA
12	A	401	HEM	C3A-C2A-CAA-CBA
12	A	402	HEM	C1A-C2A-CAA-CBA
12	A	402	HEM	C3A-C2A-CAA-CBA
12	A	402	HEM	C2A-CAA-CBA-CGA
12	A	402	HEM	C2D-C3D-CAD-CBD
12	A	402	HEM	C4D-C3D-CAD-CBD
12	a	401	HEM	C1A-C2A-CAA-CBA
12	a	401	HEM	C3A-C2A-CAA-CBA
12	a	401	HEM	C3D-CAD-CBD-CGD
13	A	403	PEE	C17-C18-C19-C20
13	A	403	PEE	C1-O3P-P-O2P
13	A	403	PEE	C1-O3P-P-O1P
13	A	403	PEE	C4-O4P-P-O1P
13	A	403	PEE	O4P-C4-C5-N
13	A	403	PEE	C38-C39-C40-C41
13	D	502	PEE	C37-C38-C39-C40
13	a	403	PEE	C4-O4P-P-O3P
13	a	403	PEE	C4-O4P-P-O2P
13	a	403	PEE	C4-O4P-P-O1P
14	B	401	HEC	C2D-C3D-CAD-CBD
14	B	401	HEC	C4D-C3D-CAD-CBD
16	D	501	CDL	CA2-C1-CB2-OB2
16	D	501	CDL	OA6-CA4-CA6-OA8
16	D	501	CDL	C11-CA5-OA6-CA4
16	D	501	CDL	CB2-OB2-PB2-OB3
16	D	501	CDL	CB2-OB2-PB2-OB4
16	D	501	CDL	CB2-OB2-PB2-OB5
16	D	501	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
16	D	501	CDL	CB3-OB5-PB2-OB4
16	D	501	CDL	OB5-CB3-CB4-OB6
16	a	404	CDL	CB2-C1-CA2-OA2
16	a	404	CDL	C11-CA5-OA6-CA4
16	a	404	CDL	CB2-OB2-PB2-OB3
13	A	403	PEE	O5-C30-O3-C3
16	D	501	CDL	OA7-CA5-OA6-CA4
16	a	404	CDL	OA7-CA5-OA6-CA4
13	A	403	PEE	C31-C30-O3-C3
16	D	501	CDL	C31-CA7-OA8-CA6
16	D	501	CDL	C71-CB7-OB8-CB6
12	A	401	HEM	C4D-C3D-CAD-CBD
16	D	501	CDL	OA9-CA7-OA8-CA6
16	D	501	CDL	OB9-CB7-OB8-CB6
16	D	501	CDL	O1-C1-CB2-OB2
16	a	404	CDL	O1-C1-CA2-OA2
16	a	404	CDL	C31-CA7-OA8-CA6
16	a	404	CDL	C71-CB7-OB8-CB6
16	D	501	CDL	CB7-C71-C72-C73
13	a	403	PEE	C30-C31-C32-C33
16	D	501	CDL	CB5-C51-C52-C53
16	a	404	CDL	OA9-CA7-OA8-CA6
12	A	401	HEM	C2D-C3D-CAD-CBD
13	A	403	PEE	C1-O3P-P-O4P
13	D	502	PEE	C1-O3P-P-O4P
16	D	501	CDL	CB3-OB5-PB2-OB2
16	a	404	CDL	CA3-OA5-PA1-OA2
13	D	502	PEE	C10-C11-C12-C13
16	D	501	CDL	C32-C33-C34-C35
13	D	502	PEE	C21-C22-C23-C24
13	D	502	PEE	C40-C41-C42-C43
16	D	501	CDL	C74-C75-C76-C77
13	D	502	PEE	C11-C12-C13-C14
13	a	403	PEE	C37-C38-C39-C40
13	A	403	PEE	C12-C13-C14-C15
13	a	403	PEE	C33-C34-C35-C36
16	a	404	CDL	OB9-CB7-OB8-CB6
16	a	404	CDL	C14-C15-C16-C17
13	a	403	PEE	C34-C35-C36-C37
13	A	403	PEE	C14-C15-C16-C17
13	D	502	PEE	C34-C35-C36-C37
13	D	502	PEE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
16	a	404	CDL	C74-C75-C76-C77
13	D	502	PEE	C22-C23-C24-C25
13	A	403	PEE	C19-C20-C21-C22
13	D	502	PEE	C23-C24-C25-C26
16	a	404	CDL	C54-C55-C56-C57
12	A	402	HEM	C3D-CAD-CBD-CGD
16	D	501	CDL	C11-C12-C13-C14
13	a	403	PEE	C39-C40-C41-C42
13	a	403	PEE	C22-C23-C24-C25
16	a	404	CDL	C72-C73-C74-C75
16	a	404	CDL	C51-C52-C53-C54
16	a	404	CDL	C32-C33-C34-C35
16	a	404	CDL	C52-C53-C54-C55
13	D	502	PEE	C15-C16-C17-C18
12	a	402	HEM	C4D-C3D-CAD-CBD
16	D	501	CDL	C71-C72-C73-C74
13	A	403	PEE	C30-C31-C32-C33
16	D	501	CDL	OB5-CB3-CB4-CB6
13	a	403	PEE	C11-C12-C13-C14
16	D	501	CDL	C73-C74-C75-C76
13	D	502	PEE	C13-C14-C15-C16
13	a	403	PEE	C1-C2-C3-O3
16	D	501	CDL	C13-C14-C15-C16
13	a	403	PEE	C35-C36-C37-C38
16	D	501	CDL	C51-C52-C53-C54
13	A	403	PEE	C23-C24-C25-C26
12	a	402	HEM	C2D-C3D-CAD-CBD
16	a	404	CDL	O1-C1-CB2-OB2
16	D	501	CDL	C12-C13-C14-C15
16	a	404	CDL	C12-C13-C14-C15
16	a	404	CDL	C75-C76-C77-C78
13	A	403	PEE	C4-O4P-P-O3P
13	D	502	PEE	C32-C33-C34-C35
13	A	403	PEE	O2-C2-C3-O3
13	D	502	PEE	C42-C43-C44-C45
12	A	401	HEM	C3D-CAD-CBD-CGD
16	a	404	CDL	OB5-CB3-CB4-CB6
13	D	502	PEE	C39-C40-C41-C42
13	a	403	PEE	C32-C33-C34-C35
13	a	403	PEE	C42-C43-C44-C45
13	A	403	PEE	C1-C2-C3-O3
16	D	501	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
16	a	404	CDL	OB5-CB3-CB4-OB6
13	a	403	PEE	C41-C42-C43-C44
13	A	403	PEE	C15-C16-C17-C18
13	A	403	PEE	C2-C3-O3-C30
13	a	403	PEE	C13-C14-C15-C16
16	D	501	CDL	CB4-CB3-OB5-PB2
13	A	403	PEE	C4-O4P-P-O2P
13	D	502	PEE	C1-O3P-P-O2P
16	a	404	CDL	CA3-OA5-PA1-OA3
16	a	404	CDL	CA3-OA5-PA1-OA4
16	a	404	CDL	CB3-OB5-PB2-OB4
16	a	404	CDL	CA5-C11-C12-C13
13	a	403	PEE	C5-C4-O4P-P
16	a	404	CDL	OA5-CA3-CA4-OA6
13	a	403	PEE	C40-C41-C42-C43
13	a	403	PEE	O2-C2-C3-O3
13	A	403	PEE	C31-C32-C33-C34
16	D	501	CDL	C75-C76-C77-C78
16	a	404	CDL	OA5-CA3-CA4-CA6
16	a	404	CDL	C31-C32-C33-C34
16	D	501	CDL	CA2-OA2-PA1-OA5
16	D	501	CDL	CA3-OA5-PA1-OA2
16	a	404	CDL	CA2-OA2-PA1-OA5
16	a	404	CDL	CB2-OB2-PB2-OB5
12	a	402	HEM	CAD-CBD-CGD-O2D
16	a	404	CDL	OB6-CB4-CB6-OB8
16	D	501	CDL	C15-C16-C17-C18
16	a	404	CDL	CA2-C1-CB2-OB2
12	A	401	HEM	CAD-CBD-CGD-O1D
12	a	402	HEM	CAD-CBD-CGD-O1D
16	a	404	CDL	C71-C72-C73-C74
13	D	502	PEE	C38-C39-C40-C41
13	a	403	PEE	C14-C15-C16-C17
13	a	403	PEE	C38-C39-C40-C41
13	A	403	PEE	C22-C23-C24-C25
14	b	401	HEC	CAD-CBD-CGD-O2D
13	A	403	PEE	C36-C37-C38-C39
13	a	403	PEE	C18-C19-C20-C21
12	A	401	HEM	CAD-CBD-CGD-O2D
13	a	403	PEE	C36-C37-C38-C39
14	b	401	HEC	CAD-CBD-CGD-O1D
16	D	501	CDL	C54-C55-C56-C57

*Continued on next page...*

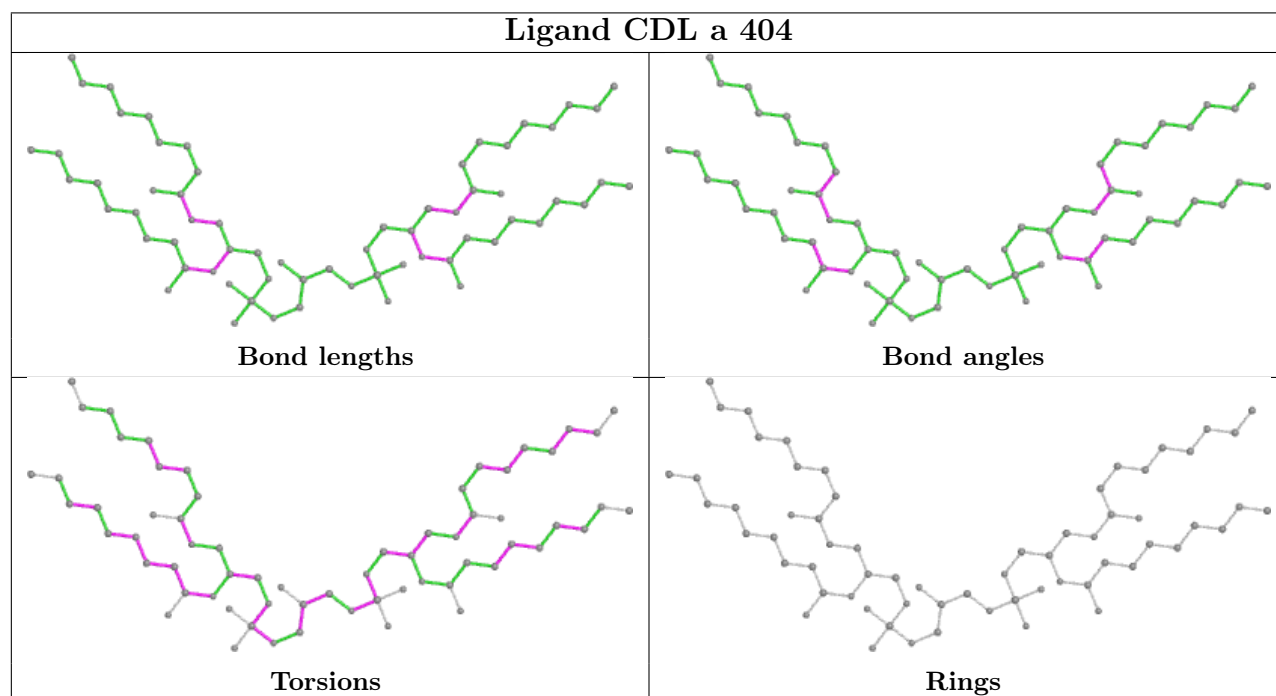
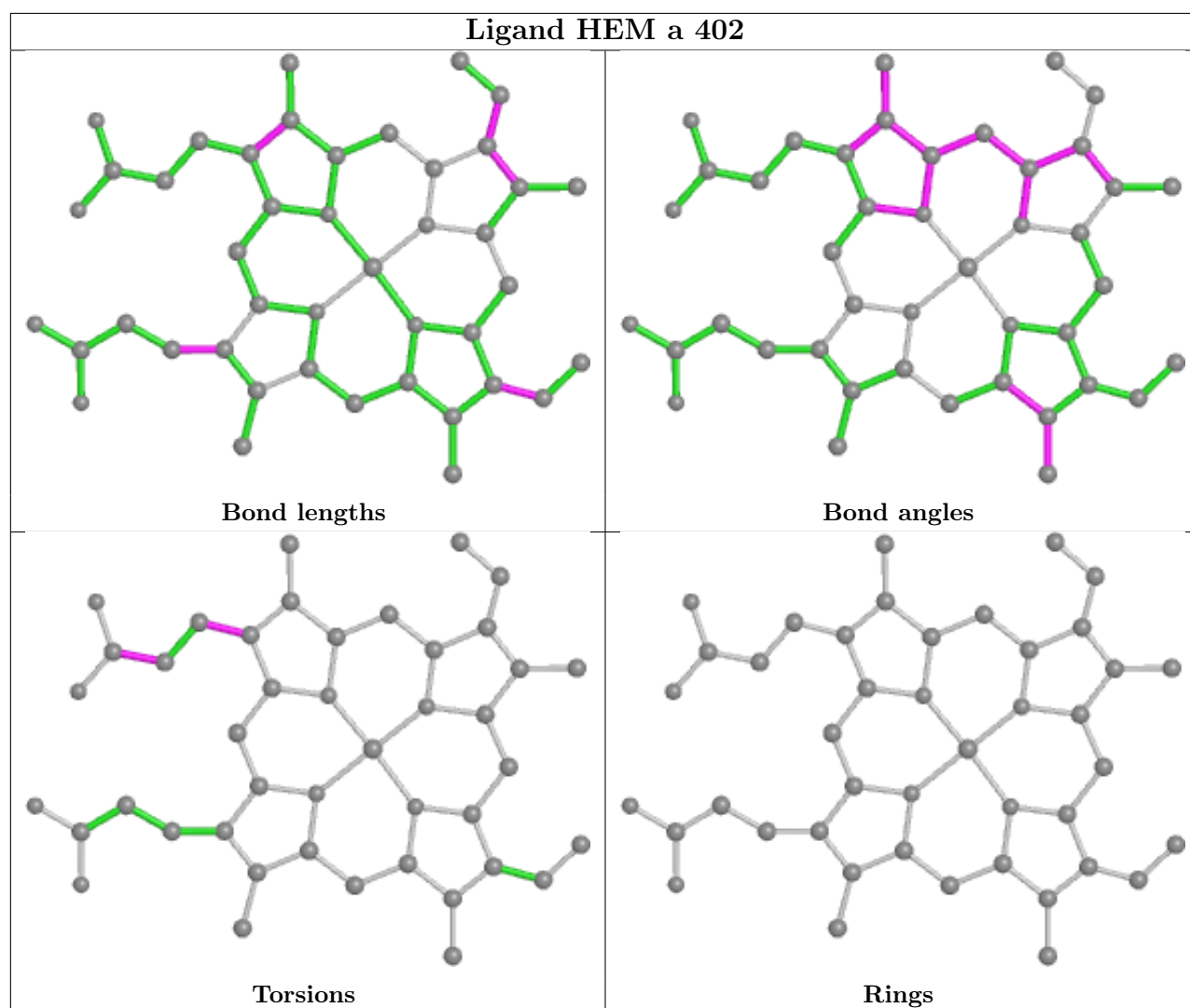
*Continued from previous page...*

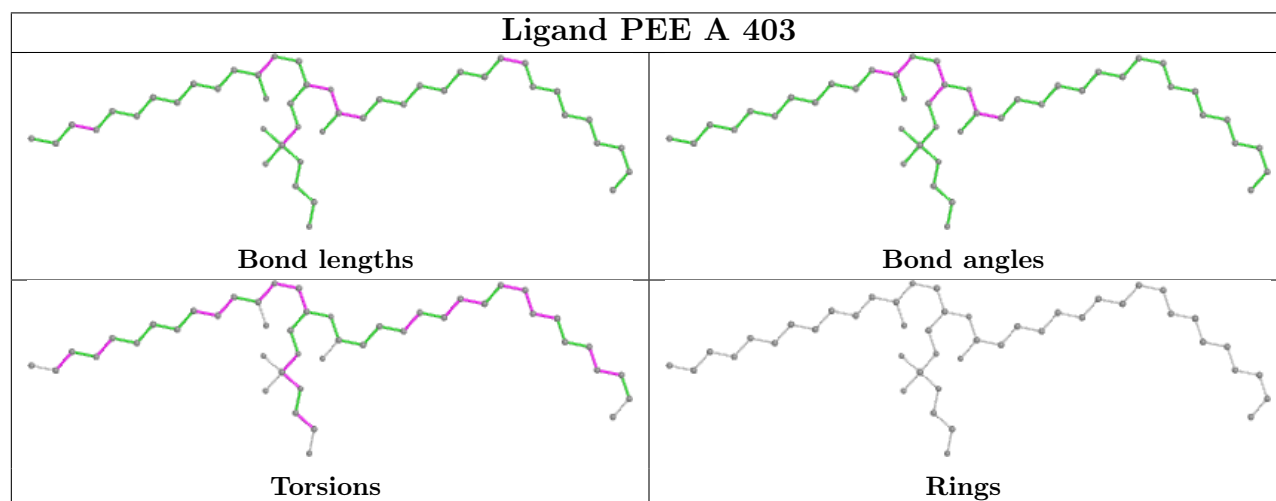
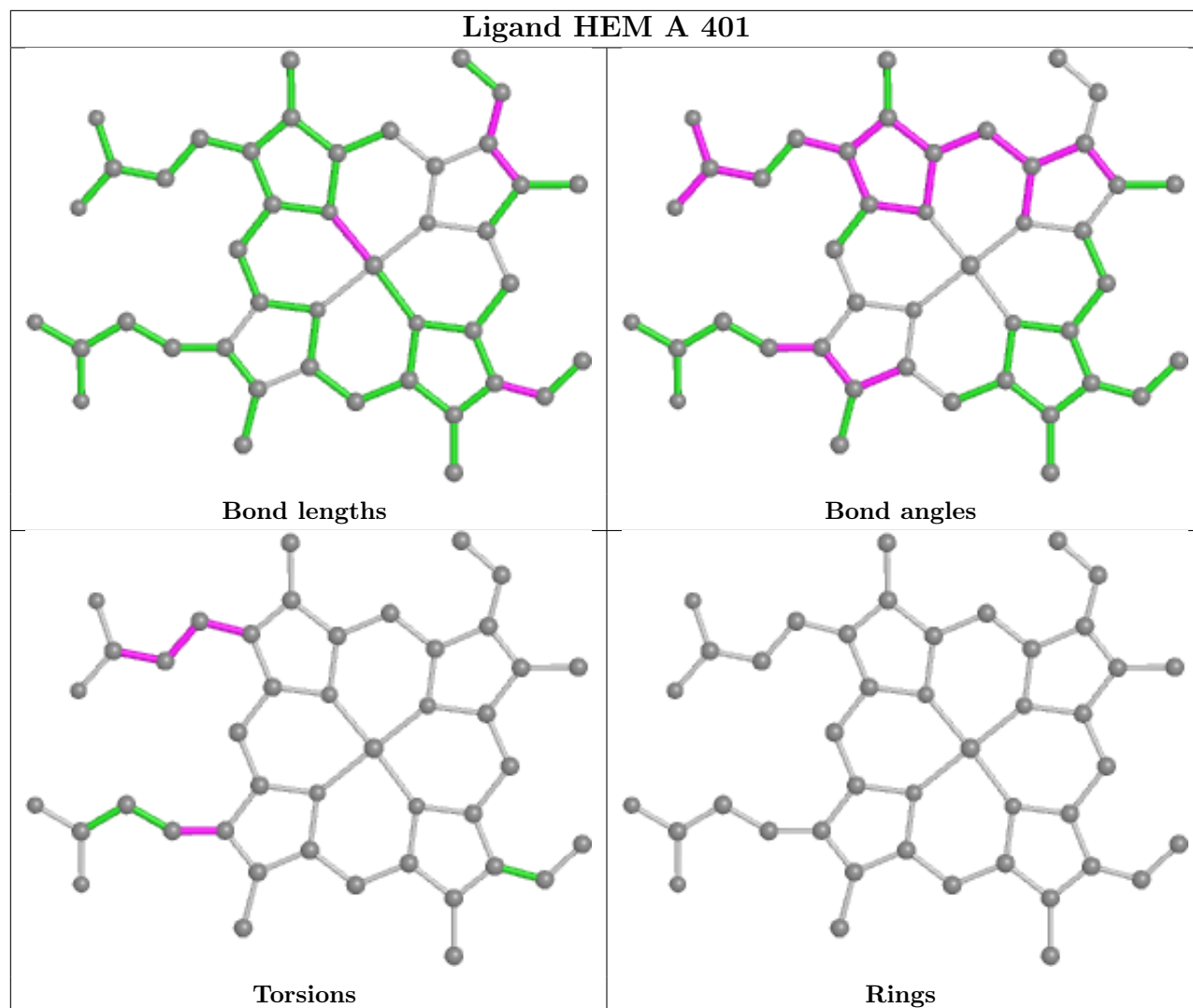
Mol	Chain	Res	Type	Atoms
16	D	501	CDL	OB6-CB4-CB6-OB8
16	D	501	CDL	CB3-CB4-CB6-OB8
16	a	404	CDL	CB3-OB5-PB2-OB2
14	b	401	HEC	CAA-CBA-CGA-O2A
16	a	404	CDL	CA2-OA2-PA1-OA3
16	a	404	CDL	C11-C12-C13-C14
12	a	401	HEM	CAD-CBD-CGD-O2D
12	A	402	HEM	CAD-CBD-CGD-O1D
16	a	404	CDL	C12-C11-CA5-OA6
13	A	403	PEE	C18-C19-C20-C21
12	A	402	HEM	CAD-CBD-CGD-O2D

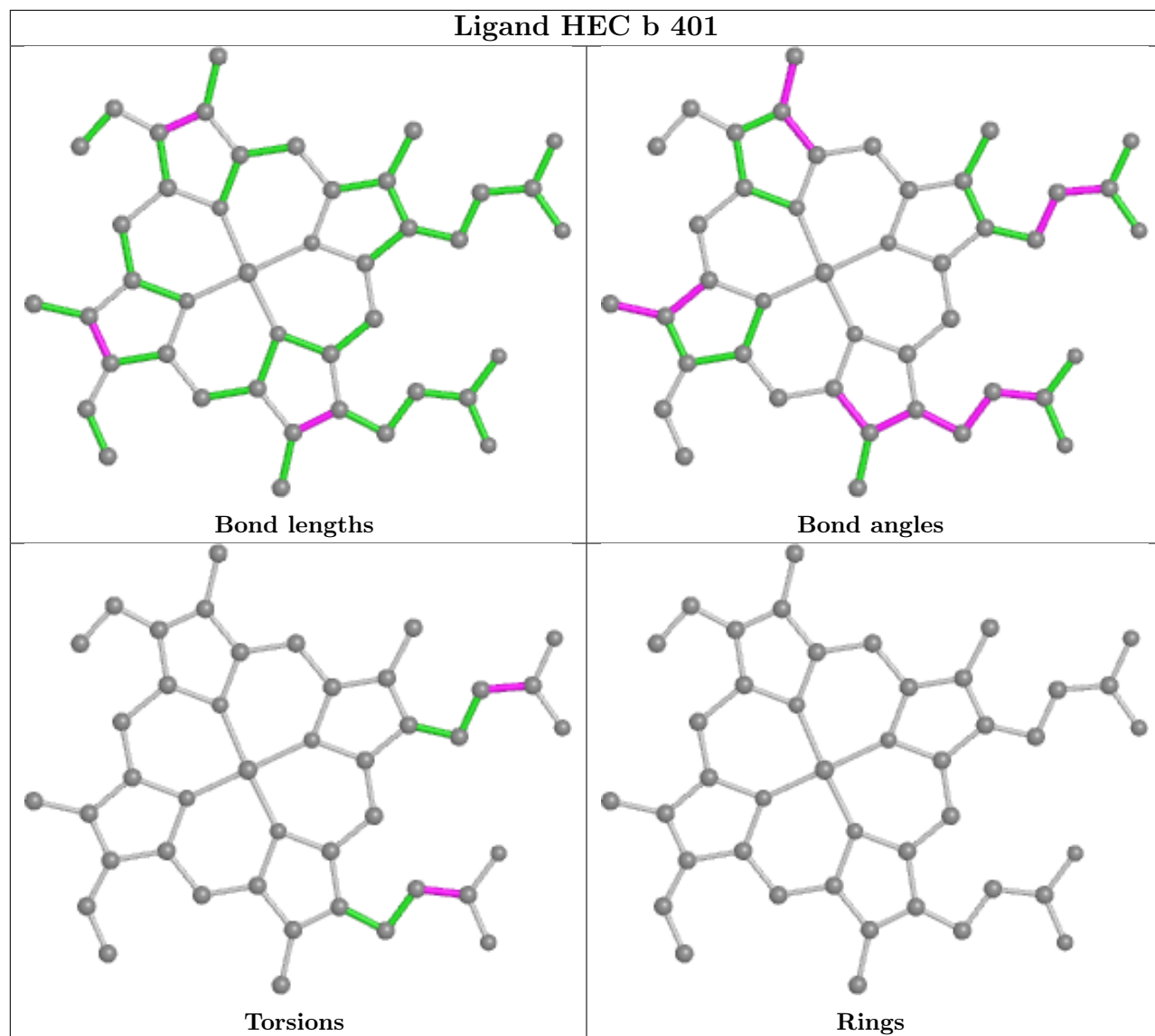
There are no ring outliers.

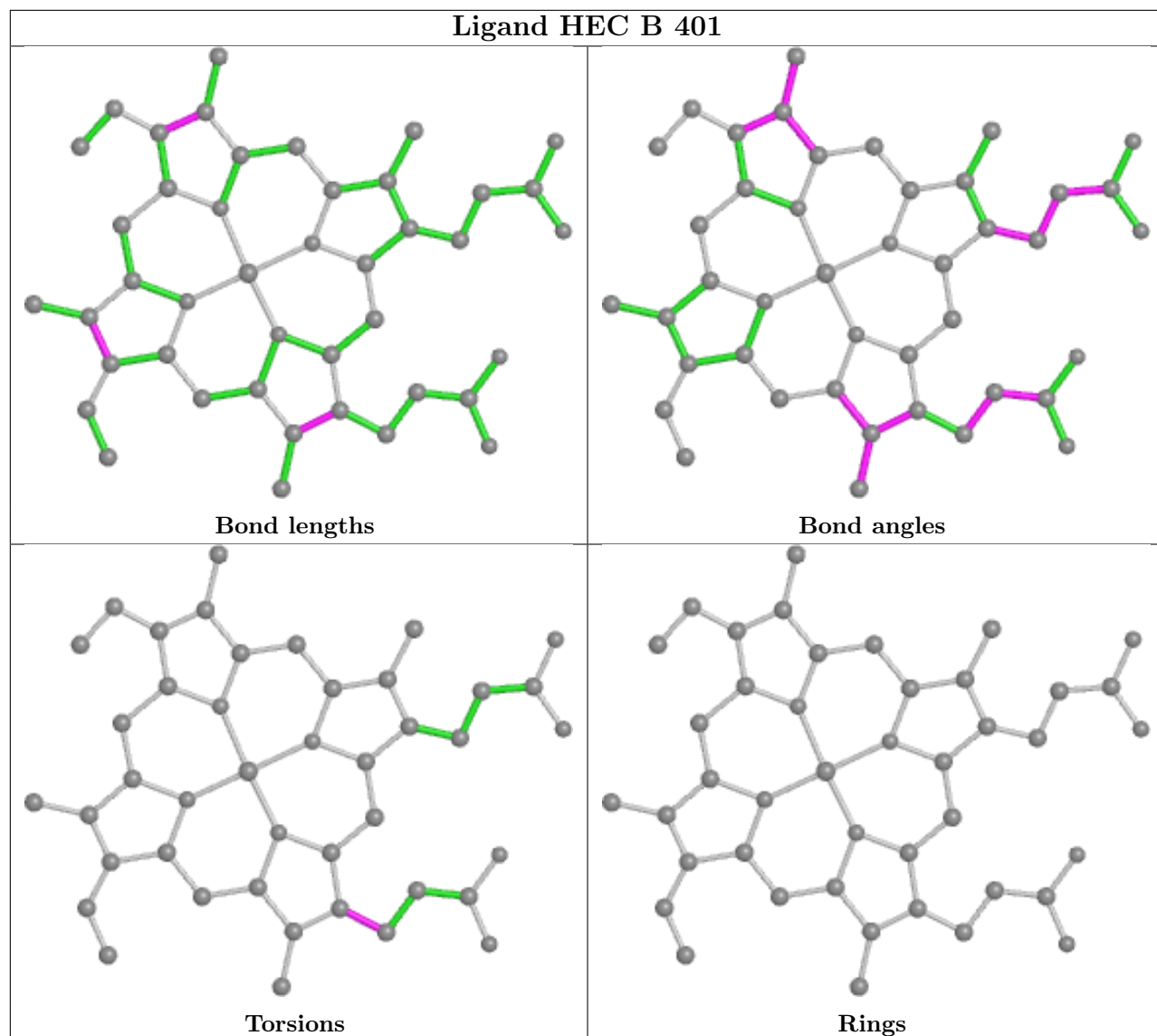
No monomer is involved in short contacts.

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

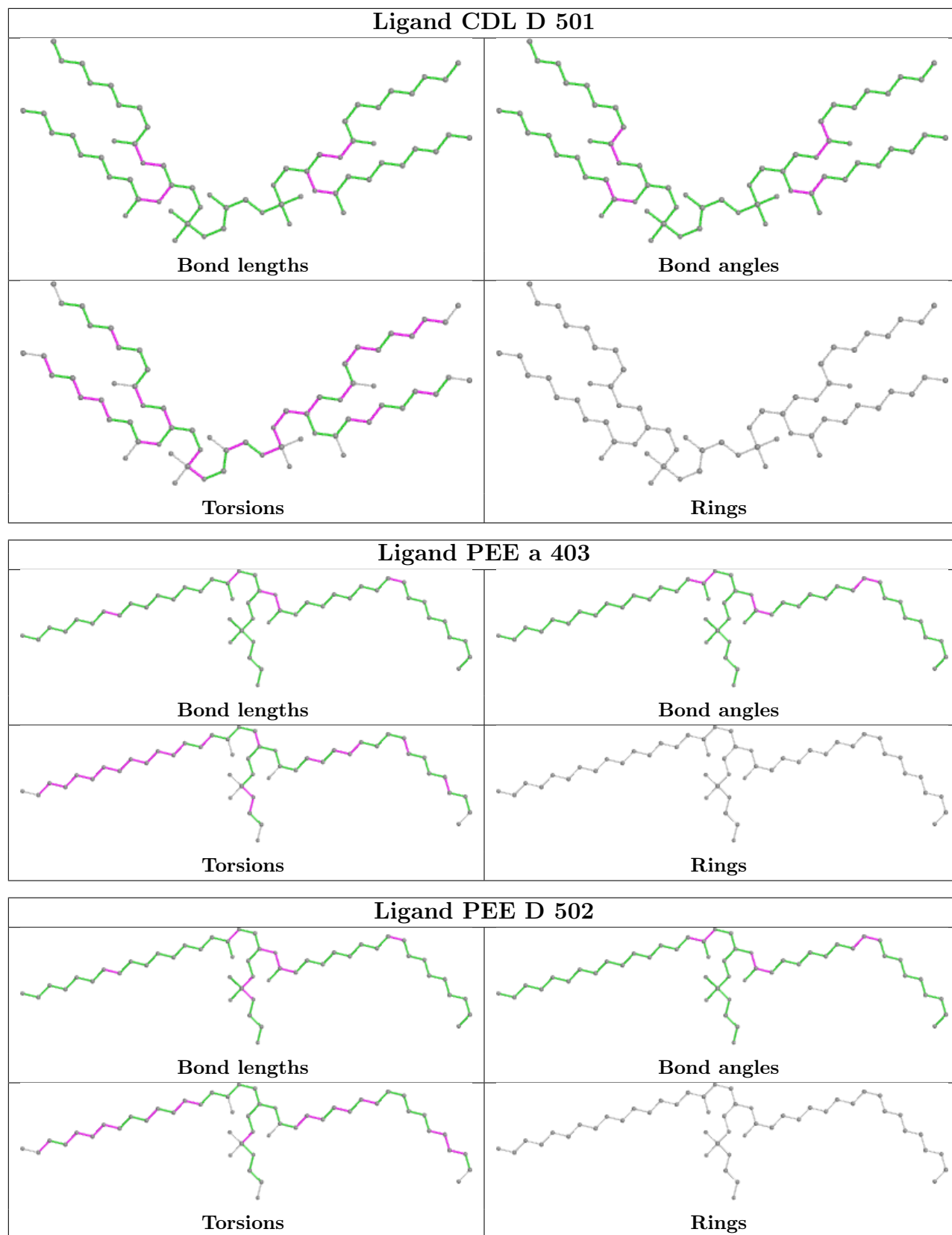


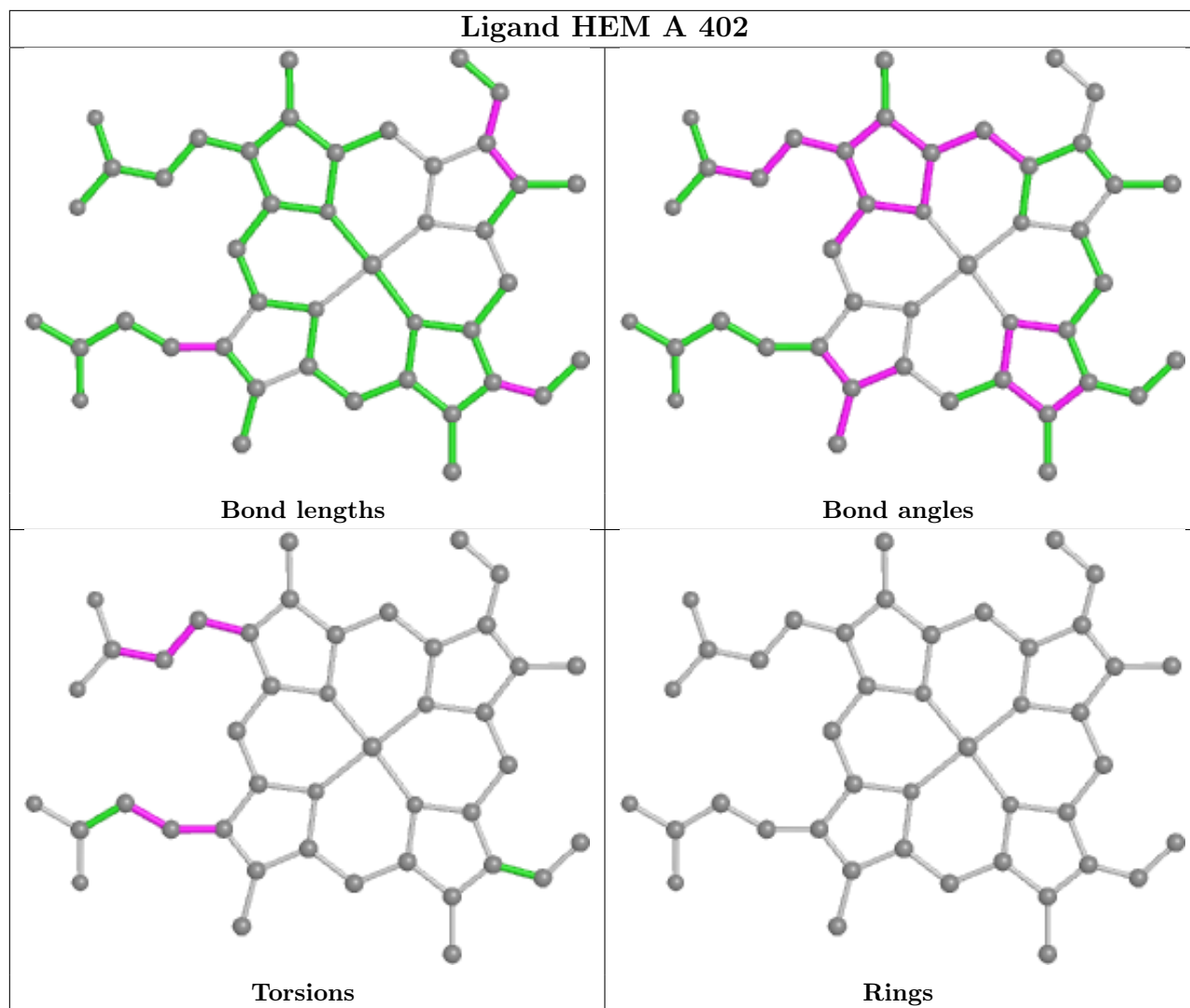


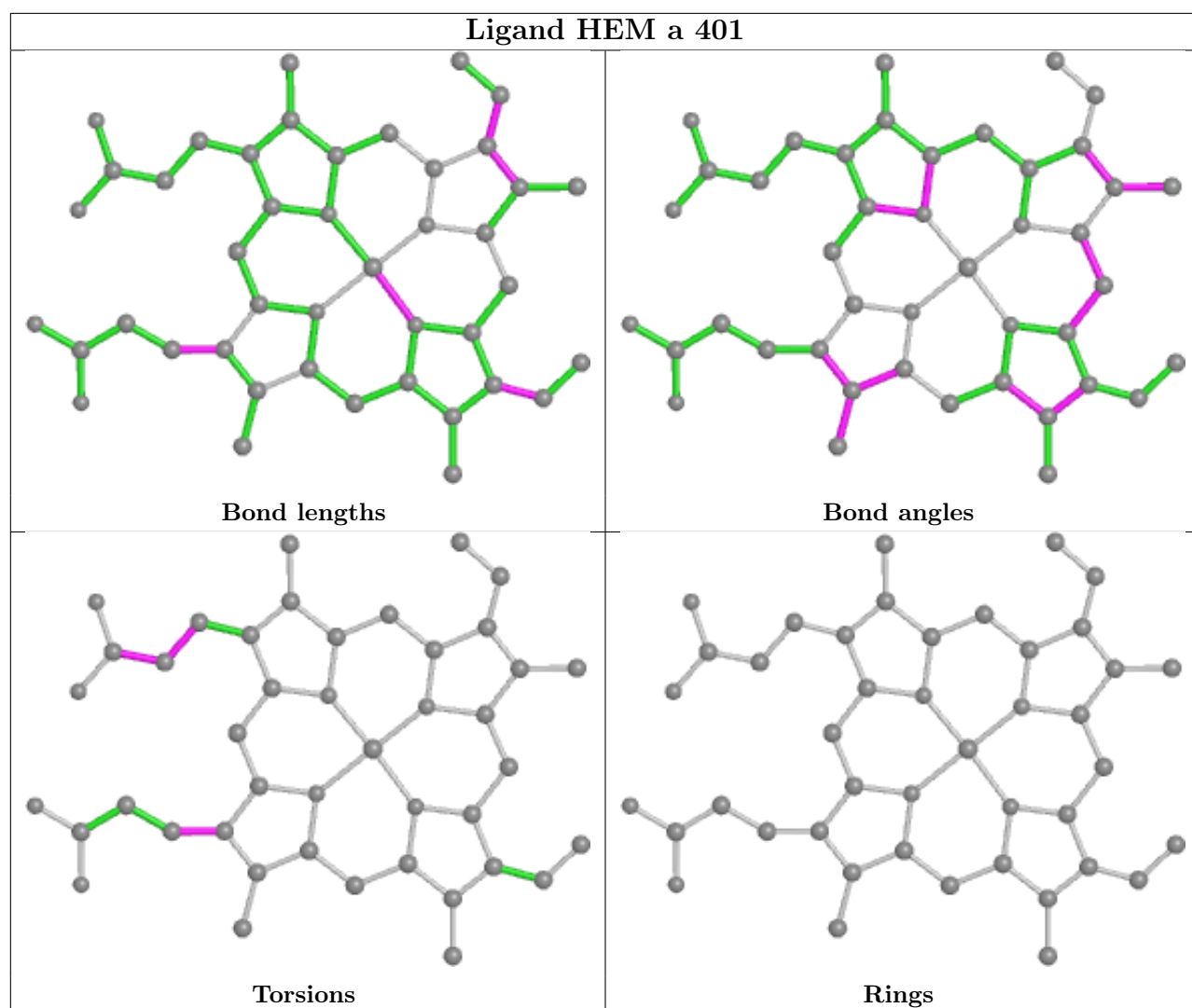












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

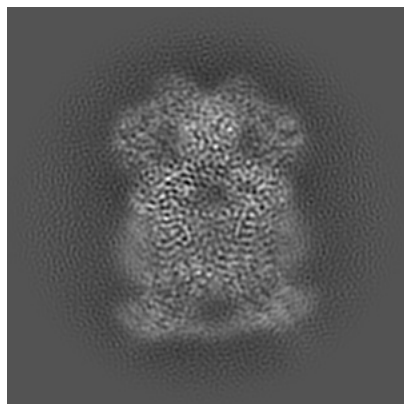
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35618. These allow visual inspection of the internal detail of the map and identification of artifacts.

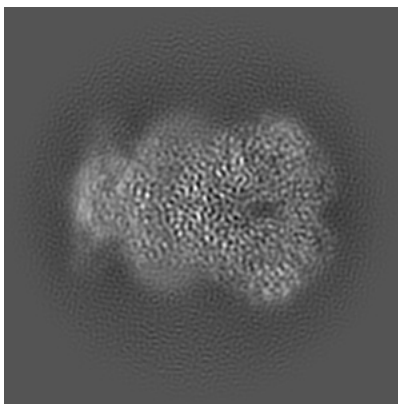
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

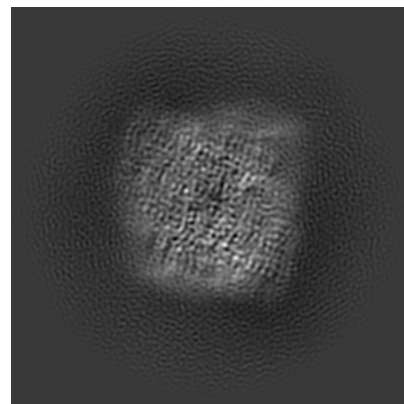
#### 6.1.1 Primary map



X

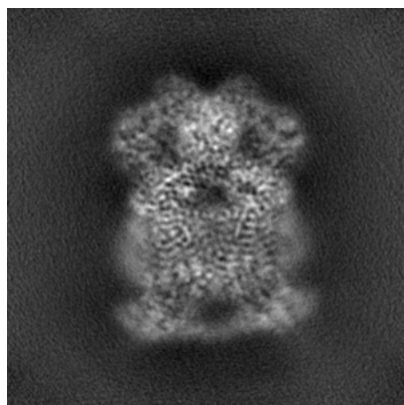


Y

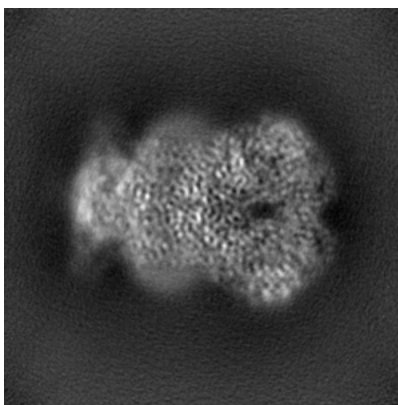


Z

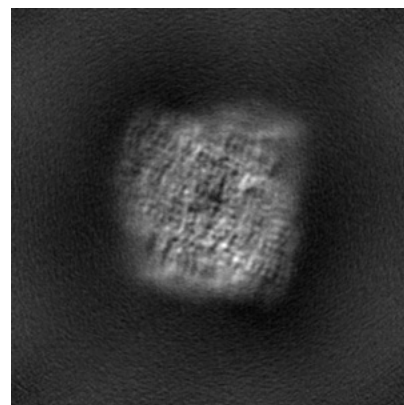
#### 6.1.2 Raw map



X



Y

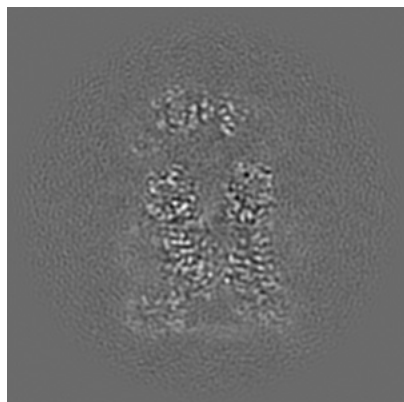


Z

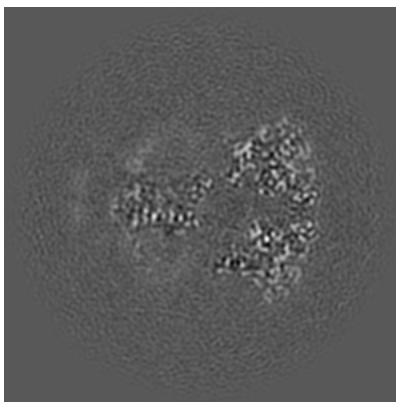
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

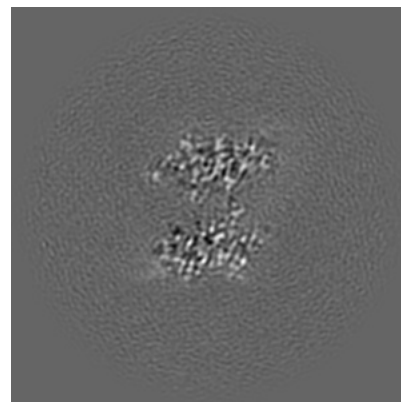
### 6.2.1 Primary map



X Index: 140

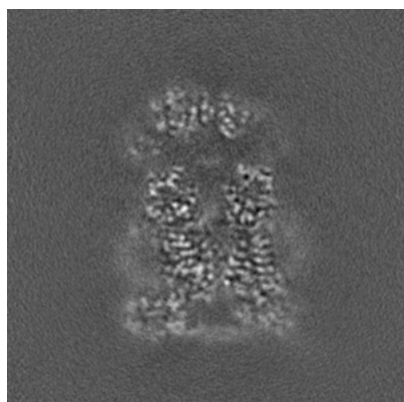


Y Index: 140

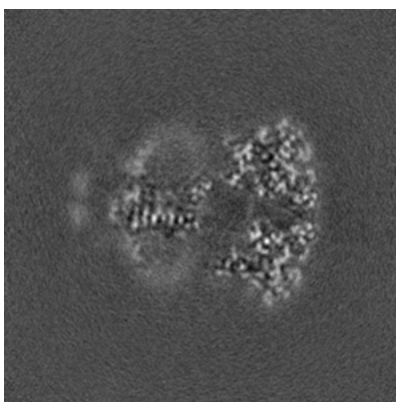


Z Index: 140

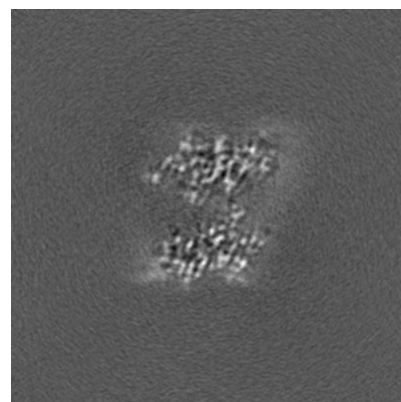
### 6.2.2 Raw map



X Index: 140



Y Index: 140

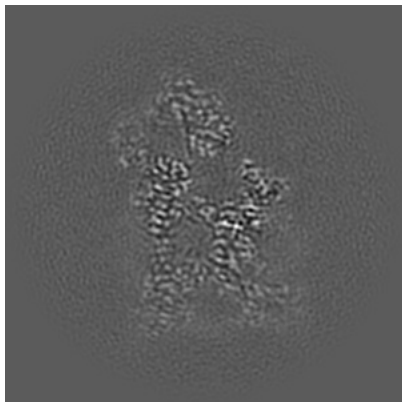


Z Index: 140

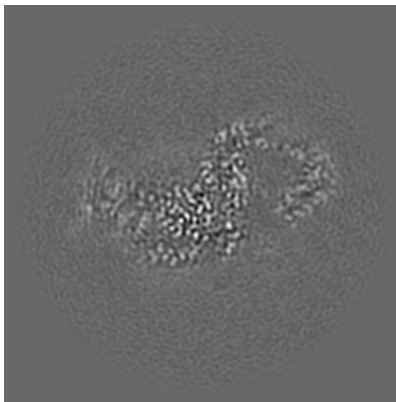
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

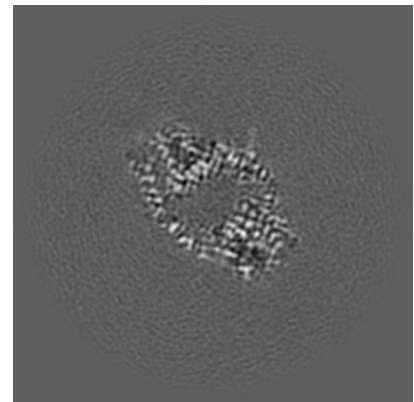
### 6.3.1 Primary map



X Index: 153

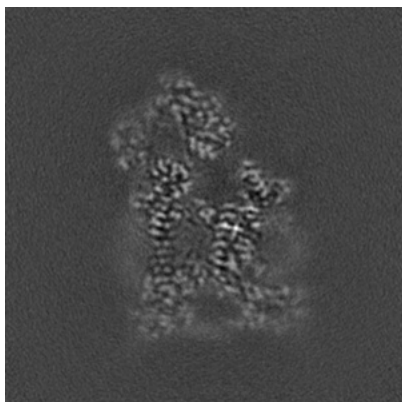


Y Index: 117

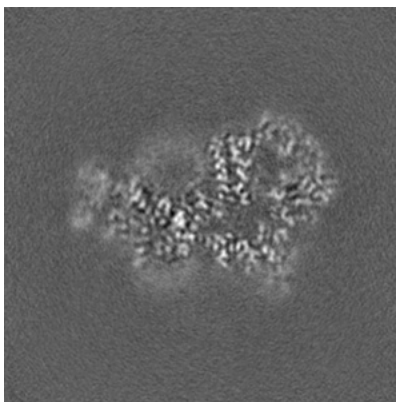


Z Index: 164

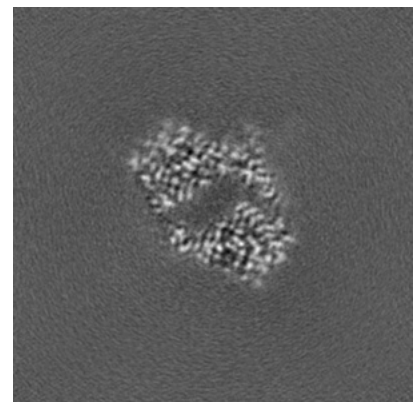
### 6.3.2 Raw map



X Index: 153



Y Index: 125



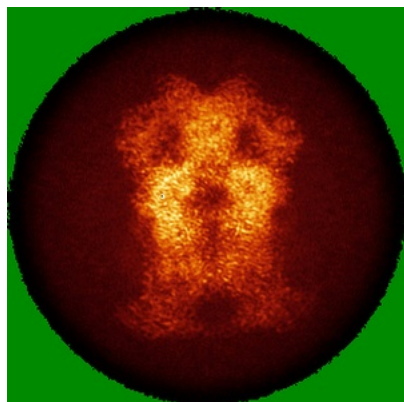
Z Index: 160

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

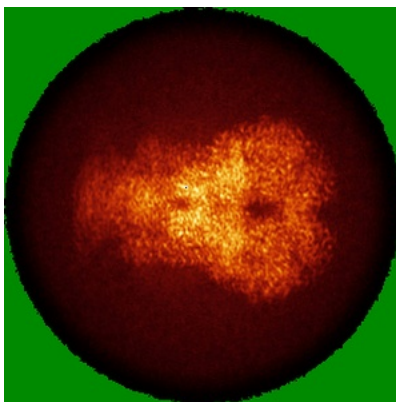


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

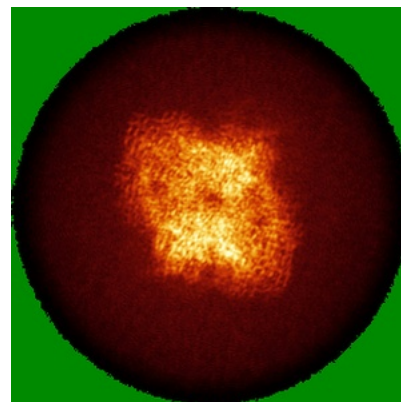
### 6.4.1 Primary map



X

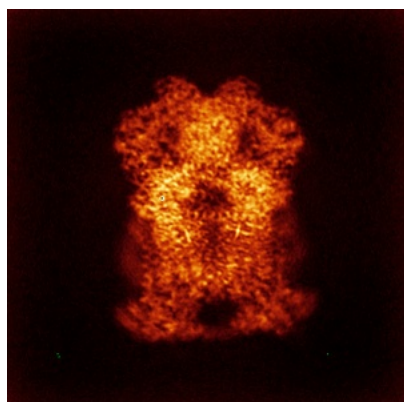


Y

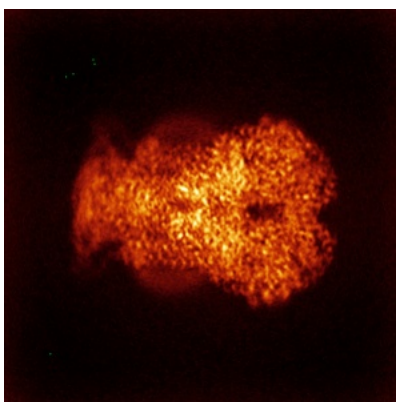


Z

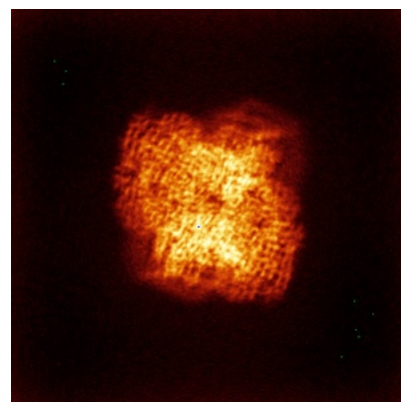
### 6.4.2 Raw map



X



Y

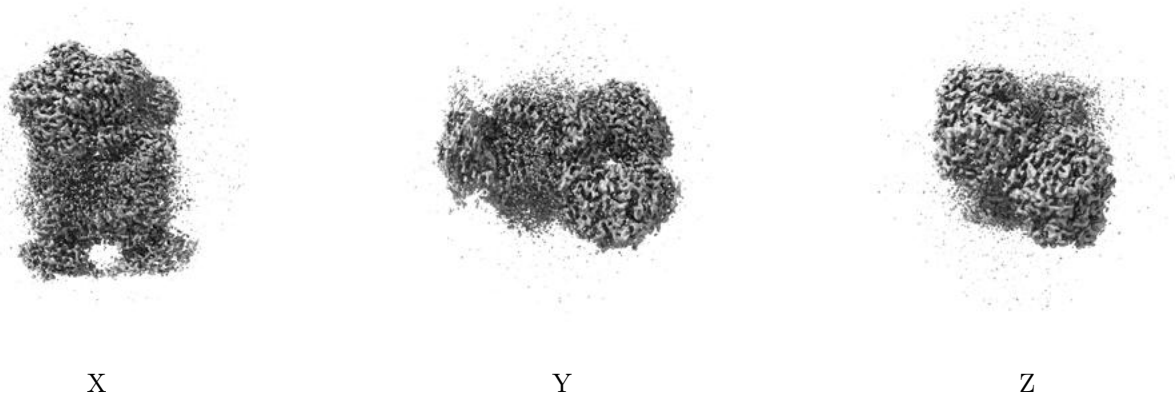


Z

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.

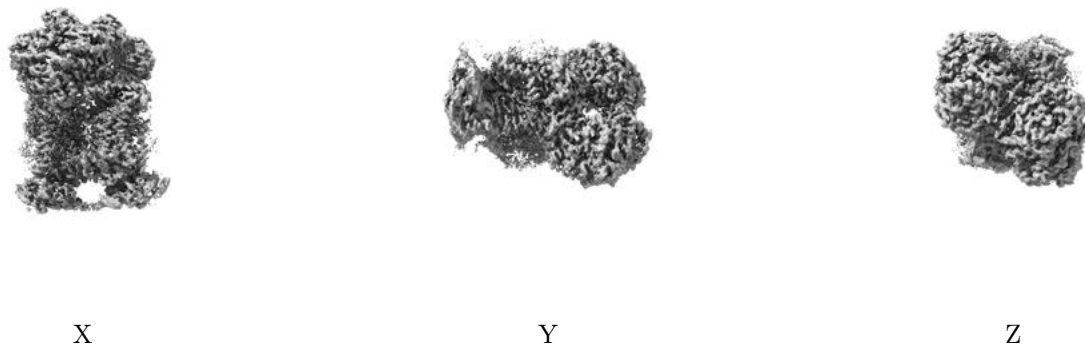
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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



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](#)

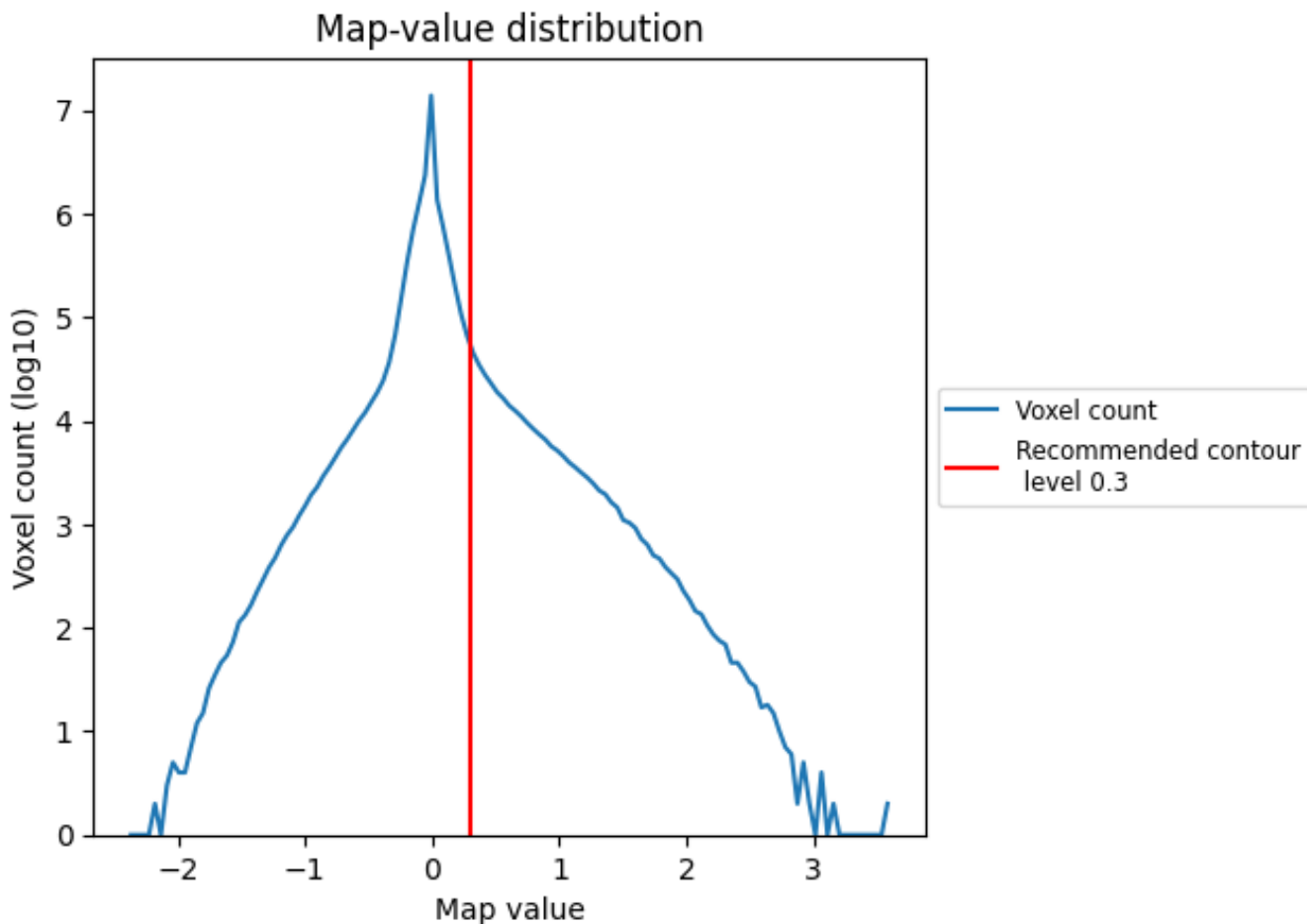
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

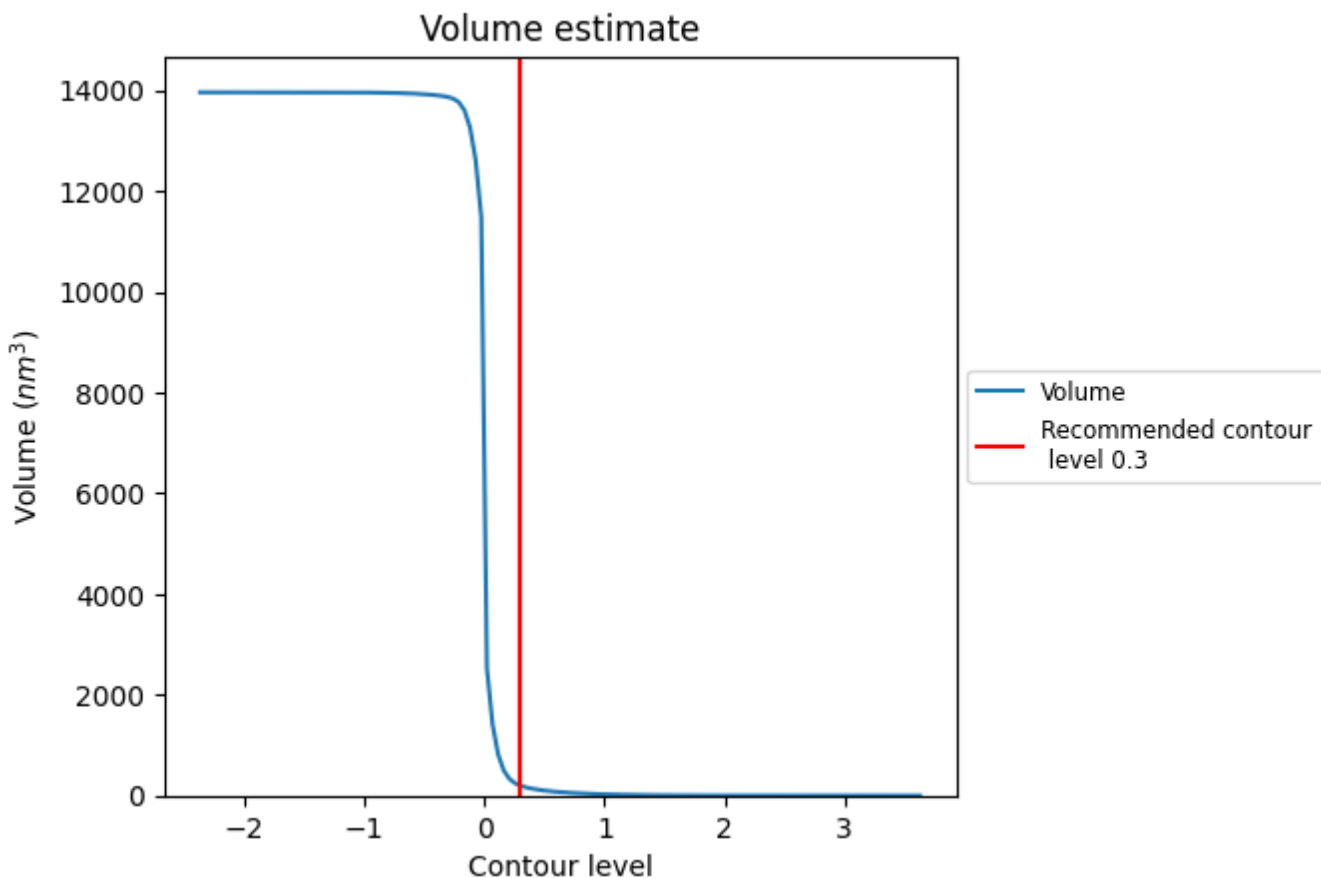
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

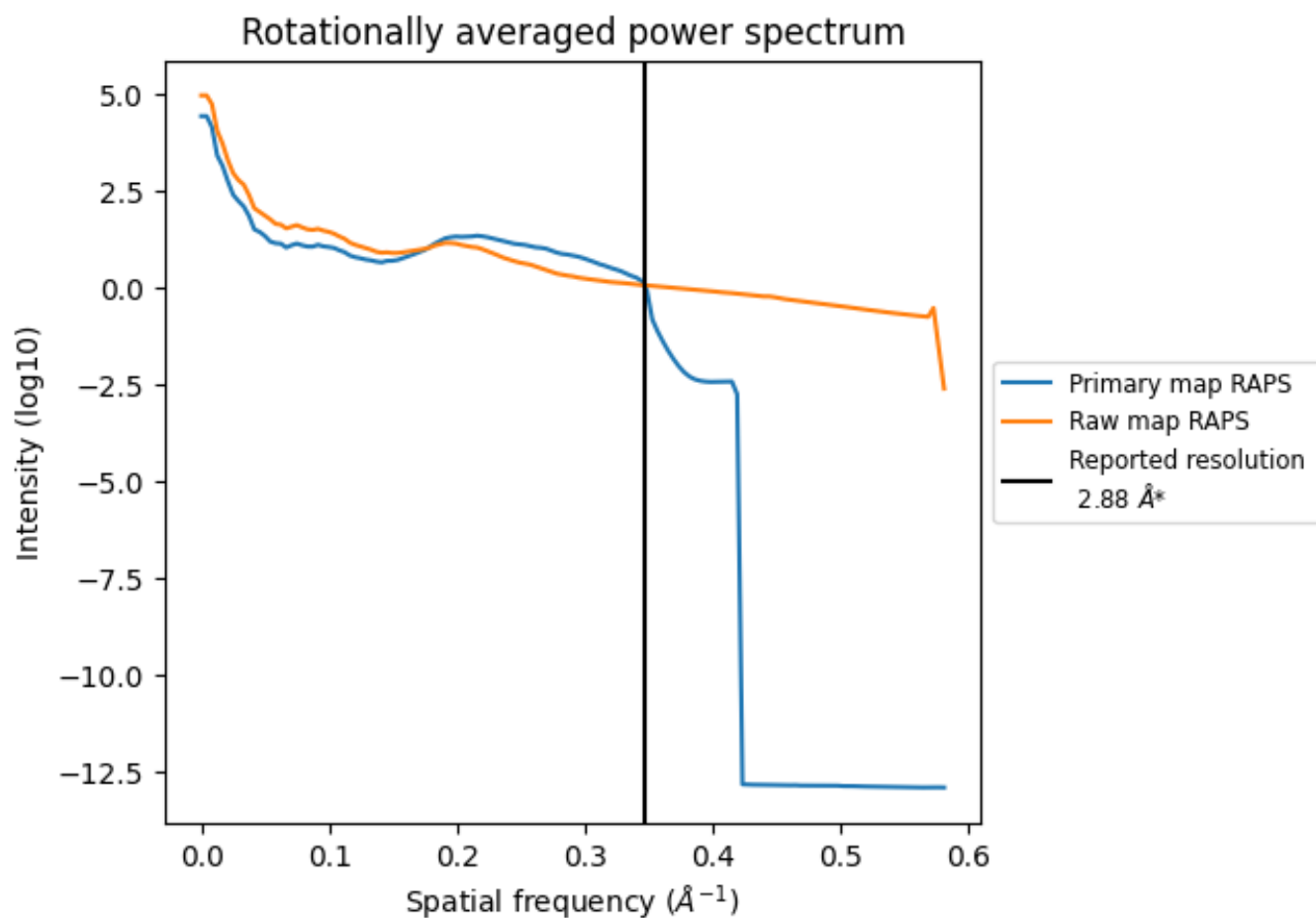
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 196 nm<sup>3</sup>; this corresponds to an approximate mass of 177 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](#)

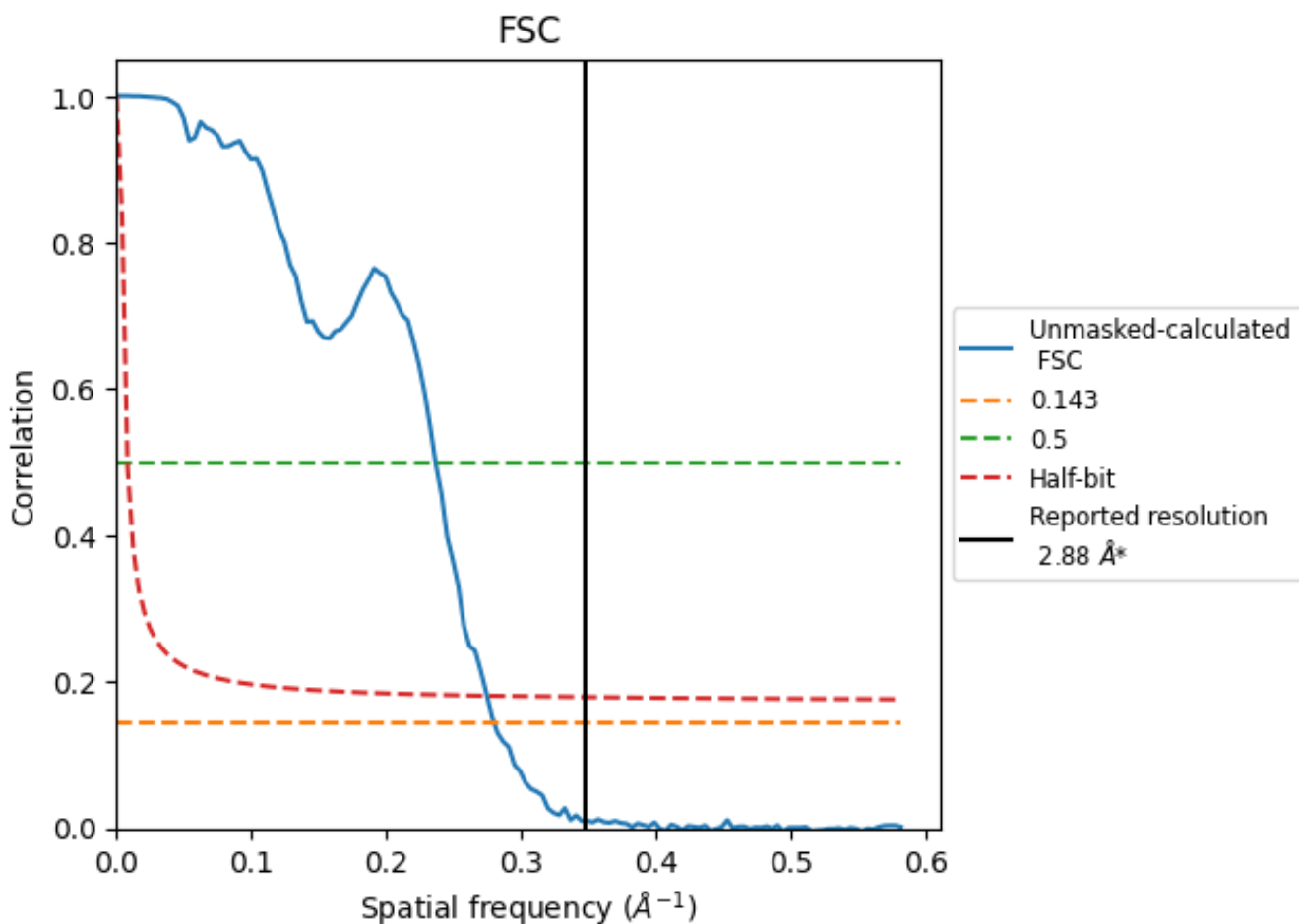


\*Reported resolution corresponds to spatial frequency of 0.347 Å<sup>-1</sup>

## 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 0.347 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

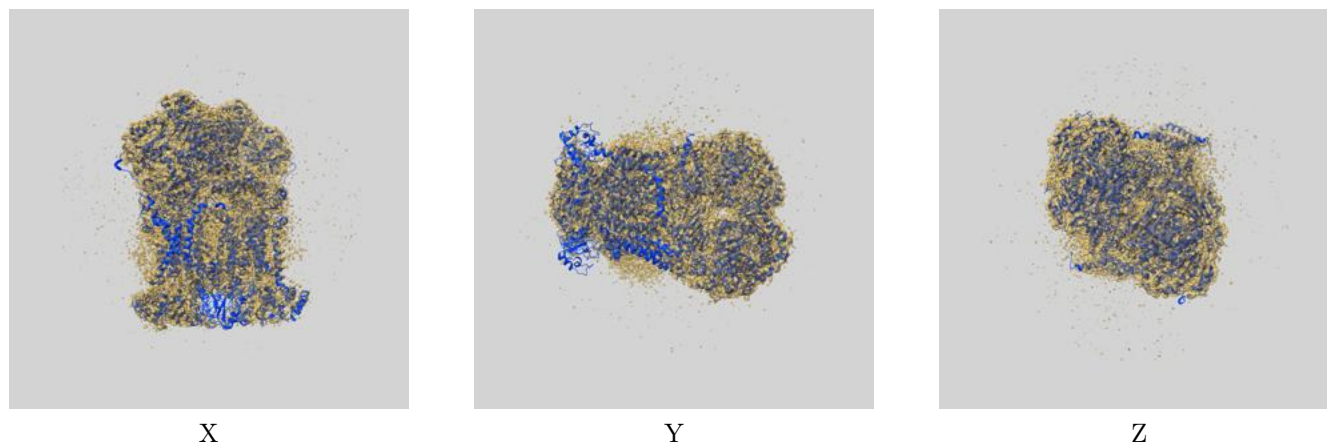
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.57	4.23	3.64

\*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 3.57 differs from the reported value 2.88 by more than 10 %

## 9 Map-model fit [i](#)

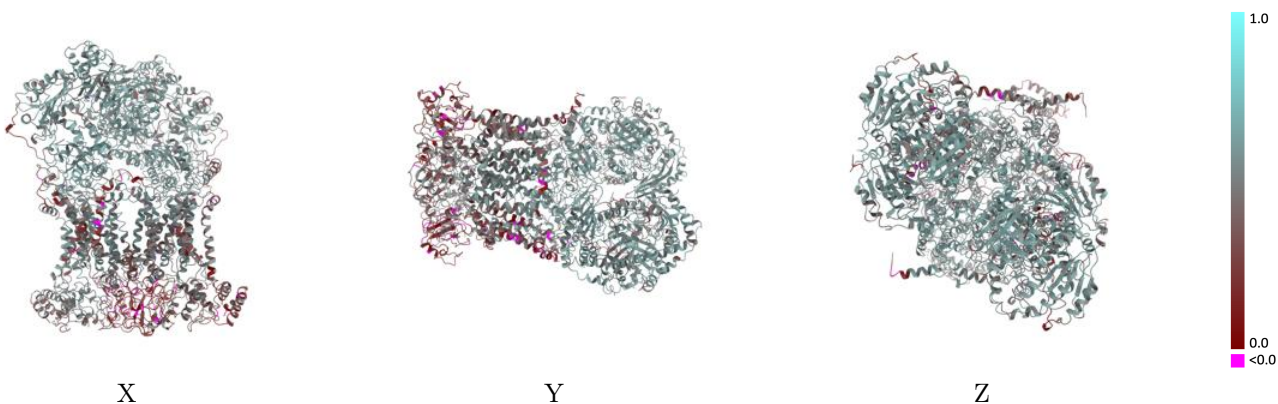
This section contains information regarding the fit between EMDB map EMD-35618 and PDB model 8IOG. Per-residue inclusion information can be found in section 3 on page 10.

### 9.1 Map-model overlay [i](#)



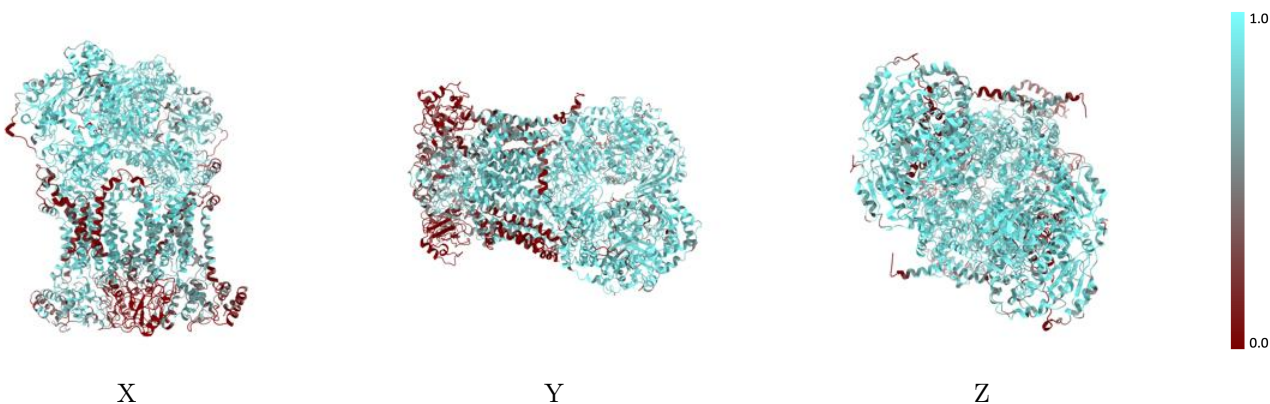
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



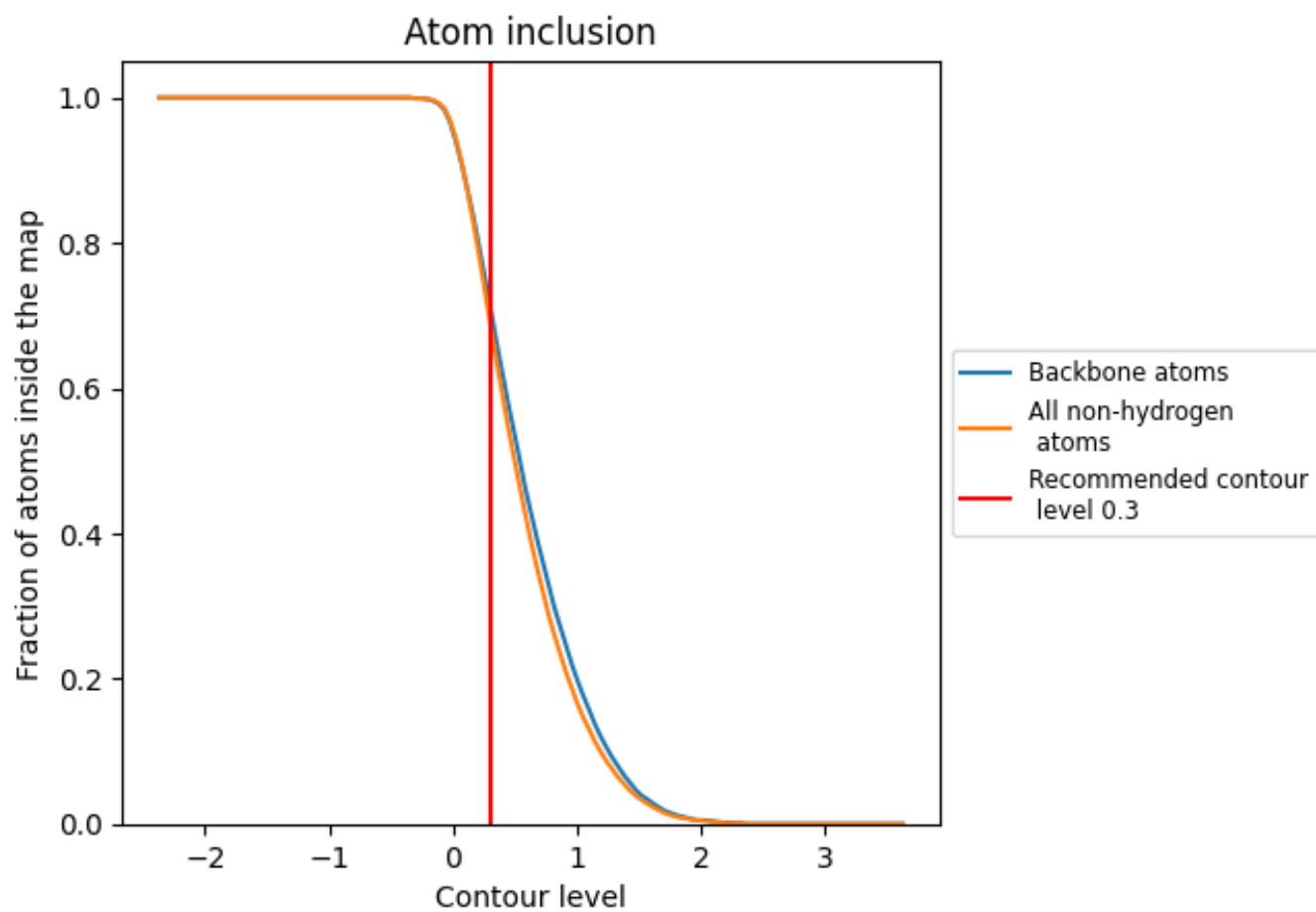
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

## 9.4 Atom inclusion [i](#)

















































At the recommended contour level, 71% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6880	 0.4770
A	 0.8720	 0.5310
B	 0.6660	 0.4620
C	 0.1280	 0.2640
D	 0.8340	 0.5480
E	 0.8810	 0.5630
F	 0.4340	 0.3910
G	 0.8770	 0.5590
H	 0.7710	 0.5100
I	 0.3130	 0.3820
J	 0.0360	 0.2290
K	 0.4540	 0.3630
a	 0.8170	 0.5000
b	 0.6050	 0.4310
c	 0.0930	 0.2300
d	 0.8480	 0.5490
e	 0.8870	 0.5660
f	 0.2460	 0.3040
g	 0.8050	 0.5230
h	 0.4910	 0.4020
i	 0.2080	 0.3260
j	 0.0250	 0.1960
k	 0.4090	 0.3600

