



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 12:13 AM EDT

PDB ID : 9C7H / pdb_00009c7h
EMDB ID : EMD-45282
Title : Cryo-EM structure of respiratory supercomplex III
Authors : Zhang, Z.; Maharjan, R.; Tringides, M.
Deposited on : 2024-06-10
Resolution : 2.78 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

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:

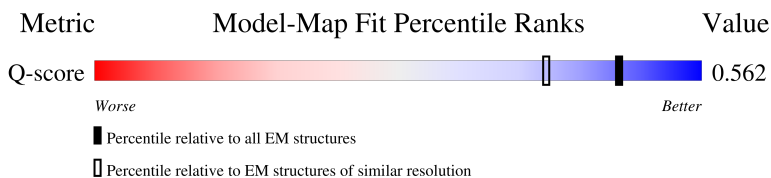
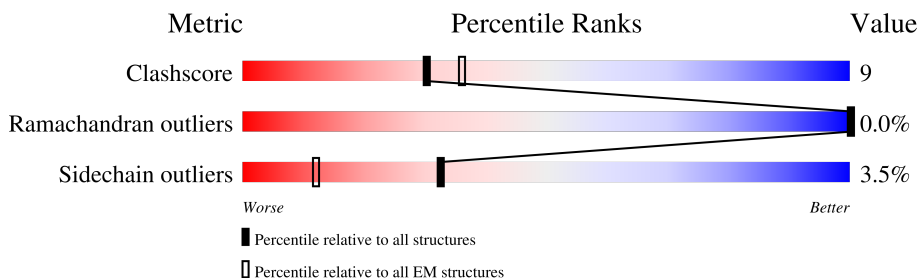
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.78 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.



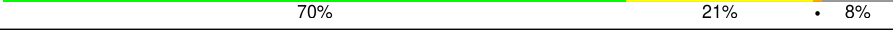
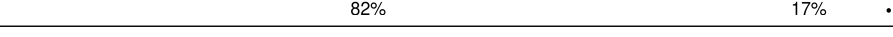
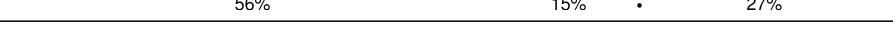
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10754 (2.28 - 3.28)

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	0	91	47% 27% 25%
1	Ab	91	52% 22% • 25%
2	1	64	78% 16% 6%
2	Ac	64	84% 9% 6%

Continued on next page...

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Mol	Chain	Length	Quality of chain
3	2	299	
3	4	299	
3	Ae	299	
3	Af	299	
4	3	56	
4	Ad	56	
5	5	480	
5	u	480	
6	6	453	
6	v	453	
7	7	379	
7	w	379	
8	8	326	
8	x	326	
9	9	111	
9	y	111	
10	Aa	82	
10	z	82	

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
11	FES	2	301	-	-	X	-
11	FES	4	301	-	-	X	-
13	HEC	8	401	X	-	-	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 32776 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	68	Total	C	N	O	S	0	0
			561	341	101	114	5		
1	Ab	68	Total	C	N	O	S	0	0
			561	341	101	114	5		

- Molecule 2 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	60	Total	C	N	O	0	0
			493	322	87	84		
2	Ac	60	Total	C	N	O	0	0
			493	322	87	84		

- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	195	Total	C	N	O	S	0	0
			1513	953	264	289	7		
3	4	196	Total	C	N	O	S	0	0
			1515	954	265	289	7		
3	Af	39	Total	C	N	O	S	0	0
			275	172	53	47	3		
3	Ae	39	Total	C	N	O	S	0	0
			271	169	52	47	3		

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	51	Total	C	N	O	S	0	0
			417	279	74	63	1		
4	Ad	51	Total	C	N	O	S	0	0
			417	279	74	63	1		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	435	Total	C	N	O	S	0	0
			3374	2105	594	656	19		
5	u	435	Total	C	N	O	S	0	0
			3373	2105	594	655	19		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	418	Total	C	N	O	S	0	0
			3140	1966	556	610	8		
6	v	418	Total	C	N	O	S	0	0
			3140	1966	556	610	8		

- Molecule 7 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
7	w	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		

- Molecule 8 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	239	Total	C	N	O	S	0	0
			1903	1215	328	345	15		
8	x	238	Total	C	N	O	S	0	0
			1896	1211	326	343	16		

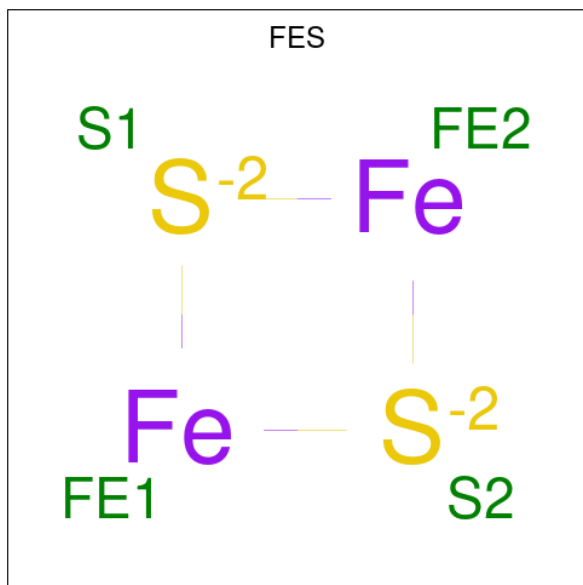
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	101	Total	C	N	O	S	0	0
			893	572	157	162	2		
9	y	101	Total	C	N	O	S	0	0
			893	572	157	162	2		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 8.

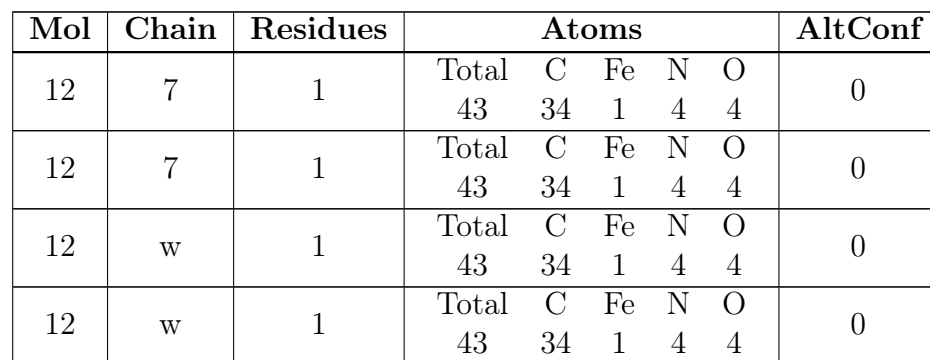
Mol	Chain	Residues	Atoms					AltConf	Trace
10	z	79	Total	C	N	O	S	0	0
			666	434	122	108	2		
10	Aa	79	Total	C	N	O	S	0	0
			666	434	122	108	2		

- Molecule 11 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
11	2	1	Total	Fe	S	0
			4	2	2	
11	4	1	Total	Fe	S	0
			4	2	2	

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



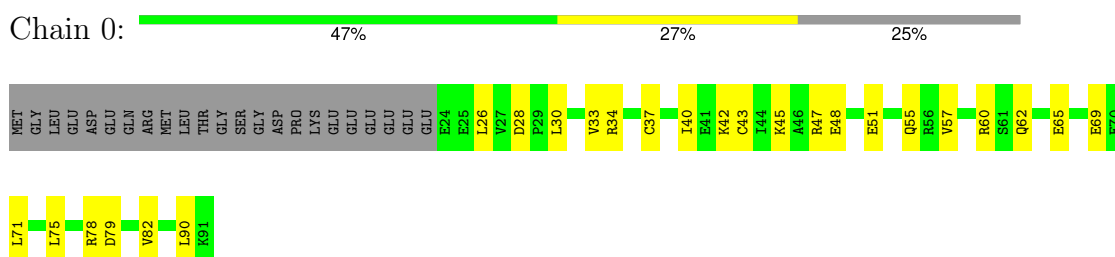
- # HEC
-
- The chemical structure of HEC (Hexaethylcyclotriazine) is shown. It features a central Fe atom coordinated by four N atoms in a porphyrin-like ring. The substituents are labeled with green text: CBC, GAC, CMC, C2C, C3C, C4C, CHC, C3B, C4B, C2B, C1B, CHB, CMB, CMA, C3A, C4A, C2A, C1A, CHA, C3D, C4D, C2D, C1D, CHD, CMD, CBD, CAD, CBA, CAA, CGD, CGA, O2D, O1D, O2A, O1A. The central Fe atom is labeled with a purple 'Fe' and the bond to the N atoms is labeled with a purple 'FE'. The N atoms are labeled with blue 'N' and the bond to the Fe atom is labeled with a blue 'N'. The bond to the C atoms is labeled with a blue 'C'.

Mol	Chain	Residues	Atoms					AltConf
13	8	1	Total 43	C 34	Fe 1	N 4	O 4	0
13	x	1	Total 43	C 34	Fe 1	N 4	O 4	0

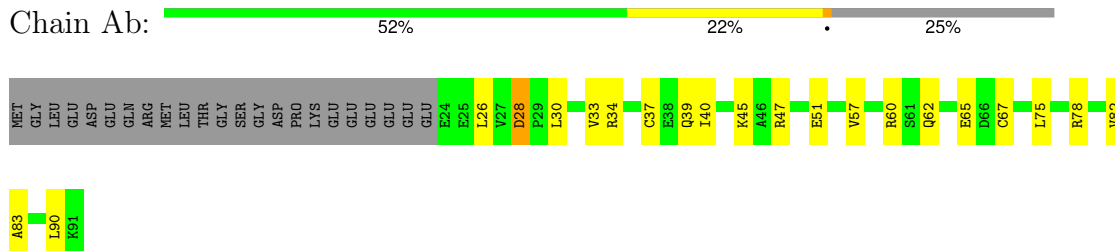
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

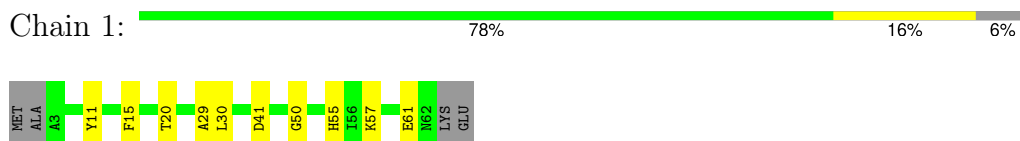
- Molecule 1: Cytochrome b-c1 complex subunit 6, mitochondrial



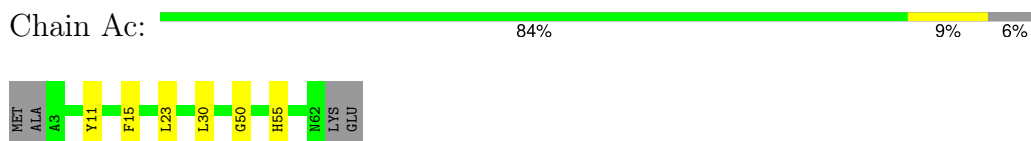
- Molecule 1: Cytochrome b-c1 complex subunit 6, mitochondrial



- Molecule 2: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

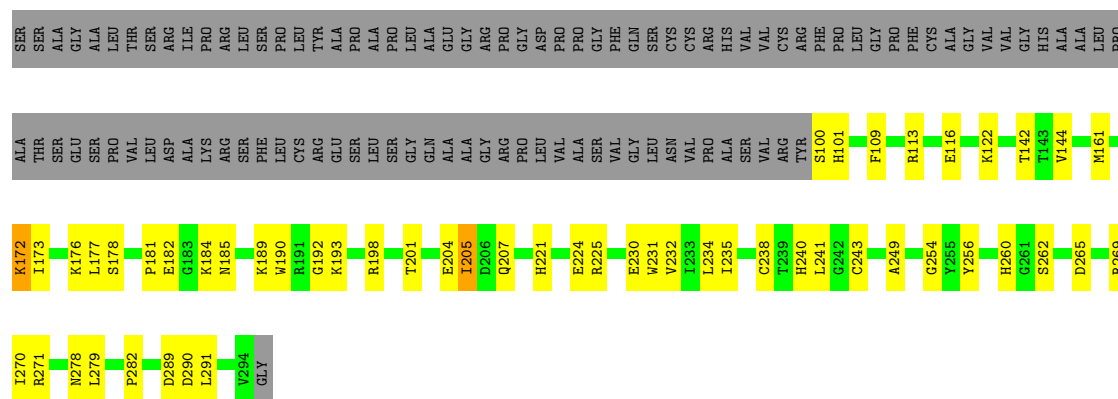


- Molecule 2: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

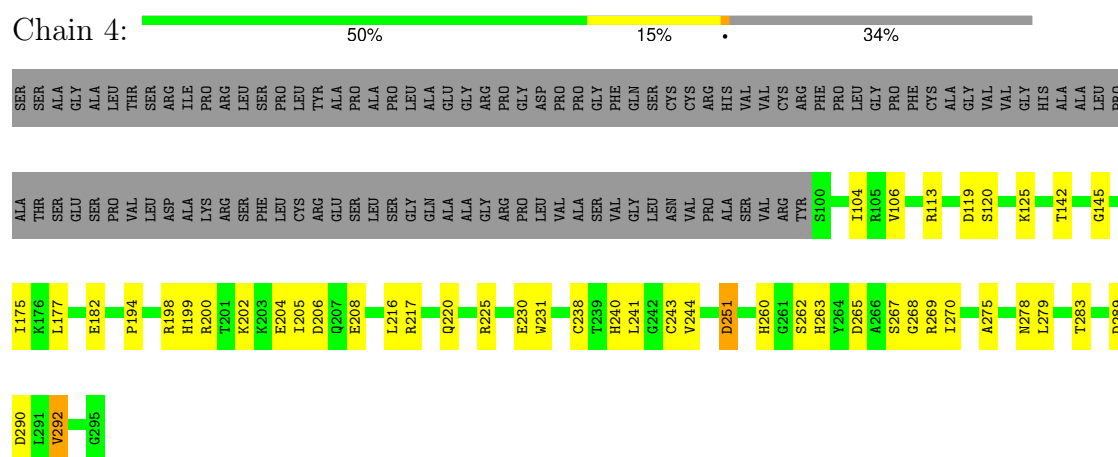


- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

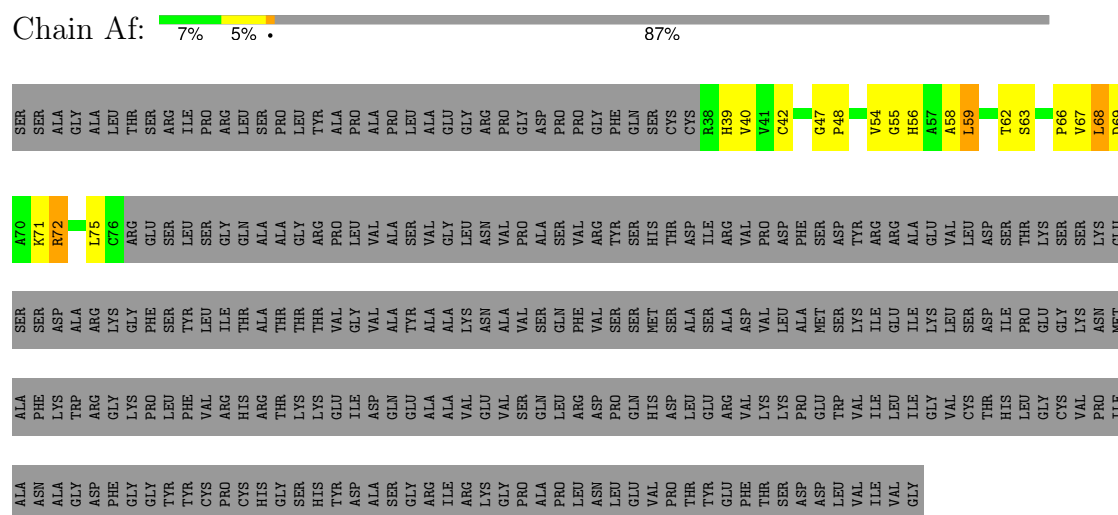




- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1



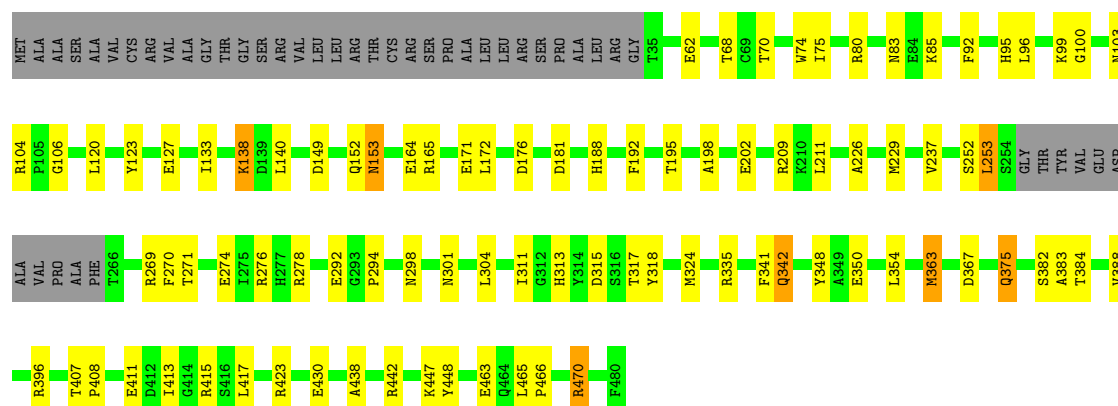
- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1



- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

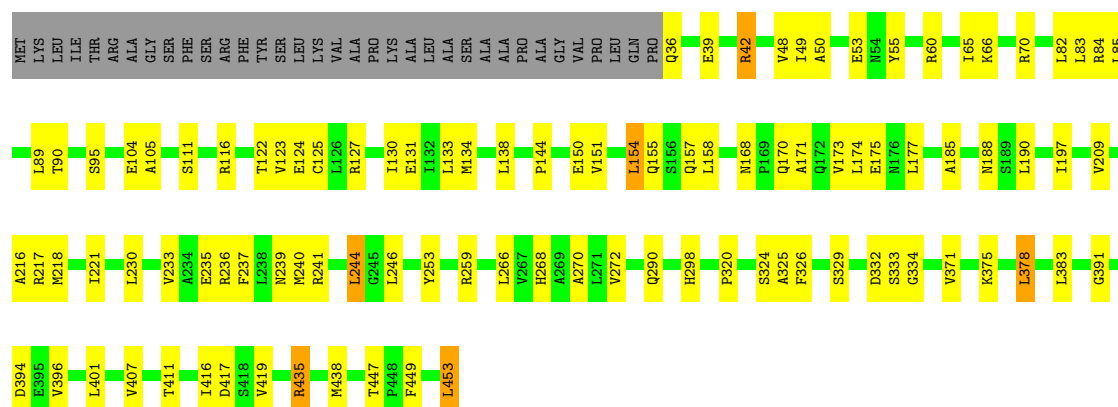


Chain u:  72% 17% 9%



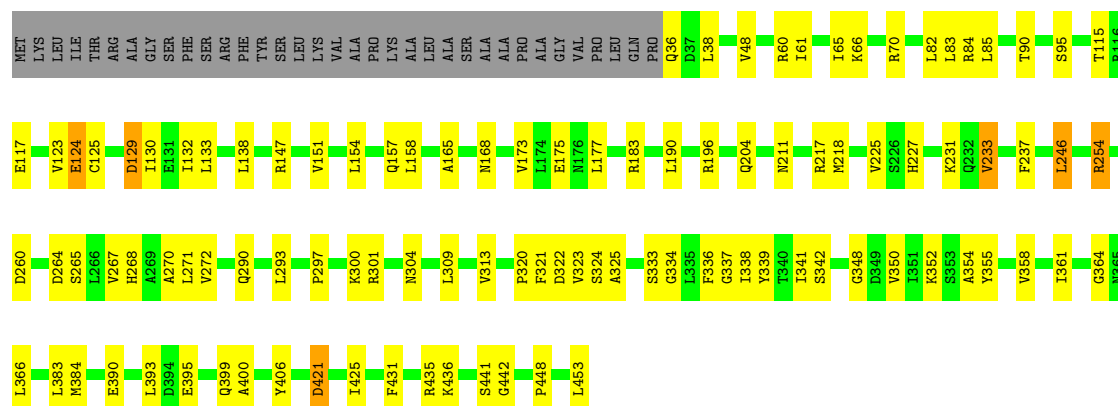
- Molecule 6: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 6:  70% 21% 8%

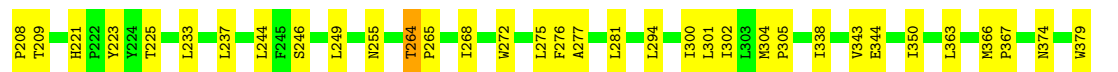
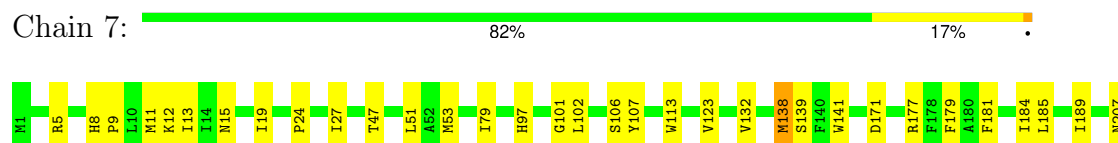


- Molecule 6: Cytochrome b-c1 complex subunit 2, mitochondrial

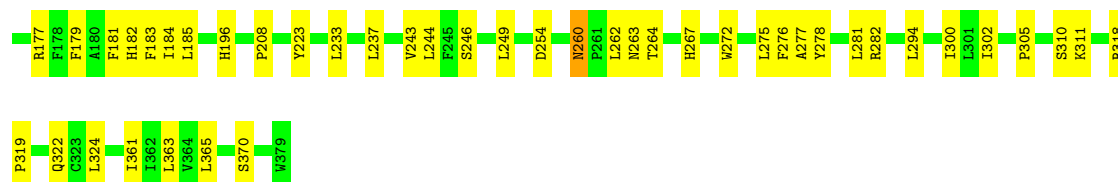
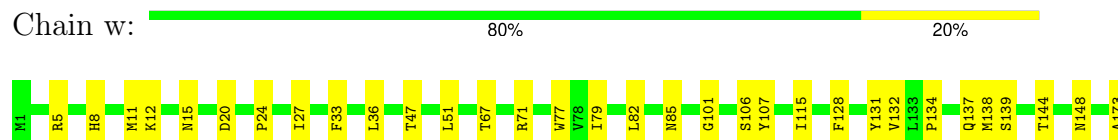
Chain v:  69% 22% 8%



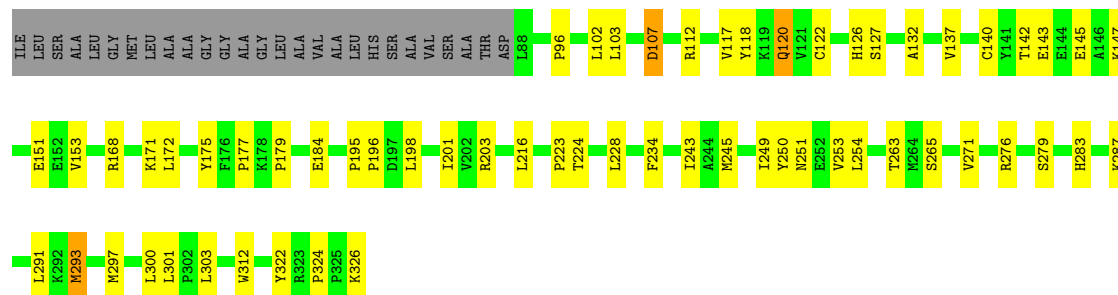
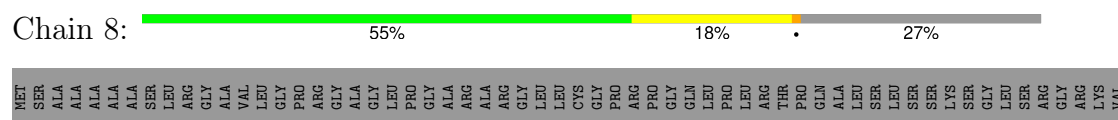
- Molecule 7: Cytochrome b



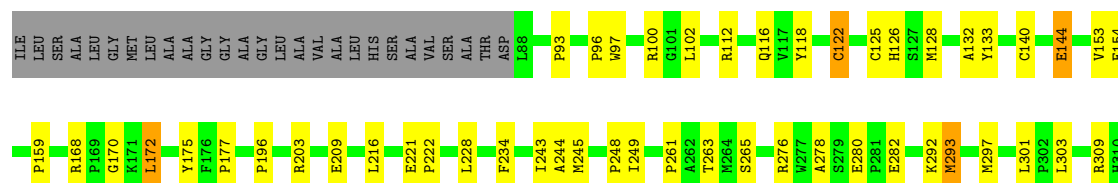
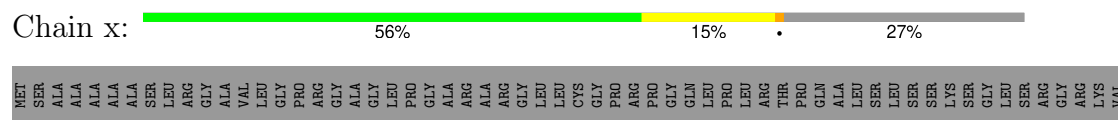
• Molecule 7: Cytochrome b



• Molecule 8: Cytochrome c1



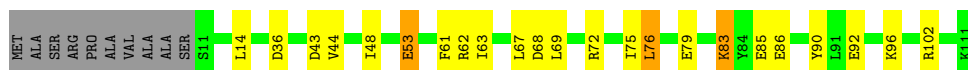
• Molecule 8: Cytochrome c1





- Molecule 9: Cytochrome b-c1 complex subunit 7

Chain 9: 70% 18% 9%



- Molecule 9: Cytochrome b-c1 complex subunit 7

Chain y: 75% 15% 9%



- Molecule 10: Cytochrome b-c1 complex subunit 8

Chain z: 77% 18% 2%



- Molecule 10: Cytochrome b-c1 complex subunit 8

Chain Aa: 80% 15% 2%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43845	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	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.408	Depositor
Minimum map value	-0.717	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	547.84, 547.84, 547.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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	0	0.19	0/567	0.32	0/759
1	Ab	0.12	0/567	0.27	0/759
2	1	0.14	0/506	0.25	0/683
2	Ac	0.12	0/506	0.21	0/683
3	2	0.13	0/1546	0.27	0/2093
3	4	0.11	0/1548	0.25	0/2094
3	Ae	0.21	0/277	0.55	0/379
3	Af	0.20	0/281	0.52	0/383
4	3	0.14	0/433	0.32	0/593
4	Ad	0.14	0/433	0.30	0/593
5	5	0.14	0/3442	0.27	0/4667
5	u	0.14	0/3441	0.27	0/4667
6	6	0.13	0/3192	0.28	0/4322
6	v	0.15	0/3192	0.29	0/4322
7	7	0.16	0/3123	0.29	0/4269
7	w	0.17	0/3123	0.32	0/4269
8	8	0.15	0/1961	0.27	0/2660
8	x	0.14	0/1954	0.26	0/2652
9	9	0.13	0/913	0.25	0/1223
9	y	0.13	0/913	0.25	0/1223
10	Aa	0.14	0/688	0.24	0/931
10	z	0.16	0/688	0.29	0/931
All	All	0.15	0/33294	0.28	0/45155

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	0	561	0	540	21	0
1	Ab	561	0	540	16	0
2	1	493	0	491	6	0
2	Ac	493	0	491	3	0
3	2	1513	0	1495	36	0
3	4	1515	0	1496	38	0
3	Ae	271	0	265	22	0
3	Af	275	0	276	19	0
4	3	417	0	414	5	0
4	Ad	417	0	414	8	0
5	5	3374	0	3272	82	0
5	u	3373	0	3272	57	0
6	6	3140	0	3121	67	0
6	v	3140	0	3121	64	0
7	7	3025	0	3090	45	0
7	w	3025	0	3090	53	0
8	8	1903	0	1850	45	0
8	x	1896	0	1845	40	0
9	9	893	0	888	14	0
9	y	893	0	888	10	0
10	Aa	666	0	663	9	0
10	z	666	0	663	12	0
11	2	4	0	0	2	0
11	4	4	0	0	3	0
12	7	86	0	60	7	0
12	w	86	0	60	8	0
13	8	43	0	31	3	0
13	x	43	0	32	5	0
All	All	32776	0	32368	584	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 9.

All (584) 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)
3:Af:47:GLY:HA2	3:Af:67:VAL:HG12	1.58	0.84
6:v:320:PRO:HB3	3:Af:75:LEU:HB3	1.61	0.82
1:Ab:75:LEU:HD23	1:Ab:78:ARG:HH12	1.45	0.80
7:w:67:THR:O	7:w:71:ARG:HB2	1.83	0.78
3:Ae:47:GLY:HA3	3:Ae:66:PRO:HA	1.65	0.78
3:Af:47:GLY:HA3	3:Af:66:PRO:HA	1.67	0.77
5:5:338:CYS:HB2	5:5:368:MET:HE3	1.70	0.74
8:x:97:TRP:HB2	8:x:100:ARG:HG3	1.69	0.74
7:7:138:MET:HE1	7:7:268:ILE:HA	1.70	0.73
5:u:363:MET:HE3	10:z:6:GLY:HA3	1.70	0.73
6:v:70:ARG:HD2	6:v:117:GLU:HG2	1.69	0.73
6:v:115:THR:HG22	3:Af:63:SER:HB2	1.73	0.70
3:Ae:55:GLY:HA3	3:Ae:59:LEU:HB3	1.73	0.70
6:6:111:SER:HB3	3:Ae:59:LEU:HG	1.72	0.70
6:6:155:GLN:NE2	6:6:197:ILE:O	2.23	0.70
3:Ae:47:GLY:HA2	3:Ae:67:VAL:HG12	1.74	0.69
2:Ac:11:TYR:HA	2:Ac:15:PHE:HB2	1.74	0.69
1:0:34:ARG:HD3	1:0:78:ARG:HH21	1.56	0.68
9:y:53:GLU:OE2	10:z:12:ARG:NH1	2.26	0.68
6:6:216:ALA:HB3	6:6:244:LEU:H	1.58	0.68
4:3:45:VAL:O	4:3:49:ASN:ND2	2.25	0.68
8:8:184:GLU:HG3	8:x:159:PRO:HB2	1.76	0.67
8:x:216:LEU:HB3	8:x:249:ILE:HD11	1.76	0.67
3:4:120:SER:HA	5:5:269:ARG:HE	1.58	0.67
6:v:61:ILE:HD11	6:v:225:VAL:HG21	1.76	0.67
6:6:131:GLU:HA	6:6:134:MET:HE3	1.75	0.66
7:w:237:LEU:HD13	8:x:297:MET:HG2	1.76	0.66
5:u:298:ASN:O	5:u:301:ASN:ND2	2.26	0.66
6:v:304:ASN:HD21	3:Af:71:LYS:HG3	1.61	0.65
10:Aa:37:ASN:OD1	10:Aa:40:ARG:NH1	2.30	0.65
5:5:179:MET:HE1	5:5:282:LEU:HD13	1.77	0.65
7:7:8:HIS:HB3	7:7:11:MET:HB2	1.78	0.65
12:w:401:HEM:HMC1	12:w:401:HEM:HBC2	1.80	0.64
3:Ae:46:LEU:O	3:Ae:48:PRO:HD2	1.97	0.64
5:u:103:ASN:OD1	5:u:153:ASN:ND2	2.31	0.64
9:y:68:ASP:OD2	9:y:72:ARG:NH1	2.31	0.64
5:5:276:ARG:NH2	5:5:466:PRO:O	2.30	0.64
5:u:317:THR:HA	6:v:157:GLN:HE22	1.63	0.64
12:7:401:HEM:HMC1	12:7:401:HEM:HBC2	1.78	0.64
8:8:203:ARG:HB2	8:8:279:SER:HB2	1.80	0.63
3:4:125:LYS:HD3	5:5:292:GLU:HG2	1.80	0.63
3:4:225:ARG:NH2	3:4:279:LEU:O	2.22	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:7:402:HEM:HMC2	12:7:402:HEM:HBC2	1.79	0.63
9:9:68:ASP:OD2	9:9:72:ARG:NH1	2.32	0.63
3:4:243:CYS:HA	7:w:264:THR:HG21	1.81	0.62
3:Af:42:CYS:HA	3:Af:48:PRO:HG2	1.80	0.62
1:Ab:28:ASP:OD1	1:Ab:28:ASP:N	2.31	0.62
6:6:174:LEU:HD11	3:Ae:67:VAL:HB	1.81	0.62
8:8:265:SER:HB3	1:Ab:90:LEU:HD11	1.80	0.62
9:y:69:LEU:HD11	9:y:76:LEU:HD13	1.80	0.62
3:Af:68:LEU:HD13	3:Af:69:ASP:H	1.64	0.62
7:7:237:LEU:HD13	8:8:297:MET:HG2	1.82	0.62
5:u:470:ARG:NH2	7:w:20:ASP:OD1	2.33	0.62
3:Af:55:GLY:HA3	3:Af:59:LEU:HB3	1.82	0.62
3:4:220:GLN:HE21	3:4:278:ASN:HD22	1.48	0.61
12:w:402:HEM:HMC2	12:w:402:HEM:HBC2	1.82	0.61
3:2:262:SER:OG	11:2:301:FES:S2	2.55	0.61
7:7:53:MET:HB3	7:w:177:ARG:HD3	1.82	0.61
7:7:281:LEU:HB2	7:7:294:LEU:HD12	1.81	0.61
5:u:226:ALA:HB2	5:u:253:LEU:HB3	1.83	0.61
7:w:246:SER:HB2	7:w:249:LEU:HB2	1.82	0.61
7:7:132:VAL:HA	7:7:139:SER:HB3	1.81	0.61
1:0:90:LEU:HD21	8:x:265:SER:HB2	1.83	0.61
3:4:216:LEU:HD13	3:4:269:ARG:HD2	1.82	0.61
2:1:20:THR:HG22	4:3:23:MET:HE2	1.84	0.60
5:5:317:THR:HA	6:6:157:GLN:HE22	1.67	0.60
3:2:185:ASN:HB2	3:2:198:ARG:HE	1.67	0.60
6:6:90:THR:HG23	6:6:95:SER:HA	1.83	0.60
5:5:80:ARG:NH2	5:5:268:CYS:SG	2.74	0.60
8:8:228:LEU:HD11	8:8:234:PHE:HB2	1.83	0.60
7:7:102:LEU:HD22	7:7:304:MET:HE2	1.84	0.60
7:7:246:SER:HB2	7:7:249:LEU:HB2	1.83	0.60
8:x:228:LEU:HD11	8:x:234:PHE:HB2	1.82	0.60
1:Ab:37:CYS:O	1:Ab:40:ILE:N	2.33	0.60
8:8:245:MET:SD	13:8:401:HEC:NA	2.75	0.60
7:w:137:GLN:NE2	7:w:263:ASN:O	2.35	0.60
7:7:338:ILE:HD11	7:7:350:ILE:HG22	1.83	0.59
6:v:395:GLU:OE2	6:v:399:GLN:NE2	2.32	0.59
7:w:85:ASN:HD22	7:w:243:VAL:HG22	1.68	0.59
3:2:172:LYS:HA	3:2:190:TRP:HE1	1.67	0.59
5:u:274:GLU:HG2	10:z:18:SER:HB2	1.83	0.59
8:x:118:TYR:HA	8:x:122:CYS:SG	2.42	0.59
1:0:30:LEU:HD21	1:0:34:ARG:HH21	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:138:LEU:HD12	6:6:233:VAL:HG22	1.85	0.59
6:v:138:LEU:HD12	6:v:233:VAL:HG22	1.85	0.59
6:v:300:LYS:HD2	6:v:301:ARG:HG3	1.84	0.58
7:w:5:ARG:NH1	7:w:15:ASN:OD1	2.34	0.58
3:2:225:ARG:NH2	3:2:279:LEU:O	2.36	0.58
3:4:217:ARG:NH1	3:4:275:ALA:O	2.35	0.58
5:5:165:ARG:NH1	5:5:208:VAL:O	2.36	0.58
5:5:222:GLN:O	5:5:225:LYS:NZ	2.32	0.58
6:6:70:ARG:HH22	6:6:332:ASP:HB2	1.67	0.58
5:u:68:THR:HG21	6:v:384:MET:HG2	1.85	0.58
6:v:196:ARG:NH2	6:v:204:GLN:OE1	2.30	0.58
3:2:243:CYS:HA	7:7:264:THR:HG21	1.86	0.58
7:w:319:PRO:HB3	10:z:48:ARG:HH21	1.69	0.58
6:6:123:VAL:HB	6:6:133:LEU:HD23	1.85	0.58
8:8:224:THR:OG1	1:Ab:67:CYS:SG	2.61	0.58
7:w:8:HIS:HB3	7:w:11:MET:HB2	1.86	0.58
6:6:60:ARG:HG3	6:6:124:GLU:HB3	1.85	0.58
9:9:53:GLU:OE2	10:Aa:12:ARG:NH1	2.37	0.58
10:z:37:ASN:OD1	10:z:40:ARG:NH1	2.35	0.57
5:5:375:GLN:OE1	5:5:378:ARG:NH1	2.37	0.57
5:u:195:THR:HG21	5:u:269:ARG:H	1.70	0.57
8:8:107:ASP:OD1	8:8:107:ASP:N	2.23	0.57
6:v:84:ARG:NH2	6:v:190:LEU:O	2.32	0.57
3:Af:67:VAL:HG22	3:Af:68:LEU:H	1.70	0.57
6:6:53:GLU:OE2	6:6:127:ARG:NH1	2.37	0.57
7:7:5:ARG:NH1	7:7:15:ASN:OD1	2.37	0.57
6:v:217:ARG:NH2	6:v:246:LEU:O	2.38	0.57
3:Ae:68:LEU:HD13	3:Ae:69:ASP:H	1.69	0.57
1:0:69:GLU:OE2	10:z:72:ARG:NH1	2.38	0.56
7:w:281:LEU:HB2	7:w:294:LEU:HD12	1.87	0.56
6:v:90:THR:HG23	6:v:95:SER:HA	1.86	0.56
5:5:96:LEU:HA	5:5:99:LYS:HG2	1.86	0.56
5:5:274:GLU:HG2	10:Aa:18:SER:HB2	1.86	0.56
6:6:378:LEU:HD13	6:6:416:ILE:HD12	1.86	0.56
12:7:402:HEM:HMB1	12:7:402:HEM:HBB2	1.86	0.56
9:9:83:LYS:HB2	9:9:86:GLU:HG2	1.87	0.56
6:v:82:LEU:HD13	6:v:158:LEU:HD11	1.88	0.56
1:0:28:ASP:HB3	8:x:263:THR:HB	1.87	0.56
3:2:249:ALA:HB3	3:2:256:TYR:HB3	1.86	0.56
5:u:62:GLU:OE2	5:u:423:ARG:NH1	2.35	0.56
5:u:104:ARG:NH1	5:u:149:ASP:OD2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:w:402:HEM:HBB2	12:w:402:HEM:HMB1	1.86	0.56
3:4:175:ILE:HB	3:4:292:VAL:HG13	1.87	0.56
8:x:153:VAL:HG21	8:x:177:PRO:HG2	1.87	0.56
4:Ad:45:VAL:O	4:Ad:49:ASN:ND2	2.39	0.56
7:w:24:PRO:HB2	7:w:27:ILE:HG23	1.88	0.55
7:w:51:LEU:HD13	12:w:401:HEM:HBD1	1.89	0.55
5:u:123:TYR:OH	5:u:411:GLU:OE1	2.24	0.55
7:w:196:HIS:HE1	12:w:402:HEM:ND	2.04	0.55
7:w:173:ALA:O	7:w:177:ARG:HG2	2.05	0.55
3:Af:72:ARG:HH12	3:Af:75:LEU:HB2	1.71	0.55
7:7:207:ASN:ND2	7:7:209:THR:OG1	2.39	0.55
6:v:129:ASP:OD1	6:v:129:ASP:N	2.40	0.55
7:w:101:GLY:HA2	7:w:106:SER:HB2	1.88	0.55
9:9:69:LEU:HD11	9:9:76:LEU:HD13	1.89	0.55
5:u:188:HIS:NE2	5:u:348:TYR:OH	2.38	0.55
6:v:348:GLY:HA2	6:v:448:PRO:HD3	1.89	0.55
4:3:9:ARG:HG3	5:u:384:THR:HG21	1.87	0.55
5:5:318:TYR:HE1	3:Ae:54:VAL:HG23	1.72	0.55
7:7:24:PRO:HB2	7:7:27:ILE:HG23	1.89	0.55
5:u:318:TYR:CE1	3:Af:55:GLY:HA2	2.42	0.55
6:v:82:LEU:HD21	6:v:151:VAL:HG13	1.89	0.55
3:4:113:ARG:HH21	5:5:271:THR:HG21	1.71	0.54
5:5:318:TYR:CE1	3:Ae:55:GLY:HA2	2.42	0.54
8:8:126:HIS:ND1	8:8:196:PRO:O	2.40	0.54
10:Aa:78:TYR:CG	1:Ab:65:GLU:HB3	2.42	0.54
5:5:341:PHE:HB2	5:5:358:PHE:HB3	1.88	0.54
1:0:71:LEU:O	1:0:75:LEU:HG	2.07	0.54
7:7:237:LEU:HB2	8:8:297:MET:HG2	1.90	0.54
6:v:341:ILE:HG21	3:Af:72:ARG:HD3	1.89	0.54
3:4:230:GLU:HG2	3:4:231:TRP:CD1	2.43	0.54
5:5:378:ARG:NH2	5:5:387:GLU:OE1	2.40	0.54
9:9:36:ASP:OD2	9:9:62:ARG:NH1	2.40	0.54
1:0:78:ARG:HH11	1:0:78:ARG:HB3	1.72	0.54
5:5:96:LEU:HD13	5:5:156:LEU:HD22	1.89	0.54
6:6:66:LYS:O	6:6:217:ARG:NH2	2.36	0.54
6:6:85:LEU:HD12	6:6:158:LEU:HD12	1.89	0.54
3:Ae:42:CYS:HA	3:Ae:48:PRO:HG3	1.89	0.54
1:0:60:ARG:NH1	1:0:65:GLU:OE2	2.41	0.54
3:2:100:SER:O	3:2:101:HIS:ND1	2.40	0.54
5:5:328:LEU:HB2	5:5:375:GLN:HG3	1.90	0.53
6:6:320:PRO:HG3	3:Ae:75:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:x:125:CYS:SG	13:x:401:HEC:HAC	2.49	0.53
6:v:271:LEU:HD22	6:v:453:LEU:HD13	1.91	0.53
5:5:282:LEU:HD12	5:5:460:GLY:HA2	1.90	0.53
6:6:42:ARG:HH11	6:6:42:ARG:HB2	1.71	0.53
6:6:324:SER:HB3	3:Ae:68:LEU:HD23	1.91	0.53
12:w:401:HEM:HMB1	12:w:401:HEM:HBB2	1.90	0.53
7:w:82:LEU:HD23	7:w:243:VAL:HG21	1.91	0.53
5:5:112:GLU:O	5:5:115:SER:OG	2.22	0.53
5:5:190:THR:HB	5:5:275:ILE:HG13	1.91	0.53
8:8:126:HIS:HE1	8:8:196:PRO:HD2	1.74	0.53
6:6:168:ASN:HB2	6:6:170:GLN:HE22	1.74	0.53
5:u:388:VAL:HG21	5:u:438:ALA:HA	1.90	0.53
3:4:119:ASP:OD1	3:4:119:ASP:N	2.41	0.53
6:v:65:ILE:HG12	6:v:218:MET:HG2	1.91	0.53
5:5:315:ASP:OD1	5:5:316:SER:N	2.42	0.52
5:5:396:ARG:NE	5:5:430:GLU:OE2	2.41	0.52
6:v:324:SER:HB3	3:Af:68:LEU:HD23	1.91	0.52
6:v:123:VAL:HB	6:v:133:LEU:HD23	1.90	0.52
5:5:311:ILE:HD12	5:5:375:GLN:HB3	1.92	0.52
5:5:388:VAL:HG21	5:5:438:ALA:HA	1.92	0.52
5:u:318:TYR:HD2	5:u:324:MET:HE1	1.74	0.52
6:v:66:LYS:O	6:v:217:ARG:NH1	2.43	0.52
7:7:107:TYR:HB2	7:7:305:PRO:HG3	1.90	0.52
8:8:118:TYR:HA	8:8:122:CYS:SG	2.49	0.52
5:u:304:LEU:HD13	5:u:354:LEU:HD22	1.90	0.52
2:Ac:23:LEU:HD22	4:Ad:23:MET:HE1	1.92	0.52
1:0:37:CYS:SG	1:0:78:ARG:HA	2.49	0.52
7:w:128:PHE:O	7:w:132:VAL:HG23	2.10	0.52
12:7:401:HEM:HMB1	12:7:401:HEM:HBB2	1.92	0.52
7:w:300:ILE:HD11	7:w:363:LEU:HD21	1.92	0.52
1:0:30:LEU:HB2	8:x:265:SER:OG	2.10	0.52
7:7:101:GLY:HA2	7:7:106:SER:HB2	1.92	0.52
6:v:165:ALA:O	6:v:168:ASN:ND2	2.42	0.52
5:u:318:TYR:HE1	3:Af:54:VAL:HG23	1.75	0.51
5:u:278:ARG:NH2	5:u:463:GLU:OE1	2.43	0.51
8:x:112:ARG:HB2	8:x:140:CYS:HB2	1.93	0.51
7:w:107:TYR:HB2	7:w:305:PRO:HG3	1.93	0.51
9:y:92:GLU:HG2	9:y:96:LYS:HE3	1.93	0.51
2:1:29:ALA:HA	3:2:144:VAL:HG13	1.92	0.51
3:4:220:GLN:HE21	3:4:278:ASN:ND2	2.07	0.51
6:v:190:LEU:HD13	3:Af:62:THR:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:w:115:ILE:HB	7:w:196:HIS:HD2	1.76	0.51
7:w:138:MET:HE1	7:w:267:HIS:O	2.10	0.51
3:4:244:VAL:HG23	7:w:264:THR:HG23	1.92	0.51
5:5:366:ASP:HB2	5:5:464:GLN:HG2	1.93	0.51
6:6:266:LEU:HD13	3:Ae:72:ARG:HE	1.76	0.51
9:9:43:ASP:OD2	9:9:102:ARG:NH1	2.44	0.51
7:w:131:TYR:O	7:w:134:PRO:HD2	2.11	0.51
3:2:289:ASP:OD1	3:2:289:ASP:N	2.44	0.51
3:4:202:LYS:NZ	3:4:206:ASP:OD1	2.40	0.51
5:5:412:ASP:OD2	5:5:423:ARG:NE	2.44	0.51
8:8:127:SER:HB2	8:8:179:PRO:HD3	1.92	0.51
8:8:243:ILE:HG12	8:8:245:MET:H	1.74	0.51
2:1:11:TYR:HA	2:1:15:PHE:HB2	1.93	0.50
3:2:230:GLU:HG2	3:2:231:TRP:CD1	2.47	0.50
7:7:47:THR:HG23	7:7:79:ILE:HG23	1.94	0.50
3:2:265:ASP:HB3	3:2:271:ARG:HH11	1.76	0.50
5:u:140:LEU:HD22	5:u:237:VAL:HG12	1.93	0.50
7:7:272:TRP:HA	7:7:275:LEU:HG	1.93	0.50
9:9:92:GLU:HG2	9:9:96:LYS:HE3	1.94	0.50
6:v:364:GLY:HA2	6:v:425:ILE:HD13	1.93	0.50
6:6:449:PHE:CZ	6:v:183:ARG:HB2	2.46	0.50
5:5:152:GLN:HG2	5:5:253:LEU:HD13	1.94	0.50
6:6:259:ARG:NH2	6:6:447:THR:O	2.45	0.50
8:8:216:LEU:HB3	8:8:249:ILE:HD11	1.94	0.50
7:w:272:TRP:HA	7:w:275:LEU:HG	1.93	0.50
2:1:41:ASP:OD1	8:x:292:LYS:NZ	2.41	0.49
5:u:152:GLN:NE2	5:u:252:SER:OG	2.44	0.49
6:v:211:ASN:HB3	6:v:246:LEU:HB2	1.94	0.49
1:Ab:37:CYS:HB3	1:Ab:78:ARG:HG3	1.94	0.49
5:5:104:ARG:NH2	5:5:145:GLU:OE2	2.45	0.49
7:w:244:LEU:HD12	8:x:293:MET:HG2	1.93	0.49
3:2:176:LYS:NZ	3:2:178:SER:OG	2.42	0.49
3:4:270:ILE:HG22	3:4:278:ASN:OD1	2.12	0.49
5:5:75:ILE:HG23	5:5:229:MET:HG2	1.94	0.49
8:8:96:PRO:HD3	1:Ab:83:ALA:O	2.12	0.49
8:8:245:MET:SD	13:8:401:HEC:NB	2.86	0.49
6:v:85:LEU:HD12	6:v:158:LEU:HD12	1.93	0.49
1:Ab:33:VAL:HG12	1:Ab:82:VAL:HG22	1.95	0.49
1:0:26:LEU:HD11	8:x:261:PRO:HB3	1.94	0.49
6:6:190:LEU:HD13	3:Ae:62:THR:HB	1.94	0.49
7:7:8:HIS:O	7:7:12:LYS:N	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:362:ASN:N	5:5:362:ASN:OD1	2.45	0.49
6:6:233:VAL:HG23	6:6:236:ARG:HH12	1.77	0.49
7:w:182:HIS:HE1	12:w:401:HEM:C1B	2.28	0.49
8:x:168:ARG:HG2	8:x:170:GLY:H	1.76	0.49
3:4:145:GLY:HA3	8:8:300:LEU:HD21	1.95	0.49
3:4:194:PRO:HG3	7:w:262:LEU:HA	1.95	0.49
5:u:83:ASN:OD1	5:u:85:LYS:HG2	2.13	0.49
6:v:125:CYS:SG	6:v:133:LEU:HD22	2.53	0.49
7:w:47:THR:HG23	7:w:79:ILE:HG23	1.95	0.49
10:Aa:73:LYS:HG3	10:Aa:78:TYR:HE2	1.77	0.49
1:0:33:VAL:HG12	1:0:82:VAL:HG22	1.94	0.48
3:2:260:HIS:CD2	7:7:343:VAL:HB	2.47	0.48
5:5:422:ARG:NH2	5:5:428:GLU:OE1	2.45	0.48
5:u:276:ARG:O	10:z:15:ILE:HA	2.13	0.48
8:8:103:LEU:HD22	8:8:291:LEU:HB2	1.95	0.48
8:8:322:TYR:HB2	9:9:61:PHE:CD1	2.48	0.48
3:4:289:ASP:OD1	3:4:289:ASP:N	2.36	0.48
7:7:244:LEU:HD12	8:8:293:MET:HG2	1.95	0.48
8:8:265:SER:OG	1:Ab:30:LEU:HB2	2.13	0.48
7:7:15:ASN:HA	7:7:19:ILE:HB	1.95	0.48
6:v:264:ASP:OD1	6:v:265:SER:N	2.46	0.48
3:4:262:SER:OG	11:4:301:FES:S1	2.60	0.48
7:w:310:SER:HB2	7:w:370:SER:HB3	1.94	0.48
5:u:70:THR:HG21	5:u:407:THR:HA	1.95	0.48
3:2:182:GLU:HG3	3:2:201:THR:HG22	1.95	0.48
6:6:39:GLU:O	6:6:50:ALA:HA	2.13	0.48
6:6:82:LEU:HD13	6:6:158:LEU:HD11	1.94	0.48
6:6:171:ALA:O	6:6:175:GLU:HG2	2.14	0.48
7:7:138:MET:HE2	7:7:138:MET:HA	1.94	0.48
8:8:324:PRO:HB2	8:8:326:LYS:HG2	1.94	0.48
3:4:290:ASP:OD1	3:4:290:ASP:N	2.47	0.48
7:7:9:PRO:O	7:7:13:ILE:HG12	2.14	0.48
5:u:396:ARG:NE	5:u:430:GLU:OE2	2.44	0.48
6:6:82:LEU:HD21	6:6:151:VAL:HG13	1.95	0.48
5:u:172:LEU:HD21	5:u:202:GLU:HB3	1.95	0.48
6:v:293:LEU:HB3	6:v:309:LEU:HG	1.96	0.48
6:6:116:ARG:NH1	6:6:188:ASN:O	2.47	0.48
6:6:138:LEU:HD13	6:6:237:PHE:HB2	1.95	0.48
6:6:70:ARG:HG3	6:6:185:ALA:HB1	1.96	0.47
5:u:120:LEU:HD13	5:u:133:ILE:HG12	1.96	0.47
8:x:221:GLU:HG2	8:x:222:PRO:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:52:GLN:HE21	5:5:56:GLY:HA2	1.78	0.47
5:5:324:MET:O	5:5:330:SER:OG	2.32	0.47
6:v:60:ARG:CZ	6:v:124:GLU:HG2	2.44	0.47
3:4:260:HIS:HB2	11:4:301:FES:S1	2.54	0.47
5:u:447:LYS:HE3	5:u:448:TYR:CE2	2.49	0.47
6:6:253:TYR:HE2	6:6:435:ARG:HB3	1.80	0.47
8:8:112:ARG:HB2	8:8:140:CYS:HB2	1.95	0.47
8:8:223:PRO:HB2	1:Ab:67:CYS:HB2	1.96	0.47
8:8:153:VAL:HG21	8:8:177:PRO:HG2	1.96	0.47
5:u:294:PRO:HG3	5:u:448:TYR:CZ	2.50	0.47
6:v:138:LEU:HD13	6:v:237:PHE:HB2	1.96	0.47
6:v:60:ARG:CZ	6:v:390:GLU:HG3	2.44	0.47
6:v:321:PHE:HD2	6:v:323:VAL:HG13	1.80	0.47
6:v:338:ILE:HG21	6:v:354:ALA:HB1	1.95	0.47
5:5:283:PRO:HB2	5:5:284:LEU:HD12	1.97	0.47
8:x:243:ILE:HG12	8:x:245:MET:H	1.80	0.47
7:7:179:PHE:HE2	7:w:179:PHE:HE2	1.62	0.46
3:Ae:47:GLY:O	3:Ae:50:CYS:HB2	2.15	0.46
3:2:235:ILE:HG13	3:2:282:PRO:HD3	1.96	0.46
7:7:221:HIS:O	7:7:225:THR:OG1	2.25	0.46
6:v:267:VAL:HG22	6:v:442:GLY:HA3	1.97	0.46
3:2:177:LEU:HB2	3:2:290:ASP:HA	1.97	0.46
5:5:131:TYR:HH	5:5:224:TYR:HH	1.63	0.46
5:5:234:ALA:N	5:5:410:CYS:SG	2.89	0.46
6:6:375:LYS:NZ	6:6:419:VAL:O	2.40	0.46
8:8:102:LEU:O	8:8:287:LYS:HD2	2.16	0.46
6:v:297:PRO:HB2	3:Af:71:LYS:HE3	1.96	0.46
1:0:45:LYS:O	1:0:48:GLU:HG2	2.15	0.46
6:6:371:VAL:HG12	6:6:375:LYS:HE3	1.97	0.46
7:7:106:SER:HB3	12:7:402:HEM:HBD2	1.96	0.46
3:4:106:VAL:HG22	5:5:275:ILE:HD11	1.97	0.46
7:w:223:TYR:HB3	8:x:312:TRP:CZ2	2.50	0.46
3:4:238:CYS:SG	3:4:240:HIS:HB3	2.55	0.46
6:6:55:TYR:HA	6:6:127:ARG:HH12	1.81	0.46
6:6:65:ILE:HG12	6:6:218:MET:HG2	1.97	0.46
6:6:144:PRO:HG3	6:6:209:VAL:HG11	1.96	0.46
6:6:407:VAL:HG13	6:6:411:THR:HB	1.97	0.46
7:w:71:ARG:NH2	8:x:278:ALA:O	2.49	0.46
5:5:192:PHE:O	5:5:195:THR:OG1	2.27	0.46
8:8:132:ALA:HA	8:8:175:TYR:HA	1.97	0.46
9:y:43:ASP:OD2	9:y:102:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:241:LEU:HD12	3:4:260:HIS:HE1	1.80	0.46
6:v:177:LEU:HD11	6:v:272:VAL:HG22	1.98	0.46
3:Ae:55:GLY:CA	3:Ae:59:LEU:HB3	2.45	0.46
3:2:221:HIS:O	3:2:224:GLU:HG2	2.15	0.46
5:5:61:SER:HA	5:5:233:ALA:O	2.16	0.46
6:6:235:GLU:O	6:6:239:ASN:ND2	2.49	0.46
8:x:203:ARG:CZ	8:x:280:GLU:HG2	2.46	0.46
3:2:260:HIS:HB2	11:2:301:FES:S2	2.55	0.46
6:6:233:VAL:HG23	6:6:236:ARG:NH1	2.31	0.45
5:u:74:TRP:CZ2	5:u:411:GLU:HA	2.52	0.45
8:x:118:TYR:CZ	8:x:128:MET:HG3	2.50	0.45
3:2:176:LYS:HA	3:2:291:LEU:HD23	1.98	0.45
8:8:251:ASN:ND2	1:Ab:26:LEU:O	2.49	0.45
5:5:70:THR:HB	5:5:410:CYS:SG	2.56	0.45
6:v:361:ILE:HD12	6:v:366:LEU:HD13	1.98	0.45
8:x:133:TYR:HB2	8:x:172:LEU:HA	1.97	0.45
5:u:92:PHE:O	5:u:96:LEU:HG	2.16	0.45
5:5:195:THR:HG21	5:5:269:ARG:H	1.81	0.45
7:7:138:MET:HB2	7:7:255:ASN:HD22	1.81	0.45
13:x:401:HEC:HHA	13:x:401:HEC:HBA1	1.98	0.45
3:2:173:ILE:HG23	3:2:190:TRP:HD1	1.82	0.45
3:2:181:PRO:HD2	3:2:184:LYS:HD2	1.99	0.45
3:4:241:LEU:HB2	11:4:301:FES:S2	2.57	0.45
1:0:65:GLU:HB3	10:z:78:TYR:CG	2.52	0.45
6:v:431:PHE:O	6:v:436:LYS:NZ	2.50	0.45
5:5:384:THR:HG21	4:Ad:9:ARG:HG3	1.98	0.45
6:6:270:ALA:O	6:6:438:MET:HA	2.17	0.45
5:u:165:ARG:HD3	5:u:209:ARG:HA	1.98	0.45
3:2:142:THR:OG1	8:x:303:LEU:HB3	2.17	0.45
8:8:120:GLN:HG2	8:8:254:LEU:HD13	1.98	0.45
8:x:248:PRO:HG2	13:x:401:HEC:HBB2	1.99	0.45
1:Ab:34:ARG:HD3	1:Ab:78:ARG:HE	1.81	0.45
2:Ac:50:GLY:H	2:Ac:55:HIS:CD2	2.35	0.45
2:1:57:LYS:O	2:1:61:GLU:HG2	2.16	0.45
6:6:177:LEU:HD11	6:6:272:VAL:HG22	1.97	0.45
6:v:358:VAL:HG11	6:v:431:PHE:CD2	2.51	0.45
6:v:173:VAL:HG21	6:v:268:HIS:HB2	1.98	0.44
1:0:37:CYS:O	1:0:40:ILE:HB	2.18	0.44
3:2:113:ARG:HH12	5:u:271:THR:HG21	1.81	0.44
3:2:189:LYS:HD2	3:2:192:GLY:HA2	1.99	0.44
3:4:270:ILE:HD13	3:4:275:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:335:ARG:HB2	5:5:337:LEU:HG	1.98	0.44
6:6:89:LEU:HD21	6:6:154:LEU:HD12	1.99	0.44
6:6:221:ILE:HG12	6:6:396:VAL:HG12	2.00	0.44
6:6:326:PHE:CE2	3:Ae:65:SER:HB2	2.52	0.44
7:7:223:TYR:HB3	8:8:312:TRP:CZ2	2.52	0.44
5:u:99:LYS:HE3	5:u:164:GLU:OE2	2.17	0.44
5:u:407:THR:HB	5:u:408:PRO:HD3	1.99	0.44
6:v:260:ASP:HB3	6:v:441:SER:HA	1.99	0.44
7:w:8:HIS:O	7:w:12:LYS:N	2.40	0.44
5:5:180:ARG:HH21	5:5:342:GLN:HE22	1.63	0.44
5:5:383:ALA:HB3	5:5:442:ARG:HG3	1.99	0.44
6:6:125:CYS:SG	6:6:133:LEU:HD22	2.57	0.44
8:x:126:HIS:ND1	8:x:196:PRO:O	2.50	0.44
3:4:205:ILE:HD11	3:4:230:GLU:HA	1.99	0.44
5:u:465:LEU:HD12	5:u:466:PRO:HD2	1.99	0.44
6:v:272:VAL:HA	6:v:337:GLY:HA3	1.99	0.44
3:2:240:HIS:O	3:2:241:LEU:HD23	2.17	0.44
5:u:311:ILE:HD12	5:u:375:GLN:HB3	1.98	0.44
7:w:302:ILE:O	7:w:305:PRO:HD2	2.17	0.44
5:5:71:VAL:HG21	5:5:144:VAL:HG22	2.00	0.44
7:7:113:TRP:NE1	7:7:301:LEU:O	2.35	0.44
9:9:63:ILE:O	9:9:67:LEU:HG	2.17	0.44
6:v:60:ARG:HG2	6:v:393:LEU:HD22	2.00	0.44
3:2:161:MET:C	7:7:177:ARG:HH21	2.25	0.44
3:2:270:ILE:HG22	3:2:278:ASN:OD1	2.17	0.44
3:4:251:ASP:OD1	3:4:263:HIS:ND1	2.51	0.44
5:5:405:GLY:C	5:5:408:PRO:HD2	2.43	0.44
5:5:428:GLU:OE2	5:5:432:ARG:NH2	2.35	0.44
7:w:33:PHE:HA	7:w:36:LEU:HB2	1.99	0.44
8:x:244:ALA:HB3	13:x:401:HEC:HBD2	1.99	0.44
3:2:204:GLU:O	3:2:207:GLN:HG3	2.18	0.44
6:6:104:GLU:HG2	3:Ae:56:HIS:ND1	2.33	0.44
6:6:375:LYS:HD3	6:6:417:ASP:HA	2.00	0.44
5:u:274:GLU:CD	5:u:276:ARG:HE	2.26	0.44
5:5:304:LEU:HD22	5:5:354:LEU:HD21	2.00	0.44
8:8:198:LEU:HD22	8:8:201:ILE:HG21	2.00	0.44
6:v:313:VAL:HG11	6:v:350:VAL:HG13	2.00	0.44
7:w:260:ASN:HD22	7:w:262:LEU:H	1.64	0.44
9:y:83:LYS:HB2	9:y:86:GLU:HG2	2.00	0.44
3:2:193:LYS:HE2	3:2:193:LYS:HB2	1.90	0.43
3:4:142:THR:OG1	8:8:303:LEU:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:390:ARG:HG3	6:6:105:ALA:HA	1.99	0.43
8:8:250:TYR:CZ	8:8:253:VAL:HG23	2.52	0.43
1:Ab:47:ARG:O	1:Ab:51:GLU:HG2	2.18	0.43
5:5:114:GLU:HG2	6:6:298:HIS:HB2	2.00	0.43
7:7:374:ASN:HA	7:7:379:TRP:HD1	1.82	0.43
7:w:27:ILE:HA	7:w:208:PRO:HD3	2.00	0.43
4:Ad:51:LYS:HE3	4:Ad:52:PHE:CE2	2.53	0.43
3:2:265:ASP:OD1	3:2:269:ARG:N	2.52	0.43
7:7:276:PHE:CG	7:7:277:ALA:N	2.86	0.43
7:7:366:MET:HB3	7:7:367:PRO:HD3	2.00	0.43
5:u:165:ARG:NH2	5:u:211:LEU:O	2.45	0.43
5:u:383:ALA:H	5:u:442:ARG:HD3	1.83	0.43
7:w:237:LEU:HD22	8:x:301:LEU:HD11	2.01	0.43
5:u:335:ARG:NH2	5:u:367:ASP:OD2	2.50	0.43
7:w:318:ARG:O	7:w:322:GLN:HG3	2.18	0.43
10:z:46:ILE:HG23	10:z:47:LEU:HD22	2.00	0.43
3:2:198:ARG:HH12	3:2:254:GLY:HA2	1.83	0.43
5:5:233:ALA:HB1	5:5:237:VAL:HG11	2.00	0.43
7:7:51:LEU:HD13	12:7:401:HEM:HBD1	1.99	0.43
7:7:141:TRP:CD1	7:7:265:PRO:HD3	2.53	0.43
3:Af:56:HIS:C	3:Af:58:ALA:H	2.26	0.43
4:Ad:39:ARG:HB2	4:Ad:52:PHE:CE1	2.54	0.43
1:0:34:ARG:HD3	1:0:78:ARG:NH2	2.29	0.43
5:5:174:GLU:O	5:5:177:SER:OG	2.33	0.43
6:6:154:LEU:HD23	6:6:157:GLN:HB3	2.01	0.43
2:1:50:GLY:H	2:1:55:HIS:CD2	2.37	0.43
3:2:109:PHE:O	3:2:113:ARG:HG3	2.19	0.43
5:5:67:PRO:HB2	6:6:383:LEU:HD13	2.00	0.43
5:5:74:TRP:CZ2	5:5:411:GLU:HA	2.54	0.43
5:5:241:GLN:HA	5:5:244:ASP:OD2	2.19	0.43
6:6:125:CYS:SG	6:6:130:ILE:HA	2.59	0.43
6:6:453:LEU:HD13	6:6:453:LEU:HA	1.86	0.43
8:x:209:GLU:OE1	8:x:276:ARG:NE	2.29	0.43
1:Ab:37:CYS:SG	1:Ab:78:ARG:HA	2.59	0.43
1:0:47:ARG:O	1:0:51:GLU:HG2	2.18	0.43
7:7:237:LEU:HD22	8:8:301:LEU:HD11	2.01	0.43
6:v:421:ASP:OD1	6:v:421:ASP:N	2.50	0.43
5:u:342:GLN:HE21	5:u:342:GLN:HB2	1.60	0.43
8:x:132:ALA:HA	8:x:175:TYR:HA	2.00	0.43
5:5:167:VAL:O	5:5:171:GLU:HG2	2.19	0.43
5:5:233:ALA:HB3	5:5:242:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:123:VAL:HG22	7:7:189:ILE:HD13	2.01	0.42
8:8:137:VAL:HG13	8:8:143:GLU:HA	2.01	0.42
7:w:185:LEU:HA	7:w:185:LEU:HD23	1.82	0.42
3:2:198:ARG:HB3	3:2:232:VAL:HG13	2.00	0.42
7:7:302:ILE:O	7:7:305:PRO:HD2	2.19	0.42
6:v:290:GLN:HB2	6:v:336:PHE:HE1	1.83	0.42
6:v:48:VAL:HG11	6:v:400:ALA:HB1	2.01	0.42
1:Ab:57:VAL:HG22	1:Ab:65:GLU:HG3	2.00	0.42
4:3:23:MET:O	4:3:27:VAL:HG23	2.18	0.42
7:7:97:HIS:HE1	12:7:402:HEM:NA	2.17	0.42
6:v:383:LEU:HD23	6:v:383:LEU:HA	1.92	0.42
7:w:276:PHE:CG	7:w:277:ALA:N	2.87	0.42
7:w:361:ILE:HG12	7:w:365:LEU:HD12	2.01	0.42
6:6:230:LEU:O	6:6:233:VAL:HG12	2.19	0.42
7:7:185:LEU:HD23	7:7:185:LEU:HA	1.83	0.42
6:v:132:ILE:HD12	6:v:132:ILE:H	1.84	0.42
7:w:138:MET:HE3	7:w:254:ASP:HB2	2.02	0.42
8:x:96:PRO:HA	8:x:100:ARG:HH21	1.84	0.42
8:x:322:TYR:HB2	9:y:61:PHE:CD1	2.55	0.42
3:4:204:GLU:O	3:4:208:GLU:HG2	2.19	0.42
3:4:225:ARG:NH1	3:4:267:SER:O	2.52	0.42
5:5:317:THR:HA	6:6:157:GLN:NE2	2.33	0.42
8:8:122:CYS:HB3	13:8:401:HEC:CHC	2.49	0.42
5:u:75:ILE:HG12	5:u:229:MET:HG2	2.01	0.42
8:x:112:ARG:HG2	8:x:116:GLN:HE21	1.85	0.42
8:x:126:HIS:HE1	8:x:196:PRO:HD2	1.85	0.42
8:8:142:THR:HG23	8:8:145:GLU:H	1.85	0.42
5:5:104:ARG:NH1	5:5:149:ASP:OD2	2.51	0.42
5:5:363:MET:HE1	10:Aa:7:HIS:CG	2.55	0.42
6:6:42:ARG:HD3	6:6:48:VAL:HG22	2.02	0.42
7:7:344:GLU:HG3	10:Aa:67:PHE:HE1	1.84	0.42
5:u:192:PHE:O	5:u:198:ALA:HB2	2.19	0.42
6:v:38:LEU:HD23	6:v:406:TYR:CD2	2.54	0.42
7:w:144:THR:O	7:w:148:ASN:HB2	2.19	0.42
9:y:110:LYS:NZ	4:Ad:3:SER:O	2.49	0.42
6:6:104:GLU:HA	3:Ae:56:HIS:HE1	1.84	0.42
7:7:27:ILE:HA	7:7:208:PRO:HD3	2.01	0.42
7:w:33:PHE:HA	7:w:36:LEU:HD12	2.02	0.42
8:x:309:ARG:HG3	10:z:27:PHE:CE2	2.54	0.42
10:Aa:51:PRO:HB2	10:Aa:52:PRO:HD3	2.02	0.42
5:5:422:ARG:HH22	5:5:428:GLU:CD	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:u:80:ARG:HD2	5:u:127:GLU:HG2	2.02	0.42
3:4:265:ASP:OD1	3:4:269:ARG:N	2.48	0.41
5:5:473:SER:HA	5:5:476:PHE:CE1	2.55	0.41
5:u:100:GLY:HA3	5:u:106:GLY:HA2	2.02	0.41
5:u:270:PHE:CG	5:u:292:GLU:HB2	2.55	0.41
9:y:85:GLU:CD	9:y:85:GLU:H	2.28	0.41
10:Aa:19:LEU:HD22	10:Aa:23:GLU:HB2	2.02	0.41
3:4:198:ARG:HD2	3:4:200:ARG:HG2	2.01	0.41
5:5:84:GLU:O	5:5:207:ASN:ND2	2.53	0.41
5:5:120:LEU:HD13	5:5:133:ILE:HG12	2.02	0.41
6:v:290:GLN:HG3	6:v:325:ALA:HB3	2.01	0.41
7:w:77:TRP:CD2	8:x:282:GLU:HG3	2.55	0.41
7:w:324:LEU:HD23	7:w:324:LEU:HA	1.92	0.41
6:6:174:LEU:HD13	3:Ae:64:GLU:HB3	2.02	0.41
7:7:181:PHE:HA	7:7:184:ILE:HG22	2.03	0.41
8:8:168:ARG:HH12	8:8:171:LYS:HG2	1.85	0.41
3:Ae:72:ARG:O	3:Ae:72:ARG:HD3	2.20	0.41
4:Ad:39:ARG:HA	4:Ad:42:LEU:HB2	2.03	0.41
3:2:234:LEU:HD22	3:2:279:LEU:HB2	2.01	0.41
5:5:388:VAL:O	5:5:392:LYS:HG3	2.21	0.41
6:6:333:SER:OG	6:6:334:GLY:N	2.53	0.41
8:8:172:LEU:H	8:8:172:LEU:HD12	1.85	0.41
6:v:254:ARG:O	6:v:435:ARG:NH1	2.53	0.41
7:w:278:TYR:CE2	7:w:282:ARG:HD3	2.56	0.41
8:8:322:TYR:HB2	9:9:61:PHE:CE1	2.55	0.41
9:9:44:VAL:O	9:9:48:ILE:HG12	2.20	0.41
6:v:355:TYR:OH	6:v:436:LYS:HE3	2.21	0.41
8:x:144:GLU:H	8:x:144:GLU:CD	2.28	0.41
3:4:182:GLU:HA	3:4:199:HIS:HB3	2.02	0.41
5:5:180:ARG:O	5:5:183:VAL:HG12	2.21	0.41
5:5:303:PRO:O	5:5:306:VAL:HB	2.21	0.41
6:6:320:PRO:C	3:Ae:72:ARG:HH22	2.29	0.41
1:0:51:GLU:O	1:0:55:GLN:HG2	2.21	0.41
3:2:205:ILE:HD13	3:2:205:ILE:HA	1.90	0.41
5:5:215:ASP:OD1	5:5:215:ASP:N	2.53	0.41
8:8:117:VAL:HG11	8:8:271:VAL:HB	2.01	0.41
5:u:62:GLU:HB2	5:u:413:ILE:HD11	2.02	0.41
1:0:28:ASP:OD1	1:0:28:ASP:N	2.52	0.41
1:0:79:ASP:HB3	8:x:93:PRO:HG2	2.03	0.41
5:5:407:THR:HB	5:5:408:PRO:HD3	2.02	0.41
9:9:85:GLU:H	9:9:85:GLU:CD	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:16:ASN:HD22	5:u:382:SER:HA	1.85	0.41
5:5:76:ASP:HB2	5:5:418:LEU:HD22	2.03	0.41
5:5:304:LEU:HD13	5:5:354:LEU:HD22	2.01	0.41
5:5:392:LYS:O	5:5:396:ARG:HG3	2.20	0.41
6:6:90:THR:OG1	6:6:150:GLU:OE2	2.36	0.41
6:6:173:VAL:HG21	6:6:268:HIS:HB2	2.02	0.41
6:6:290:GLN:HG3	6:6:325:ALA:HB3	2.03	0.41
6:6:391:GLY:HA2	6:6:394:ASP:OD2	2.20	0.41
7:7:300:ILE:HD11	7:7:363:LEU:HD21	2.03	0.41
5:u:315:ASP:HB3	5:u:318:TYR:CE1	2.56	0.41
6:v:138:LEU:HB3	6:v:237:PHE:CG	2.56	0.41
6:v:333:SER:OG	6:v:334:GLY:N	2.53	0.41
6:v:399:GLN:HG2	3:Af:39:HIS:HD2	1.85	0.41
8:x:249:ILE:HG23	13:x:401:HEC:HBB1	2.03	0.41
9:y:107:GLU:HA	9:y:110:LYS:HD3	2.02	0.41
4:Ad:38:TRP:C	4:Ad:40:LEU:H	2.29	0.41
1:0:57:VAL:HG22	1:0:65:GLU:HG3	2.02	0.41
8:8:147:LYS:O	8:8:151:GLU:HG2	2.21	0.41
9:9:79:GLU:CD	9:9:79:GLU:H	2.28	0.41
6:v:348:GLY:O	6:v:352:LYS:HG2	2.21	0.41
10:z:49:VAL:O	10:z:52:PRO:HD2	2.20	0.41
5:5:284:LEU:CD2	5:5:339:GLN:HG3	2.51	0.40
5:5:292:GLU:OE1	5:5:351:THR:OG1	2.38	0.40
9:9:36:ASP:OD1	9:9:90:TYR:OH	2.22	0.40
5:u:253:LEU:HD13	5:u:253:LEU:HA	1.86	0.40
7:w:132:VAL:HA	7:w:139:SER:HB3	2.03	0.40
6:6:84:ARG:NH2	6:6:190:LEU:O	2.42	0.40
5:u:138:LYS:H	5:u:138:LYS:HG3	1.67	0.40
5:u:153:ASN:OD1	5:u:153:ASN:N	2.51	0.40
6:v:270:ALA:HB2	6:v:339:TYR:CD2	2.57	0.40
7:w:181:PHE:HA	7:w:184:ILE:HG22	2.03	0.40
3:4:177:LEU:HB3	3:4:231:TRP:CZ2	2.57	0.40
3:4:177:LEU:HB3	3:4:231:TRP:CH2	2.56	0.40
3:4:241:LEU:HD12	3:4:260:HIS:CE1	2.55	0.40
5:5:274:GLU:HA	5:5:456:VAL:O	2.21	0.40
8:8:195:PRO:HA	8:8:196:PRO:HD3	1.97	0.40
5:u:278:ARG:NH2	10:z:9:THR:O	2.55	0.40
6:v:138:LEU:HD11	6:v:233:VAL:HG13	2.03	0.40
3:4:225:ARG:HH12	3:4:268:GLY:C	2.30	0.40
5:5:68:THR:HG22	5:5:136:LEU:HD23	2.03	0.40
5:5:188:HIS:NE2	5:5:348:TYR:OH	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:316:SER:N	5:5:339:GLN:O	2.54	0.40
5:u:313:HIS:HE1	3:Af:56:HIS:HB2	1.87	0.40
3:2:122:LYS:HB2	3:2:122:LYS:HE3	1.85	0.40
5:5:186:TYR:O	5:5:190:THR:HG22	2.22	0.40
6:6:174:LEU:HD23	6:6:174:LEU:HA	1.85	0.40
8:8:283:HIS:O	8:8:287:LYS:HG2	2.22	0.40
5:u:324:MET:HE3	5:u:324:MET:HB2	1.98	0.40
7:w:183:PHE:CZ	12:w:401:HEM:HBC1	2.57	0.40
8:x:311:LYS:HA	8:x:311:LYS:HD3	1.76	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	66/91 (72%)	63 (96%)	3 (4%)	0	100	100
1	Ab	66/91 (72%)	64 (97%)	2 (3%)	0	100	100
2	1	58/64 (91%)	57 (98%)	1 (2%)	0	100	100
2	Ac	58/64 (91%)	57 (98%)	1 (2%)	0	100	100
3	2	193/299 (64%)	187 (97%)	6 (3%)	0	100	100
3	4	194/299 (65%)	191 (98%)	3 (2%)	0	100	100
3	Ae	37/299 (12%)	30 (81%)	7 (19%)	0	100	100
3	Af	37/299 (12%)	30 (81%)	7 (19%)	0	100	100
4	3	49/56 (88%)	47 (96%)	2 (4%)	0	100	100
4	Ad	49/56 (88%)	48 (98%)	1 (2%)	0	100	100
5	5	431/480 (90%)	418 (97%)	13 (3%)	0	100	100
5	u	431/480 (90%)	421 (98%)	10 (2%)	0	100	100
6	6	416/453 (92%)	409 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	v	416/453 (92%)	402 (97%)	13 (3%)	1 (0%)	43	70
7	7	377/379 (100%)	371 (98%)	6 (2%)	0	100	100
7	w	377/379 (100%)	371 (98%)	6 (2%)	0	100	100
8	8	237/326 (73%)	232 (98%)	5 (2%)	0	100	100
8	x	236/326 (72%)	231 (98%)	5 (2%)	0	100	100
9	9	99/111 (89%)	97 (98%)	2 (2%)	0	100	100
9	y	99/111 (89%)	98 (99%)	1 (1%)	0	100	100
10	Aa	77/82 (94%)	77 (100%)	0	0	100	100
10	z	77/82 (94%)	77 (100%)	0	0	100	100
All	All	4080/5280 (77%)	3978 (98%)	101 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	v	322	ASP

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	0	65/85 (76%)	62 (95%)	3 (5%)	24	55
1	Ab	65/85 (76%)	60 (92%)	5 (8%)	12	33
2	1	49/52 (94%)	48 (98%)	1 (2%)	48	77
2	Ac	49/52 (94%)	48 (98%)	1 (2%)	48	77
3	2	166/245 (68%)	162 (98%)	4 (2%)	43	74
3	4	165/245 (67%)	161 (98%)	4 (2%)	43	74
3	Ae	28/245 (11%)	25 (89%)	3 (11%)	6	19
3	Af	29/245 (12%)	25 (86%)	4 (14%)	3	11
4	3	40/46 (87%)	37 (92%)	3 (8%)	12	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Ad	40/46 (87%)	38 (95%)	2 (5%)	22	51
5	5	363/397 (91%)	350 (96%)	13 (4%)	31	63
5	u	363/397 (91%)	348 (96%)	15 (4%)	27	59
6	6	329/355 (93%)	314 (95%)	15 (5%)	24	55
6	v	329/355 (93%)	314 (95%)	15 (5%)	24	55
7	7	332/332 (100%)	328 (99%)	4 (1%)	63	84
7	w	332/332 (100%)	329 (99%)	3 (1%)	70	87
8	8	203/259 (78%)	198 (98%)	5 (2%)	42	73
8	x	203/259 (78%)	196 (97%)	7 (3%)	32	65
9	9	93/99 (94%)	88 (95%)	5 (5%)	20	48
9	y	93/99 (94%)	89 (96%)	4 (4%)	26	57
10	Aa	70/73 (96%)	68 (97%)	2 (3%)	37	70
10	z	70/73 (96%)	68 (97%)	2 (3%)	37	70
All	All	3476/4376 (79%)	3356 (96%)	120 (4%)	32	64

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	42	LYS
1	0	43	CYS
1	0	62	GLN
2	1	30	LEU
3	2	116	GLU
3	2	172	LYS
3	2	205	ILE
3	2	238	CYS
4	3	13	LEU
4	3	18	ILE
4	3	39	ARG
3	4	104	ILE
3	4	251	ASP
3	4	283	THR
3	4	292	VAL
5	5	85	LYS
5	5	95	HIS
5	5	142	LYS
5	5	164	GLU

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Mol	Chain	Res	Type
5	5	207	ASN
5	5	215	ASP
5	5	247	GLN
5	5	266	THR
5	5	313	HIS
5	5	327	THR
5	5	350	GLU
5	5	362	ASN
5	5	363	MET
6	6	36	GLN
6	6	42	ARG
6	6	49	ILE
6	6	83	LEU
6	6	122	THR
6	6	154	LEU
6	6	240	MET
6	6	241	ARG
6	6	244	LEU
6	6	246	LEU
6	6	329	SER
6	6	378	LEU
6	6	401	LEU
6	6	435	ARG
6	6	453	LEU
7	7	138	MET
7	7	171	ASP
7	7	233	LEU
7	7	264	THR
8	8	107	ASP
8	8	120	GLN
8	8	263	THR
8	8	276	ARG
8	8	293	MET
9	9	14	LEU
9	9	53	GLU
9	9	75	ILE
9	9	76	LEU
9	9	83	LYS
5	u	95	HIS
5	u	138	LYS
5	u	153	ASN
5	u	171	GLU

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Mol	Chain	Res	Type
5	u	176	ASP
5	u	181	ASP
5	u	253	LEU
5	u	341	PHE
5	u	342	GLN
5	u	350	GLU
5	u	363	MET
5	u	375	GLN
5	u	415	ARG
5	u	417	LEU
5	u	470	ARG
6	v	36	GLN
6	v	83	LEU
6	v	124	GLU
6	v	129	ASP
6	v	130	ILE
6	v	147	ARG
6	v	154	LEU
6	v	175	GLU
6	v	227	HIS
6	v	231	LYS
6	v	233	VAL
6	v	246	LEU
6	v	254	ARG
6	v	342	SER
6	v	421	ASP
7	w	233	LEU
7	w	260	ASN
7	w	311	LYS
8	x	102	LEU
8	x	122	CYS
8	x	144	GLU
8	x	154	GLU
8	x	172	LEU
8	x	293	MET
8	x	320	LEU
9	y	13	TRP
9	y	14	LEU
9	y	75	ILE
9	y	83	LYS
10	z	47	LEU
10	z	65	GLN

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Mol	Chain	Res	Type
3	Af	40	VAL
3	Af	59	LEU
3	Af	68	LEU
3	Af	72	ARG
3	Ae	46	LEU
3	Ae	59	LEU
3	Ae	68	LEU
10	Aa	19	LEU
10	Aa	65	GLN
1	Ab	28	ASP
1	Ab	39	GLN
1	Ab	45	LYS
1	Ab	60	ARG
1	Ab	62	GLN
2	Ac	30	LEU
4	Ad	13	LEU
4	Ad	39	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	62	GLN
2	1	55	HIS
3	2	156	GLN
3	4	220	GLN
3	4	240	HIS
5	5	52	GLN
5	5	66	GLN
5	5	152	GLN
5	5	170	GLN
5	5	247	GLN
5	5	313	HIS
5	5	323	HIS
5	5	342	GLN
5	5	402	HIS
5	5	464	GLN
5	5	469	ASN
6	6	36	GLN
6	6	75	ASN
6	6	157	GLN
6	6	168	ASN
6	6	170	GLN

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Mol	Chain	Res	Type
6	6	232	GLN
6	6	319	GLN
6	6	327	ASN
6	6	443	ASN
7	7	97	HIS
7	7	196	HIS
7	7	207	ASN
7	7	255	ASN
7	7	260	ASN
8	8	91	HIS
8	8	283	HIS
8	8	310	HIS
9	9	23	ASN
5	u	222	GLN
5	u	323	HIS
5	u	469	ASN
6	v	157	GLN
6	v	168	ASN
6	v	268	HIS
6	v	290	GLN
6	v	304	ASN
6	v	311	GLN
6	v	372	GLN
7	w	85	ASN
7	w	207	ASN
7	w	255	ASN
7	w	260	ASN
7	w	267	HIS
7	w	312	GLN
8	x	241	GLN
8	x	266	GLN
9	y	23	ASN
3	Af	39	HIS
3	Ae	39	HIS
10	Aa	65	GLN
1	Ab	39	GLN
1	Ab	62	GLN
1	Ab	80	HIS
2	Ac	55	HIS

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$
13	HEC	8	401	8	50,50,50	1.76	5 (10%)	68,82,82	1.18	2 (2%)
12	HEM	w	401	7	50,50,50	1.38	8 (16%)	67,82,82	1.08	4 (5%)
12	HEM	7	401	7	50,50,50	1.40	8 (16%)	67,82,82	1.04	1 (1%)
12	HEM	7	402	-	50,50,50	1.36	8 (16%)	67,82,82	1.06	4 (5%)
11	FES	2	301	3	0,4,4	-	-	-	-	-
12	HEM	w	402	-	50,50,50	1.34	9 (18%)	67,82,82	1.09	6 (8%)
13	HEC	x	401	8	50,50,50	1.73	5 (10%)	68,82,82	1.24	5 (7%)
11	FES	4	301	3	0,4,4	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	HEC	8	401	8	1/1/3/7	1/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	HEM	w	401	7	-	2/14/54/54	-
12	HEM	7	401	7	-	1/14/54/54	-
12	HEM	7	402	-	-	0/14/54/54	-
12	HEM	w	402	-	-	0/14/54/54	-
11	FES	2	301	3	-	-	0/1/1/1
13	HEC	x	401	8	-	2/14/54/54	-
11	FES	4	301	3	-	-	0/1/1/1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	x	401	HEC	C3D-C2D	7.84	1.53	1.36
13	8	401	HEC	C3D-C2D	7.65	1.53	1.36
13	8	401	HEC	FE-ND	4.23	2.07	1.94
13	x	401	HEC	FE-ND	4.14	2.07	1.94
13	8	401	HEC	FE-NB	3.88	2.06	1.94
12	w	401	HEM	FE-ND	3.45	2.05	1.94
13	x	401	HEC	FE-NB	3.36	2.05	1.94
13	8	401	HEC	FE-NA	3.34	2.06	1.95
12	7	402	HEM	FE-ND	3.32	2.05	1.94
12	7	401	HEM	FE-NA	3.29	2.06	1.95
12	w	402	HEM	FE-ND	3.28	2.05	1.94
12	w	401	HEM	FE-NC	3.24	2.05	1.95
13	x	401	HEC	FE-NA	3.16	2.05	1.95
12	7	401	HEM	FE-ND	3.13	2.04	1.94
12	w	402	HEM	CAB-C3B	3.06	1.55	1.47
12	7	401	HEM	CAB-C3B	3.04	1.55	1.47
12	7	401	HEM	FE-NB	3.03	2.04	1.94
12	w	402	HEM	CAC-C3C	3.02	1.55	1.47
12	7	402	HEM	CAB-C3B	3.01	1.55	1.47
12	w	401	HEM	CAB-C3B	2.99	1.55	1.47
12	w	401	HEM	CAC-C3C	2.95	1.55	1.47
12	7	402	HEM	CAC-C3C	2.94	1.55	1.47
12	7	402	HEM	FE-NA	2.92	2.04	1.95
12	7	401	HEM	CAC-C3C	2.91	1.55	1.47
13	8	401	HEC	FE-NC	2.90	2.04	1.95
12	7	402	HEM	FE-NB	2.73	2.03	1.94
12	w	401	HEM	FE-NB	2.70	2.03	1.94
12	7	401	HEM	FE-NC	2.67	2.04	1.95
13	x	401	HEC	FE-NC	2.63	2.03	1.95
12	w	402	HEM	FE-NC	2.52	2.03	1.95
12	w	402	HEM	FE-NA	2.49	2.03	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	7	402	HEM	FE-NC	2.44	2.03	1.95
12	w	401	HEM	FE-NA	2.38	2.03	1.95
12	w	402	HEM	FE-NB	2.32	2.02	1.94
12	w	401	HEM	C2A-C3A	-2.09	1.33	1.38
12	7	401	HEM	C2A-C3A	-2.09	1.33	1.38
12	w	402	HEM	CMC-C2C	2.08	1.55	1.50
12	7	401	HEM	CMB-C2B	2.05	1.55	1.50
12	w	401	HEM	CMB-C2B	2.04	1.55	1.50
12	7	402	HEM	CMC-C2C	2.03	1.54	1.50
12	w	402	HEM	C2A-C3A	-2.03	1.33	1.38
12	w	402	HEM	CMB-C2B	2.02	1.54	1.50
12	7	402	HEM	CMB-C2B	2.01	1.54	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	x	401	HEC	C1D-ND-C4D	5.27	111.44	105.21
13	8	401	HEC	C1D-ND-C4D	5.03	111.16	105.21
13	x	401	HEC	C2A-C1A-NA	-2.44	107.97	110.32
12	w	402	HEM	C4D-ND-C1D	2.42	108.07	105.21
12	w	401	HEM	C2A-C1A-NA	-2.34	107.56	110.15
12	w	402	HEM	C1B-NB-C4B	2.31	107.94	105.21
12	7	402	HEM	C4D-ND-C1D	2.29	107.92	105.21
12	w	402	HEM	C3D-C4D-ND	-2.23	107.73	110.17
12	7	402	HEM	C1B-NB-C4B	2.12	107.72	105.21
12	7	402	HEM	C3D-C4D-ND	-2.12	107.85	110.17
13	x	401	HEC	C3C-C4C-NC	-2.10	107.82	110.15
12	w	402	HEM	C2A-C1A-NA	-2.10	107.82	110.15
12	w	402	HEM	CBD-CAD-C3D	-2.09	106.75	112.53
12	w	401	HEM	C1B-NB-C4B	2.08	107.67	105.21
13	x	401	HEC	CHA-C4D-ND	2.07	126.66	124.42
12	7	402	HEM	C2A-C1A-NA	-2.07	107.85	110.15
13	x	401	HEC	CAA-CBA-CGA	-2.05	108.24	113.67
13	8	401	HEC	CHA-C4D-ND	2.04	126.62	124.42
12	w	401	HEM	C4D-ND-C1D	2.04	107.62	105.21
12	7	401	HEM	CAD-CBD-CGD	-2.03	108.29	113.67
12	w	402	HEM	C3B-C2B-C1B	2.01	107.92	106.41
12	w	401	HEM	CAD-CBD-CGD	-2.01	108.33	113.67

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	8	401	HEC	NA

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	7	401	HEM	C3D-CAD-CBD-CGD
12	w	401	HEM	C3D-CAD-CBD-CGD
13	x	401	HEC	C1A-C2A-CAA-CBA
12	w	401	HEM	C1A-C2A-CAA-CBA
13	x	401	HEC	C3A-C2A-CAA-CBA
13	8	401	HEC	CAD-CBD-CGD-O2D

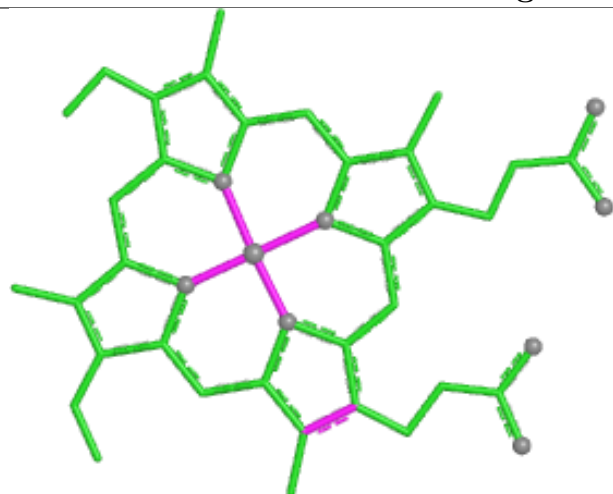
There are no ring outliers.

8 monomers are involved in 28 short contacts:

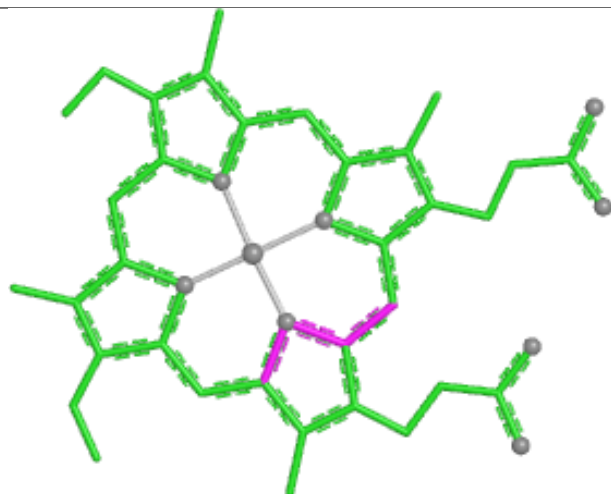
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	8	401	HEC	3	0
12	w	401	HEM	5	0
12	7	401	HEM	3	0
12	7	402	HEM	4	0
11	2	301	FES	2	0
12	w	402	HEM	3	0
13	x	401	HEC	5	0
11	4	301	FES	3	0

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.

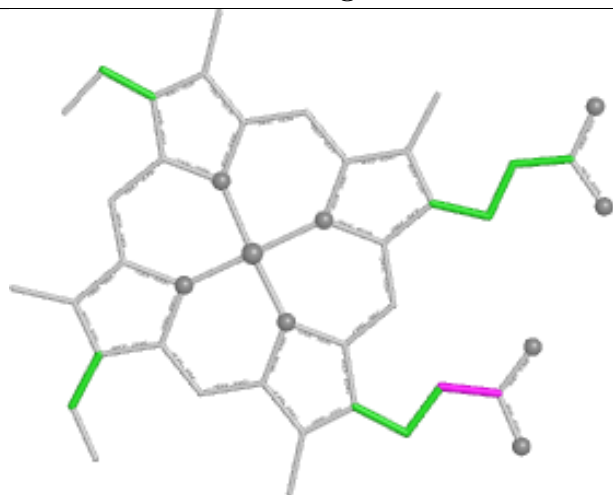
Ligand HEC 8 401



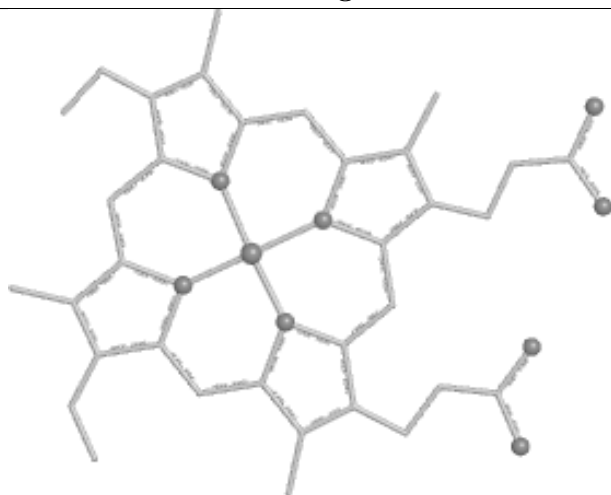
Bond lengths



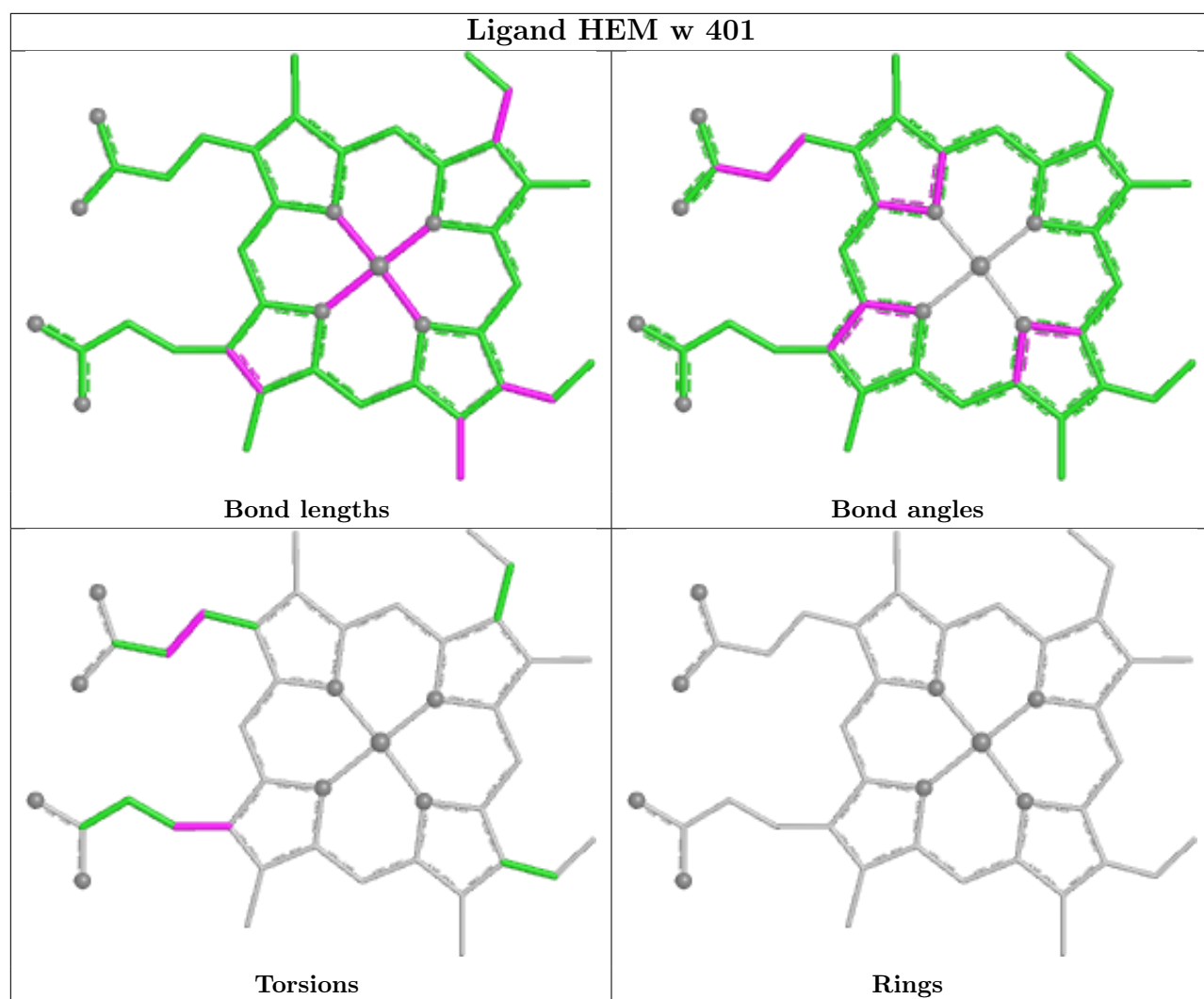
Bond angles

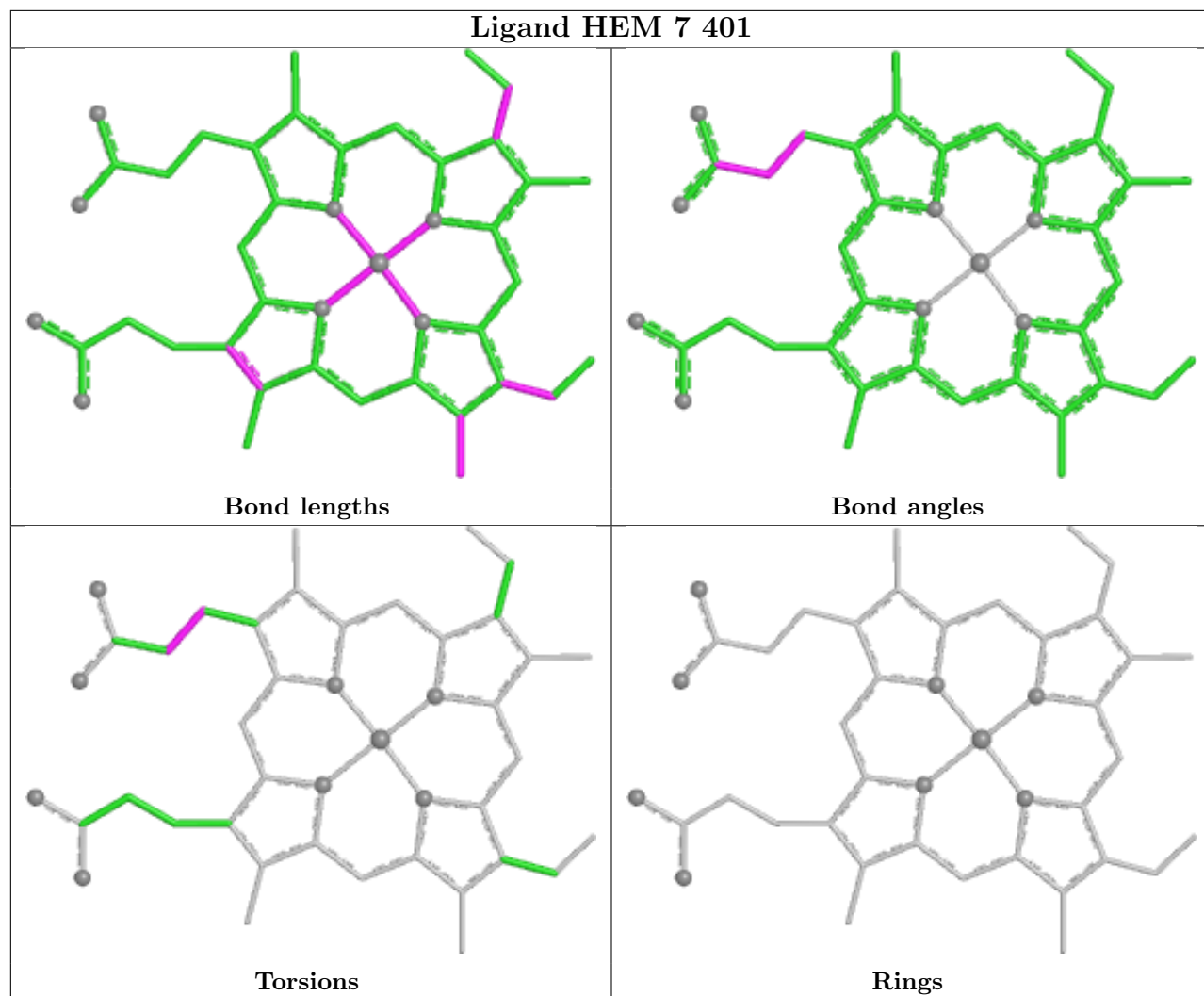


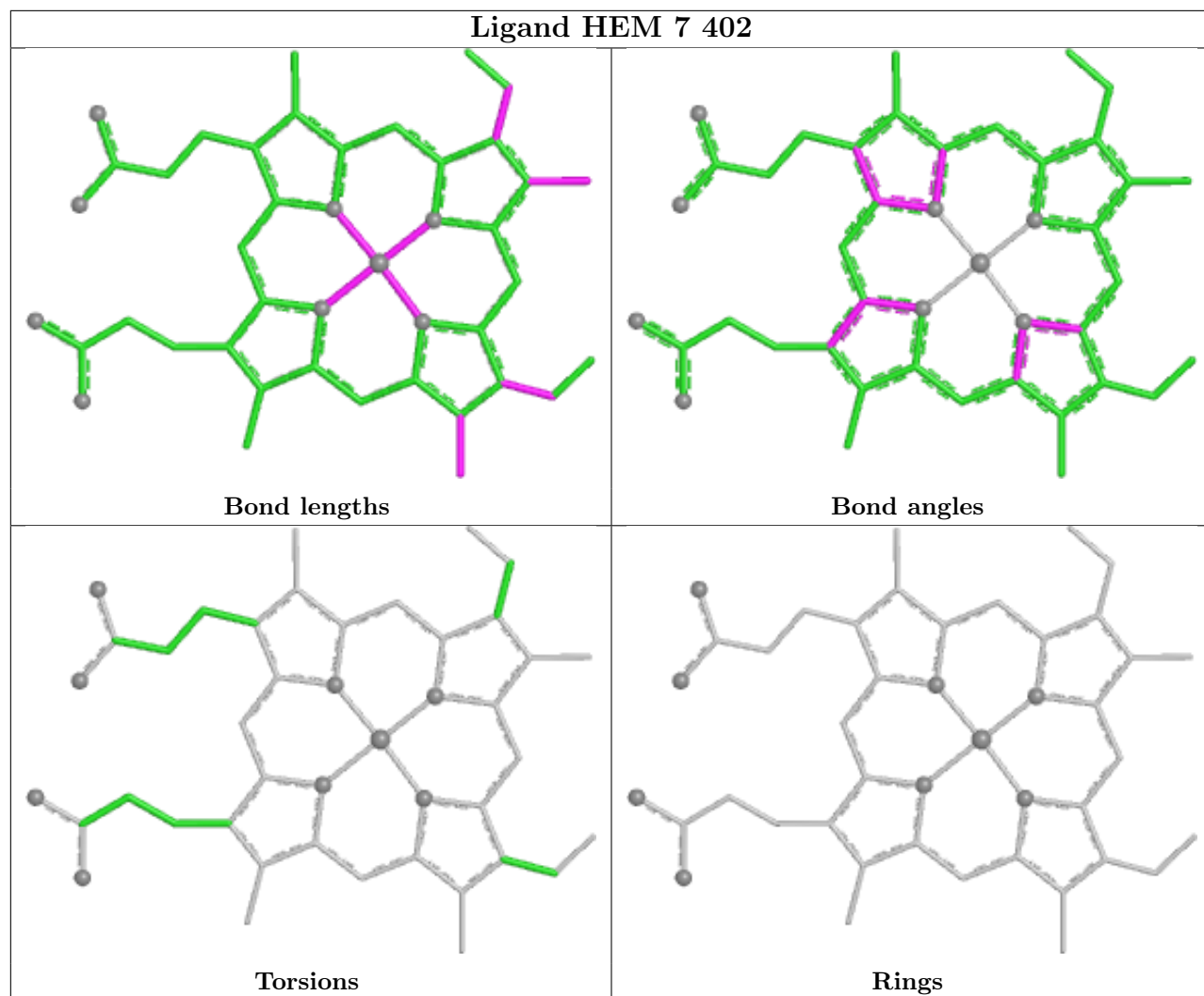
Torsions

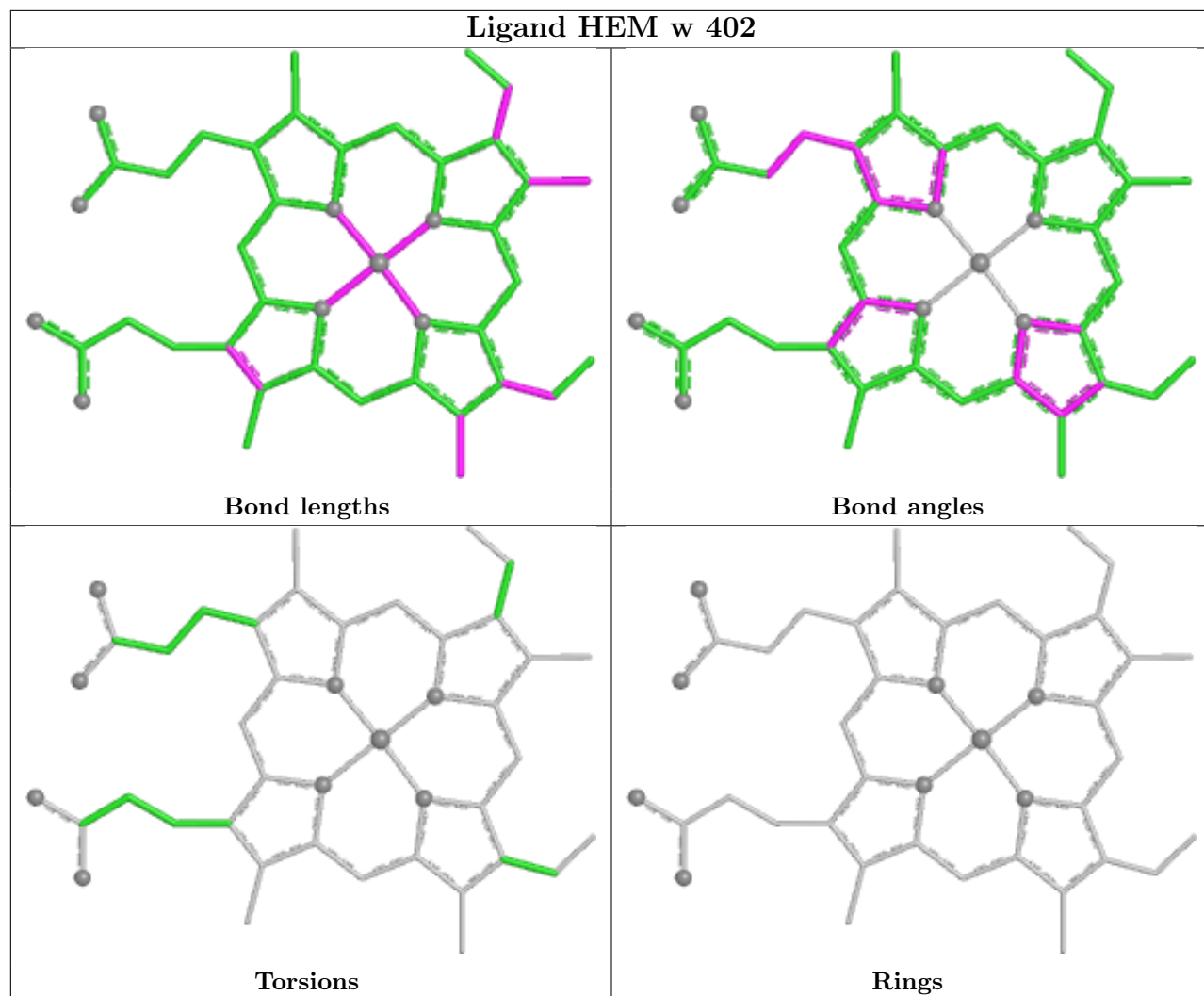


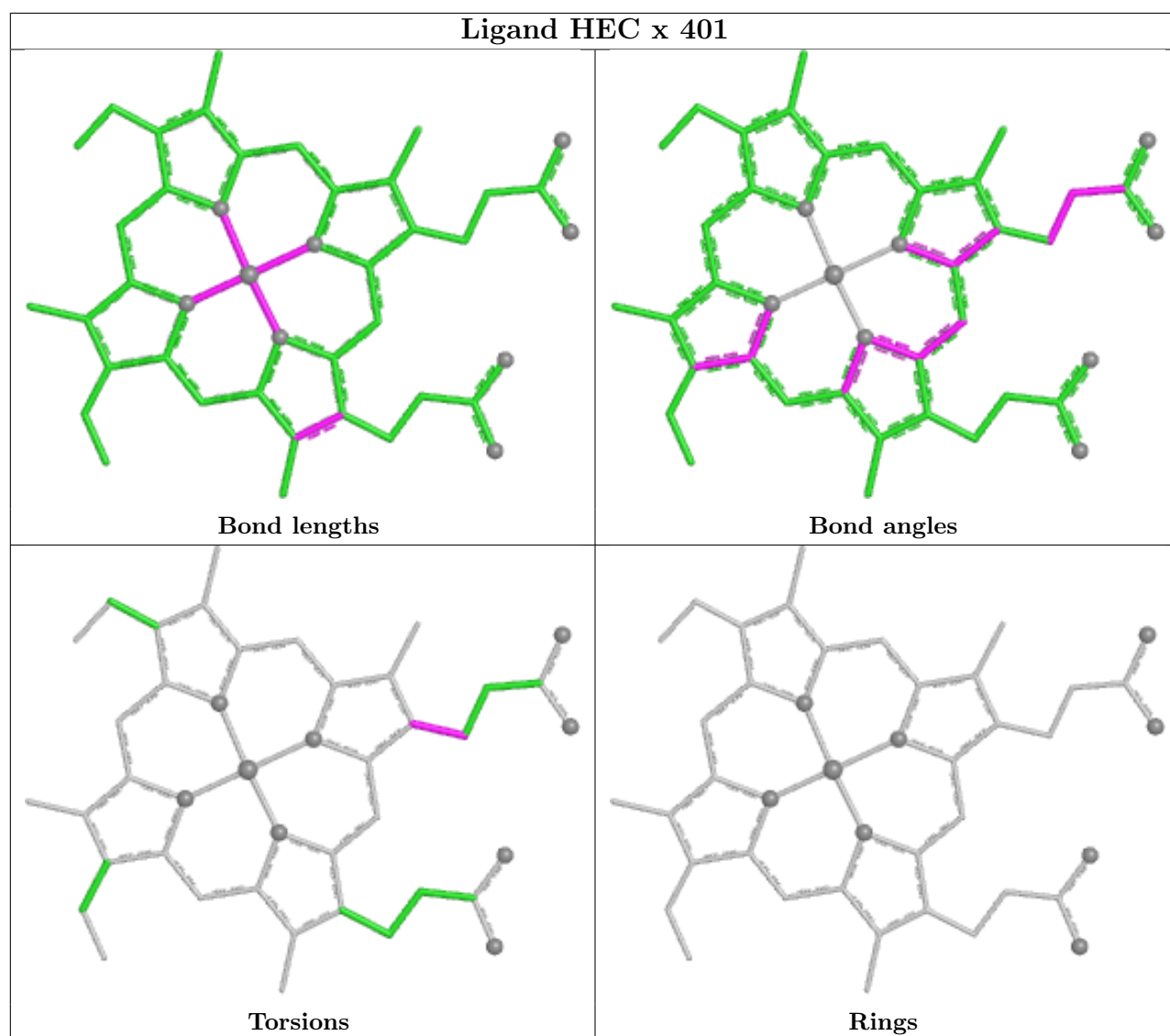
Rings











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.

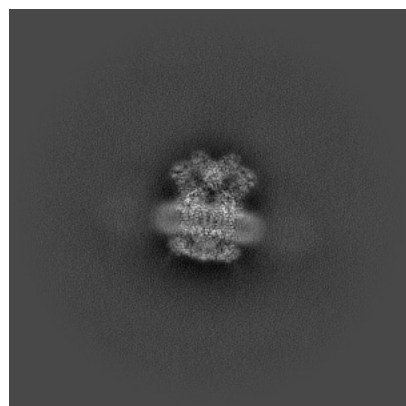
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45282. These allow visual inspection of the internal detail of the map and identification of artifacts.

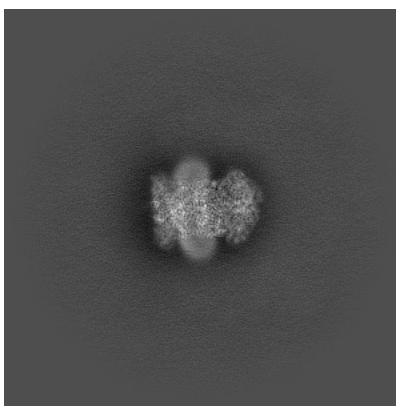
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

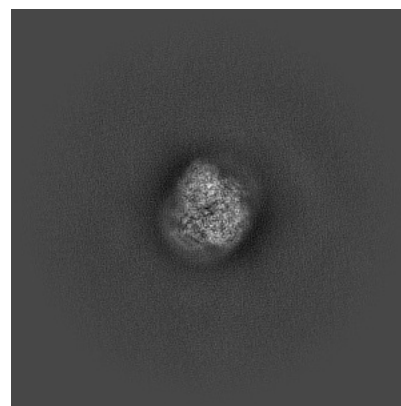
6.1.1 Primary map



X

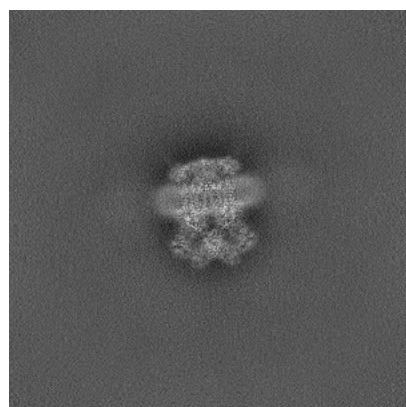


Y

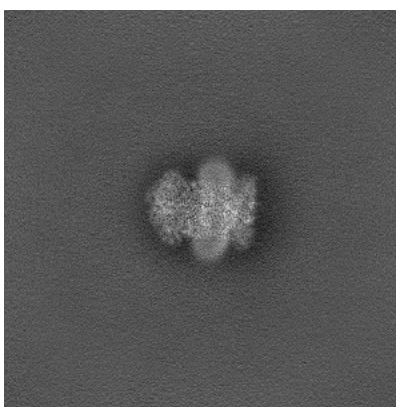


Z

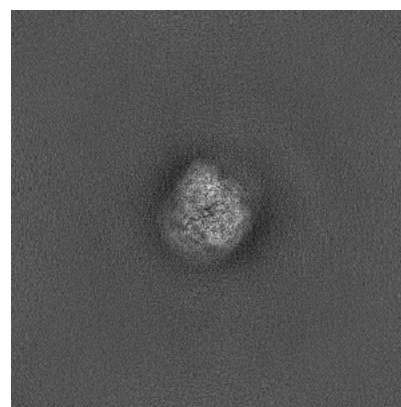
6.1.2 Raw map



X



Y

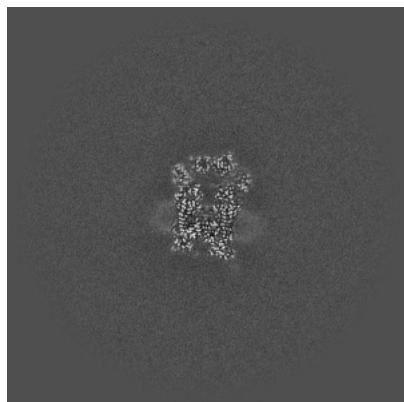


Z

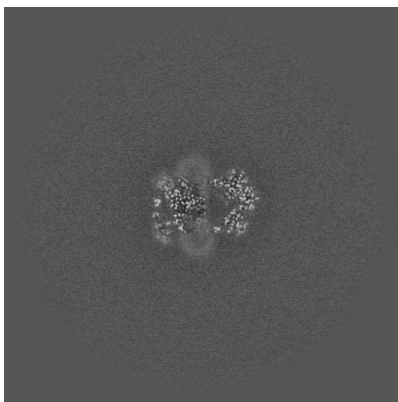
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

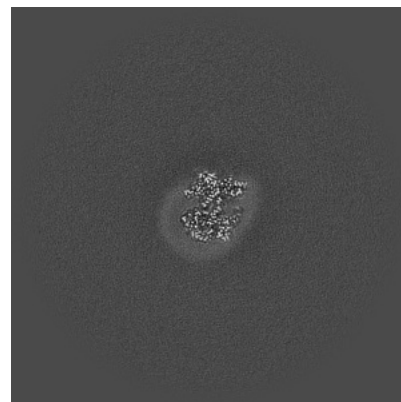
6.2.1 Primary map



X Index: 256

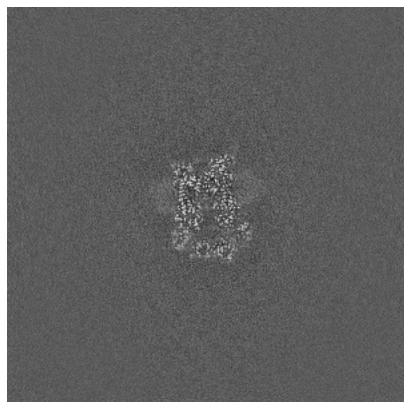


Y Index: 256

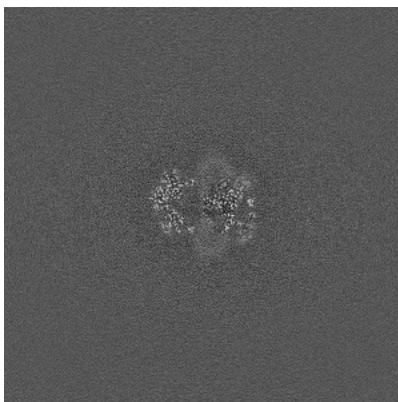


Z Index: 256

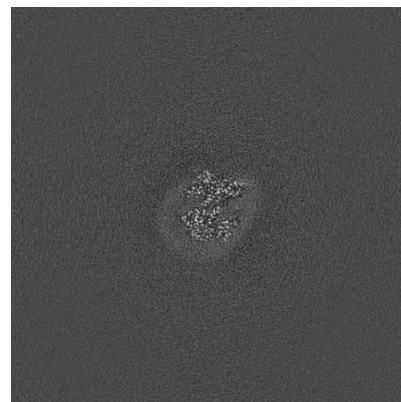
6.2.2 Raw map



X Index: 256



Y Index: 256

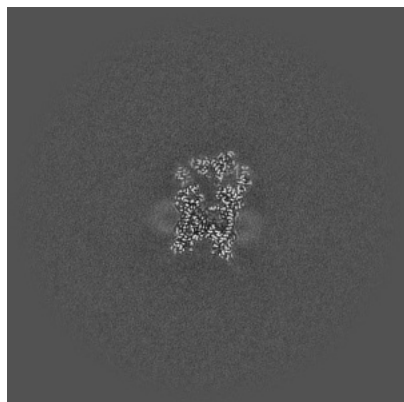


Z Index: 256

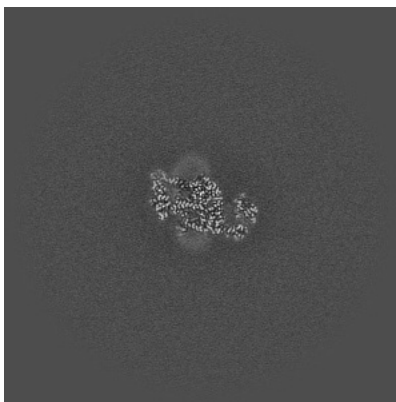
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

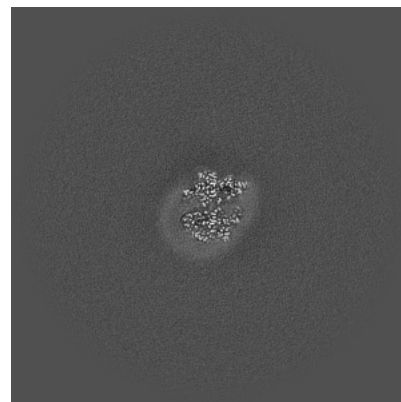
6.3.1 Primary map



X Index: 253

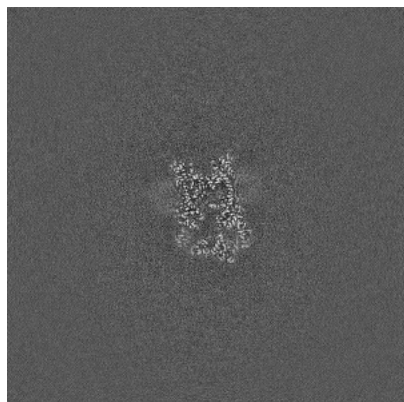


Y Index: 277

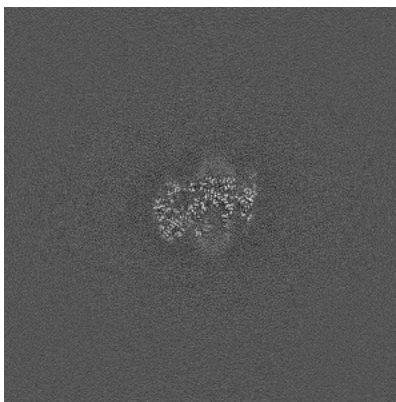


Z Index: 257

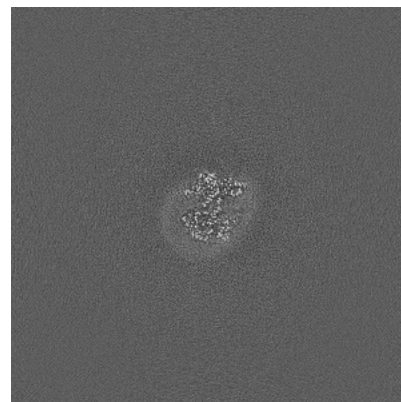
6.3.2 Raw map



X Index: 253



Y Index: 270

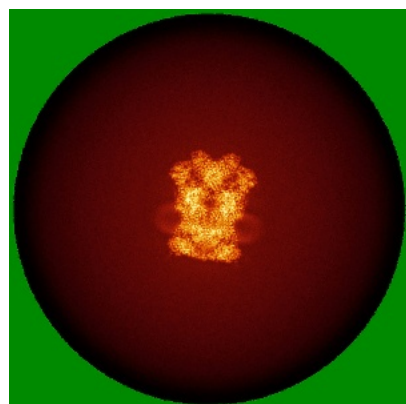


Z Index: 255

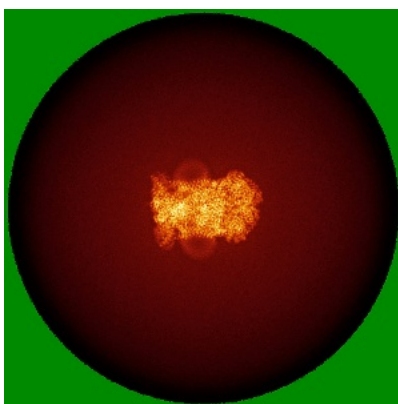
The images above show the largest variance slices of the map in three orthogonal directions.

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

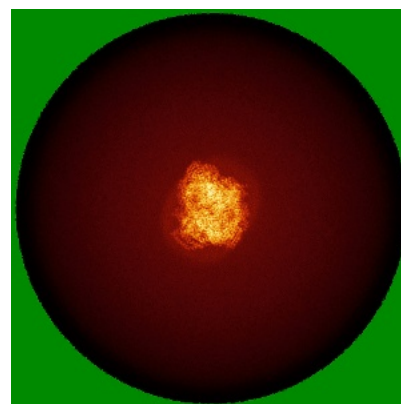
6.4.1 Primary map



X

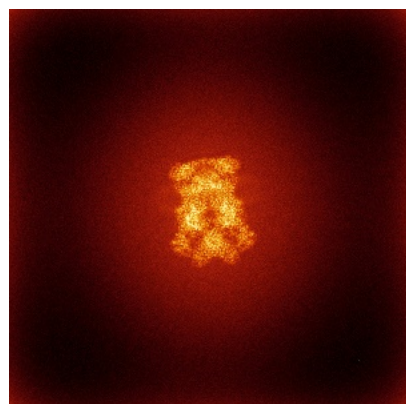


Y

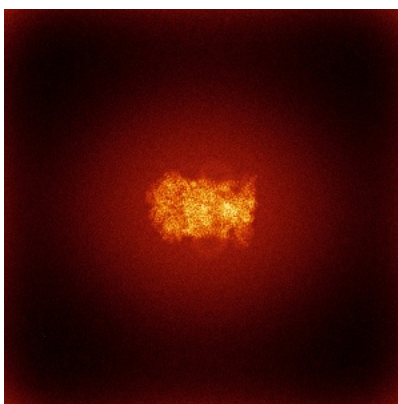


Z

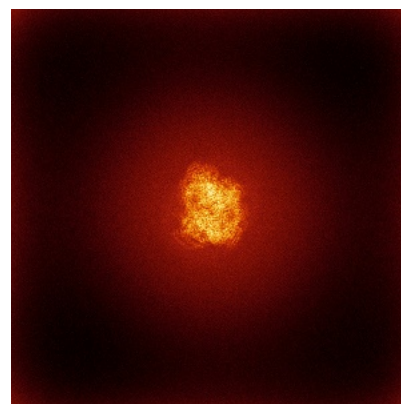
6.4.2 Raw map



X



Y

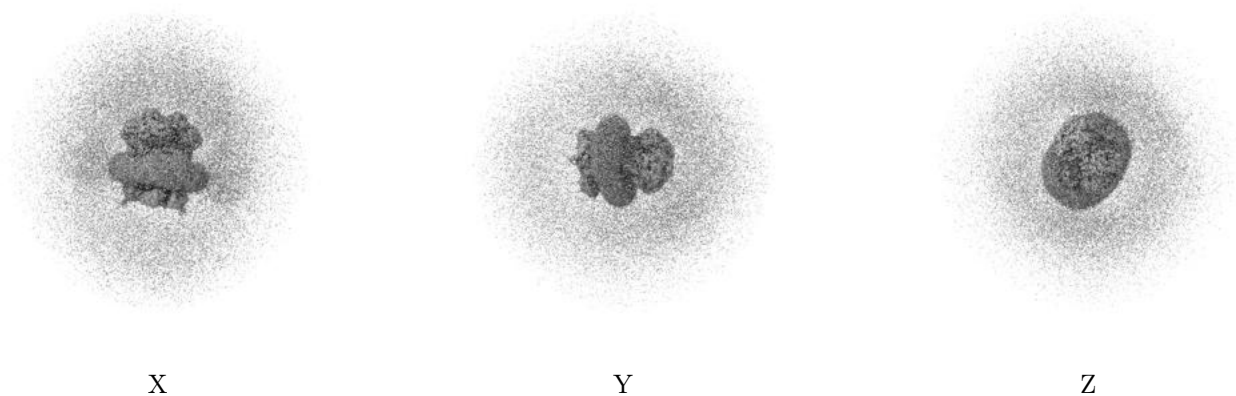


Z

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.

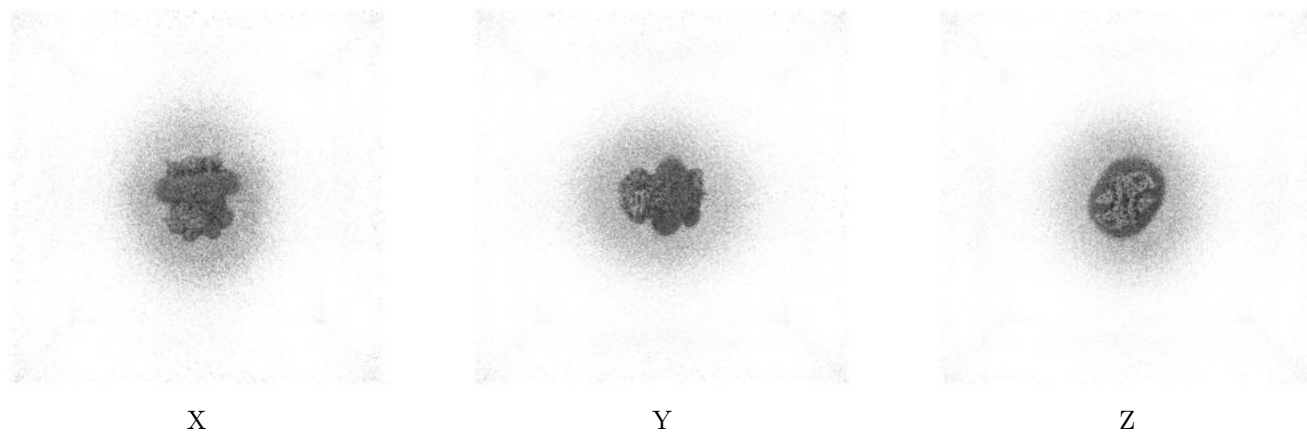
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

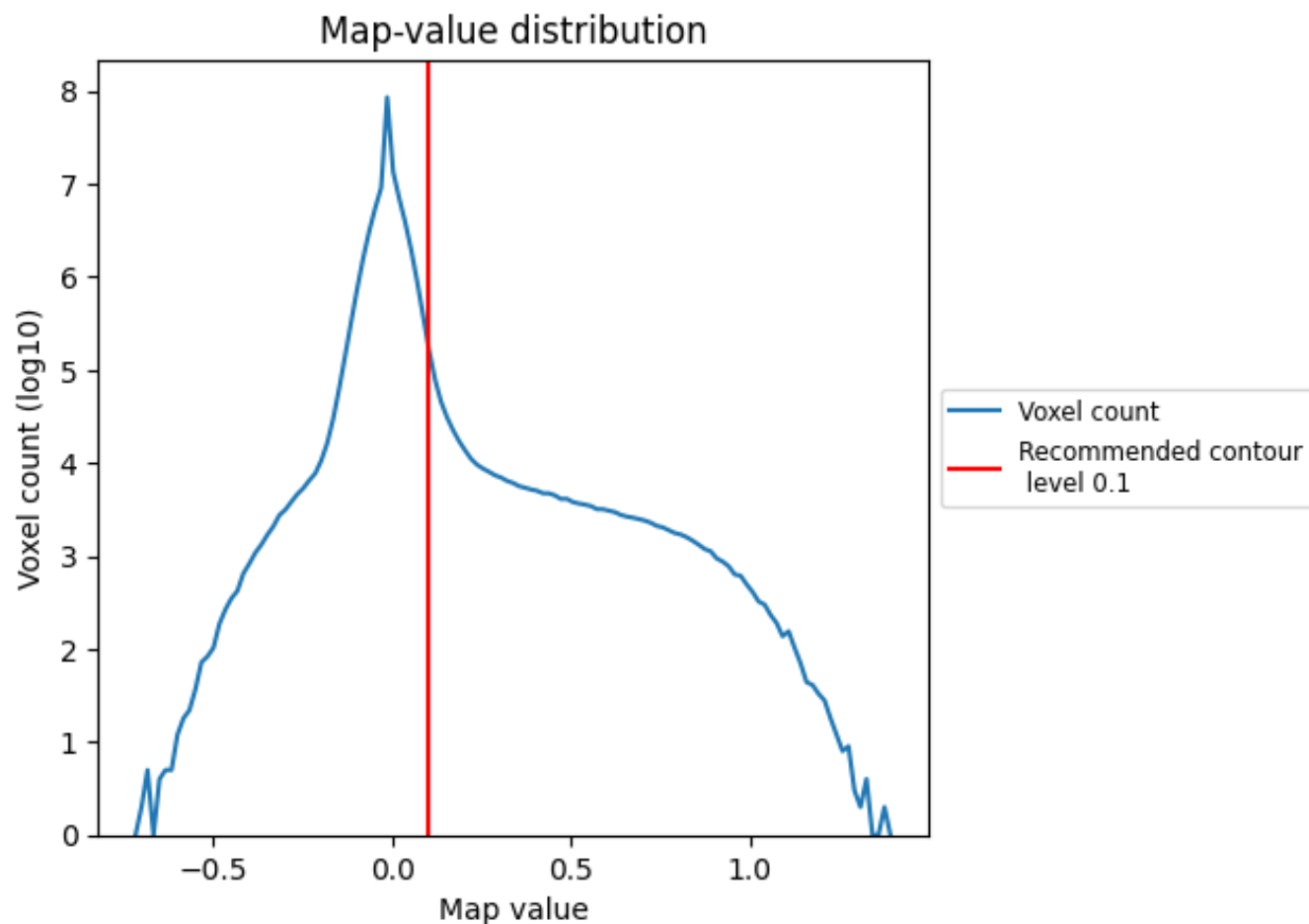
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

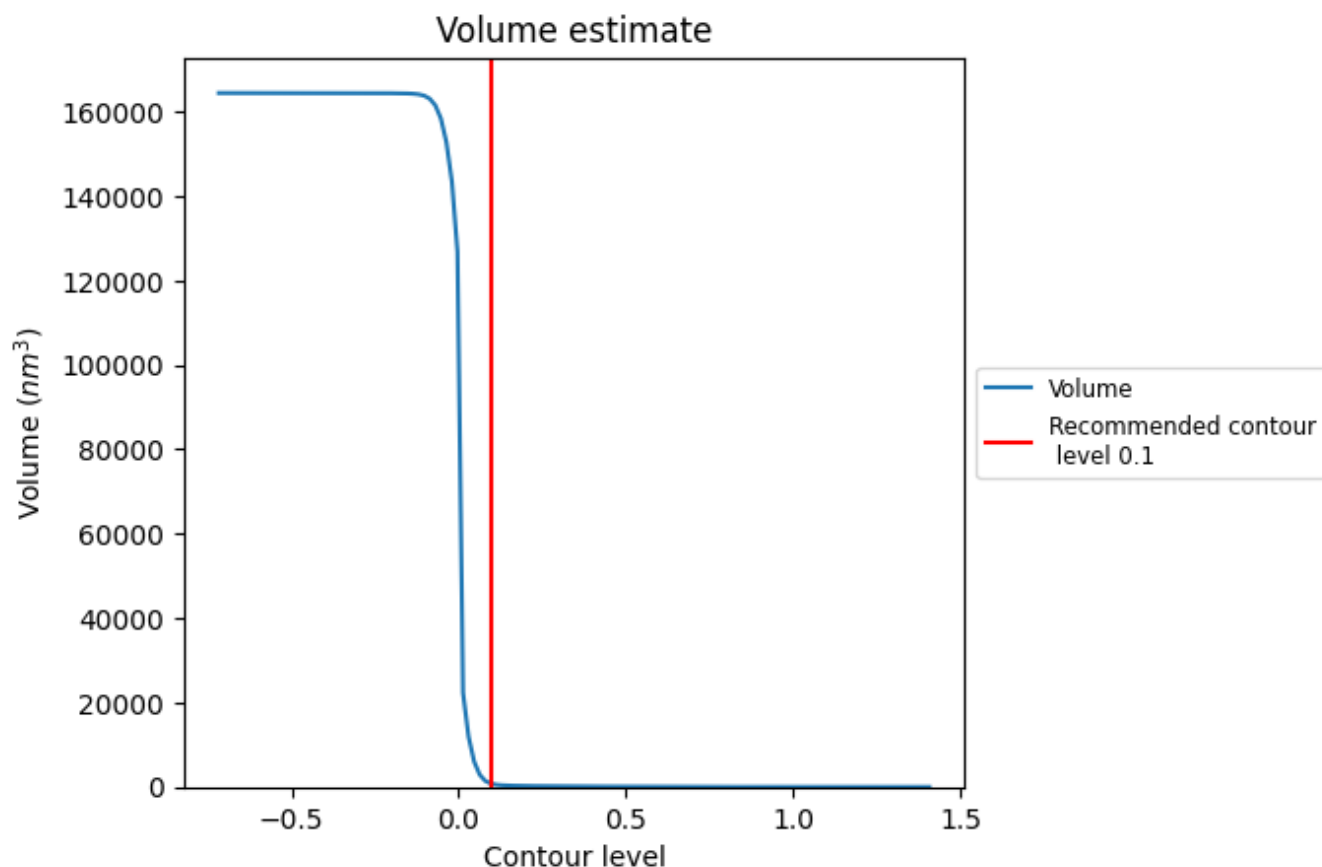
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

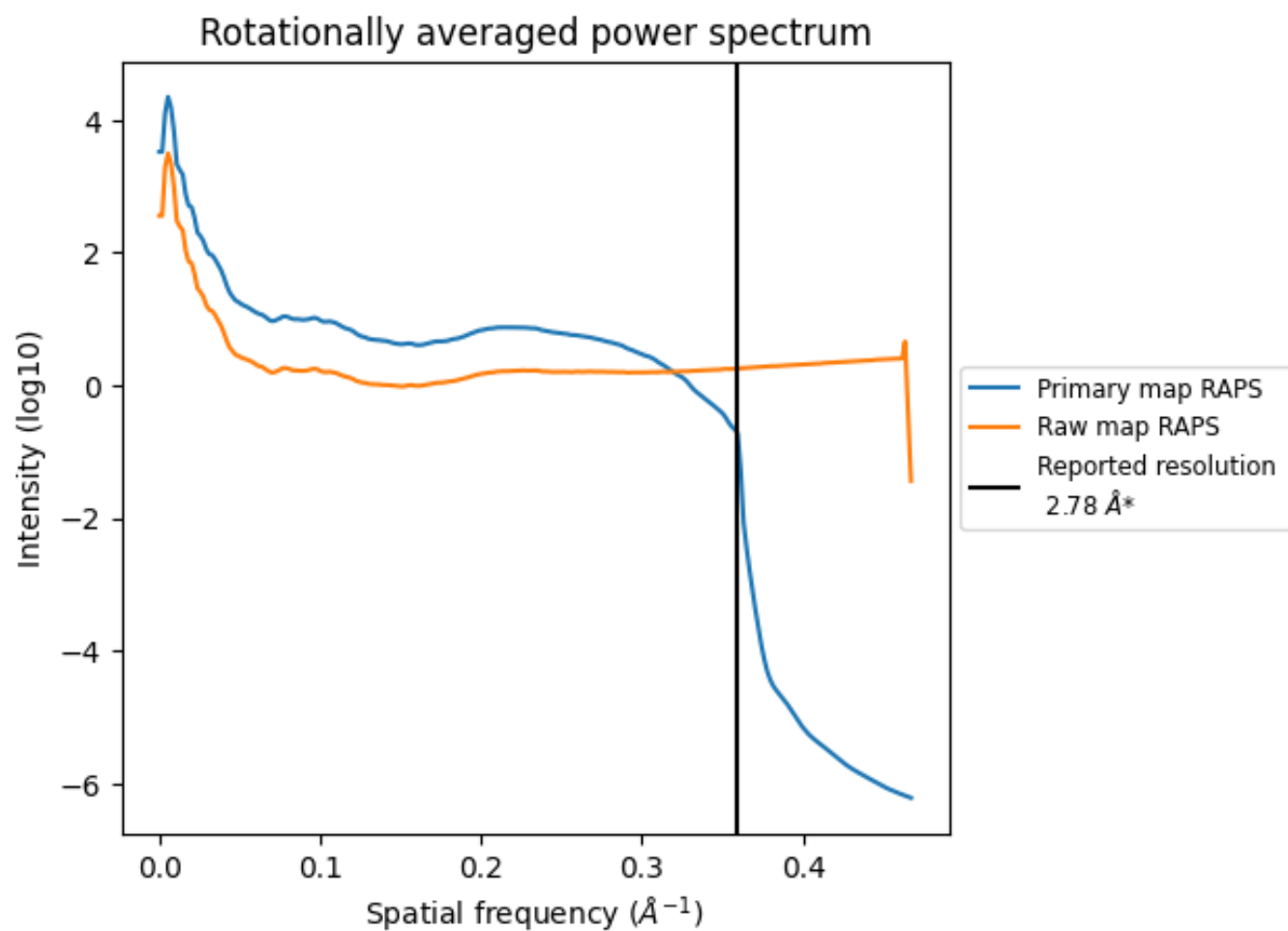
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 740 nm^3 ; this corresponds to an approximate mass of 668 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 ⓘ

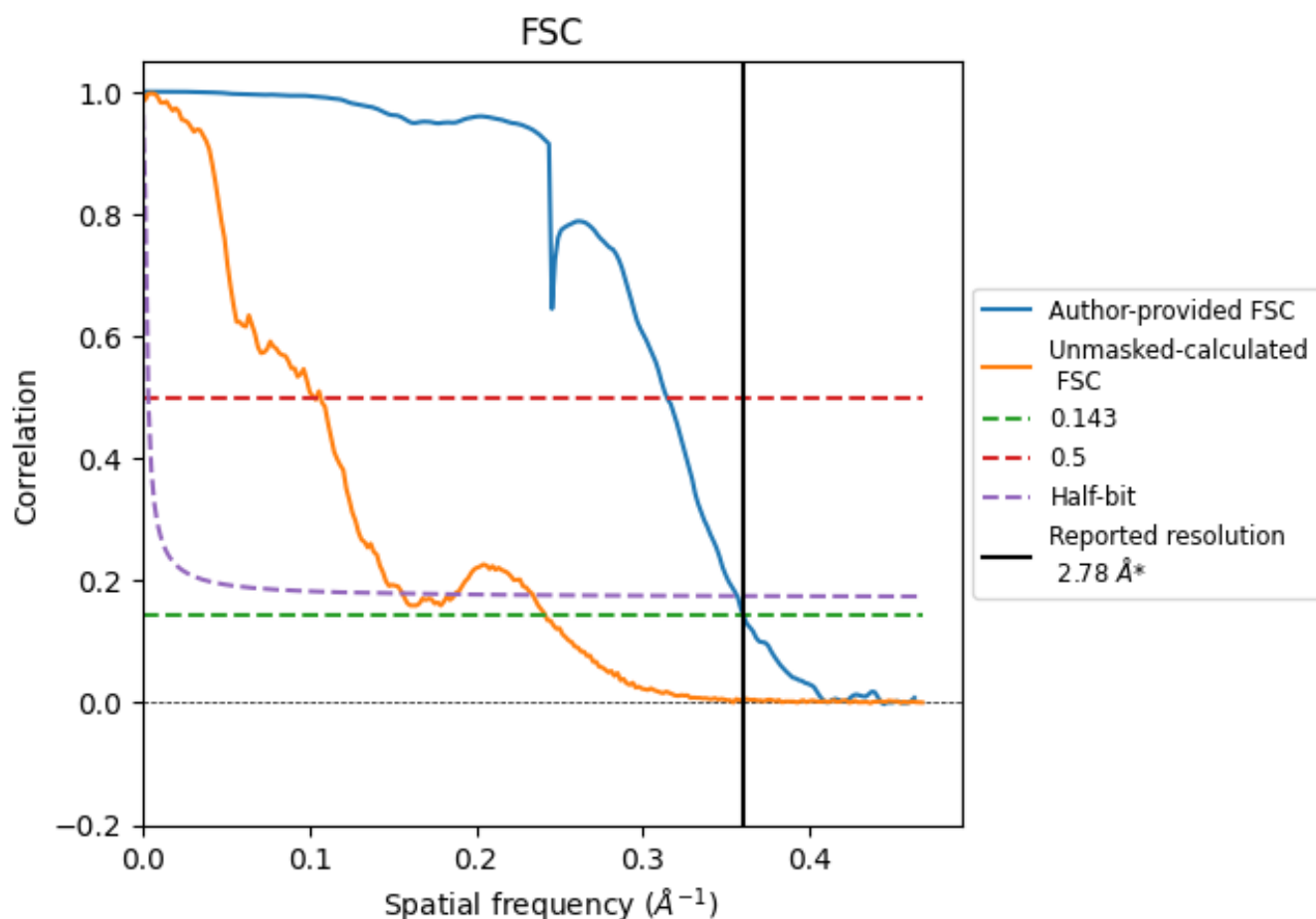


*Reported resolution corresponds to spatial frequency of 0.360 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.360 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

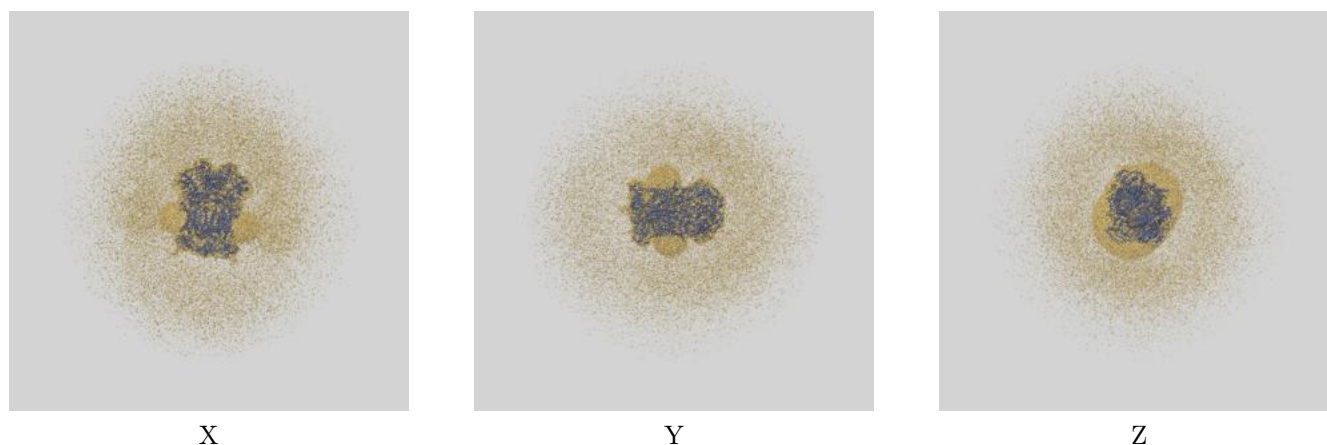
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	2.78	3.18	2.81
Unmasked-calculated*	4.14	9.74	6.42

*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 4.14 differs from the reported value 2.78 by more than 10 %

9 Map-model fit [i](#)

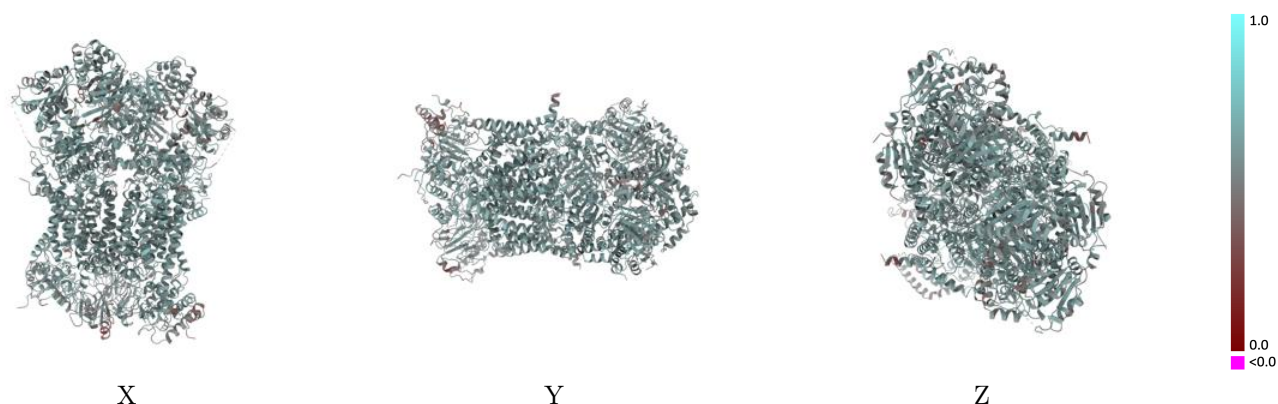
This section contains information regarding the fit between EMDB map EMD-45282 and PDB model 9C7H. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



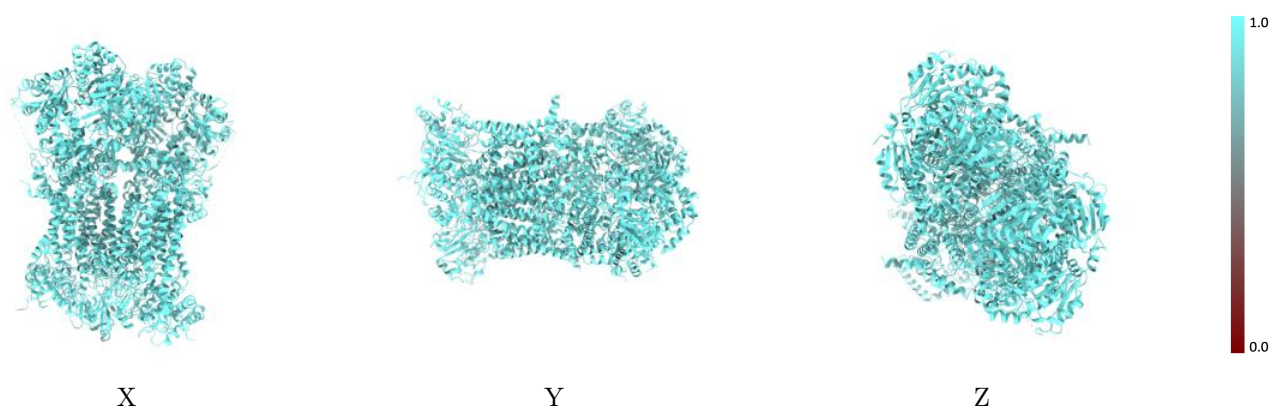
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



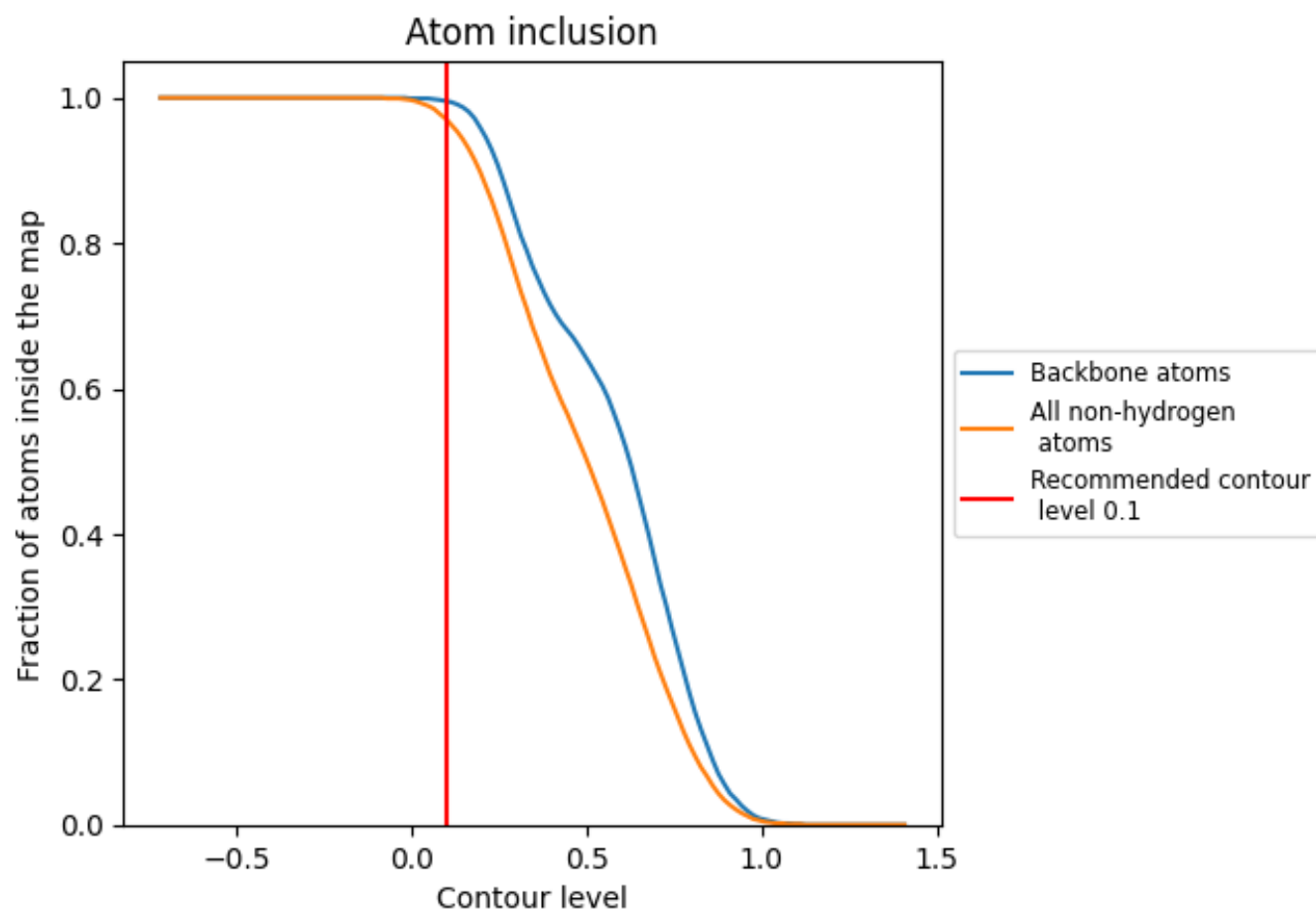
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 97% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9700	 0.5620
0	 0.9270	 0.4850
1	 0.9850	 0.5790
2	 0.9480	 0.5240
3	 0.9880	 0.5590
4	 0.9480	 0.5220
5	 0.9750	 0.5700
6	 0.9760	 0.5660
7	 0.9840	 0.5850
8	 0.9760	 0.5750
9	 0.9580	 0.5680
Aa	 0.9780	 0.5630
Ab	 0.9230	 0.4900
Ac	 0.9730	 0.5590
Ad	 0.9750	 0.5560
Ae	 0.7960	 0.3980
Af	 0.8250	 0.4080
u	 0.9750	 0.5690
v	 0.9730	 0.5630
w	 0.9860	 0.5870
x	 0.9770	 0.5730
y	 0.9560	 0.5670
z	 0.9860	 0.5730

