



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 09:25 PM UTC

PDB ID : 9W2X / pdb_00009w2x
EMDB ID : EMD-65583
Title : Cryo-EM structure of complex III on the bovine heart submitochondrial particles, III-1
Authors : Nakano, A.; Masuya, T.; Akisada, S.; Ishikawa-Fukuda, M.; Mitsuoka, K.; Miyoshi, H.; Murai, M.; Yokoyama, K.
Deposited on : 2025-07-28
Resolution : 2.20 Å (reported)
Based on initial model : 1SQB

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

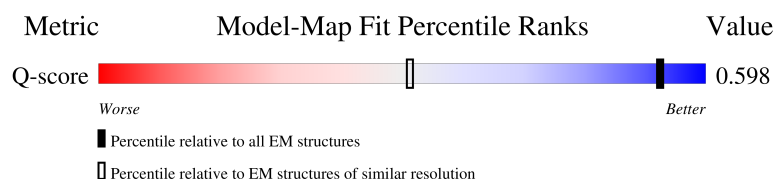
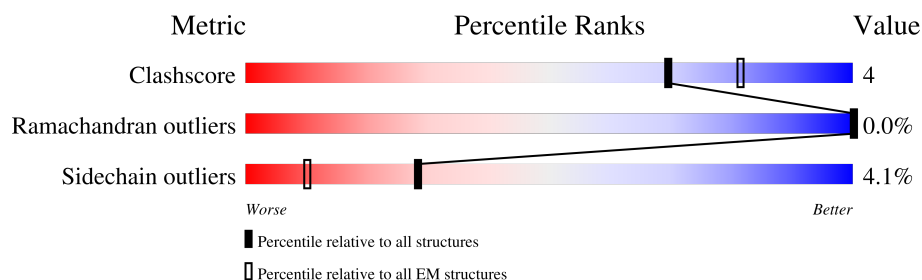
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

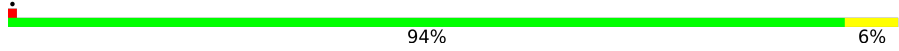

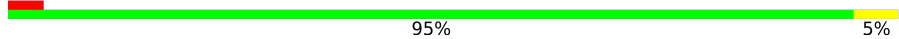
The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3184 (1.71 - 2.70)

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

Mol	Chain	Length	Quality of chain
1	A	446	
1	L	446	
2	B	425	

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Mol	Chain	Length	Quality of chain
2	M	425	
3	C	378	
3	N	378	
4	D	241	
4	O	241	
5	E	196	
5	P	196	
6	F	105	
6	Q	105	
7	G	75	
7	R	75	
8	H	67	
8	S	67	
9	I	57	
9	T	57	
10	J	61	
10	U	61	
11	K	52	
11	V	52	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	FES	E	200	-	-	X	-
14	FES	P	200	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 66121 atoms, of which 32847 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-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	446	Total	C	H	N	O	S	0	0
			6815	2161	3357	609	668	20		
1	L	446	Total	C	H	N	O	S	0	0
			6815	2161	3357	609	668	20		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	425	Total	C	H	N	O	S	0	0
			6344	1998	3163	564	612	7		
2	M	425	Total	C	H	N	O	S	0	0
			6345	1998	3164	564	612	7		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	378	Total	C	H	N	O	S	0	0
			6071	2013	3068	471	501	18		
3	N	378	Total	C	H	N	O	S	0	0
			6071	2013	3068	471	501	18		

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	241	Total	C	H	N	O	S	0	0
			3789	1225	1870	330	349	15		
4	O	241	Total	C	H	N	O	S	0	0
			3789	1225	1870	330	349	15		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	196	Total	C	H	N	O	S	0	0
			3026	957	1507	263	291	8		
5	P	196	Total	C	H	N	O	S	0	0
			3026	957	1507	263	291	8		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	105	Total	C	H	N	O	S	0	0
			1818	576	907	165	168	2		
6	Q	105	Total	C	H	N	O	S	0	0
			1818	576	907	165	168	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	56	ASP	ASN	conflict	UNP P00129
Q	56	ASP	ASN	conflict	UNP P00129

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	75	Total	C	H	N	O	S	0	0
			1265	410	636	118	100	1		
7	R	75	Total	C	H	N	O	S	0	0
			1265	410	636	118	100	1		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	67	Total	C	H	N	O	S	0	0
			1085	332	537	99	112	5		
8	S	67	Total	C	H	N	O	S	0	0
			1085	332	537	99	112	5		

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	57	Total	C	H	N	O	S	0	0
			844	253	437	77	75	2		
9	T	57	Total	C	H	N	O	S	0	0
			844	253	437	77	75	2		

- | Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|---------|---------|---------|-------|
| 10 | J | 61 | Total
1008 | C
329 | H
505 | N
87 | O
87 | 0 | 0 |
| 10 | U | 61 | Total
1008 | C
329 | H
505 | N
87 | O
87 | 0 | 0 |

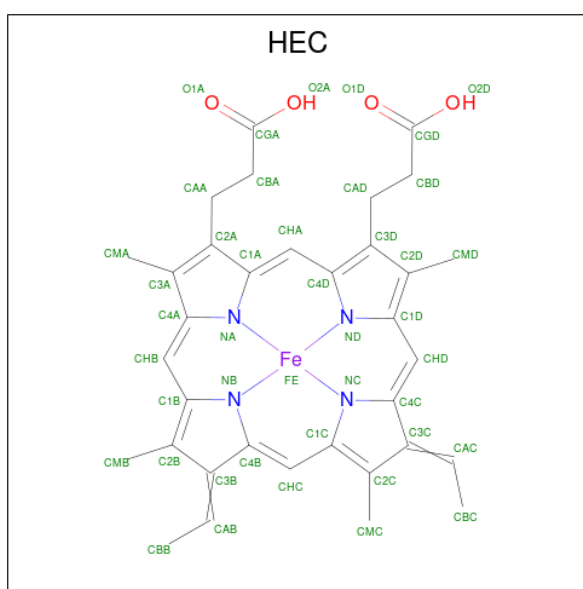
- | Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|---------|---------|---------|-------|
| 11 | K | 52 | Total
862 | C
282 | H
436 | N
77 | O
67 | 0 | 0 |
| 11 | V | 52 | Total
862 | C
282 | H
436 | N
77 | O
67 | 0 | 0 |

Chain	Residue	Modelled	Actual	Comment	Reference
K	22	GLN	SER	conflict	UNP P07552
K	38	SER	TRP	conflict	UNP P07552
V	22	GLN	SER	conflict	UNP P07552
V	38	SER	TRP	conflict	UNP P07552

- # HEM
-
- The diagram illustrates the chemical structure of Hemoglobin (HEM). It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The iron atom is also coordinated by a heme group (O1A, O2A, O1D, O2D) and a proximal histidine residue (C1A). The heme group is shown in red, while the rest of the structure is in green. The structure includes various side chains and a heme group, with labels for atoms and bonds.

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

- Molecule 13 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
13	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

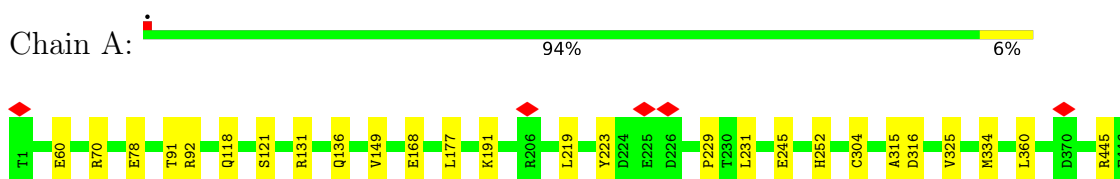


Mol	Chain	Residues	Atoms			AltConf
14	E	1	Total	Fe	S	0
			4	2	2	
14	P	1	Total	Fe	S	0
			4	2	2	

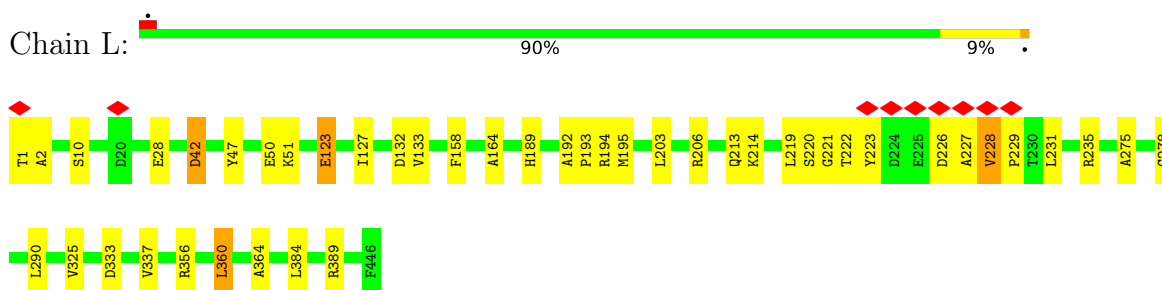
3 Residue-property plots

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.

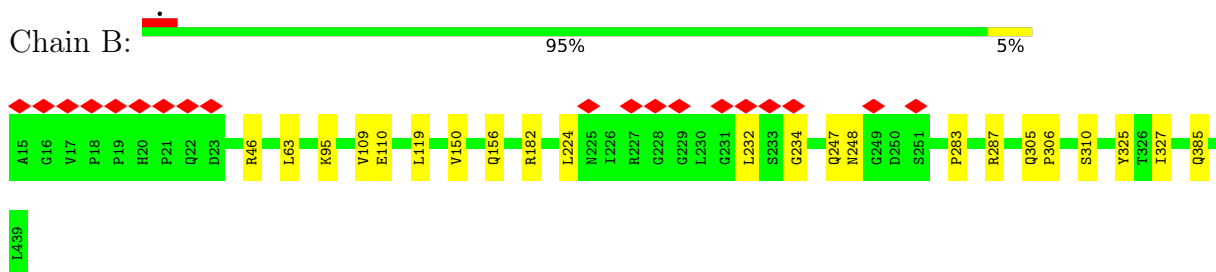
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



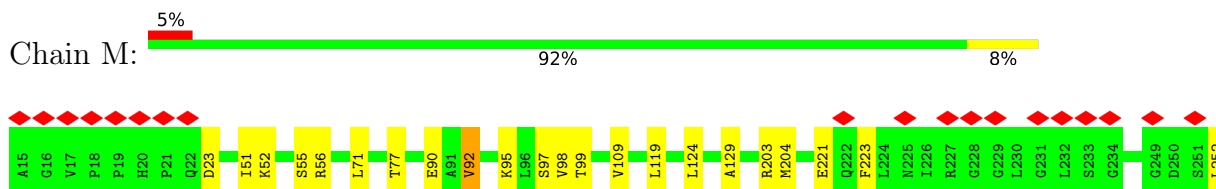
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



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



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





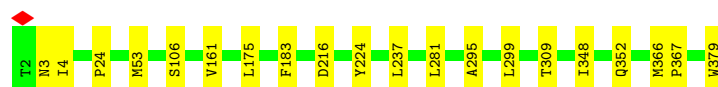
• Molecule 3: Cytochrome b

Chain C: 95% 5%



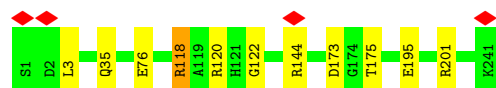
• Molecule 3: Cytochrome b

Chain N: 95% 5%



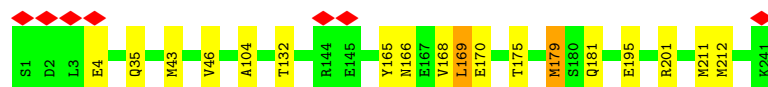
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D: 95% 5%



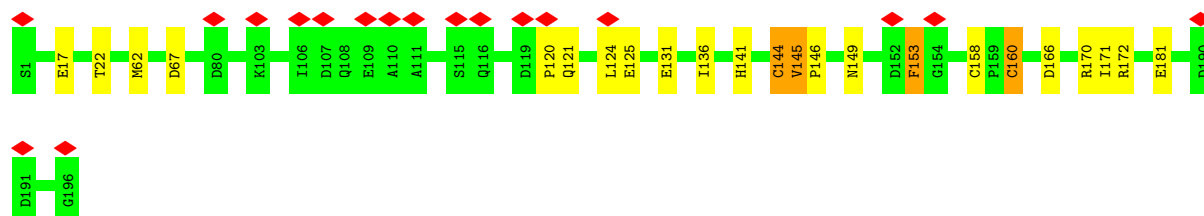
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain O: 93% 7%



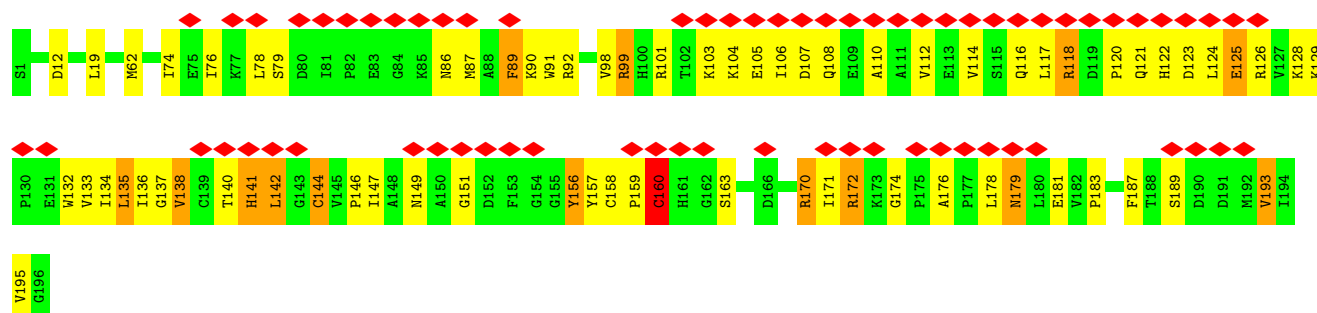
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E: 9% 88% 10%

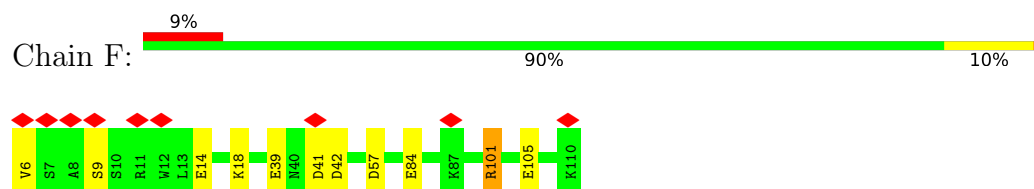


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

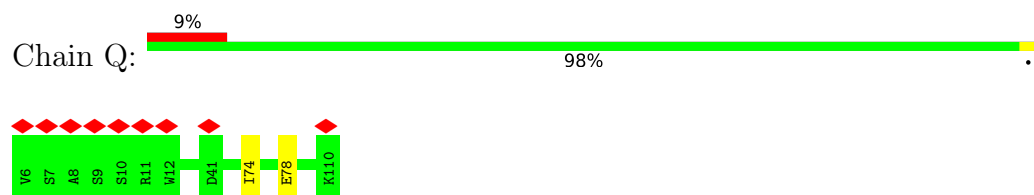
Chain P: 35% 64% 29% 7%



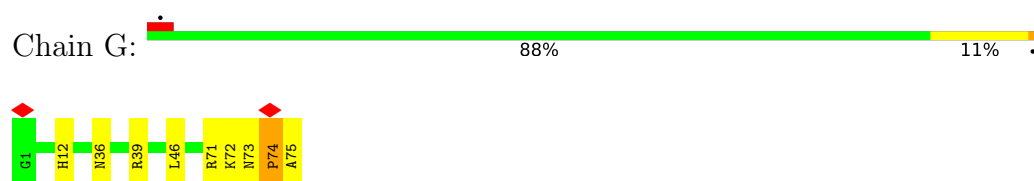
- Molecule 6: Cytochrome b-c1 complex subunit 7



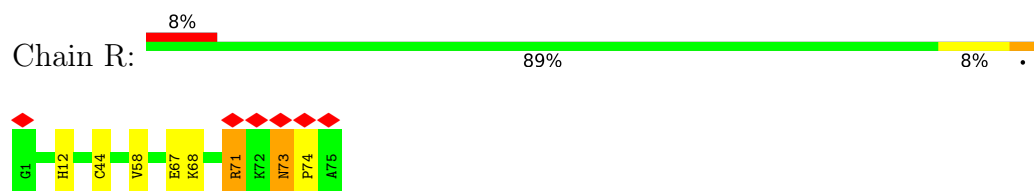
- Molecule 6: Cytochrome b-c1 complex subunit 7



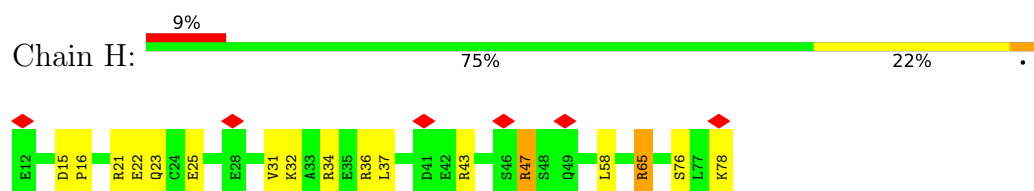
- Molecule 7: Cytochrome b-c1 complex subunit 8



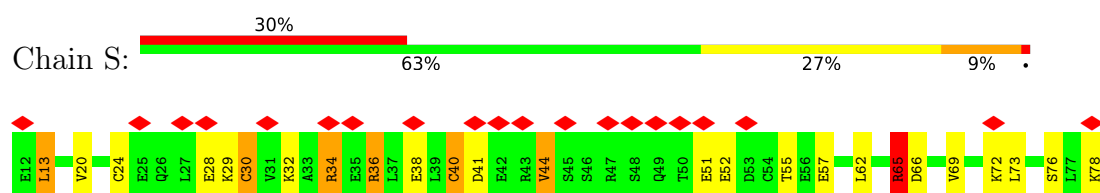
- Molecule 7: Cytochrome b-c1 complex subunit 8



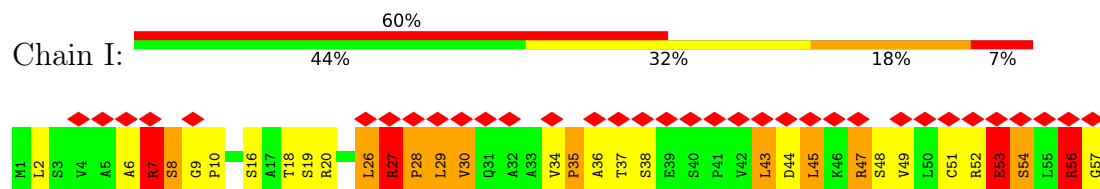
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



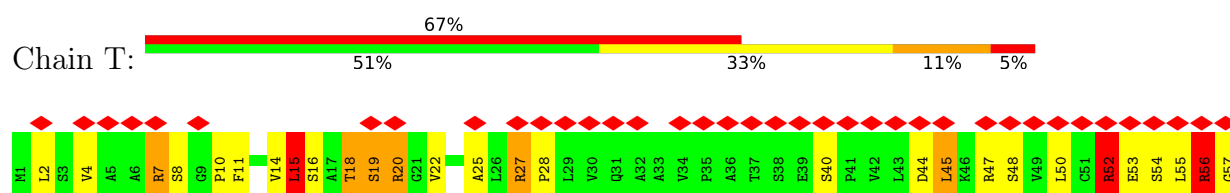
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



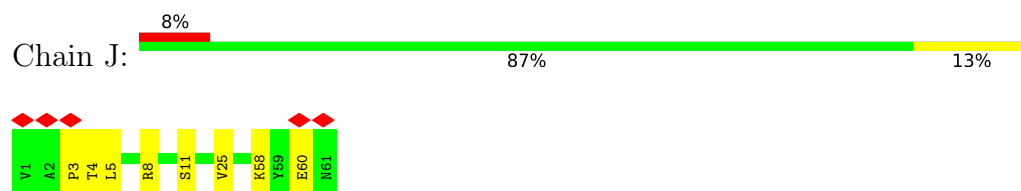
• Molecule 9: Cytochrome b-c1 complex subunit 9



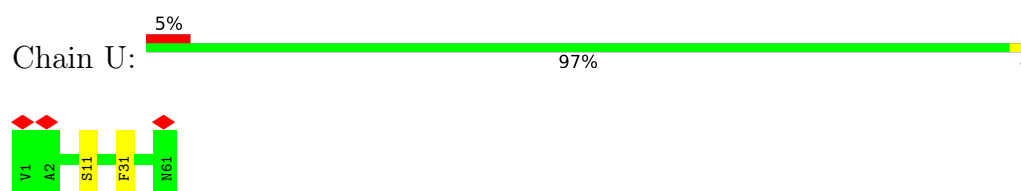
• Molecule 9: Cytochrome b-c1 complex subunit 9



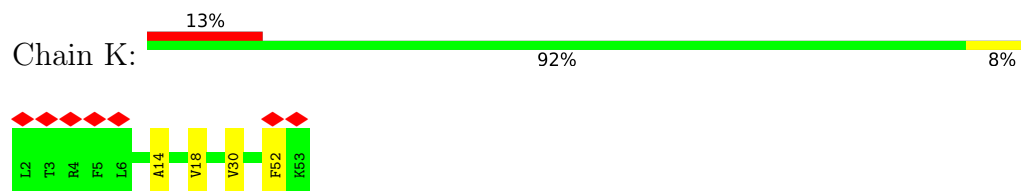
• Molecule 10: Cytochrome b-c1 complex subunit 9



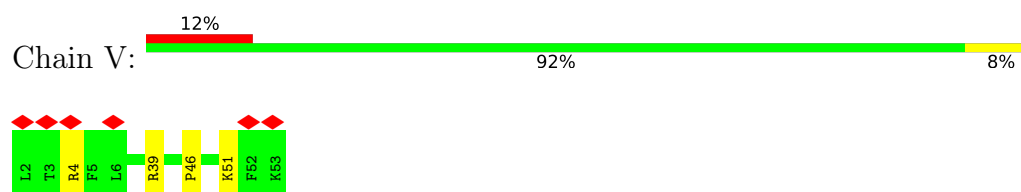
• Molecule 10: Cytochrome b-c1 complex subunit 9



• Molecule 11: Cytochrome b-c1 complex subunit 10



• Molecule 11: Cytochrome b-c1 complex subunit 10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	477031	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.043	Depositor
Minimum map value	-0.685	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	654.0, 654.0, 654.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, FES, HEC

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	0.23	0/3531	0.44	0/4792
1	L	0.41	1/3531 (0.0%)	0.65	7/4792 (0.1%)
2	B	0.14	0/3241	0.36	0/4398
2	M	0.26	0/3241	0.49	1/4398 (0.0%)
3	C	0.18	0/3100	0.40	0/4242
3	N	0.17	0/3100	0.40	0/4242
4	D	0.38	0/1978	0.62	1/2684 (0.0%)
4	O	0.34	0/1978	0.59	1/2684 (0.0%)
5	E	0.45	0/1553	0.76	4/2100 (0.2%)
5	P	0.85	0/1553	1.21	9/2100 (0.4%)
6	F	0.17	0/930	0.39	0/1246
6	Q	0.16	0/930	0.41	0/1246
7	G	0.40	0/650	0.62	1/878 (0.1%)
7	R	0.39	0/650	0.63	0/878
8	H	0.89	0/553	1.35	0/741
8	S	0.92	0/553	1.36	1/741 (0.1%)
9	I	1.01	0/412	1.63	8/558 (1.4%)
9	T	1.21	3/412 (0.7%)	1.94	17/558 (3.0%)
10	J	0.18	0/516	0.41	0/696
10	U	0.17	0/516	0.36	0/696
11	K	0.17	0/440	0.38	0/600
11	V	0.44	0/440	0.63	1/600 (0.2%)
All	All	0.40	4/33808 (0.0%)	0.66	51/45870 (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	L	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	M	0	1
4	D	0	3
5	P	0	7
7	G	0	1
7	R	0	1
8	H	0	6
8	S	0	3
9	I	0	5
9	T	0	7
All	All	0	37

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	360	LEU	C-O	-7.43	1.15	1.24
9	T	20	ARG	N-CA	6.31	1.53	1.46
9	T	19	SER	CA-CB	-5.63	1.45	1.53
9	T	19	SER	CA-C	5.46	1.59	1.53

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	T	10	PRO	N-CD-CG	-11.81	85.48	103.20
5	P	157	TYR	N-CA-CB	11.53	128.67	110.57
9	T	10	PRO	CB-CG-CD	9.49	136.49	106.10
9	T	20	ARG	N-CA-C	9.03	124.12	109.76
9	T	19	SER	N-CA-C	8.68	121.53	109.29
5	E	144	CYS	CB-CA-C	-8.51	93.46	110.30
9	I	35	PRO	N-CA-C	-8.23	98.37	110.80
9	T	27	ARG	N-CA-C	-7.92	101.09	108.22
9	T	56	ARG	CG-CD-NE	-7.59	95.29	112.00
9	I	27	ARG	N-CA-C	-7.51	101.39	108.07
9	I	27	ARG	CB-CA-C	7.41	119.80	110.76
9	I	28	PRO	N-CA-CB	-7.34	97.66	102.65
2	M	92	VAL	O-C-N	-7.00	113.82	122.57
9	T	54	SER	N-CA-C	-6.80	104.24	112.54
5	P	160	CYS	N-CA-CB	-6.66	100.36	110.01
9	T	18	THR	CA-C-O	-6.51	111.20	120.51
1	L	360	LEU	CA-C-O	-6.51	114.17	121.00
9	T	28	PRO	N-CA-C	6.35	121.24	110.95
5	P	156	TYR	N-CA-CB	-6.31	99.58	111.00
9	T	10	PRO	CA-CB-CG	-6.27	92.58	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	364	ALA	CA-C-O	-6.06	114.00	120.42
5	P	89	PHE	N-CA-CB	-5.96	100.21	111.00
5	P	147	ILE	CA-C-O	-5.96	115.52	122.13
9	T	18	THR	N-CA-CB	-5.90	100.53	110.49
11	V	46	PRO	N-CA-C	5.76	121.71	113.47
9	I	6	ALA	N-CA-C	-5.71	104.96	111.07
9	I	29	LEU	N-CA-C	-5.66	105.12	113.61
9	T	53	GLU	N-CA-C	-5.62	107.01	112.97
4	D	122	GLY	CA-C-O	-5.57	116.28	121.18
5	P	159	PRO	N-CA-C	-5.54	106.94	113.86
5	E	120	PRO	CA-N-CD	-5.49	104.31	112.00
9	I	7	ARG	N-CA-C	-5.48	102.64	110.59
1	L	214	LYS	CB-CA-C	-5.48	102.25	110.90
9	T	7	ARG	N-CA-C	-5.46	103.32	110.53
9	T	20	ARG	N-CA-CB	-5.41	101.56	109.95
5	E	145	VAL	N-CA-C	-5.37	97.28	108.88
5	P	151	GLY	CA-C-O	-5.32	118.32	122.52
1	L	222	THR	OG1-CB-CG2	5.29	119.88	109.30
8	S	24	CYS	CB-CA-C	-5.25	101.92	110.85
9	T	27	ARG	CB-CA-C	5.23	117.12	110.22
5	E	144	CYS	N-CA-CB	5.22	119.73	111.43
5	P	147	ILE	N-CA-C	-5.18	104.35	110.21
9	T	25	ALA	CA-C-O	-5.18	115.89	121.38
9	I	53	GLU	N-CA-C	-5.16	106.96	113.20
1	L	290	LEU	CA-C-N	5.12	127.10	120.44
1	L	290	LEU	C-N-CA	5.12	127.10	120.44
1	L	278	GLY	N-CA-C	5.11	120.92	112.84
4	O	104	ALA	N-CA-C	-5.08	103.34	110.35
9	T	10	PRO	CA-N-CD	5.06	119.09	112.00
7	G	74	PRO	CA-C-O	-5.05	115.82	121.23
5	P	160	CYS	CA-C-O	-5.03	115.54	120.82

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	118	ARG	Sidechain
4	D	120	ARG	Sidechain
4	D	144	ARG	Sidechain
7	G	71	ARG	Sidechain
8	H	21	ARG	Sidechain
8	H	34	ARG	Sidechain

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Mol	Chain	Res	Type	Group
8	H	36	ARG	Sidechain
8	H	43	ARG	Sidechain
8	H	47	ARG	Sidechain
8	H	65	ARG	Sidechain
9	I	27	ARG	Sidechain
9	I	47	ARG	Sidechain
9	I	52	ARG	Sidechain
9	I	56	ARG	Sidechain
9	I	7	ARG	Sidechain
1	L	206	ARG	Sidechain
1	L	235	ARG	Sidechain
1	L	356	ARG	Sidechain
2	M	56	ARG	Sidechain
5	P	101	ARG	Sidechain
5	P	118	ARG	Sidechain
5	P	126	ARG	Sidechain
5	P	170	ARG	Sidechain
5	P	172	ARG	Sidechain
5	P	92	ARG	Sidechain
5	P	99	ARG	Sidechain
7	R	71	ARG	Sidechain
8	S	34	ARG	Sidechain
8	S	36	ARG	Sidechain
8	S	65	ARG	Sidechain
9	T	15	LEU	Mainchain
9	T	20	ARG	Sidechain
9	T	27	ARG	Sidechain
9	T	47	ARG	Sidechain
9	T	52	ARG	Sidechain
9	T	56	ARG	Sidechain
9	T	7	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3458	3357	3356	15	0
1	L	3458	3357	3356	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3181	3163	3160	24	0
2	M	3181	3164	3160	20	0
3	C	3003	3068	3065	11	0
3	N	3003	3068	3065	12	0
4	D	1919	1870	1868	4	0
4	O	1919	1870	1868	11	0
5	E	1519	1507	1503	13	0
5	P	1519	1507	1503	33	0
6	F	911	907	904	7	0
6	Q	911	907	904	1	0
7	G	629	636	636	2	0
7	R	629	636	636	1	0
8	H	548	537	530	5	0
8	S	548	537	529	5	0
9	I	407	437	437	39	0
9	T	407	437	437	17	0
10	J	503	505	505	4	0
10	U	503	505	505	1	0
11	K	426	436	433	3	0
11	V	426	436	433	2	0
12	C	86	0	60	9	0
12	N	86	0	60	10	0
13	D	43	0	30	2	0
13	O	43	0	29	3	0
14	E	4	0	0	2	0
14	P	4	0	0	2	0
All	All	33274	32847	32972	237	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 4.

All (237) 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)
12:N:401:HEM:HMC2	12:N:401:HEM:HBC2	1.63	0.81
12:C:401:HEM:HBC2	12:C:401:HEM:HMC2	1.63	0.81
12:C:402:HEM:HMC1	12:C:402:HEM:HBC2	1.62	0.80
8:H:15:ASP:OD1	8:H:16:PRO:HD2	1.81	0.79
12:N:402:HEM:HBC2	12:N:402:HEM:HMC1	1.65	0.78
4:O:4:GLU:OE2	4:O:4:GLU:N	2.16	0.78
1:L:360:LEU:HD21	9:T:56:ARG:HD3	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:17:GLU:N	5:E:17:GLU:OE2	2.19	0.75
12:N:401:HEM:HMB2	12:N:401:HEM:HBB2	1.68	0.75
2:M:77:THR:OG1	2:M:129:ALA:O	2.04	0.74
12:N:402:HEM:HMB2	12:N:402:HEM:HBB2	1.69	0.74
12:C:402:HEM:HBB2	12:C:402:HEM:HMB2	1.69	0.74
1:L:189:HIS:CE1	1:L:228:VAL:HG11	2.22	0.74
9:I:19:SER:HB2	9:I:57:GLY:HA2	1.69	0.74
12:C:401:HEM:HBB2	12:C:401:HEM:HMB2	1.69	0.72
2:B:109:VAL:HG22	2:B:119:LEU:HD23	1.72	0.70
5:P:76:ILE:HG21	5:P:87:MET:HE1	1.74	0.69
8:H:15:ASP:OD1	8:H:16:PRO:CD	2.41	0.69
2:B:95:LYS:HE2	9:I:57:GLY:HA3	1.75	0.67
8:S:40:CYS:O	8:S:44:VAL:HG23	1.95	0.67
5:E:121:GLN:NE2	5:E:125:GLU:OE1	2.28	0.66
1:L:50:GLU:OE2	1:L:50:GLU:N	2.28	0.66
4:O:35:GLN:HB2	4:O:169:LEU:HD21	1.77	0.66
1:A:70:ARG:NE	1:A:78:GLU:OE2	2.29	0.64
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.29	0.64
4:D:76:GLU:OE2	4:D:76:GLU:N	2.30	0.64
2:M:385:GLN:HA	9:T:2:LEU:HD11	1.79	0.64
2:M:376:GLU:OE2	2:M:376:GLU:N	2.29	0.63
1:A:131:ARG:NH2	1:A:177:LEU:O	2.31	0.63
1:L:189:HIS:HE1	1:L:228:VAL:HG11	1.63	0.62
5:P:141:HIS:CE1	5:P:142:LEU:HD12	2.35	0.62
11:K:14:ALA:O	11:K:18:VAL:HG23	2.00	0.61
4:O:195:GLU:OE2	4:O:201:ARG:NH1	2.33	0.61
9:I:18:THR:OG1	9:I:57:GLY:N	2.33	0.60
5:E:160:CYS:HB2	14:E:200:FES:S1	2.41	0.60
5:P:171:ILE:HD11	5:P:176:ALA:HB3	1.84	0.59
9:T:19:SER:HB2	9:T:57:GLY:HA3	1.85	0.58
5:E:131:GLU:OE2	5:E:131:GLU:N	2.36	0.58
5:P:98:VAL:HG22	5:P:134:ILE:HG13	1.86	0.58
3:C:53:MET:HE1	5:E:62:MET:SD	2.44	0.57
2:M:99:THR:HG23	9:T:14:VAL:HG22	1.85	0.57
5:P:170:ARG:HA	5:P:179:ASN:HD22	1.70	0.57
5:P:158:CYS:C	5:P:160:CYS:SG	2.89	0.56
9:I:20:ARG:HD2	9:I:51:CYS:HA	1.87	0.56
5:E:136:ILE:HD12	5:E:181:GLU:HG2	1.86	0.56
2:M:92:VAL:HG21	2:M:119:LEU:HD11	1.86	0.56
12:C:401:HEM:HBB2	12:C:401:HEM:CMB	2.36	0.55
4:D:195:GLU:OE2	4:D:201:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLN:HB3	9:I:36:ALA:CB	2.36	0.55
12:C:402:HEM:HBC2	12:C:402:HEM:CMC	2.36	0.55
9:I:19:SER:HB2	9:I:57:GLY:CA	2.36	0.55
1:A:118:GLN:HG2	1:A:219:LEU:HD13	1.89	0.55
2:B:95:LYS:HG2	9:I:57:GLY:C	2.32	0.54
2:B:63:LEU:O	2:B:182:ARG:NE	2.40	0.54
2:B:327:ILE:CD1	9:I:29:LEU:HD12	2.37	0.54
5:P:124:LEU:HD12	5:P:125:GLU:N	2.22	0.54
12:C:402:HEM:HBB2	12:C:402:HEM:CMB	2.38	0.54
12:N:401:HEM:HBB2	12:N:401:HEM:CMB	2.37	0.54
5:P:163:SER:HA	5:P:174:GLY:HA3	1.90	0.54
12:N:402:HEM:HBB2	12:N:402:HEM:CMB	2.37	0.54
9:T:45:LEU:N	9:T:45:LEU:HD23	2.22	0.54
4:D:3:LEU:HD12	4:D:3:LEU:O	2.08	0.53
1:L:193:PRO:HD3	1:L:221:GLY:HA2	1.91	0.53
5:P:114:VAL:HG12	5:P:120:PRO:HB2	1.91	0.53
1:A:304:CYS:HB3	1:A:334:MET:HE3	1.91	0.53
1:L:228:VAL:N	1:L:229:PRO:CD	2.72	0.53
2:B:109:VAL:CG2	2:B:119:LEU:HD23	2.38	0.53
3:N:237:LEU:HA	4:O:212:MET:HE3	1.90	0.53
2:B:283:PRO:HD2	9:I:30:VAL:HG11	1.91	0.53
6:F:39:GLU:OE2	6:F:39:GLU:N	2.30	0.53
5:P:74:ILE:HD12	5:P:91:TRP:HB2	1.91	0.53
12:N:402:HEM:HBC2	12:N:402:HEM:CMC	2.36	0.52
5:E:141:HIS:O	14:E:200:FES:S2	2.67	0.52
1:L:42:ASP:OD1	1:L:384:LEU:HD22	2.10	0.52
9:I:45:LEU:N	9:I:45:LEU:HD23	2.24	0.51
8:S:20:VAL:HG12	8:S:69:VAL:HG22	1.92	0.51
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.44	0.50
1:L:195:MET:HE2	1:L:219:LEU:HD21	1.91	0.50
1:L:195:MET:HE2	1:L:219:LEU:CD2	2.41	0.50
3:N:53:MET:HE1	5:P:62:MET:SD	2.50	0.50
5:P:142:LEU:HB2	14:P:200:FES:S2	2.51	0.50
3:C:177:ARG:HH11	3:C:177:ARG:HG2	1.76	0.50
1:L:123:GLU:O	1:L:127:ILE:HG23	2.12	0.50
5:P:137:GLY:O	5:P:138:VAL:HG23	2.12	0.50
3:N:24:PRO:O	3:N:224:TYR:OH	2.25	0.50
1:L:132:ASP:OD1	1:L:133:VAL:N	2.45	0.49
2:M:52:LYS:HG2	2:M:203:ARG:HB3	1.93	0.49
9:T:50:LEU:HD12	9:T:52:ARG:NH2	2.28	0.49
12:C:401:HEM:HBC2	12:C:401:HEM:CMC	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:401:HEM:HBC2	12:N:401:HEM:CMC	2.38	0.49
4:O:175:THR:HG23	8:S:78:LYS:HD2	1.93	0.49
2:B:46:ARG:NH2	2:B:110:GLU:OE1	2.46	0.48
2:M:71:LEU:HA	9:T:15:LEU:HD22	1.94	0.48
9:I:19:SER:OG	9:I:20:ARG:N	2.46	0.48
5:E:124:LEU:HD12	5:E:125:GLU:N	2.29	0.48
2:B:95:LYS:HE2	9:I:57:GLY:O	2.14	0.48
5:P:78:LEU:HD22	5:P:132:TRP:CE3	2.48	0.48
1:A:315:ALA:O	1:A:316:ASP:OD2	2.31	0.48
3:C:171:ASP:OD1	3:C:172:LYS:N	2.42	0.48
5:E:144:CYS:HB2	5:E:146:PRO:HD3	1.96	0.48
1:L:192:ALA:HA	1:L:219:LEU:HD23	1.96	0.48
2:M:109:VAL:HG22	2:M:119:LEU:HD23	1.95	0.48
1:L:275:ALA:HB1	9:T:55:LEU:HD21	1.96	0.48
5:P:105:GLU:HA	5:P:108:GLN:HG2	1.96	0.48
3:C:240:MET:HE3	3:C:240:MET:HA	1.95	0.47
2:M:71:LEU:HD23	9:T:15:LEU:HD22	1.95	0.47
13:O:301:HEC:HMC1	13:O:301:HEC:HBC3	1.96	0.47
2:M:71:LEU:CD2	9:T:15:LEU:HD13	2.44	0.47
12:C:402:HEM:HHA	12:C:402:HEM:HBA2	1.95	0.47
7:G:74:PRO:O	7:G:75:ALA:HB3	2.15	0.47
1:L:360:LEU:HD21	9:T:56:ARG:CD	2.42	0.47
2:B:95:LYS:HE2	9:I:57:GLY:CA	2.41	0.47
5:P:74:ILE:HD11	5:P:89:PHE:CE2	2.50	0.47
1:A:223:TYR:CE1	1:A:229:PRO:CD	2.98	0.47
2:B:95:LYS:HE2	9:I:57:GLY:C	2.40	0.47
1:L:47:TYR:CZ	1:L:231:LEU:HD11	2.50	0.47
9:I:19:SER:HB3	9:I:57:GLY:O	2.14	0.47
2:M:366:ALA:O	2:M:370:MET:HE3	2.15	0.47
7:R:73:ASN:N	7:R:74:PRO:CD	2.78	0.47
2:B:325:TYR:CD1	9:I:28:PRO:CG	2.98	0.46
2:B:156:GLN:HE22	9:I:29:LEU:HB2	1.80	0.46
1:A:60:GLU:OE1	2:B:287:ARG:NH2	2.44	0.46
5:E:166:ASP:OD1	5:E:170:ARG:N	2.44	0.46
8:H:15:ASP:OD1	8:H:16:PRO:N	2.49	0.46
5:P:118:ARG:HH22	5:P:174:GLY:H	1.63	0.46
1:L:42:ASP:O	1:L:194:ARG:NH2	2.49	0.46
1:L:227:ALA:HB1	1:L:229:PRO:HD2	1.96	0.46
3:C:3:ASN:OD1	3:C:4:ILE:N	2.49	0.46
2:B:95:LYS:HD2	9:I:56:ARG:O	2.16	0.46
1:L:28:GLU:OE1	1:L:389:ARG:NH1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:71:LEU:HD22	9:T:15:LEU:HD13	1.98	0.46
5:P:187:PHE:HA	5:P:193:VAL:HG12	1.98	0.46
3:C:112:THR:HG22	3:C:196:HIS:CE1	2.51	0.45
1:A:91:THR:HG22	1:A:92:ARG:N	2.31	0.45
10:J:3:PRO:O	10:J:8:ARG:NH2	2.45	0.45
5:P:87:MET:HE2	5:P:98:VAL:HB	1.97	0.45
3:C:348:ILE:O	3:C:352:GLN:HG3	2.16	0.45
1:A:136:GLN:HB3	9:I:36:ALA:HB3	1.98	0.45
6:F:14:GLU:HA	6:F:14:GLU:OE2	2.17	0.45
9:I:8:SER:HB2	9:I:26:LEU:HB3	1.99	0.45
4:O:35:GLN:CB	4:O:169:LEU:HD21	2.44	0.45
5:P:117:LEU:HD22	5:P:170:ARG:HB3	1.99	0.45
9:T:56:ARG:HG3	9:T:57:GLY:N	2.31	0.45
2:B:305:GLN:N	2:B:305:GLN:OE1	2.50	0.45
1:A:191:LYS:HE3	1:A:191:LYS:HA	1.99	0.44
9:I:47:ARG:HH22	9:I:49:VAL:HA	1.82	0.44
2:B:156:GLN:NE2	9:I:29:LEU:HD13	2.32	0.44
10:J:25:VAL:HG11	11:K:30:VAL:HG13	2.00	0.44
1:L:1:THR:HG23	1:L:2:ALA:N	2.32	0.44
9:T:50:LEU:HD12	9:T:52:ARG:CZ	2.47	0.44
5:E:171:ILE:O	5:E:171:ILE:HG23	2.16	0.44
4:O:166:ASN:ND2	8:S:13:LEU:HD23	2.33	0.44
5:P:117:LEU:HD23	5:P:172:ARG:HH11	1.81	0.44
9:I:27:ARG:HA	9:I:27:ARG:CZ	2.47	0.44
9:I:27:ARG:HD3	9:I:28:PRO:HD3	1.99	0.44
1:L:333:ASP:O	1:L:337:VAL:HG23	2.17	0.44
4:O:211:MET:HE1	10:U:31:PHE:CE2	2.52	0.44
2:B:232:LEU:HD12	2:B:234:GLY:H	1.82	0.44
11:K:52:PHE:O	11:K:52:PHE:CG	2.71	0.44
2:M:221:GLU:HA	2:M:221:GLU:OE2	2.17	0.44
4:O:43:MET:CE	4:O:46:VAL:HG21	2.47	0.44
5:E:145:VAL:O	5:E:146:PRO:C	2.59	0.44
3:N:106:SER:HB3	12:N:401:HEM:HBD2	2.00	0.44
5:E:153:PHE:CE1	5:E:172:ARG:HB2	2.53	0.44
3:N:309:THR:O	3:N:309:THR:OG1	2.33	0.44
6:F:41:ASP:OD1	6:F:41:ASP:N	2.50	0.43
2:M:393:THR:OG1	2:M:397:THR:OG1	2.34	0.43
4:O:132:THR:HA	4:O:179:MET:HE1	2.00	0.43
5:P:135:LEU:HD23	5:P:181:GLU:O	2.18	0.43
2:B:310:SER:HB3	9:I:28:PRO:HB3	2.00	0.43
5:P:12:ASP:OD1	5:P:12:ASP:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:87:MET:HE3	5:P:89:PHE:HB2	1.99	0.43
3:C:224:TYR:O	3:C:228:ASP:OD1	2.36	0.43
3:N:216:ASP:OD1	3:N:216:ASP:C	2.61	0.43
11:V:39:ARG:H	11:V:39:ARG:HD3	1.83	0.43
6:Q:78:GLU:OE1	6:Q:78:GLU:C	2.62	0.43
5:P:146:PRO:HB2	5:P:156:TYR:HB3	2.00	0.43
1:A:168:GLU:OE1	1:A:168:GLU:N	2.49	0.43
2:B:150:VAL:HG11	9:I:47:ARG:HG2	2.01	0.43
2:B:327:ILE:HD12	9:I:28:PRO:O	2.18	0.43
9:I:34:VAL:HB	9:I:35:PRO:HD3	2.00	0.43
13:O:301:HEC:CBB	13:O:301:HEC:HHC	2.49	0.43
6:F:105:GLU:OE1	11:V:4:ARG:NH2	2.51	0.43
10:J:58:LYS:HA	10:J:58:LYS:HE2	2.01	0.43
2:M:318:ASP:OD1	2:M:318:ASP:N	2.51	0.43
6:F:57:ASP:OD2	6:F:57:ASP:N	2.52	0.43
8:S:30:CYS:SG	8:S:65:ARG:HA	2.59	0.43
6:F:84:GLU:OE2	6:F:84:GLU:N	2.49	0.43
2:B:385:GLN:HG2	9:I:2:LEU:HD13	2.01	0.42
3:C:177:ARG:HH11	3:C:177:ARG:CG	2.31	0.42
2:M:124:LEU:HD12	2:M:223:PHE:HB3	2.01	0.42
13:D:301:HEC:HMC1	13:D:301:HEC:CBC	2.49	0.42
1:L:158:PHE:O	1:L:164:ALA:HB2	2.19	0.42
10:J:4:THR:HG22	10:J:5:LEU:H	1.84	0.42
1:A:252:HIS:CE1	9:I:43:LEU:HD13	2.54	0.42
13:D:301:HEC:HBB2	13:D:301:HEC:HMB3	2.01	0.42
1:L:227:ALA:C	1:L:229:PRO:HD2	2.45	0.42
5:P:144:CYS:HB3	14:P:200:FES:S2	2.59	0.42
2:B:306:PRO:HB3	9:I:35:PRO:HB2	2.02	0.42
13:O:301:HEC:HMC1	13:O:301:HEC:CBC	2.50	0.42
9:T:45:LEU:HD23	9:T:45:LEU:H	1.85	0.42
3:N:281:LEU:C	3:N:281:LEU:HD13	2.45	0.42
9:I:9:GLY:N	9:I:10:PRO:HD2	2.35	0.41
2:B:247:GLN:O	2:B:248:ASN:ND2	2.51	0.41
5:P:136:ILE:HD11	5:P:183:PRO:HB3	2.02	0.41
5:P:140:THR:OG1	5:P:176:ALA:HB1	2.20	0.41
8:H:25:GLU:HG3	8:H:65:ARG:HG3	2.02	0.41
4:O:165:TYR:CD2	4:O:168:VAL:CG1	3.03	0.41
5:P:107:ASP:O	5:P:110:ALA:HB3	2.21	0.41
9:I:27:ARG:HD3	9:I:28:PRO:CD	2.51	0.41
2:M:90:GLU:HG2	9:T:56:ARG:HE	1.85	0.41
5:P:74:ILE:HG23	5:P:195:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:98:VAL:HG13	5:P:134:ILE:CD1	2.50	0.41
5:P:171:ILE:HB	5:P:179:ASN:HA	2.01	0.41
3:C:111:GLU:H	3:C:111:GLU:CD	2.29	0.41
3:C:223:TYR:O	3:C:226:ILE:HG22	2.20	0.41
9:I:19:SER:HB3	9:I:57:GLY:C	2.46	0.41
3:N:183:PHE:CZ	12:N:402:HEM:HBC1	2.55	0.41
5:P:108:GLN:O	5:P:112:VAL:HG23	2.21	0.41
9:T:52:ARG:HA	9:T:52:ARG:HD3	1.91	0.41
1:A:360:LEU:CD2	9:I:56:ARG:HB3	2.51	0.41
1:L:51:LYS:C	1:L:51:LYS:HD2	2.46	0.41
1:A:445:ARG:HD2	1:A:445:ARG:H	1.86	0.41
8:H:37:LEU:HD22	8:H:58:LEU:HA	2.03	0.41
3:N:348:ILE:O	3:N:352:GLN:HG3	2.21	0.41
1:L:192:ALA:CA	1:L:219:LEU:HD23	2.51	0.41
2:M:23:ASP:OD1	2:M:23:ASP:N	2.48	0.41
3:N:3:ASN:OD1	3:N:4:ILE:N	2.53	0.41
9:I:8:SER:HB3	9:I:26:LEU:HB2	2.03	0.40
9:I:45:LEU:HD23	9:I:45:LEU:H	1.86	0.40
3:N:366:MET:HB2	3:N:367:PRO:HD3	2.03	0.40
9:I:53:GLU:O	9:I:54:SER:CB	2.69	0.40
2:M:51:ILE:HG12	2:M:204:MET:HE3	2.04	0.40
9:I:20:ARG:NH1	9:I:48:SER:CB	2.85	0.40
2:M:309:VAL:HG23	2:M:326:THR:HG22	2.03	0.40
4:D:173:ASP:OD1	4:D:175:THR:OG1	2.30	0.40
3:N:295:ALA:O	3:N:299:LEU:HD23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	444/446 (100%)	431 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	444/446 (100%)	433 (98%)	11 (2%)	0	100	100
2	B	423/425 (100%)	412 (97%)	11 (3%)	0	100	100
2	M	423/425 (100%)	414 (98%)	9 (2%)	0	100	100
3	C	376/378 (100%)	367 (98%)	9 (2%)	0	100	100
3	N	376/378 (100%)	367 (98%)	9 (2%)	0	100	100
4	D	239/241 (99%)	233 (98%)	6 (2%)	0	100	100
4	O	239/241 (99%)	233 (98%)	6 (2%)	0	100	100
5	E	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
5	P	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
6	F	103/105 (98%)	103 (100%)	0	0	100	100
6	Q	103/105 (98%)	103 (100%)	0	0	100	100
7	G	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
7	R	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
8	H	65/67 (97%)	65 (100%)	0	0	100	100
8	S	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
9	I	55/57 (96%)	50 (91%)	4 (7%)	1 (2%)	6	4
9	T	55/57 (96%)	46 (84%)	8 (14%)	1 (2%)	6	4
10	J	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
10	U	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
11	K	50/52 (96%)	47 (94%)	3 (6%)	0	100	100
11	V	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
All	All	4162/4206 (99%)	4044 (97%)	116 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	I	54	SER
9	T	56	ARG

5.3.2 Protein sidechains ⓘ

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	370/370 (100%)	365 (99%)	5 (1%)	59	75
1	L	370/370 (100%)	360 (97%)	10 (3%)	39	53
2	B	332/332 (100%)	331 (100%)	1 (0%)	86	93
2	M	332/332 (100%)	325 (98%)	7 (2%)	47	63
3	C	326/326 (100%)	321 (98%)	5 (2%)	57	73
3	N	326/326 (100%)	323 (99%)	3 (1%)	70	84
4	D	206/206 (100%)	204 (99%)	2 (1%)	68	81
4	O	206/206 (100%)	202 (98%)	4 (2%)	50	66
5	E	168/168 (100%)	162 (96%)	6 (4%)	31	42
5	P	168/168 (100%)	141 (84%)	27 (16%)	2	2
6	F	96/96 (100%)	92 (96%)	4 (4%)	26	36
6	Q	96/96 (100%)	95 (99%)	1 (1%)	68	81
7	G	66/66 (100%)	62 (94%)	4 (6%)	17	20
7	R	66/66 (100%)	59 (89%)	7 (11%)	6	6
8	H	64/64 (100%)	57 (89%)	7 (11%)	6	6
8	S	64/64 (100%)	43 (67%)	21 (33%)	0	0
9	I	44/44 (100%)	31 (70%)	13 (30%)	0	0
9	T	44/44 (100%)	31 (70%)	13 (30%)	0	0
10	J	51/51 (100%)	49 (96%)	2 (4%)	28	39
10	U	51/51 (100%)	50 (98%)	1 (2%)	48	64
11	K	42/42 (100%)	42 (100%)	0	100	100
11	V	42/42 (100%)	41 (98%)	1 (2%)	43	58
All	All	3530/3530 (100%)	3386 (96%)	144 (4%)	28	37

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	A	149	VAL
1	A	231	LEU
1	A	245	GLU
1	A	325	VAL
2	B	224	LEU

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Mol	Chain	Res	Type
3	C	20	ASP
3	C	175	LEU
3	C	177	ARG
3	C	184	ILE
3	C	379	TRP
4	D	35	GLN
4	D	118	ARG
5	E	22	THR
5	E	67	ASP
5	E	149	ASN
5	E	153	PHE
5	E	158	CYS
5	E	160	CYS
6	F	6	VAL
6	F	9	SER
6	F	18	LYS
6	F	101	ARG
7	G	12	HIS
7	G	46	LEU
7	G	72	LYS
7	G	73	ASN
8	H	22	GLU
8	H	23	GLN
8	H	31	VAL
8	H	32	LYS
8	H	47	ARG
8	H	76	SER
8	H	78	LYS
9	I	7	ARG
9	I	8	SER
9	I	16	SER
9	I	26	LEU
9	I	27	ARG
9	I	30	VAL
9	I	37	THR
9	I	38	SER
9	I	43	LEU
9	I	44	ASP
9	I	45	LEU
9	I	53	GLU
9	I	56	ARG
10	J	11	SER

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Mol	Chain	Res	Type
10	J	60	GLU
1	L	10	SER
1	L	42	ASP
1	L	123	GLU
1	L	203	LEU
1	L	213	GLN
1	L	220	SER
1	L	223	TYR
1	L	226	ASP
1	L	228	VAL
1	L	325	VAL
2	M	55	SER
2	M	95	LYS
2	M	97	SER
2	M	98	VAL
2	M	252	LEU
2	M	310	SER
2	M	329	GLN
3	N	161	VAL
3	N	175	LEU
3	N	379	TRP
4	O	169	LEU
4	O	170	GLU
4	O	179	MET
4	O	181	GLN
5	P	19	LEU
5	P	79	SER
5	P	86	ASN
5	P	90	LYS
5	P	99	ARG
5	P	103	LYS
5	P	104	LYS
5	P	106	ILE
5	P	116	GLN
5	P	121	GLN
5	P	122	HIS
5	P	123	ASP
5	P	125	GLU
5	P	128	LYS
5	P	129	LYS
5	P	133	VAL
5	P	135	LEU

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Mol	Chain	Res	Type
5	P	138	VAL
5	P	141	HIS
5	P	142	LEU
5	P	144	CYS
5	P	149	ASN
5	P	160	CYS
5	P	178	LEU
5	P	179	ASN
5	P	189	SER
5	P	193	VAL
6	Q	74	ILE
7	R	12	HIS
7	R	44	CYS
7	R	58	VAL
7	R	67	GLU
7	R	68	LYS
7	R	71	ARG
7	R	73	ASN
8	S	13	LEU
8	S	28	GLU
8	S	29	LYS
8	S	30	CYS
8	S	32	LYS
8	S	34	ARG
8	S	36	ARG
8	S	38	GLU
8	S	40	CYS
8	S	41	ASP
8	S	44	VAL
8	S	51	GLU
8	S	52	GLU
8	S	55	THR
8	S	57	GLU
8	S	62	LEU
8	S	65	ARG
8	S	66	ASP
8	S	72	LYS
8	S	73	LEU
8	S	76	SER
9	T	4	VAL
9	T	8	SER
9	T	11	PHE

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Mol	Chain	Res	Type
9	T	15	LEU
9	T	16	SER
9	T	18	THR
9	T	22	VAL
9	T	40	SER
9	T	44	ASP
9	T	45	LEU
9	T	48	SER
9	T	52	ARG
9	T	56	ARG
10	U	11	SER
11	V	51	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	119	ASN
1	A	267	ASN
1	A	289	HIS
1	A	311	ASN
1	A	341	GLN
2	B	156	GLN
2	B	248	ASN
2	B	276	GLN
3	C	201	HIS
4	D	14	HIS
1	L	189	HIS
1	L	243	HIS
1	L	252	HIS
1	L	289	HIS
1	L	341	GLN
2	M	59	ASN
2	M	192	HIS
2	M	198	HIS
2	M	329	GLN
3	N	44	GLN
3	N	312	GLN
4	O	31	GLN
4	O	166	ASN
5	P	86	ASN
5	P	121	GLN

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Mol	Chain	Res	Type
5	P	141	HIS
5	P	161	HIS
5	P	164	HIS
6	Q	79	GLN
8	S	23	GLN
10	U	37	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	$\# Z > 2$
14	FES	P	200	5	0,4,4	-	-	-		
13	HEC	O	301	4	46,50,50	1.85	6 (13%)	58,82,82	1.10	5 (8%)
12	HEM	C	402	3	50,50,50	1.46	6 (12%)	67,82,82	1.06	3 (4%)
12	HEM	N	401	3	50,50,50	1.38	6 (12%)	67,82,82	1.04	3 (4%)
12	HEM	N	402	3	50,50,50	1.40	6 (12%)	67,82,82	1.07	4 (5%)
14	FES	E	200	5	0,4,4	-	-	-		
12	HEM	C	401	3	50,50,50	1.40	7 (14%)	67,82,82	1.05	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	HEC	D	301	4	46,50,50	1.86	5 (10%)	58,82,82	1.05	3 (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
14	FES	P	200	5	-	-	0/1/1/1
13	HEC	O	301	4	-	2/14/54/54	-
12	HEM	C	402	3	-	5/14/54/54	-
12	HEM	N	401	3	-	5/14/54/54	-
12	HEM	N	402	3	-	3/14/54/54	-
14	FES	E	200	5	-	-	0/1/1/1
12	HEM	C	401	3	-	4/14/54/54	-
13	HEC	D	301	4	-	2/14/54/54	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	301	HEC	CAB-C3B	6.23	1.55	1.35
13	O	301	HEC	CAC-C3C	6.19	1.55	1.35
13	D	301	HEC	CAC-C3C	6.18	1.55	1.35
13	O	301	HEC	CAB-C3B	6.18	1.55	1.35
13	D	301	HEC	CBC-CAC	-4.19	1.34	1.49
13	O	301	HEC	CBB-CAB	-4.18	1.34	1.49
13	O	301	HEC	CBC-CAC	-4.18	1.34	1.49
13	D	301	HEC	CBB-CAB	-4.17	1.34	1.49
12	C	402	HEM	FE-ND	3.45	2.05	1.94
12	C	402	HEM	FE-NB	3.42	2.05	1.94
12	C	402	HEM	FE-NA	3.37	2.06	1.95
12	C	402	HEM	FE-NC	3.36	2.06	1.95
12	N	402	HEM	FE-NB	3.30	2.05	1.94
12	N	401	HEM	FE-NB	3.27	2.05	1.94
12	C	401	HEM	FE-ND	3.25	2.04	1.94
12	N	401	HEM	FE-ND	3.22	2.04	1.94
12	C	401	HEM	FE-NA	3.13	2.05	1.95
12	C	401	HEM	FE-NB	3.12	2.04	1.94
12	N	402	HEM	FE-NC	3.07	2.05	1.95
12	N	402	HEM	FE-ND	3.06	2.04	1.94
12	N	402	HEM	FE-NA	2.94	2.04	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	N	401	HEM	CAB-C3B	2.94	1.55	1.47
12	N	401	HEM	CAC-C3C	2.91	1.55	1.47
12	N	402	HEM	CAB-C3B	2.91	1.55	1.47
12	C	401	HEM	CAB-C3B	2.91	1.55	1.47
12	C	402	HEM	CAB-C3B	2.90	1.55	1.47
12	C	402	HEM	CAC-C3C	2.89	1.55	1.47
12	C	401	HEM	FE-NC	2.88	2.04	1.95
12	N	402	HEM	CAC-C3C	2.88	1.55	1.47
12	C	401	HEM	CAC-C3C	2.88	1.55	1.47
12	N	401	HEM	FE-NC	2.74	2.04	1.95
12	N	401	HEM	FE-NA	2.74	2.04	1.95
13	O	301	HEC	C3B-C2B	-2.17	1.33	1.41
12	C	401	HEM	C2A-C3A	-2.02	1.33	1.38
13	O	301	HEC	C3C-C2C	-2.01	1.34	1.41
13	D	301	HEC	C3D-C2D	-2.00	1.33	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	301	HEC	CBB-CAB-C3B	-2.73	121.98	127.43
13	O	301	HEC	C2A-C1A-NA	-2.47	107.94	110.32
13	D	301	HEC	CAA-CBA-CGA	-2.37	107.37	113.67
12	N	402	HEM	C3B-C2B-C1B	2.31	108.14	106.41
12	N	402	HEM	C4D-ND-C1D	2.29	107.92	105.21
13	D	301	HEC	CBB-CAB-C3B	-2.27	122.90	127.43
13	D	301	HEC	CBC-CAC-C3C	-2.26	122.91	127.43
12	C	401	HEM	C4D-ND-C1D	2.20	107.81	105.21
12	C	401	HEM	C3B-C2B-C1B	2.19	108.05	106.41
12	N	401	HEM	C4D-ND-C1D	2.17	107.78	105.21
12	C	402	HEM	C4D-ND-C1D	2.17	107.78	105.21
12	C	402	HEM	C3B-C2B-C1B	2.16	108.03	106.41
13	O	301	HEC	CBC-CAC-C3C	-2.13	123.17	127.43
12	C	401	HEM	C1B-NB-C4B	2.08	107.67	105.21
12	C	402	HEM	C3D-C4D-ND	-2.08	107.89	110.17
12	N	402	HEM	C1B-NB-C4B	2.06	107.64	105.21
12	N	401	HEM	C1B-NB-C4B	2.04	107.62	105.21
13	O	301	HEC	C3D-C4D-ND	-2.04	107.89	110.15
12	N	402	HEM	C3D-C4D-ND	-2.04	107.94	110.17
12	N	401	HEM	C3B-C2B-C1B	2.03	107.94	106.41
13	O	301	HEC	CAA-CBA-CGA	-2.02	108.32	113.67

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	402	HEM	C1A-C2A-CAA-CBA
12	N	402	HEM	C3D-CAD-CBD-CGD
12	C	402	HEM	C3D-CAD-CBD-CGD
13	D	301	HEC	C1A-C2A-CAA-CBA
12	N	401	HEM	C4D-C3D-CAD-CBD
12	N	401	HEM	C2D-C3D-CAD-CBD
13	D	301	HEC	C3A-C2A-CAA-CBA
12	N	401	HEM	C2A-CAA-CBA-CGA
12	C	402	HEM	C3A-C2A-CAA-CBA
12	C	401	HEM	CAA-CBA-CGA-O1A
12	N	401	HEM	C3D-CAD-CBD-CGD
12	C	401	HEM	CAA-CBA-CGA-O2A
13	O	301	HEC	C3D-CAD-CBD-CGD
12	C	402	HEM	CAA-CBA-CGA-O2A
12	C	402	HEM	CAA-CBA-CGA-O1A
12	N	402	HEM	CAA-CBA-CGA-O2A
12	C	401	HEM	C2A-CAA-CBA-CGA
12	N	401	HEM	CAA-CBA-CGA-O1A
12	N	402	HEM	CAA-CBA-CGA-O1A
12	C	401	HEM	CAD-CBD-CGD-O2D
13	O	301	HEC	CAD-CBD-CGD-O2D

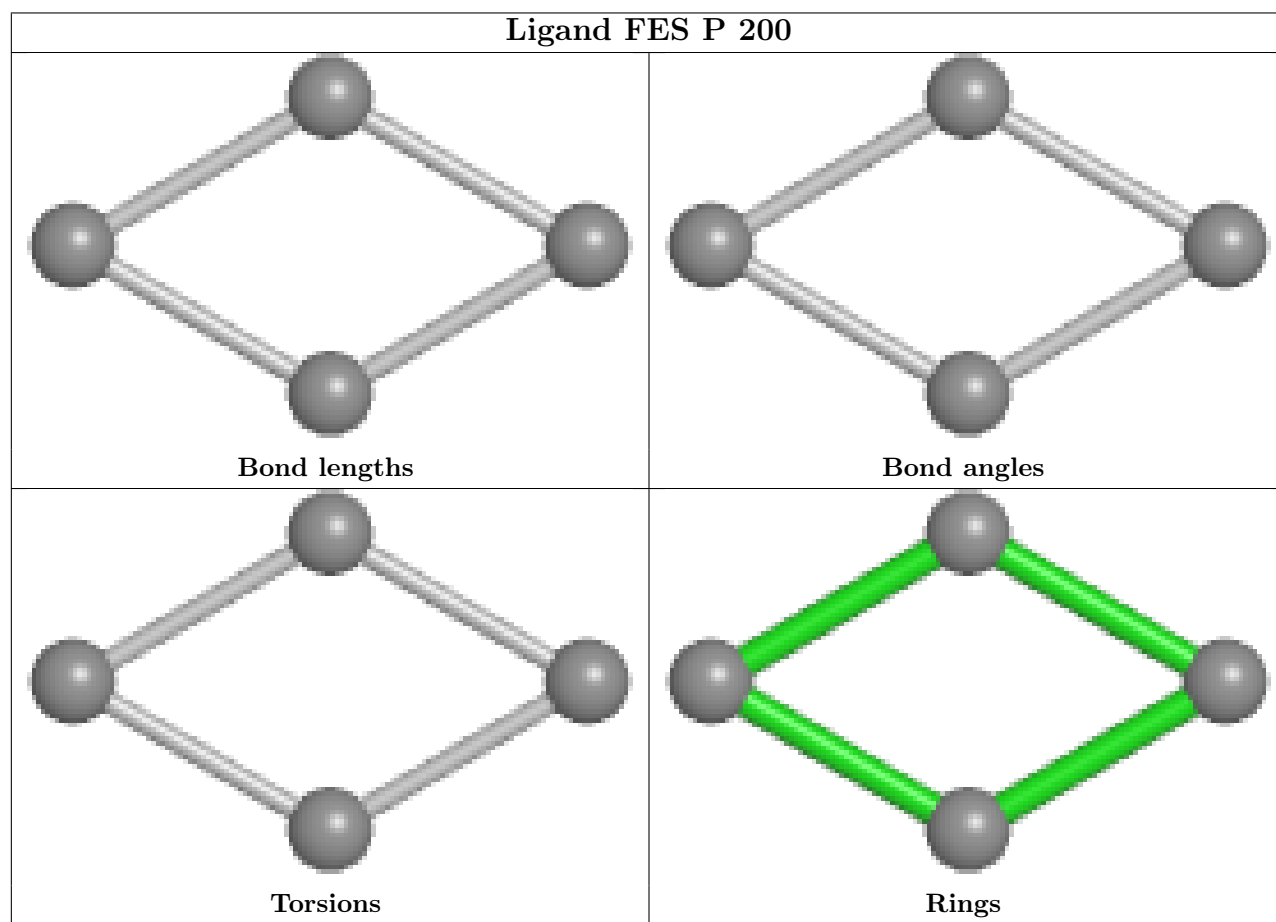
There are no ring outliers.

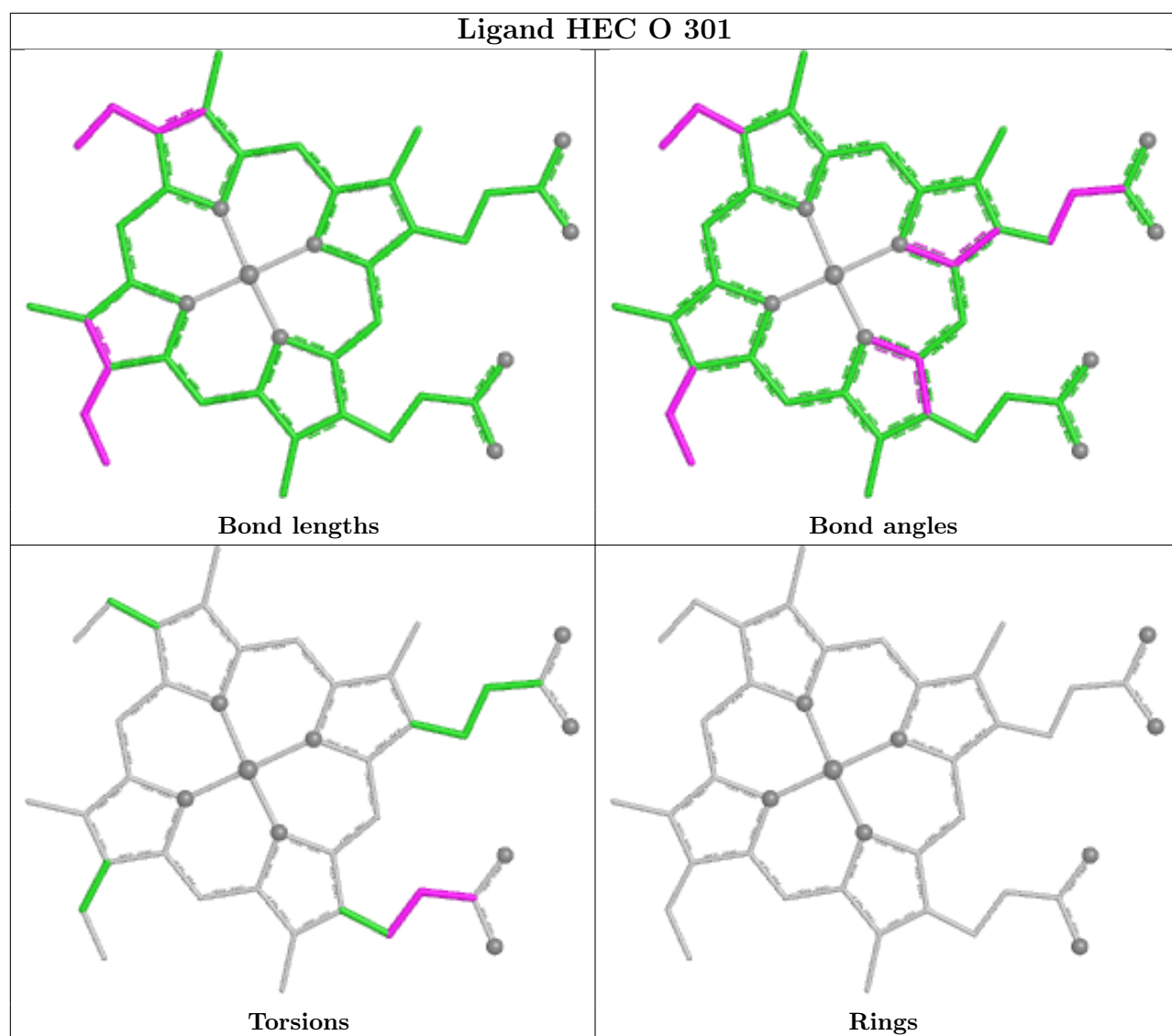
8 monomers are involved in 28 short contacts:

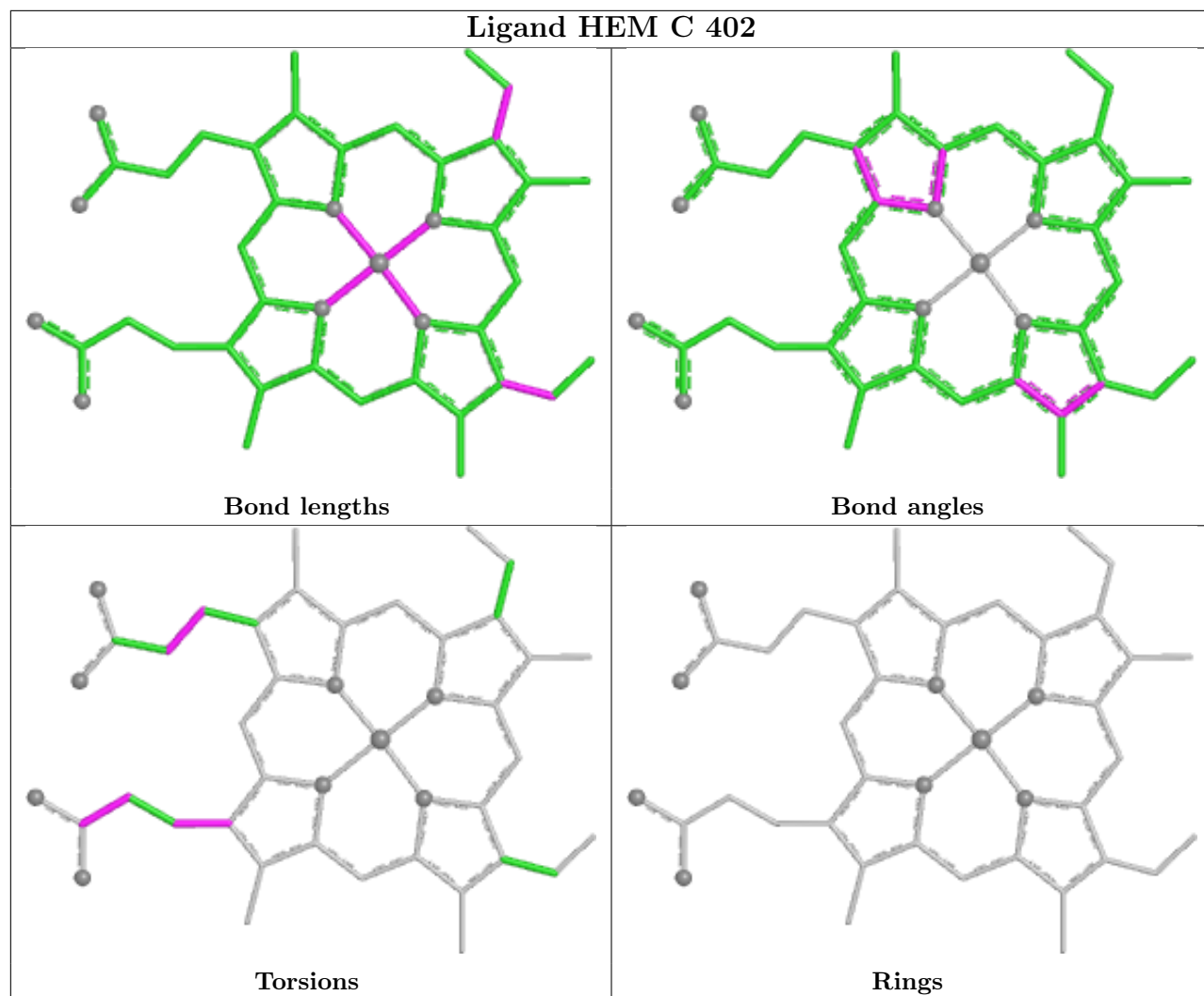
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	P	200	FES	2	0
13	O	301	HEC	3	0
12	C	402	HEM	5	0
12	N	401	HEM	5	0
12	N	402	HEM	5	0
14	E	200	FES	2	0
12	C	401	HEM	4	0
13	D	301	HEC	2	0

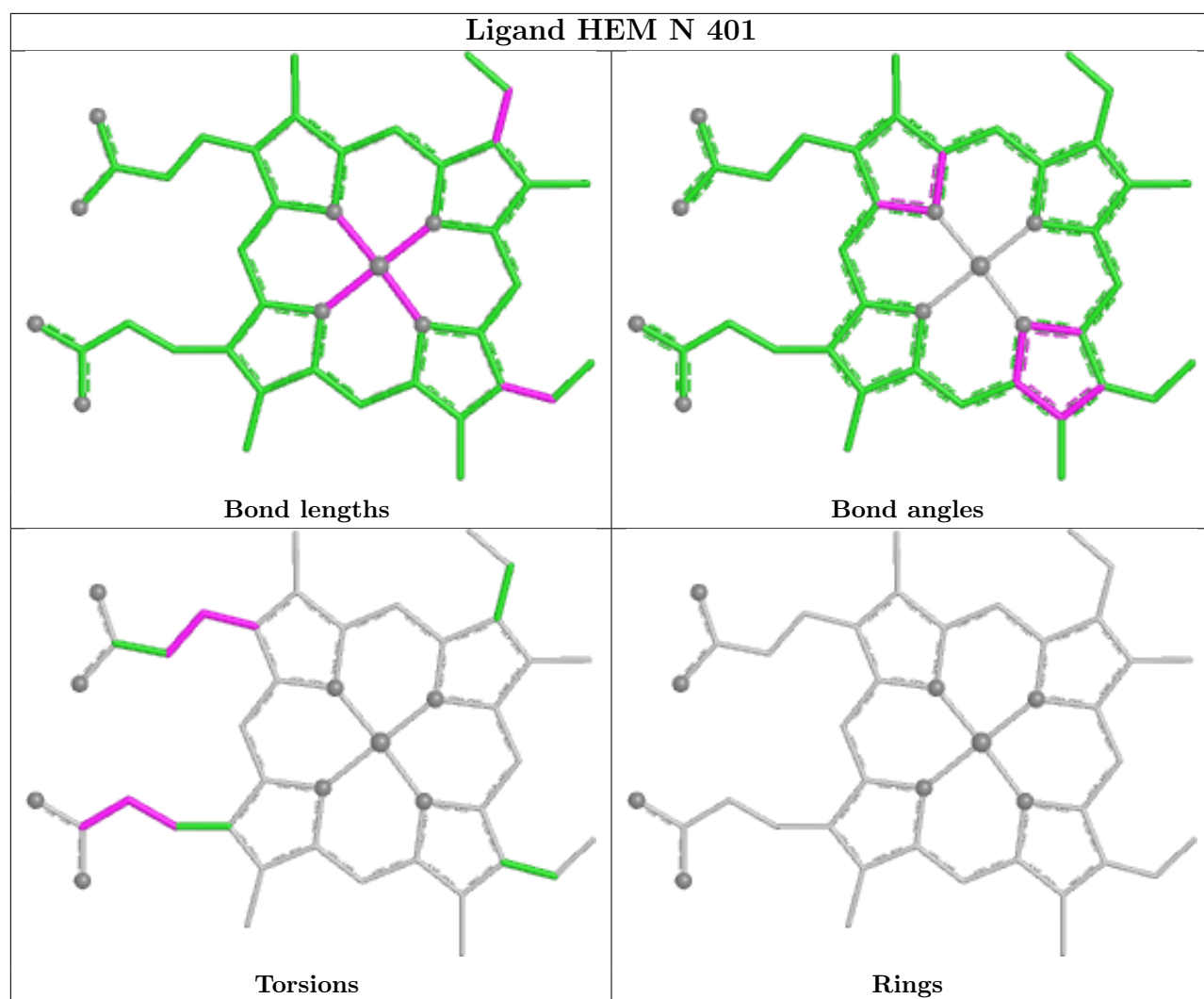
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

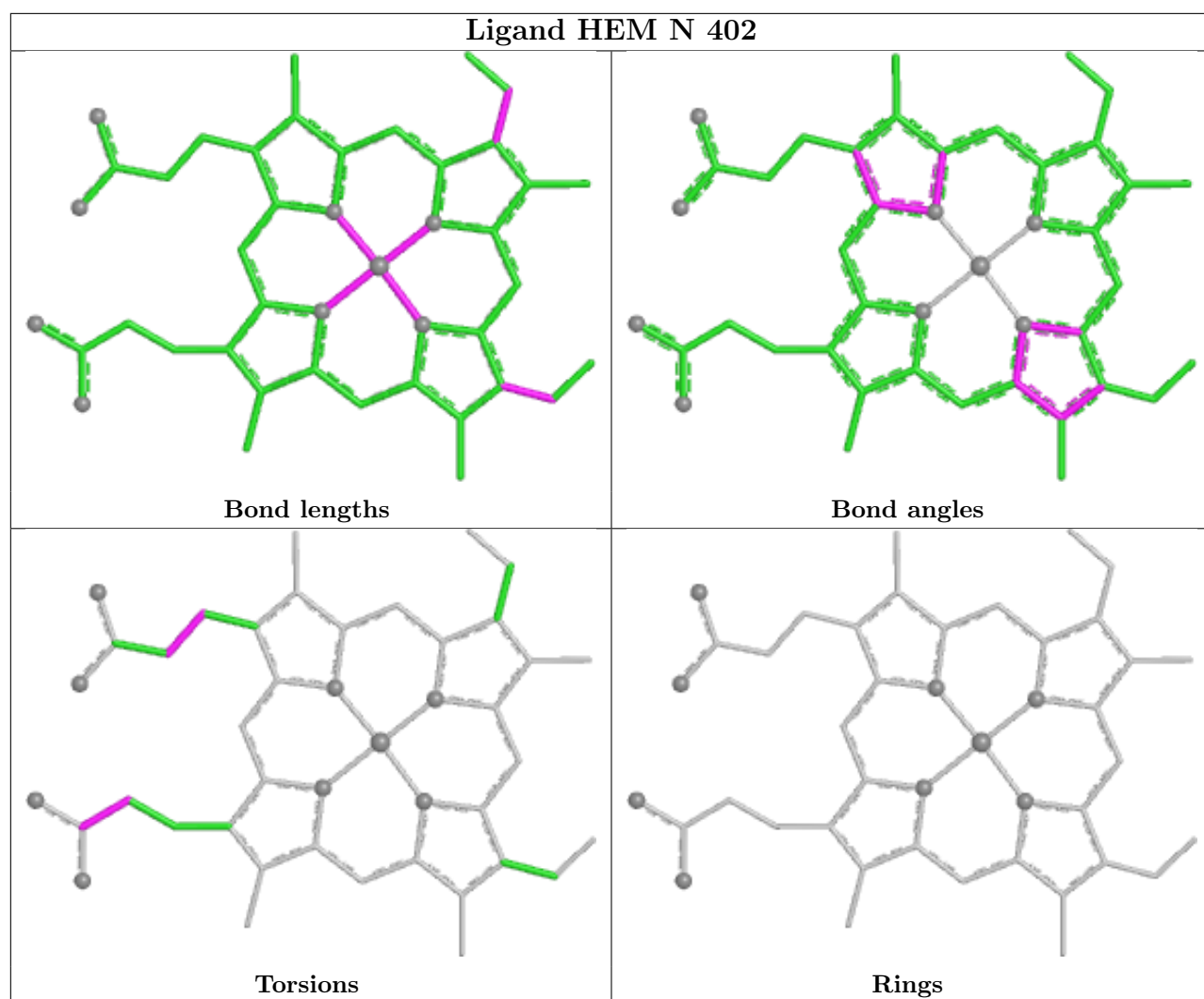
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

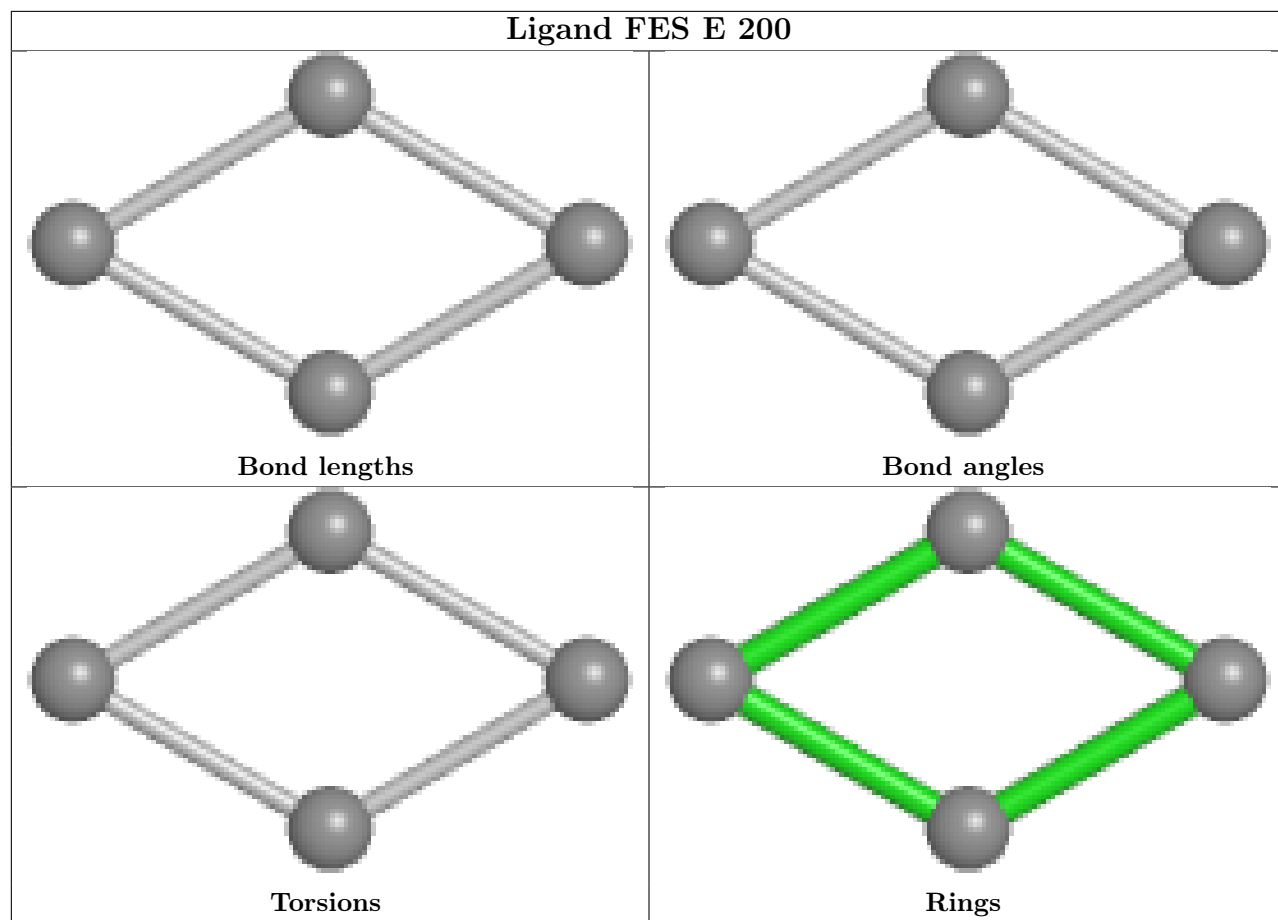


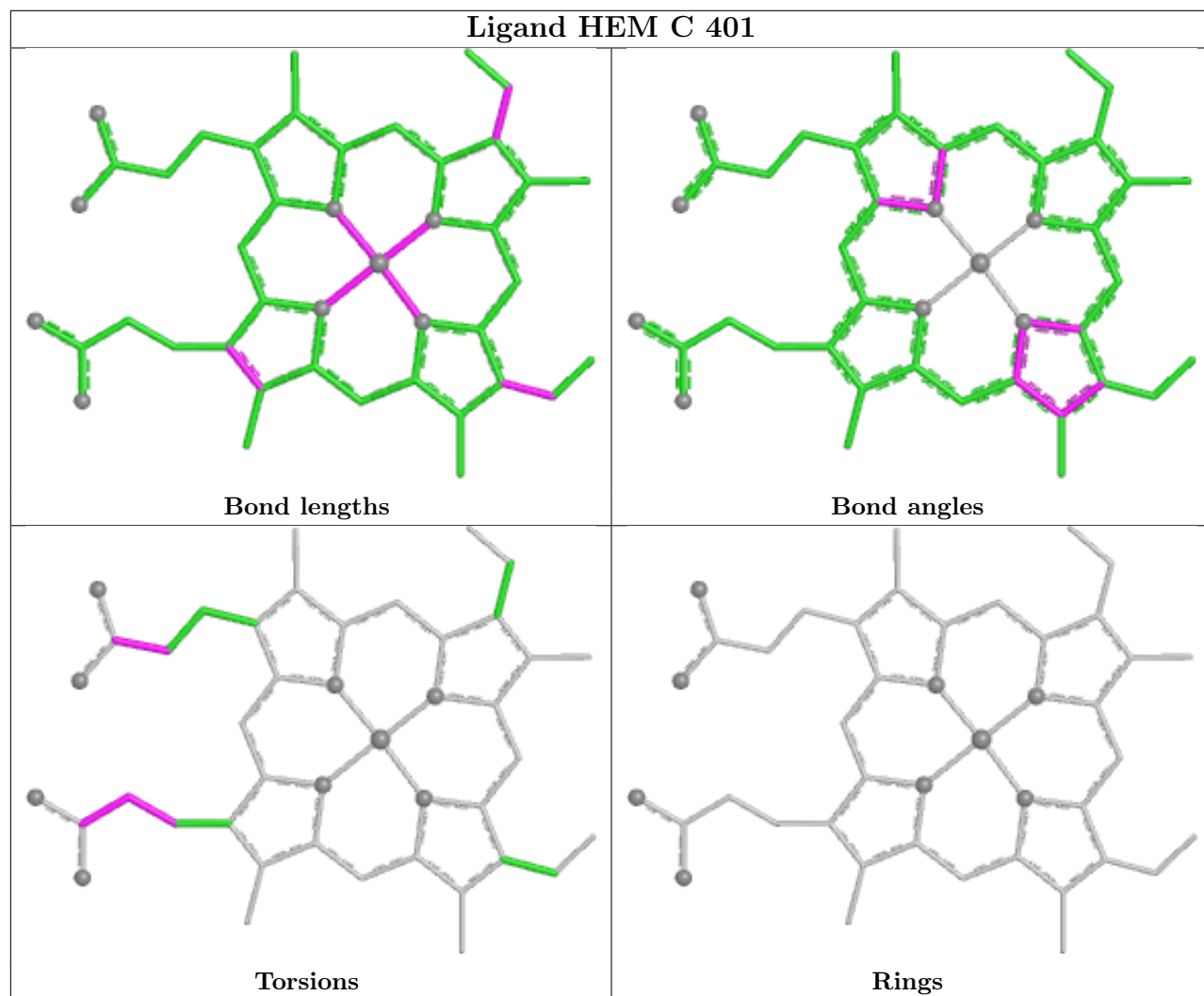


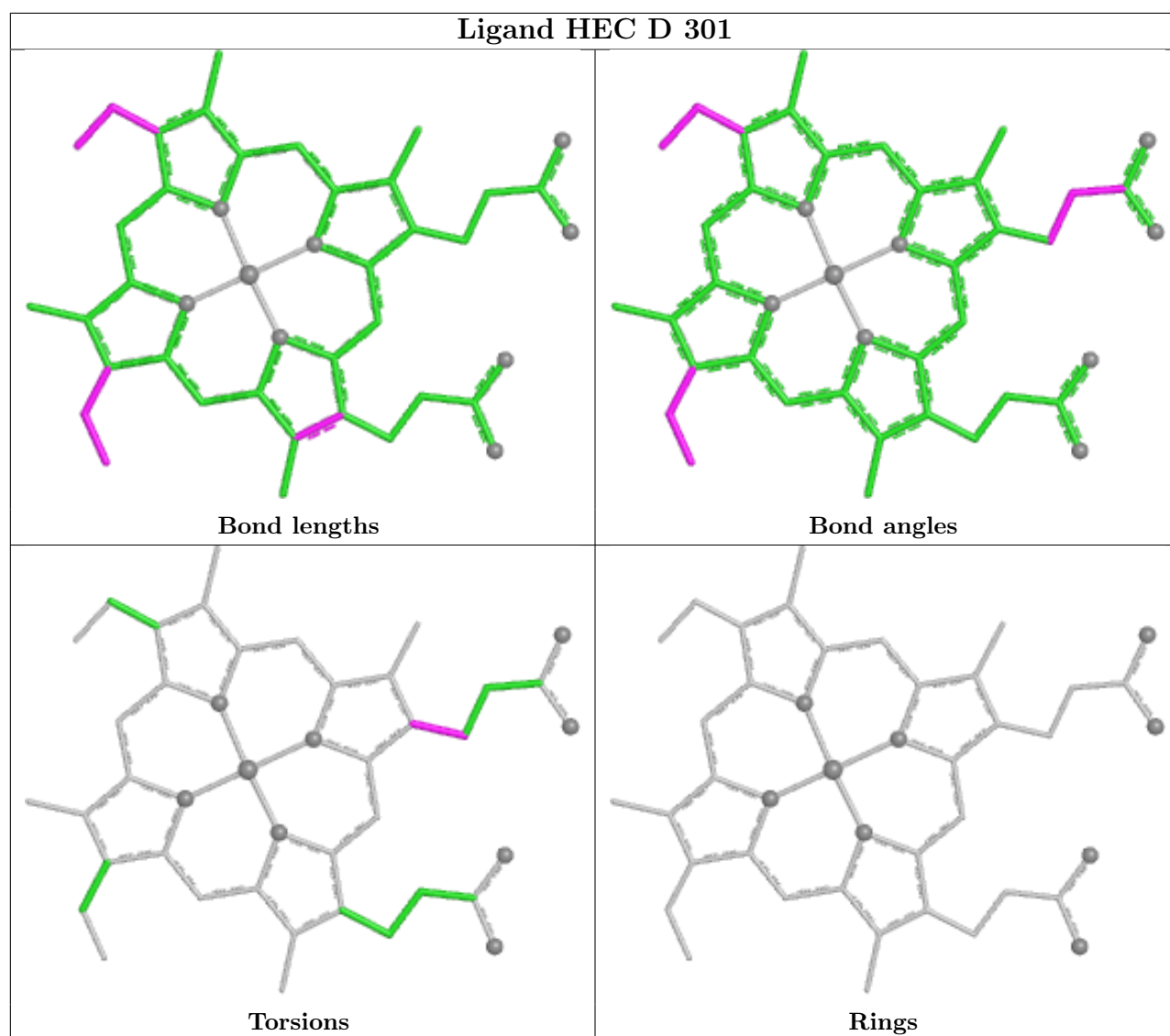












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

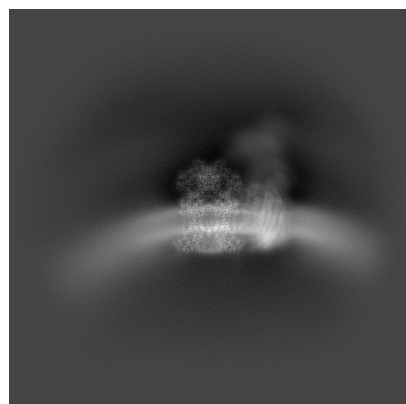
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65583. These allow visual inspection of the internal detail of the map and identification of artifacts.

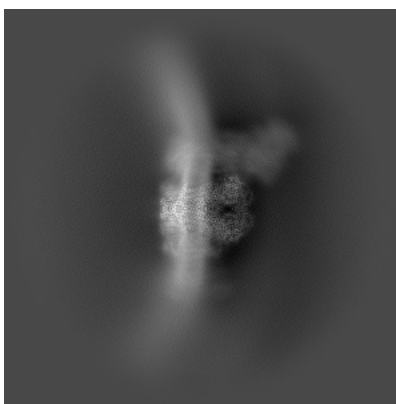
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

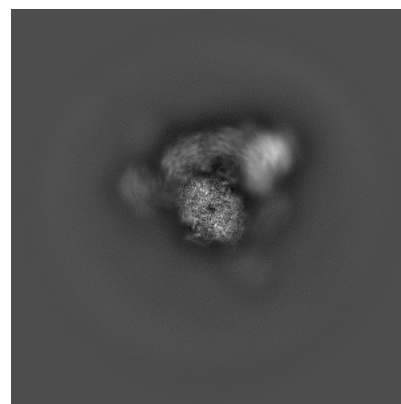
6.1.1 Primary map



X

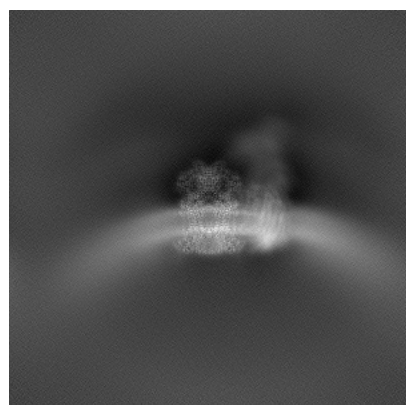


Y

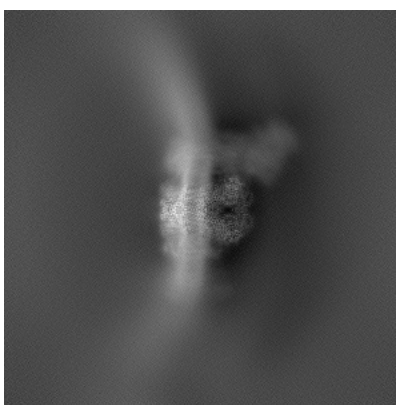


Z

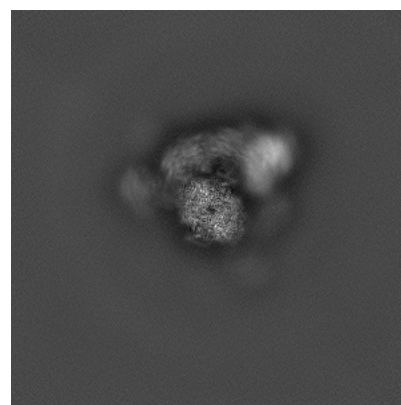
6.1.2 Raw map



X



Y

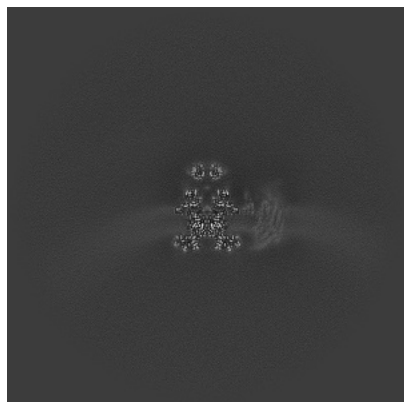


Z

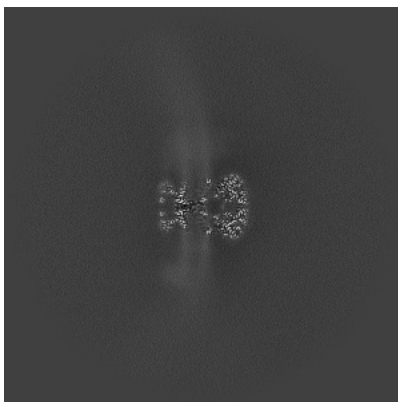
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

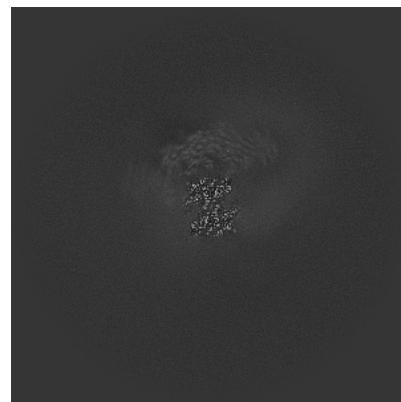
6.2.1 Primary map



X Index: 300

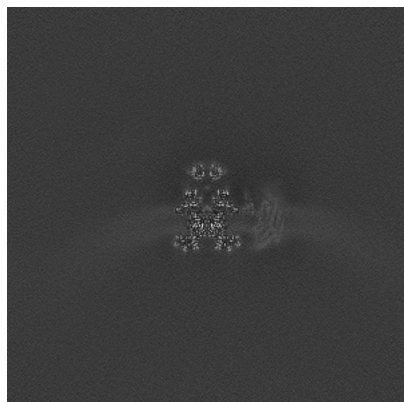


Y Index: 300

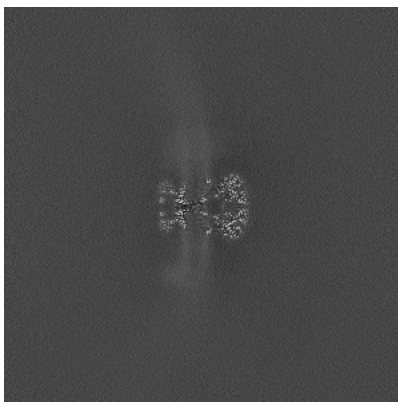


Z Index: 300

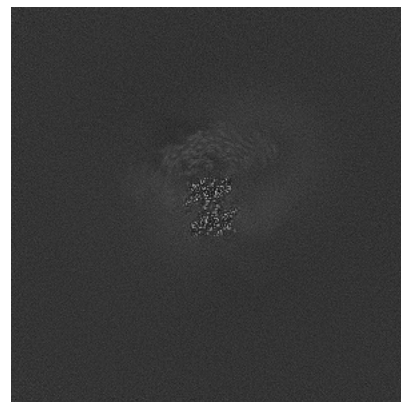
6.2.2 Raw map



X Index: 300



Y Index: 300

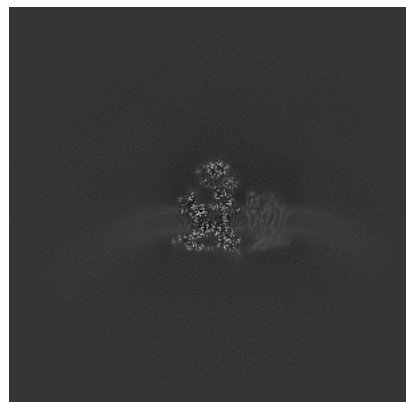


Z Index: 300

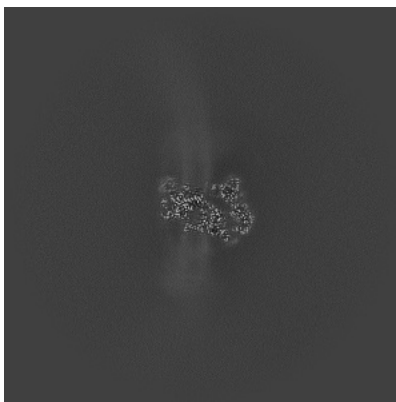
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

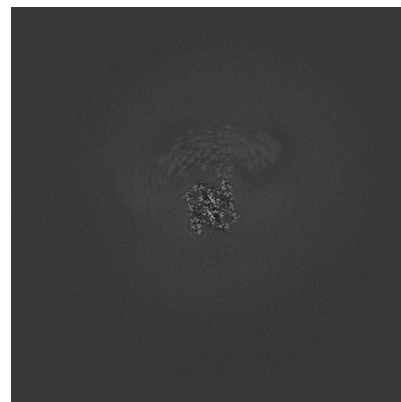
6.3.1 Primary map



X Index: 293

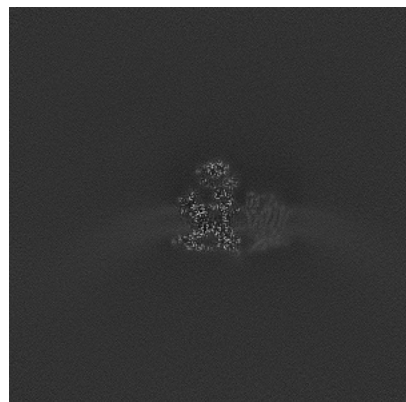


Y Index: 311

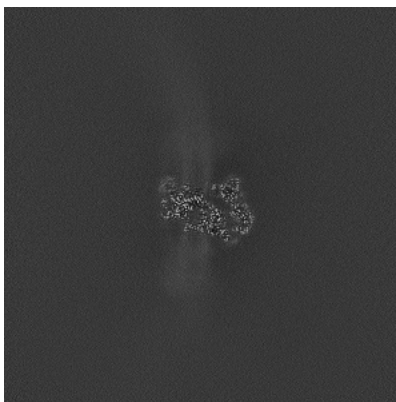


Z Index: 271

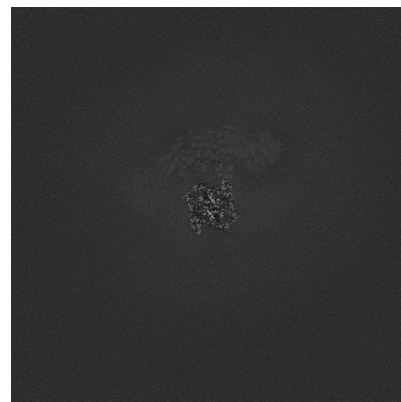
6.3.2 Raw map



X Index: 293



Y Index: 311

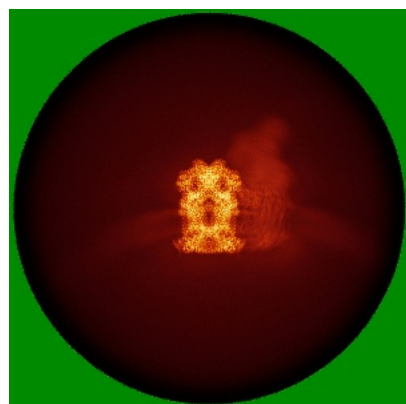


Z Index: 271

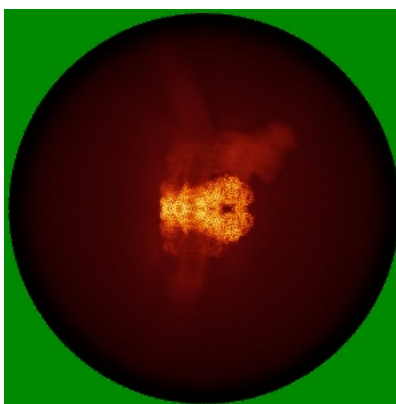
The images above show the largest variance slices of the map in three orthogonal directions.

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

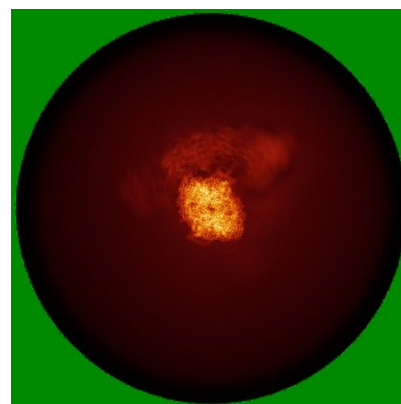
6.4.1 Primary map



X

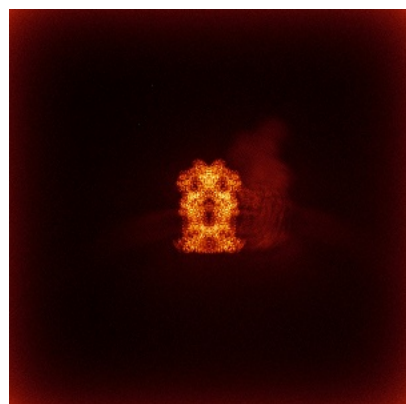


Y

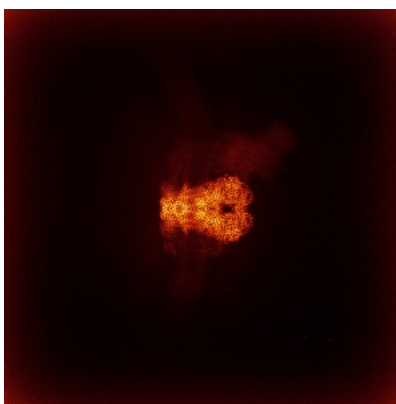


Z

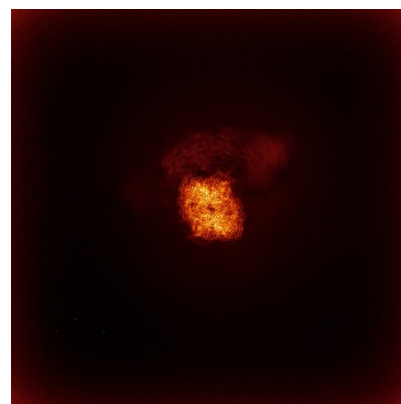
6.4.2 Raw map



X



Y

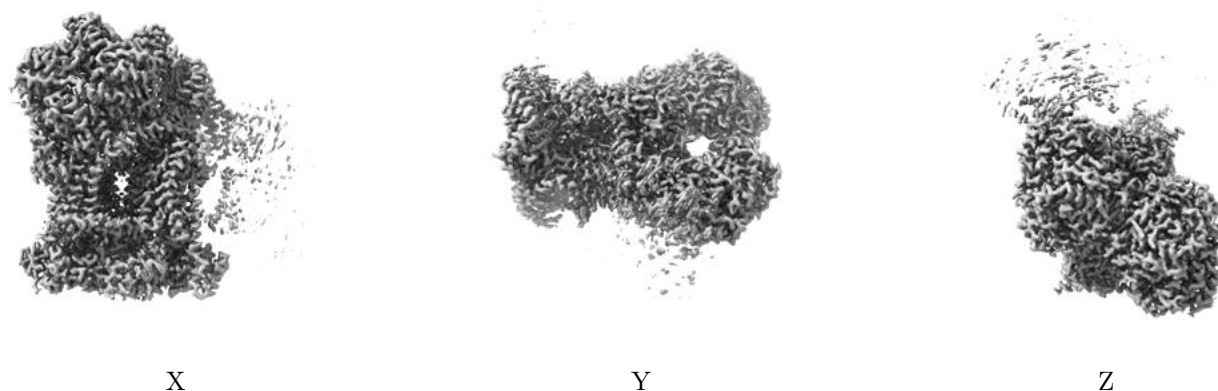


Z

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.

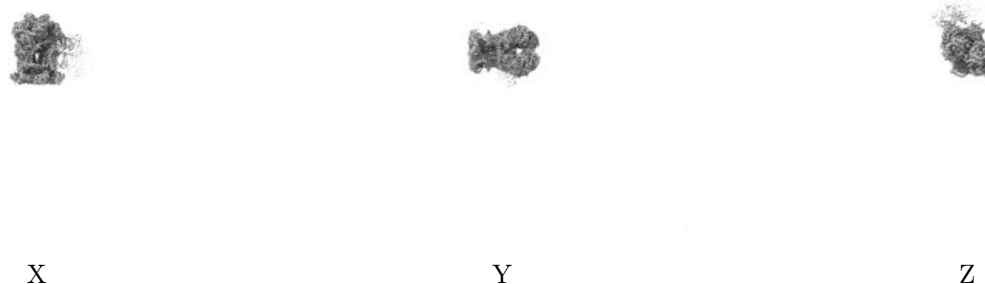
6.5 Orthogonal surface views [i](#)

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.

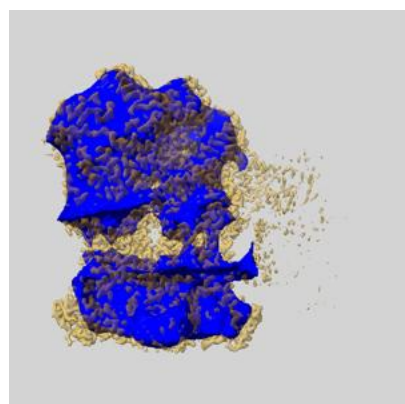
6.6 Mask visualisation [i](#)

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

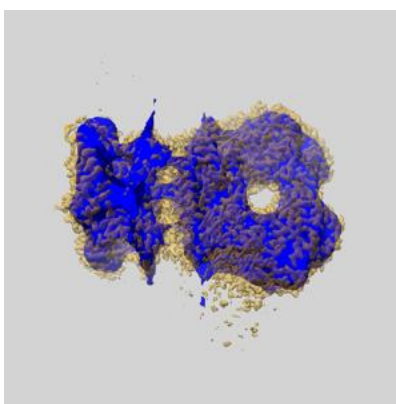
A mask typically either:

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

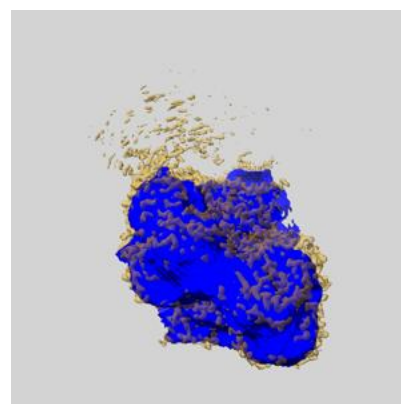
6.6.1 emd_65583_msk_1.map [i](#)



X



Y

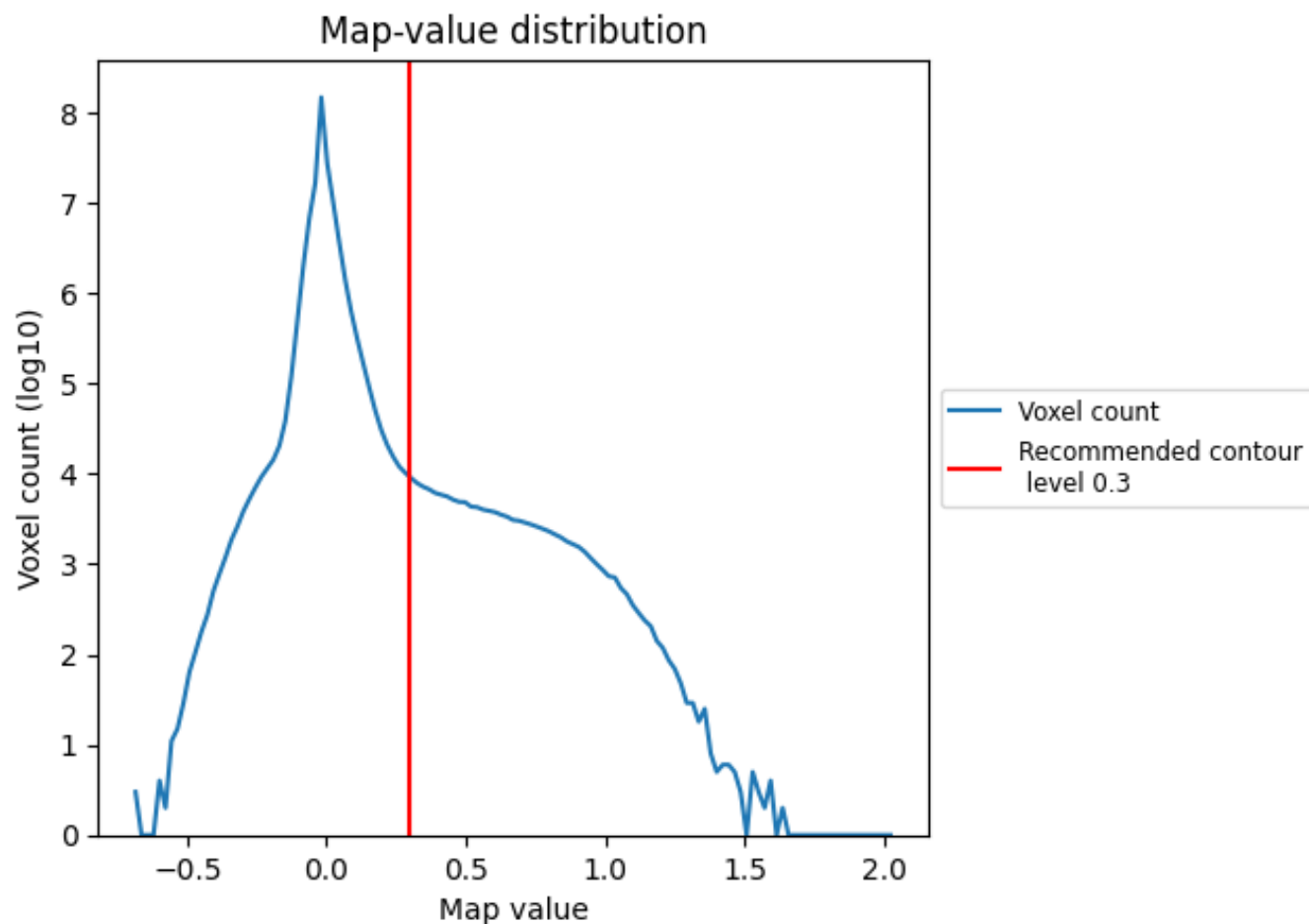


Z

7 Map analysis [i](#)

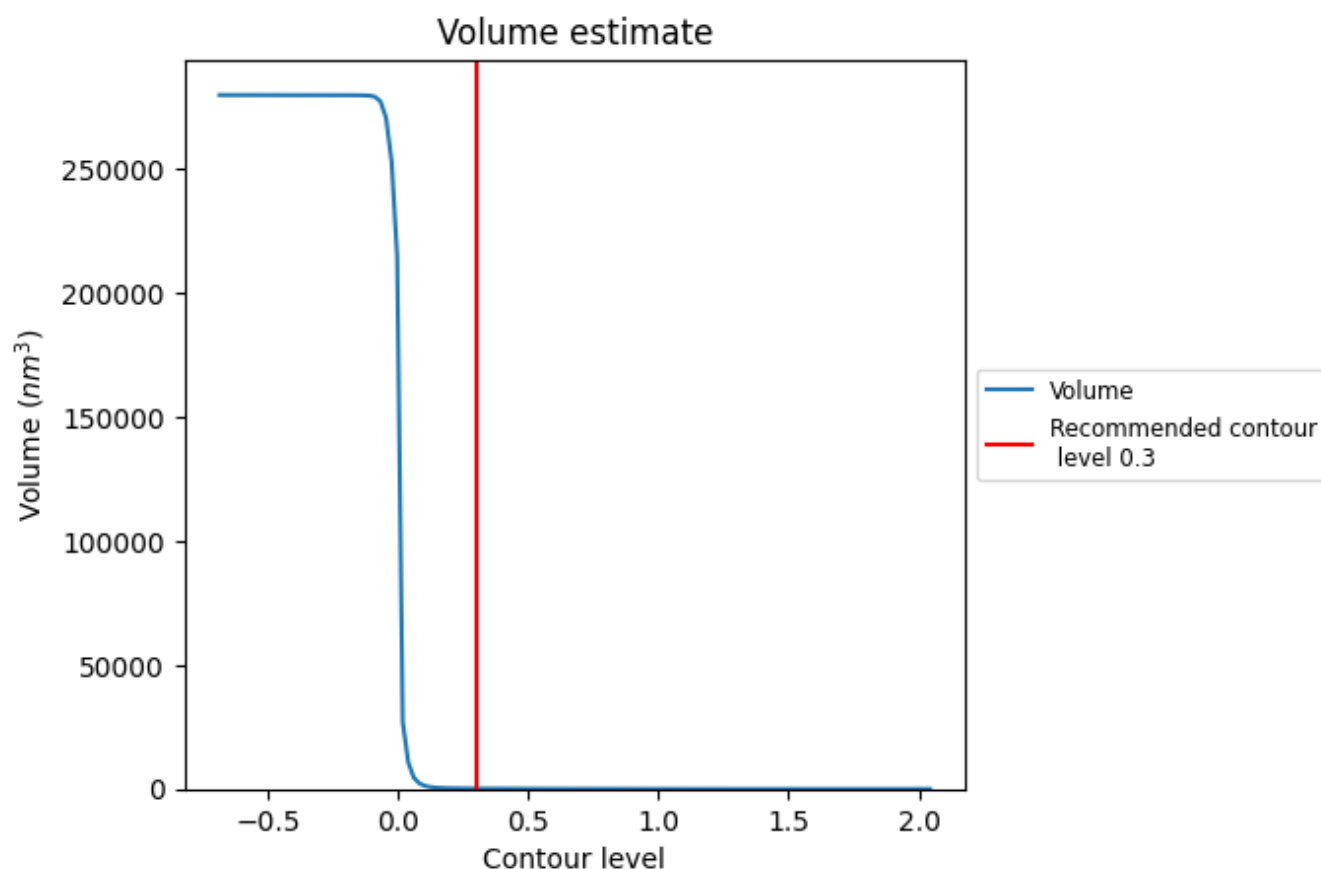
This section contains the results of statistical analysis of the map.

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.

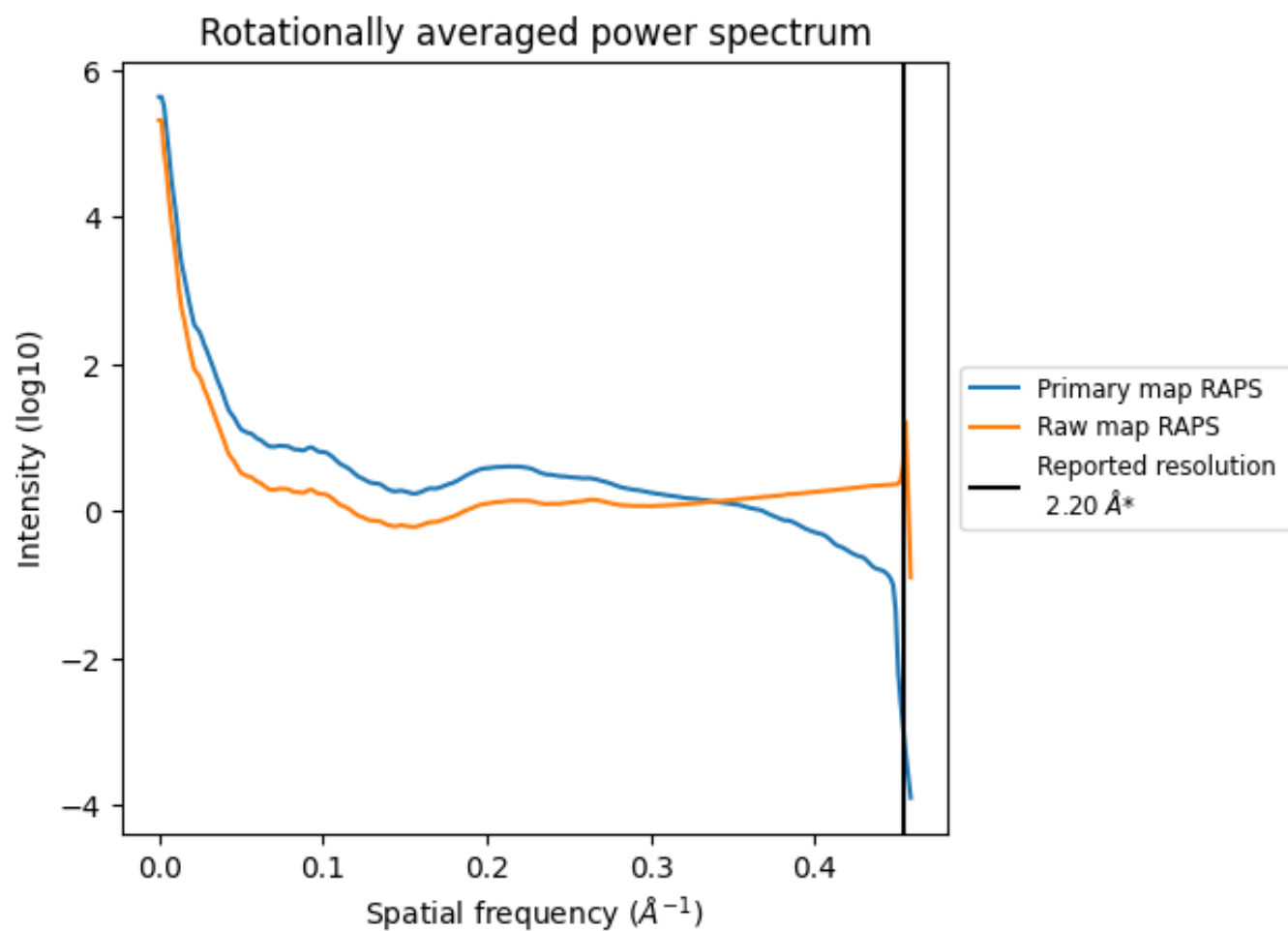
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 166 nm^3 ; this corresponds to an approximate mass of 150 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 ⓘ

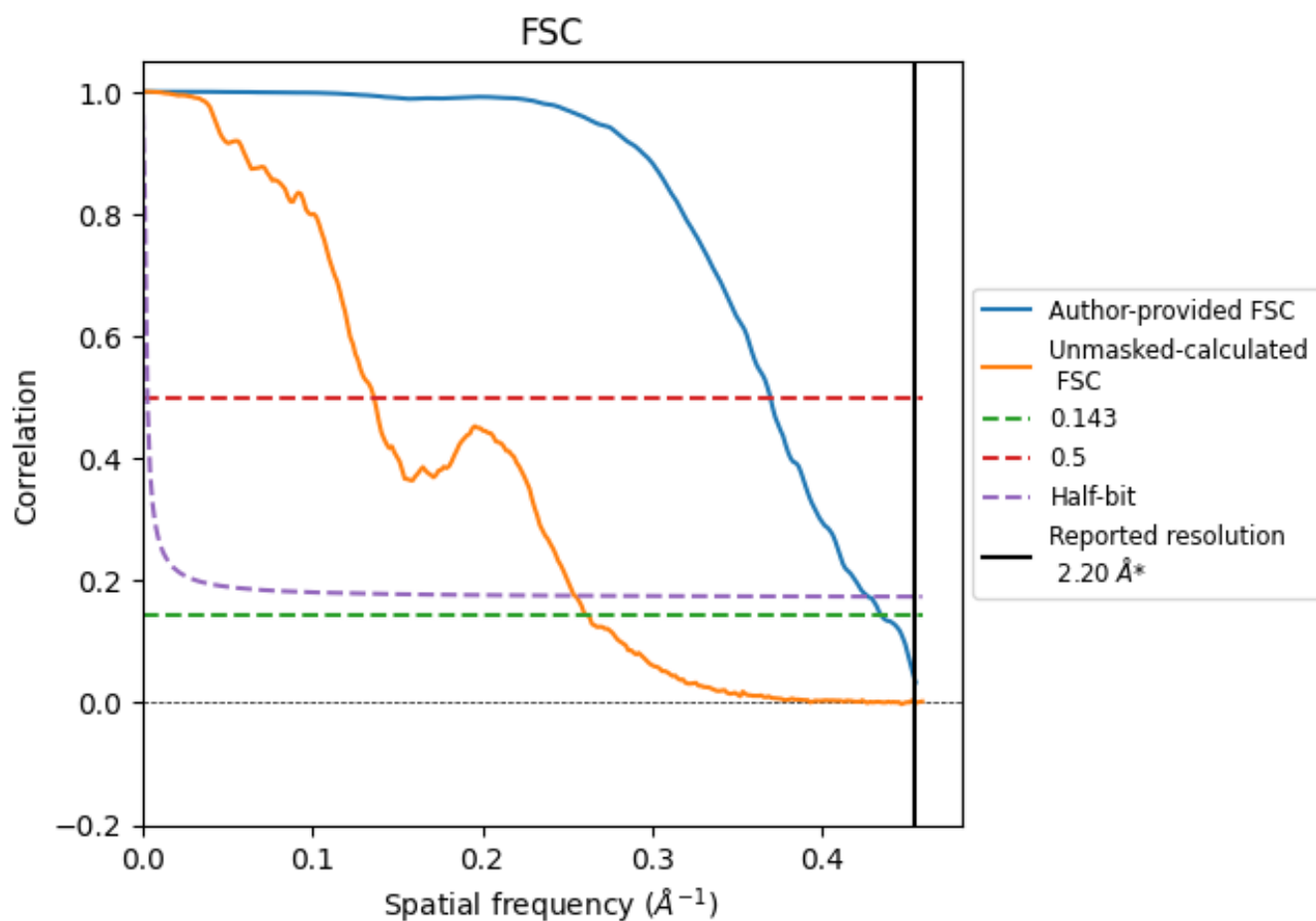


*Reported resolution corresponds to spatial frequency of 0.455 \AA^{-1}

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 0.455 Å⁻¹

8.2 Resolution estimates [i](#)

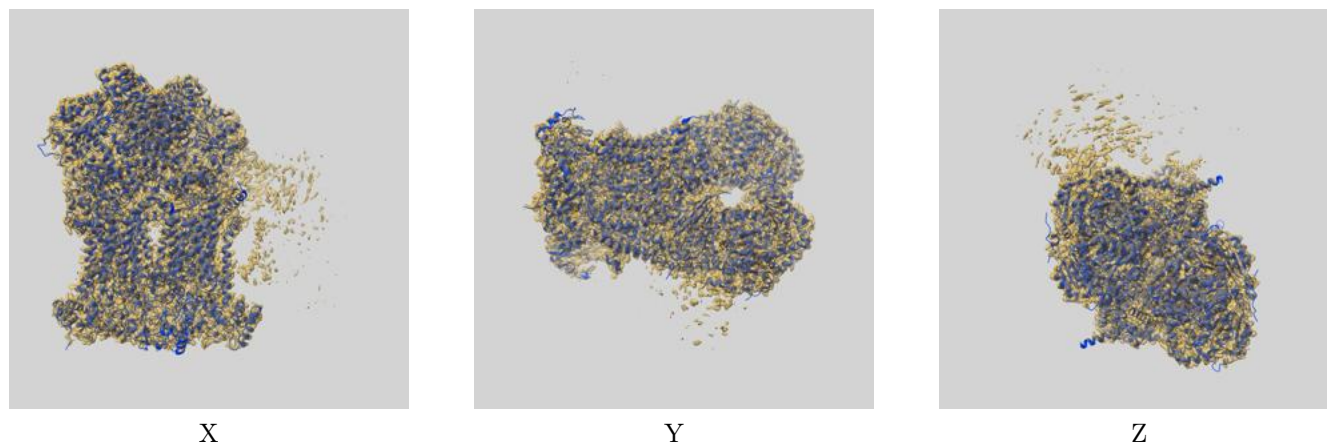
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.30	2.71	2.34
Unmasked-calculated*	3.82	7.34	3.93

*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 3.82 differs from the reported value 2.2 by more than 10 %

9 Map-model fit [i](#)

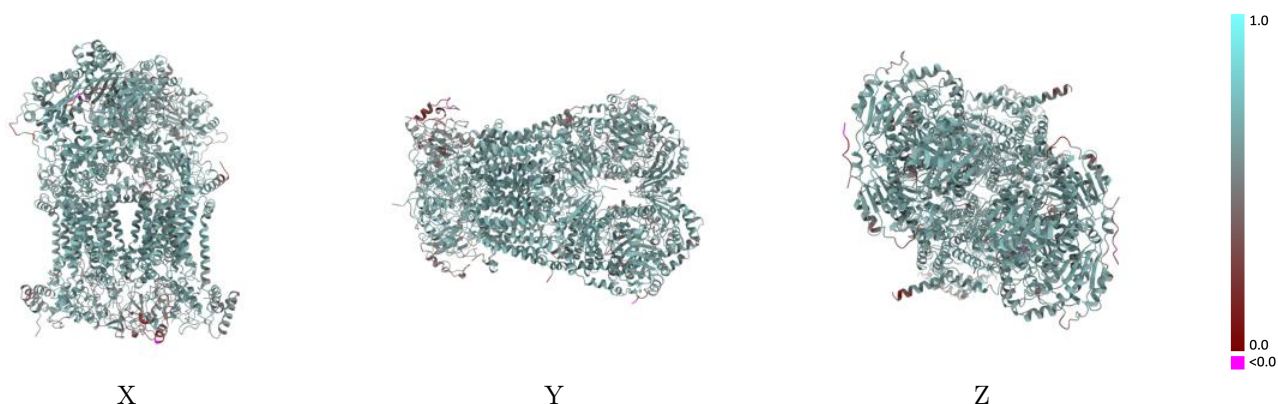
This section contains information regarding the fit between EMDB map EMD-65583 and PDB model 9W2X. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



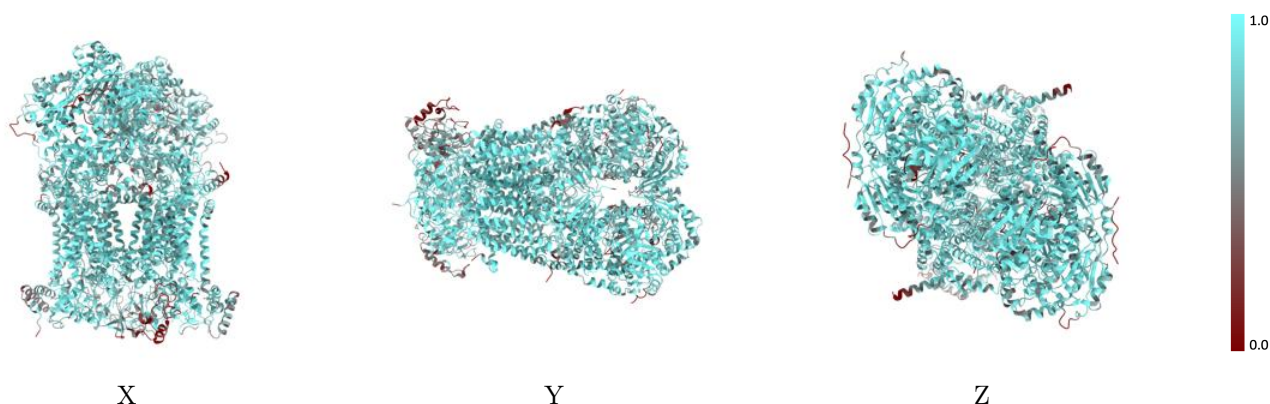
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



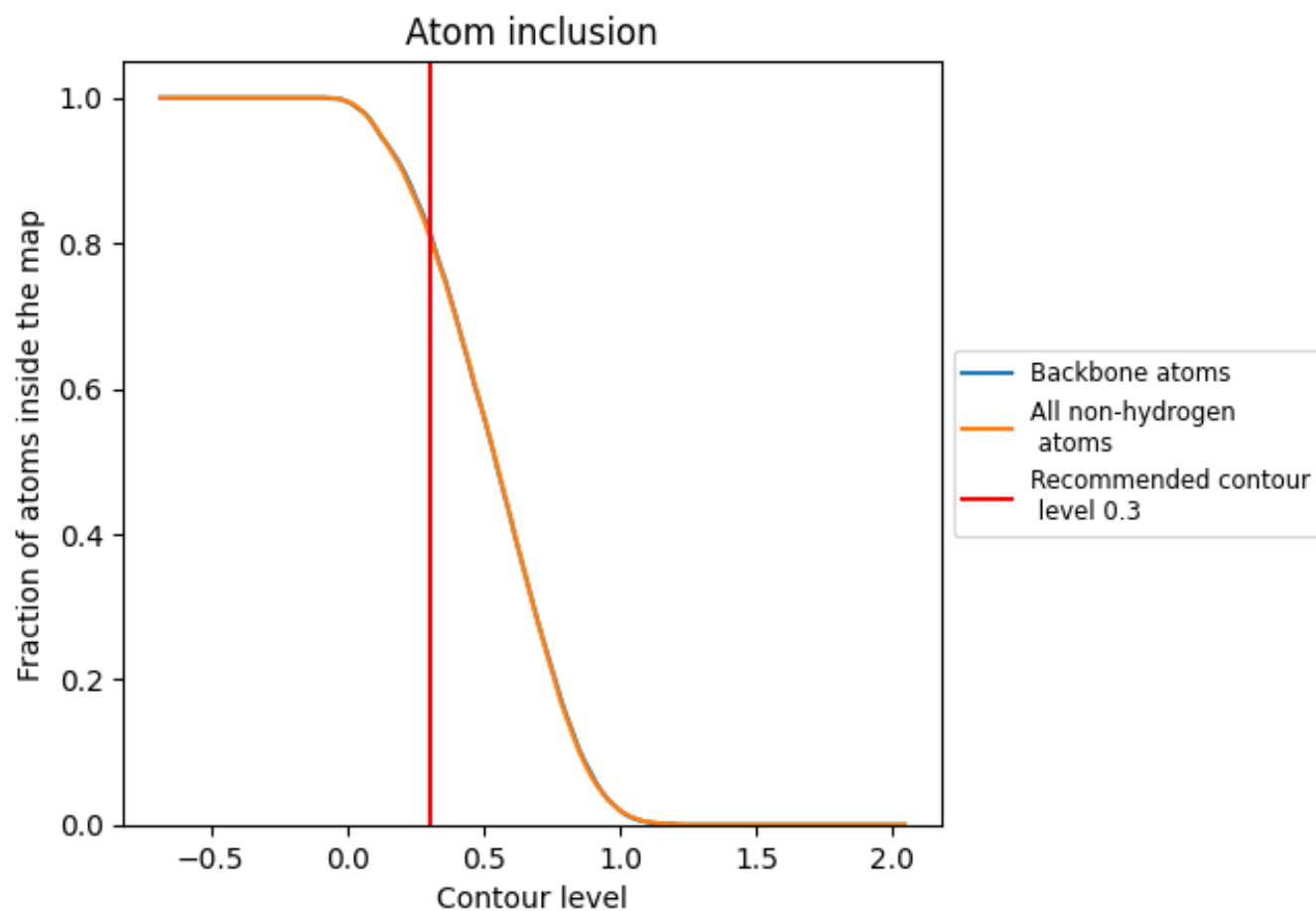
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



At the recommended contour level, 82% of all backbone atoms, 81% 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	 0.8120	 0.5980
A	 0.8810	 0.6250
B	 0.8530	 0.6040
C	 0.9040	 0.6420
D	 0.8910	 0.6190
E	 0.7420	 0.5470
F	 0.7890	 0.5980
G	 0.8220	 0.5940
H	 0.6750	 0.5420
I	 0.3570	 0.3980
J	 0.8190	 0.5990
K	 0.7270	 0.5720
L	 0.8540	 0.6190
M	 0.8340	 0.6030
N	 0.9040	 0.6430
O	 0.8730	 0.6130
P	 0.5640	 0.4960
Q	 0.7950	 0.5900
R	 0.8020	 0.5870
S	 0.5020	 0.4880
T	 0.3010	 0.3730
U	 0.8210	 0.5990
V	 0.7200	 0.5730

