



## Full wwPDB EM Validation Report ⓘ

Dec 22, 2022 – 03:18 am GMT

PDB ID : 7OY2  
EMDB ID : EMD-13108  
Title : High resolution structure of cytochrome bd-II oxidase from E. coli  
Authors : Grund, T.N.; Wu, D.; Bald, D.; Michel, H.; Safarian, S.  
Deposited on : 2021-06-23  
Resolution : 2.06 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

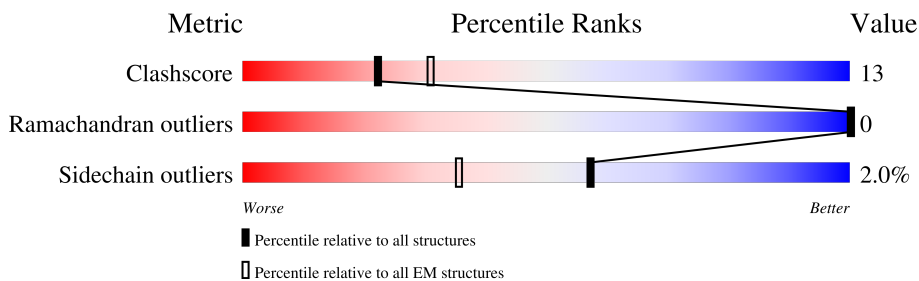
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.06 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	B	378	
2	C	514	
3	X	61	

## 2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 7166 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 bd-II ubiquinol oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	376	2980	2006	473	481	20	0	0

- Molecule 2 is a protein called Cytochrome bd-II ubiquinol oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	454	3620	2392	591	611	26	0	0

- Molecule 3 is a protein called Putative cytochrome bd-II ubiquinol oxidase subunit AppX.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	X	28	237	166	34	34	3	0	0

There are 31 discrepancies between the modelled and reference sequences:

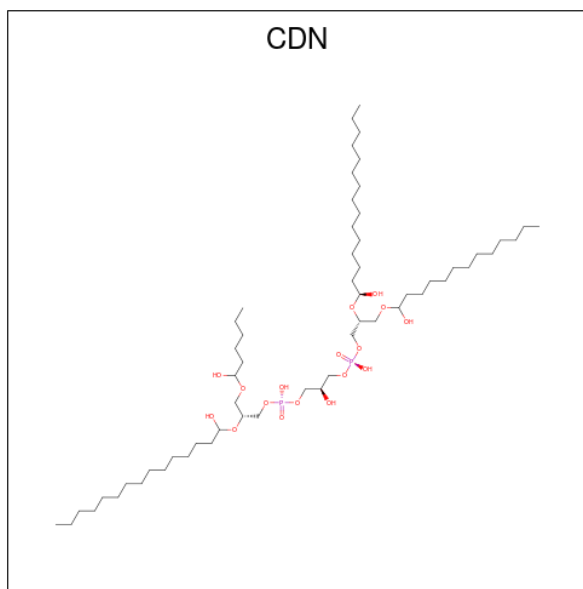
Chain	Residue	Modelled	Actual	Comment	Reference
X	31	ILE	-	expression tag	UNP P24244
X	32	GLU	-	expression tag	UNP P24244
X	33	GLY	-	expression tag	UNP P24244
X	34	ARG	-	expression tag	UNP P24244
X	35	GLY	-	expression tag	UNP P24244
X	36	THR	-	expression tag	UNP P24244
X	37	SER	-	expression tag	UNP P24244
X	38	GLY	-	expression tag	UNP P24244
X	39	SER	-	expression tag	UNP P24244
X	40	SER	-	expression tag	UNP P24244
X	41	GLY	-	expression tag	UNP P24244
X	42	SER	-	expression tag	UNP P24244
X	43	GLY	-	expression tag	UNP P24244
X	44	SER	-	expression tag	UNP P24244
X	45	GLY	-	expression tag	UNP P24244

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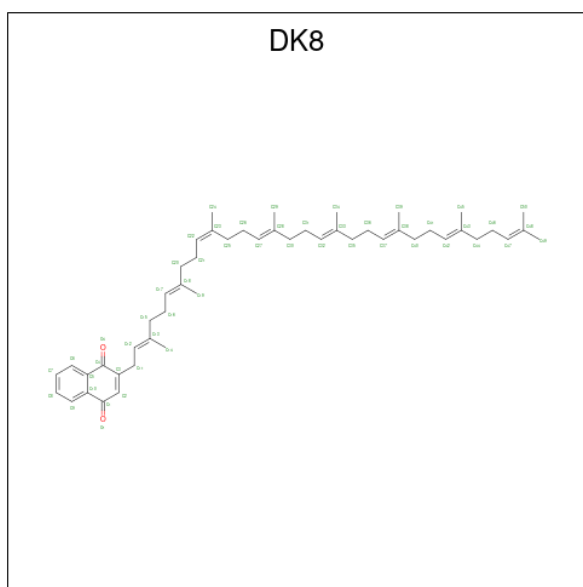
Chain	Residue	Modelled	Actual	Comment	Reference
X	46	GLY	-	expression tag	UNP P24244
X	47	SER	-	expression tag	UNP P24244
X	48	GLY	-	expression tag	UNP P24244
X	49	SER	-	expression tag	UNP P24244
X	50	GLY	-	expression tag	UNP P24244
X	51	GLY	-	expression tag	UNP P24244
X	52	GLY	-	expression tag	UNP P24244
X	53	GLY	-	expression tag	UNP P24244
X	54	TRP	-	expression tag	UNP P24244
X	55	SER	-	expression tag	UNP P24244
X	56	HIS	-	expression tag	UNP P24244
X	57	PRO	-	expression tag	UNP P24244
X	58	GLN	-	expression tag	UNP P24244
X	59	PHE	-	expression tag	UNP P24244
X	60	GLU	-	expression tag	UNP P24244
X	61	LYS	-	expression tag	UNP P24244

- Molecule 4 is CARDIOLIPIN (three-letter code: CDN) (formula:  $C_{58}H_{120}O_{17}P_2$ ) (labeled as "Ligand of Interest" by depositor).



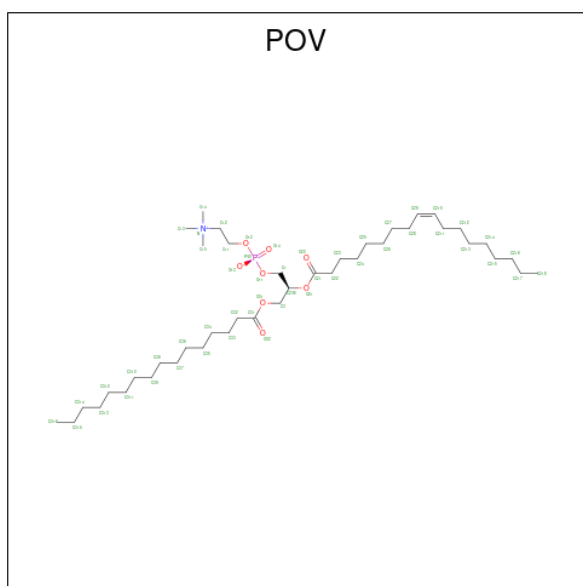
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
4	B	1	69	50	17	2	0

- Molecule 5 is 2-[(2 {E},6 {E},10 {Z},14 {E},18 {E},22 {E},26 {E})-3,7,11,15,19,23,27,31-octamethyldotriaconta-2,6,10,14,18,22,26,30-octaenyl]naphthalene-1,4-dione (three-letter code: DK8) (formula:  $C_{50}H_{70}O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
5	B	1	52	50	2	0

- Molecule 6 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (three-letter code: POV) (formula:  $C_{42}H_{82}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



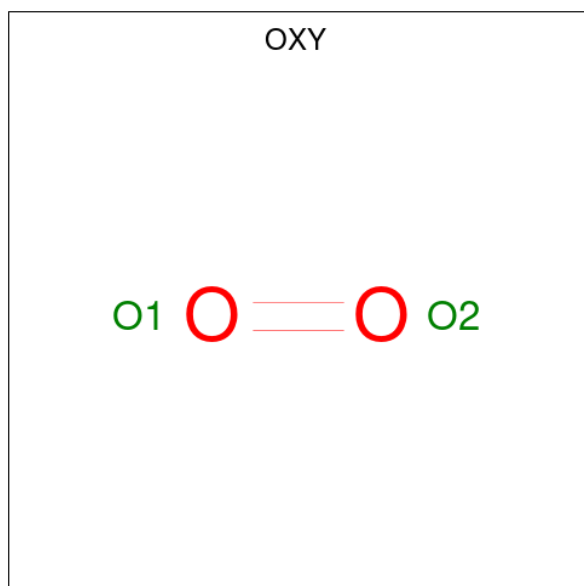
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	C	1	52	42	1	8	1	0

- Molecule 7 is HEME B/C (three-letter code: HEB) (formula:  $C_{34}H_{34}FeN_4O_4$ ) (labeled as



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
8	C	1	44	34	1	4	5	0

- Molecule 9 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



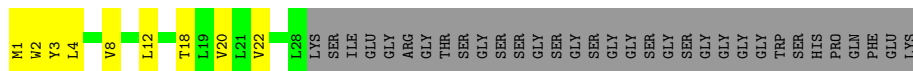
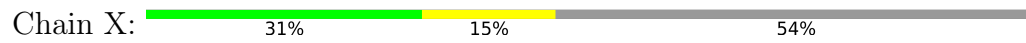
Mol	Chain	Residues	Atoms		AltConf
9	C	1	Total	O	0
			2	2	

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		AltConf
10	B	10	Total	O	0
			10	10	
10	C	14	Total	O	0
			14	14	







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	533309	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 ( $e^-/\text{\AA}^2$ )	108	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.166	Depositor
Minimum map value	-0.062	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	214.272, 214.272, 214.272	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEB, OXY, HDD, DK8, CDN, POV

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	B	0.31	0/3073	0.47	0/4197
2	C	0.34	0/3723	0.48	1/5060 (0.0%)
3	X	0.29	0/245	0.43	0/336
All	All	0.33	0/7041	0.47	1/9593 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	445	GLU	CB-CA-C	5.72	121.85	110.40

There are no chirality outliers.

There are no planarity outliers.

### 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	B	2980	0	3066	64	0
2	C	3620	0	3630	111	0
3	X	237	0	254	7	0
4	B	69	0	96	3	0
5	B	52	0	0	0	0
6	C	52	0	82	3	0
7	C	86	0	64	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	44	0	31	8	0
9	C	2	0	0	1	0
10	B	10	0	0	0	0
10	C	14	0	0	1	0
All	All	7166	0	7223	182	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 13.

All (182) 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:C:185:VAL:CG1	2:C:237:LEU:HD21	1.49	1.39
2:C:185:VAL:HG12	2:C:237:LEU:CD2	1.51	1.36
2:C:185:VAL:CG1	2:C:237:LEU:CD2	2.05	1.32
2:C:185:VAL:HG11	2:C:237:LEU:HD21	1.26	1.10
2:C:185:VAL:HG12	2:C:237:LEU:HD22	1.27	1.08
2:C:185:VAL:HB	2:C:237:LEU:HD23	1.48	0.95
2:C:185:VAL:CB	2:C:237:LEU:CD2	2.48	0.90
2:C:185:VAL:CB	2:C:237:LEU:HD23	2.04	0.87
2:C:253:LEU:O	2:C:257:GLU:HG2	1.74	0.87
2:C:84:TYR:HB2	2:C:462:ALA:HB1	1.58	0.86
2:C:246:ALA:HA	2:C:253:LEU:HD12	1.59	0.82
2:C:441:TRP:CE2	7:C:602:HEB:HAB2	2.15	0.81
2:C:99:GLU:OE1	2:C:144:ILE:HB	1.82	0.79
7:C:602:HEB:HBC1	7:C:602:HEB:HMC1	1.64	0.77
2:C:246:ALA:CA	2:C:253:LEU:HD12	2.15	0.76
2:C:449:GLN:NE2	7:C:602:HEB:O1D	2.14	0.75
2:C:441:TRP:HB3	7:C:602:HEB:HMB3	1.70	0.73
2:C:185:VAL:HB	2:C:237:LEU:CD2	2.13	0.73
1:B:202:LEU:HD21	1:B:206:ARG:HH11	1.53	0.73
2:C:250:PRO:HB2	2:C:310:LEU:HD22	1.73	0.71
1:B:142:LEU:HD13	1:B:222:LEU:HD11	1.73	0.70
1:B:190:LEU:HG	1:B:287:PRO:HB2	1.75	0.69
1:B:147:PHE:O	1:B:316:SER:OG	2.11	0.68
2:C:88:VAL:HG11	2:C:453:ILE:HG13	1.75	0.68
1:B:356:TRP:O	1:B:360:LYS:HG2	1.94	0.68
4:B:401:CDN:H332	4:B:401:CDN:H111	1.75	0.67
2:C:108:SER:O	10:C:701:HOH:O	2.12	0.67
2:C:181:GLN:HB3	3:X:2:TRP:HB2	1.76	0.66
1:B:32:ILE:HG12	1:B:188:LEU:HG	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:99:GLU:OE1	9:C:605:OXY:O1	2.15	0.65
1:B:30:MET:O	1:B:127:SER:HB3	1.97	0.64
2:C:430:LEU:HD23	6:C:601:POV:H28A	1.79	0.64
1:B:343:VAL:HA	2:C:101:LEU:HD21	1.79	0.64
2:C:448:ARG:HH22	7:C:602:HEB:C4D	2.11	0.64
1:B:281:ALA:HA	1:B:284:ARG:HE	1.62	0.62
2:C:160:ASP:HB2	2:C:167:GLU:HG3	1.81	0.62
8:C:604:HDD:HMC1	8:C:604:HDD:HBC1	1.81	0.61
2:C:110:PHE:HD1	2:C:113:LEU:HD12	1.66	0.60
1:B:294:ALA:O	1:B:298:GLN:HG2	2.01	0.60
1:B:167:PRO:HB2	1:B:221:TRP:HH2	1.65	0.60
2:C:323:MET:HB3	2:C:347:LEU:HD13	1.83	0.60
1:B:22:PHE:CE1	1:B:64:LEU:HB2	2.38	0.59
2:C:13:ALA:CB	7:C:602:HEB:HMA2	2.33	0.59
2:C:41:VAL:HG22	2:C:123:LYS:HG3	1.84	0.59
2:C:20:PHE:CD1	7:C:602:HEB:HBB1	2.38	0.58
2:C:235:LEU:HA	7:C:603:HEB:HBB3	1.84	0.58
2:C:108:SER:OG	8:C:604:HDD:O2A	2.20	0.58
2:C:311:MET:HG2	2:C:380:ILE:HG13	1.86	0.58
3:X:1:MET:HE1	3:X:3:TYR:HB2	1.86	0.57
1:B:102:LEU:HD21	2:C:65:LEU:HD13	1.86	0.57
1:B:281:ALA:HB2	1:B:284:ARG:HH11	1.70	0.57
2:C:146:ASN:HA	2:C:180:SER:HB3	1.87	0.56
2:C:254:ALA:HB1	2:C:259:GLU:OE1	2.05	0.56
1:B:342:ILE:HD13	2:C:98:MET:SD	2.45	0.56
1:B:96:SER:HB2	1:B:126:GLY:HA2	1.88	0.56
2:C:310:LEU:O	2:C:314:THR:HG23	2.06	0.56
2:C:23:VAL:HG22	8:C:604:HDD:HAD1	1.89	0.54
1:B:28:PHE:HB3	1:B:183:GLN:HG3	1.90	0.54
2:C:448:ARG:HH12	7:C:602:HEB:HBD2	1.72	0.53
1:B:110:ILE:HB	1:B:115:TRP:CD1	2.43	0.53
1:B:338:ILE:HD13	2:C:171:PHE:HB2	1.89	0.53
2:C:234:THR:HG21	7:C:603:HEB:HBC1	1.89	0.53
2:C:246:ALA:CB	2:C:253:LEU:HD12	2.38	0.53
2:C:387:PHE:O	2:C:391:ARG:HG2	2.07	0.53
2:C:205:TRP:CE2	6:C:601:POV:H33A	2.44	0.52
1:B:201:GLN:O	1:B:205:LYS:HG2	2.10	0.52
2:C:192:TYR:HB3	2:C:226:PHE:CE2	2.45	0.52
3:X:1:MET:HE3	3:X:4:LEU:H	1.75	0.52
2:C:315:TYR:CZ	2:C:319:GLN:NE2	2.78	0.51
1:B:65:ILE:HD13	8:C:604:HDD:HBA2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:441:TRP:CD2	7:C:602:HEB:HAB2	2.46	0.51
1:B:167:PRO:HB2	1:B:221:TRP:CH2	2.46	0.51
2:C:69:THR:O	2:C:73:MET:HG2	2.11	0.51
1:B:231:LEU:HD21	1:B:234:GLN:HB3	1.93	0.50
2:C:396:CYS:HB2	2:C:436:ALA:HB2	1.92	0.50
1:B:275:PRO:HG3	1:B:297:MET:SD	2.51	0.50
2:C:23:VAL:HG22	8:C:604:HDD:CAD	2.40	0.50
2:C:355:MET:HE2	2:C:461:SER:HB3	1.93	0.50
1:B:79:TYR:OH	2:C:77:PHE:HB2	2.13	0.49
1:B:346:PHE:CE1	2:C:102:MET:HG2	2.47	0.49
2:C:225:VAL:HG21	3:X:20:VAL:HG11	1.94	0.49
1:B:47:ARG:HH12	1:B:374:GLU:HG3	1.77	0.49
1:B:5:GLU:HG3	1:B:236:ALA:HB1	1.95	0.49
1:B:186:VAL:HG13	1:B:282:ILE:HD11	1.94	0.49
2:C:244:GLU:OE2	2:C:244:GLU:HA	2.12	0.48
2:C:181:GLN:HG2	3:X:3:TYR:CZ	2.48	0.48
2:C:9:ARG:HD2	7:C:602:HEB:O2A	2.14	0.47
2:C:378:GLY:O	2:C:450:PRO:HG3	2.14	0.47
2:C:359:ARG:HD3	2:C:360:TYR:CZ	2.48	0.47
2:C:359:ARG:HD3	2:C:360:TYR:CE1	2.50	0.47
2:C:441:TRP:CD1	7:C:603:HEB:HAD2	2.49	0.46
2:C:441:TRP:CG	7:C:603:HEB:HAD2	2.51	0.46
2:C:144:ILE:HG13	7:C:602:HEB:HMC1	1.96	0.46
1:B:147:PHE:CE1	1:B:314:MET:HG2	2.50	0.46
2:C:434:TRP:HB3	6:C:601:POV:H21E	1.97	0.46
1:B:240:SER:HA	1:B:328:ASP:HA	1.98	0.46
1:B:36:LEU:HD11	1:B:46:ARG:HD3	1.97	0.46
2:C:51:MET:HG2	2:C:215:VAL:HG13	1.98	0.46
2:C:110:PHE:CD1	2:C:113:LEU:HD12	2.48	0.46
2:C:185:VAL:CB	2:C:237:LEU:HD21	2.21	0.46
1:B:46:ARG:HD2	1:B:120:ASP:OD2	2.16	0.45
1:B:314:MET:HB3	1:B:324:LEU:HB2	1.97	0.45
1:B:112:ASP:OD1	1:B:114:ARG:NH1	2.45	0.45
1:B:135:GLY:HA3	1:B:173:GLY:HA2	1.97	0.45
2:C:102:MET:HE2	2:C:143:TRP:HE1	1.82	0.45
2:C:441:TRP:HB3	7:C:602:HEB:CMB	2.42	0.45
2:C:243:TYR:O	2:C:247:GLN:HG2	2.15	0.45
1:B:287:PRO:HD2	4:B:401:CDN:HA22	1.99	0.45
1:B:222:LEU:HA	1:B:226:ILE:HD12	1.99	0.45
1:B:168:PHE:HB3	1:B:169:PRO:HD3	1.97	0.45
2:C:43:THR:HB	2:C:45:LYS:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:434:TRP:O	2:C:438:GLU:HG2	2.16	0.45
2:C:246:ALA:HB1	2:C:253:LEU:HD12	1.98	0.45
2:C:335:ASN:ND2	2:C:340:VAL:HG21	2.31	0.45
1:B:230:VAL:HG23	1:B:253:ALA:HB1	1.99	0.45
1:B:8:ARG:HD3	1:B:327:TRP:HA	1.98	0.45
1:B:360:LYS:HB3	1:B:360:LYS:HE3	1.66	0.44
2:C:41:VAL:HG21	2:C:127:LEU:HD22	1.99	0.44
7:C:602:HEB:HMC1	7:C:602:HEB:CBC	2.40	0.44
7:C:602:HEB:HMB1	7:C:602:HEB:HAB	1.72	0.44
1:B:8:ARG:HG2	1:B:330:THR:HG21	1.98	0.44
1:B:192:THR:O	1:B:364:ARG:NH2	2.49	0.44
2:C:84:TYR:HA	2:C:457:LEU:HD21	1.99	0.44
2:C:184:PHE:O	2:C:188:VAL:HG22	2.18	0.44
2:C:415:LYS:HB3	2:C:418:GLN:HB2	1.98	0.44
1:B:309:LEU:O	1:B:312:PHE:N	2.51	0.43
2:C:5:ILE:HG12	2:C:463:HIS:CG	2.53	0.43
3:X:18:THR:O	3:X:22:VAL:HG23	2.18	0.43
1:B:146:PRO:HA	1:B:318:VAL:HG13	1.99	0.43
2:C:183:LYS:NZ	7:C:603:HEB:O2D	2.49	0.43
2:C:314:THR:O	2:C:318:LEU:HG	2.18	0.43
8:C:604:HDD:HMD2	8:C:604:HDD:HAD2	1.77	0.43
1:B:3:ASP:N	1:B:3:ASP:OD1	2.51	0.43
2:C:424:LYS:O	2:C:428:TRP:HD1	2.02	0.43
2:C:241:SER:O	2:C:245:VAL:HG13	2.18	0.43
2:C:13:ALA:HB1	7:C:602:HEB:HMA2	1.99	0.43
2:C:18:TYR:HD2	2:C:69:THR:HG21	1.84	0.43
2:C:23:VAL:HG13	8:C:604:HDD:HMD2	2.00	0.43
2:C:84:TYR:O	2:C:88:VAL:HG22	2.19	0.43
1:B:257:ASN:ND2	1:B:310:PHE:O	2.43	0.43
1:B:62:VAL:HA	1:B:65:ILE:HD12	2.01	0.43
2:C:28:GLY:HA2	2:C:192:TYR:HD1	1.83	0.43
2:C:231:ILE:O	2:C:235:LEU:HG	2.19	0.43
2:C:144:ILE:HD12	2:C:144:ILE:HA	1.95	0.42
4:B:401:CDN:H532	4:B:401:CDN:H561	1.76	0.42
1:B:270:LEU:O	1:B:274:CYS:HB2	2.20	0.42
1:B:278:THR:O	1:B:282:ILE:HG12	2.20	0.42
1:B:17:VAL:O	1:B:21:VAL:HG23	2.19	0.42
2:C:100:ALA:HA	2:C:104:PHE:HB2	2.01	0.42
2:C:102:MET:CE	2:C:143:TRP:HE1	2.33	0.42
1:B:33:GLY:HA3	1:B:127:SER:OG	2.20	0.42
1:B:22:PHE:CD1	1:B:64:LEU:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LYS:HB3	1:B:117:LYS:HE3	1.51	0.41
1:B:335:THR:O	1:B:339:MET:HG2	2.20	0.41
1:B:342:ILE:HG21	2:C:98:MET:HG2	2.02	0.41
2:C:74:GLU:HB2	8:C:604:HDD:HMA1	2.02	0.41
1:B:128:LEU:O	1:B:131:PRO:HD2	2.21	0.41
1:B:8:ARG:NH1	1:B:238:GLY:O	2.48	0.41
1:B:75:TRP:CD1	1:B:330:THR:HG22	2.55	0.41
2:C:437:ILE:HG23	7:C:603:HEB:HMD2	2.02	0.41
7:C:603:HEB:HMB1	7:C:603:HEB:HBB2	2.01	0.41
2:C:209:ARG:HB2	2:C:211:ARG:HG2	2.03	0.41
2:C:183:LYS:HE2	2:C:183:LYS:HB2	1.90	0.41
2:C:441:TRP:CZ2	7:C:603:HEB:HBD1	2.55	0.41
3:X:8:VAL:O	3:X:12:LEU:HG	2.21	0.41
1:B:265:TRP:O	1:B:269:LEU:HG	2.21	0.41
2:C:325:TRP:O	2:C:329:GLN:HG2	2.20	0.41
2:C:189:MET:SD	2:C:233:GLY:HA3	2.61	0.40
2:C:325:TRP:CZ3	2:C:364:MET:HG3	2.56	0.40
2:C:475:LEU:HD23	2:C:475:LEU:HA	1.93	0.40
1:B:33:GLY:HA2	1:B:123:LEU:CD2	2.51	0.40
1:B:227:ASP:HB3	1:B:249:VAL:HG12	2.03	0.40
2:C:178:PRO:HB2	2:C:244:GLU:OE1	2.20	0.40
2:C:345:ARG:HD3	2:C:345:ARG:HA	1.86	0.40
2:C:92:PHE:HZ	7:C:602:HEB:HAC	1.86	0.40
2:C:373:GLN:HA	2:C:376:MET:HB2	2.03	0.40
2:C:437:ILE:HA	7:C:603:HEB:HMD2	2.03	0.40
7:C:602:HEB:HHC	7:C:602:HEB:HBB2	2.03	0.40
7:C:602:HEB:O2D	7:C:602:HEB:HHA	2.22	0.40
1:B:344:LEU:HD23	1:B:344:LEU:HA	1.77	0.40
2:C:56:GLY:HA2	2:C:59:PHE:HB3	2.03	0.40
2:C:317:ARG:HG2	2:C:320:ARG:NH1	2.36	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	B	374/378 (99%)	370 (99%)	4 (1%)	0	100	100
2	C	450/514 (88%)	447 (99%)	3 (1%)	0	100	100
3	X	26/61 (43%)	26 (100%)	0	0	100	100
All	All	850/953 (89%)	843 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	316/318 (99%)	308 (98%)	8 (2%)	47	41
2	C	372/422 (88%)	366 (98%)	6 (2%)	62	59
3	X	27/48 (56%)	27 (100%)	0	100	100
All	All	715/788 (91%)	701 (98%)	14 (2%)	57	51

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4	TYR
1	B	72	PHE
1	B	114	ARG
1	B	227	ASP
1	B	255	MET
1	B	286	ARG
1	B	353	TYR
1	B	368	GLU
2	C	20	PHE
2	C	65	LEU
2	C	140	SER
2	C	236	GLN
2	C	311	MET

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Mol	Chain	Res	Type
2	C	313	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	319	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

7 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
5	DK8	B	402	-	53,53,53	2.10	18 (33%)	65,67,67	1.94	19 (29%)
7	HEB	C	602	2	35,50,50	4.19	16 (45%)	32,82,82	4.96	11 (34%)
4	CDN	B	401	-	68,68,76	0.91	2 (2%)	70,80,88	0.84	2 (2%)
8	HDD	C	604	9,2	41,52,52	2.00	15 (36%)	31,89,89	2.81	14 (45%)
7	HEB	C	603	2	35,50,50	4.25	15 (42%)	32,82,82	4.79	15 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	POV	C	601	-	51,51,51	1.08	6 (11%)	57,59,59	1.01	2 (3%)
9	OXY	C	605	8	1,1,1	0.13	0	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DK8	B	402	-	-	10/47/63/63	0/2/2/2
7	HEB	C	602	2	-	5/12/94/94	-
4	CDN	B	401	-	-	35/79/79/87	-
8	HDD	C	604	9,2	-	0/5/89/89	0/1/9/9
7	HEB	C	603	2	-	6/12/94/94	-
6	POV	C	601	-	-	22/55/55/55	-

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	603	HEB	C3C-C2C	-12.16	1.23	1.40
7	C	602	HEB	C3C-C2C	-10.76	1.25	1.40
7	C	602	HEB	CHA-C4D	10.15	1.54	1.37
7	C	603	HEB	CHA-C4D	9.53	1.53	1.37
7	C	602	HEB	C4D-ND	8.70	1.53	1.36
7	C	603	HEB	C4D-ND	8.10	1.52	1.36
7	C	603	HEB	CHD-C1D	6.95	1.49	1.37
7	C	602	HEB	CHD-C1D	6.86	1.49	1.37
7	C	603	HEB	C4B-NB	6.48	1.49	1.36
7	C	602	HEB	C4B-NB	6.26	1.48	1.36
7	C	603	HEB	CHB-C1B	6.22	1.48	1.37
7	C	602	HEB	C3B-C2B	-6.07	1.23	1.36
7	C	602	HEB	CHB-C1B	5.78	1.47	1.37
7	C	603	HEB	C1B-NB	5.71	1.47	1.36
5	B	402	DK8	C10-C1	5.53	1.57	1.48
5	B	402	DK8	C2-C3	5.51	1.48	1.34
7	C	602	HEB	CHC-C4B	5.47	1.47	1.37
7	C	603	HEB	CHC-C4B	5.43	1.46	1.37
7	C	602	HEB	C1B-NB	5.31	1.46	1.36
7	C	603	HEB	C3B-C2B	-5.28	1.25	1.36
7	C	603	HEB	CHC-C1C	5.23	1.51	1.40
5	B	402	DK8	C5-C4	4.81	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	602	HEB	CHC-C1C	4.76	1.50	1.40
7	C	603	HEB	C2A-C3A	-4.57	1.24	1.37
8	C	604	HDD	O1D-CGD	4.38	1.42	1.35
7	C	602	HEB	C2A-C3A	-4.32	1.24	1.37
8	C	604	HDD	O1D-C3D	-4.30	1.39	1.46
8	C	604	HDD	C3C-C2C	4.15	1.46	1.40
7	C	603	HEB	CHB-C4A	3.89	1.48	1.40
4	B	401	CDN	OA6-CA4	-3.71	1.39	1.44
7	C	602	HEB	C1D-ND	3.61	1.43	1.36
7	C	603	HEB	C1D-ND	3.39	1.43	1.36
7	C	602	HEB	CBC-CAC	3.38	1.51	1.29
7	C	603	HEB	CBC-CAC	3.37	1.51	1.29
5	B	402	DK8	C39-C38	3.35	1.59	1.50
5	B	402	DK8	C15-C13	3.34	1.58	1.51
8	C	604	HDD	C3B-C2B	3.23	1.44	1.40
7	C	602	HEB	CHB-C4A	3.11	1.47	1.40
8	C	604	HDD	CAA-C2A	-3.11	1.47	1.52
7	C	602	HEB	CHA-C1A	3.07	1.47	1.40
8	C	604	HDD	C4D-ND	-3.07	1.32	1.37
5	B	402	DK8	O1-C1	-2.98	1.17	1.24
4	B	401	CDN	OB6-CB4	-2.94	1.40	1.44
5	B	402	DK8	C45-C43	2.91	1.58	1.50
5	B	402	DK8	C36-C37	2.79	1.59	1.50
5	B	402	DK8	C2-C1	2.75	1.50	1.44
8	C	604	HDD	FE-ND	-2.70	1.85	1.95
5	B	402	DK8	O4-C4	-2.67	1.17	1.23
6	C	601	POV	O21-C21	2.61	1.41	1.34
5	B	402	DK8	C11-C12	2.61	1.54	1.50
5	B	402	DK8	C40-C38	2.56	1.56	1.51
5	B	402	DK8	C11-C3	2.52	1.53	1.51
5	B	402	DK8	C19-C18	2.51	1.57	1.50
8	C	604	HDD	CHD-C1D	-2.48	1.32	1.36
8	C	604	HDD	C1D-ND	-2.45	1.33	1.37
6	C	601	POV	O31-C31	2.43	1.40	1.33
8	C	604	HDD	C2A-C3A	2.38	1.44	1.37
5	B	402	DK8	C27-C28	2.38	1.38	1.33
8	C	604	HDD	C4C-NC	-2.32	1.31	1.36
8	C	604	HDD	C1A-CHA	2.27	1.47	1.41
7	C	603	HEB	CHA-C1A	2.25	1.45	1.40
6	C	601	POV	P-O11	2.24	1.68	1.59
6	C	601	POV	O31-C3	-2.22	1.40	1.45
6	C	601	POV	O21-C2	-2.22	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	602	HEB	C3C-CAC	2.20	1.52	1.47
5	B	402	DK8	C14-C13	2.10	1.56	1.50
5	B	402	DK8	C31-C32	2.09	1.57	1.50
6	C	601	POV	C15-N	-2.07	1.44	1.50
8	C	604	HDD	C1C-NC	-2.07	1.31	1.36
5	B	402	DK8	C35-C33	2.07	1.55	1.51
8	C	604	HDD	C4C-CHD	2.05	1.46	1.41
8	C	604	HDD	C1A-NA	-2.04	1.32	1.36

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	602	HEB	C1D-C2D-C3D	18.17	123.72	108.61
7	C	603	HEB	C1D-C2D-C3D	18.03	123.60	108.61
7	C	602	HEB	C1B-C2B-C3B	14.63	120.77	108.61
7	C	603	HEB	C1B-C2B-C3B	14.26	120.47	108.61
8	C	604	HDD	C4A-C3A-C2A	-8.01	101.42	107.00
7	C	602	HEB	C3B-C4B-NB	-7.59	98.61	114.98
8	C	604	HDD	CBA-CAA-C2A	-7.29	100.18	112.62
7	C	603	HEB	C3D-C4D-ND	-6.93	100.03	114.98
7	C	602	HEB	C3D-C4D-ND	-6.81	100.28	114.98
7	C	603	HEB	C3B-C4B-NB	-6.61	100.72	114.98
5	B	402	DK8	C11-C12-C13	-6.18	116.50	126.79
7	C	603	HEB	CMB-C2B-C1B	-4.83	115.61	124.73
5	B	402	DK8	C11-C3-C4	4.39	120.45	116.88
7	C	602	HEB	CBA-CAA-C2A	-4.30	105.36	112.60
7	C	602	HEB	CBB-CAB-C3B	-4.24	106.67	112.88
7	C	602	HEB	CMB-C2B-C1B	-4.05	117.07	124.73
6	C	601	POV	O21-C21-C22	3.96	120.03	111.50
7	C	602	HEB	CAD-CBD-CGD	-3.92	105.17	113.60
8	C	604	HDD	C3C-C4C-NC	3.87	114.22	109.21
5	B	402	DK8	C26-C27-C28	-3.74	118.65	127.66
8	C	604	HDD	CMB-C2B-C3B	3.71	131.62	124.68
5	B	402	DK8	C41-C42-C43	-3.63	118.92	127.66
5	B	402	DK8	C31-C32-C33	-3.54	119.13	127.66
7	C	603	HEB	CMD-C2D-C1D	-3.52	118.07	124.73
5	B	402	DK8	C11-C3-C2	-3.50	118.70	123.30
7	C	602	HEB	CMD-C2D-C1D	-3.46	118.19	124.73
8	C	604	HDD	C4C-CHD-C1D	-3.22	123.74	130.12
5	B	402	DK8	C21-C22-C23	-3.21	119.94	127.66
8	C	604	HDD	C2D-C1D-CHD	-3.19	119.01	124.28
8	C	604	HDD	CAD-CBD-CGD	-3.12	99.74	104.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	602	HEB	CMD-C2D-C3D	-2.96	118.09	126.12
5	B	402	DK8	C50-C48-C49	2.96	121.14	114.60
8	C	604	HDD	C2B-C3B-C4B	-2.93	104.85	106.90
5	B	402	DK8	C16-C17-C18	-2.89	120.70	127.66
7	C	603	HEB	CMD-C2D-C3D	-2.88	118.32	126.12
8	C	604	HDD	CHD-C1D-ND	2.88	128.42	124.20
8	C	604	HDD	CMC-C2C-C3C	2.82	129.95	124.68
7	C	603	HEB	CAA-CBA-CGA	-2.73	106.11	113.76
5	B	402	DK8	C19-C18-C20	2.66	119.74	115.27
5	B	402	DK8	C34-C33-C35	2.65	119.73	115.27
8	C	604	HDD	C1A-CHA-C4D	-2.61	124.94	130.12
8	C	604	HDD	CMA-C3A-C4A	2.60	132.47	128.46
8	C	604	HDD	O1D-C3D-CAD	2.60	107.90	103.01
7	C	603	HEB	CBB-CAB-C3B	2.60	116.68	112.88
5	B	402	DK8	C29-C28-C30	2.57	119.59	115.27
6	C	601	POV	O31-C31-C32	2.54	119.87	111.91
7	C	602	HEB	C4D-C3D-C2D	-2.54	103.76	113.64
7	C	603	HEB	CAA-C2A-C3A	-2.54	119.96	127.25
5	B	402	DK8	C14-C13-C15	2.49	119.47	115.27
5	B	402	DK8	C46-C47-C48	-2.41	119.51	127.75
5	B	402	DK8	C36-C37-C38	-2.38	121.94	127.66
7	C	603	HEB	C4D-C3D-C2D	-2.36	104.45	113.64
5	B	402	DK8	C39-C38-C40	2.34	119.20	115.27
5	B	402	DK8	C45-C43-C44	2.25	119.05	115.27
4	B	401	CDN	C12-C11-CA5	-2.20	108.29	113.38
4	B	401	CDN	C72-C71-CB7	-2.19	108.32	113.38
5	B	402	DK8	C24-C23-C25	2.18	118.94	115.27
7	C	603	HEB	CBD-CAD-C3D	-2.17	106.66	112.62
5	B	402	DK8	C5-C4-C3	2.11	119.48	116.62
8	C	604	HDD	CMD-C2D-C1D	-2.06	108.97	112.63
7	C	603	HEB	CAD-CBD-CGD	-2.06	109.18	113.60
7	C	603	HEB	CBA-CAA-C2A	2.05	116.06	112.60
7	C	603	HEB	C4B-CHC-C1C	2.03	124.17	118.67

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	401	CDN	CB2-OB2-PB2-OB5
4	B	401	CDN	CB2-OB2-PB2-OB3
4	B	401	CDN	CB2-OB2-PB2-OB4
4	B	401	CDN	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
4	B	401	CDN	C72-C71-CB7-OB9
4	B	401	CDN	CA3-OA5-PA1-OA2
4	B	401	CDN	C31-CA7-OA8-CA6
4	B	401	CDN	OA7-CA5-OA6-CA4
5	B	402	DK8	C18-C20-C21-C22
5	B	402	DK8	C23-C25-C26-C27
6	C	601	POV	C11-O12-P-O13
6	C	601	POV	C22-C21-O21-C2
7	C	603	HEB	C4B-C3B-CAB-CBB
6	C	601	POV	C32-C31-O31-C3
6	C	601	POV	O22-C21-O21-C2
6	C	601	POV	O32-C31-O31-C3
5	B	402	DK8	C28-C30-C31-C32
4	B	401	CDN	OB6-CB4-CB6-OB8
6	C	601	POV	C31-C32-C33-C34
6	C	601	POV	C11-O12-P-O11
6	C	601	POV	C24-C25-C26-C27
6	C	601	POV	C23-C24-C25-C26
5	B	402	DK8	C45-C43-C44-C46
6	C	601	POV	C214-C215-C216-C217
6	C	601	POV	C33-C34-C35-C36
4	B	401	CDN	C51-C52-C53-C54
4	B	401	CDN	C34-C35-C36-C37
5	B	402	DK8	C32-C33-C35-C36
5	B	402	DK8	C42-C43-C44-C46
4	B	401	CDN	C57-C58-C59-C60
4	B	401	CDN	C58-C59-C60-C61
6	C	601	POV	C35-C36-C37-C38
5	B	402	DK8	C24-C23-C25-C26
5	B	402	DK8	C34-C33-C35-C36
6	C	601	POV	C310-C311-C312-C313
6	C	601	POV	C34-C35-C36-C37
4	B	401	CDN	CB3-CB4-CB6-OB8
4	B	401	CDN	C59-C60-C61-C62
4	B	401	CDN	C52-C51-CB5-OB6
4	B	401	CDN	C54-C55-C56-C57
4	B	401	CDN	CB3-CB4-OB6-CB5
4	B	401	CDN	CB6-CB4-OB6-CB5
4	B	401	CDN	C14-C15-C16-C17
4	B	401	CDN	C15-C16-C17-C18
4	B	401	CDN	C32-C33-C34-C35
7	C	603	HEB	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
4	B	401	CDN	C60-C61-C62-C63
4	B	401	CDN	CA5-C11-C12-C13
6	C	601	POV	C313-C314-C315-C316
4	B	401	CDN	CB3-OB5-PB2-OB2
4	B	401	CDN	CA3-OA5-PA1-OA3
4	B	401	CDN	CA2-OA2-PA1-OA3
6	C	601	POV	C36-C37-C38-C39
4	B	401	CDN	OA5-CA3-CA4-OA6
6	C	601	POV	C11-C12-N-C14
4	B	401	CDN	C72-C71-CB7-OB8
4	B	401	CDN	OA5-CA3-CA4-CA6
5	B	402	DK8	C22-C23-C25-C26
7	C	602	HEB	C2B-C3B-CAB-CBB
7	C	602	HEB	CAA-CBA-CGA-O1A
7	C	603	HEB	CAD-CBD-CGD-O1D
4	B	401	CDN	CA7-C31-C32-C33
7	C	602	HEB	CAD-CBD-CGD-O1D
6	C	601	POV	C11-C12-N-C13
7	C	603	HEB	CAD-CBD-CGD-O2D
7	C	602	HEB	CAA-CBA-CGA-O2A
4	B	401	CDN	CA4-CA3-OA5-PA1
6	C	601	POV	O21-C2-C3-O31
6	C	601	POV	C11-C12-N-C15
7	C	602	HEB	CAD-CBD-CGD-O2D
4	B	401	CDN	C32-C31-CA7-OA9
5	B	402	DK8	C25-C26-C27-C28
4	B	401	CDN	C36-C37-C38-C39
4	B	401	CDN	CA2-OA2-PA1-OA5
7	C	603	HEB	CAA-CBA-CGA-O2A
7	C	603	HEB	CAA-CBA-CGA-O1A
6	C	601	POV	O31-C31-C32-C33
6	C	601	POV	O32-C31-C32-C33

There are no ring outliers.

6 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	602	HEB	18	0
4	B	401	CDN	3	0
8	C	604	HDD	8	0
7	C	603	HEB	9	0
6	C	601	POV	3	0

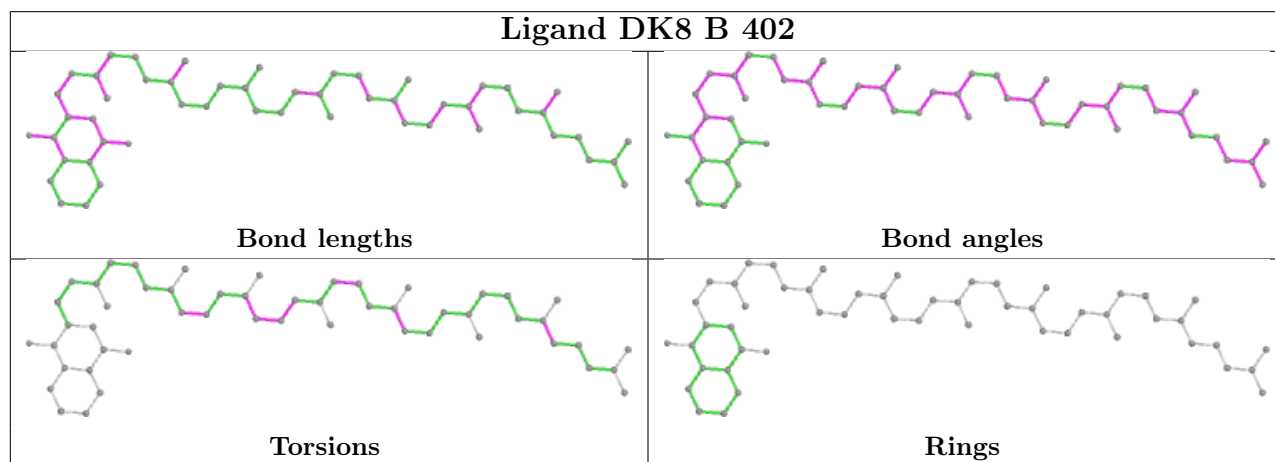
*Continued on next page...*

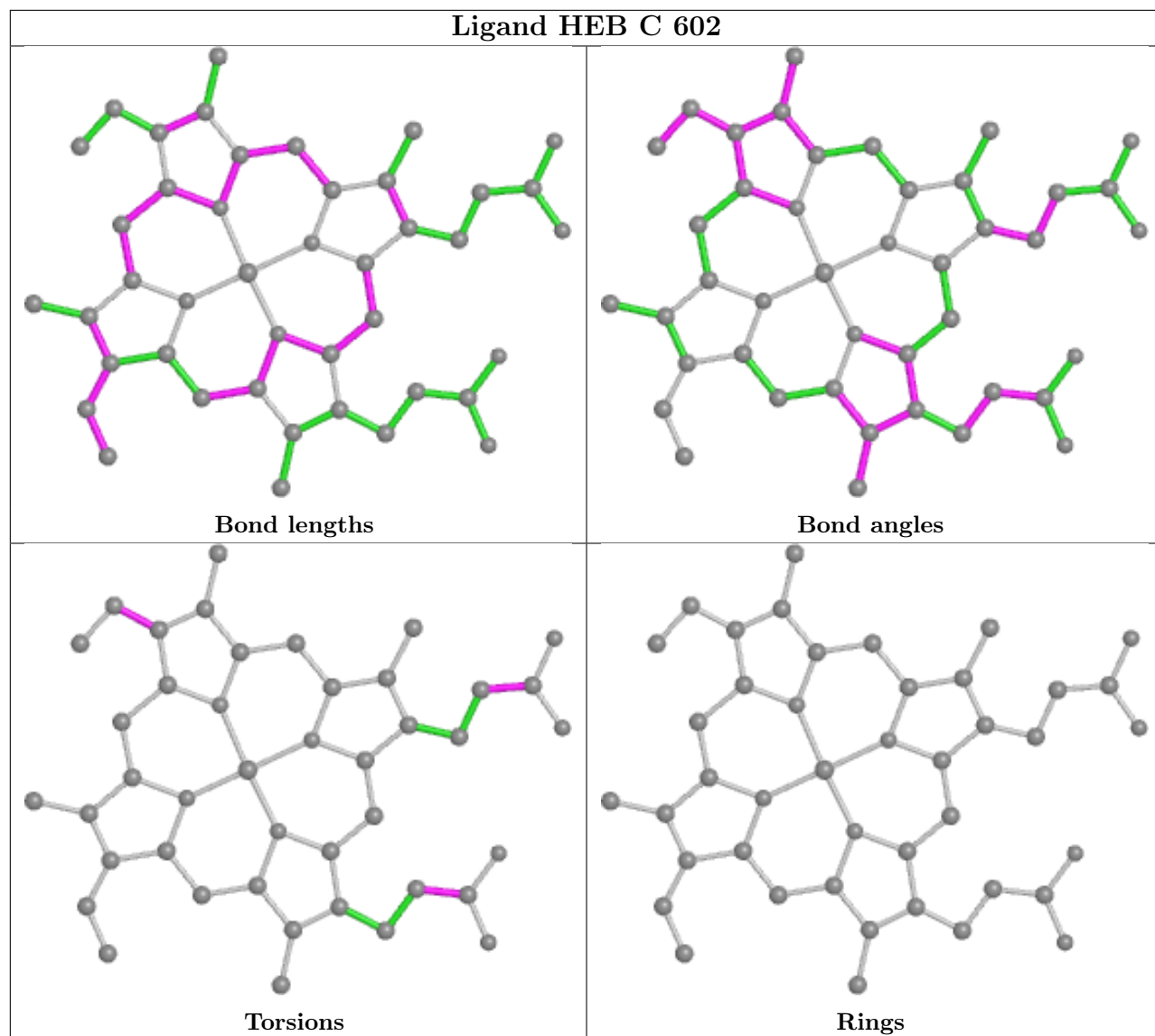


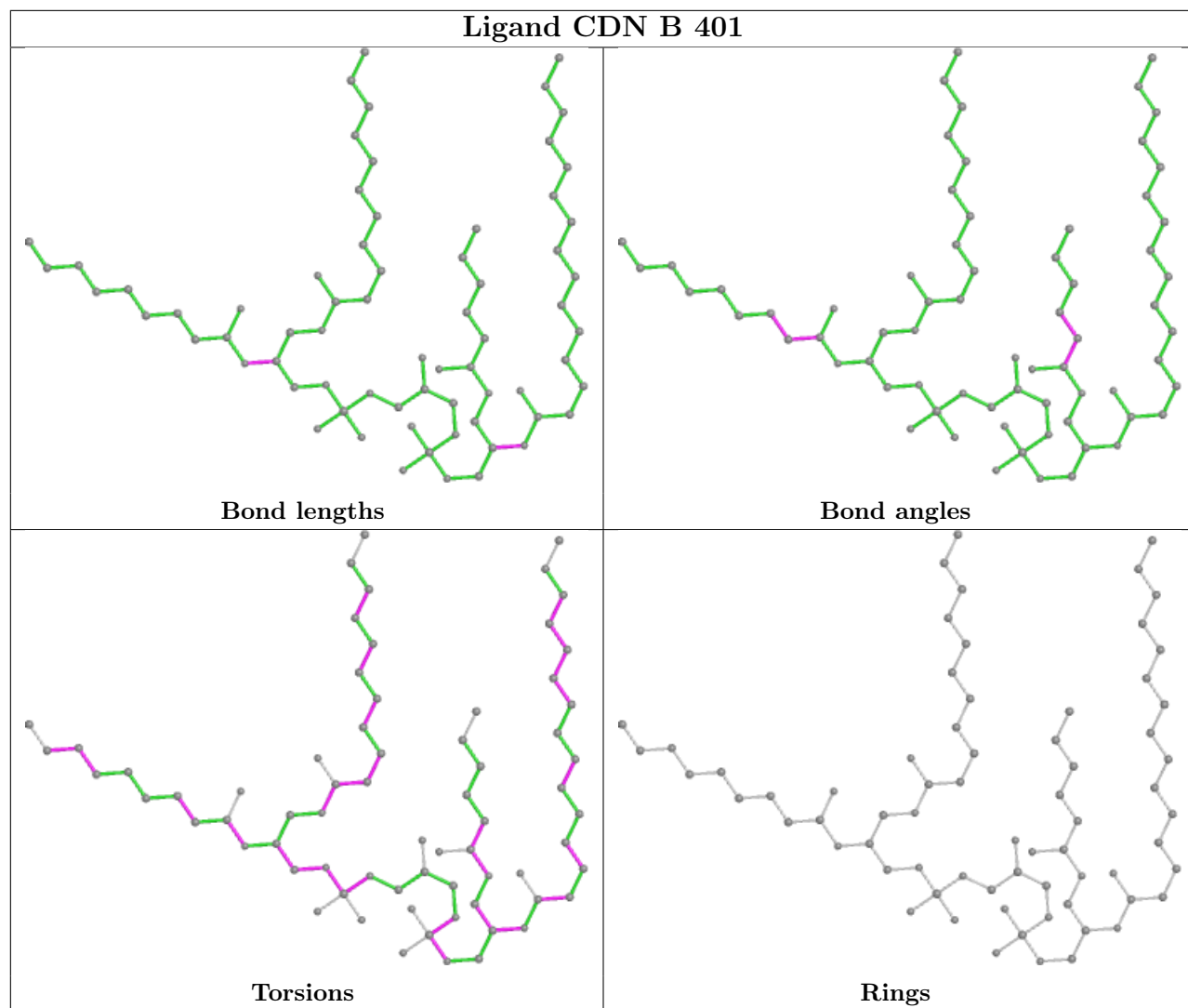
*Continued from previous page...*

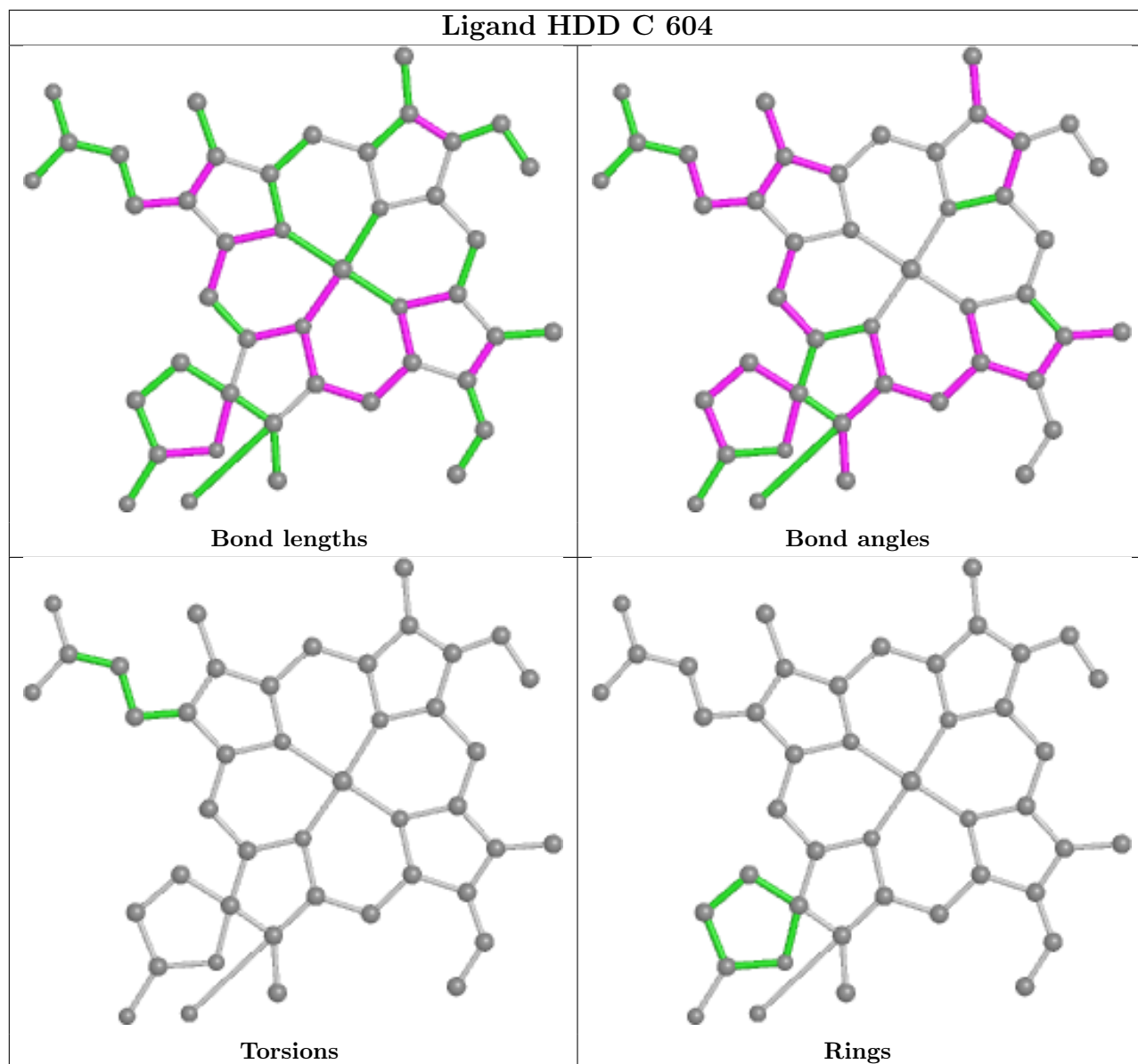
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	605	OXY	1	0

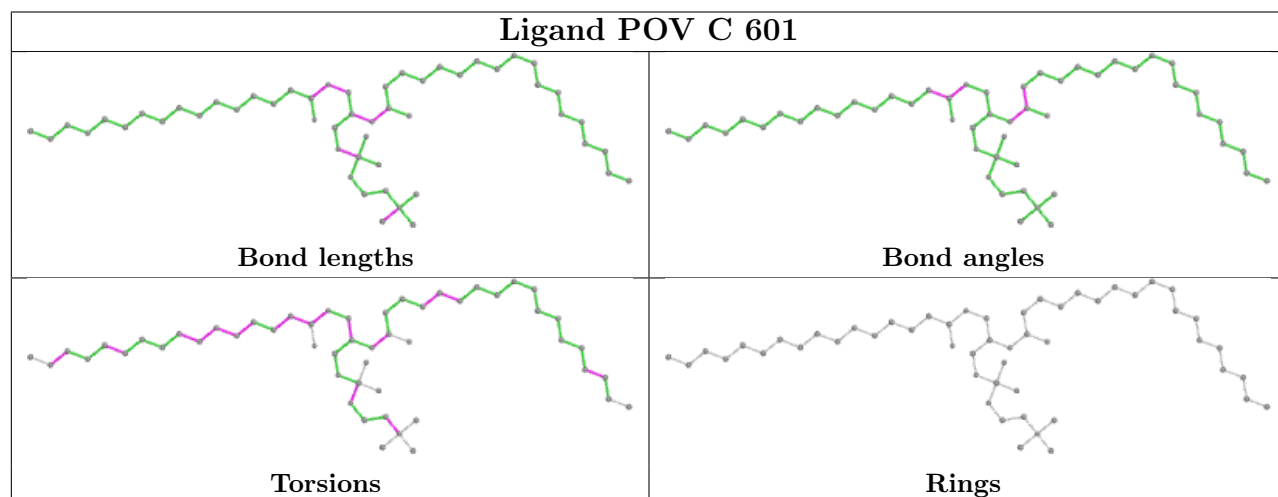
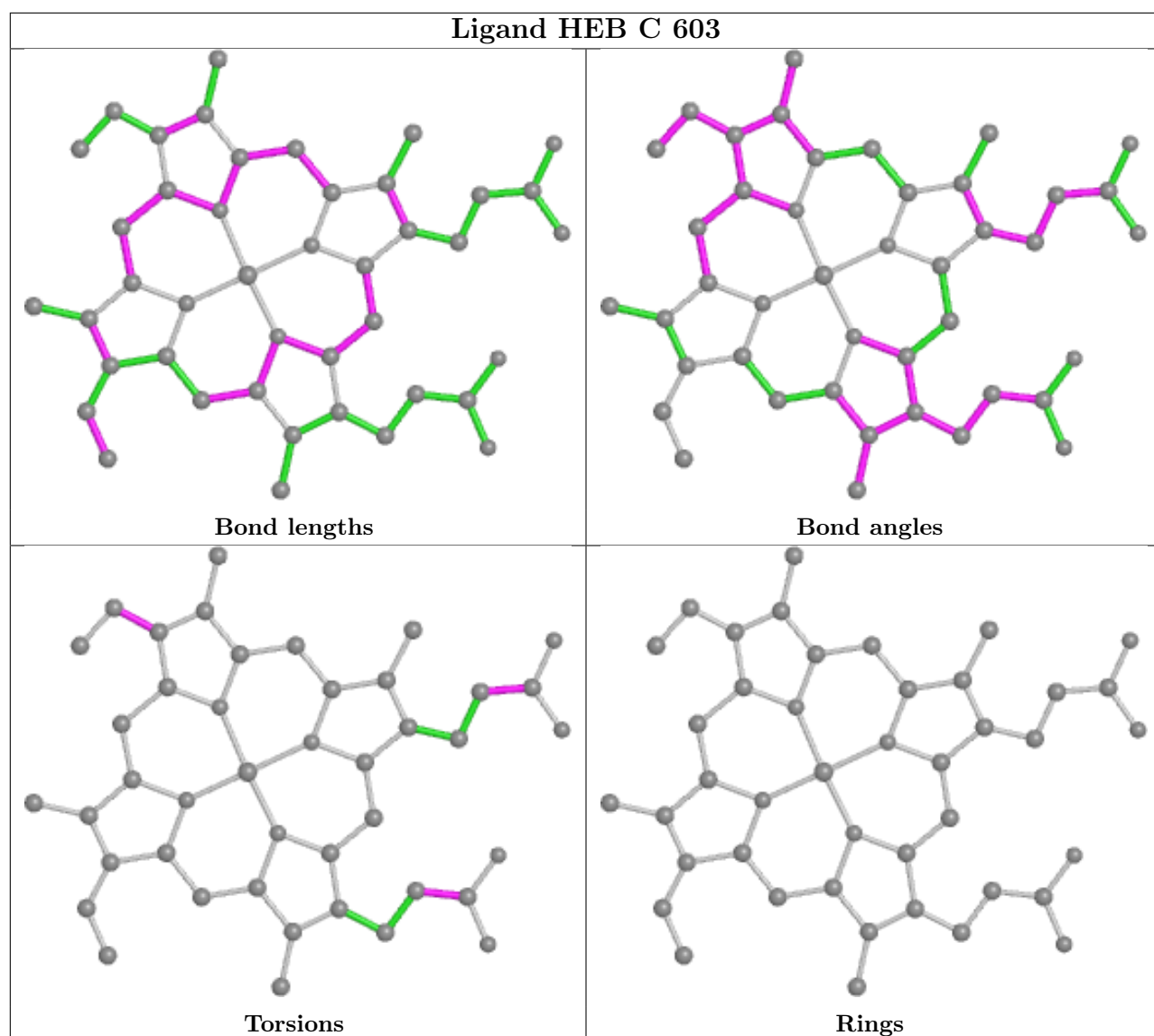
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

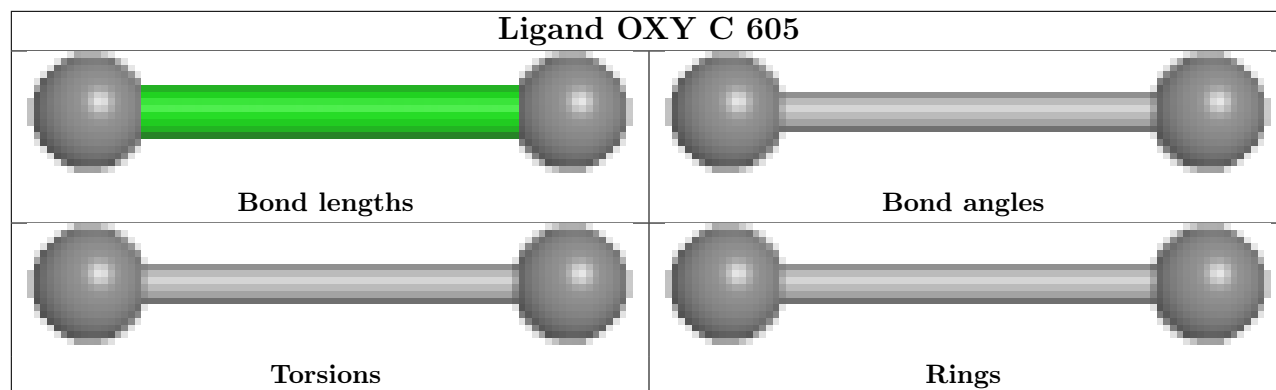












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

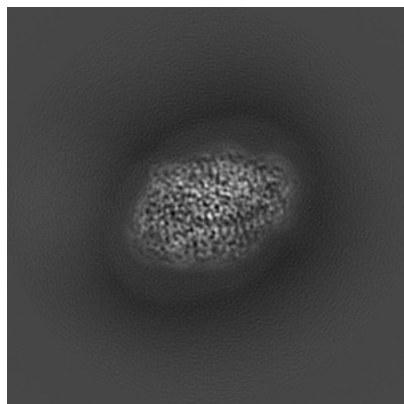
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13108. These allow visual inspection of the internal detail of the map and identification of artifacts.

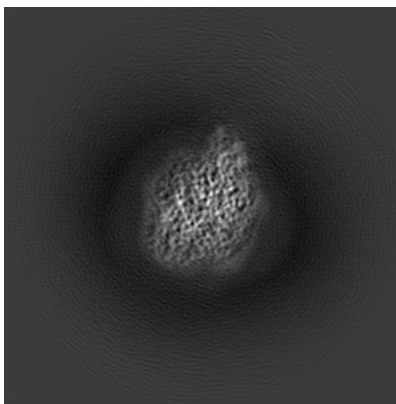
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

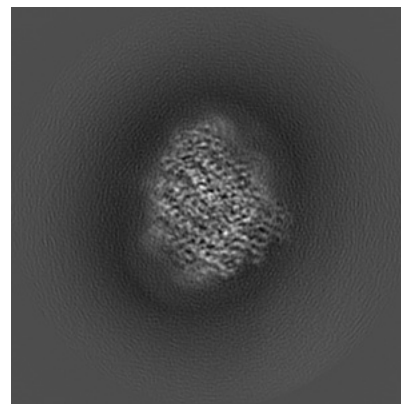
#### 6.1.1 Primary map



X

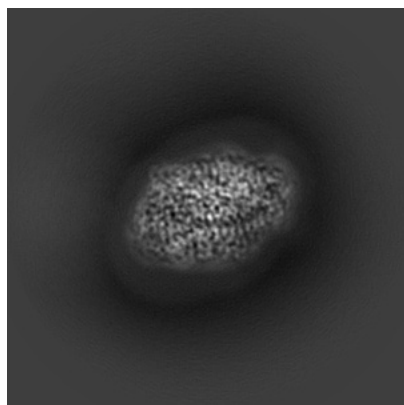


Y

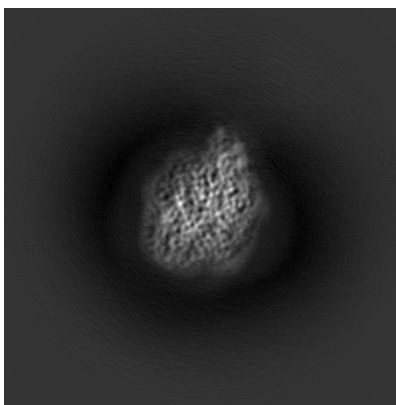


Z

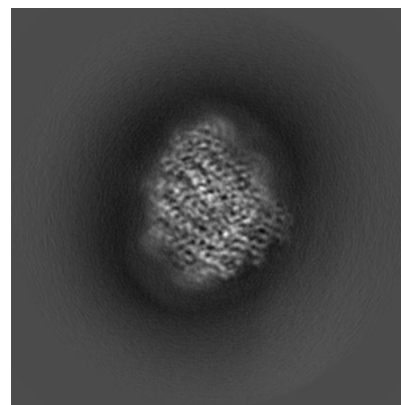
#### 6.1.2 Raw map



X



Y

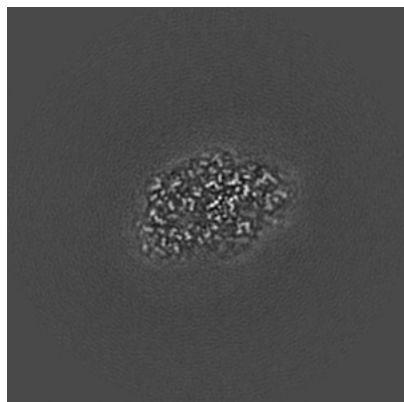


Z

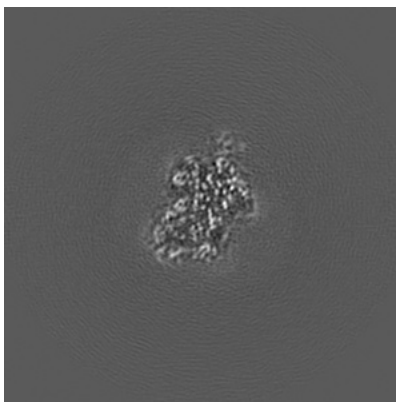
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

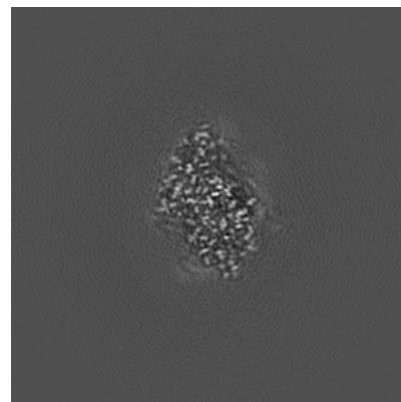
### 6.2.1 Primary map



X Index: 128

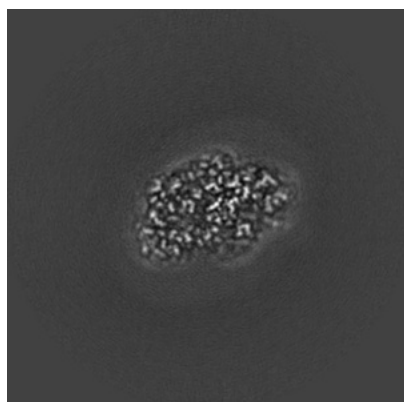


Y Index: 128

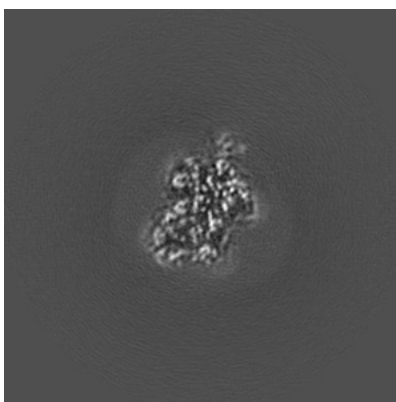


Z Index: 128

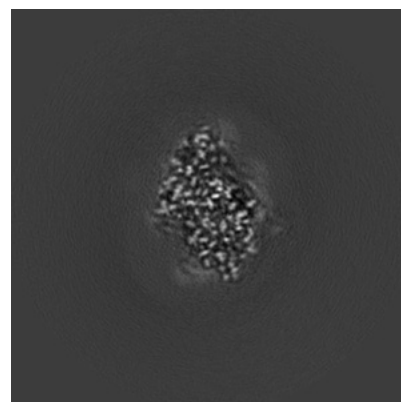
### 6.2.2 Raw map



X Index: 128



Y Index: 128



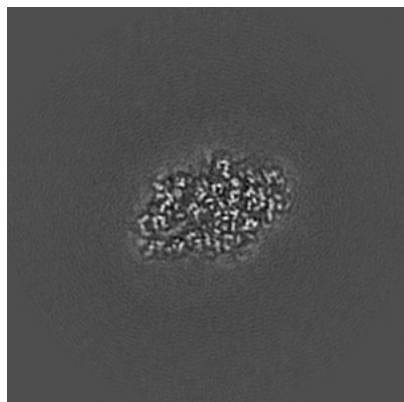
Z Index: 128

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

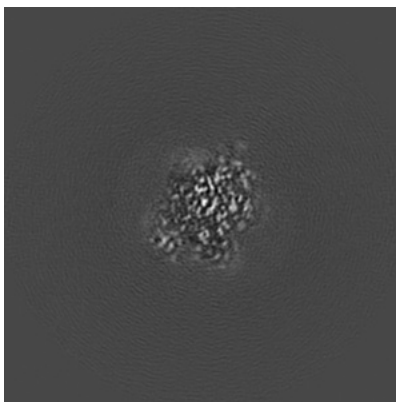


## 6.3 Largest variance slices [i](#)

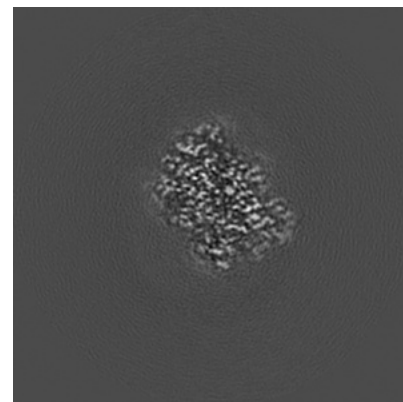
### 6.3.1 Primary map



X Index: 123

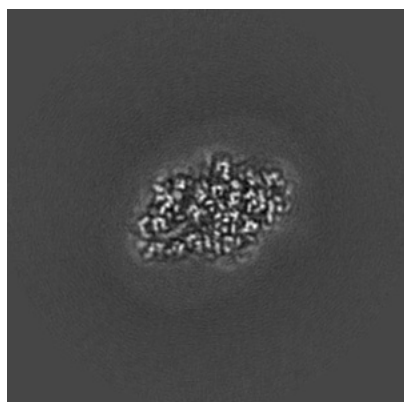


Y Index: 136

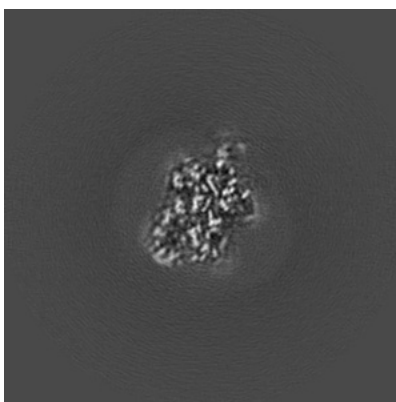


Z Index: 137

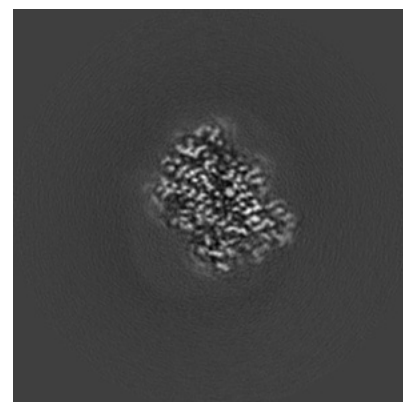
### 6.3.2 Raw map



X Index: 123



Y Index: 129



Z Index: 137

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

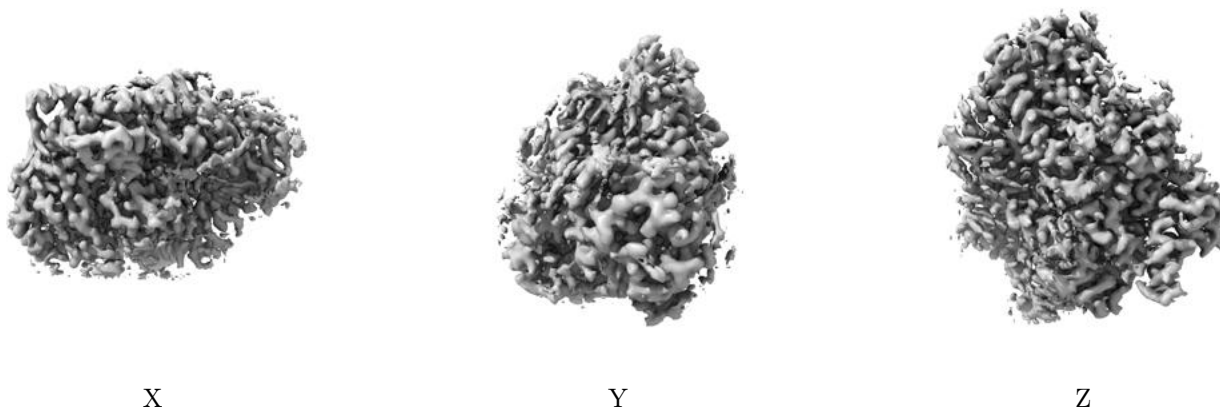
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

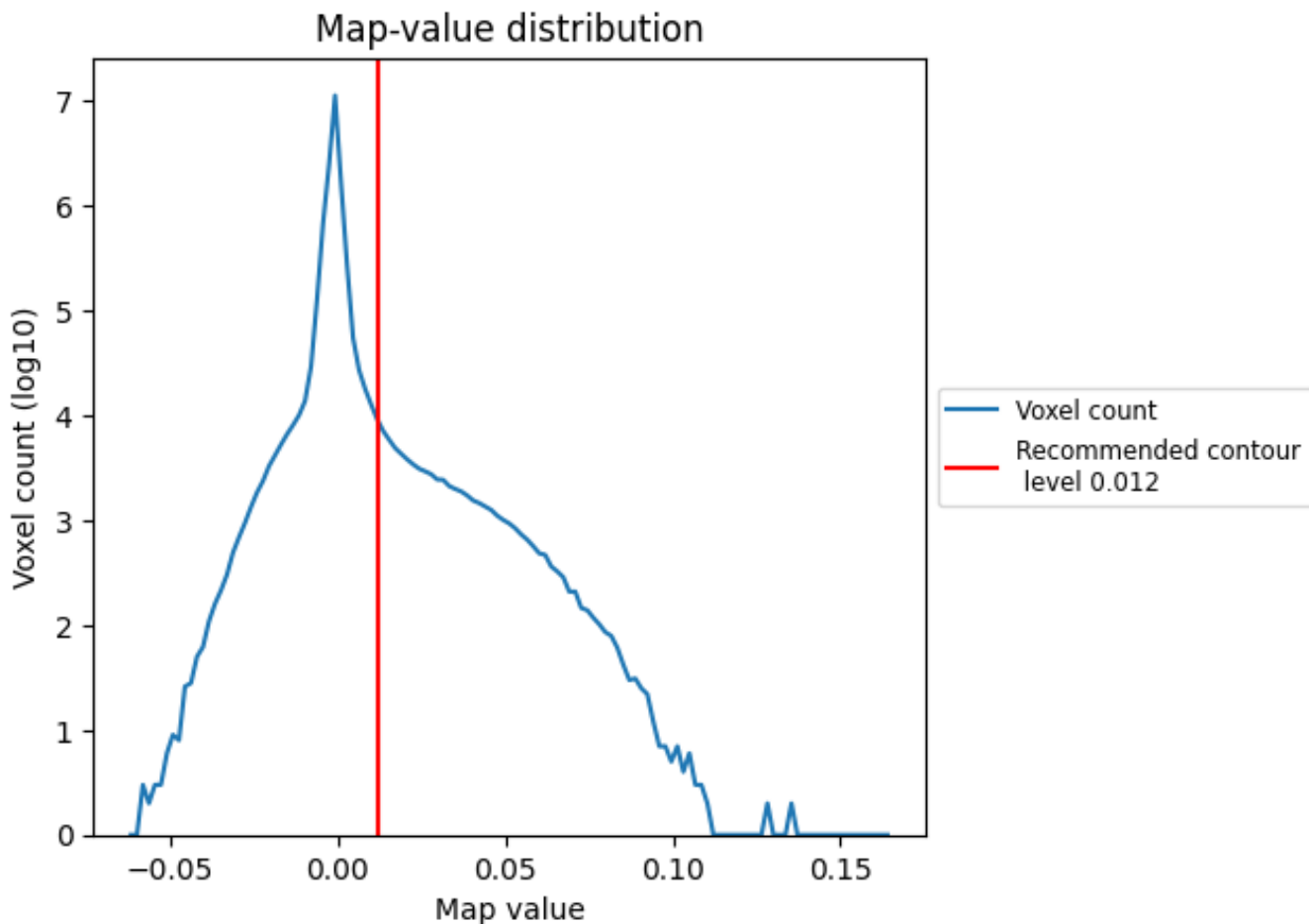
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

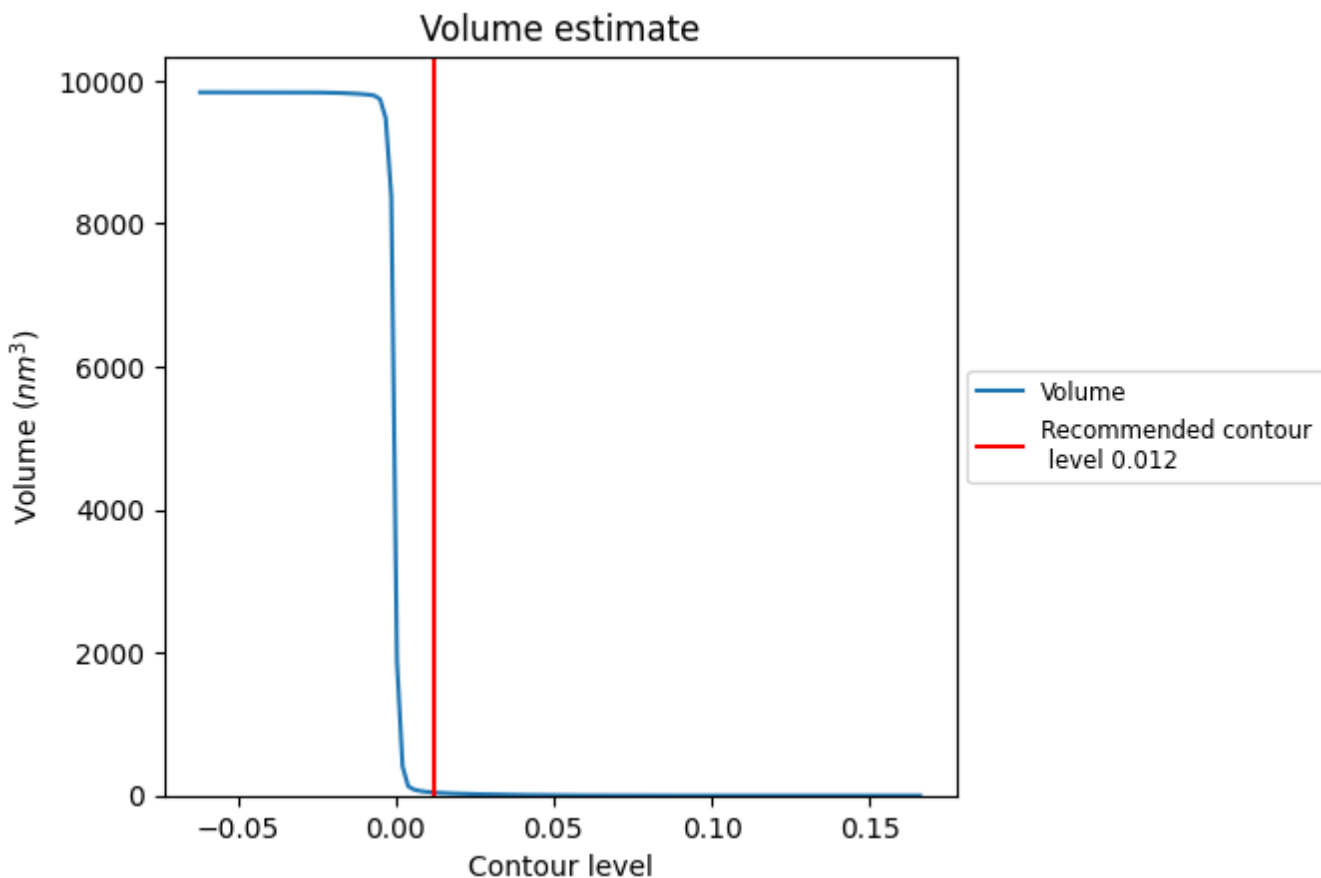
This section contains the results of statistical analysis of the map.

### 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.

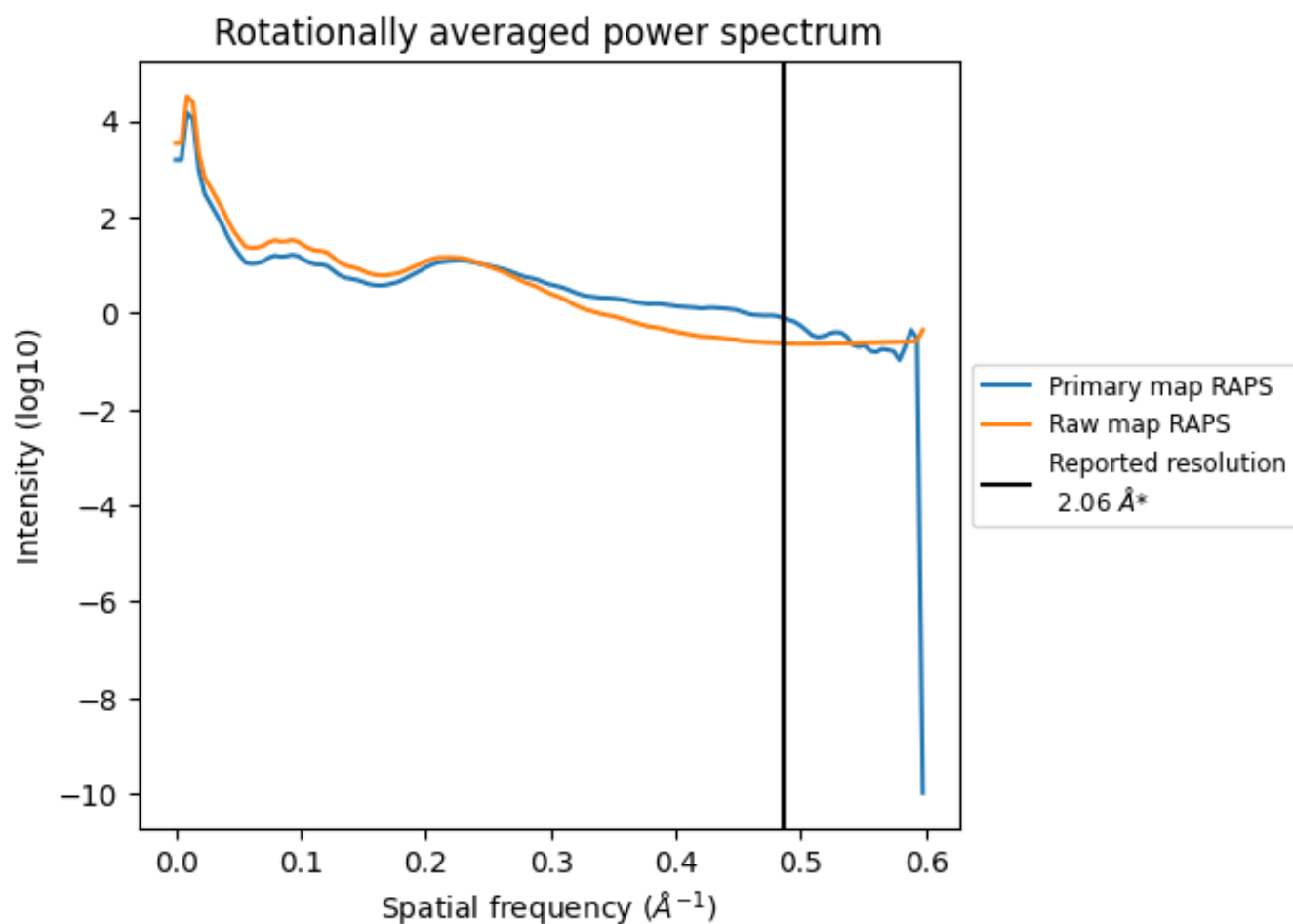
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 43 nm<sup>3</sup>; this corresponds to an approximate mass of 39 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

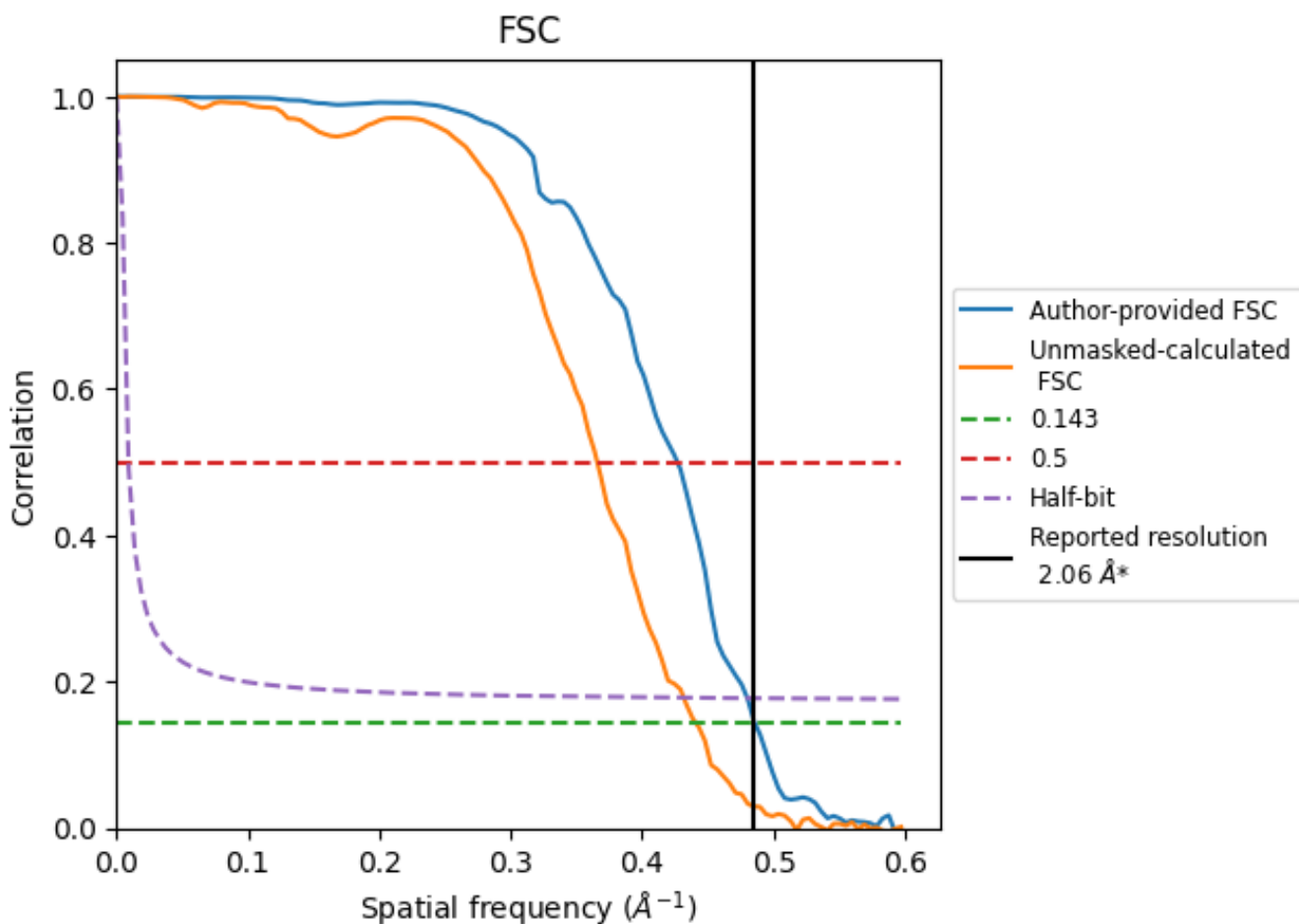


\*Reported resolution corresponds to spatial frequency of  $0.485 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.485 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

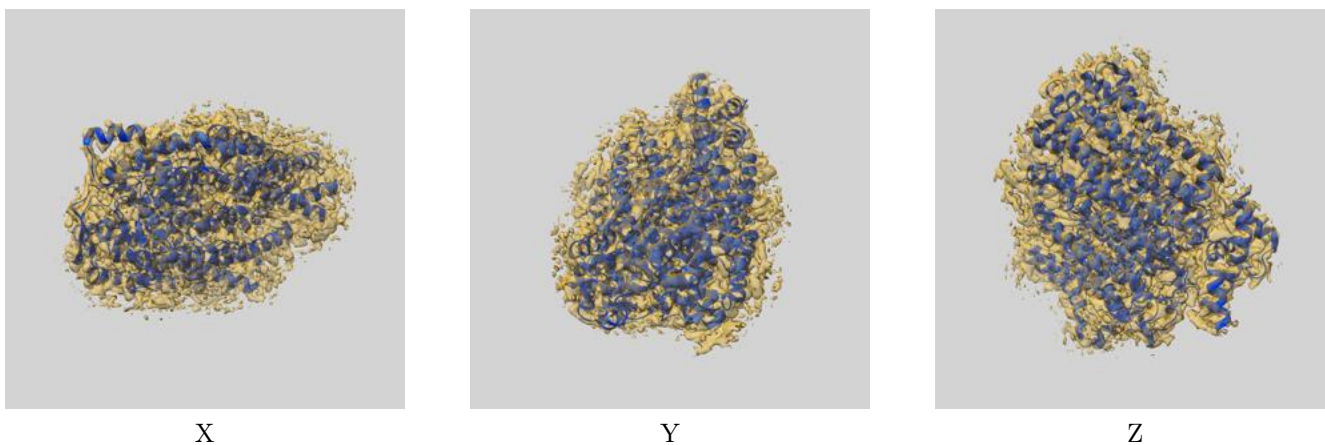
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.06	-	-
Author-provided FSC curve	2.06	2.34	2.08
Unmasked-calculated*	2.27	2.73	2.32

\*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 2.27 differs from the reported value 2.06 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-13108 and PDB model 7OY2. Per-residue inclusion information can be found in section 3 on page 8.

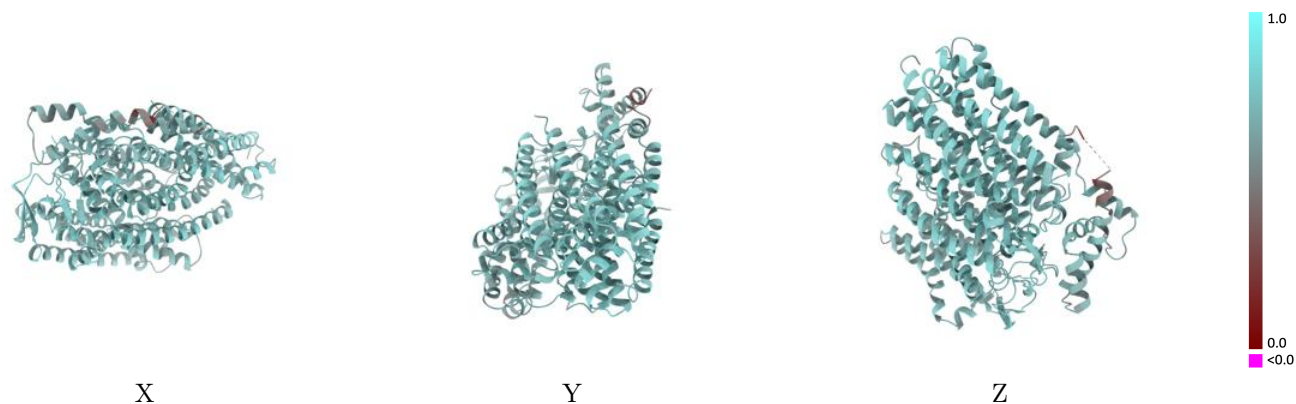
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.012 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.

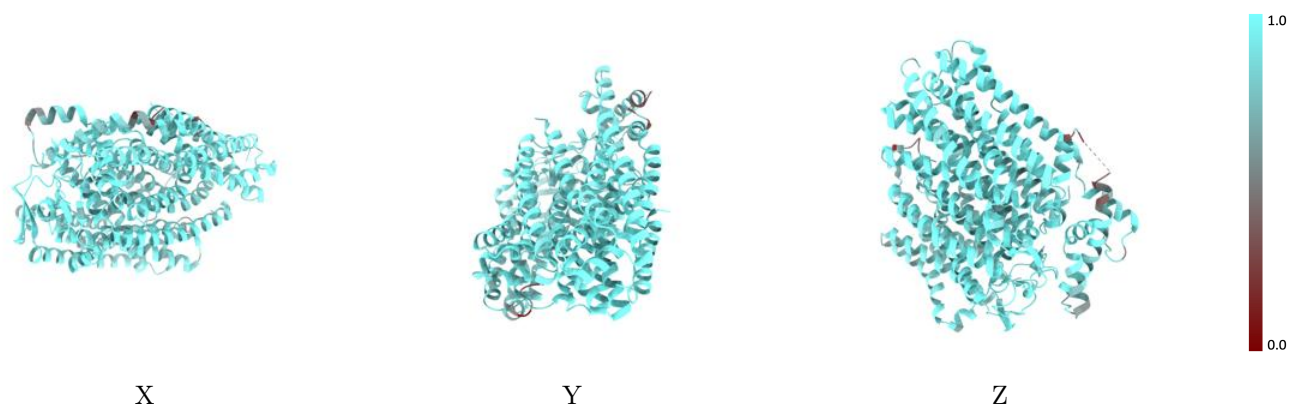


## 9.2 Q-score mapped to coordinate model [i](#)



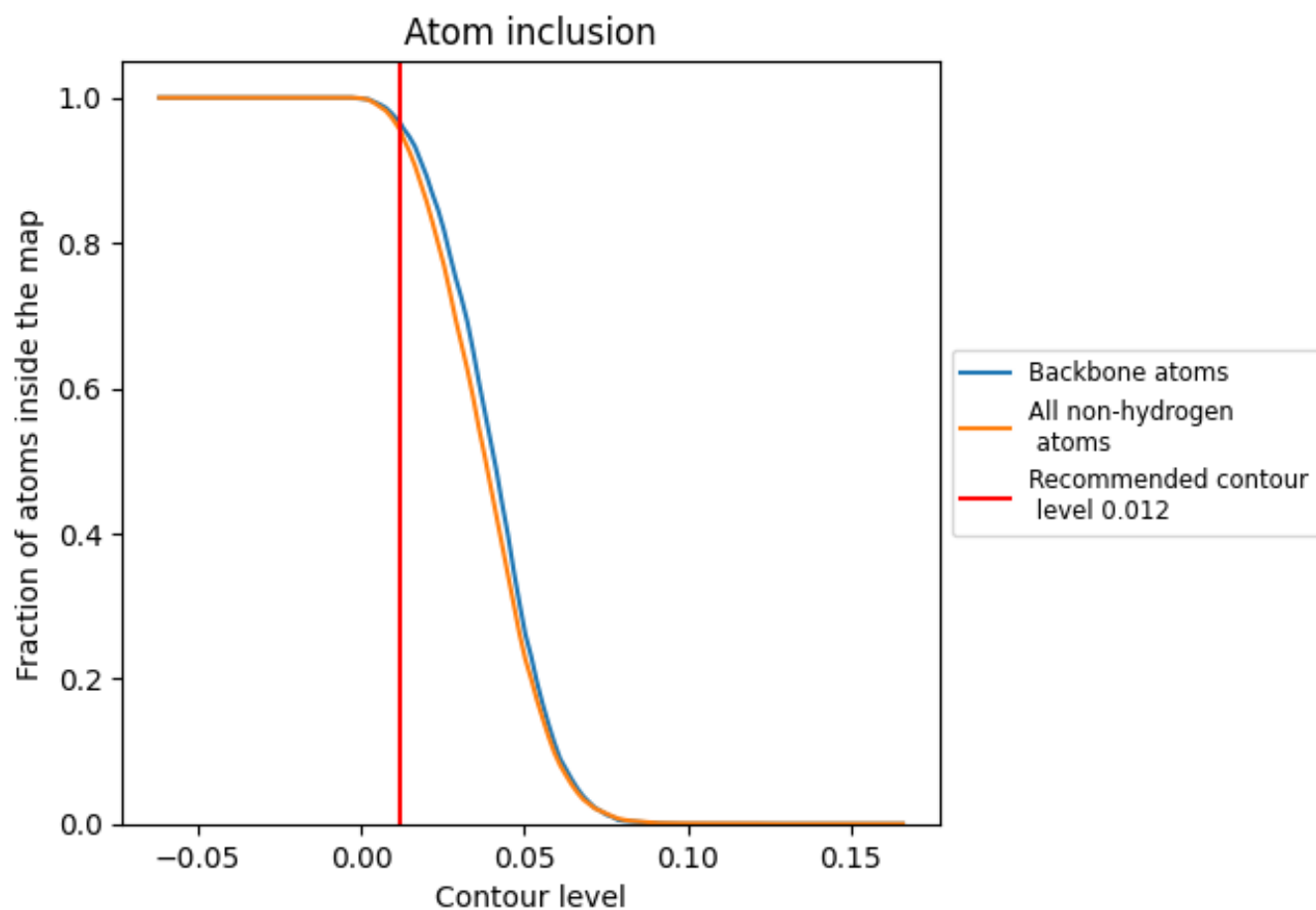
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9548	 0.7000
B	 0.9595	 0.7030
C	 0.9561	 0.6990
X	 0.9740	 0.6960

