



# Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 07:20 AM EDT

PDB ID : 7TZ6  
EMDB ID : EMD-26203  
Title : Structure of mitochondrial bc1 in complex with ck-2-68  
Authors : Xia, D.; Esser, L.; Zhou, F.; Huang, R.  
Deposited on : 2022-02-15  
Resolution : 2.88 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

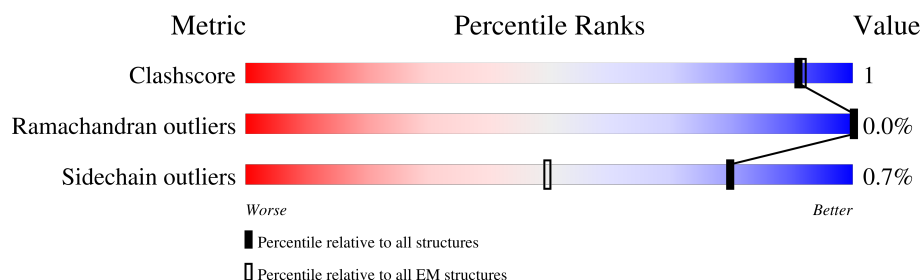
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

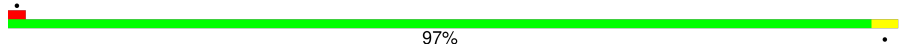
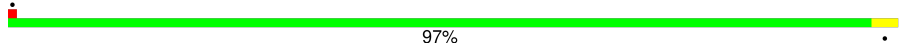
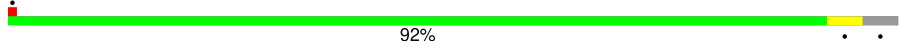
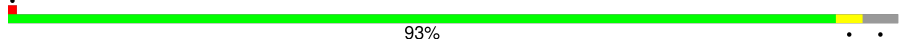
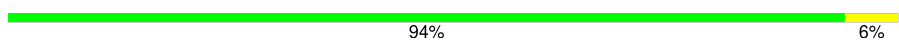
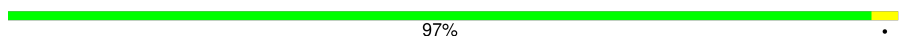
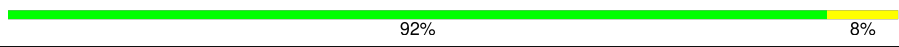
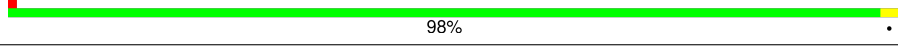
The reported resolution of this entry is 2.88 Å.

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	446	
1	N	446	
2	B	439	
2	O	439	
3	C	379	
3	P	379	
4	D	241	
4	Q	241	

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Mol	Chain	Length	Quality of chain
5	E	196	
5	R	196	
6	F	110	
6	S	110	
7	G	80	
7	T	80	
8	H	78	
8	U	78	
9	I	78	
9	V	78	
10	J	63	
10	W	63	
11	K	56	
11	X	56	

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 65124 atoms, of which 32382 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
			6812	2161	3355	609	667	20		
1	N	446	Total	C	H	N	O	S	0	0
			6812	2161	3355	609	667	20		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	423	Total	C	H	N	O	S	0	0
			6323	1993	3152	562	609	7		
2	O	423	Total	C	H	N	O	S	0	0
			6323	1993	3152	562	609	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
			6067	2013	3065	471	500	18		
3	P	378	Total	C	H	N	O	S	0	0
			6067	2013	3065	471	500	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
			3786	1225	1868	330	348	15		
4	Q	241	Total	C	H	N	O	S	0	0
			3786	1225	1868	330	348	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
			3021	957	1503	263	290	8		
5	R	196	Total	C	H	N	O	S	0	0
			3021	957	1503	263	290	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
			1816	576	906	166	166	2		
6	S	105	Total	C	H	N	O	S	0	0
			1816	576	906	166	166	2		

- 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
			1264	410	636	118	99	1		
7	T	75	Total	C	H	N	O	S	0	0
			1264	410	636	118	99	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
			1077	332	530	99	111	5		
8	U	67	Total	C	H	N	O	S	0	0
			1077	332	530	99	111	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	20	Total	C	H	N	O	0	0
			272	82	140	25	25		
9	V	20	Total	C	H	N	O	0	0
			272	82	140	25	25		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	60	Total	C	H	N	O	0	0
			988	324	493	86	85		

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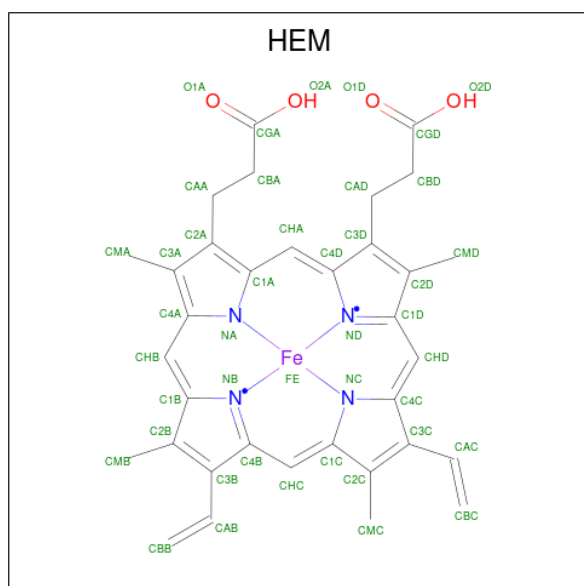
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Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	60	Total	C	H	N	O	0	0
			988	324	493	86	85		

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 10.

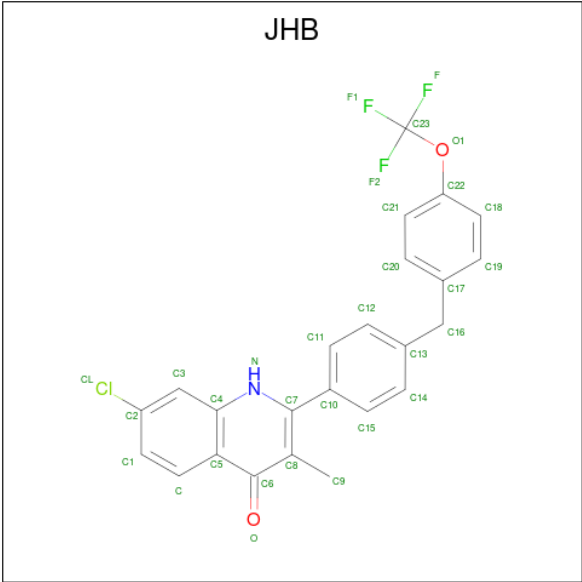
Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	52	Total 863	C 287	H 434	N 76	O 65	S 1	0	0
11	X	52	Total 863	C 287	H 434	N 76	O 65	S 1	0	0

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



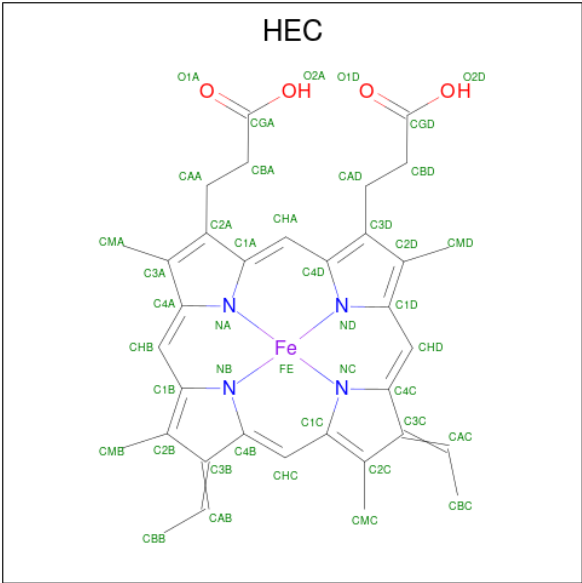
Mol	Chain	Residues	Atoms						AltConf
12	C	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0
12	C	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0
12	P	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0
12	P	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0

- Molecule 13 is 7-chloranyl-3-methyl-2-[4-[[4-(trifluoromethoxy)phenyl]methyl]phenyl]-1 {H}-quinolin-4-one (three-letter code: JHB) (formula:  $C_{24}H_{17}ClF_3NO_2$ ) (labeled as "Ligand of Interest" by depositor).



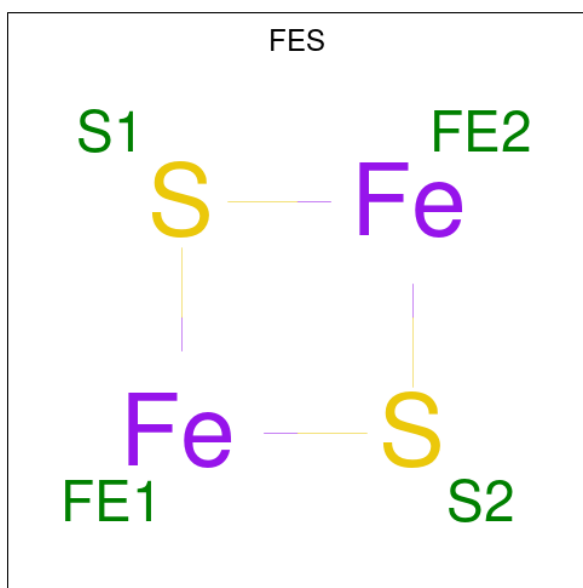
Mol	Chain	Residues	Atoms							AltConf
			Total	C	Cl	F	H	N	O	
13	C	1	48	24	1	3	17	1	2	0
13	P	1	48	24	1	3	17	1	2	0

- Molecule 14 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
14	D	1	75	34	1	32	4	4	0
14	Q	1	75	34	1	32	4	4	0

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



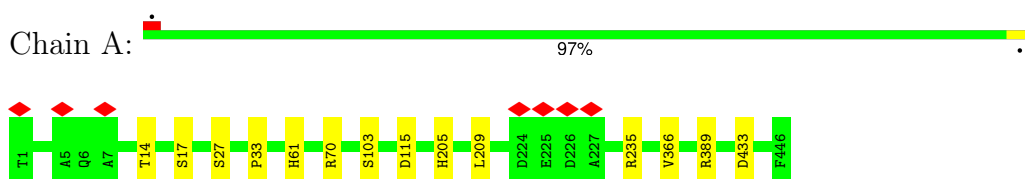
Mol	Chain	Residues	Atoms			AltConf
15	E	1	Total	Fe	S	0
			4	2	2	
15	R	1	Total	Fe	S	0
			4	2	2	



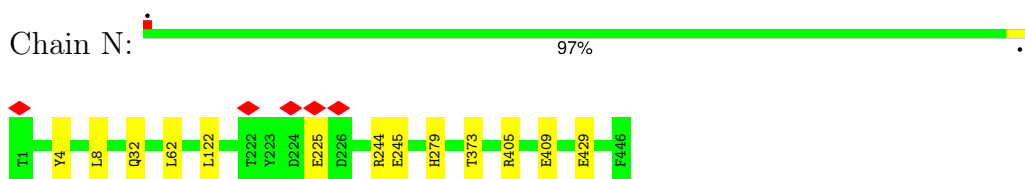
### 3 Residue-property plots

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.

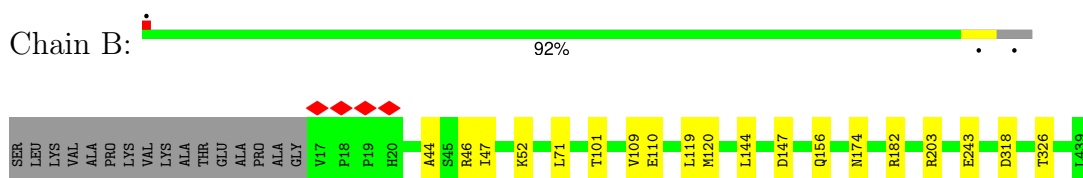
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



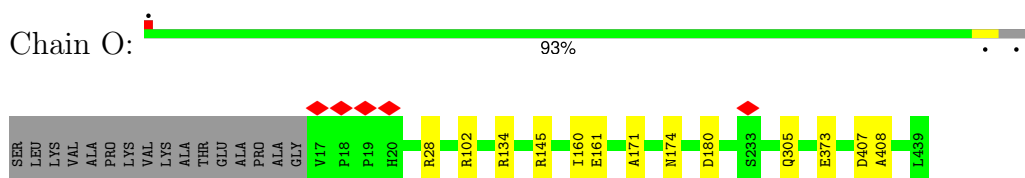
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



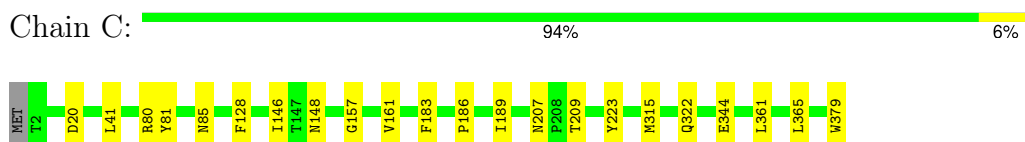
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



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

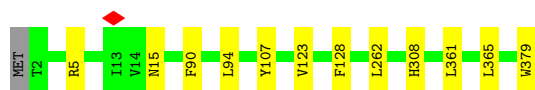


- Molecule 3: Cytochrome b



- Molecule 3: Cytochrome b

Chain P:  97%



- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:  92%



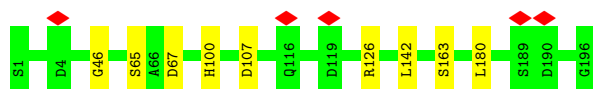
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain Q:  98%



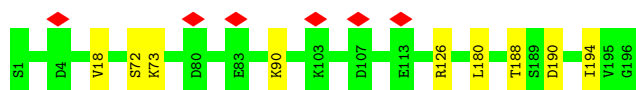
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:  95%



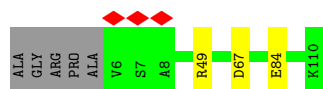
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain R:  95%



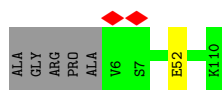
- Molecule 6: Cytochrome b-c1 complex subunit 7

Chain F:  93%



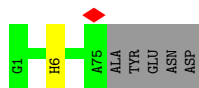
- Molecule 6: Cytochrome b-c1 complex subunit 7

Chain S:  95%



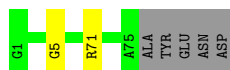
- Molecule 7: Cytochrome b-c1 complex subunit 8

Chain G: 92% 6%



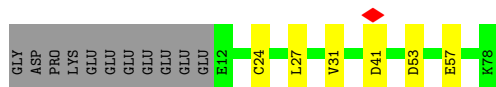
- Molecule 7: Cytochrome b-c1 complex subunit 8

Chain T: 91% 6%



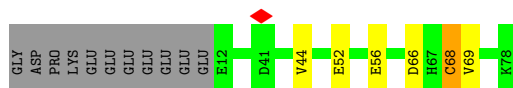
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain H: 78% 8% 14%



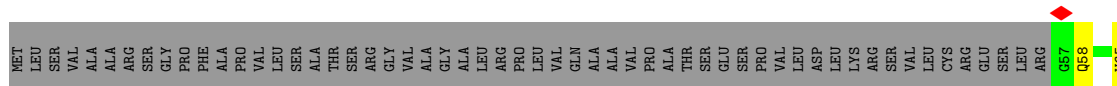
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain U: 78% 6% 14%



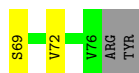
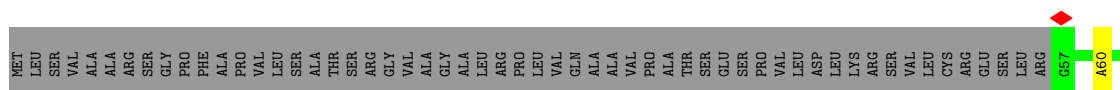
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain I: 23% 74%

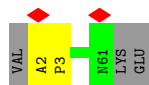


- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

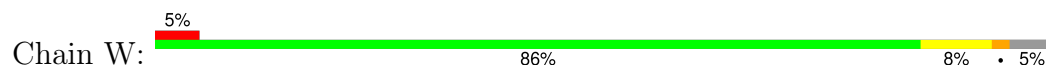
Chain V: 22% 74%



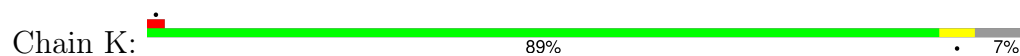
- Molecule 10: Cytochrome b-c1 complex subunit 9



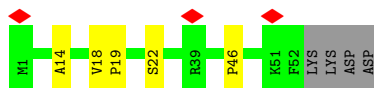
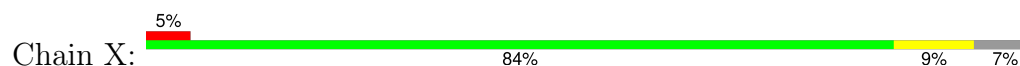
- Molecule 10: Cytochrome b-c1 complex subunit 9



- 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, C1	Depositor
Number of particles used	454182	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 ( $e^-/\text{\AA}^2$ )	50.24	Depositor
Minimum defocus (nm)	630	Depositor
Maximum defocus (nm)	2820	Depositor
Magnification	58275	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	22.098	Depositor
Minimum map value	-15.043	Depositor
Average map value	-0.015	Depositor
Map value standard deviation	0.691	Depositor
Recommended contour level	2.6	Depositor
Map size (Å)	439.296, 439.296, 439.296	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.858, 0.858, 0.858	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, JHB, HEC, 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	0.29	0/3530	0.56	0/4792
1	N	0.30	0/3530	0.60	0/4792
2	B	0.29	0/3231	0.54	0/4386
2	O	0.30	0/3231	0.60	0/4386
3	C	0.31	0/3099	0.50	0/4242
3	P	0.31	0/3099	0.58	0/4242
4	D	0.32	0/1977	0.55	0/2684
4	Q	0.34	0/1977	0.64	0/2684
5	E	0.29	0/1552	0.54	0/2100
5	R	0.30	0/1552	0.61	0/2100
6	F	0.29	0/929	0.57	0/1246
6	S	0.30	0/929	0.63	0/1246
7	G	0.31	0/649	0.62	0/878
7	T	0.32	0/649	0.65	0/878
8	H	0.26	0/552	0.58	0/741
8	U	0.30	0/552	0.66	0/741
9	I	0.24	0/133	0.55	0/182
9	V	0.26	0/133	0.60	0/182
10	J	0.29	0/508	0.52	0/686
10	W	0.33	0/508	0.66	0/686
11	K	0.29	0/445	0.58	0/610
11	X	0.29	0/445	0.65	0/610
All	All	0.30	0/33210	0.58	0/45094

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	3457	3355	3356	8	0
1	N	3457	3355	3356	8	0
2	B	3171	3152	3152	12	0
2	O	3171	3152	3152	8	0
3	C	3002	3065	3065	14	0
3	P	3002	3065	3065	5	0
4	D	1918	1868	1868	12	0
4	Q	1918	1868	1868	3	0
5	E	1518	1503	1503	5	0
5	R	1518	1503	1503	5	0
6	F	910	906	906	2	0
6	S	910	906	906	1	0
7	G	628	636	636	0	0
7	T	628	636	636	2	0
8	H	547	530	530	3	0
8	U	547	530	530	4	0
9	I	132	140	139	2	0
9	V	132	140	139	2	0
10	J	495	493	493	1	0
10	W	495	493	493	3	0
11	K	429	434	434	1	0
11	X	429	434	434	2	0
12	C	86	60	60	6	0
12	P	86	60	60	2	0
13	C	31	17	0	1	0
13	P	31	17	0	0	0
14	D	43	32	30	3	0
14	Q	43	32	30	2	0
15	E	4	0	0	1	0
15	R	4	0	0	0	0
All	All	32742	32382	32344	96	0

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

All (96) 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)
1:A:433:ASP:OD2	3:C:223:TYR:OH	2.04	0.74
4:Q:28:ARG:NE	4:Q:185:ASP:OD2	2.22	0.73
1:N:32:GLN:NE2	2:O:373:GLU:OE2	2.22	0.73
2:O:102:ARG:NH2	2:O:161:GLU:OE1	2.22	0.72
14:Q:1001:HEC:HMC1	14:Q:1001:HEC:HBC3	1.70	0.72
1:N:405:ARG:NH1	1:N:409:GLU:OE2	2.22	0.71
3:P:5:ARG:NH1	3:P:15:ASN:OD1	2.23	0.70
2:O:102:ARG:NH1	2:O:174:ASN:O	2.25	0.68
3:C:207:ASN:OD1	3:C:209:THR:OG1	2.12	0.68
4:D:191:ARG:NH2	4:D:195:GLU:OE1	2.28	0.67
8:U:68:CYS:SG	8:U:69:VAL:N	2.70	0.64
4:D:27:ARG:NH1	4:D:55:CYS:O	2.30	0.64
14:D:1001:HEC:HBC3	14:D:1001:HEC:HMC1	1.78	0.64
4:D:139:THR:OG1	8:H:41:ASP:OD2	2.08	0.63
1:N:244:ARG:NH2	1:N:429:GLU:OE2	2.32	0.62
1:A:70:ARG:NH1	1:A:115:ASP:OD2	2.36	0.58
12:C:1001:HEM:HMC1	12:C:1001:HEM:HBC2	1.84	0.58
2:B:109:VAL:CG1	2:B:119:LEU:HD23	2.34	0.58
1:N:225:GLU:N	1:N:225:GLU:OE1	2.38	0.57
12:C:1002:HEM:HBC2	12:C:1002:HEM:HMC2	1.85	0.57
12:P:1002:HEM:HMC2	12:P:1002:HEM:HBC2	1.85	0.56
5:E:126:ARG:NH2	5:E:180:LEU:O	2.38	0.56
8:H:57:GLU:N	8:H:57:GLU:OE1	2.37	0.55
4:D:72:ASP:OD1	4:D:73:GLY:N	2.40	0.55
2:B:52:LYS:O	2:B:203:ARG:NH2	2.40	0.55
3:P:107:TYR:OH	3:P:308:HIS:ND1	2.26	0.55
2:B:318:ASP:N	2:B:318:ASP:OD1	2.40	0.55
6:S:52:GLU:N	6:S:52:GLU:OE1	2.40	0.54
3:C:146:ILE:HD11	13:C:1003:JHB:C15	2.38	0.53
2:O:160:ILE:HD11	9:V:60:ALA:CB	2.39	0.53
2:B:46:ARG:NH2	2:B:110:GLU:OE1	2.41	0.53
3:C:41:LEU:HD12	12:C:1001:HEM:HBB1	1.91	0.53
12:P:1001:HEM:HMC1	12:P:1001:HEM:HBC2	1.91	0.52
8:U:44:VAL:HG11	8:U:52:GLU:O	2.10	0.52
4:Q:152:TYR:OH	8:U:66:ASP:OD2	2.24	0.52
11:X:14:ALA:O	11:X:18:VAL:HG13	2.10	0.52
1:A:27:SER:OG	1:A:205:HIS:ND1	2.38	0.51
4:D:99:GLU:OE1	4:D:99:GLU:N	2.42	0.51
5:E:163:SER:OG	15:E:1001:FES:S1	2.58	0.51
5:R:72:SER:OG	5:R:73:LYS:N	2.43	0.51
10:W:33:ARG:NH1	10:W:37:GLN:OE1	2.42	0.51
6:F:84:GLU:N	6:F:84:GLU:OE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:128:PHE:CE1	3:C:146:ILE:HD12	2.46	0.51
3:C:148:ASN:ND2	5:E:142:LEU:O	2.42	0.50
1:N:429:GLU:OE1	7:T:5:GLY:N	2.42	0.50
3:C:81:TYR:OH	4:D:118:ARG:NH1	2.45	0.50
3:P:94:LEU:HD11	3:P:123:VAL:HG11	1.94	0.49
2:B:156:GLN:NE2	9:I:58:GLN:O	2.42	0.49
3:C:315:MET:O	3:C:322:GLN:NE2	2.44	0.49
2:O:145:ARG:NH2	2:O:180:ASP:OD1	2.44	0.49
2:B:47:ILE:HD13	2:B:120:MET:CE	2.44	0.48
5:R:188:THR:HG21	5:R:194:ILE:HD12	1.95	0.48
2:B:156:GLN:OE1	2:B:156:GLN:N	2.45	0.48
1:N:4:TYR:CE2	1:N:8:LEU:HD11	2.49	0.48
4:D:126:TYR:OH	14:D:1001:HEC:O2A	2.17	0.48
2:B:71:LEU:HD12	2:B:144:LEU:HD12	1.98	0.46
3:C:186:PRO:HA	3:C:189:ILE:HD12	1.98	0.46
5:E:46:GLY:HA3	4:Q:215:LEU:HD21	1.97	0.46
3:C:183:PHE:CZ	12:C:1001:HEM:HBC1	2.52	0.45
3:C:128:PHE:CD1	3:C:146:ILE:HD12	2.51	0.45
5:E:65:SER:OG	5:E:67:ASP:OD1	2.22	0.45
2:O:407:ASP:OD1	2:O:408:ALA:N	2.50	0.45
7:T:71:ARG:NH1	8:U:56:GLU:OE2	2.50	0.45
10:W:51:LEU:HD22	10:W:51:LEU:H	1.80	0.45
12:C:1002:HEM:HMB2	12:C:1002:HEM:HBB2	1.99	0.45
11:K:14:ALA:O	11:K:18:VAL:HG23	2.17	0.44
1:A:14:THR:OG1	1:A:389:ARG:NH1	2.49	0.44
14:Q:1001:HEC:HMB1	14:Q:1001:HEC:HBB3	1.99	0.44
12:C:1001:HEM:HBB2	12:C:1001:HEM:HMB1	1.99	0.44
4:D:142:SER:OG	4:D:143:LEU:N	2.51	0.44
3:C:361:LEU:HD23	3:C:365:LEU:HD12	2.00	0.44
1:A:366:VAL:HG11	2:B:44:ALA:HB2	2.01	0.43
2:B:101:THR:HG22	9:I:65:VAL:HG22	1.98	0.43
2:B:243:GLU:N	2:B:243:GLU:OE1	2.51	0.43
9:V:69:SER:OG	9:V:72:VAL:O	2.36	0.43
1:A:33:PRO:O	1:A:103:SER:OG	2.26	0.43
4:D:19:SER:O	4:D:202:LYS:NZ	2.44	0.43
8:H:27:LEU:O	8:H:31:VAL:HG23	2.19	0.43
10:J:2:ALA:HB3	10:J:3:PRO:HD3	1.99	0.43
3:P:361:LEU:HD23	3:P:365:LEU:HD12	1.99	0.43
4:D:31:GLN:NE2	4:D:172:ASP:OD2	2.52	0.42
4:D:23:HIS:ND1	4:D:54:VAL:O	2.51	0.42
1:A:17:SER:OG	1:A:209:LEU:HD13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:4:TYR:CZ	1:N:8:LEU:HD11	2.55	0.42
10:W:2:ALA:HB3	10:W:3:PRO:HD3	2.01	0.42
1:N:62:LEU:HD13	1:N:122:LEU:HD22	2.02	0.41
5:R:126:ARG:NH2	5:R:180:LEU:O	2.50	0.41
2:B:174:ASN:N	2:B:174:ASN:OD1	2.54	0.41
6:F:49:ARG:O	2:O:134:ARG:NH2	2.53	0.41
11:X:19:PRO:O	11:X:22:SER:OG	2.28	0.41
3:C:81:TYR:O	3:C:85:ASN:ND2	2.47	0.41
3:C:157:GLY:O	3:C:161:VAL:HG23	2.20	0.41
1:A:235:ARG:NH1	5:R:18:VAL:O	2.53	0.41
3:P:262:LEU:HD21	5:R:90:LYS:HG3	2.03	0.41
4:D:116:ILE:HG12	14:D:1001:HEC:HMA3	2.02	0.40
2:O:305:GLN:OE1	2:O:305:GLN:N	2.55	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%)	430 (97%)	14 (3%)	0	100	100
1	N	444/446 (100%)	438 (99%)	6 (1%)	0	100	100
2	B	421/439 (96%)	407 (97%)	14 (3%)	0	100	100
2	O	421/439 (96%)	414 (98%)	6 (1%)	1 (0%)	44	71
3	C	376/379 (99%)	367 (98%)	9 (2%)	0	100	100
3	P	376/379 (99%)	371 (99%)	5 (1%)	0	100	100
4	D	239/241 (99%)	232 (97%)	7 (3%)	0	100	100
4	Q	239/241 (99%)	234 (98%)	5 (2%)	0	100	100
5	E	194/196 (99%)	180 (93%)	14 (7%)	0	100	100
5	R	194/196 (99%)	188 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	103/110 (94%)	102 (99%)	1 (1%)	0	100	100
6	S	103/110 (94%)	102 (99%)	1 (1%)	0	100	100
7	G	73/80 (91%)	69 (94%)	4 (6%)	0	100	100
7	T	73/80 (91%)	69 (94%)	4 (6%)	0	100	100
8	H	65/78 (83%)	64 (98%)	1 (2%)	0	100	100
8	U	65/78 (83%)	64 (98%)	1 (2%)	0	100	100
9	I	18/78 (23%)	17 (94%)	1 (6%)	0	100	100
9	V	18/78 (23%)	17 (94%)	1 (6%)	0	100	100
10	J	58/63 (92%)	55 (95%)	3 (5%)	0	100	100
10	W	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
11	K	50/56 (89%)	49 (98%)	1 (2%)	0	100	100
11	X	50/56 (89%)	46 (92%)	3 (6%)	1 (2%)	6	21
All	All	4082/4332 (94%)	3972 (97%)	108 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	O	171	ALA
11	X	46	PRO

### 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%)	369 (100%)	1 (0%)	91	97
1	N	370/370 (100%)	367 (99%)	3 (1%)	79	92
2	B	332/343 (97%)	329 (99%)	3 (1%)	75	91
2	O	332/343 (97%)	331 (100%)	1 (0%)	91	97
3	C	326/327 (100%)	322 (99%)	4 (1%)	67	87
3	P	326/327 (100%)	323 (99%)	3 (1%)	75	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	206/206 (100%)	205 (100%)	1 (0%)	86	95
4	Q	206/206 (100%)	206 (100%)	0	100	100
5	E	168/168 (100%)	166 (99%)	2 (1%)	67	87
5	R	168/168 (100%)	167 (99%)	1 (1%)	84	94
6	F	96/98 (98%)	95 (99%)	1 (1%)	73	90
6	S	96/98 (98%)	96 (100%)	0	100	100
7	G	66/70 (94%)	65 (98%)	1 (2%)	60	84
7	T	66/70 (94%)	66 (100%)	0	100	100
8	H	64/74 (86%)	62 (97%)	2 (3%)	35	67
8	U	64/74 (86%)	63 (98%)	1 (2%)	58	82
9	I	14/60 (23%)	14 (100%)	0	100	100
9	V	14/60 (23%)	14 (100%)	0	100	100
10	J	50/53 (94%)	50 (100%)	0	100	100
10	W	50/53 (94%)	48 (96%)	2 (4%)	27	58
11	K	42/46 (91%)	42 (100%)	0	100	100
11	X	42/46 (91%)	42 (100%)	0	100	100
All	All	3468/3630 (96%)	3442 (99%)	26 (1%)	80	93

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
2	B	147	ASP
2	B	182	ARG
2	B	326	THR
3	C	20	ASP
3	C	80	ARG
3	C	344	GLU
3	C	379	TRP
4	D	200	HIS
5	E	100	HIS
5	E	107	ASP
6	F	67	ASP
7	G	6	HIS
8	H	24	CYS
8	H	53	ASP

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Mol	Chain	Res	Type
1	N	245	GLU
1	N	279	HIS
1	N	373	THR
2	O	28	ARG
3	P	90	PHE
3	P	128	PHE
3	P	379	TRP
5	R	190	ASP
8	U	68	CYS
10	W	40	ASP
10	W	51	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	FES	R	1001	5	0,4,4	-	-	-		
12	HEM	P	1001	3	42,50,50	1.49	5 (11%)	46,82,82	1.28	4 (8%)
13	JHB	C	1003	-	34,34,34	0.83	0	49,50,50	0.85	1 (2%)
12	HEM	C	1001	3	42,50,50	1.48	5 (11%)	46,82,82	1.24	4 (8%)
15	FES	E	1001	5	0,4,4	-	-	-		
14	HEC	Q	1001	4	32,50,50	2.09	3 (9%)	30,82,82	2.11	5 (16%)
12	HEM	C	1002	3	42,50,50	1.46	5 (11%)	46,82,82	1.25	3 (6%)
12	HEM	P	1002	3	42,50,50	1.46	3 (7%)	46,82,82	1.21	3 (6%)
14	HEC	D	1001	4	32,50,50	2.12	3 (9%)	30,82,82	2.12	6 (20%)
13	JHB	P	1003	-	34,34,34	0.83	0	49,50,50	0.83	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FES	R	1001	5	-	-	0/1/1/1
12	HEM	P	1001	3	-	3/12/54/54	-
13	JHB	C	1003	-	-	2/13/13/13	0/4/4/4
12	HEM	C	1001	3	-	3/12/54/54	-
15	FES	E	1001	5	-	-	0/1/1/1
14	HEC	Q	1001	4	-	2/10/54/54	-
12	HEM	C	1002	3	-	4/12/54/54	-
12	HEM	P	1002	3	-	4/12/54/54	-
14	HEC	D	1001	4	-	0/10/54/54	-
13	JHB	P	1003	-	-	0/13/13/13	0/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	D	1001	HEC	C2B-C3B	-6.54	1.33	1.40
14	Q	1001	HEC	C2B-C3B	-6.35	1.33	1.40
14	D	1001	HEC	C3C-C2C	-5.81	1.34	1.40
14	Q	1001	HEC	C3C-C2C	-5.52	1.34	1.40
14	Q	1001	HEC	C3D-C2D	5.16	1.52	1.37
14	D	1001	HEC	C3D-C2D	5.11	1.52	1.37
12	P	1001	HEM	C3C-C2C	-4.30	1.34	1.40
12	P	1002	HEM	C3C-C2C	-4.22	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	1001	HEM	C3C-C2C	-4.08	1.34	1.40
12	C	1002	HEM	C3C-C2C	-3.96	1.35	1.40
12	C	1002	HEM	C3C-CAC	3.55	1.55	1.47
12	P	1001	HEM	C3C-CAC	3.53	1.55	1.47
12	C	1001	HEM	C3C-CAC	3.43	1.55	1.47
12	P	1002	HEM	C3C-CAC	3.41	1.55	1.47
12	C	1002	HEM	CAB-C3B	3.07	1.55	1.47
12	C	1001	HEM	CAB-C3B	3.05	1.55	1.47
12	P	1002	HEM	CAB-C3B	3.03	1.55	1.47
12	P	1001	HEM	CAB-C3B	3.02	1.55	1.47
12	P	1001	HEM	C3C-C4C	2.69	1.45	1.41
12	C	1001	HEM	C3C-C4C	2.66	1.45	1.41
12	C	1002	HEM	C3C-C4C	2.40	1.44	1.41
12	C	1001	HEM	CMB-C2B	2.20	1.55	1.50
12	P	1001	HEM	CMB-C2B	2.06	1.55	1.50
12	C	1002	HEM	CMB-C2B	2.05	1.55	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	Q	1001	HEC	CBB-CAB-C3B	-7.27	110.47	127.49
14	D	1001	HEC	CBB-CAB-C3B	-6.73	111.74	127.49
14	D	1001	HEC	CBC-CAC-C3C	-5.82	113.88	127.49
14	Q	1001	HEC	CBC-CAC-C3C	-5.10	115.56	127.49
14	D	1001	HEC	CBD-CAD-C3D	-3.47	106.70	112.54
14	Q	1001	HEC	CMC-C2C-C1C	-3.36	123.53	128.46
12	P	1001	HEM	C4C-CHD-C1D	2.96	126.46	122.56
14	D	1001	HEC	C1D-C2D-C3D	-2.92	104.97	107.00
12	C	1002	HEM	C4B-CHC-C1C	2.88	126.35	122.56
12	C	1001	HEM	C4B-CHC-C1C	2.76	126.21	122.56
12	C	1001	HEM	C4C-CHD-C1D	2.74	126.17	122.56
14	Q	1001	HEC	C1D-C2D-C3D	-2.69	105.12	107.00
12	P	1001	HEM	C4B-CHC-C1C	2.61	126.00	122.56
14	Q	1001	HEC	CBD-CAD-C3D	-2.60	108.16	112.54
14	D	1001	HEC	CMC-C2C-C1C	-2.58	124.68	128.46
12	P	1002	HEM	C4C-CHD-C1D	2.53	125.90	122.56
12	C	1002	HEM	C4C-CHD-C1D	2.53	125.90	122.56
12	C	1002	HEM	CBA-CAA-C2A	-2.22	108.81	112.54
12	P	1002	HEM	C4B-CHC-C1C	2.19	125.44	122.56
12	C	1001	HEM	CMC-C2C-C3C	2.14	128.95	124.68
13	C	1003	JHB	O-C6-C8	2.14	123.26	120.45
12	P	1001	HEM	CBA-CAA-C2A	-2.07	109.07	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	D	1001	HEC	CAA-CBA-CGA	-2.03	108.36	113.83
12	P	1002	HEM	C3B-C2B-C1B	2.03	107.93	106.41
12	C	1001	HEM	C4D-ND-C1D	2.01	107.58	105.21
12	P	1001	HEM	C4D-ND-C1D	2.01	107.58	105.21

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	1001	HEM	C3D-CAD-CBD-CGD
12	P	1001	HEM	C3D-CAD-CBD-CGD
12	C	1002	HEM	CAD-CBD-CGD-O1D
12	C	1001	HEM	CAD-CBD-CGD-O1D
13	C	1003	JHB	F-C23-O1-C22
12	P	1002	HEM	CAA-CBA-CGA-O1A
12	C	1001	HEM	CAD-CBD-CGD-O2D
12	P	1001	HEM	CAD-CBD-CGD-O1D
12	P	1002	HEM	CAA-CBA-CGA-O2A
12	C	1002	HEM	CAD-CBD-CGD-O2D
14	Q	1001	HEC	CAA-CBA-CGA-O2A
12	C	1002	HEM	CAA-CBA-CGA-O1A
14	Q	1001	HEC	CAA-CBA-CGA-O1A
12	P	1001	HEM	CAD-CBD-CGD-O2D
12	C	1002	HEM	CAA-CBA-CGA-O2A
12	P	1002	HEM	CAD-CBD-CGD-O2D
13	C	1003	JHB	F2-C23-O1-C22
12	P	1002	HEM	CAD-CBD-CGD-O1D

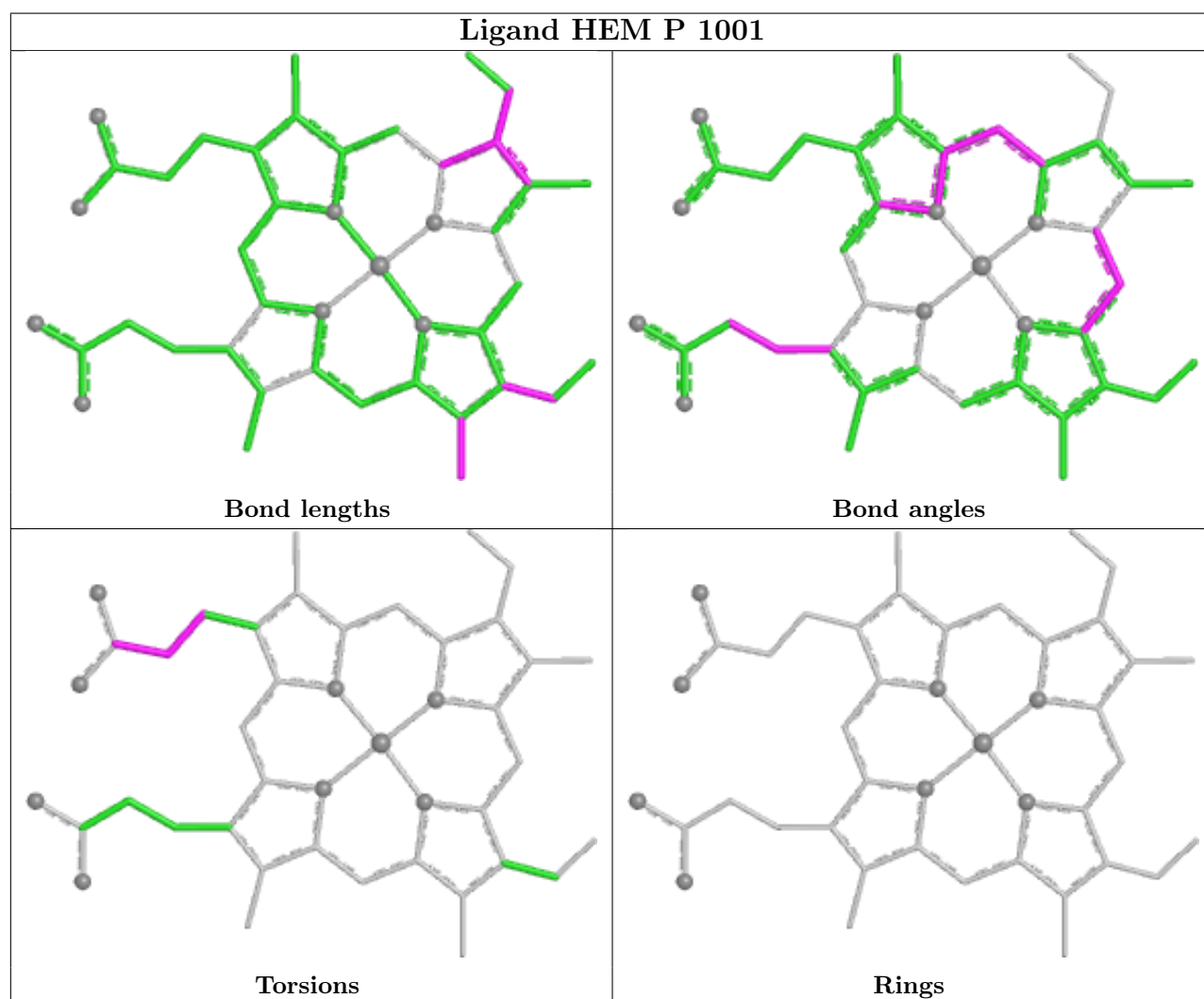
There are no ring outliers.

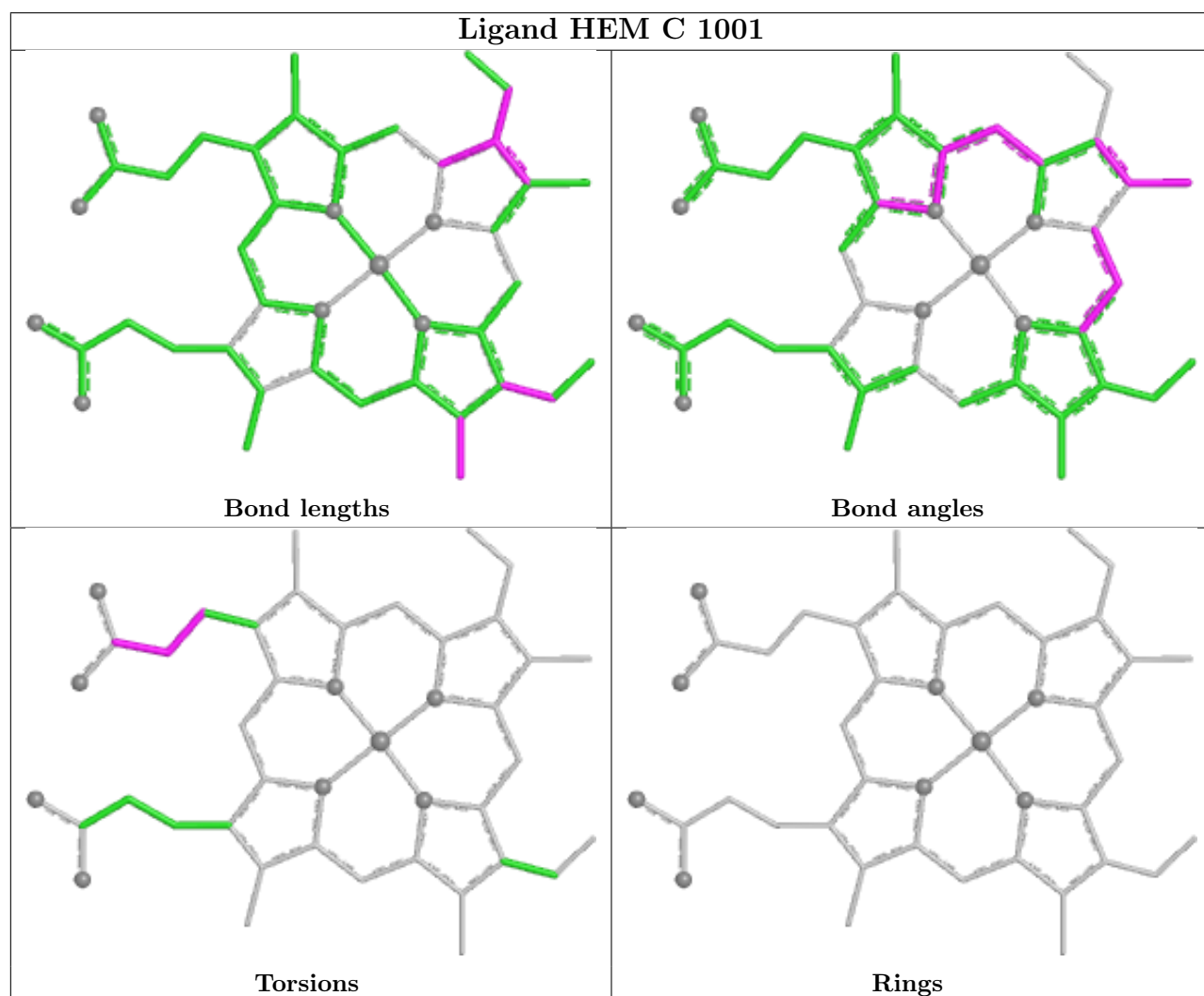
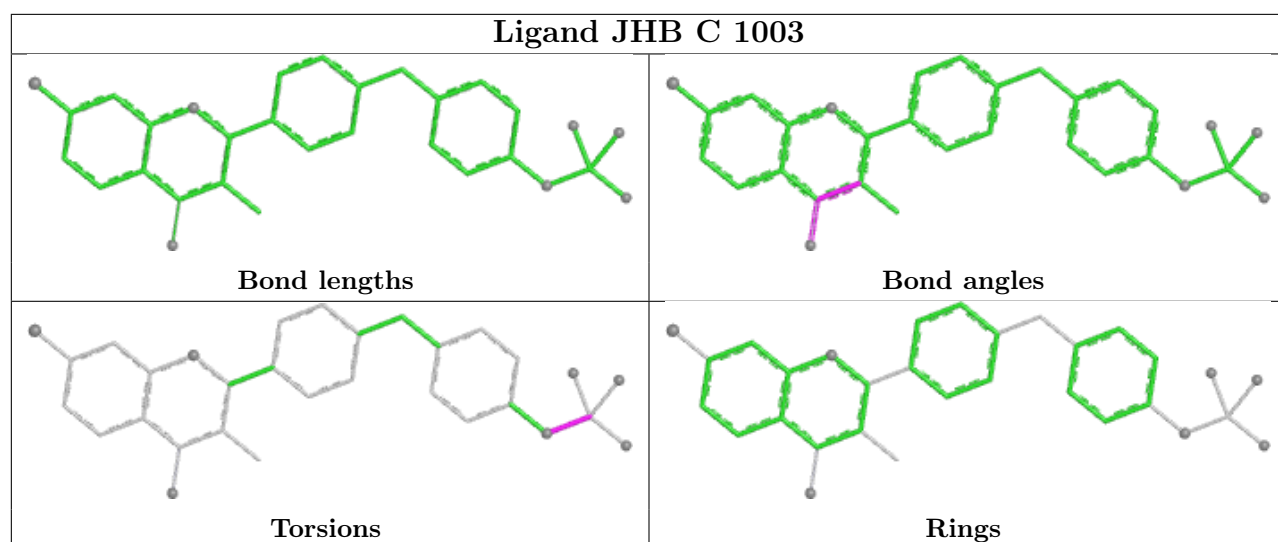
8 monomers are involved in 15 short contacts:

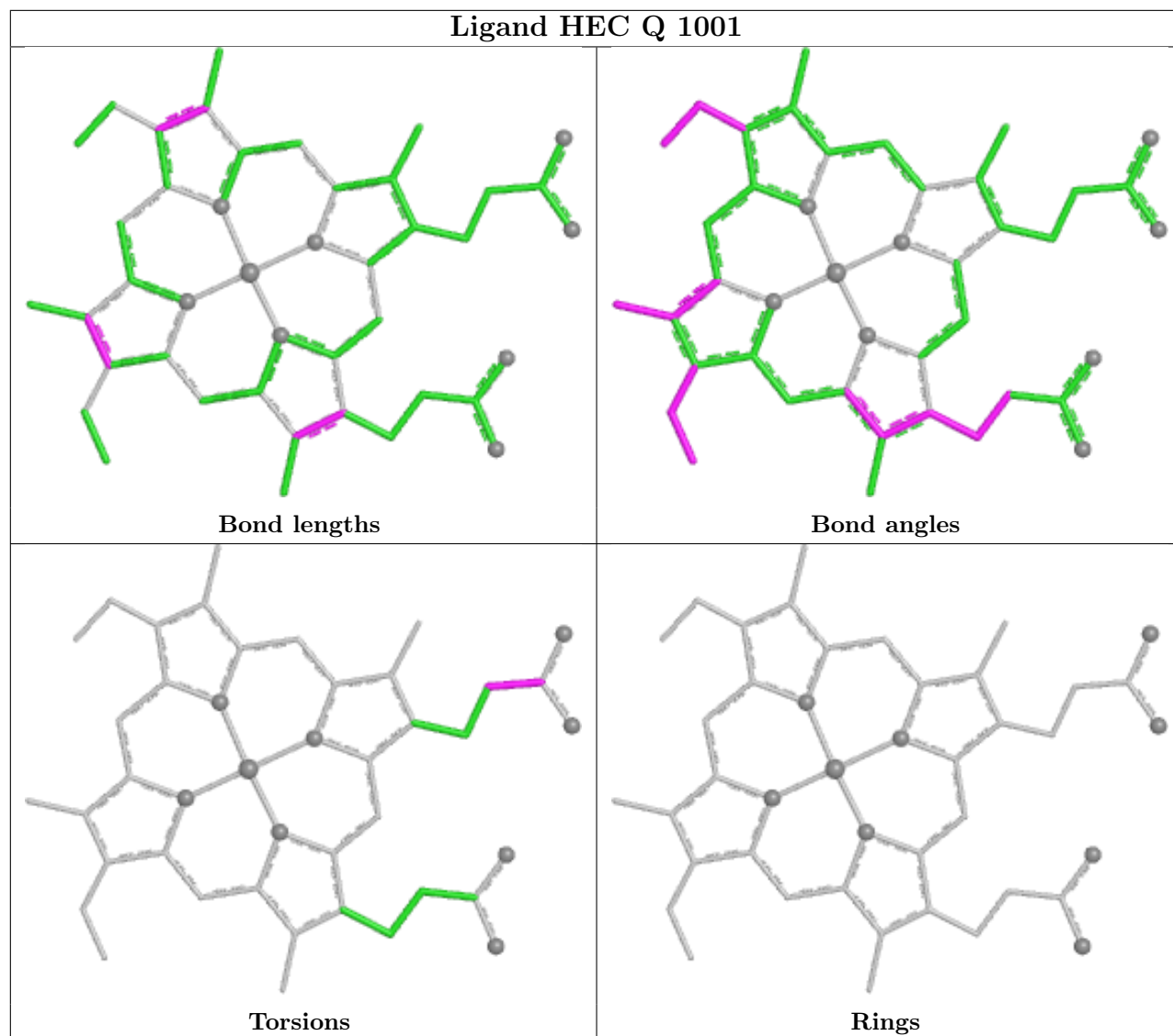
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	P	1001	HEM	1	0
13	C	1003	JHB	1	0
12	C	1001	HEM	4	0
15	E	1001	FES	1	0
14	Q	1001	HEC	2	0
12	C	1002	HEM	2	0
12	P	1002	HEM	1	0
14	D	1001	HEC	3	0

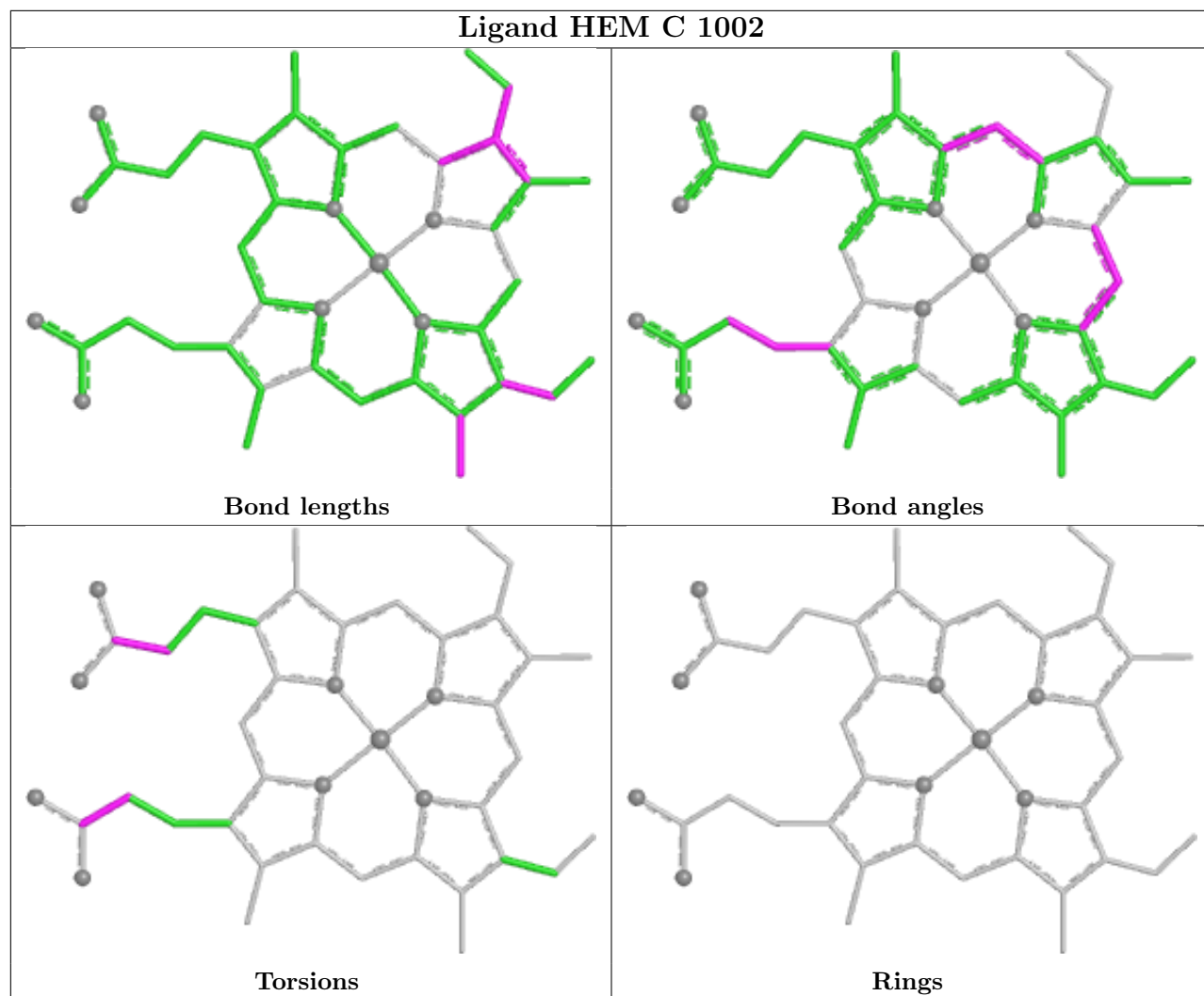


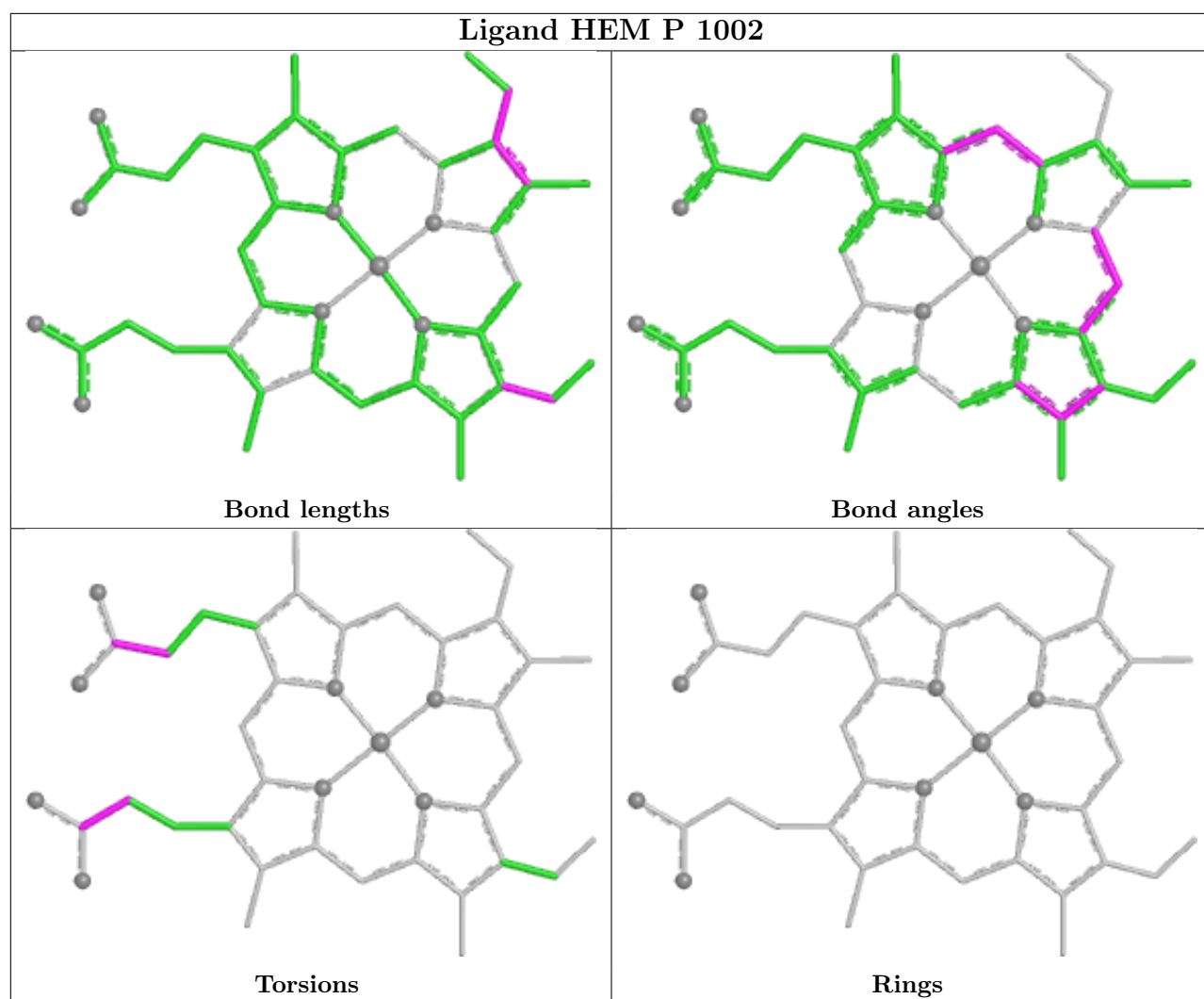
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



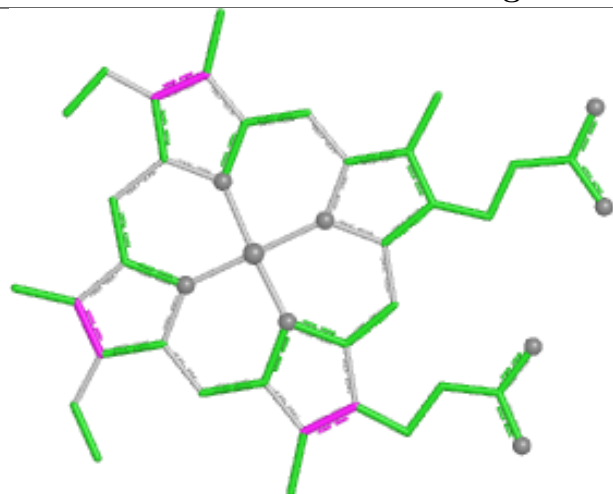




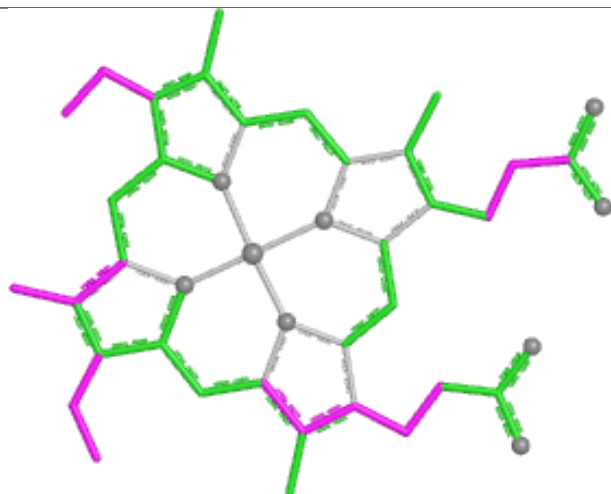




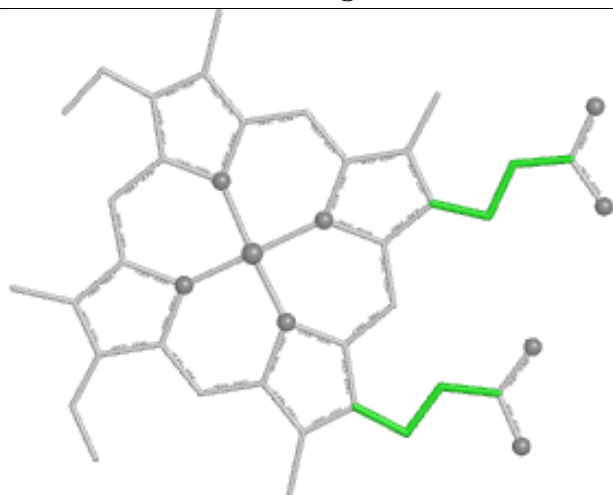
## Ligand HEC D 1001



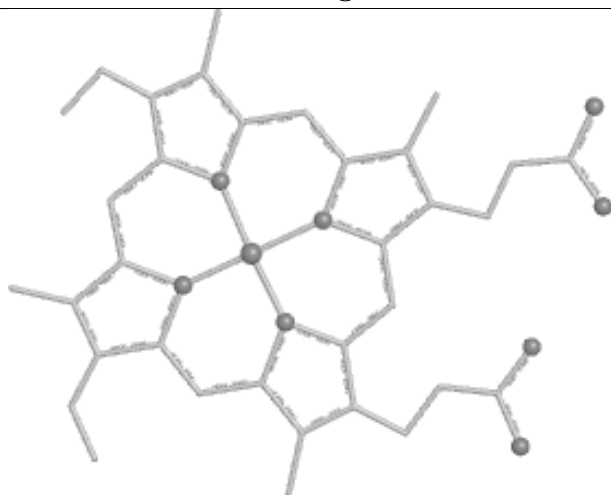
Bond lengths



Bond angles

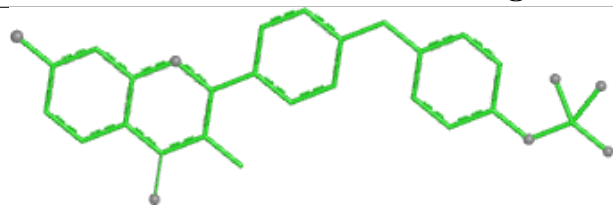


Torsions

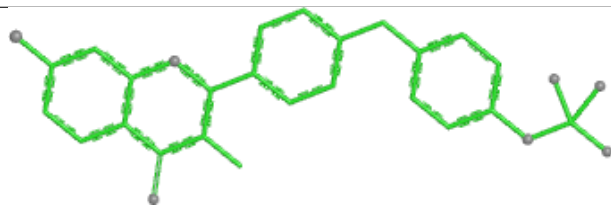


Rings

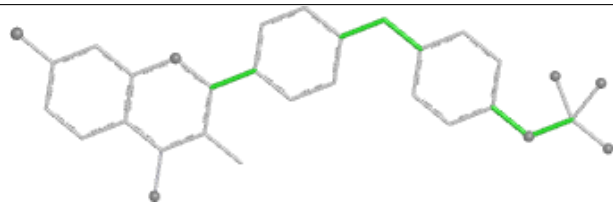
## Ligand JHB P 1003



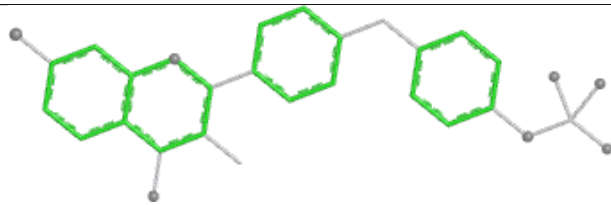
Bond lengths



Bond angles



Torsions



Rings

## 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.

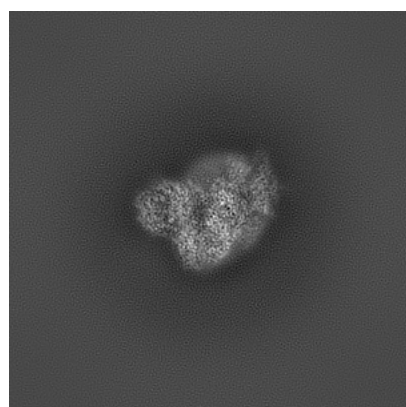
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26203. These allow visual inspection of the internal detail of the map and identification of artifacts.

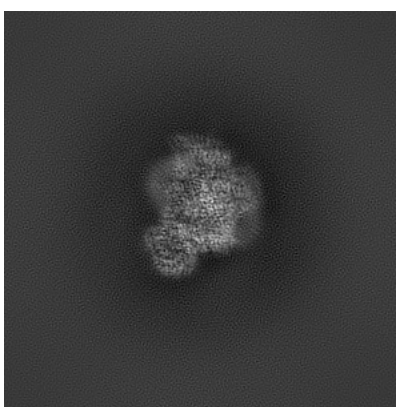
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

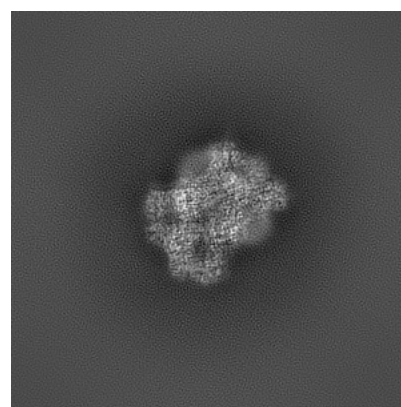
#### 6.1.1 Primary map



X



Y

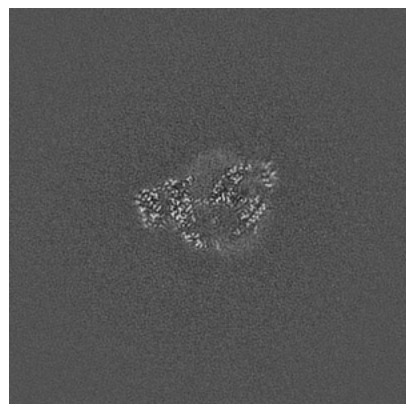


Z

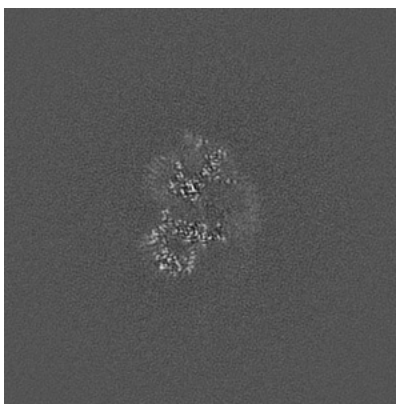
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

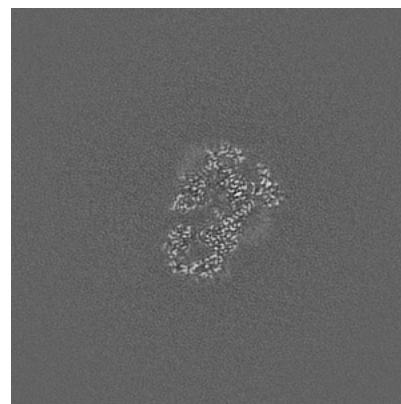
#### 6.2.1 Primary map



X Index: 256



Y Index: 256



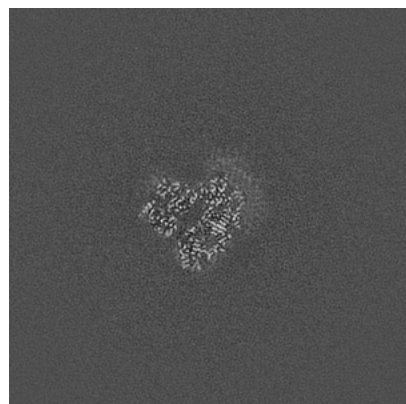
Z Index: 256



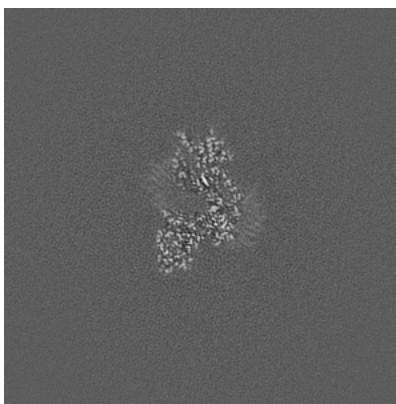
The images above show central slices of the map in three orthogonal directions.

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

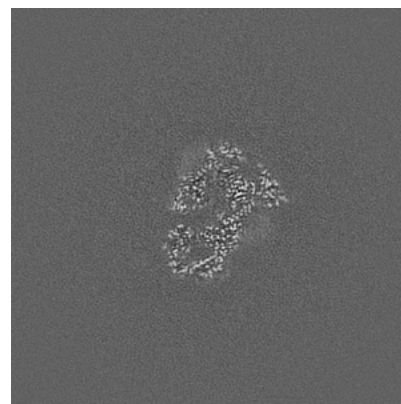
### 6.3.1 Primary map



X Index: 222



Y Index: 274

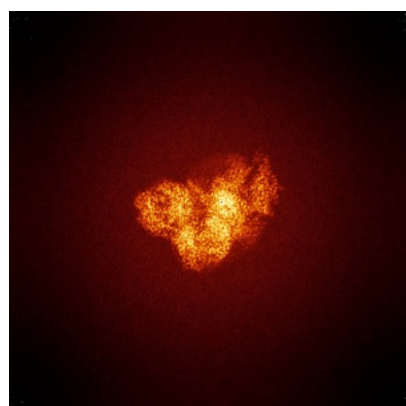


Z Index: 255

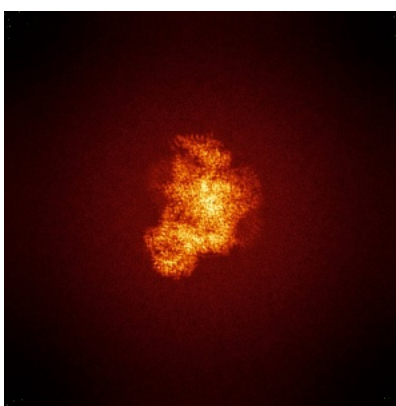
The images above show the largest variance slices of the map in three orthogonal directions.

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

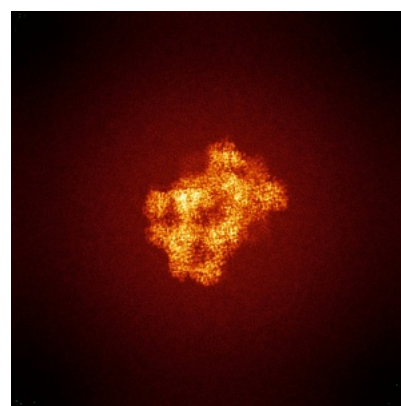
### 6.4.1 Primary map



X



Y

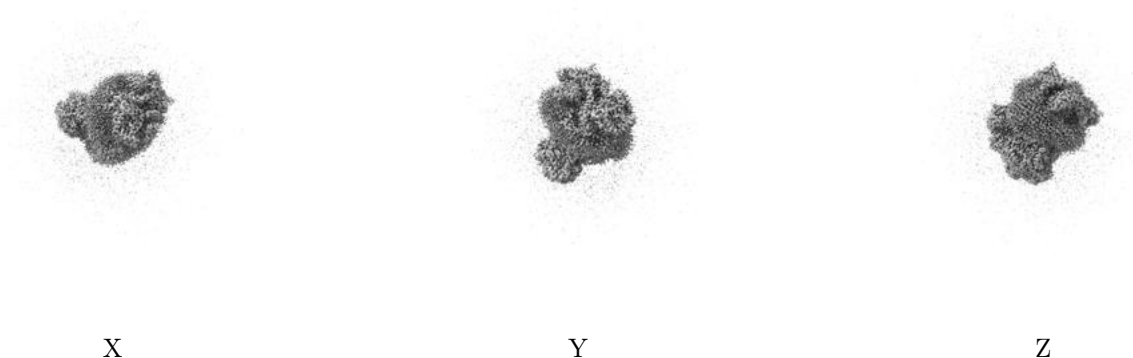


Z

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 2.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

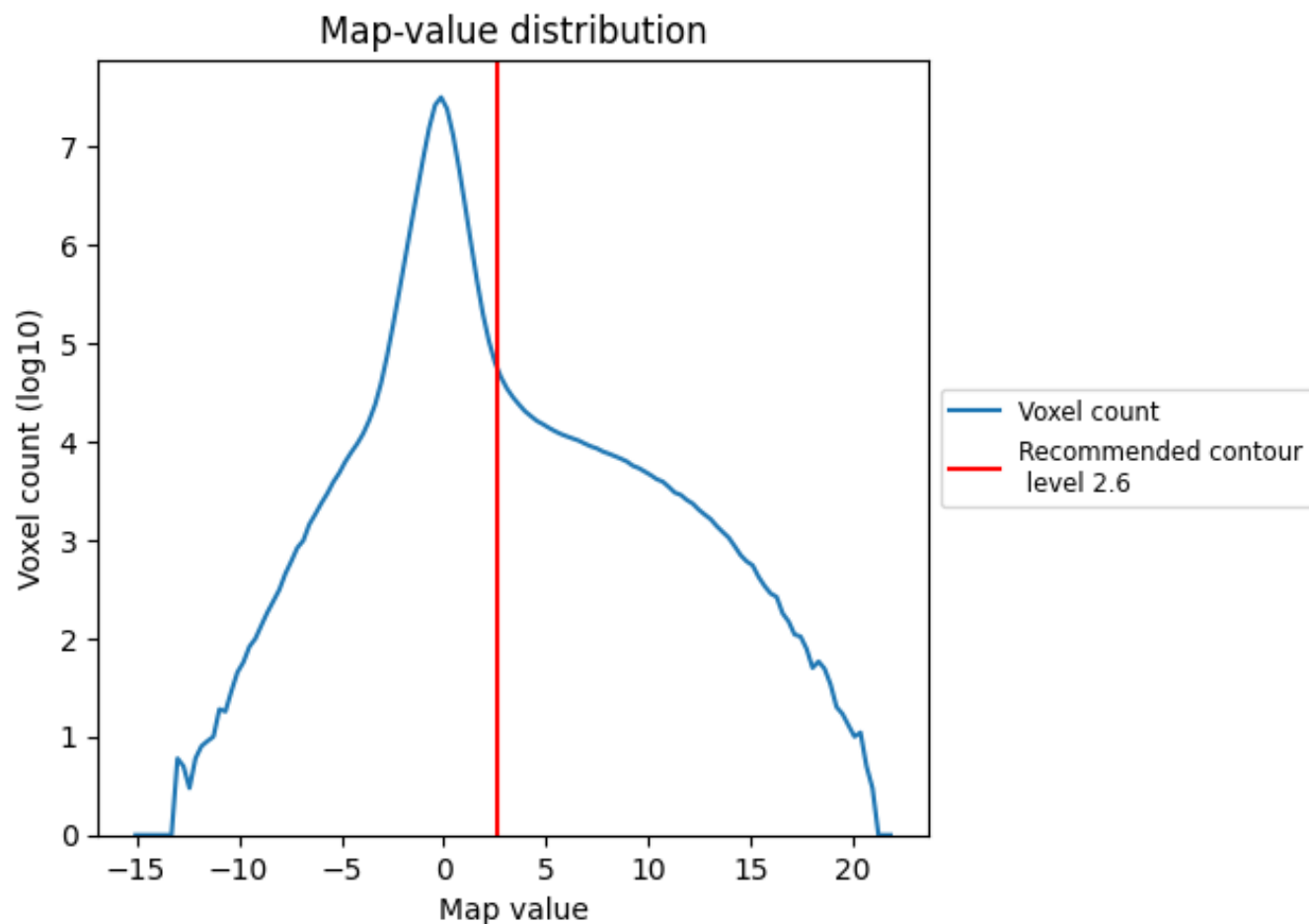
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

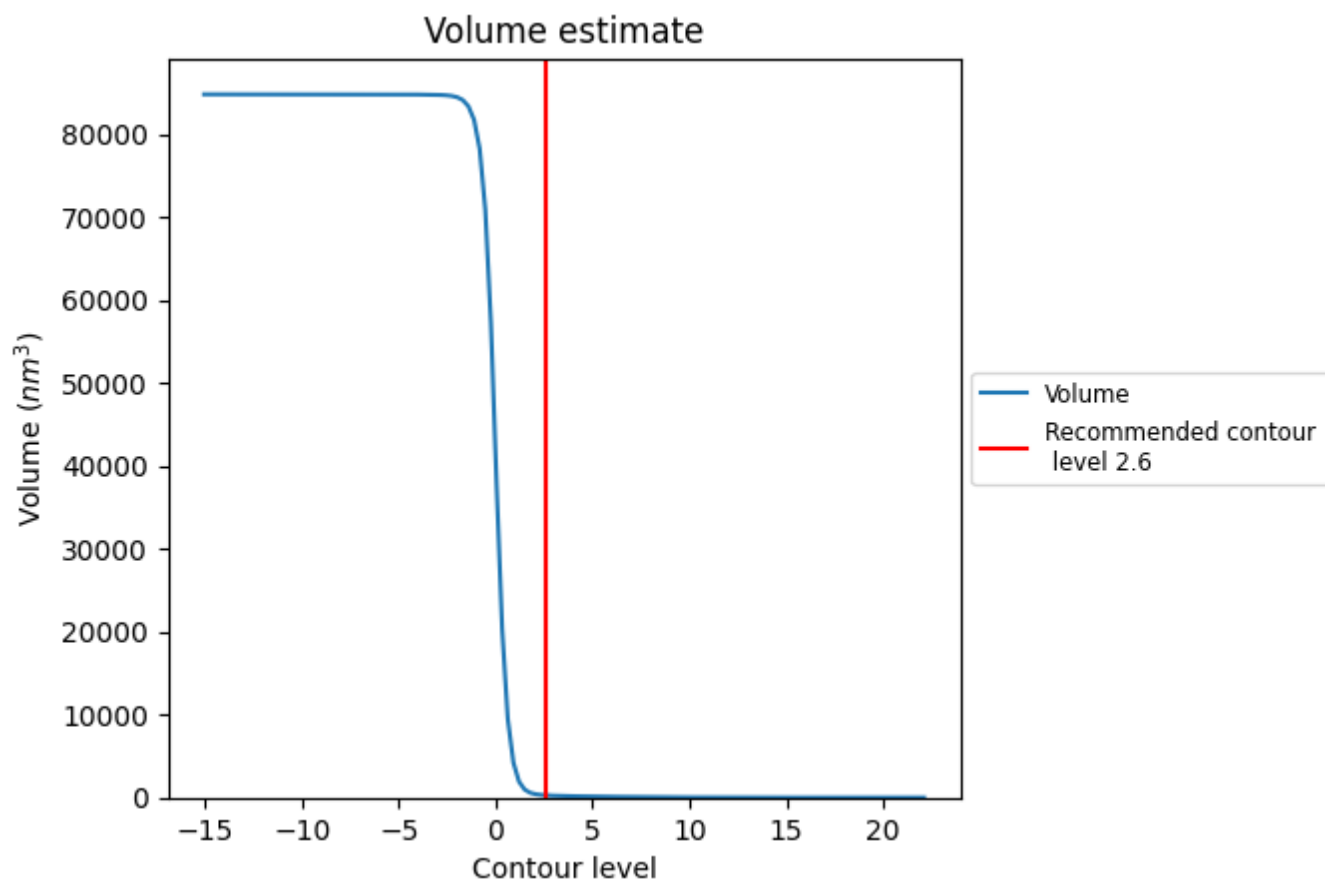
This section contains the results of statistical analysis of the map.

### 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.

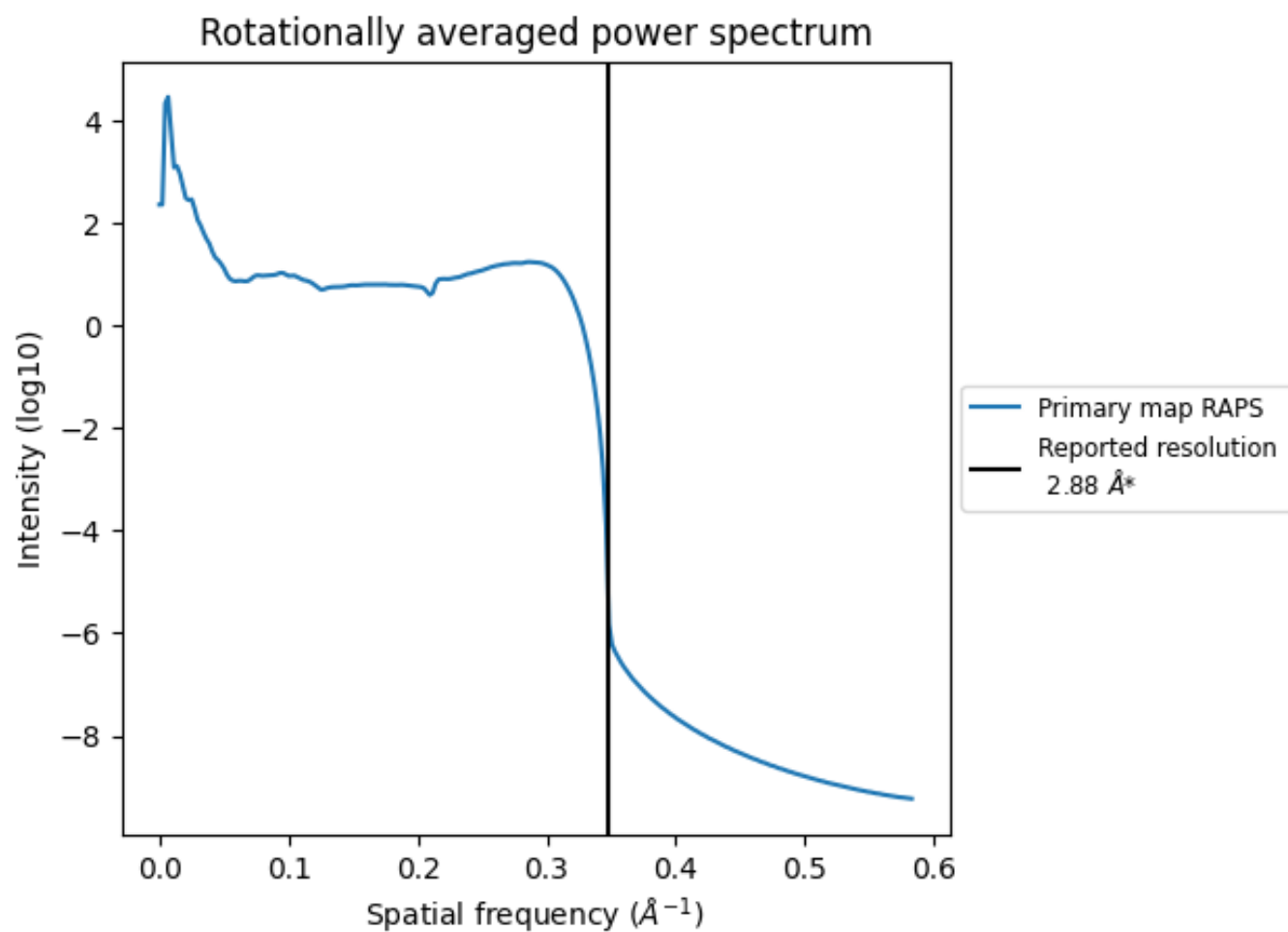
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 273 nm<sup>3</sup>; this corresponds to an approximate mass of 246 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 0.347 Å<sup>-1</sup>

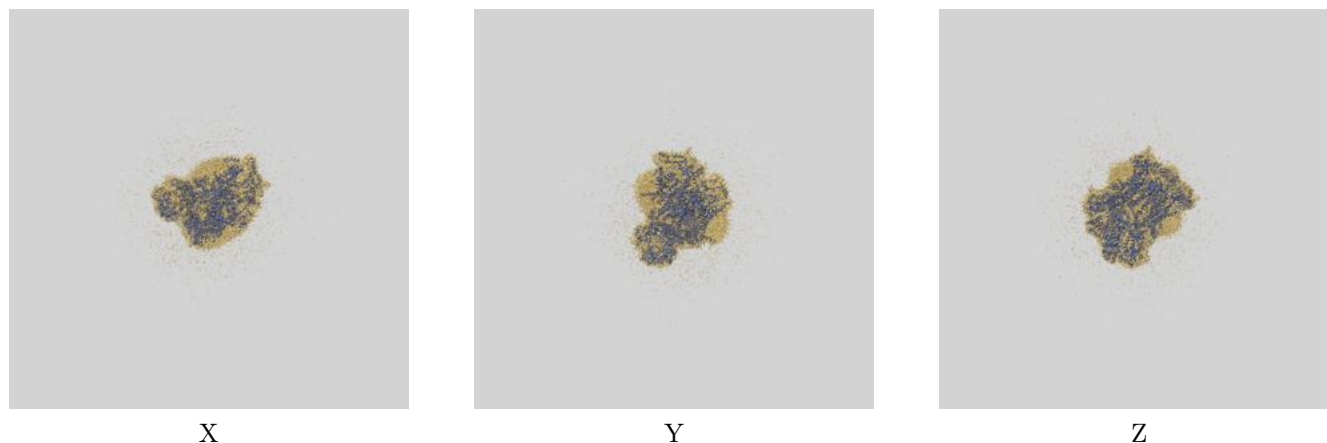
## 8 Fourier-Shell correlation ⓘ

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

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

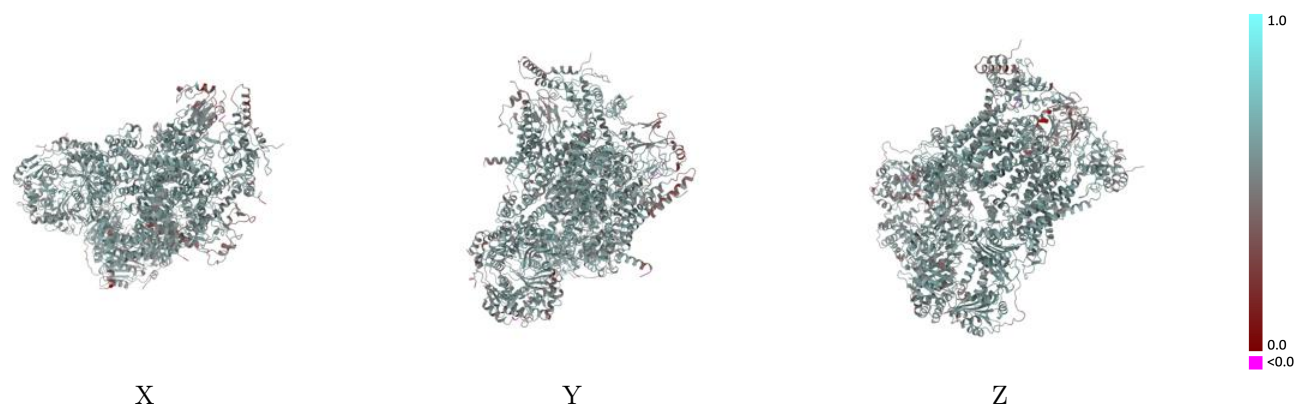
This section contains information regarding the fit between EMDB map EMD-26203 and PDB model 7TZ6. Per-residue inclusion information can be found in section [3](#) on page [9](#).

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



The images above show the 3D surface view of the map at the recommended contour level 2.6 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.

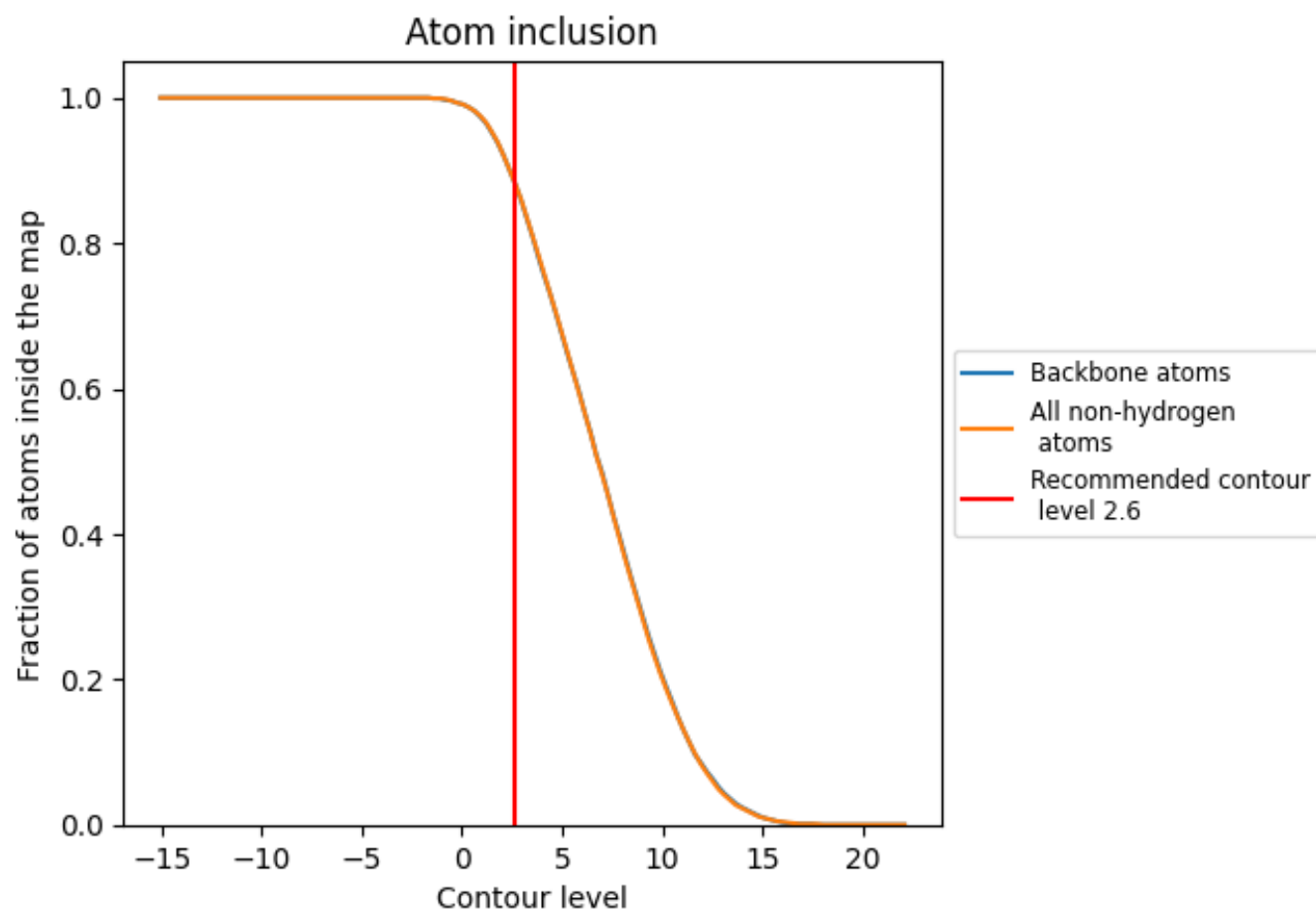
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (2.6).

















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 89% 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 (2.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8860	 0.5550
A	 0.9000	 0.5700
B	 0.9070	 0.5620
C	 0.9180	 0.5910
D	 0.9260	 0.5770
E	 0.8370	 0.5230
F	 0.8850	 0.5610
G	 0.8840	 0.5500
H	 0.8470	 0.4920
I	 0.7770	 0.5460
J	 0.8800	 0.5570
K	 0.8500	 0.5510
N	 0.8870	 0.5480
O	 0.8890	 0.5450
P	 0.9100	 0.5780
Q	 0.9160	 0.5600
R	 0.8210	 0.5050
S	 0.8580	 0.5400
T	 0.8790	 0.5370
U	 0.8220	 0.4580
V	 0.8080	 0.5510
W	 0.8510	 0.5300
X	 0.8160	 0.5340

