



Full wwPDB EM Validation Report ⓘ

Aug 7, 2026 – 08:33 AM JST

PDB ID : 9UFZ / pdb_00009ufz
EMDB ID : EMD-64127
Title : Ubiquinol Binding Site of Cytochrome bo3 from *Acinetobacter baumannii*
Authors : Li, J.; Zhu, J.P.
Deposited on : 2025-04-10
Resolution : 3.28 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:

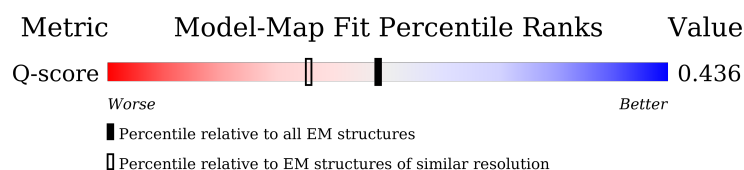
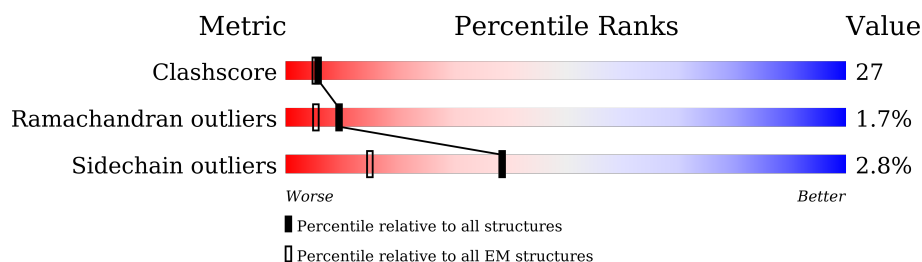
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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

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

The reported resolution of this entry is 3.28 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	14492 (2.78 - 3.78)

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

Mol	Chain	Length	Quality of chain
1	A	660	
2	B	277	
3	C	191	
4	D	97	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 10264 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 bo(3) ubiquinol oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	660	Total	C	N	O	S	1	0
			5260	3547	816	861	36		

- Molecule 2 is a protein called Ubiquinol oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	277	Total	C	N	O	S	0	0
			2195	1421	368	396	10		

- Molecule 3 is a protein called Cytochrome bo(3) ubiquinol oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	191	Total	C	N	O	S	0	0
			1530	1030	233	261	6		

- Molecule 4 is a protein called Cytochrome bo(3) ubiquinol oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	97	Total	C	N	O	S	0	0
			761	509	119	124	9		

There are 11 discrepancies between the modelled and reference sequences:

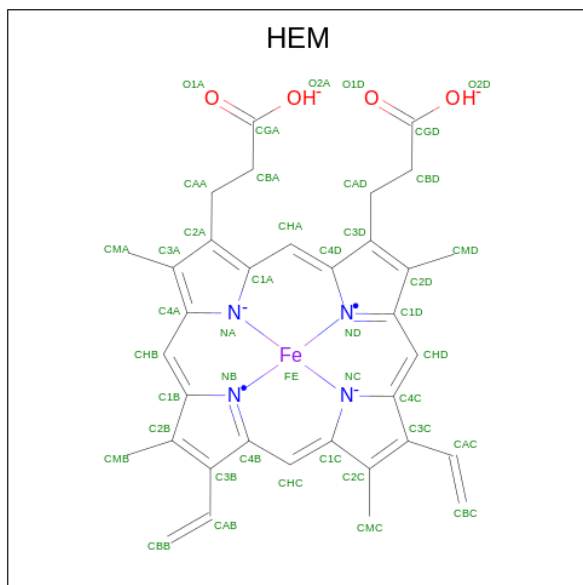
Chain	Residue	Modelled	Actual	Comment	Reference
D	13	GLY	-	expression tag	UNP V5VBE6
D	14	SER	-	expression tag	UNP V5VBE6
D	15	VAL	-	expression tag	UNP V5VBE6
D	16	LYS	-	expression tag	UNP V5VBE6
D	17	THR	-	expression tag	UNP V5VBE6
D	18	TYR	-	expression tag	UNP V5VBE6
D	19	MET	-	expression tag	UNP V5VBE6
D	20	THR	-	expression tag	UNP V5VBE6
D	26	ILE	VAL	conflict	UNP V5VBE6

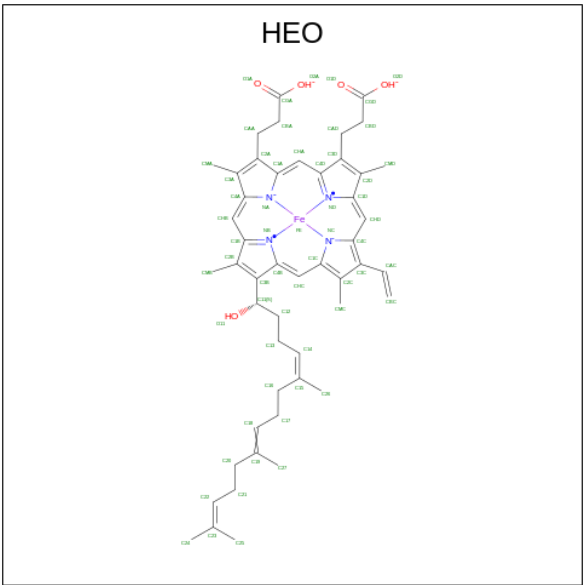
Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	30	VAL	ILE	conflict	UNP V5VBE6
D	109	HIS	-	expression tag	UNP V5VBE6

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



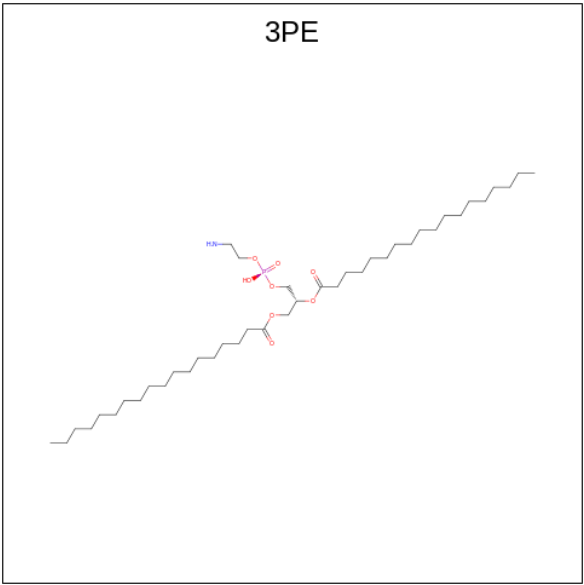


Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	Fe	N	O	0
			59	49	1	4	5	

- Molecule 7 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

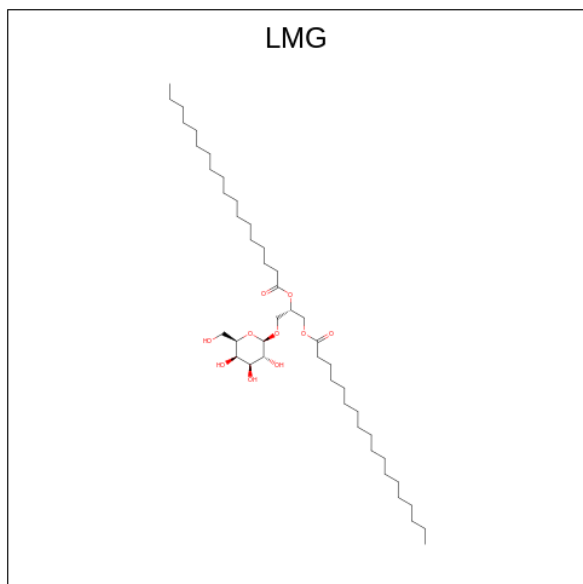
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Cu	0
			1	1	

- Molecule 8 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



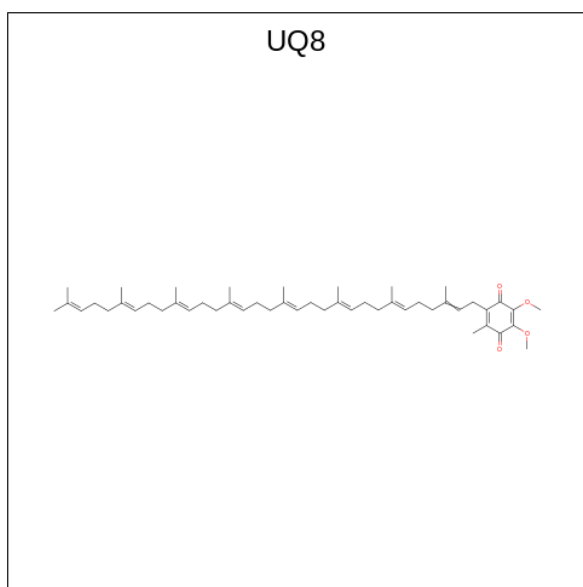
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
8	A	1	Total	C	N	O	P	0
			30	20	1	8	1	
8	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
8	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
8	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
8	C	1	Total	C	N	O	P	0
			44	34	1	8	1	

- Molecule 9 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			46	36	10	
9	A	1	Total	C	O	0
			40	30	10	
9	A	1	Total	C	O	0
			36	26	10	

- Molecule 10 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$) (labeled as "Ligand of Interest" by depositor).

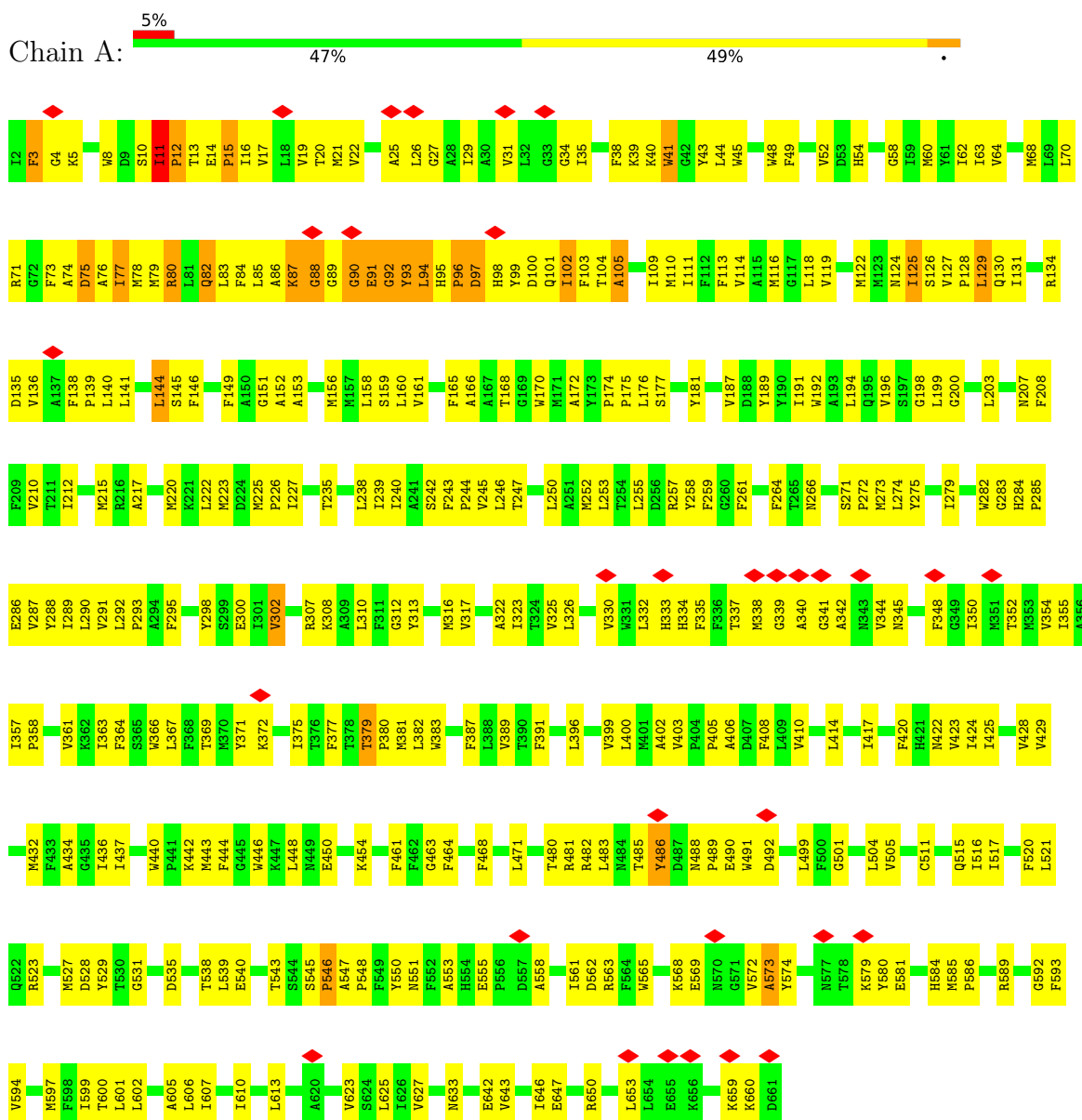


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
10	A	1	45	41	4	0

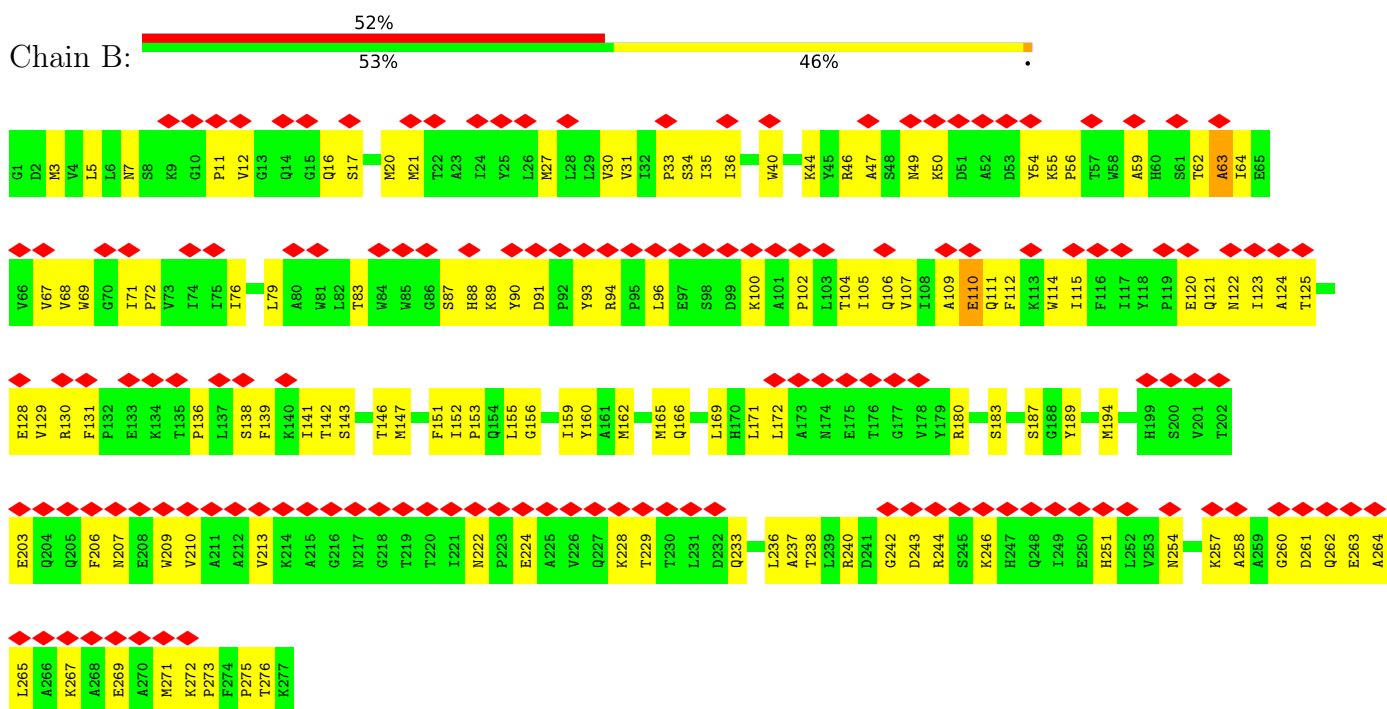
3 Residue-property plots

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.

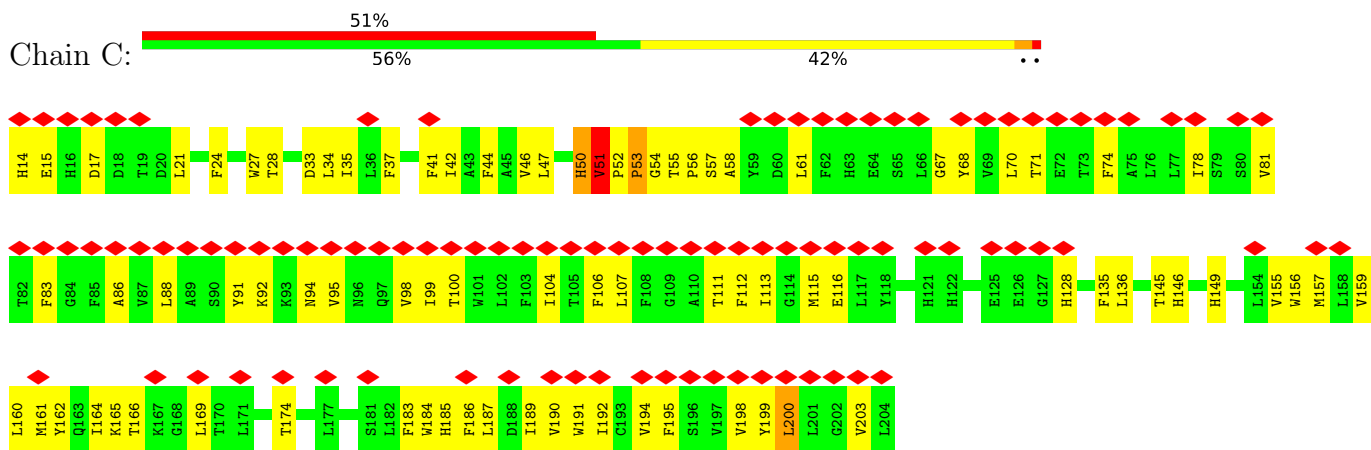
• Molecule 1: Cytochrome bo(3) ubiquinol oxidase subunit 1



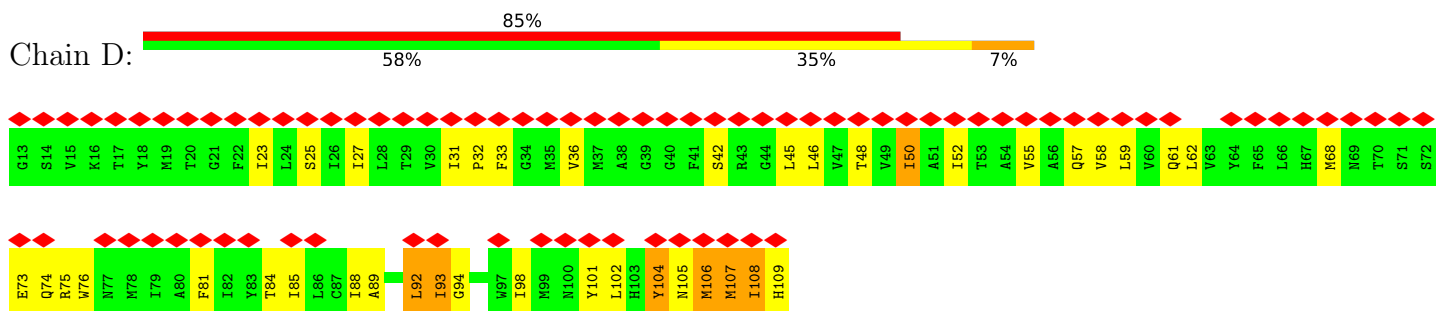
• Molecule 2: Ubiquinol oxidase subunit 2



• Molecule 3: Cytochrome bo(3) ubiquinol oxidase subunit 3



• Molecule 4: Cytochrome bo(3) ubiquinol oxidase subunit 4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48128	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.205	Depositor
Minimum map value	-0.791	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	246.0, 246.0, 246.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UQ8, CU, LMG, 3PE, HEM, HEO

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	0.37	0/5442	0.54	3/7420 (0.0%)
2	B	0.17	0/2256	0.45	0/3067
3	C	0.24	0/1582	0.48	2/2161 (0.1%)
4	D	0.24	0/778	0.52	0/1058
All	All	0.31	0/10058	0.51	5/13706 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
4	D	0	1
All	All	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ALA	N-CA-C	-5.87	105.96	114.12
3	C	51	VAL	CA-C-N	-5.76	114.45	120.38
3	C	51	VAL	C-N-CA	-5.76	114.45	120.38
1	A	11	ILE	CA-C-N	5.49	126.70	119.84
1	A	11	ILE	C-N-CA	5.49	126.70	119.84

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	302	VAL	Peptide
1	A	75	ASP	Mainchain
4	D	92	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5260	0	5258	364	0
2	B	2195	0	2179	112	0
3	C	1530	0	1511	74	0
4	D	761	0	800	43	0
5	A	43	0	30	5	0
6	A	59	0	56	12	0
7	A	1	0	0	0	0
8	A	153	0	208	16	0
8	C	95	0	147	8	0
9	A	122	0	154	11	0
10	A	45	0	59	14	0
All	All	10264	0	10402	558	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 27.

All (558) 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)
2:B:162:MET:HE1	4:D:106:MET:HE1	1.55	0.88
3:C:34:LEU:HB3	4:D:84:THR:HG21	1.59	0.83
4:D:92:LEU:O	4:D:94:GLY:N	2.13	0.81
3:C:47:LEU:O	3:C:51:VAL:HB	1.81	0.81
2:B:162:MET:HE1	4:D:106:MET:CE	2.10	0.79
1:A:26:LEU:HA	1:A:29:ILE:HG22	1.64	0.79
1:A:599:ILE:HD11	8:A:1004:3PE:H2A2	1.64	0.79
4:D:31:ILE:HG13	4:D:32:PRO:HD3	1.62	0.79
2:B:166:GLN:HB2	2:B:271:MET:HE1	1.65	0.78
1:A:58:GLY:HA3	1:A:125:ILE:HG23	1.64	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:PHE:HE1	5:A:1001:HEM:HAB	1.48	0.78
1:A:151:GLY:HA3	1:A:600:THR:HG21	1.65	0.76
1:A:144:LEU:HG	1:A:592:GLY:HA2	1.68	0.76
1:A:75:ASP:HB2	1:A:102:ILE:HG23	1.67	0.76
4:D:102:LEU:HD13	4:D:106:MET:HE2	1.67	0.76
1:A:396:LEU:HB2	2:B:31:VAL:HG21	1.67	0.75
1:A:235:THR:HG21	1:A:293:PRO:HD3	1.67	0.75
1:A:94:LEU:HD12	1:A:98[A]:HIS:ND1	2.02	0.75
1:A:284:HIS:O	1:A:287:VAL:HG12	1.85	0.75
1:A:330:VAL:HG21	1:A:355:ILE:HD11	1.69	0.75
1:A:414:LEU:HD13	1:A:471:LEU:HD22	1.69	0.75
1:A:379:THR:HG23	1:A:380:PRO:HD3	1.68	0.74
1:A:339:GLY:HA3	4:D:106:MET:SD	2.27	0.74
1:A:543:THR:O	1:A:650:ARG:NH1	2.22	0.73
1:A:102:ILE:HA	10:A:1011:UQ8:H3M	1.70	0.72
1:A:136:VAL:HG12	1:A:138:PHE:H	1.52	0.72
9:A:1009:LMG:H312	9:A:1009:LMG:H122	1.70	0.72
8:A:1004:3PE:H282	8:A:1004:3PE:H3A1	1.72	0.72
1:A:136:VAL:HG11	1:A:207:ASN:HB3	1.73	0.71
1:A:399:VAL:HG11	2:B:27:MET:HG3	1.72	0.71
3:C:195:PHE:HA	3:C:199:TYR:HD2	1.55	0.71
1:A:91:GLU:HA	1:A:485:THR:HB	1.72	0.71
1:A:425:ILE:HA	1:A:429:VAL:HB	1.73	0.71
2:B:87:SER:O	2:B:88:HIS:ND1	2.24	0.70
1:A:189:TYR:CE1	1:A:607:ILE:HG21	2.27	0.70
1:A:284:HIS:HB2	1:A:334:HIS:HE1	1.56	0.70
1:A:383:TRP:HB2	1:A:434:ALA:HB2	1.71	0.70
1:A:517:ILE:HG12	10:A:1011:UQ8:H36A	1.74	0.70
1:A:558:ALA:HA	1:A:563:ARG:HG2	1.75	0.69
3:C:146:HIS:HD2	3:C:194:VAL:HG21	1.58	0.69
2:B:83:THR:HA	2:B:87:SER:HB2	1.75	0.69
1:A:174:PRO:HG2	1:A:272:PRO:HB3	1.74	0.68
1:A:235:THR:HB	1:A:289:ILE:HG23	1.74	0.68
2:B:107:VAL:HG11	2:B:114:TRP:HE3	1.58	0.68
1:A:54:HIS:CE1	1:A:128:PRO:HB2	2.29	0.68
2:B:114:TRP:HZ2	2:B:183:SER:HB2	1.58	0.68
1:A:194:LEU:O	1:A:198:GLY:N	2.20	0.67
3:C:113:ILE:HA	3:C:116:GLU:HB2	1.76	0.67
1:A:94:LEU:HD12	1:A:98[A]:HIS:HD1	1.59	0.67
1:A:273:MET:HG3	1:A:338:MET:HE3	1.77	0.67
1:A:308:LYS:HG3	2:B:56:PRO:HA	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:TRP:HA	1:A:11:ILE:HD11	1.75	0.67
1:A:60:MET:HG2	8:A:1007:3PE:H3B1	1.75	0.67
1:A:181:TYR:HD2	2:B:146:THR:HG23	1.61	0.66
1:A:602:LEU:O	1:A:606:LEU:HD12	1.95	0.66
3:C:46:VAL:O	3:C:50:HIS:HB2	1.95	0.66
1:A:141:LEU:HD22	1:A:203:LEU:HD13	1.77	0.66
1:A:490:GLU:OE2	2:B:180:ARG:NH2	2.29	0.66
1:A:375:ILE:HB	2:B:46:ARG:HA	1.76	0.66
1:A:285:PRO:O	1:A:289:ILE:HG13	1.96	0.65
1:A:134:ARG:HH12	1:A:555:GLU:HG2	1.61	0.65
1:A:152:ALA:HB2	1:A:196:VAL:HG23	1.78	0.65
1:A:71:ARG:CZ	10:A:1011:UQ8:H4MA	2.27	0.65
2:B:62:THR:O	2:B:64:ILE:N	2.29	0.65
3:C:67:GLY:O	3:C:70:LEU:HB2	1.96	0.65
1:A:561:ILE:HD12	1:A:561:ILE:H	1.62	0.65
1:A:605:ALA:HB2	1:A:613:LEU:HD23	1.78	0.65
1:A:189:TYR:HE1	1:A:607:ILE:HG21	1.61	0.64
2:B:110:GLU:HB2	2:B:115:ILE:HD11	1.78	0.64
4:D:48:THR:O	4:D:52:ILE:HD12	1.96	0.64
2:B:159:ILE:HG21	2:B:169:LEU:HB2	1.80	0.64
2:B:146:THR:OG1	2:B:187:SER:O	2.12	0.64
1:A:417:ILE:HD13	1:A:420:PHE:HE2	1.62	0.64
2:B:165:MET:HE1	4:D:106:MET:HE3	1.78	0.64
1:A:323:ILE:HG13	1:A:358:PRO:HB2	1.79	0.63
2:B:125:THR:OG1	2:B:128:GLU:O	2.17	0.63
3:C:14:HIS:N	3:C:17:ASP:OD1	2.31	0.63
1:A:16:ILE:O	1:A:20:THR:HG23	1.98	0.63
1:A:14:GLU:O	1:A:17:VAL:HG22	1.98	0.63
1:A:545:SER:HB2	1:A:546:PRO:HD2	1.79	0.63
1:A:623:VAL:O	1:A:627:VAL:HG23	1.98	0.63
4:D:68:MET:HB2	4:D:74:GLN:HG3	1.80	0.63
4:D:89:ALA:O	4:D:93:ILE:HG22	1.98	0.63
1:A:17:VAL:O	1:A:21:MET:HG2	1.99	0.63
1:A:52:VAL:HG22	1:A:139:PRO:HB2	1.80	0.63
2:B:67:VAL:O	2:B:71:ILE:HD12	1.98	0.62
1:A:291:VAL:O	1:A:295:PHE:N	2.31	0.62
1:A:127:VAL:HB	1:A:128:PRO:HD3	1.81	0.62
1:A:244:PRO:HG3	3:C:35:ILE:HG23	1.82	0.62
1:A:242:SER:HB3	1:A:285:PRO:HB2	1.82	0.62
3:C:107:LEU:O	3:C:111:THR:HG23	1.99	0.62
1:A:80:ARG:HB2	1:A:499:LEU:HD13	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:LEU:HD11	1:A:558:ALA:HB2	1.82	0.62
1:A:332:LEU:HD13	4:D:98:ILE:HD11	1.80	0.61
1:A:274:LEU:HD21	3:C:46:VAL:HA	1.82	0.61
2:B:162:MET:CE	4:D:106:MET:HE1	2.29	0.61
1:A:245:VAL:HA	3:C:42:ILE:HD13	1.80	0.61
1:A:334:HIS:HA	6:A:1002:HEO:HAA1	1.83	0.61
1:A:5:LYS:HD2	1:A:610:ILE:HG12	1.83	0.61
1:A:62:ILE:HG12	1:A:443:MET:HE1	1.83	0.61
1:A:71:ARG:HH12	1:A:160:LEU:HD23	1.66	0.61
4:D:73:GLU:OE2	4:D:74:GLN:NE2	2.34	0.61
3:C:68:TYR:O	3:C:71:THR:OG1	2.16	0.60
1:A:191:ILE:HG23	1:A:250:LEU:HB3	1.83	0.60
1:A:350:ILE:O	1:A:354:VAL:HG23	2.01	0.60
6:A:1002:HEO:H242	2:B:72:PRO:HB3	1.82	0.60
1:A:341:GLY:H	4:D:101:TYR:HE2	1.49	0.60
1:A:116:MET:HE1	1:A:286:GLU:HG2	1.83	0.60
3:C:41:PHE:HA	3:C:44:PHE:HB2	1.84	0.60
1:A:73:PHE:CE1	5:A:1001:HEM:HAB	2.34	0.60
1:A:83:LEU:HD21	1:A:483:LEU:O	2.02	0.60
1:A:110:MET:HA	1:A:114:VAL:HB	1.83	0.60
3:C:37:PHE:HB3	4:D:88:ILE:HD11	1.83	0.60
1:A:145:SER:OG	1:A:200:GLY:O	2.20	0.59
1:A:422:ASN:HA	1:A:464:PHE:CZ	2.37	0.59
1:A:417:ILE:HA	1:A:420:PHE:CE2	2.37	0.59
1:A:75:ASP:O	1:A:79:MET:HG3	2.02	0.59
1:A:217:ALA:HB3	1:A:220:MET:HB2	1.85	0.59
4:D:81:PHE:O	4:D:85:ILE:HD12	2.03	0.59
1:A:422:ASN:HA	1:A:464:PHE:HZ	1.67	0.59
3:C:51:VAL:C	3:C:53:PRO:HD3	2.29	0.58
1:A:12:PRO:HD2	1:A:161:VAL:O	2.03	0.58
1:A:446:TRP:HH2	8:A:1007:3PE:H32	1.68	0.58
3:C:58:ALA:H	3:C:128:HIS:HE1	1.51	0.58
4:D:102:LEU:HD13	4:D:106:MET:CE	2.32	0.58
1:A:134:ARG:NH2	1:A:553:ALA:O	2.36	0.58
1:A:156:MET:HE1	1:A:165:PHE:CZ	2.39	0.58
1:A:113:PHE:HA	1:A:149:PHE:CE1	2.39	0.57
2:B:12:VAL:HG11	2:B:171:LEU:HA	1.85	0.57
1:A:371:TYR:HD1	1:A:372:LYS:HG2	1.69	0.57
8:C:301:3PE:H341	8:C:301:3PE:H221	1.86	0.57
1:A:307:ARG:HH12	2:B:54:TYR:HB3	1.69	0.57
2:B:71:ILE:HD12	2:B:71:ILE:H	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLY:O	1:A:90:GLY:C	2.48	0.57
1:A:3:PHE:CG	1:A:4:GLY:N	2.66	0.57
1:A:375:ILE:HD12	1:A:381:MET:HE2	1.87	0.57
1:A:60:MET:HE3	1:A:146:PHE:CE2	2.40	0.57
1:A:102:ILE:HA	10:A:1011:UQ8:C3M	2.34	0.57
2:B:67:VAL:HG13	2:B:71:ILE:HD11	1.86	0.57
1:A:45:TRP:HA	1:A:49:PHE:HB2	1.86	0.57
2:B:33:PRO:HD2	2:B:34:SER:H	1.70	0.57
3:C:146:HIS:NE2	3:C:190:VAL:HG13	2.20	0.57
3:C:156:TRP:CD1	8:C:301:3PE:H331	2.40	0.56
1:A:90:GLY:O	1:A:91:GLU:C	2.44	0.56
1:A:127:VAL:O	1:A:128:PRO:C	2.45	0.56
1:A:174:PRO:HG3	1:A:275:TYR:HB3	1.86	0.56
1:A:239:ILE:HG13	1:A:289:ILE:HD13	1.87	0.56
1:A:95:HIS:N	1:A:98[A]:HIS:CE1	2.73	0.56
1:A:332:LEU:HD23	1:A:348:PHE:HB2	1.88	0.56
1:A:642:GLU:O	1:A:646:ILE:HG13	2.05	0.56
3:C:183:PHE:O	3:C:187:LEU:HG	2.04	0.56
3:C:189:ILE:HA	3:C:192:ILE:HD12	1.88	0.56
1:A:594:VAL:HG11	9:A:1008:LMG:H302	1.88	0.56
2:B:79:LEU:O	2:B:83:THR:OG1	2.21	0.56
1:A:109:ILE:HA	1:A:113:PHE:HD2	1.70	0.56
1:A:442:LYS:NZ	1:A:540:GLU:O	2.39	0.56
2:B:90:TYR:HA	2:B:94:ARG:HD2	1.86	0.56
1:A:292:LEU:HA	1:A:295:PHE:HB2	1.88	0.55
2:B:224:GLU:HB2	2:B:263:GLU:HB3	1.88	0.55
1:A:580:TYR:CZ	1:A:647:GLU:HG3	2.41	0.55
1:A:130:GLN:HG2	1:A:226:PRO:HG2	1.89	0.55
1:A:283:GLY:O	1:A:287:VAL:N	2.40	0.55
8:A:1005:3PE:H382	8:A:1007:3PE:H372	1.88	0.55
1:A:82:GLN:O	1:A:85:LEU:N	2.39	0.55
2:B:169:LEU:HD21	2:B:171:LEU:HD23	1.89	0.55
1:A:377:PHE:O	1:A:454:LYS:NZ	2.39	0.55
1:A:464:PHE:HE1	1:A:468:PHE:HB2	1.71	0.55
1:A:440:TRP:HE1	1:A:446:TRP:NE1	2.04	0.55
1:A:572:VAL:O	1:A:574:TYR:N	2.40	0.55
1:A:129:LEU:HD23	1:A:551:ASN:OD1	2.07	0.55
1:A:274:LEU:HD21	3:C:46:VAL:HG22	1.89	0.55
1:A:516:ILE:O	1:A:520:PHE:N	2.40	0.55
2:B:11:PRO:HD2	2:B:172:LEU:HB3	1.89	0.54
1:A:95:HIS:HD2	1:A:98[A]:HIS:CE1	2.25	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:GLN:HB3	2:B:271:MET:HG2	1.88	0.54
2:B:273:PRO:O	2:B:276:THR:N	2.35	0.54
1:A:181:TYR:CD2	2:B:146:THR:HG23	2.43	0.54
3:C:88:LEU:O	3:C:91:TYR:HB2	2.08	0.54
1:A:68:MET:SD	1:A:153:ALA:HB1	2.48	0.54
1:A:105:ALA:HB3	10:A:1011:UQ8:H3M	1.90	0.54
1:A:424:ILE:HG21	5:A:1001:HEM:CAC	2.37	0.54
2:B:125:THR:HA	2:B:261:ASP:HA	1.88	0.54
4:D:31:ILE:HG13	4:D:32:PRO:CD	2.35	0.54
1:A:95:HIS:H	1:A:98[A]:HIS:CE1	2.27	0.54
1:A:302:VAL:HG21	1:A:366:TRP:HB2	1.89	0.53
2:B:100:LYS:H	2:B:136:PRO:HG3	1.73	0.53
1:A:170:TRP:HB3	5:A:1001:HEM:HBD1	1.90	0.53
1:A:481:ARG:NH1	6:A:1002:HEO:O2D	2.40	0.53
2:B:242:GLY:HA2	2:B:246:LYS:HD2	1.91	0.53
1:A:312:GLY:N	2:B:59:ALA:O	2.38	0.53
1:A:326:LEU:O	1:A:330:VAL:HG23	2.08	0.53
3:C:112:PHE:HA	3:C:115:MET:HE3	1.91	0.53
1:A:97:ASP:HB3	2:B:236:LEU:HG	1.91	0.53
8:A:1004:3PE:O14	8:A:1004:3PE:N	2.30	0.53
1:A:238:LEU:HD22	1:A:285:PRO:HB3	1.89	0.53
1:A:389:VAL:HA	2:B:35:ILE:HD12	1.91	0.53
1:A:511:CYS:O	1:A:515:GLN:N	2.38	0.53
3:C:61:LEU:HA	3:C:203:VAL:HG13	1.90	0.53
1:A:95:HIS:CD2	1:A:98[A]:HIS:CE1	2.97	0.53
1:A:105:ALA:HB2	1:A:165:PHE:HD2	1.74	0.53
1:A:565:TRP:O	1:A:569:GLU:HG2	2.09	0.53
2:B:111:GLN:HG2	2:B:233:GLN:HB2	1.90	0.53
2:B:114:TRP:CZ2	2:B:183:SER:HB2	2.43	0.53
2:B:222:ASN:H	2:B:260:GLY:HA2	1.74	0.53
1:A:95:HIS:H	1:A:98[A]:HIS:HE1	1.56	0.52
2:B:203:GLU:O	2:B:207:ASN:N	2.34	0.52
1:A:63:ILE:HD13	8:A:1007:3PE:H392	1.90	0.52
1:A:174:PRO:HD3	1:A:275:TYR:CD1	2.45	0.52
1:A:371:TYR:CD1	1:A:372:LYS:HG2	2.44	0.52
8:A:1004:3PE:H292	8:A:1004:3PE:H251	1.91	0.52
1:A:550:TYR:HE2	1:A:646:ILE:HD12	1.75	0.52
1:A:550:TYR:CZ	1:A:643:VAL:HG23	2.44	0.52
4:D:36:VAL:HG22	4:D:46:LEU:HD22	1.91	0.52
1:A:141:LEU:O	1:A:145:SER:N	2.32	0.52
1:A:79:MET:HA	1:A:99:TYR:HE1	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:146:HIS:CD2	3:C:194:VAL:HG21	2.42	0.52
1:A:118:LEU:HD22	1:A:436:ILE:HD11	1.90	0.52
2:B:31:VAL:O	2:B:35:ILE:HG12	2.10	0.52
2:B:122:ASN:HB3	2:B:264:ALA:HA	1.91	0.52
8:A:1004:3PE:H122	3:C:21:LEU:HD13	1.92	0.52
1:A:74:ALA:HB1	10:A:1011:UQ8:H8	1.91	0.51
3:C:195:PHE:HB3	4:D:33:PHE:HZ	1.74	0.51
1:A:291:VAL:HG11	6:A:1002:HEO:HMC1	1.93	0.51
1:A:49:PHE:HE2	9:A:1009:LMG:H381	1.75	0.51
1:A:189:TYR:CD1	1:A:607:ILE:HD13	2.45	0.51
1:A:210:VAL:HA	3:C:27:TRP:HZ3	1.74	0.51
1:A:105:ALA:HB2	1:A:165:PHE:CD2	2.45	0.51
1:A:139:PRO:HG3	1:A:586:PRO:HG3	1.93	0.51
1:A:287:VAL:O	6:A:1002:HEO:HBC1	2.09	0.51
1:A:405:PRO:HD2	2:B:87:SER:HB3	1.93	0.51
1:A:529:TYR:HB3	1:A:653:LEU:HD21	1.90	0.51
3:C:149:HIS:CD2	8:C:301:3PE:H2C2	2.45	0.51
1:A:94:LEU:HD12	1:A:98[A]:HIS:CE1	2.45	0.51
1:A:363:ILE:O	1:A:367:LEU:HB2	2.11	0.51
3:C:94:ASN:O	3:C:98:VAL:HG23	2.11	0.51
1:A:159:SER:HA	1:A:189:TYR:CE2	2.46	0.51
3:C:55:THR:HB	3:C:56:PRO:HD3	1.93	0.51
3:C:33:ASP:HB3	3:C:186:PHE:CD2	2.46	0.51
1:A:86:ALA:O	1:A:88:GLY:N	2.44	0.51
1:A:405:PRO:HG2	2:B:88:HIS:H	1.76	0.51
8:A:1007:3PE:H231	10:A:1011:UQ8:H37	1.93	0.51
1:A:253:LEU:O	1:A:257:ARG:HG3	2.11	0.51
1:A:464:PHE:CE1	1:A:468:PHE:HB2	2.46	0.51
3:C:200:LEU:HD11	4:D:50:ILE:HD11	1.93	0.51
1:A:45:TRP:HE1	9:A:1009:LMG:HC61	1.76	0.50
2:B:238:THR:H	2:B:251:HIS:CE1	2.29	0.50
1:A:64:VAL:O	1:A:68:MET:HG2	2.11	0.50
8:A:1004:3PE:H241	8:A:1004:3PE:H392	1.92	0.50
1:A:97:ASP:HA	2:B:189:TYR:CE1	2.45	0.50
2:B:123:ILE:HG22	2:B:213:VAL:HB	1.92	0.50
1:A:75:ASP:CB	1:A:102:ILE:HG23	2.37	0.50
1:A:140:LEU:HD22	1:A:589:ARG:HH21	1.77	0.50
1:A:335:PHE:HB2	1:A:338:MET:HB2	1.94	0.50
1:A:399:VAL:O	1:A:402:ALA:HB3	2.11	0.50
1:A:485:THR:O	1:A:486:TYR:HB2	2.11	0.50
1:A:87:LYS:HG3	1:A:492:ASP:OD2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ALA:HB1	2:B:88:HIS:HD2	1.77	0.50
1:A:375:ILE:O	2:B:47:ALA:N	2.44	0.50
1:A:528:ASP:O	1:A:531:GLY:N	2.41	0.50
3:C:155:VAL:O	3:C:159:VAL:HG12	2.11	0.50
1:A:95:HIS:HD2	1:A:98[A]:HIS:NE2	2.09	0.50
1:A:440:TRP:HA	1:A:443:MET:HB2	1.93	0.50
1:A:275:TYR:O	1:A:279:ILE:HG12	2.11	0.50
2:B:40:TRP:HE1	2:B:44:LYS:HD2	1.77	0.50
1:A:240:ILE:HG23	3:C:35:ILE:HG13	1.94	0.50
1:A:243:PHE:O	1:A:247:THR:HG23	2.12	0.50
1:A:255:LEU:HD23	1:A:261:PHE:CE2	2.46	0.50
1:A:403:VAL:HG12	1:A:405:PRO:HD2	1.94	0.49
1:A:550:TYR:CE1	1:A:553:ALA:HB2	2.47	0.49
2:B:102:PRO:HB3	2:B:136:PRO:HB2	1.93	0.49
1:A:223:MET:SD	1:A:317:VAL:HG11	2.52	0.49
1:A:501:GLY:O	1:A:505:VAL:HG23	2.12	0.49
3:C:200:LEU:HD12	4:D:36:VAL:HG21	1.94	0.49
1:A:568:LYS:HA	1:A:573:ALA:HB2	1.95	0.49
3:C:33:ASP:HB3	3:C:186:PHE:CE2	2.47	0.49
1:A:31:VAL:O	1:A:35:ILE:HG13	2.12	0.49
1:A:75:ASP:OD1	1:A:76:ALA:N	2.45	0.49
3:C:160:LEU:O	3:C:164:ILE:HG13	2.12	0.49
1:A:572:VAL:HG23	1:A:573:ALA:H	1.77	0.49
1:A:136:VAL:CG1	1:A:207:ASN:HB3	2.41	0.49
1:A:308:LYS:HZ2	1:A:372:LYS:HB2	1.77	0.49
2:B:123:ILE:HD12	2:B:130:ARG:HH22	1.76	0.49
1:A:85:LEU:HD12	1:A:93:TYR:CD2	2.48	0.49
1:A:330:VAL:HG12	1:A:333:HIS:CE1	2.48	0.49
1:A:93:TYR:CE1	1:A:94:LEU:HD22	2.48	0.49
4:D:23:ILE:O	4:D:27:ILE:HG23	2.11	0.49
1:A:41:TRP:CE2	9:A:1010:LMG:H291	2.48	0.48
1:A:94:LEU:HB3	1:A:99:TYR:HB2	1.95	0.48
1:A:420:PHE:HB2	6:A:1002:HEO:C2D	2.43	0.48
1:A:333:HIS:CE1	1:A:334:HIS:CE1	3.01	0.48
1:A:481:ARG:HG3	1:A:482:ARG:H	1.77	0.48
3:C:106:PHE:HB2	3:C:157:MET:HG2	1.94	0.48
3:C:184:TRP:HA	3:C:187:LEU:HD12	1.94	0.48
1:A:141:LEU:HB3	1:A:207:ASN:HD21	1.77	0.48
1:A:357:ILE:HB	1:A:358:PRO:HD3	1.95	0.48
1:A:480:THR:HG21	2:B:183:SER:O	2.13	0.48
4:D:92:LEU:C	4:D:94:GLY:N	2.71	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:PRO:HB2	2:B:146:THR:HG22	1.95	0.48
1:A:199:LEU:HD11	8:A:1004:3PE:H3B1	1.95	0.48
1:A:240:ILE:HG12	3:C:35:ILE:HD11	1.95	0.48
1:A:489:PRO:O	1:A:492:ASP:HB2	2.13	0.48
1:A:19:VAL:HA	1:A:22:VAL:HG12	1.96	0.48
1:A:192:TRP:NE1	1:A:258:TYR:OH	2.45	0.48
1:A:308:LYS:NZ	1:A:372:LYS:HB2	2.29	0.48
3:C:37:PHE:CE1	3:C:190:VAL:HB	2.48	0.48
4:D:25:SER:CB	4:D:57:GLN:HE22	2.26	0.48
2:B:5:LEU:O	2:B:17:SER:OG	2.24	0.48
2:B:112:PHE:HD1	2:B:194:MET:HE3	1.79	0.48
2:B:62:THR:HG22	2:B:63:ALA:H	1.78	0.48
1:A:95:HIS:O	1:A:96:PRO:C	2.55	0.48
1:A:298:TYR:O	1:A:302:VAL:HG22	2.14	0.48
2:B:130:ARG:HH11	2:B:210:VAL:HG13	1.78	0.48
1:A:11:ILE:H	1:A:11:ILE:HG12	1.50	0.48
1:A:20:THR:HG21	10:A:1011:UQ8:H1MA	1.96	0.48
1:A:39:LYS:NZ	1:A:41:TRP:HB2	2.29	0.48
1:A:488:ASN:H	1:A:491:TRP:HE1	1.61	0.47
1:A:290:LEU:HB3	1:A:428:VAL:HG21	1.95	0.47
2:B:142:THR:OG1	2:B:143:SER:N	2.47	0.47
1:A:14:GLU:OE2	1:A:98[A]:HIS:CD2	2.67	0.47
1:A:25:ALA:O	1:A:26:LEU:HB2	2.13	0.47
1:A:38:PHE:HB3	8:A:1005:3PE:H222	1.96	0.47
2:B:33:PRO:HA	2:B:36:ILE:HB	1.97	0.47
1:A:14:GLU:O	1:A:15:PRO:C	2.57	0.47
1:A:39:LYS:HD2	1:A:39:LYS:HA	1.64	0.47
9:A:1008:LMG:H162	9:A:1009:LMG:H132	1.97	0.47
1:A:227:ILE:HD12	1:A:310:LEU:HD13	1.96	0.47
1:A:259:PHE:CZ	8:C:302:3PE:H261	2.49	0.47
1:A:158:LEU:HA	1:A:161:VAL:HG22	1.96	0.47
1:A:302:VAL:HG12	1:A:381:MET:HE1	1.96	0.47
1:A:82:GLN:C	1:A:84:PHE:N	2.72	0.47
1:A:125:ILE:O	1:A:129:LEU:HD11	2.14	0.47
1:A:129:LEU:HD13	1:A:540:GLU:CB	2.44	0.47
1:A:271:SER:OG	1:A:273:MET:SD	2.73	0.47
1:A:284:HIS:ND1	1:A:333:HIS:HE1	2.12	0.47
1:A:593:PHE:O	1:A:597:MET:HB3	2.13	0.47
2:B:107:VAL:HB	2:B:141:ILE:HG23	1.97	0.47
1:A:54:HIS:CD2	1:A:135:ASP:HA	2.49	0.47
1:A:82:GLN:O	1:A:84:PHE:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:O	10:A:1011:UQ8:H16A	2.14	0.47
1:A:87:LYS:O	1:A:87:LYS:HG2	2.15	0.46
1:A:105:ALA:HB3	10:A:1011:UQ8:C3M	2.45	0.46
1:A:627:VAL:HG22	8:A:1006:3PE:H241	1.97	0.46
1:A:659:LYS:HG3	1:A:660:LYS:HG3	1.96	0.46
1:A:111:ILE:HG21	1:A:170:TRP:CZ3	2.50	0.46
1:A:361:VAL:HG11	2:B:69:TRP:CD2	2.50	0.46
1:A:464:PHE:CD1	1:A:464:PHE:C	2.91	0.46
1:A:14:GLU:OE2	1:A:98[A]:HIS:HD2	1.98	0.46
1:A:192:TRP:HB2	1:A:607:ILE:HD11	1.98	0.46
1:A:517:ILE:O	1:A:520:PHE:HB3	2.15	0.46
1:A:127:VAL:O	1:A:129:LEU:N	2.49	0.46
1:A:215:MET:HE3	1:A:215:MET:HB3	1.86	0.46
1:A:252:MET:SD	3:C:46:VAL:HG21	2.55	0.46
1:A:463:GLY:HA2	1:A:504:LEU:HD23	1.97	0.46
4:D:81:PHE:O	4:D:84:THR:OG1	2.28	0.46
2:B:155:LEU:HG	2:B:171:LEU:HD13	1.96	0.46
1:A:255:LEU:HD21	8:C:302:3PE:H392	1.98	0.46
1:A:138:PHE:CZ	3:C:28:THR:HB	2.51	0.46
1:A:174:PRO:HG2	1:A:175:PRO:HD3	1.98	0.46
1:A:264:PHE:CG	1:A:275:TYR:HB2	2.51	0.46
1:A:338:MET:O	1:A:338:MET:HG3	2.16	0.46
1:A:26:LEU:HA	1:A:29:ILE:CG2	2.42	0.46
1:A:222:LEU:HD11	4:D:76:TRP:HZ2	1.81	0.46
1:A:450:GLU:O	1:A:454:LYS:HG2	2.16	0.46
1:A:579:LYS:HB3	1:A:581:GLU:OE2	2.16	0.46
1:A:579:LYS:HD2	1:A:579:LYS:HA	1.80	0.46
10:A:1011:UQ8:H15	10:A:1011:UQ8:H12A	1.63	0.46
2:B:93:TYR:CZ	2:B:159:ILE:HD13	2.51	0.46
2:B:124:ALA:HB3	2:B:262:GLN:HB2	1.98	0.46
2:B:228:LYS:HZ1	2:B:262:GLN:HG2	1.82	0.45
3:C:95:VAL:HG13	3:C:164:ILE:HG22	1.98	0.45
1:A:127:VAL:O	1:A:130:GLN:N	2.50	0.45
1:A:140:LEU:HD22	1:A:589:ARG:NH2	2.31	0.45
1:A:340:ALA:HB3	1:A:345:ASN:HD21	1.80	0.45
3:C:51:VAL:HG22	3:C:135:PHE:CD1	2.52	0.45
3:C:70:LEU:HD11	4:D:33:PHE:HB3	1.98	0.45
8:A:1007:3PE:H2	8:A:1007:3PE:H341	1.98	0.45
2:B:50:LYS:HA	2:B:50:LYS:HD3	1.79	0.45
3:C:195:PHE:O	3:C:199:TYR:HB2	2.16	0.45
1:A:633:ASN:OD1	1:A:633:ASN:N	2.44	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:146:HIS:CE1	3:C:191:TRP:CD1	3.04	0.45
1:A:337:THR:HG22	2:B:160:TYR:HD1	1.81	0.45
1:A:461:PHE:C	1:A:463:GLY:H	2.24	0.45
2:B:105:ILE:O	2:B:139:PHE:HA	2.17	0.45
1:A:174:PRO:HD3	1:A:275:TYR:HD1	1.81	0.45
1:A:76:ALA:O	1:A:80:ARG:HG2	2.17	0.45
2:B:107:VAL:HA	2:B:115:ILE:O	2.17	0.45
3:C:47:LEU:HD22	3:C:198:VAL:HG22	1.98	0.45
1:A:483:LEU:HD12	1:A:483:LEU:HA	1.78	0.44
1:A:82:GLN:CD	1:A:485:THR:HG22	2.42	0.44
1:A:122:MET:HB3	1:A:122:MET:HE3	1.84	0.44
1:A:358:PRO:HA	1:A:361:VAL:HG22	1.99	0.44
1:A:100:ASP:HA	1:A:103:PHE:CE2	2.53	0.44
2:B:46:ARG:NE	2:B:49:ASN:HD21	2.15	0.44
3:C:145:THR:HG23	8:C:301:3PE:H2G2	1.98	0.44
3:C:186:PHE:O	3:C:190:VAL:HG12	2.17	0.44
9:A:1009:LMG:HC2	9:A:1009:LMG:HC71	1.52	0.44
2:B:257:LYS:NZ	2:B:258:ALA:H	2.15	0.44
2:B:271:MET:HE3	2:B:271:MET:HB2	1.88	0.44
3:C:57:SER:OG	3:C:58:ALA:N	2.50	0.44
6:A:1002:HEO:H212	6:A:1002:HEO:H18	1.56	0.44
2:B:120:GLU:HG2	2:B:121:GLN:N	2.31	0.44
1:A:159:SER:HA	1:A:189:TYR:HE2	1.83	0.44
1:A:82:GLN:NE2	1:A:485:THR:HG22	2.32	0.44
1:A:259:PHE:CE2	8:C:302:3PE:H242	2.53	0.44
1:A:34:GLY:O	1:A:38:PHE:HB2	2.18	0.44
1:A:95:HIS:H	1:A:95:HIS:CD2	2.34	0.44
1:A:129:LEU:HD13	1:A:540:GLU:HB2	1.98	0.44
1:A:168:THR:OG1	1:A:172:ALA:HA	2.18	0.44
1:A:246:LEU:HB2	1:A:282:TRP:CD1	2.53	0.44
1:A:308:LYS:HD3	1:A:369:THR:O	2.18	0.44
1:A:625:LEU:HD21	8:A:1004:3PE:H252	2.00	0.44
1:A:288:TYR:O	1:A:292:LEU:HB2	2.17	0.43
1:A:322:ALA:HA	1:A:325:VAL:HG12	2.00	0.43
1:A:332:LEU:HD13	4:D:98:ILE:CD1	2.47	0.43
9:A:1009:LMG:H362	9:A:1010:LMG:H321	2.00	0.43
1:A:14:GLU:O	1:A:17:VAL:N	2.51	0.43
1:A:291:VAL:HG21	6:A:1002:HEO:HMC2	2.00	0.43
2:B:104:THR:HA	2:B:138:SER:HB3	1.98	0.43
3:C:157:MET:O	3:C:161:MET:HG3	2.18	0.43
1:A:48:TRP:HB3	1:A:60:MET:SD	2.59	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:GLY:O	1:A:90:GLY:N	2.45	0.43
1:A:189:TYR:CD1	1:A:607:ILE:HG21	2.52	0.43
1:A:550:TYR:CE2	1:A:646:ILE:HD12	2.52	0.43
3:C:78:ILE:O	3:C:81:VAL:HG12	2.18	0.43
1:A:444:PHE:C	1:A:546:PRO:HD3	2.43	0.43
2:B:272:LYS:HB3	2:B:272:LYS:HE2	1.80	0.43
3:C:47:LEU:HG	3:C:51:VAL:HG23	2.00	0.43
1:A:74:ALA:O	1:A:78:MET:HE2	2.18	0.43
1:A:379:THR:O	1:A:383:TRP:HD1	2.02	0.43
1:A:406:ALA:O	1:A:410:VAL:HG22	2.18	0.43
3:C:14:HIS:HB3	3:C:15:GLU:H	1.57	0.43
3:C:95:VAL:O	3:C:99:ILE:HG12	2.18	0.43
1:A:119:VAL:HG13	1:A:293:PRO:HG3	2.00	0.43
1:A:259:PHE:CD1	1:A:259:PHE:N	2.86	0.43
1:A:330:VAL:HG13	1:A:352:THR:OG1	2.19	0.43
1:A:420:PHE:HA	1:A:423:VAL:HG22	1.99	0.43
1:A:539:LEU:HD23	1:A:539:LEU:HA	1.82	0.43
9:A:1008:LMG:H162	9:A:1009:LMG:H111	2.00	0.43
2:B:240:ARG:NE	2:B:240:ARG:HA	2.33	0.43
1:A:76:ALA:O	1:A:77:ILE:C	2.59	0.43
1:A:91:GLU:O	1:A:92:GLY:C	2.62	0.43
1:A:100:ASP:O	1:A:101:GLN:C	2.62	0.43
1:A:364:PHE:HB3	2:B:68:VAL:HG22	2.00	0.43
1:A:574:TYR:HD2	1:A:650:ARG:HH22	1.67	0.43
4:D:42:SER:HB2	4:D:45:LEU:HB3	2.00	0.43
4:D:75:ARG:O	4:D:75:ARG:HG3	2.19	0.43
1:A:43:TYR:CD2	1:A:44:LEU:HD12	2.54	0.43
1:A:225:MET:O	1:A:313:TYR:OH	2.35	0.43
1:A:333:HIS:HE1	1:A:334:HIS:CE1	2.37	0.43
3:C:162:TYR:O	3:C:166:THR:HG22	2.18	0.43
4:D:102:LEU:HA	4:D:105:ASN:ND2	2.34	0.43
4:D:105:ASN:CG	4:D:106:MET:N	2.77	0.43
6:A:1002:HEO:H22	2:B:30:VAL:HG21	2.00	0.43
3:C:100:THR:O	3:C:104:ILE:HG23	2.19	0.43
3:C:149:HIS:NE2	8:C:301:3PE:H2C2	2.34	0.43
1:A:166:ALA:HB2	1:A:187:VAL:HA	2.01	0.42
1:A:424:ILE:O	1:A:428:VAL:N	2.50	0.42
2:B:243:ASP:HB2	2:B:244:ARG:HD2	2.01	0.42
1:A:39:LYS:HZ1	1:A:41:TRP:HB2	1.84	0.42
1:A:284:HIS:NE2	1:A:330:VAL:HG11	2.33	0.42
1:A:382:LEU:HD23	1:A:382:LEU:HA	1.79	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:ILE:HD13	1:A:515:GLN:HE22	1.85	0.42
1:A:94:LEU:HD12	1:A:94:LEU:HA	1.75	0.42
1:A:103:PHE:CD1	1:A:103:PHE:C	2.97	0.42
1:A:372:LYS:O	2:B:54:TYR:HA	2.19	0.42
1:A:446:TRP:CE3	1:A:523:ARG:HB2	2.54	0.42
1:A:563:ARG:HA	1:A:563:ARG:HD2	1.80	0.42
2:B:152:ILE:O	2:B:156:GLY:N	2.52	0.42
3:C:70:LEU:HD22	3:C:74:PHE:CZ	2.55	0.42
3:C:136:LEU:HD23	3:C:136:LEU:HA	1.90	0.42
1:A:340:ALA:HB1	1:A:344:VAL:HG23	2.00	0.42
1:A:517:ILE:O	1:A:521:LEU:HD12	2.19	0.42
1:A:538:THR:OG1	1:A:540:GLU:HG2	2.18	0.42
10:A:1011:UQ8:H22	10:A:1011:UQ8:H25	1.85	0.42
3:C:92:LYS:HB3	3:C:92:LYS:HE2	1.83	0.42
4:D:107:MET:HE2	4:D:107:MET:HB2	1.74	0.42
1:A:408:PHE:HB2	2:B:16:GLN:HE22	1.84	0.42
1:A:432:MET:O	1:A:436:ILE:HG13	2.20	0.42
3:C:192:ILE:HG21	4:D:57:GLN:HB3	2.02	0.42
1:A:35:ILE:HG23	1:A:40:LYS:O	2.19	0.42
1:A:337:THR:HG22	2:B:160:TYR:CD1	2.54	0.42
2:B:87:SER:C	2:B:89:LYS:H	2.27	0.42
2:B:100:LYS:HA	2:B:100:LYS:HD3	1.72	0.42
4:D:58:VAL:O	4:D:62:LEU:HD12	2.18	0.42
4:D:101:TYR:CE1	4:D:104:TYR:HE2	2.38	0.42
4:D:101:TYR:HA	4:D:104:TYR:HD2	1.84	0.42
1:A:73:PHE:CE2	1:A:77:ILE:HD11	2.55	0.42
1:A:488:ASN:ND2	2:B:180:ARG:HE	2.18	0.42
9:A:1008:LMG:H372	9:A:1008:LMG:H402	1.76	0.42
2:B:254:ASN:OD1	2:B:254:ASN:N	2.53	0.42
1:A:27:GLY:O	1:A:31:VAL:HG22	2.19	0.42
1:A:45:TRP:HZ3	1:A:593:PHE:HD2	1.68	0.42
1:A:109:ILE:HA	1:A:113:PHE:CD2	2.54	0.42
1:A:156:MET:HE1	1:A:165:PHE:HZ	1.83	0.42
1:A:176:LEU:HD21	2:B:187:SER:C	2.44	0.42
1:A:561:ILE:HG22	1:A:562:ASP:OD1	2.19	0.42
2:B:129:VAL:HG22	2:B:131:PHE:HD1	1.85	0.42
2:B:152:ILE:HG22	2:B:155:LEU:HB3	2.02	0.42
1:A:103:PHE:CE2	1:A:482:ARG:HB3	2.55	0.42
1:A:113:PHE:HA	1:A:149:PHE:HE1	1.83	0.42
1:A:535:ASP:HB3	1:A:565:TRP:HZ3	1.85	0.42
2:B:109:ALA:HA	2:B:114:TRP:HA	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:51:VAL:HA	3:C:135:PHE:HB2	2.01	0.42
1:A:291:VAL:HG13	6:A:1002:HEO:CBC	2.50	0.42
1:A:585:MET:HB3	1:A:585:MET:HE3	1.79	0.42
2:B:76:ILE:HD13	2:B:76:ILE:HA	1.82	0.42
2:B:96:LEU:HD23	2:B:136:PRO:HB3	2.02	0.42
3:C:162:TYR:HA	3:C:165:LYS:HE2	2.01	0.42
1:A:20:THR:HA	10:A:1011:UQ8:C10	2.49	0.41
1:A:208:PHE:O	1:A:212:ILE:HG13	2.20	0.41
1:A:391:PHE:CE2	6:A:1002:HEO:H14	2.56	0.41
1:A:175:PRO:HD3	1:A:272:PRO:HB3	2.02	0.41
2:B:265:LEU:HD21	2:B:269:GLU:H	1.85	0.41
4:D:105:ASN:O	4:D:109:HIS:HE1	2.03	0.41
1:A:14:GLU:O	1:A:16:ILE:N	2.53	0.41
1:A:130:GLN:NE2	1:A:300:GLU:OE2	2.54	0.41
1:A:170:TRP:CD1	5:A:1001:HEM:HAD2	2.54	0.41
1:A:310:LEU:HD23	1:A:369:THR:OG1	2.20	0.41
3:C:51:VAL:O	3:C:53:PRO:HD3	2.20	0.41
3:C:185:HIS:O	3:C:189:ILE:HG13	2.20	0.41
1:A:192:TRP:CD1	1:A:607:ILE:HG13	2.56	0.41
1:A:363:ILE:HA	1:A:366:TRP:NE1	2.35	0.41
2:B:206:PHE:HA	2:B:209:TRP:CD1	2.56	0.41
4:D:92:LEU:HB3	4:D:93:ILE:H	1.76	0.41
1:A:82:GLN:C	1:A:84:PHE:H	2.29	0.41
1:A:266:ASN:HB3	2:B:276:THR:HG21	2.03	0.41
1:A:548:PRO:C	1:A:550:TYR:H	2.29	0.41
2:B:17:SER:O	2:B:21:MET:HG2	2.20	0.41
2:B:55:LYS:HE3	2:B:55:LYS:HB3	1.80	0.41
2:B:147:MET:HG2	2:B:162:MET:HA	2.03	0.41
1:A:130:GLN:O	1:A:539:LEU:HB2	2.21	0.41
1:A:440:TRP:CE2	1:A:448:LEU:HD21	2.55	0.41
1:A:565:TRP:HA	1:A:568:LYS:HD3	2.02	0.41
3:C:83:PHE:O	3:C:86:ALA:HB3	2.21	0.41
1:A:54:HIS:HB2	1:A:124:ASN:OD1	2.21	0.41
1:A:355:ILE:O	1:A:358:PRO:HD2	2.21	0.41
1:A:400:LEU:HD22	2:B:20:MET:HG3	2.03	0.41
3:C:24:PHE:O	3:C:28:THR:HG22	2.20	0.41
1:A:312:GLY:O	1:A:316:MET:HG2	2.20	0.41
9:A:1009:LMG:H121	9:A:1010:LMG:H182	2.02	0.41
1:A:62:ILE:CG1	1:A:443:MET:HE1	2.49	0.40
1:A:527:MET:HB2	1:A:529:TYR:CZ	2.55	0.40
2:B:88:HIS:O	2:B:94:ARG:NH2	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:SER:HB3	1:A:253:LEU:HD21	2.03	0.40
2:B:237:ALA:HA	2:B:251:HIS:CE1	2.56	0.40
1:A:124:ASN:CG	1:A:208:PHE:HZ	2.29	0.40
1:A:298:TYR:CZ	1:A:387:PHE:CG	3.10	0.40
10:A:1011:UQ8:H20	10:A:1011:UQ8:H17A	1.76	0.40
2:B:229:THR:HG22	2:B:229:THR:O	2.21	0.40
3:C:169:LEU:HD22	3:C:174:THR:HG22	2.04	0.40
3:C:192:ILE:HD11	4:D:61:GLN:HG3	2.03	0.40
1:A:12:PRO:CB	1:A:17:VAL:HG21	2.51	0.40
1:A:146:PHE:O	1:A:149:PHE:HB3	2.21	0.40
1:A:601:LEU:HD12	1:A:601:LEU:HA	1.89	0.40
4:D:55:VAL:O	4:D:59:LEU:HD23	2.22	0.40
6:A:1002:HEO:H22	2:B:30:VAL:CG2	2.51	0.40
2:B:3:MET:HG3	2:B:7:ASN:OD1	2.21	0.40
2:B:151:PHE:CZ	2:B:153:PRO:HG3	2.56	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	659/660 (100%)	563 (85%)	86 (13%)	10 (2%)	8	33
2	B	275/277 (99%)	231 (84%)	39 (14%)	5 (2%)	6	30
3	C	189/191 (99%)	173 (92%)	12 (6%)	4 (2%)	5	26
4	D	95/97 (98%)	86 (90%)	7 (7%)	2 (2%)	5	26
All	All	1218/1225 (99%)	1053 (86%)	144 (12%)	21 (2%)	9	30

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	PRO
1	A	546	PRO
2	B	63	ALA
2	B	275	PRO
3	C	53	PRO
4	D	93	ILE
1	A	90	GLY
1	A	93	TYR
1	A	573	ALA
4	D	108	ILE
2	B	91	ASP
3	C	52	PRO
3	C	54	GLY
1	A	486	TYR
2	B	110	GLU
3	C	200	LEU
2	B	267	LYS
1	A	92	GLY
1	A	15	PRO
1	A	88	GLY
1	A	547	ALA

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	540/539 (100%)	518 (96%)	22 (4%)	27	55
2	B	231/231 (100%)	231 (100%)	0	100	100
3	C	168/168 (100%)	166 (99%)	2 (1%)	63	75
4	D	84/84 (100%)	79 (94%)	5 (6%)	17	46
All	All	1023/1022 (100%)	994 (97%)	29 (3%)	38	62

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	10	SER
1	A	11	ILE
1	A	13	THR
1	A	41	TRP
1	A	77	ILE
1	A	80	ARG
1	A	82	GLN
1	A	87	LYS
1	A	91	GLU
1	A	94	LEU
1	A	96	PRO
1	A	97	ASP
1	A	102	ILE
1	A	104	THR
1	A	125	ILE
1	A	126	SER
1	A	129	LEU
1	A	131	ILE
1	A	144	LEU
1	A	379	THR
1	A	584	HIS
3	C	50	HIS
3	C	51	VAL
4	D	50	ILE
4	D	104	TYR
4	D	106	MET
4	D	107	MET
4	D	108	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	101	GLN
1	A	130	GLN
1	A	522	GLN
2	B	168	HIS
3	C	63	HIS
3	C	146	HIS
4	D	74	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	3PE	A	1005	-	29,29,50	0.34	0	32,34,55	0.41	0
8	3PE	C	301	-	50,50,50	0.28	0	53,55,55	0.32	0
9	LMG	A	1010	-	36,36,55	0.89	0	44,44,63	1.20	3 (6%)
8	3PE	A	1004	-	50,50,50	0.28	0	53,55,55	0.37	0
8	3PE	A	1006	-	35,35,50	0.31	0	38,40,55	0.48	0
9	LMG	A	1009	-	40,40,55	0.84	0	48,48,63	1.29	5 (10%)
10	UQ8	A	1011	-	45,45,53	1.26	2 (4%)	54,57,67	1.67	13 (24%)
6	HEO	A	1002	1	65,66,66	2.38	25 (38%)	81,102,102	2.97	35 (43%)
9	LMG	A	1008	-	46,46,55	0.79	0	54,54,63	1.28	6 (11%)
8	3PE	C	302	-	43,43,50	0.29	0	46,48,55	0.33	0
8	3PE	A	1007	-	35,35,50	0.32	0	38,40,55	0.38	0
5	HEM	A	1001	1	50,50,50	1.58	7 (14%)	66,82,82	1.79	15 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	3PE	A	1005	-	-	3/33/33/54	-
8	3PE	C	301	-	-	12/54/54/54	-
9	LMG	A	1010	-	-	17/31/51/70	0/1/1/1
8	3PE	A	1004	-	-	5/54/54/54	-
8	3PE	A	1006	-	-	7/39/39/54	-
9	LMG	A	1009	-	-	25/35/55/70	0/1/1/1
10	UQ8	A	1011	-	-	12/42/66/75	0/1/1/1
6	HEO	A	1002	1	-	10/34/74/74	-
9	LMG	A	1008	-	-	20/41/61/70	0/1/1/1
8	3PE	C	302	-	-	8/47/47/54	-
8	3PE	A	1007	-	-	6/39/39/54	-
5	HEM	A	1001	1	-	9/14/54/54	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1011	UQ8	C6-C1	7.31	1.48	1.35
6	A	1002	HEO	C3B-C2B	5.63	1.47	1.34
5	A	1001	HEM	FE-NB	5.27	2.11	1.94
6	A	1002	HEO	C2A-C3A	5.20	1.47	1.36
6	A	1002	HEO	C3D-C2D	4.99	1.47	1.36
6	A	1002	HEO	C4D-ND	4.75	1.48	1.38
6	A	1002	HEO	C4B-NB	4.70	1.48	1.40
6	A	1002	HEO	C1D-ND	4.69	1.48	1.40
6	A	1002	HEO	C1C-NC	4.60	1.48	1.39
6	A	1002	HEO	C1B-NB	4.49	1.48	1.38
6	A	1002	HEO	C4C-NC	4.31	1.48	1.39
6	A	1002	HEO	C1A-NA	4.23	1.48	1.39
6	A	1002	HEO	C4A-NA	4.15	1.47	1.39
5	A	1001	HEM	FE-NC	3.97	2.08	1.95
5	A	1001	HEM	C4D-ND	-3.37	1.34	1.40
6	A	1002	HEO	CHA-C1A	3.33	1.44	1.38
5	A	1001	HEM	C1B-NB	-3.32	1.34	1.40
6	A	1002	HEO	CHB-C4A	3.25	1.44	1.38
10	A	1011	UQ8	C4-C3	3.22	1.49	1.36
6	A	1002	HEO	CHD-C1D	3.05	1.44	1.38
6	A	1002	HEO	CHC-C4B	2.85	1.44	1.38
6	A	1002	HEO	C4B-C3B	2.68	1.49	1.44
5	A	1001	HEM	C3C-C4C	-2.66	1.41	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1002	HEO	C4D-C3D	2.54	1.49	1.45
6	A	1002	HEO	CHA-C4D	2.52	1.45	1.39
5	A	1001	HEM	C1C-C2C	-2.45	1.40	1.45
5	A	1001	HEM	FE-ND	-2.39	1.87	1.94
6	A	1002	HEO	CHD-C4C	2.37	1.44	1.39
6	A	1002	HEO	CHB-C1B	2.35	1.44	1.39
6	A	1002	HEO	C1B-C2B	2.26	1.48	1.44
6	A	1002	HEO	C3C-C4C	2.20	1.47	1.42
6	A	1002	HEO	C1C-C2C	2.19	1.48	1.43
6	A	1002	HEO	CHC-C1C	2.15	1.44	1.39
6	A	1002	HEO	C1D-C2D	2.08	1.48	1.44

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1002	HEO	C4A-NA-C1A	-7.56	97.94	105.35
6	A	1002	HEO	C4B-NB-C1B	-7.54	97.28	105.07
6	A	1002	HEO	C4C-NC-C1C	-7.35	98.15	105.35
6	A	1002	HEO	C1D-ND-C4D	-7.27	97.56	105.07
6	A	1002	HEO	C3C-C4C-NC	6.33	114.14	110.25
6	A	1002	HEO	C2A-C1A-NA	6.14	116.29	110.32
6	A	1002	HEO	C3D-C4D-ND	6.02	116.18	110.36
6	A	1002	HEO	C3B-C4B-NB	5.96	116.90	109.84
6	A	1002	HEO	C2B-C1B-NB	5.57	116.56	109.88
6	A	1002	HEO	C2D-C1D-ND	5.50	116.35	109.84
5	A	1001	HEM	CHC-C4B-NB	4.87	129.71	124.42
6	A	1002	HEO	C13-C12-C11	-4.71	107.27	114.35
5	A	1001	HEM	CHD-C1D-ND	4.55	129.36	124.42
6	A	1002	HEO	C2C-C1C-NC	4.49	116.92	110.08
5	A	1001	HEM	C1B-NB-C4B	3.91	109.11	105.07
6	A	1002	HEO	C3C-C2C-C1C	-3.67	102.73	107.16
6	A	1002	HEO	C3A-C4A-NA	3.61	116.35	109.69
5	A	1001	HEM	CHD-C4C-NC	3.54	128.27	124.44
5	A	1001	HEM	CAD-CBD-CGD	-3.50	106.06	113.60
5	A	1001	HEM	CHB-C1B-NB	3.39	128.55	124.37
5	A	1001	HEM	CHA-C4D-ND	3.38	128.54	124.37
10	A	1011	UQ8	C27-C28-C29	-3.35	119.59	127.66
5	A	1001	HEM	CAA-CBA-CGA	-3.32	106.45	113.60
6	A	1002	HEO	C4C-CHD-C1D	-3.30	118.51	126.34
6	A	1002	HEO	CHB-C1B-C2B	-3.29	119.84	124.98
10	A	1011	UQ8	C12-C13-C14	-3.17	120.03	127.66
10	A	1011	UQ8	C7-C8-C9	-3.16	121.52	126.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	HEM	CHD-C1D-C2D	-3.14	120.07	124.98
6	A	1002	HEO	CHC-C1C-C2C	-3.09	118.52	127.24
10	A	1011	UQ8	C10-C9-C11	3.08	120.45	115.27
10	A	1011	UQ8	C35-C34-C36	3.05	120.40	115.27
9	A	1010	LMG	O6-C1-O1	-2.95	102.98	109.97
6	A	1002	HEO	C1C-CHC-C4B	-2.95	119.35	126.34
6	A	1002	HEO	C4A-CHB-C1B	-2.92	119.77	126.06
6	A	1002	HEO	CHA-C4D-C3D	-2.89	120.59	124.84
6	A	1002	HEO	CAD-CBD-CGD	-2.89	107.39	113.60
6	A	1002	HEO	CHA-C1A-C2A	-2.86	120.30	124.94
10	A	1011	UQ8	C15-C14-C16	2.85	120.07	115.27
10	A	1011	UQ8	C37-C36-C34	-2.84	109.97	114.62
6	A	1002	HEO	C1A-CHA-C4D	-2.80	120.02	126.06
10	A	1011	UQ8	C17-C18-C19	-2.79	120.93	127.66
10	A	1011	UQ8	C30-C29-C31	2.77	119.93	115.27
6	A	1002	HEO	CHB-C4A-C3A	-2.77	119.67	125.48
6	A	1002	HEO	C13-C14-C15	-2.76	121.02	127.66
6	A	1002	HEO	CAD-C3D-C4D	2.75	129.47	124.66
10	A	1011	UQ8	C32-C33-C34	-2.75	121.04	127.66
5	A	1001	HEM	C4C-NC-C1C	2.70	107.99	105.35
6	A	1002	HEO	CHD-C1D-C2D	-2.61	119.48	126.73
9	A	1008	LMG	O6-C1-O1	-2.61	103.79	109.97
6	A	1002	HEO	C26-C15-C16	2.56	119.57	115.27
5	A	1001	HEM	C4C-CHD-C1D	-2.47	120.74	126.06
6	A	1002	HEO	C17-C18-C19	-2.45	121.77	127.66
10	A	1011	UQ8	C20-C19-C21	2.44	119.38	115.27
9	A	1009	LMG	O3-C3-C2	-2.40	104.79	110.35
9	A	1009	LMG	C38-C37-C36	-2.38	102.35	114.42
9	A	1009	LMG	O6-C5-C4	2.37	114.00	109.69
9	A	1008	LMG	C38-C37-C36	-2.35	102.49	114.42
6	A	1002	HEO	CAA-CBA-CGA	-2.33	108.60	113.60
6	A	1002	HEO	C25-C23-C24	2.31	119.71	114.60
10	A	1011	UQ8	C22-C23-C24	-2.29	122.14	127.66
9	A	1008	LMG	O2-C2-C1	-2.27	104.52	110.05
9	A	1009	LMG	O2-C2-C1	-2.26	104.55	110.05
9	A	1008	LMG	O3-C3-C2	-2.26	105.13	110.35
9	A	1010	LMG	O3-C3-C2	-2.22	105.22	110.35
10	A	1011	UQ8	C25-C24-C26	2.19	118.96	115.27
5	A	1001	HEM	C1A-CHA-C4D	-2.19	121.13	126.34
6	A	1002	HEO	CHC-C4B-C3B	-2.19	120.16	125.80
5	A	1001	HEM	C4A-NA-C1A	2.18	107.48	105.35
6	A	1002	HEO	C27-C19-C20	2.15	118.89	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	HEM	CHA-C1A-NA	2.13	127.76	123.85
9	A	1010	LMG	O2-C2-C1	-2.09	104.96	110.05
5	A	1001	HEM	C1C-CHC-C4B	-2.08	121.56	126.06
9	A	1009	LMG	O7-C10-O9	-2.08	118.67	123.70
6	A	1002	HEO	CBC-CAC-C3C	-2.07	117.34	127.62
6	A	1002	HEO	C21-C22-C23	-2.03	120.83	127.75
9	A	1008	LMG	O1-C7-C8	-2.01	106.04	110.90
9	A	1008	LMG	C1-O6-C5	-2.01	109.74	113.69

There are no chirality outliers.

All (134) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	HEM	C2B-C3B-CAB-CBB
5	A	1001	HEM	C4B-C3B-CAB-CBB
6	A	1002	HEO	C2C-C3C-CAC-CBC
6	A	1002	HEO	C4C-C3C-CAC-CBC
6	A	1002	HEO	C19-C20-C21-C22
8	A	1006	3PE	O22-C21-O21-C2
8	A	1006	3PE	C22-C21-O21-C2
8	A	1007	3PE	O32-C31-O31-C3
8	A	1007	3PE	C32-C31-O31-C3
8	C	301	3PE	C2-C1-O11-P
8	C	301	3PE	C12-C11-O13-P
8	C	301	3PE	O21-C2-C3-O31
8	C	302	3PE	C12-C11-O13-P
8	C	302	3PE	O32-C31-O31-C3
8	C	302	3PE	C32-C31-O31-C3
9	A	1008	LMG	C2-C1-O1-C7
9	A	1008	LMG	O6-C1-O1-C7
9	A	1009	LMG	C2-C1-O1-C7
9	A	1009	LMG	O6-C1-O1-C7
9	A	1009	LMG	C11-C10-O7-C8
10	A	1011	UQ8	C19-C21-C22-C23
9	A	1009	LMG	O9-C10-O7-C8
10	A	1011	UQ8	C30-C29-C31-C32
10	A	1011	UQ8	C28-C29-C31-C32
10	A	1011	UQ8	C14-C16-C17-C18
10	A	1011	UQ8	C34-C36-C37-C38
9	A	1008	LMG	C11-C10-O7-C8
9	A	1010	LMG	O6-C5-C6-O5
9	A	1009	LMG	C29-C28-O8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	1009	LMG	C28-C29-C30-C31
8	C	301	3PE	C21-C22-C23-C24
5	A	1001	HEM	C3D-CAD-CBD-CGD
10	A	1011	UQ8	C29-C31-C32-C33
9	A	1010	LMG	C29-C28-O8-C9
9	A	1008	LMG	C17-C18-C19-C20
8	C	302	3PE	C2-C1-O11-P
9	A	1008	LMG	C30-C31-C32-C33
5	A	1001	HEM	C2A-CAA-CBA-CGA
9	A	1009	LMG	C4-C5-C6-O5
9	A	1008	LMG	C18-C19-C20-C21
9	A	1008	LMG	C33-C34-C35-C36
9	A	1009	LMG	C29-C30-C31-C32
8	A	1004	3PE	C31-C32-C33-C34
6	A	1002	HEO	C15-C16-C17-C18
9	A	1008	LMG	C16-C17-C18-C19
9	A	1008	LMG	O9-C10-O7-C8
6	A	1002	HEO	C2A-CAA-CBA-CGA
9	A	1009	LMG	C33-C34-C35-C36
9	A	1010	LMG	C11-C10-O7-C8
9	A	1009	LMG	O1-C7-C8-O7
9	A	1010	LMG	C4-C5-C6-O5
8	A	1004	3PE	C29-C2A-C2B-C2C
9	A	1008	LMG	C32-C33-C34-C35
9	A	1008	LMG	C13-C14-C15-C16
9	A	1009	LMG	C11-C12-C13-C14
9	A	1010	LMG	O10-C28-O8-C9
9	A	1010	LMG	C11-C12-C13-C14
8	C	301	3PE	C1-C2-C3-O31
9	A	1009	LMG	O1-C7-C8-C9
9	A	1009	LMG	C7-C8-C9-O8
9	A	1010	LMG	O1-C7-C8-C9
9	A	1010	LMG	C7-C8-C9-O8
9	A	1008	LMG	C8-C7-O1-C1
9	A	1009	LMG	O10-C28-O8-C9
9	A	1009	LMG	C34-C35-C36-C37
8	A	1004	3PE	C35-C36-C37-C38
9	A	1008	LMG	C36-C37-C38-C39
8	C	301	3PE	C3B-C3C-C3D-C3E
9	A	1009	LMG	C8-C9-O8-C28
9	A	1008	LMG	C19-C20-C21-C22
9	A	1009	LMG	C38-C39-C40-C41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	1010	LMG	C30-C31-C32-C33
9	A	1010	LMG	O9-C10-O7-C8
8	A	1005	3PE	C22-C23-C24-C25
9	A	1008	LMG	O1-C7-C8-C9
10	A	1011	UQ8	C20-C19-C21-C22
8	A	1007	3PE	C3B-C3C-C3D-C3E
9	A	1008	LMG	O1-C7-C8-O7
10	A	1011	UQ8	C18-C19-C21-C22
9	A	1010	LMG	C16-C17-C18-C19
9	A	1009	LMG	C30-C31-C32-C33
8	A	1005	3PE	O11-C1-C2-C3
8	C	301	3PE	O11-C1-C2-C3
8	A	1004	3PE	C26-C27-C28-C29
8	C	301	3PE	O11-C1-C2-O21
9	A	1010	LMG	O1-C7-C8-O7
9	A	1010	LMG	O7-C8-C9-O8
10	A	1011	UQ8	C35-C34-C36-C37
8	C	301	3PE	C11-O13-P-O11
6	A	1002	HEO	O11-C11-C12-C13
8	A	1006	3PE	C12-C11-O13-P
9	A	1010	LMG	C14-C15-C16-C17
9	A	1009	LMG	O7-C8-C9-O8
9	A	1010	LMG	C17-C18-C19-C20
8	A	1006	3PE	C2-C1-O11-P
8	A	1005	3PE	O11-C1-C2-O21
9	A	1009	LMG	O8-C28-C29-C30
8	A	1006	3PE	C11-O13-P-O11
8	A	1007	3PE	C11-O13-P-O11
8	C	302	3PE	C11-O13-P-O11
5	A	1001	HEM	CAA-CBA-CGA-O1A
9	A	1009	LMG	O10-C28-C29-C30
5	A	1001	HEM	CAD-CBD-CGD-O1D
9	A	1009	LMG	C35-C36-C37-C38
9	A	1009	LMG	C37-C38-C39-C40
8	A	1007	3PE	C38-C39-C3A-C3B
5	A	1001	HEM	CAA-CBA-CGA-O2A
10	A	1011	UQ8	C5-C4-O4-C4M
5	A	1001	HEM	CAD-CBD-CGD-O2D
8	C	301	3PE	C32-C33-C34-C35
6	A	1002	HEO	CAD-CBD-CGD-O2D
9	A	1008	LMG	C15-C16-C17-C18
10	A	1011	UQ8	C33-C34-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	1008	LMG	C12-C13-C14-C15
6	A	1002	HEO	CAD-CBD-CGD-O1D
5	A	1001	HEM	C4C-C3C-CAC-CBC
8	C	301	3PE	C25-C26-C27-C28
9	A	1010	LMG	O8-C28-C29-C30
9	A	1008	LMG	O7-C10-C11-C12
6	A	1002	HEO	C4D-C3D-CAD-CBD
8	C	302	3PE	C24-C25-C26-C27
9	A	1009	LMG	C31-C32-C33-C34
9	A	1008	LMG	O9-C10-C11-C12
9	A	1009	LMG	O6-C5-C6-O5
8	A	1006	3PE	C11-O13-P-O14
8	A	1007	3PE	C11-O13-P-O14
8	C	302	3PE	C21-C22-C23-C24
6	A	1002	HEO	C3B-C11-C12-C13
8	A	1004	3PE	C12-C11-O13-P
9	A	1010	LMG	O10-C28-C29-C30
8	C	302	3PE	C23-C24-C25-C26
10	A	1011	UQ8	C13-C14-C16-C17
8	C	301	3PE	O21-C21-C22-C23
8	A	1006	3PE	O21-C21-C22-C23

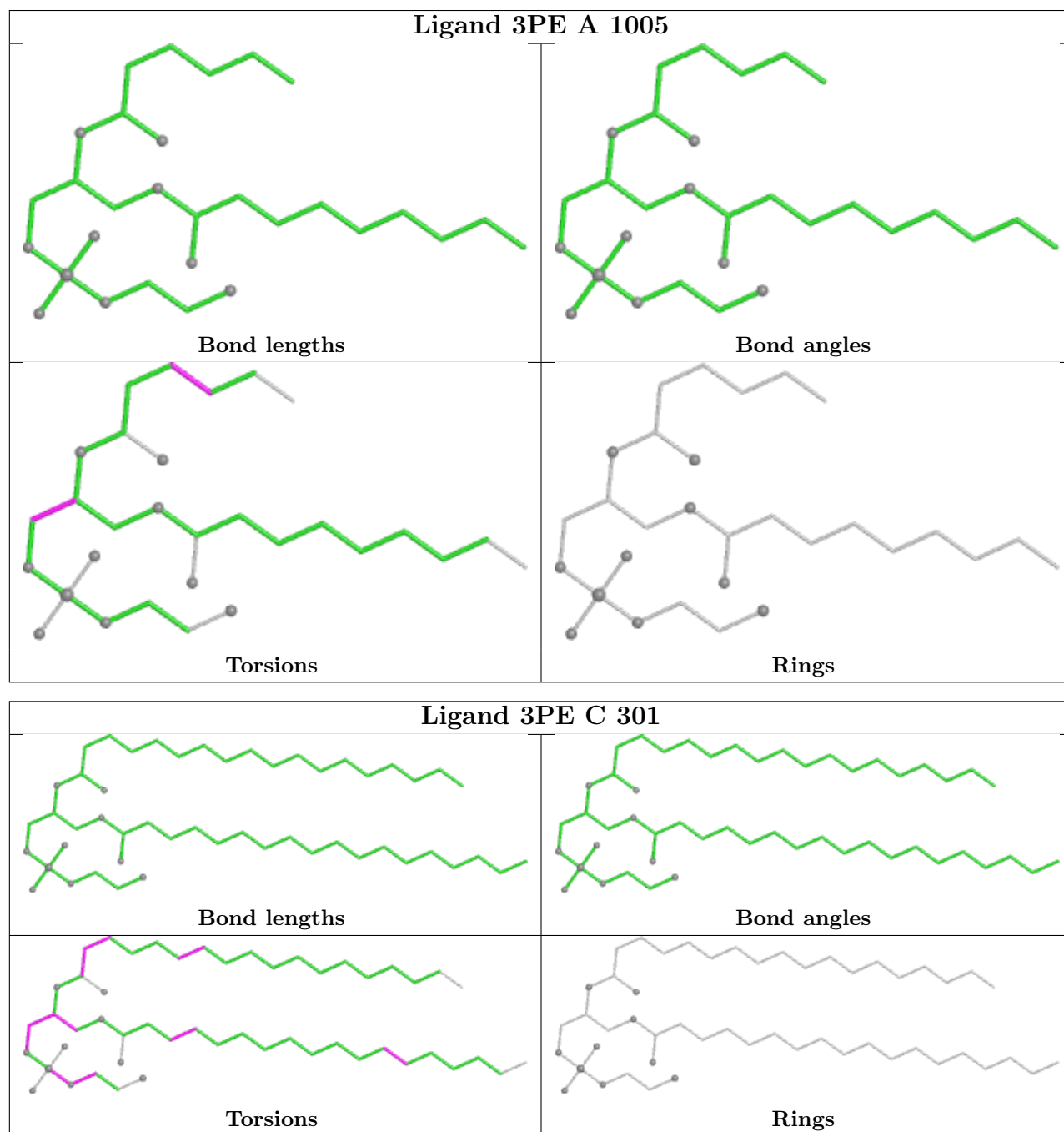
There are no ring outliers.

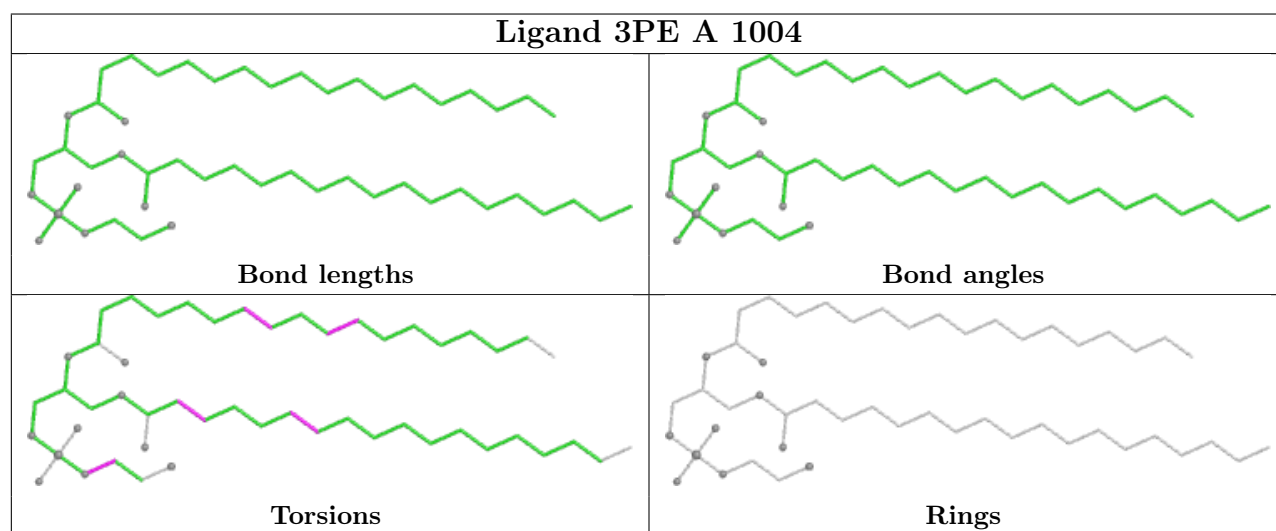
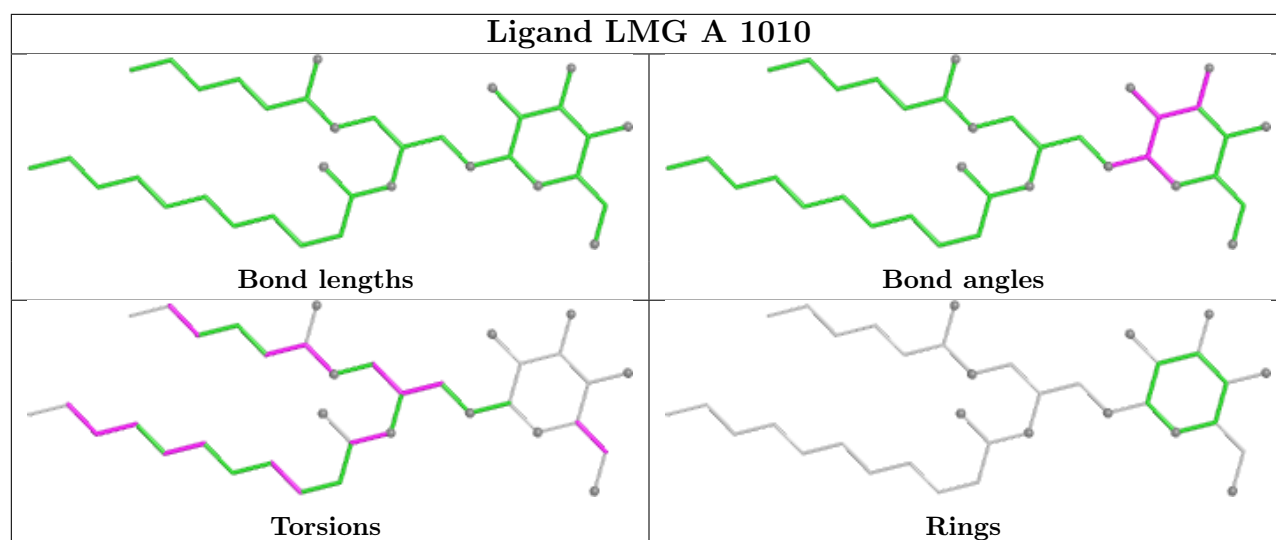
12 monomers are involved in 65 short contacts:

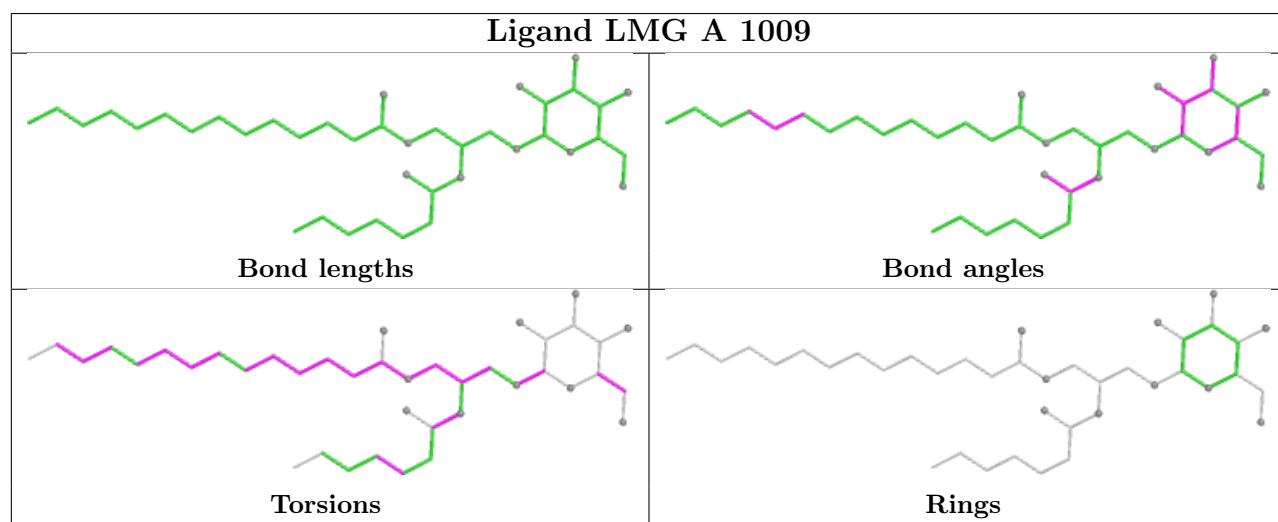
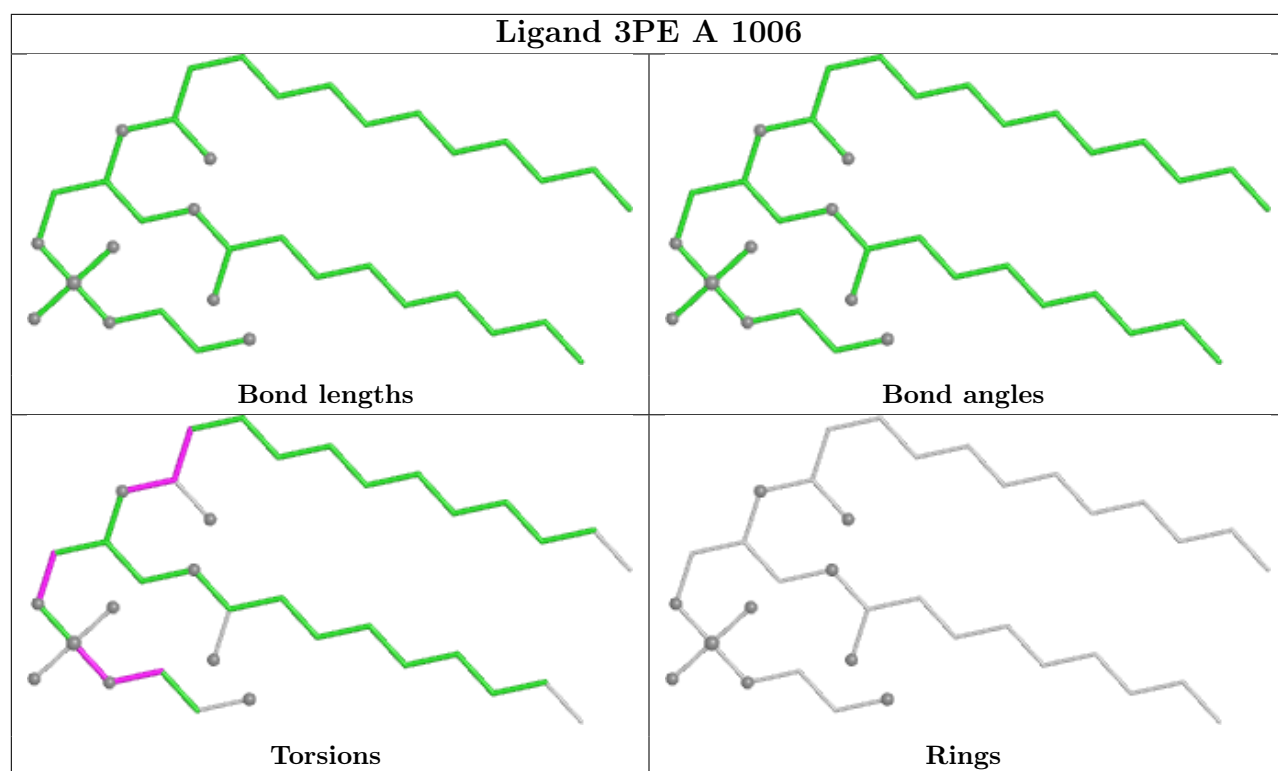
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1005	3PE	2	0
8	C	301	3PE	5	0
9	A	1010	LMG	3	0
8	A	1004	3PE	8	0
8	A	1006	3PE	1	0
9	A	1009	LMG	8	0
10	A	1011	UQ8	14	0
6	A	1002	HEO	12	0
9	A	1008	LMG	4	0
8	C	302	3PE	3	0
8	A	1007	3PE	6	0
5	A	1001	HEM	5	0

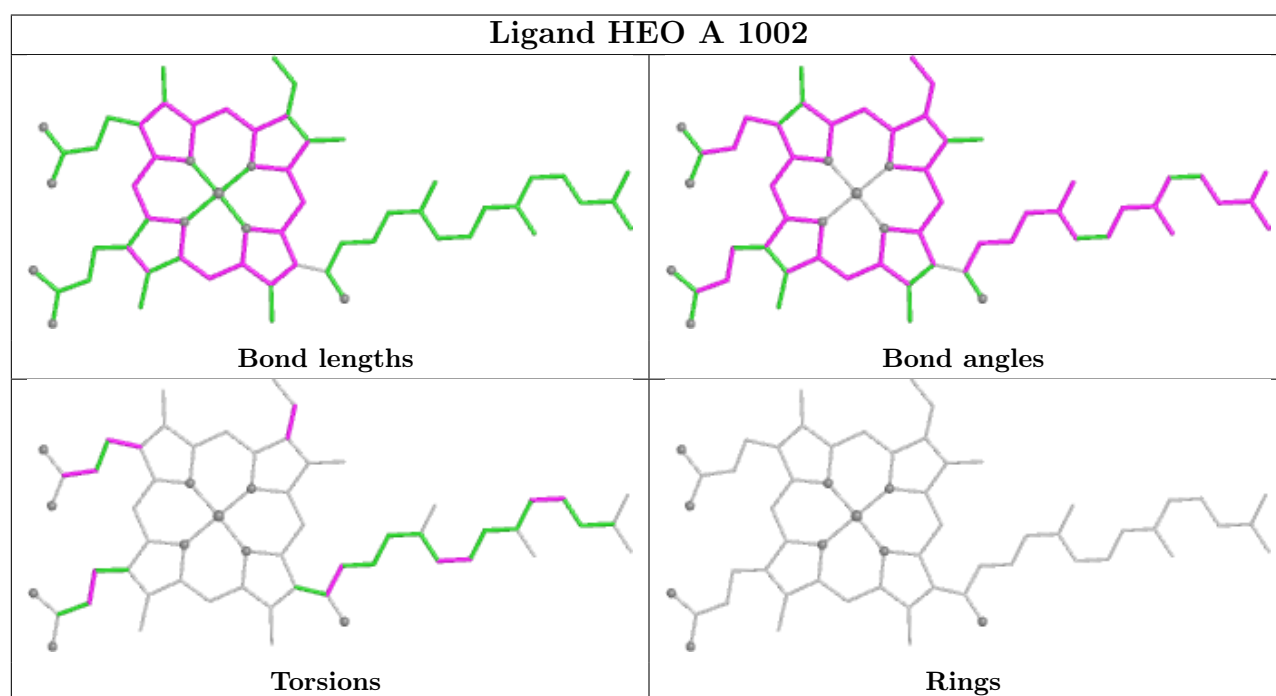
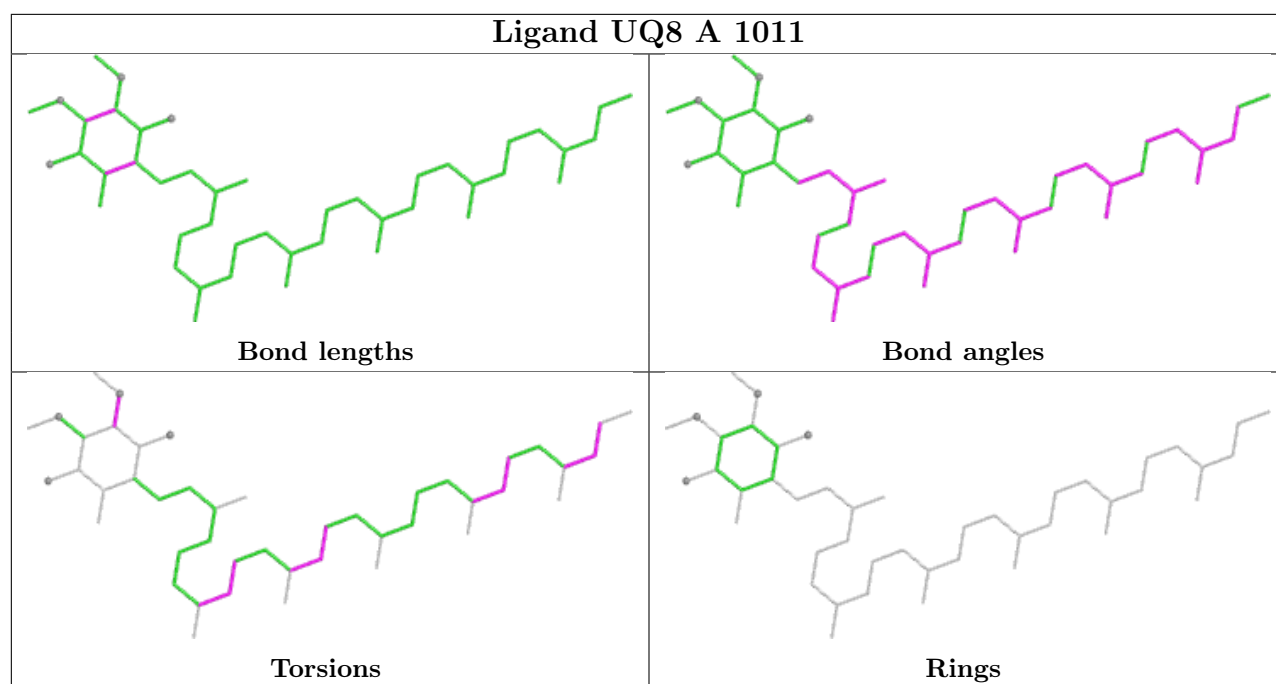
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

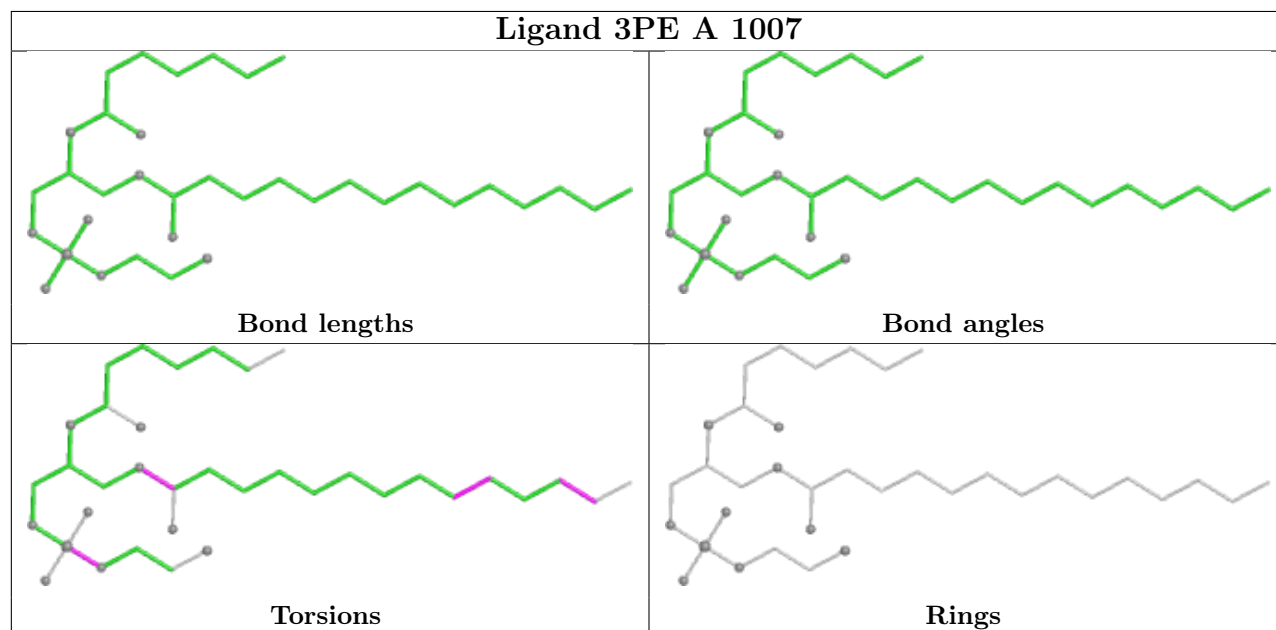
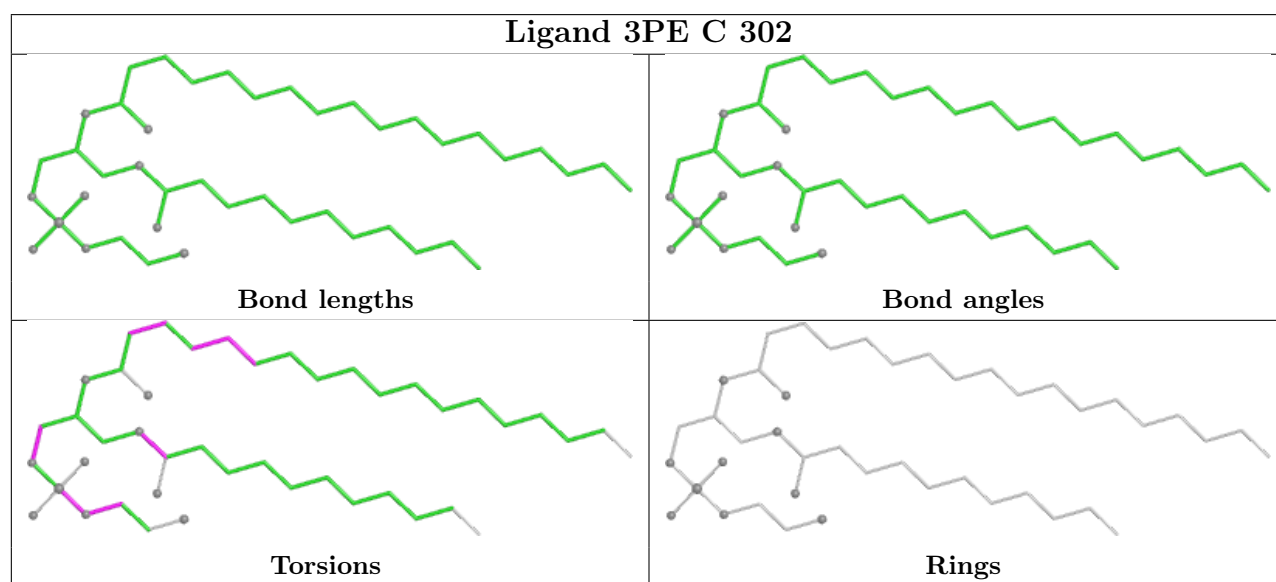
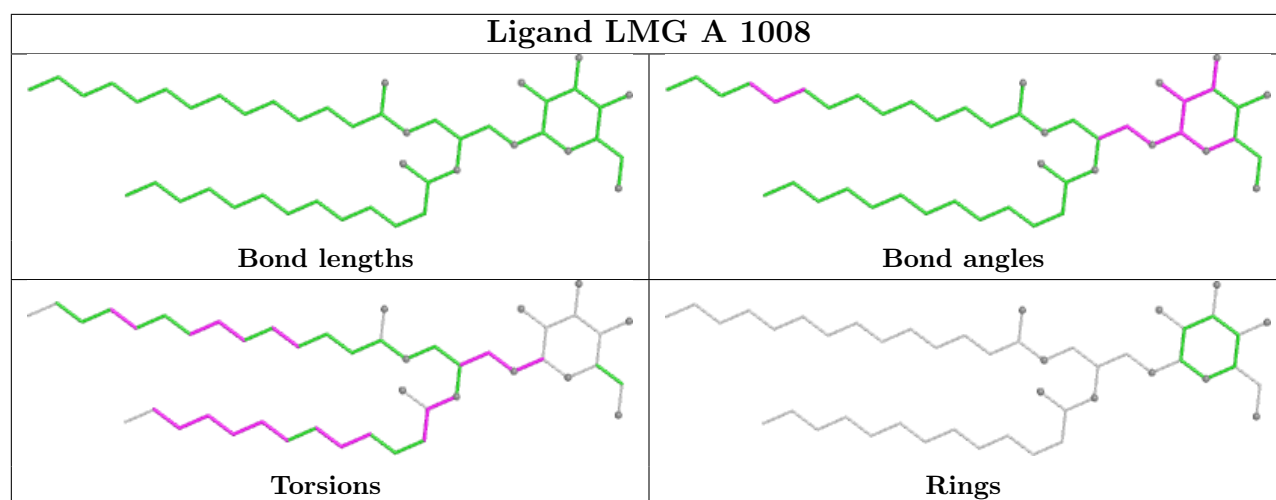
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

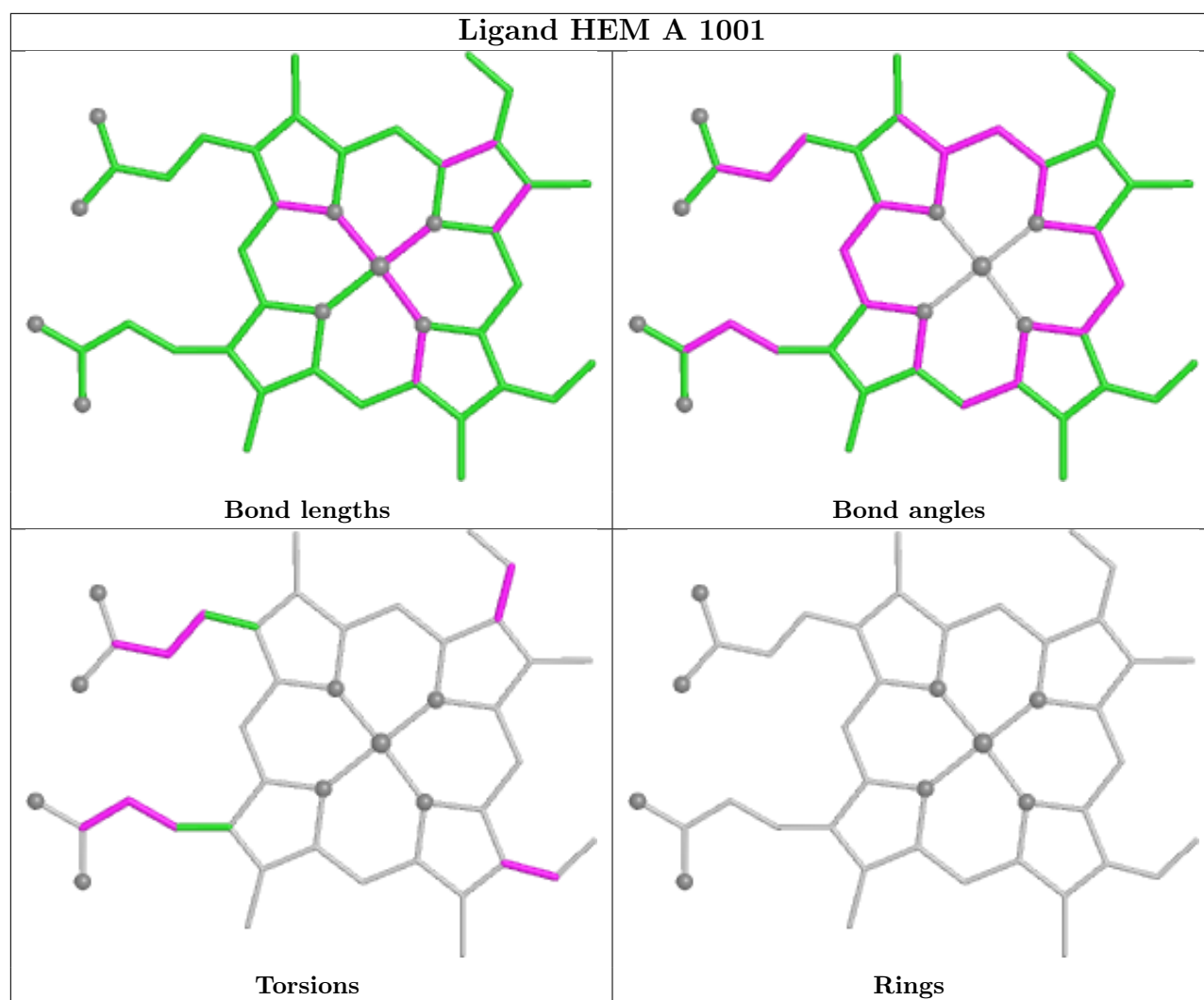












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

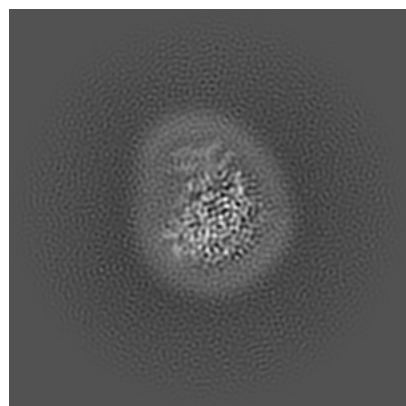
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64127. These allow visual inspection of the internal detail of the map and identification of artifacts.

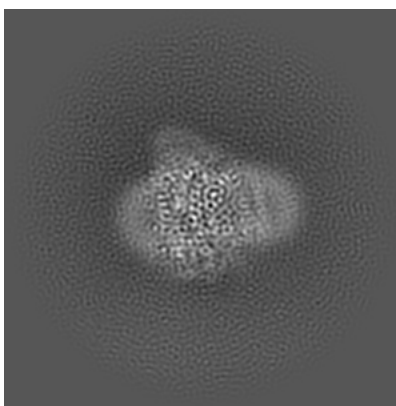
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

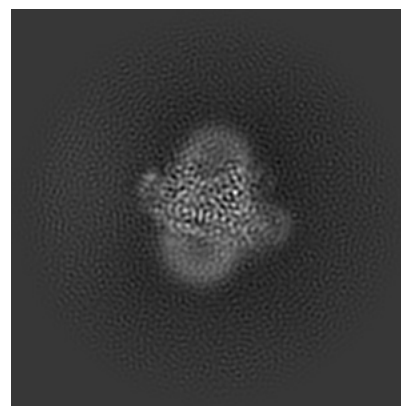
6.1.1 Primary map



X

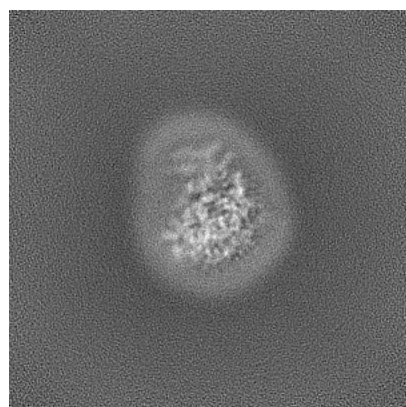


Y

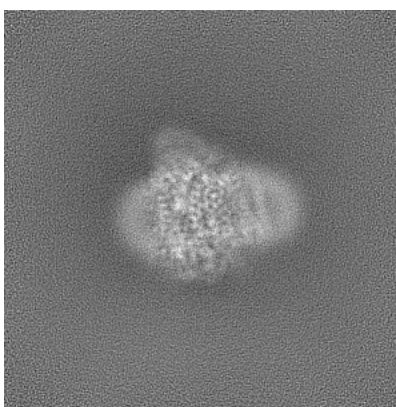


Z

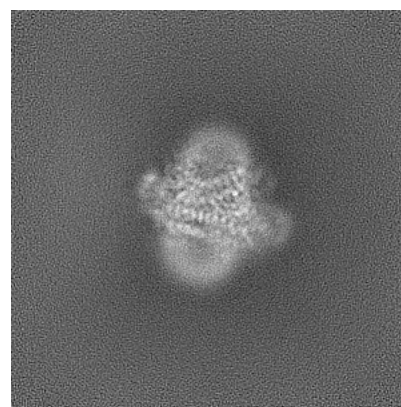
6.1.2 Raw map



X



Y

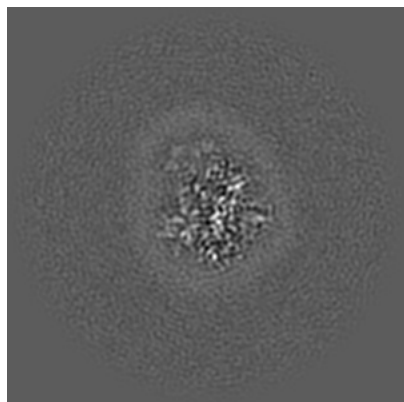


Z

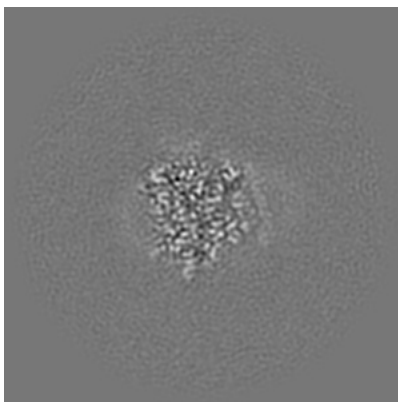
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

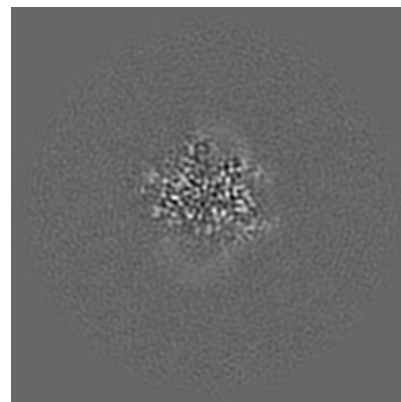
6.2.1 Primary map



X Index: 150

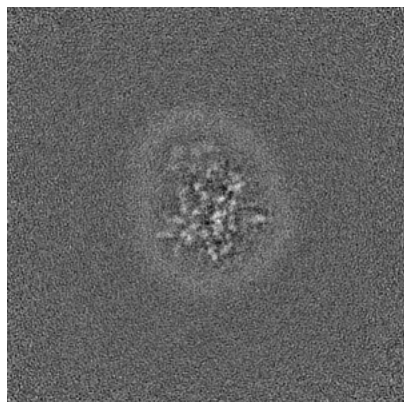


Y Index: 150

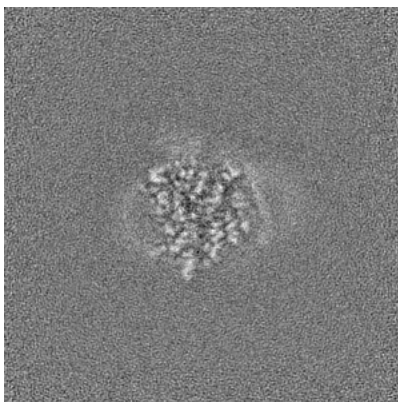


Z Index: 150

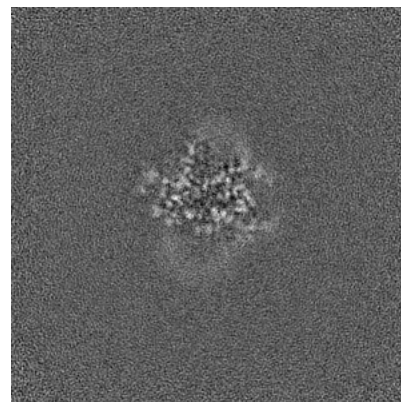
6.2.2 Raw map



X Index: 150



Y Index: 150

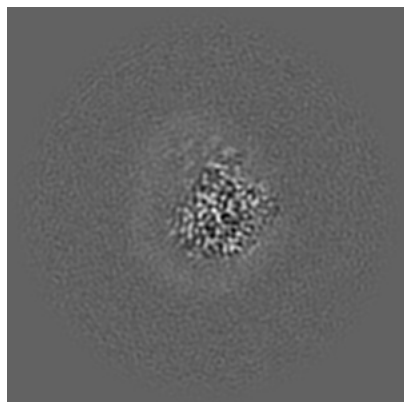


Z Index: 150

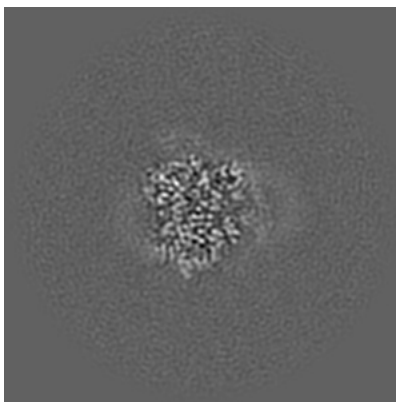
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

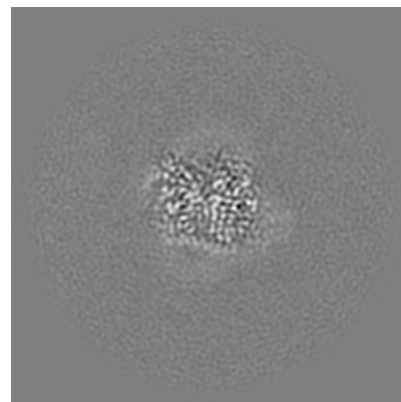
6.3.1 Primary map



X Index: 132

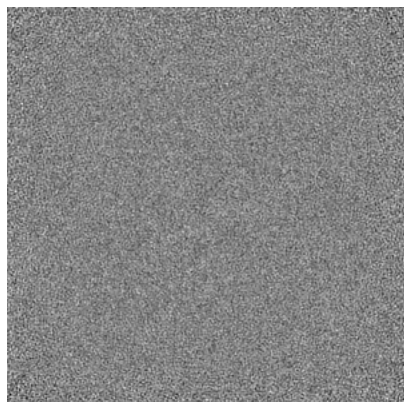


Y Index: 148

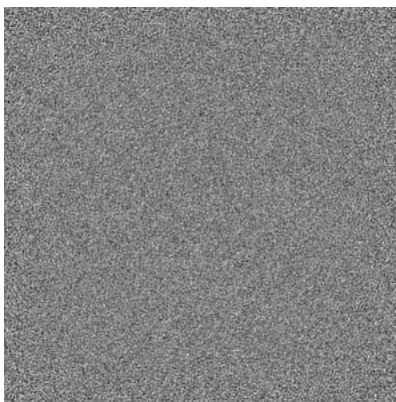


Z Index: 130

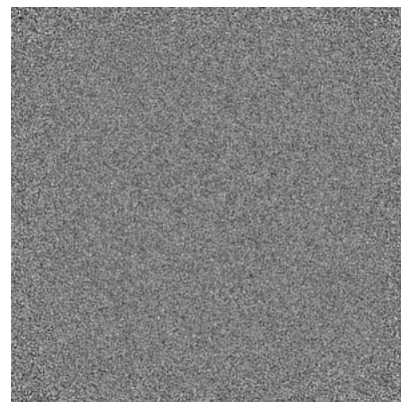
6.3.2 Raw map



X Index: 0



Y Index: 0

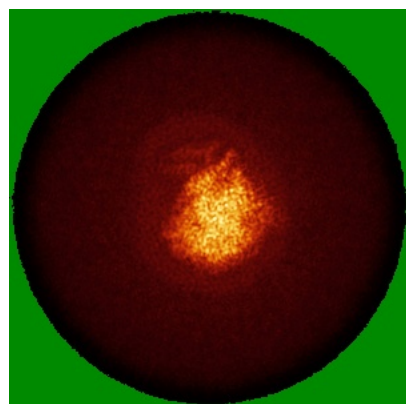


Z Index: 0

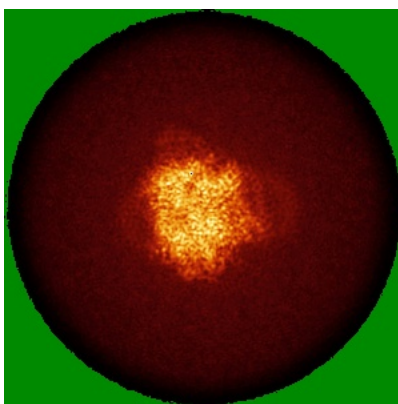
The images above show the largest variance slices of the map in three orthogonal directions.

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

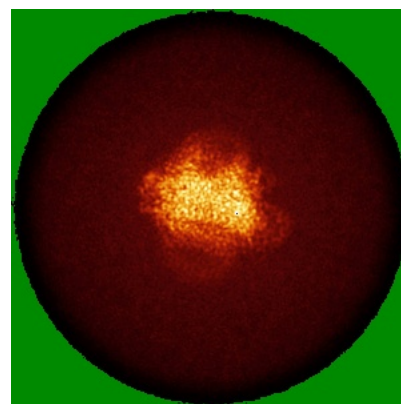
6.4.1 Primary map



X

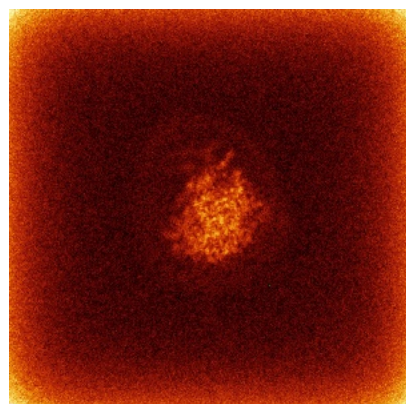


Y

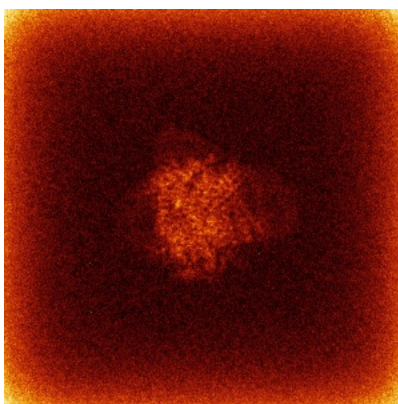


Z

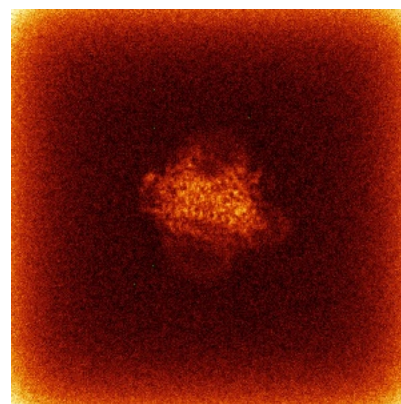
6.4.2 Raw map



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.

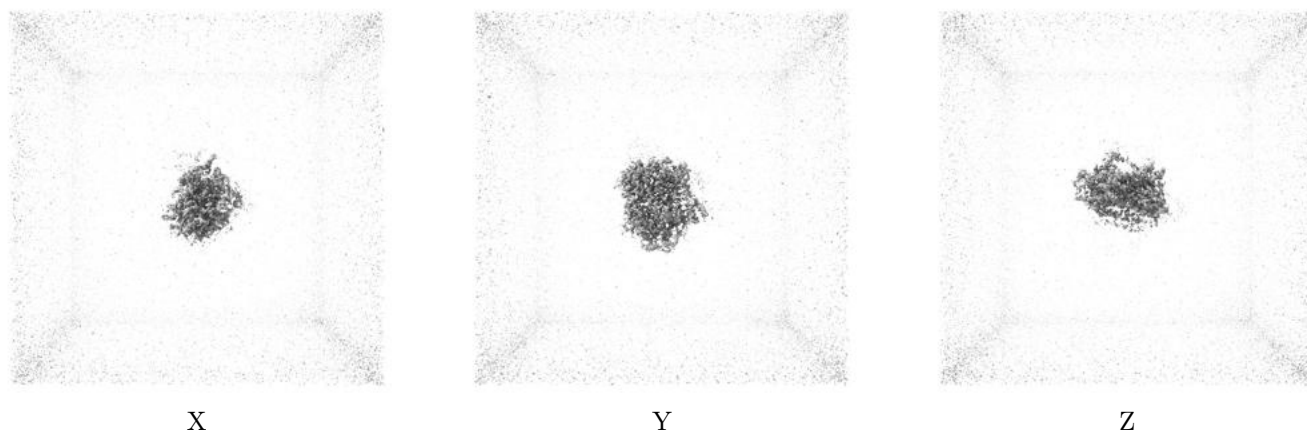
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

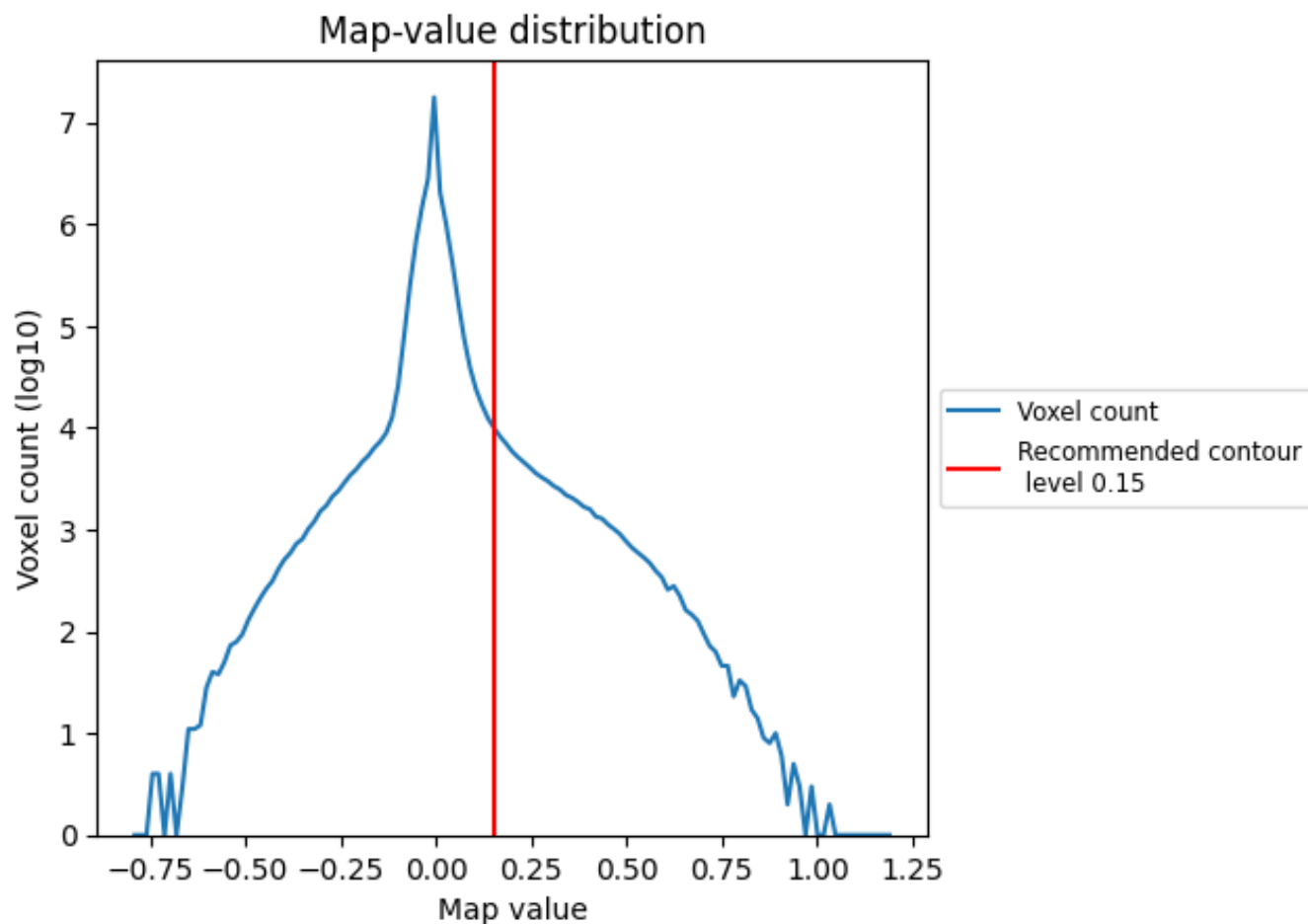
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

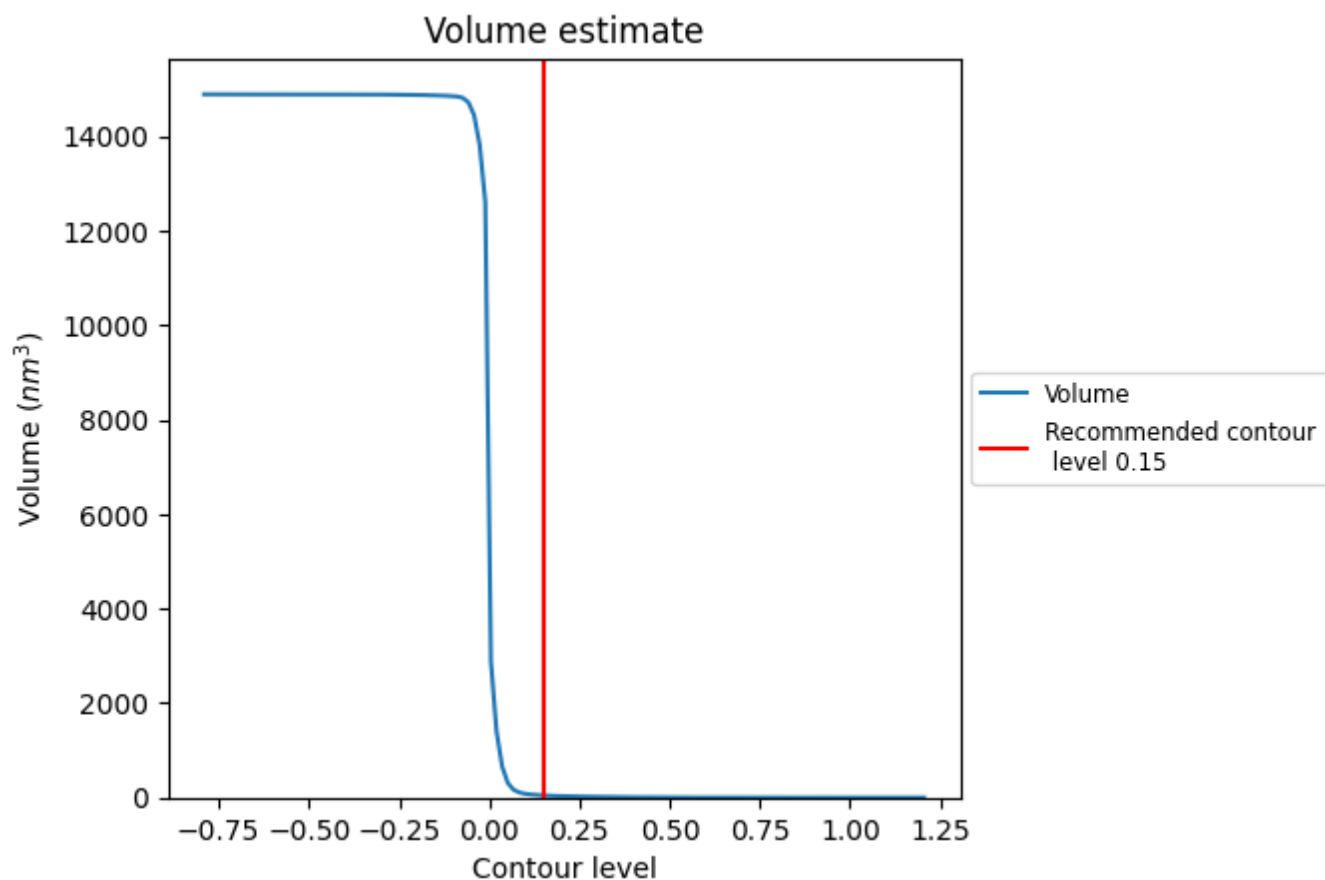
This section contains the results of statistical analysis of the map.

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.

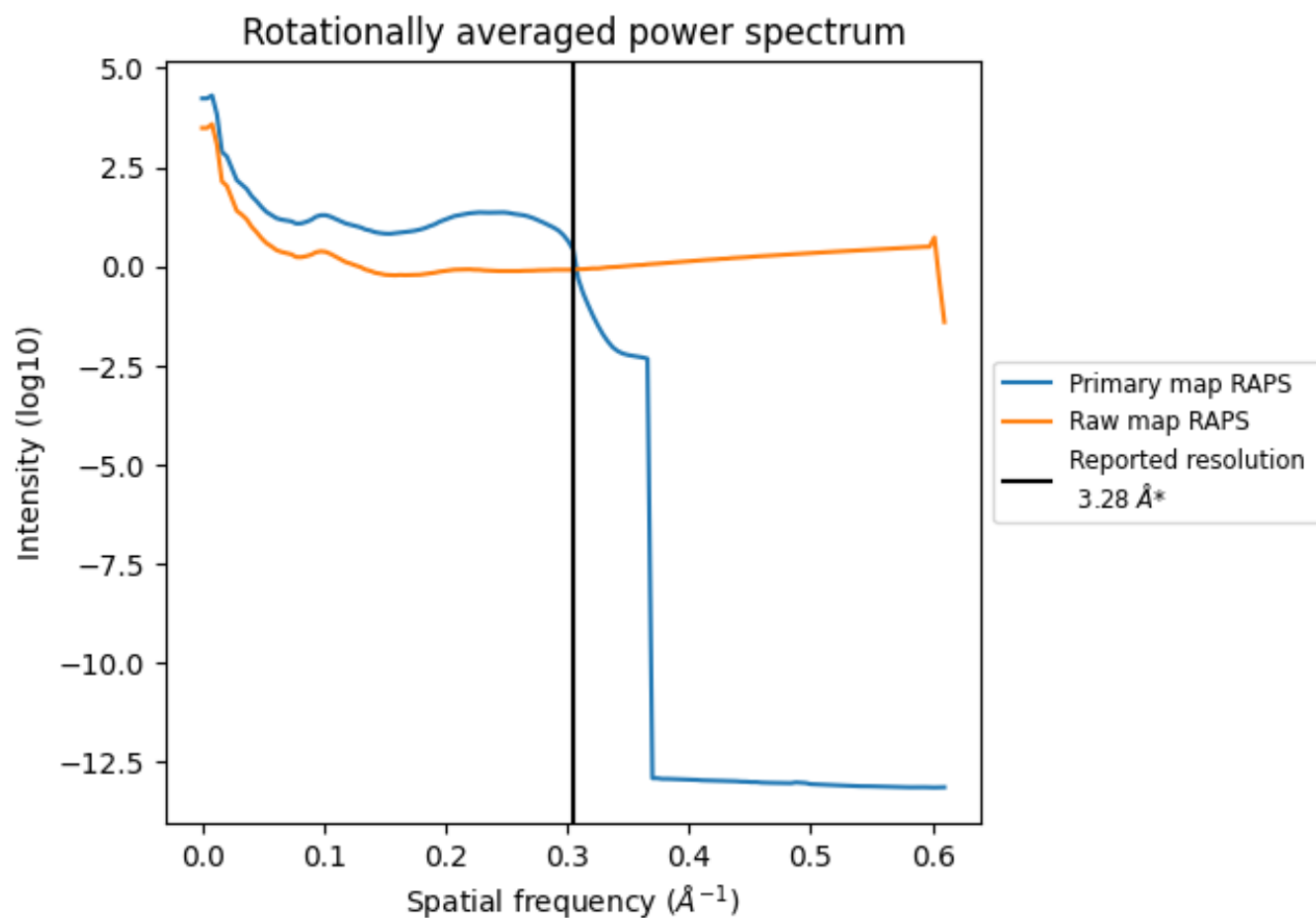
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 45 nm³; this corresponds to an approximate mass of 41 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 ⓘ

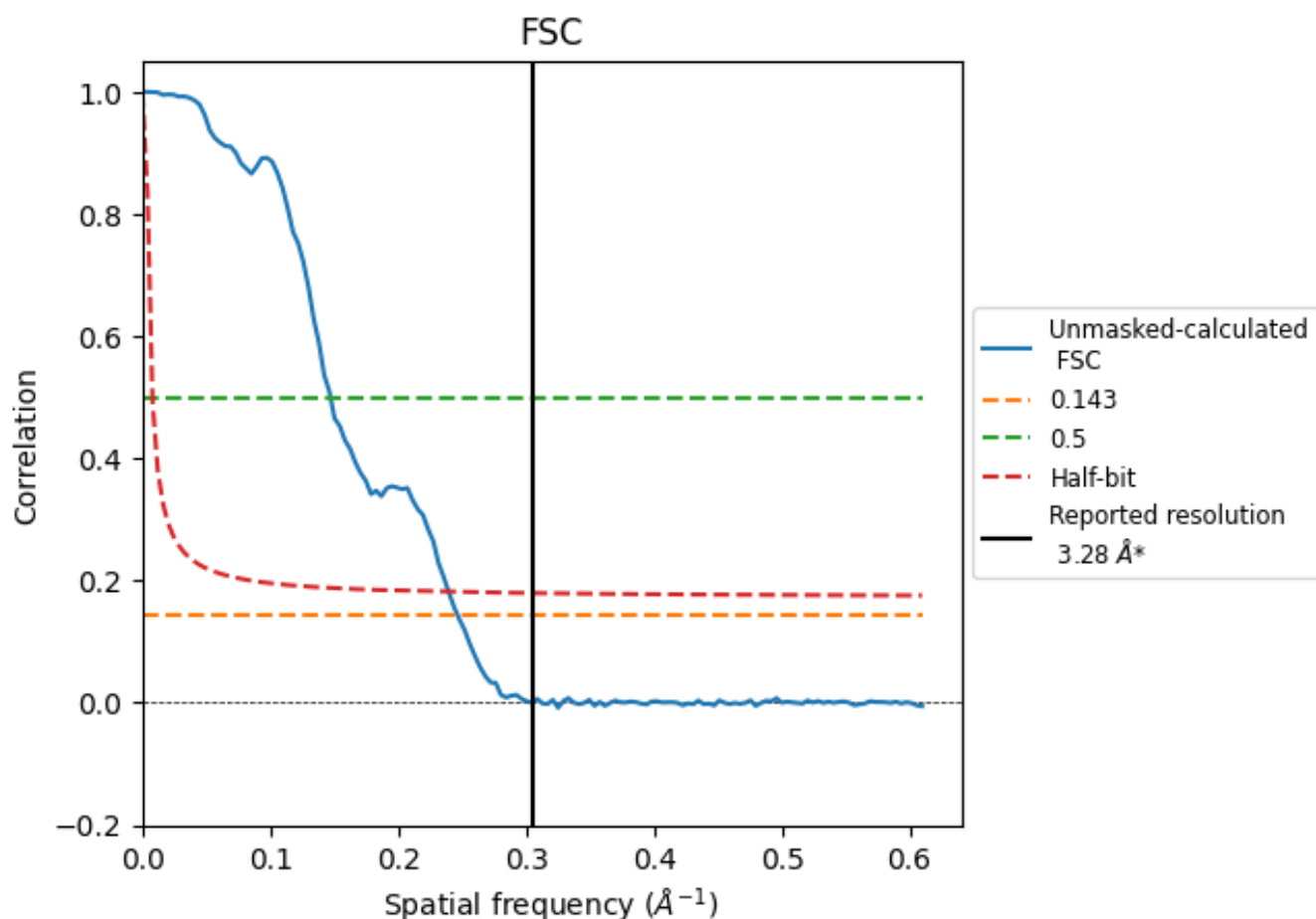


*Reported resolution corresponds to spatial frequency of 0.305 Å⁻¹

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 0.305 Å⁻¹

8.2 Resolution estimates [i](#)

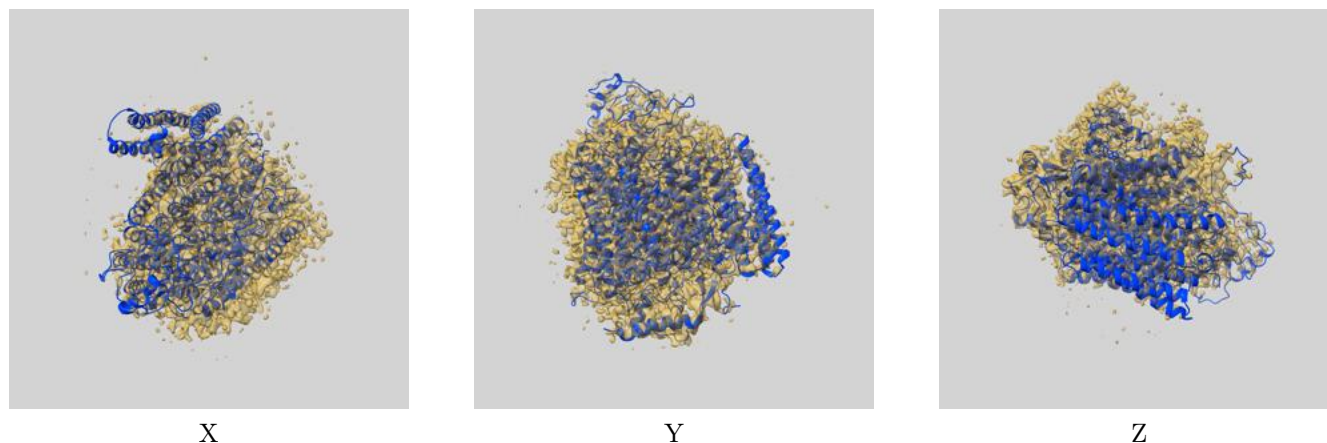
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.06	6.79	4.17

*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 4.06 differs from the reported value 3.28 by more than 10 %

9 Map-model fit [i](#)

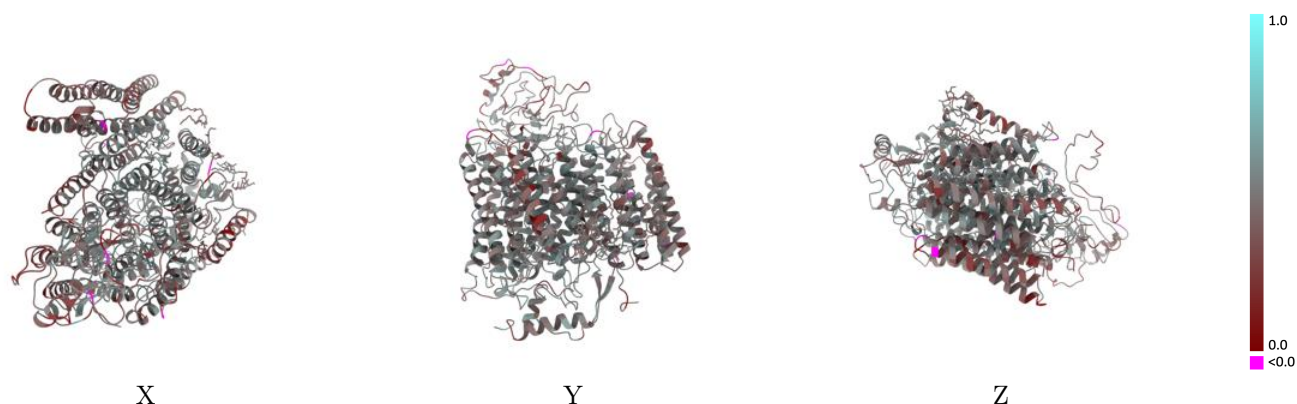
This section contains information regarding the fit between EMDB map EMD-64127 and PDB model 9UFZ. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



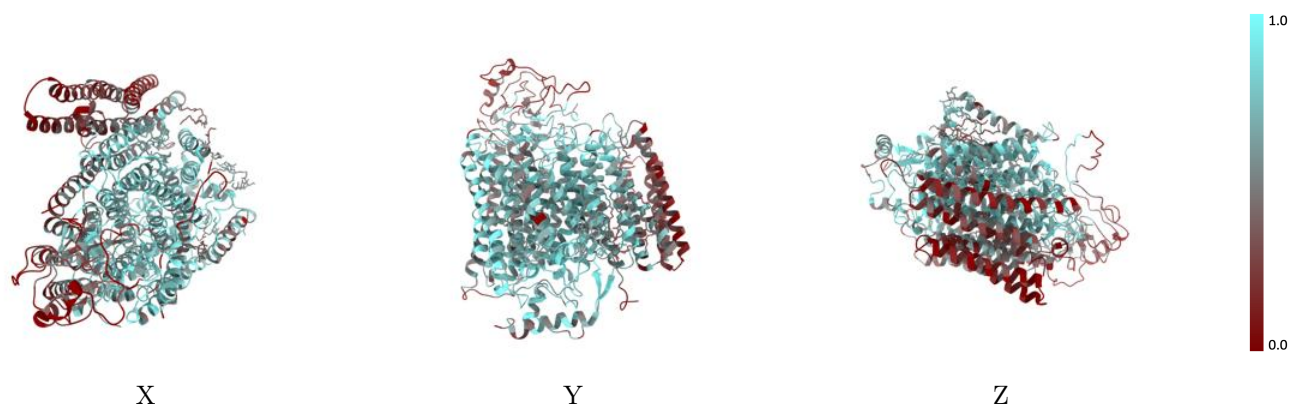
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



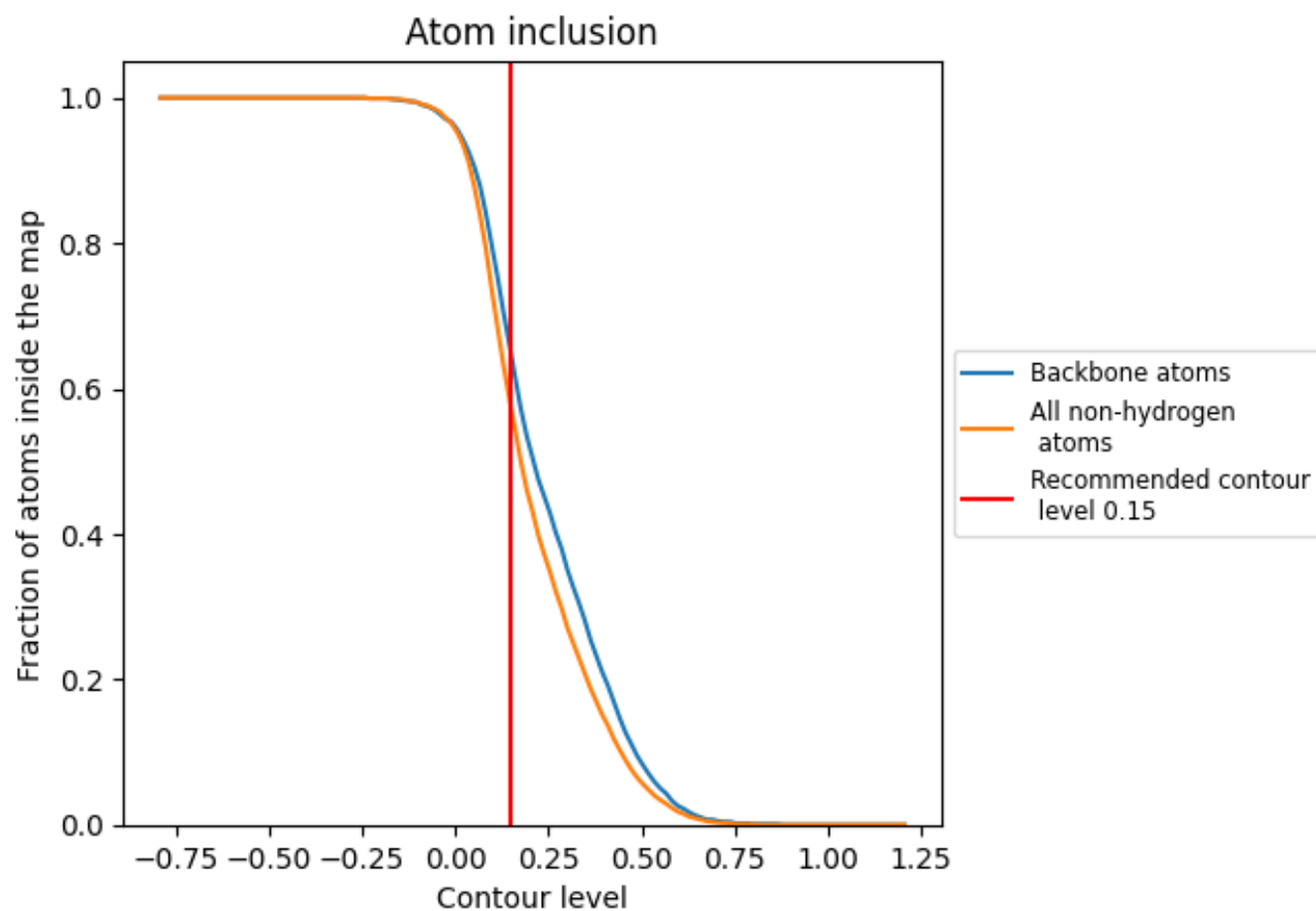
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 57% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5720	0.4360
A	0.7270	0.4690
B	0.4060	0.3940
C	0.4270	0.4170
D	0.2080	0.3490

