



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:58 AM UTC

PDB ID : 6GIQ / pdb_00006giq
EMDB ID : EMD-0004
Title : Saccharomyces cerevisiae respiratory supercomplex III2IV
Authors : Rathore, S.; Berndtsson, J.; Conrad, J.; Ott, M.
Deposited on : 2018-05-15
Resolution : 3.23 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:

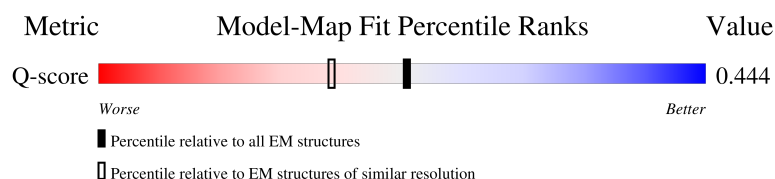
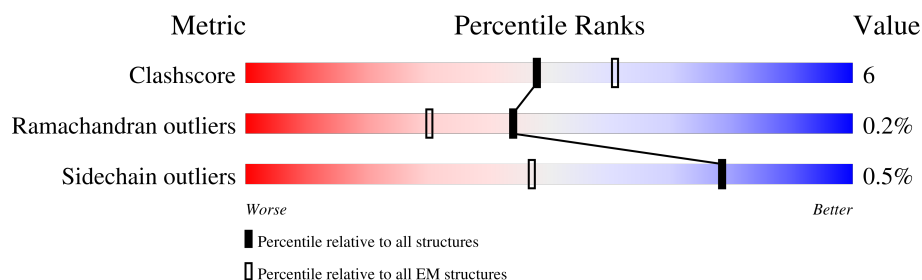
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.23 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	14612 (2.73 - 3.73)

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	457	 81% 12% 6%
1	L	457	 81% 13% 6%
2	B	368	 81% 15% .
2	M	368	 80% 15% .

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Mol	Chain	Length	Quality of chain
3	C	385	
3	N	385	
4	D	309	
4	O	309	
5	E	215	
5	P	215	
6	F	147	
6	Q	147	
7	G	127	
7	R	127	
8	H	94	
8	S	94	
9	I	66	
9	T	66	
10	U	77	
10	V	77	
11	a	534	
12	b	251	
13	c	269	
14	d	155	
15	e	153	
16	f	148	
17	g	60	
18	h	78	
19	i	59	

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Mol	Chain	Length	Quality of chain
20	j	83	
21	k	129	
22	m	31	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	FES	E	301	-	-	X	-
29	FES	P	302	-	-	X	-

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 44120 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 BJ4_G0001550.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3344	2110	576	652	6		
1	L	431	Total	C	N	O	S	0	0
			3344	2110	576	652	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		
2	M	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		
3	N	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		

- Molecule 4 is a protein called BJ4_G0049990.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	248	Total	C	N	O	S	0	0
			1961	1249	340	363	9		
4	O	248	Total	C	N	O	S	0	0
			1961	1249	340	363	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		
5	P	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		

- Molecule 6 is a protein called QCR6 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	74	Total	C	N	O	S	0	0
			624	391	108	123	2		
6	Q	75	Total	C	N	O	S	0	0
			633	396	109	126	2		

- Molecule 7 is a protein called Complex III subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		
7	R	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		

- Molecule 8 is a protein called BJ4_G0028260.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	93	Total	C	N	O	S	0	0
			773	510	131	130	2		
8	S	93	Total	C	N	O	S	0	0
			773	510	131	130	2		

- Molecule 9 is a protein called HLJ1_G0021680.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	54	Total	C	N	O	0	0
			442	295	74	73		
9	T	54	Total	C	N	O	0	0
			443	295	74	74		

- Molecule 10 is a protein called BJ4_G0023510.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	44	Total	C	N	O	S	0	0
			347	230	58	57	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	51	Total	C	N	O	S	0	0
			406	272	66	66	2		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	522	Total	C	N	O	S	0	0
			4058	2711	630	696	21		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	b	235	Total	C	N	O	S	0	0
			1879	1237	284	348	10		

- Molecule 13 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	262	Total	C	N	O	S	0	0
			2087	1395	332	346	14		

- Molecule 14 is a protein called BJ4_G0018620.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	49	Total	C	N	O	S	0	0
			390	244	63	82	1		

- Molecule 15 is a protein called BJ4_G0046460.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	96	Total	C	N	O	S	0	0
			733	468	128	134	3		

- Molecule 16 is a protein called BJ4_G0024040.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	99	Total	C	N	O	S	0	0
			828	533	134	160	1		

- Molecule 17 is a protein called BJ4_G0043230.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	g	29	Total	C	N	O	0	0
			229	160	33	36		

- Molecule 18 is a protein called BJ4_G0038800.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	h	31	Total	C	N	O	S	0	0
			246	169	40	36	1		

- Molecule 19 is a protein called Cytochrome c oxidase polypeptide VIIA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	i	49	Total	C	N	O	S	0	0
			411	270	72	66	3		

- Molecule 20 is a protein called BJ4_G0035470.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	j	57	Total	C	N	O	S	0	0
			482	313	79	85	5		

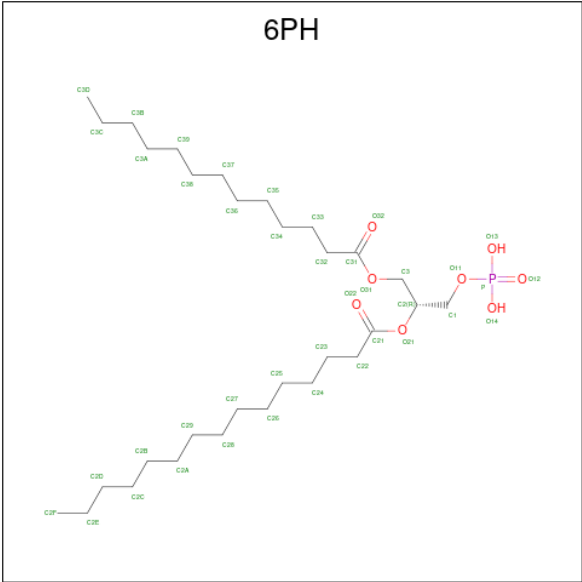
- Molecule 21 is a protein called Cytochrome c oxidase subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	k	18	Total	C	N	O	0	0
			90	54	18	18		

- Molecule 22 is a protein called Unknown Cox subunit.

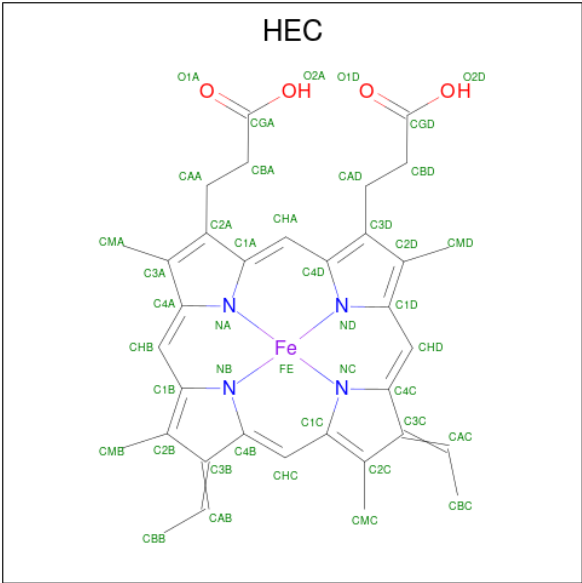
Mol	Chain	Residues	Atoms				AltConf	Trace
22	m	31	Total	C	N	O	0	0
			155	93	31	31		

- Molecule 23 is (1R)-2-(phosphonoxy)-1-[(tridecanoyloxy)methyl]ethyl pentadecanoate (CCD ID: 6PH) (formula: C₃₁H₆₁O₈P).



Mol	Chain	Residues	Atoms				AltConf
23	C	1	Total	C	O	P	0
			40	31	8	1	
23	N	1	Total	C	O	P	0
			40	31	8	1	

- Molecule 24 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



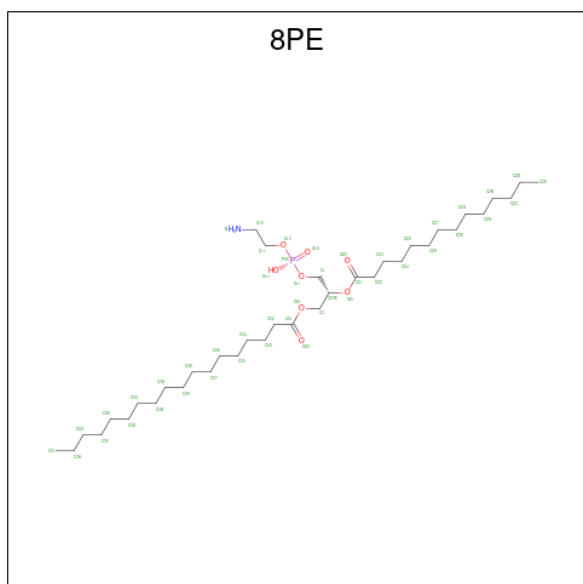
Mol	Chain	Residues	Atoms					AltConf
24	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
24	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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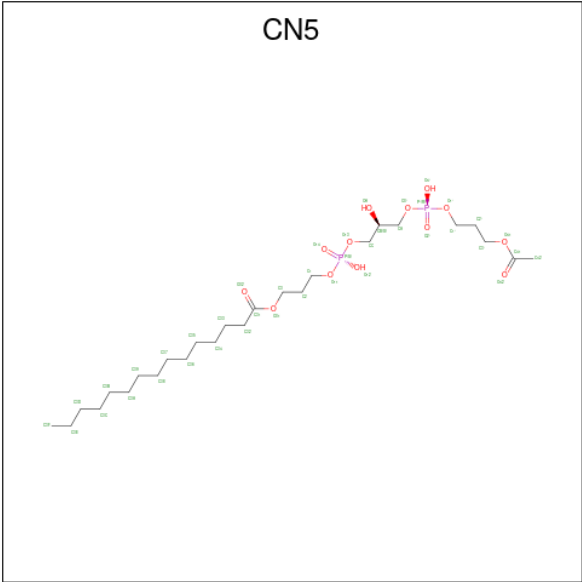
Mol	Chain	Residues	Atoms					AltConf
24	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
24	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
24	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
24	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 25 is (2R)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(tetradecanoyloxy)propyl octadecanoate (CCD ID: 8PE) (formula: C₃₇H₇₄NO₈P).



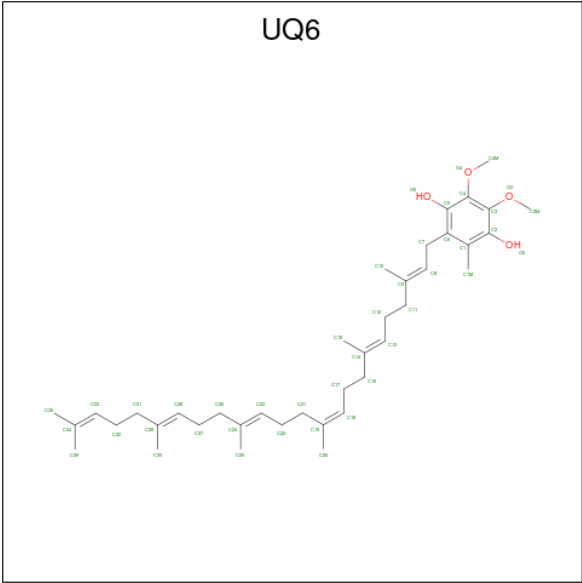
Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
25	N	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 26 is (5S,11R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-4,6,10,12,16-pentaoxa-5,11-di phosphaoctadec-1-yl pentadecanoate (CCD ID: CN5) (formula: C₂₆H₅₂O₁₃P₂).



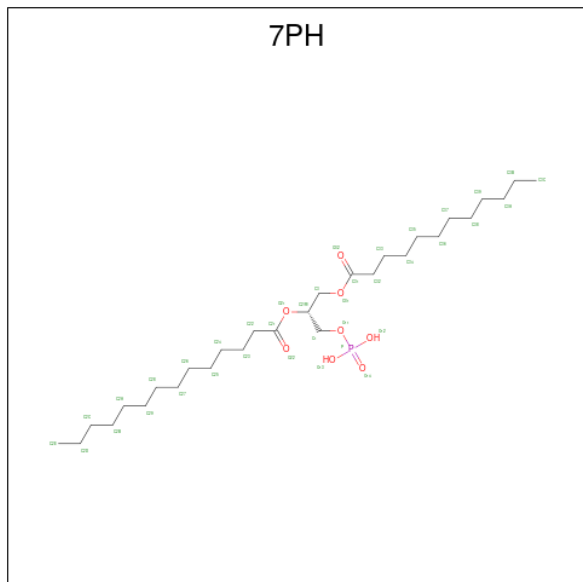
Mol	Chain	Residues	Atoms				AltConf
26	C	1	Total	C	O	P	0
			41	26	13	2	

- Molecule 27 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXA ENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula: C₃₉H₆₀O₄).



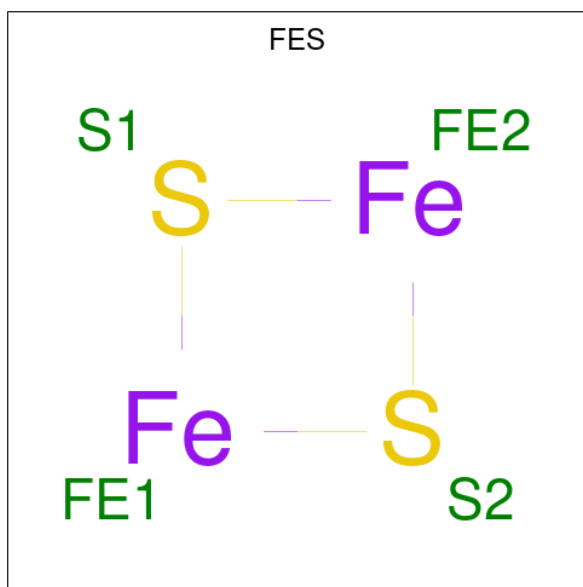
Mol	Chain	Residues	Atoms				AltConf
27	C	1	Total	C	O		0
			43	39	4		
27	N	1	Total	C	O		0
			43	39	4		

- Molecule 28 is (1R)-2-(dodecanoyloxy)-1-[(phosphonoxy)methyl]ethyl tetradecanoate (CCD ID: 7PH) (formula: $C_{29}H_{57}O_8P$).



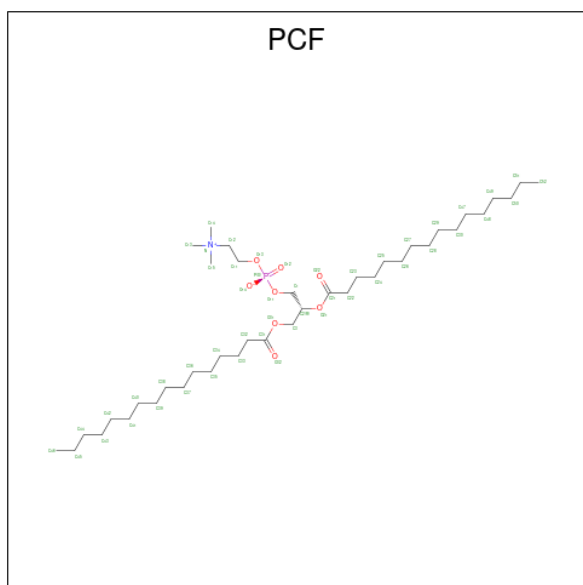
Mol	Chain	Residues	Atoms				AltConf
28	D	1	Total	C	O	P	0
			38	29	8	1	
28	P	1	Total	C	O	P	0
			38	29	8	1	

- Molecule 29 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



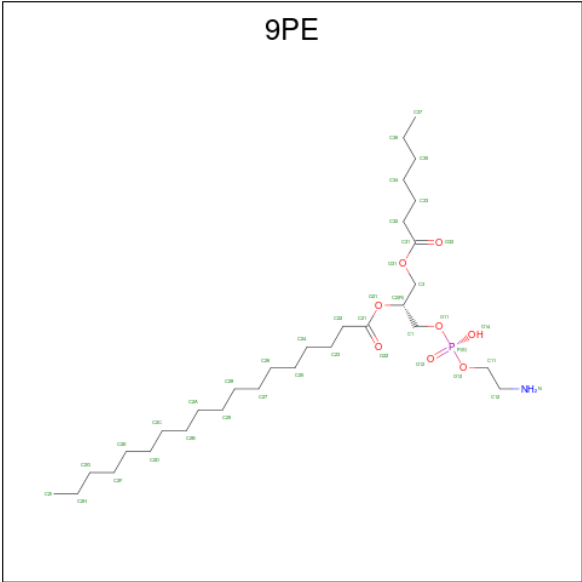
Mol	Chain	Residues	Atoms			AltConf
29	E	1	Total	Fe	S	0
			4	2	2	
29	P	1	Total	Fe	S	0
			4	2	2	

- Molecule 30 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (CCD ID: PCF) (formula: C₄₀H₈₀NO₈P).



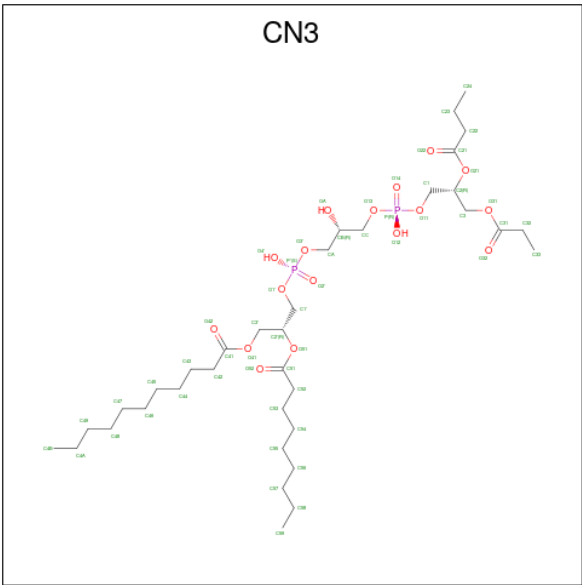
Mol	Chain	Residues	Atoms					AltConf
30	I	1	Total	C	N	O	P	0
			35	25	1	8	1	
30	T	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 31 is (1R)-2-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(heptanoyloxy)methyl]ethyl octadecanoate (CCD ID: 9PE) (formula: C₃₀H₆₀NO₈P).



Mol	Chain	Residues	Atoms					AltConf
31	N	1	Total	C	N	O	P	0
			40	30	1	8	1	
31	N	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 32 is (2R,5S,11R,14R)-5,8,11-trihydroxy-2-(nonanoyloxy)-5,11-dioxido-16-oxo-14-[(propanoyloxy)methyl]-4,6,10,12,15-pentaoxa-5,11-diphosphanadec-1-yl undecanoate (CCD ID: CN3) (formula: C₃₆H₆₈O₁₇P₂).

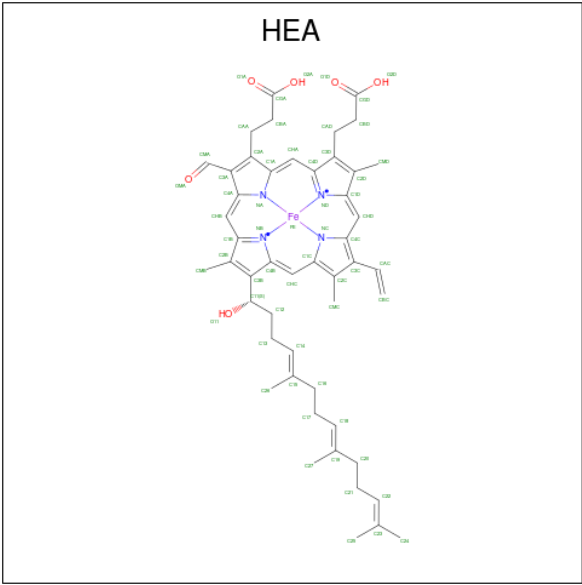


Mol	Chain	Residues	Atoms				AltConf
32	N	1	Total	C	O	P	0
			55	36	17	2	

- Molecule 33 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

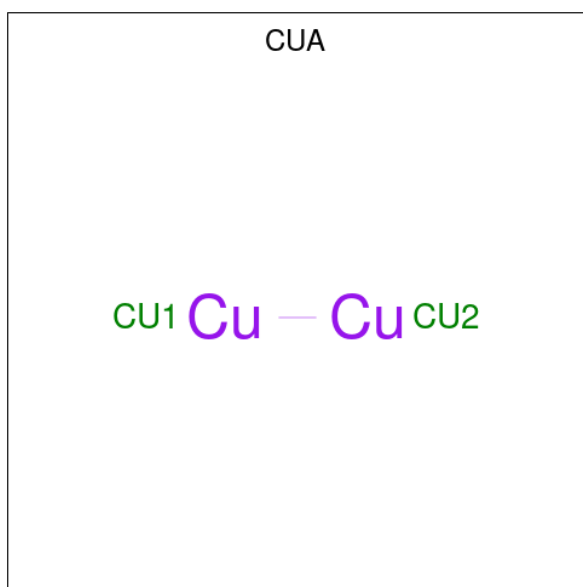
Mol	Chain	Residues	Atoms		AltConf
33	a	1	Total	Cu	0
			1	1	

- Molecule 34 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
34	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
34	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 35 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).

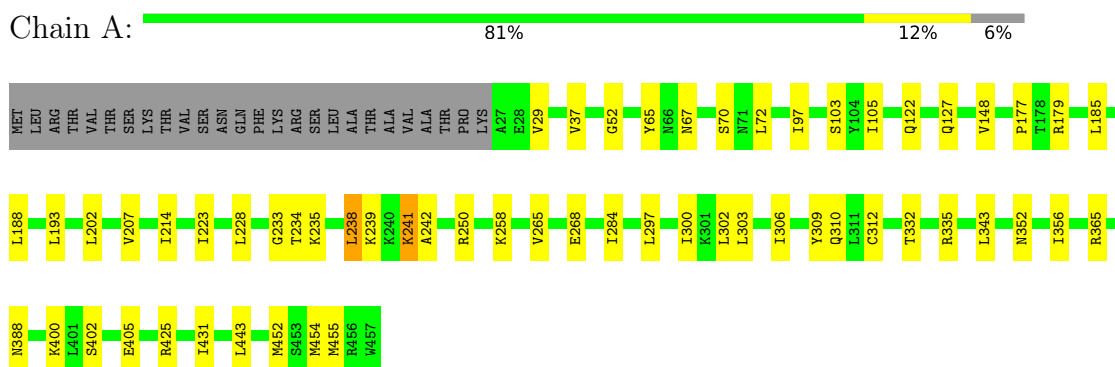


Mol	Chain	Residues	Atoms		AltConf
35	b	1	Total	Cu	0
			2	2	

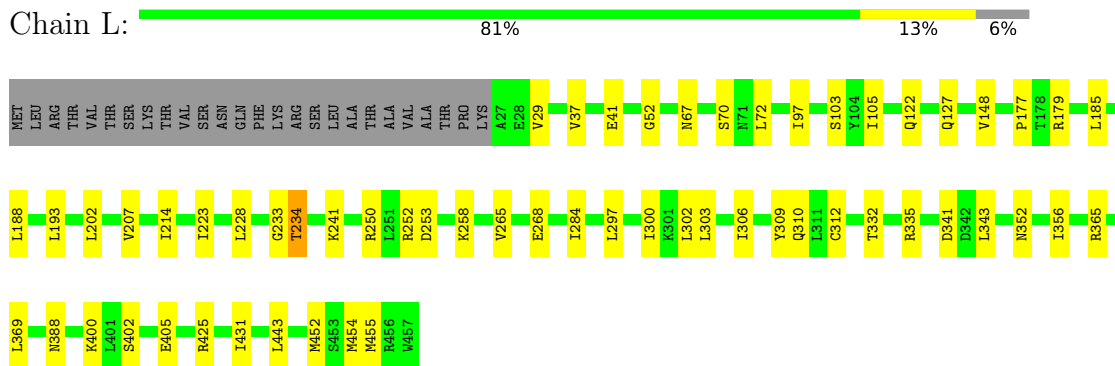
3 Residue-property plots

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

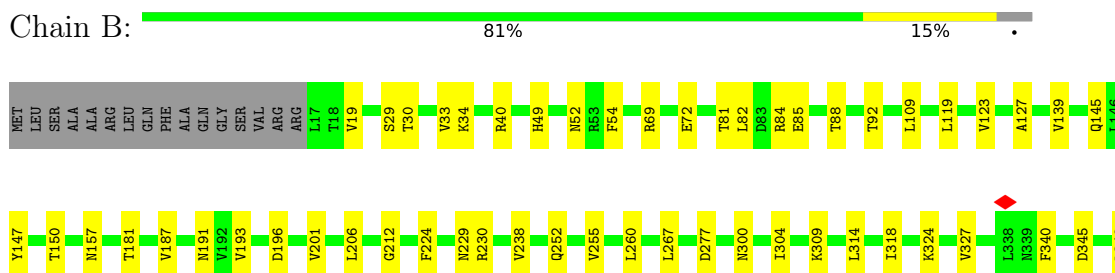
- Molecule 1: BJ4_G0001550.mRNA.1.CDS.1

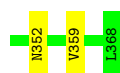


- Molecule 1: BJ4_G0001550.mRNA.1.CDS.1



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





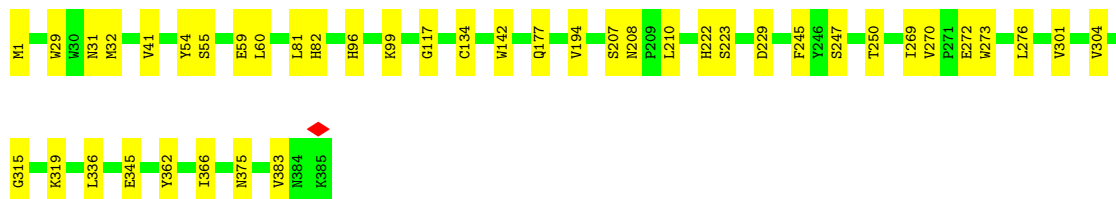
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M: 80% 15%



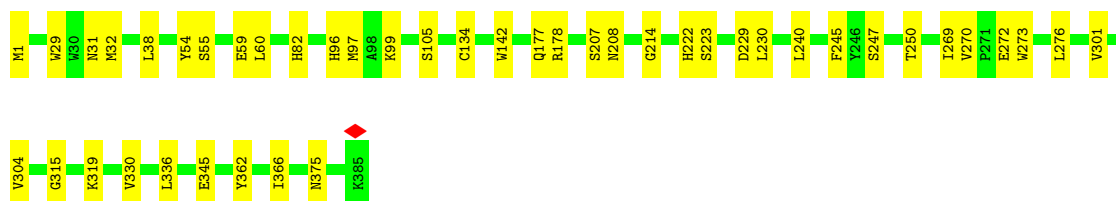
- Molecule 3: Cytochrome b

Chain C: 89% 11%



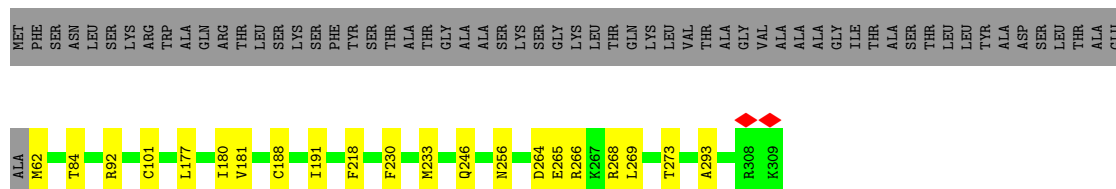
- Molecule 3: Cytochrome b

Chain N: 89% 11%

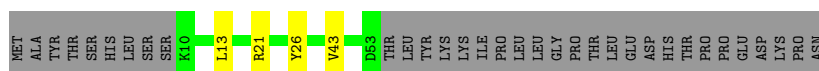


- Molecule 4: BJ4_G0049990.mRNA.1.CDS.1

Chain D: 73% 7% 20%

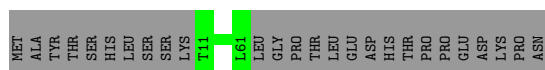


- Molecule 4: BJ4_G0049990.mRNA.1.CDS.1



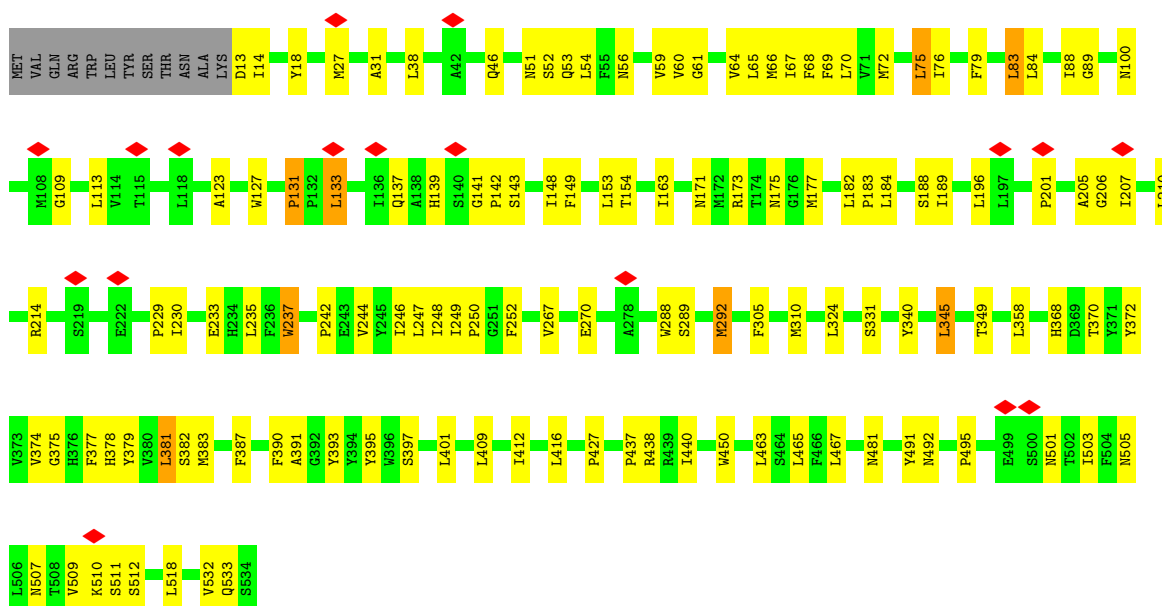
• Molecule 10: BJ4_G0023510.mRNA.1.CDS.1

Chain V: 66% 34%



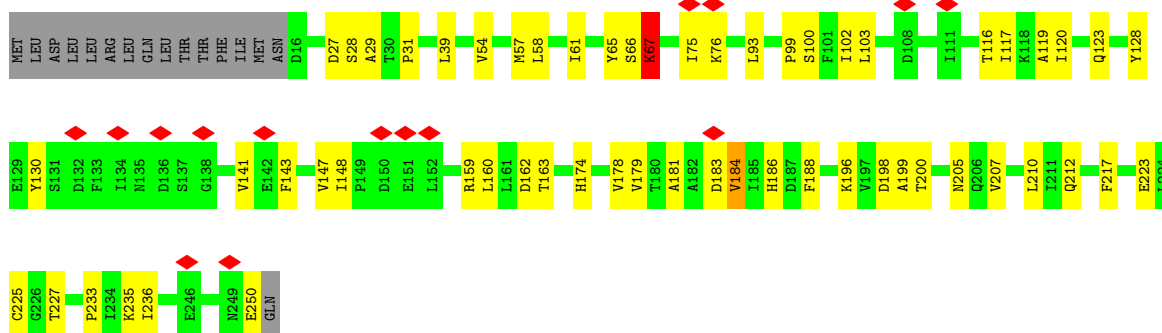
• Molecule 11: Cytochrome c oxidase subunit 1

Chain a: 73% 23% ..



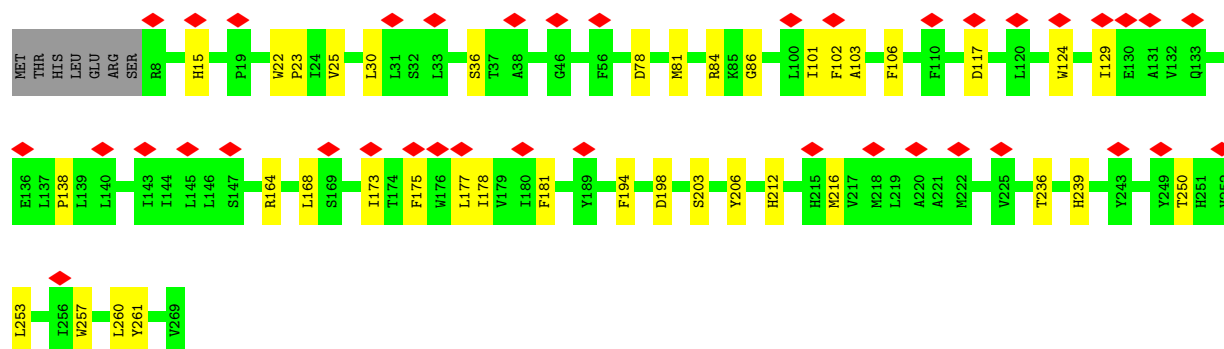
• Molecule 12: Cytochrome c oxidase subunit 2

Chain b: 6% 71% 22% 6%

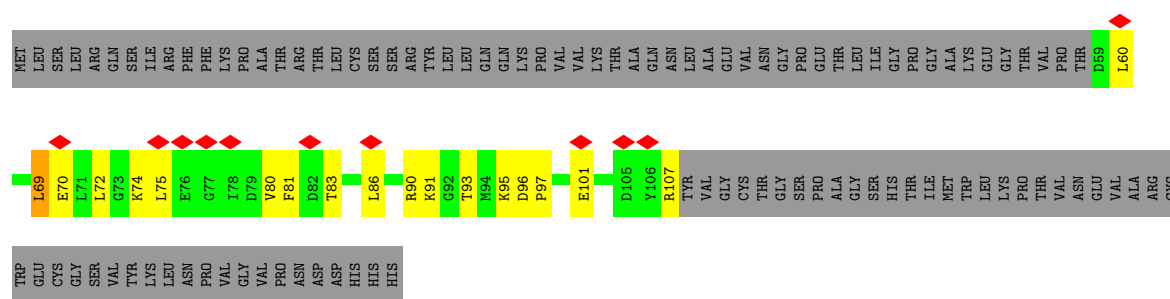


• Molecule 13: Cytochrome c oxidase subunit 3

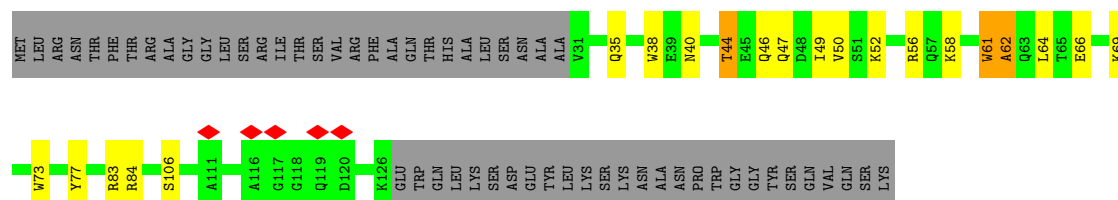
Chain c: 14% 83% 14%



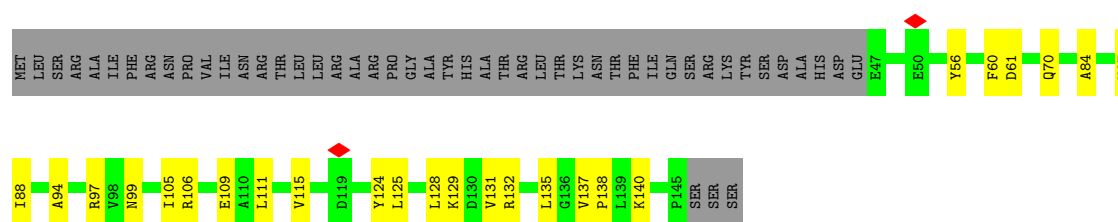
- Molecule 14: BJ4_G0018620.mRNA.1.CDS.1



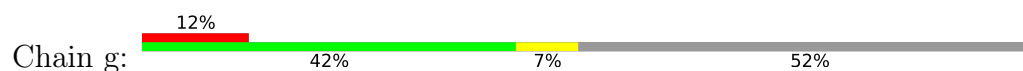
- Molecule 15: BJ4_G0046460.mRNA.1.CDS.1

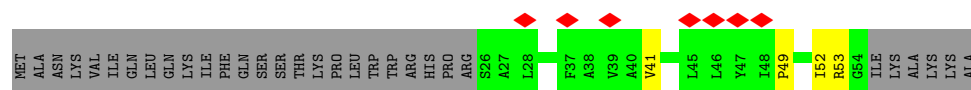


- Molecule 16: BJ4_G0024040.mRNA.1.CDS.1

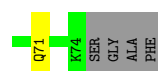
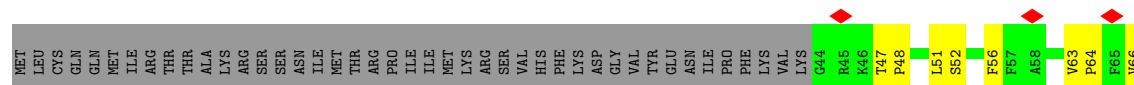


- Molecule 17: BJ4_G0043230.mRNA.1.CDS.1





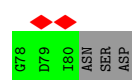
• Molecule 18: BJ4_G0038800.mRNA.1.CDS.1



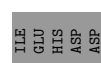
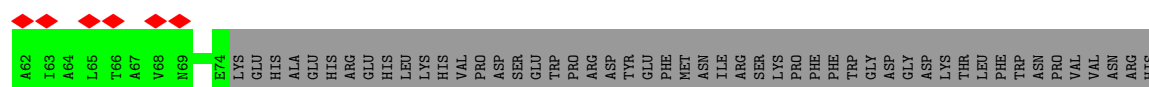
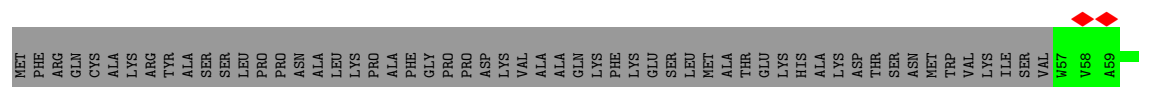
• Molecule 19: Cytochrome c oxidase polypeptide VIIA



• Molecule 20: BJ4_G0035470.mRNA.1.CDS.1



• Molecule 21: Cytochrome c oxidase subunit



• Molecule 22: Unknown Cox subunit



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	203271	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.423	Depositor
Minimum map value	-1.223	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.33	Depositor
Map size (Å)	392.19998, 392.19998, 392.19998	wwPDB
Map dimensions	370, 370, 370	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 8PE, UQ6, 9PE, 6PH, FES, HEA, CUA, PCF, CN3, CN5, 7PH, CU, HEC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/3405	0.60	0/4615
1	L	0.39	0/3405	0.62	2/4615 (0.0%)
2	B	0.38	0/2781	0.60	0/3764
2	M	0.38	0/2781	0.60	0/3764
3	C	0.43	0/3192	0.60	2/4354 (0.0%)
3	N	0.43	0/3192	0.60	2/4354 (0.0%)
4	D	0.37	0/2022	0.50	0/2751
4	O	0.37	0/2022	0.50	0/2751
5	E	0.23	0/1444	0.44	0/1957
5	P	0.23	0/1444	0.44	0/1957
6	F	0.29	0/638	0.57	0/858
6	Q	0.32	0/647	0.55	0/870
7	G	0.38	0/1040	0.62	0/1408
7	R	0.38	0/1040	0.62	0/1408
8	H	0.36	0/804	0.66	0/1088
8	S	0.36	0/804	0.66	0/1088
9	I	0.34	0/455	0.49	0/614
9	T	0.31	0/456	0.51	0/615
10	U	0.30	0/358	0.76	0/483
10	V	0.35	0/419	0.74	0/567
11	a	0.40	0/4183	0.84	5/5712 (0.1%)
12	b	0.29	0/1931	0.69	2/2641 (0.1%)
13	c	0.26	0/2158	0.62	0/2956
14	d	0.33	0/394	0.96	4/529 (0.8%)
15	e	0.36	0/750	0.86	2/1017 (0.2%)
16	f	0.33	0/845	0.76	0/1143
17	g	0.33	0/237	0.67	0/327
18	h	0.25	0/255	0.64	0/343
19	i	0.26	0/422	0.60	0/564
20	j	0.27	0/499	0.74	1/675 (0.1%)
21	k	0.14	0/89	0.37	0/123
All	All	0.36	0/44112	0.63	20/59911 (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
3	C	0	2
3	N	0	2
11	a	0	3
12	b	0	3
13	c	0	1
15	e	0	2
20	j	0	1
All	All	0	14

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	234	THR	CA-C-N	8.77	134.90	120.86
1	L	234	THR	C-N-CA	8.77	134.90	120.86
3	N	222	HIS	CA-C-N	6.05	133.09	121.54
3	N	222	HIS	C-N-CA	6.05	133.09	121.54
3	C	222	HIS	CA-C-N	6.03	133.05	121.54
3	C	222	HIS	C-N-CA	6.03	133.05	121.54
14	d	60	LEU	CA-C-N	5.91	132.33	123.05
14	d	60	LEU	C-N-CA	5.91	132.33	123.05
14	d	81	PHE	CA-C-N	5.58	132.19	121.54
14	d	81	PHE	C-N-CA	5.58	132.19	121.54
11	a	237	TRP	CA-CB-CG	-5.56	103.03	113.60
12	b	29	ALA	CA-C-N	5.35	134.84	121.80
12	b	29	ALA	C-N-CA	5.35	134.84	121.80
20	j	38	VAL	N-CA-C	5.22	120.20	109.34
11	a	237	TRP	CB-CA-C	5.12	118.92	110.88
15	e	61	TRP	CA-C-N	5.12	131.32	121.54
15	e	61	TRP	C-N-CA	5.12	131.32	121.54
11	a	518	LEU	CA-C-N	5.02	131.13	121.54
11	a	518	LEU	C-N-CA	5.02	131.13	121.54
11	a	292	MET	CG-SD-CE	-5.00	89.89	100.90

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	223	SER	Mainchain
3	C	272	GLU	Peptide
3	N	223	SER	Mainchain
3	N	272	GLU	Peptide
11	a	131	PRO	Peptide
11	a	133	LEU	Peptide
11	a	288	TRP	Peptide
12	b	183	ASP	Peptide
12	b	66	SER	Peptide
12	b	67	LYS	Peptide
13	c	203	SER	Peptide
15	e	44	THR	Peptide
15	e	62	ALA	Peptide
20	j	37	CYS	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	3344	0	3323	36	0
1	L	3344	0	3323	37	0
2	B	2735	0	2774	33	0
2	M	2735	0	2774	35	0
3	C	3090	0	3128	28	0
3	N	3090	0	3129	33	0
4	D	1961	0	1890	25	0
4	O	1961	0	1890	30	0
5	E	1411	0	1388	12	0
5	P	1411	0	1388	10	0
6	F	624	0	581	7	0
6	Q	633	0	587	6	0
7	G	1019	0	1034	9	0
7	R	1019	0	1034	9	0
8	H	773	0	736	5	0
8	S	773	0	736	8	0
9	I	442	0	440	3	0
9	T	443	0	440	6	0
10	U	347	0	345	3	0
10	V	406	0	414	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	a	4058	0	4084	96	0
12	b	1879	0	1860	42	0
13	c	2087	0	2076	23	0
14	d	390	0	387	9	0
15	e	733	0	709	17	0
16	f	828	0	807	20	0
17	g	229	0	237	3	0
18	h	246	0	249	7	0
19	i	411	0	415	7	0
20	j	482	0	445	5	0
21	k	90	0	46	0	0
22	m	155	0	33	0	0
23	C	40	0	59	1	0
23	N	40	0	59	5	0
24	C	86	0	64	11	0
24	D	43	0	32	17	0
24	N	86	0	64	13	0
24	O	43	0	32	8	0
25	C	47	0	73	0	0
25	N	47	0	73	1	0
26	C	41	0	50	3	0
27	C	43	0	58	1	0
27	N	43	0	58	3	0
28	D	38	0	55	3	0
28	P	38	0	55	4	0
29	E	4	0	0	2	0
29	P	4	0	0	2	0
30	I	35	0	44	0	0
30	T	35	0	44	1	0
31	N	80	0	118	0	0
32	N	55	0	66	3	0
33	a	1	0	0	0	0
34	a	120	0	108	9	0
35	b	2	0	0	0	0
All	All	44120	0	43814	519	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 6.

All (519) 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)
4:O:101:CYS:SG	24:O:401:HEC:HAB	1.47	1.51
4:O:101:CYS:SG	24:O:401:HEC:CAB	2.12	1.35
4:D:101:CYS:SG	24:D:401:HEC:CAB	2.17	1.31
24:D:401:HEC:HMB3	24:D:401:HEC:HBB3	1.34	1.05
3:N:105:SER:OG	24:N:404:HEC:O2D	1.81	0.97
4:D:101:CYS:SG	24:D:401:HEC:HAB	2.08	0.91
16:f:111:LEU:O	16:f:115:VAL:HB	1.71	0.90
4:O:218:PHE:HE1	24:O:401:HEC:O2A	1.55	0.89
4:D:101:CYS:SG	24:D:401:HEC:CBB	2.63	0.86
16:f:125:LEU:O	16:f:129:LYS:HB2	1.74	0.86
4:D:218:PHE:HE1	24:D:401:HEC:O2A	1.58	0.86
4:O:218:PHE:CE1	24:O:401:HEC:O2A	2.30	0.84
24:C:403:HEC:HBB2	24:C:403:HEC:HMB3	1.62	0.82
11:a:65:LEU:O	11:a:69:PHE:HB2	1.82	0.79
6:F:131:GLN:O	6:F:135:ASP:HB2	1.84	0.78
4:O:101:CYS:CB	24:O:401:HEC:HAB	2.13	0.78
11:a:66:MET:HG2	34:a:602:HEA:HBC1	1.66	0.78
16:f:124:TYR:O	16:f:128:LEU:HB2	1.85	0.77
11:a:381:LEU:HD23	34:a:603:HEA:HBC2	1.67	0.77
3:N:105:SER:HB3	24:N:404:HEC:HBD2	1.69	0.75
4:D:218:PHE:CE1	24:D:401:HEC:O2A	2.40	0.74
24:D:401:HEC:HBA2	24:D:401:HEC:HHA	1.70	0.73
24:N:404:HEC:HBC2	24:N:404:HEC:HMC3	1.71	0.72
8:H:31:PRO:HA	8:H:34:GLN:HB3	1.74	0.70
16:f:56:TYR:O	16:f:60:PHE:HB2	1.91	0.70
8:S:31:PRO:HA	8:S:34:GLN:HB3	1.74	0.69
3:N:105:SER:CB	24:N:404:HEC:HBD2	2.22	0.69
12:b:116:THR:HG21	20:j:58:LEU:H	1.58	0.68
1:L:202:LEU:HB3	1:L:233:GLY:HA2	1.75	0.68
1:A:241:LYS:HB2	1:A:241:LYS:NZ	2.09	0.67
1:A:241:LYS:HB2	1:A:241:LYS:HZ3	1.59	0.67
24:C:403:HEC:HBC2	24:C:403:HEC:CMC	2.24	0.67
12:b:117:ILE:HD11	12:b:128:TYR:HB3	1.75	0.67
11:a:14:ILE:O	11:a:18:TYR:HB2	1.96	0.65
4:O:230:PHE:H	4:O:233:MET:HE3	1.60	0.65
11:a:205:ALA:HB2	13:c:101:ILE:HG13	1.78	0.65
11:a:175:ASN:ND2	14:d:83:THR:O	2.30	0.65
4:D:230:PHE:H	4:D:233:MET:HE3	1.60	0.65
11:a:177:MET:HE2	11:a:183:PRO:HD3	1.78	0.65
11:a:370:THR:HG23	11:a:372:TYR:H	1.62	0.65
20:j:45:PHE:O	20:j:49:LYS:HB2	1.97	0.65
1:L:365:ARG:NH2	2:M:72:GLU:OE2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:89:GLY:HA2	11:a:510:LYS:HE2	1.79	0.64
24:C:403:HEC:HBB2	24:C:403:HEC:CMB	2.27	0.64
14:d:70:GLU:O	14:d:74:LYS:HB2	1.98	0.64
1:A:365:ARG:NH2	2:B:72:GLU:OE2	2.30	0.64
11:a:378:HIS:O	11:a:382:SER:HB3	1.98	0.63
24:C:403:HEC:HBC2	24:C:403:HEC:HMC3	1.78	0.63
5:P:183:SER:OG	29:P:302:FES:S1	2.56	0.63
14:d:93:THR:HG22	14:d:95:LYS:H	1.63	0.63
24:D:401:HEC:HMB3	24:D:401:HEC:CBB	2.17	0.63
11:a:67:ILE:HD11	34:a:602:HEA:HHD	1.78	0.63
11:a:532:VAL:HG11	14:d:86:LEU:H	1.63	0.63
18:h:47:THR:HG23	18:h:51:LEU:H	1.65	0.62
3:C:345:GLU:OE2	4:D:62:MET:N	2.33	0.62
11:a:79:PHE:O	11:a:83:LEU:HB3	2.00	0.61
11:a:331:SER:HA	12:b:67:LYS:HG3	1.82	0.61
4:D:101:CYS:CA	24:D:401:HEC:HAB	2.31	0.61
4:D:101:CYS:SG	24:D:401:HEC:C3B	2.89	0.61
4:O:188:CYS:SG	4:O:256:ASN:ND2	2.72	0.61
11:a:133:LEU:O	11:a:137:GLN:NE2	2.34	0.60
11:a:267:VAL:HB	12:b:76:LYS:HE2	1.83	0.60
11:a:505:ASN:HB2	11:a:511:SER:HA	1.81	0.60
4:D:188:CYS:SG	4:D:256:ASN:ND2	2.72	0.60
3:N:32:MET:HE1	32:N:408:CN3:H43A	1.83	0.60
16:f:94:ALA:HA	16:f:97:ARG:HE	1.67	0.60
1:A:300:ILE:HG22	1:A:302:LEU:H	1.67	0.59
24:N:404:HEC:HAA2	27:N:405:UQ6:H3M2	1.83	0.59
1:L:300:ILE:HG22	1:L:302:LEU:H	1.67	0.59
3:N:315:GLY:O	3:N:319:LYS:NZ	2.35	0.59
11:a:375:GLY:O	11:a:379:TYR:HB2	2.02	0.59
19:i:41:ILE:O	19:i:45:GLU:HB2	2.02	0.59
11:a:68:PHE:HB3	11:a:154:THR:HG21	1.85	0.59
1:A:284:ILE:O	1:A:365:ARG:NH1	2.36	0.59
2:B:33:VAL:HG11	2:B:109:LEU:HD11	1.85	0.59
1:L:122:GLN:OE1	1:L:127:GLN:NE2	2.36	0.59
26:C:405:CN5:H3AB	23:N:402:6PH:H2FA	1.84	0.59
1:A:122:GLN:OE1	1:A:127:GLN:NE2	2.36	0.59
1:A:250:ARG:NH1	1:A:443:LEU:O	2.36	0.59
2:M:33:VAL:HG11	2:M:109:LEU:HD11	1.85	0.59
1:A:148:VAL:HG22	1:A:179:ARG:HG3	1.85	0.58
5:E:69:ALA:HA	9:I:29:GLN:HE21	1.67	0.58
1:L:148:VAL:HG22	1:L:179:ARG:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LEU:O	2:B:69:ARG:NH2	2.36	0.58
5:E:183:SER:OG	29:E:301:FES:S1	2.56	0.58
11:a:349:THR:HG21	12:b:54:VAL:HG21	1.85	0.58
1:L:284:ILE:O	1:L:365:ARG:NH1	2.36	0.58
2:M:145:GLN:OE1	2:M:229:ASN:ND2	2.37	0.58
11:a:100:ASN:HB3	13:c:25:VAL:HG11	1.84	0.58
2:B:145:GLN:OE1	2:B:229:ASN:ND2	2.37	0.58
3:C:315:GLY:O	3:C:319:LYS:NZ	2.35	0.58
24:D:401:HEC:HBB3	24:D:401:HEC:CMB	2.17	0.57
14:d:69:LEU:HA	14:d:72:LEU:HB2	1.85	0.57
3:C:194:VAL:CG2	24:C:403:HEC:HBB3	2.34	0.57
1:L:250:ARG:NH1	1:L:443:LEU:O	2.36	0.57
1:L:352:ASN:ND2	1:L:452:MET:O	2.35	0.57
4:O:83:GLU:HA	9:T:44:ASN:HD21	1.69	0.57
6:Q:106:LYS:O	6:Q:110:GLN:NE2	2.36	0.57
5:E:53:ARG:HH22	9:I:8:LYS:HE2	1.69	0.57
12:b:141:VAL:HG11	12:b:250:GLU:HB2	1.87	0.57
11:a:358:LEU:HD23	34:a:603:HEA:HBA1	1.85	0.57
1:A:303:LEU:HA	1:A:306:ILE:HG22	1.87	0.57
13:c:81:MET:SD	13:c:84:ARG:NH1	2.77	0.57
2:B:318:ILE:HD11	2:B:340:PHE:HB3	1.87	0.57
4:D:269:LEU:HD22	28:D:402:7PH:H1	1.87	0.57
1:L:356:ILE:HD13	1:L:454:MET:HE1	1.87	0.57
20:j:73:LYS:HE3	20:j:75:ILE:HD12	1.86	0.57
1:A:356:ILE:HD13	1:A:454:MET:HE1	1.87	0.57
3:N:247:SER:OG	3:N:250:THR:OG1	2.23	0.56
3:C:31:ASN:HD21	3:C:229:ASP:HA	1.70	0.56
7:G:5:PHE:HA	7:G:8:ILE:HG22	1.87	0.56
1:L:303:LEU:HA	1:L:306:ILE:HG22	1.87	0.56
11:a:109:GLY:HA3	11:a:153:LEU:HD11	1.87	0.56
14:d:69:LEU:HD22	14:d:80:VAL:HA	1.85	0.56
1:A:352:ASN:ND2	1:A:452:MET:O	2.35	0.56
2:B:252:GLN:NE2	2:B:345:ASP:O	2.39	0.56
2:M:252:GLN:NE2	2:M:345:ASP:O	2.39	0.56
4:O:269:LEU:HD22	28:P:301:7PH:H1	1.87	0.56
12:b:186:HIS:HA	12:b:223:GLU:HB3	1.85	0.56
11:a:184:LEU:O	11:a:188:SER:HB2	2.06	0.56
12:b:119:ALA:H	12:b:179:VAL:HG12	1.68	0.56
2:B:150:THR:HG22	2:B:352:ASN:HD22	1.70	0.56
1:L:37:VAL:HB	1:L:207:VAL:HG22	1.88	0.56
2:M:150:THR:HG22	2:M:352:ASN:HD22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:375:ASN:HB3	7:R:8:ILE:HD12	1.88	0.55
11:a:38:LEU:HG	11:a:46:GLN:HG3	1.88	0.55
12:b:120:ILE:HG13	12:b:181:ALA:HA	1.87	0.55
14:d:90:ARG:NH2	14:d:97:PRO:O	2.38	0.55
19:i:33:TRP:O	19:i:37:HIS:HB3	2.06	0.55
3:N:31:ASN:HD21	3:N:229:ASP:HA	1.70	0.55
2:B:267:LEU:HD13	2:B:304:ILE:HD12	1.88	0.55
14:d:101:GLU:O	14:d:107:ARG:NH1	2.39	0.55
1:A:29:VAL:HG21	1:A:400:LYS:HD3	1.89	0.55
3:C:247:SER:OG	3:C:250:THR:OG1	2.23	0.55
1:L:29:VAL:HG21	1:L:400:LYS:HD3	1.89	0.55
2:M:318:ILE:HD11	2:M:340:PHE:HB3	1.87	0.55
1:L:223:ILE:HG23	1:L:228:LEU:HD23	1.89	0.55
11:a:270:GLU:H	12:b:76:LYS:HB3	1.71	0.55
3:C:117:GLY:O	24:C:403:HEC:HMC2	2.07	0.55
4:D:92:ARG:HH22	4:D:246:GLN:HE21	1.55	0.55
4:O:92:ARG:HH22	4:O:246:GLN:HE21	1.55	0.55
1:A:238:LEU:HD13	1:A:238:LEU:N	2.22	0.55
2:M:267:LEU:HD13	2:M:304:ILE:HD12	1.88	0.55
7:R:5:PHE:HA	7:R:8:ILE:HG22	1.88	0.55
1:A:37:VAL:HB	1:A:207:VAL:HG22	1.88	0.54
5:P:181:HIS:HB2	29:P:302:FES:S1	2.48	0.54
11:a:173:ARG:HH12	11:a:182:LEU:HD11	1.72	0.54
3:C:32:MET:HB2	3:C:96:HIS:HD1	1.73	0.54
11:a:324:LEU:HD11	12:b:57:MET:HB3	1.87	0.54
3:N:54:TYR:OH	3:N:134:CYS:O	2.24	0.54
11:a:61:GLY:O	11:a:65:LEU:HB3	2.08	0.54
3:C:375:ASN:HB3	7:G:8:ILE:HD12	1.90	0.54
3:N:32:MET:HB2	3:N:96:HIS:HD1	1.73	0.54
15:e:38:TRP:NE1	15:e:40:ASN:O	2.41	0.54
11:a:412:ILE:HG13	11:a:467:LEU:HD21	1.90	0.54
2:B:260:LEU:HD22	2:B:267:LEU:HD11	1.90	0.53
12:b:174:HIS:HD2	12:b:210:LEU:HB3	1.73	0.53
15:e:73:TRP:O	15:e:77:TYR:HB2	2.08	0.53
24:N:404:HEC:HBC2	24:N:404:HEC:CMC	2.37	0.53
11:a:52:SER:H	12:b:227:THR:HA	1.73	0.53
2:M:260:LEU:HD22	2:M:267:LEU:HD11	1.90	0.53
8:S:80:LEU:HD13	8:S:89:LEU:HD23	1.91	0.53
1:A:241:LYS:HG3	1:A:242:ALA:N	2.24	0.53
4:D:181:VAL:HG12	4:D:191:ILE:HG13	1.90	0.53
3:N:59:GLU:HG3	3:N:60:LEU:HG	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:80:LEU:HD13	8:H:89:LEU:HD23	1.91	0.53
1:A:223:ILE:HG23	1:A:228:LEU:HD23	1.89	0.53
5:E:181:HIS:HB2	29:E:301:FES:S1	2.47	0.53
11:a:324:LEU:HD21	12:b:57:MET:HG3	1.91	0.53
11:a:368:HIS:HB3	12:b:196:LYS:HD3	1.91	0.53
11:a:492:ASN:HB3	11:a:495:PRO:HD2	1.90	0.53
11:a:391:ALA:O	11:a:395:TYR:HB2	2.09	0.53
11:a:503:ILE:HD12	11:a:533:GLN:HG3	1.90	0.53
4:O:181:VAL:HG12	4:O:191:ILE:HG13	1.90	0.53
11:a:465:LEU:HD21	34:a:602:HEA:H272	1.90	0.53
3:C:59:GLU:HG3	3:C:60:LEU:HG	1.90	0.52
4:D:265:GLU:OE2	4:D:268:ARG:NH2	2.42	0.52
5:P:70:GLY:HA3	28:P:301:7PH:H35	1.91	0.52
11:a:53:GLN:NE2	18:h:71:GLN:OE1	2.43	0.52
3:C:270:VAL:HG13	3:C:276:LEU:HD11	1.91	0.52
24:D:401:HEC:HBA2	24:D:401:HEC:CHA	2.37	0.52
11:a:84:LEU:HB2	11:a:189:ILE:HD11	1.92	0.52
15:e:66:GLU:HA	15:e:69:LYS:HB3	1.90	0.52
1:L:297:LEU:O	2:M:69:ARG:NH2	2.43	0.52
3:N:330:VAL:HG13	25:N:406:8PE:H3CA	1.92	0.52
11:a:391:ALA:O	11:a:395:TYR:CB	2.57	0.52
13:c:175:PHE:HA	13:c:178:ILE:HG12	1.90	0.52
15:e:61:TRP:HZ2	16:f:99:ASN:HA	1.75	0.52
1:A:402:SER:OG	1:A:405:GLU:OE1	2.28	0.52
11:a:54:LEU:HD13	18:h:71:GLN:HB3	1.93	0.51
11:a:509:VAL:HG13	11:a:510:LYS:HD2	1.91	0.51
1:L:67:ASN:HD21	1:L:177:PRO:HD2	1.76	0.51
2:M:19:VAL:HG12	2:M:187:VAL:HB	1.93	0.51
11:a:64:VAL:HG13	11:a:113:LEU:HD11	1.91	0.51
11:a:133:LEU:HB2	12:b:184:VAL:HG22	1.92	0.51
3:C:41:VAL:HG22	27:C:406:UQ6:H203	1.93	0.51
12:b:148:ILE:HD13	12:b:162:ASP:HB3	1.91	0.51
3:N:270:VAL:HG13	3:N:276:LEU:HD11	1.91	0.51
11:a:139:HIS:HE1	11:a:214:ARG:HD2	1.76	0.51
11:a:390:PHE:HE1	34:a:602:HEA:H242	1.76	0.51
12:b:198:ASP:H	12:b:205:ASN:HD21	1.58	0.51
14:d:91:LYS:HD2	14:d:96:ASP:HB3	1.91	0.51
11:a:244:VAL:HA	11:a:247:LEU:HD12	1.93	0.51
12:b:99:PRO:HA	12:b:102:ILE:HG22	1.91	0.51
4:D:101:CYS:SG	24:D:401:HEC:HBB3	2.49	0.51
13:c:138:PRO:O	13:c:261:TYR:OH	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:40:ARG:HD3	2:M:85:GLU:HG2	1.93	0.51
12:b:179:VAL:HG21	12:b:188:PHE:HE1	1.76	0.51
13:c:236:THR:H	13:c:239:HIS:HB3	1.76	0.51
1:A:67:ASN:HD21	1:A:177:PRO:HD2	1.76	0.51
2:B:40:ARG:HD3	2:B:85:GLU:HG2	1.93	0.51
2:B:147:TYR:OH	2:B:277:ASP:OD2	2.29	0.51
1:L:402:SER:OG	1:L:405:GLU:OE1	2.28	0.51
11:a:345:LEU:HD12	12:b:58:LEU:HD11	1.93	0.51
3:C:117:GLY:C	24:C:403:HEC:HBC3	2.37	0.50
7:G:115:LYS:NZ	7:G:119:GLU:OE2	2.44	0.50
2:M:147:TYR:OH	2:M:277:ASP:OD2	2.29	0.50
13:c:194:PHE:O	13:c:206:TYR:OH	2.26	0.50
16:f:106:ARG:NE	16:f:109:GLU:OE2	2.42	0.50
24:C:403:HEC:CMB	24:C:403:HEC:CBB	2.89	0.50
11:a:438:ARG:NH1	34:a:603:HEA:O1D	2.43	0.50
18:h:52:SER:O	18:h:56:PHE:CB	2.59	0.50
11:a:56:ASN:HA	11:a:59:VAL:HG22	1.93	0.50
12:b:65:TYR:HB3	12:b:67:LYS:HD3	1.93	0.50
12:b:159:ARG:HG2	12:b:160:LEU:HG	1.92	0.50
7:R:115:LYS:NZ	7:R:119:GLU:OE2	2.44	0.50
20:j:37:CYS:O	20:j:39:ASN:N	2.44	0.50
11:a:171:ASN:HD22	13:c:86:GLY:HA3	1.77	0.50
2:B:19:VAL:HG12	2:B:187:VAL:HB	1.93	0.50
16:f:94:ALA:HB2	16:f:97:ARG:HH11	1.76	0.50
11:a:491:TYR:O	16:f:70:GLN:NE2	2.45	0.50
11:a:507:ASN:ND2	11:a:532:VAL:H	2.10	0.50
4:D:101:CYS:CB	24:D:401:HEC:HAB	2.40	0.50
4:O:293:ALA:HB1	8:S:34:GLN:HG2	1.94	0.50
12:b:163:THR:H	12:b:235:LYS:HE3	1.76	0.50
4:O:181:VAL:HG21	4:O:256:ASN:HA	1.95	0.49
4:O:265:GLU:OE2	4:O:268:ARG:NH2	2.42	0.49
1:A:202:LEU:HB3	1:A:233:GLY:HA2	1.93	0.49
32:N:408:CN3:O14	4:O:288:LYS:NZ	2.37	0.49
12:b:198:ASP:OD1	12:b:199:ALA:N	2.45	0.49
18:h:52:SER:O	18:h:56:PHE:HB2	2.12	0.49
11:a:463:LEU:HD13	15:e:106:SER:HB3	1.93	0.49
11:a:206:GLY:HA3	11:a:235:LEU:HD21	1.94	0.49
3:C:54:TYR:OH	3:C:134:CYS:O	2.24	0.49
11:a:409:LEU:HA	11:a:412:ILE:HG12	1.95	0.49
3:N:207:SER:HB3	24:N:404:HEC:O2D	2.13	0.49
17:g:52:ILE:HG23	17:g:53:ARG:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:26:PHE:HB2	10:U:43:VAL:HG22	1.94	0.49
12:b:28:SER:O	19:i:48:TYR:OH	2.31	0.49
4:D:84:THR:OG1	4:D:264:ASP:OD1	2.31	0.49
4:O:84:THR:OG1	4:O:264:ASP:OD1	2.31	0.49
4:O:273:THR:HG23	28:P:301:7PH:H32	1.95	0.49
10:U:13:LEU:HD13	10:U:21:ARG:HD3	1.95	0.49
11:a:61:GLY:O	11:a:65:LEU:CB	2.61	0.48
12:b:198:ASP:HB2	12:b:200:THR:HG23	1.95	0.48
26:C:405:CN5:H3E	23:N:402:6PH:H2B	1.95	0.48
11:a:123:ALA:H	11:a:143:SER:HB2	1.77	0.48
4:O:113:ARG:HD3	5:P:90:ALA:HB2	1.96	0.48
9:T:13:ARG:HB2	9:T:16:VAL:HG12	1.95	0.48
3:N:29:TRP:O	3:N:99:LYS:NZ	2.47	0.48
15:e:35:GLN:HE22	15:e:56:ARG:HH12	1.61	0.48
3:C:29:TRP:O	3:C:99:LYS:NZ	2.47	0.48
4:D:181:VAL:HG21	4:D:256:ASN:HA	1.95	0.48
2:M:81:THR:OG1	2:M:88:THR:OG1	2.32	0.48
5:P:186:ASP:OD1	5:P:190:ARG:N	2.41	0.48
13:c:15:HIS:NE2	13:c:78:ASP:O	2.47	0.48
6:F:77:GLN:HG2	6:F:145:LYS:HB3	1.96	0.48
1:L:455:MET:HE1	23:N:402:6PH:H1	1.96	0.48
1:A:455:MET:HE1	23:C:401:6PH:H1	1.96	0.48
3:C:210:LEU:HD12	7:G:79:HIS:HD2	1.79	0.48
3:C:362:TYR:HA	3:C:366:ILE:HB	1.95	0.48
2:B:81:THR:OG1	2:B:88:THR:OG1	2.32	0.47
4:D:273:THR:HG23	28:D:402:7PH:H32	1.95	0.47
5:E:95:GLU:HG3	5:E:213:ILE:HG22	1.96	0.47
3:N:362:TYR:HA	3:N:366:ILE:HB	1.95	0.47
1:A:241:LYS:NZ	1:A:241:LYS:CB	2.73	0.47
2:M:181:THR:HB	2:M:212:GLY:H	1.79	0.47
12:b:163:THR:HB	12:b:235:LYS:HG2	1.95	0.47
15:e:62:ALA:H	15:e:64:LEU:HD23	1.79	0.47
16:f:61:ASP:HA	16:f:97:ARG:HH12	1.78	0.47
3:N:97:MET:HG2	24:N:404:HEC:HBC2	1.97	0.47
6:Q:100:GLU:OE2	6:Q:104:ARG:NH2	2.45	0.47
6:F:95:VAL:HG12	6:F:130:LEU:HD11	1.96	0.47
24:N:404:HEC:HHA	24:N:404:HEC:O2A	2.15	0.47
13:c:164:ARG:HE	13:c:168:LEU:HG	1.80	0.47
11:a:131:PRO:HG2	11:a:229:PRO:HB3	1.95	0.47
12:b:178:VAL:HG21	20:j:58:LEU:HD13	1.97	0.47
5:P:95:GLU:HG3	5:P:213:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:196:LEU:HD23	11:a:246:ILE:HG13	1.97	0.46
15:e:69:LYS:HE3	16:f:138:PRO:HG3	1.97	0.46
17:g:49:PRO:HA	17:g:52:ILE:HG22	1.98	0.46
5:E:107:VAL:HB	5:E:118:ILE:HB	1.95	0.46
7:G:53:ASN:OD1	7:G:53:ASN:N	2.49	0.46
12:b:130:TYR:HE2	12:b:143:PHE:HE1	1.62	0.46
1:A:332:THR:HG21	1:A:343:LEU:HD11	1.97	0.46
7:R:53:ASN:OD1	7:R:53:ASN:N	2.49	0.46
8:S:47:ASN:OD1	8:S:50:ARG:NH1	2.49	0.46
11:a:481:ASN:HB2	15:e:84:ARG:HH22	1.80	0.46
16:f:132:ARG:HG2	16:f:137:VAL:HG23	1.97	0.46
2:B:181:THR:HB	2:B:212:GLY:H	1.79	0.46
8:H:47:ASN:OD1	8:H:50:ARG:NH1	2.49	0.46
3:N:245:PHE:O	4:O:266:ARG:NH2	2.48	0.46
4:O:63:THR:OG1	4:O:66:GLU:OE1	2.30	0.46
4:O:104:CYS:SG	24:O:401:HEC:HAC	2.56	0.46
5:P:49:ALA:O	5:P:53:ARG:NE	2.45	0.46
5:P:107:VAL:HB	5:P:118:ILE:HB	1.95	0.46
6:Q:78:LEU:HD13	6:Q:142:LEU:HD22	1.97	0.46
11:a:66:MET:HG3	11:a:70:LEU:HG	1.97	0.46
12:b:61:ILE:O	12:b:65:TYR:HB2	2.16	0.46
1:A:268:GLU:OE2	1:A:425:ARG:NE	2.47	0.46
5:E:49:ALA:O	5:E:53:ARG:NE	2.45	0.46
11:a:237:TRP:CE3	11:a:237:TRP:HA	2.51	0.46
2:B:230:ARG:NH1	2:B:359:VAL:O	2.47	0.46
6:F:117:LEU:HG	6:F:119:HIS:HB3	1.98	0.46
2:M:230:ARG:NH1	2:M:359:VAL:O	2.48	0.46
3:N:38:LEU:HB2	23:N:402:6PH:H2C	1.98	0.46
11:a:310:MET:HB3	12:b:93:LEU:HD13	1.97	0.46
11:a:501:ASN:HA	11:a:512:SER:HB3	1.98	0.45
11:a:141:GLY:O	11:a:143:SER:N	2.44	0.45
3:N:345:GLU:OE2	4:O:62:MET:N	2.49	0.45
9:T:4:SER:OG	9:T:5:SER:N	2.49	0.45
11:a:507:ASN:ND2	11:a:532:VAL:O	2.43	0.45
6:Q:103:GLU:OE1	6:Q:104:ARG:NH1	2.50	0.45
1:L:332:THR:HG21	1:L:343:LEU:HD11	1.97	0.45
7:R:88:LEU:O	7:R:93:TRP:NE1	2.48	0.45
11:a:27:MET:HE3	11:a:27:MET:HB2	1.78	0.45
11:a:230:ILE:HD11	12:b:200:THR:HG21	1.98	0.45
12:b:75:ILE:HG13	12:b:76:LYS:H	1.82	0.45
4:D:293:ALA:HB3	8:H:31:PRO:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:b:217:PHE:HB2	12:b:236:ILE:HG23	1.99	0.45
1:L:253:ASP:OD2	8:S:22:LYS:NZ	2.49	0.45
1:A:65:TYR:HD2	15:e:38:TRP:HA	1.82	0.45
11:a:72:MET:O	11:a:76:ILE:HG22	2.17	0.45
11:a:383:MET:O	11:a:387:PHE:HB2	2.16	0.45
18:h:63:VAL:HA	18:h:66:VAL:HG22	1.99	0.45
11:a:75:LEU:HD23	11:a:250:PRO:HB2	1.98	0.45
16:f:88:ILE:HD13	16:f:128:LEU:HD21	1.99	0.45
3:C:82:HIS:NE2	24:C:402:HEC:ND	2.65	0.44
3:C:301:VAL:HA	3:C:304:VAL:HG22	1.98	0.44
1:L:265:VAL:HG12	1:L:431:ILE:HG22	1.98	0.44
1:L:356:ILE:HD12	10:U:26:TYR:HE1	1.82	0.44
11:a:393:TYR:O	11:a:397:SER:HB3	2.17	0.44
7:G:88:LEU:O	7:G:93:TRP:NE1	2.48	0.44
3:N:82:HIS:NE2	24:N:403:HEC:ND	2.65	0.44
3:N:301:VAL:HA	3:N:304:VAL:HG22	1.98	0.44
4:O:77:SER:O	9:T:47:LYS:NZ	2.44	0.44
11:a:381:LEU:CD1	34:a:602:HEA:HAC	2.47	0.44
1:A:265:VAL:HG12	1:A:431:ILE:HG22	1.98	0.44
6:F:77:GLN:O	6:F:81:LEU:HB2	2.17	0.44
11:a:233:GLU:OE1	11:a:292:MET:HE1	2.18	0.44
13:c:117:ASP:HB3	13:c:124:TRP:HZ2	1.82	0.44
34:a:603:HEA:HHA	34:a:603:HEA:HAD1	1.73	0.44
2:M:84:ARG:NH1	2:M:157:ASN:O	2.51	0.44
2:M:201:VAL:HG13	2:M:206:LEU:HD23	2.00	0.44
3:N:214:GLY:HA2	7:R:79:HIS:HE1	1.82	0.44
2:M:193:VAL:HG23	2:M:196:ASP:HB2	1.99	0.44
13:c:81:MET:HA	13:c:84:ARG:HD2	1.99	0.44
15:e:49:ILE:HG22	15:e:52:LYS:H	1.83	0.44
24:C:403:HEC:HHA	24:C:403:HEC:O2A	2.18	0.44
11:a:242:PRO:O	11:a:246:ILE:HG12	2.17	0.44
19:i:50:GLU:O	19:i:54:ARG:HB2	2.17	0.44
2:B:84:ARG:NH1	2:B:157:ASN:O	2.51	0.44
1:L:41:GLU:OE2	1:L:400:LYS:NZ	2.41	0.43
7:R:85:HIS:O	8:S:50:ARG:NH1	2.49	0.43
26:C:405:CN5:H2'	26:C:405:CN5:H1A	1.99	0.43
5:E:72:LYS:NZ	5:E:76:GLU:OE2	2.50	0.43
32:N:408:CN3:H55	32:N:408:CN3:H52A	1.74	0.43
16:f:84:ALA:HB3	16:f:87:VAL:HG23	2.00	0.43
2:B:201:VAL:HG13	2:B:206:LEU:HD23	2.00	0.43
7:G:85:HIS:O	8:H:50:ARG:NH1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:VAL:HG23	2:B:196:ASP:HB2	1.99	0.43
4:D:92:ARG:HH22	4:D:246:GLN:NE2	2.17	0.43
5:E:123:PRO:HA	5:E:126:ILE:HD12	1.99	0.43
5:P:123:PRO:HA	5:P:126:ILE:HD12	2.00	0.43
1:A:309:TYR:HE2	3:C:1:MET:HG2	1.83	0.43
2:B:29:SER:HA	2:B:191:ASN:HB2	2.01	0.43
1:L:103:SER:OG	1:L:388:ASN:ND2	2.52	0.43
24:N:404:HEC:HBB2	24:N:404:HEC:HMB3	2.00	0.43
3:C:273:TRP:HA	3:C:276:LEU:HD23	2.01	0.43
4:D:177:LEU:HD22	4:D:180:ILE:HG21	2.00	0.43
2:M:309:LYS:HG3	2:M:348:LEU:HD23	2.01	0.43
3:N:240:LEU:HD23	28:P:301:7PH:H28	2.01	0.43
2:B:34:LYS:HG2	2:B:88:THR:HG22	2.00	0.43
6:F:94:LEU:HD23	6:F:130:LEU:HA	2.01	0.43
1:L:252:ARG:HD2	8:S:21:GLN:HE21	1.84	0.43
3:N:273:TRP:HA	3:N:276:LEU:HD23	2.01	0.43
4:O:218:PHE:CD1	24:O:401:HEC:O2A	2.70	0.43
11:a:131:PRO:HB3	11:a:210:LEU:HD11	2.00	0.43
13:c:250:THR:HA	13:c:253:LEU:HB2	2.01	0.43
1:A:103:SER:OG	1:A:388:ASN:ND2	2.52	0.43
3:C:194:VAL:HG22	24:C:403:HEC:HBB3	1.98	0.43
11:a:13:ASP:OD1	11:a:13:ASP:N	2.52	0.43
12:b:147:VAL:HG12	12:b:233:PRO:HD2	2.00	0.43
1:A:239:LYS:HD2	15:e:46:GLN:HA	2.01	0.43
3:C:81:LEU:HD21	28:D:402:7PH:H26A	1.99	0.43
1:L:268:GLU:OE2	1:L:425:ARG:NE	2.47	0.43
2:M:34:LYS:HG2	2:M:88:THR:HG22	2.00	0.43
2:M:255:VAL:HG23	2:M:314:LEU:HD13	2.01	0.43
1:L:309:TYR:HE2	3:N:1:MET:HG2	1.84	0.43
2:M:29:SER:HA	2:M:191:ASN:HB2	2.01	0.43
24:N:404:HEC:HBB2	24:N:404:HEC:CMB	2.49	0.43
13:c:102:PHE:CZ	13:c:260:LEU:HB2	2.53	0.43
3:C:383:VAL:HG22	7:G:101:PRO:HG3	2.00	0.42
1:L:454:MET:HE3	1:L:454:MET:HB2	1.78	0.42
3:N:142:TRP:HB3	3:N:269:ILE:HD12	2.02	0.42
27:N:405:UQ6:H301	27:N:405:UQ6:H321	1.79	0.42
11:a:340:TYR:CE2	11:a:390:PHE:HB3	2.54	0.42
12:b:31:PRO:HD3	12:b:212:GLN:HE21	1.84	0.42
13:c:129:ILE:HD11	13:c:198:ASP:HB3	2.00	0.42
16:f:132:ARG:HA	16:f:135:LEU:HB2	2.00	0.42
1:A:454:MET:HE3	1:A:454:MET:HB2	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:ASN:O	2:B:304:ILE:HG12	2.19	0.42
4:D:101:CYS:CB	24:D:401:HEC:CAB	2.94	0.42
1:A:72:LEU:HD23	1:A:193:LEU:HD21	2.01	0.42
3:C:142:TRP:HB3	3:C:269:ILE:HD12	2.02	0.42
2:B:54:PHE:CD1	2:B:123:VAL:HG21	2.55	0.42
4:O:177:LEU:HD22	4:O:180:ILE:HG21	2.00	0.42
30:T:101:PCF:H143	30:T:101:PCF:H111	1.89	0.42
11:a:148:ILE:HG12	11:a:207:ILE:HG23	2.01	0.42
2:B:255:VAL:HG23	2:B:314:LEU:HD13	2.01	0.42
3:N:97:MET:HG2	24:N:404:HEC:CBC	2.49	0.42
12:b:67:LYS:HD2	12:b:67:LYS:HA	1.88	0.42
15:e:44:THR:HB	15:e:46:GLN:H	1.85	0.42
1:L:72:LEU:HD23	1:L:193:LEU:HD21	2.01	0.42
11:a:65:LEU:HD12	11:a:113:LEU:HD22	2.01	0.42
11:a:249:ILE:HD12	11:a:252:PHE:HD2	1.85	0.42
12:b:27:ASP:OD1	19:i:44:ARG:NE	2.53	0.42
15:e:83:ARG:HH22	16:f:106:ARG:NH1	2.18	0.42
1:A:185:LEU:HA	1:A:188:LEU:HD13	2.01	0.42
1:L:341:ASP:N	1:L:341:ASP:OD1	2.52	0.42
2:M:150:THR:HG22	2:M:352:ASN:ND2	2.35	0.42
2:M:300:ASN:O	2:M:304:ILE:HG12	2.20	0.42
11:a:51:ASN:OD1	11:a:51:ASN:N	2.53	0.42
11:a:427:PRO:HB3	11:a:450:TRP:HB3	2.00	0.42
11:a:437:PRO:HG2	11:a:440:ILE:HB	2.00	0.42
12:b:39:LEU:HD11	12:b:100:SER:HA	2.02	0.42
24:D:401:HEC:HMC3	24:D:401:HEC:HBC3	2.02	0.42
11:a:201:PRO:HB2	13:c:101:ILE:HB	2.01	0.42
16:f:125:LEU:O	16:f:129:LYS:CB	2.58	0.42
2:B:309:LYS:HG3	2:B:348:LEU:HD23	2.01	0.42
7:G:63:LEU:HD13	7:G:103:LEU:HD13	2.02	0.42
9:I:17:PHE:O	9:I:21:ILE:HG12	2.19	0.42
2:M:49:HIS:HE1	2:M:127:ALA:HA	1.84	0.42
12:b:123:GLN:NE2	12:b:225:CYS:SG	2.93	0.42
13:c:212:HIS:HB2	13:c:257:TRP:CH2	2.55	0.42
1:A:52:GLY:HA3	1:A:105:ILE:HA	2.02	0.41
2:B:54:PHE:HD1	2:B:123:VAL:HG21	1.84	0.41
2:M:139:VAL:HG12	2:M:238:VAL:HG21	2.02	0.41
7:R:63:LEU:HD13	7:R:103:LEU:HD13	2.02	0.41
15:e:58:LYS:HE2	15:e:64:LEU:HD13	2.02	0.41
1:L:369:LEU:HD21	2:M:72:GLU:HG3	2.02	0.41
2:M:54:PHE:HD1	2:M:123:VAL:HG21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:255:VAL:HG12	2:M:321:THR:HG21	2.02	0.41
4:O:101:CYS:CA	24:O:401:HEC:HAB	2.50	0.41
11:a:149:PHE:CE2	13:c:36:SER:HB2	2.55	0.41
16:f:128:LEU:HA	16:f:131:VAL:HB	2.02	0.41
19:i:33:TRP:O	19:i:37:HIS:CB	2.68	0.41
2:B:30:THR:HG22	2:B:92:THR:HG23	2.02	0.41
3:C:55:SER:OG	3:N:177:GLN:NE2	2.53	0.41
1:L:70:SER:HB3	1:L:97:ILE:HD12	2.03	0.41
9:T:5:SER:OG	9:T:6:LEU:N	2.51	0.41
13:c:103:ALA:HA	13:c:106:PHE:HB3	2.02	0.41
1:A:310:GLN:NE2	1:A:312:CYS:O	2.54	0.41
2:M:54:PHE:CD1	2:M:123:VAL:HG21	2.55	0.41
4:O:92:ARG:HH22	4:O:246:GLN:NE2	2.17	0.41
16:f:109:GLU:OE1	16:f:140:LYS:NZ	2.39	0.41
2:B:119:LEU:HA	2:B:123:VAL:HB	2.02	0.41
3:N:207:SER:OG	3:N:208:ASN:N	2.54	0.41
6:Q:122:ASP:OD1	6:Q:122:ASP:N	2.53	0.41
11:a:184:LEU:O	11:a:188:SER:CB	2.67	0.41
15:e:47:GLN:HB2	15:e:50:VAL:HG22	2.01	0.41
1:L:250:ARG:HB2	8:S:26:SER:HB3	2.03	0.41
1:L:258:LYS:HG2	1:L:335:ARG:HG2	2.03	0.41
13:c:173:ILE:O	13:c:177:LEU:CB	2.68	0.41
3:C:177:GLN:NE2	3:N:55:SER:OG	2.53	0.41
2:M:119:LEU:HA	2:M:123:VAL:HB	2.02	0.41
4:O:209:PRO:HA	4:O:210:PRO:HD3	1.91	0.41
2:B:139:VAL:HG12	2:B:238:VAL:HG21	2.02	0.41
3:C:207:SER:OG	3:C:208:ASN:N	2.54	0.41
3:C:245:PHE:O	4:D:266:ARG:NH2	2.53	0.41
5:P:134:MET:HB3	5:P:140:PRO:HB3	2.03	0.41
11:a:60:VAL:HG23	11:a:127:TRP:HA	2.02	0.41
11:a:374:VAL:HA	11:a:377:PHE:CE1	2.56	0.41
13:c:22:TRP:CD1	13:c:23:PRO:HD2	2.56	0.41
2:B:150:THR:HG22	2:B:352:ASN:ND2	2.35	0.41
5:E:134:MET:HB3	5:E:140:PRO:HB3	2.03	0.41
1:L:52:GLY:HA3	1:L:105:ILE:HA	2.02	0.41
1:L:185:LEU:HA	1:L:188:LEU:HD13	2.01	0.41
1:L:310:GLN:NE2	1:L:312:CYS:O	2.54	0.41
11:a:31:ALA:HB3	18:h:64:PRO:HG2	2.03	0.41
11:a:88:ILE:HD11	11:a:173:ARG:HG2	2.03	0.41
11:a:340:TYR:CZ	11:a:390:PHE:HB3	2.56	0.41
5:E:132:VAL:HG21	5:E:192:ARG:HH12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:136:ASP:HB3	4:O:145:LYS:HG3	2.03	0.41
19:i:38:MET:HA	19:i:41:ILE:HG22	2.02	0.41
2:B:324:LYS:HA	2:B:327:VAL:HG22	2.03	0.40
1:A:70:SER:HB3	1:A:97:ILE:HD12	2.03	0.40
6:F:92:LYS:HA	6:F:95:VAL:HG22	2.03	0.40
1:L:341:ASP:HB3	1:L:443:LEU:HD13	2.02	0.40
2:M:50:LEU:O	2:M:54:PHE:HB2	2.21	0.40
4:O:292:TRP:HZ3	7:R:83:LEU:HD11	1.86	0.40
1:A:258:LYS:HG2	1:A:335:ARG:HG2	2.03	0.40
2:B:52:ASN:HD22	2:B:82:LEU:HD22	1.86	0.40
4:D:101:CYS:HA	24:D:401:HEC:HAB	2.02	0.40
2:M:30:THR:HG22	2:M:92:THR:HG23	2.02	0.40
27:N:405:UQ6:H251	27:N:405:UQ6:H271	1.81	0.40
6:Q:108:GLN:NE2	6:Q:121:GLU:OE1	2.54	0.40
11:a:289:SER:HB3	11:a:305:PHE:CD2	2.57	0.40
11:a:310:MET:HB3	12:b:93:LEU:HD22	2.02	0.40
15:e:61:TRP:CZ2	16:f:99:ASN:HA	2.55	0.40
5:E:82:MET:O	3:N:178:ARG:NH2	2.45	0.40
2:M:35:VAL:HG22	2:M:185:LEU:HB3	2.04	0.40
2:M:52:ASN:HD22	2:M:82:LEU:HD22	1.86	0.40
3:N:230:LEU:HD13	23:N:402:6PH:H26A	2.03	0.40
13:c:30:LEU:HB3	17:g:41:VAL:HG11	2.04	0.40
13:c:181:PHE:HD2	13:c:216:MET:HE1	1.87	0.40
2:B:49:HIS:HE1	2:B:127:ALA:HA	1.84	0.40
2:B:224:PHE:O	2:B:352:ASN:ND2	2.50	0.40
11:a:72:MET:HE1	11:a:246:ILE:HB	2.02	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	A	429/457 (94%)	405 (94%)	23 (5%)	1 (0%)	43	72
1	L	429/457 (94%)	404 (94%)	24 (6%)	1 (0%)	43	72
2	B	350/368 (95%)	336 (96%)	14 (4%)	0	100	100
2	M	350/368 (95%)	336 (96%)	14 (4%)	0	100	100
3	C	383/385 (100%)	368 (96%)	15 (4%)	0	100	100
3	N	383/385 (100%)	368 (96%)	15 (4%)	0	100	100
4	D	246/309 (80%)	241 (98%)	5 (2%)	0	100	100
4	O	246/309 (80%)	241 (98%)	5 (2%)	0	100	100
5	E	183/215 (85%)	172 (94%)	11 (6%)	0	100	100
5	P	183/215 (85%)	172 (94%)	11 (6%)	0	100	100
6	F	72/147 (49%)	71 (99%)	1 (1%)	0	100	100
6	Q	73/147 (50%)	71 (97%)	2 (3%)	0	100	100
7	G	124/127 (98%)	119 (96%)	4 (3%)	1 (1%)	16	47
7	R	124/127 (98%)	119 (96%)	4 (3%)	1 (1%)	16	47
8	H	91/94 (97%)	85 (93%)	6 (7%)	0	100	100
8	S	91/94 (97%)	85 (93%)	6 (7%)	0	100	100
9	I	52/66 (79%)	50 (96%)	2 (4%)	0	100	100
9	T	52/66 (79%)	50 (96%)	2 (4%)	0	100	100
10	U	42/77 (54%)	38 (90%)	4 (10%)	0	100	100
10	V	49/77 (64%)	43 (88%)	6 (12%)	0	100	100
11	a	520/534 (97%)	460 (88%)	59 (11%)	1 (0%)	43	72
12	b	233/251 (93%)	204 (88%)	27 (12%)	2 (1%)	14	44
13	c	260/269 (97%)	242 (93%)	18 (7%)	0	100	100
14	d	47/155 (30%)	38 (81%)	9 (19%)	0	100	100
15	e	94/153 (61%)	83 (88%)	11 (12%)	0	100	100
16	f	97/148 (66%)	88 (91%)	9 (9%)	0	100	100
17	g	27/60 (45%)	26 (96%)	1 (4%)	0	100	100
18	h	29/78 (37%)	27 (93%)	1 (3%)	1 (3%)	3	18
19	i	47/59 (80%)	47 (100%)	0	0	100	100
20	j	55/83 (66%)	46 (84%)	8 (14%)	1 (2%)	6	31
21	k	16/129 (12%)	14 (88%)	2 (12%)	0	100	100
All	All	5377/6409 (84%)	5049 (94%)	319 (6%)	9 (0%)	44	72

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	5	PHE
7	R	5	PHE
12	b	67	LYS
12	b	184	VAL
20	j	38	VAL
1	L	234	THR
11	a	142	PRO
1	A	234	THR
18	h	48	PRO

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	A	370/393 (94%)	366 (99%)	4 (1%)	65	77
1	L	370/393 (94%)	368 (100%)	2 (0%)	81	84
2	B	301/313 (96%)	301 (100%)	0	100	100
2	M	301/313 (96%)	301 (100%)	0	100	100
3	C	338/338 (100%)	337 (100%)	1 (0%)	86	87
3	N	338/338 (100%)	337 (100%)	1 (0%)	86	87
4	D	206/251 (82%)	206 (100%)	0	100	100
4	O	206/251 (82%)	206 (100%)	0	100	100
5	E	151/179 (84%)	151 (100%)	0	100	100
5	P	151/179 (84%)	151 (100%)	0	100	100
6	F	67/131 (51%)	67 (100%)	0	100	100
6	Q	68/131 (52%)	68 (100%)	0	100	100
7	G	110/111 (99%)	110 (100%)	0	100	100
7	R	110/111 (99%)	110 (100%)	0	100	100
8	H	77/78 (99%)	77 (100%)	0	100	100
8	S	77/78 (99%)	77 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	44/54 (82%)	44 (100%)	0	100	100
9	T	45/54 (83%)	45 (100%)	0	100	100
10	U	35/66 (53%)	35 (100%)	0	100	100
10	V	42/66 (64%)	42 (100%)	0	100	100
11	a	436/447 (98%)	428 (98%)	8 (2%)	51	71
12	b	208/224 (93%)	206 (99%)	2 (1%)	68	78
13	c	221/228 (97%)	221 (100%)	0	100	100
14	d	44/135 (33%)	42 (96%)	2 (4%)	24	55
15	e	73/127 (58%)	73 (100%)	0	100	100
16	f	88/131 (67%)	87 (99%)	1 (1%)	65	77
17	g	23/51 (45%)	23 (100%)	0	100	100
18	h	24/67 (36%)	24 (100%)	0	100	100
19	i	41/50 (82%)	41 (100%)	0	100	100
20	j	51/74 (69%)	51 (100%)	0	100	100
All	All	4616/5362 (86%)	4595 (100%)	21 (0%)	78	84

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	ILE
1	A	235	LYS
1	A	238	LEU
1	A	241	LYS
3	C	336	LEU
1	L	214	ILE
1	L	241	LYS
3	N	336	LEU
11	a	75	LEU
11	a	83	LEU
11	a	163	ILE
11	a	248	ILE
11	a	345	LEU
11	a	381	LEU
11	a	401	LEU
11	a	416	LEU
12	b	103	LEU
12	b	207	VAL

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Mol	Chain	Res	Type
14	d	69	LEU
14	d	75	LEU
16	f	105	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	102	GLN
1	A	126	GLN
1	A	130	ASN
1	A	154	ASN
1	A	156	HIS
1	A	231	GLN
1	A	271	ASN
1	A	317	HIS
1	A	350	GLN
1	A	352	ASN
1	A	388	ASN
2	B	49	HIS
2	B	60	ASN
2	B	136	GLN
2	B	170	GLN
3	C	57	ASN
3	C	177	GLN
3	C	222	HIS
4	D	78	HIS
4	D	95	GLN
4	D	127	ASN
4	D	141	GLN
4	D	170	GLN
4	D	246	GLN
4	D	256	ASN
5	E	181	HIS
6	F	119	HIS
7	G	3	GLN
7	G	79	HIS
9	I	29	GLN
1	L	42	HIS
1	L	102	GLN
1	L	126	GLN
1	L	130	ASN

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Mol	Chain	Res	Type
1	L	154	ASN
1	L	156	HIS
1	L	199	ASN
1	L	231	GLN
1	L	271	ASN
1	L	317	HIS
1	L	350	GLN
1	L	352	ASN
1	L	388	ASN
2	M	49	HIS
2	M	60	ASN
2	M	136	GLN
2	M	170	GLN
3	N	57	ASN
3	N	177	GLN
4	O	78	HIS
4	O	79	ASN
4	O	95	GLN
4	O	127	ASN
4	O	141	GLN
4	O	170	GLN
4	O	246	GLN
4	O	256	ASN
5	P	106	ASN
5	P	141	GLN
5	P	181	HIS
6	Q	84	HIS
6	Q	132	HIS
7	R	3	GLN
7	R	79	HIS
9	T	44	ASN
11	a	46	GLN
11	a	49	HIS
11	a	53	GLN
11	a	62	HIS
11	a	81	ASN
11	a	291	HIS
11	a	360	ASN
11	a	411	GLN
11	a	429	HIS
11	a	492	ASN
11	a	507	ASN

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Mol	Chain	Res	Type
12	b	42	ASN
12	b	123	GLN
12	b	174	HIS
12	b	212	GLN
13	c	141	ASN
13	c	156	HIS
13	c	185	GLN
13	c	232	ASN
16	f	70	GLN
16	f	117	ASN
20	j	35	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 1 is monoatomic - leaving 25 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	$\# Z > 2$
29	FES	P	302	-	0,4,4	-	-	-		
23	6PH	N	402	-	39,39,39	0.50	0	42,44,44	1.14	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	7PH	D	402	-	37,37,37	0.54	0	40,42,42	1.10	2 (5%)
31	9PE	N	407	-	39,39,39	0.44	0	42,44,44	1.10	2 (4%)
26	CN5	C	405	-	40,40,40	1.04	2 (5%)	44,48,48	1.01	2 (4%)
34	HEA	a	603	-	67,67,67	1.25	7 (10%)	81,103,103	1.72	20 (24%)
29	FES	E	301	-	0,4,4	-	-	-	-	-
30	PCF	I	101	-	34,34,49	0.67	0	40,42,57	0.62	0
23	6PH	C	401	-	39,39,39	0.51	0	42,44,44	1.14	2 (4%)
30	PCF	T	101	-	34,34,49	0.67	0	40,42,57	0.62	0
25	8PE	C	404	-	46,46,46	0.44	0	49,51,51	1.18	2 (4%)
24	HEC	C	403	3	46,50,50	2.22	19 (41%)	58,82,82	2.11	16 (27%)
27	UQ6	C	406	-	43,43,43	0.43	0	54,55,55	1.57	10 (18%)
24	HEC	D	401	4	46,50,50	1.98	16 (34%)	58,82,82	2.05	18 (31%)
25	8PE	N	406	-	46,46,46	0.42	0	49,51,51	1.16	2 (4%)
24	HEC	C	402	3	46,50,50	1.94	8 (17%)	58,82,82	1.05	4 (6%)
24	HEC	N	404	3	46,50,50	1.72	10 (21%)	58,82,82	1.59	10 (17%)
35	CUA	b	301	-	0,1,1	-	-	-	-	-
32	CN3	N	408	-	54,54,54	0.49	0	60,66,66	1.32	5 (8%)
34	HEA	a	602	11	67,67,67	1.26	8 (11%)	81,103,103	1.56	13 (16%)
28	7PH	P	301	-	37,37,37	0.53	0	40,42,42	1.10	2 (5%)
31	9PE	N	401	-	39,39,39	0.43	0	42,44,44	1.14	2 (4%)
24	HEC	O	401	4	46,50,50	2.04	17 (36%)	58,82,82	1.99	13 (22%)
24	HEC	N	403	3	46,50,50	1.94	8 (17%)	58,82,82	1.05	4 (6%)
27	UQ6	N	405	-	43,43,43	0.59	1 (2%)	54,55,55	1.56	12 (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
29	FES	P	302	-	-	-	0/1/1/1
23	6PH	N	402	-	-	10/41/41/41	-
28	7PH	D	402	-	-	16/39/39/39	-
31	9PE	N	407	-	-	16/43/43/43	-
26	CN5	C	405	-	-	17/44/44/44	-
34	HEA	a	603	-	-	15/36/76/76	-
29	FES	E	301	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PCF	I	101	-	-	14/38/38/53	-
23	6PH	C	401	-	-	10/41/41/41	-
30	PCF	T	101	-	-	14/38/38/53	-
25	8PE	C	404	-	-	20/50/50/50	-
24	HEC	C	403	3	-	7/14/54/54	-
27	UQ6	C	406	-	-	11/39/39/39	0/1/1/1
24	HEC	D	401	4	-	6/14/54/54	-
25	8PE	N	406	-	-	25/50/50/50	-
24	HEC	C	402	3	-	5/14/54/54	-
24	HEC	N	404	3	-	7/14/54/54	-
32	CN3	N	408	-	-	34/65/65/65	-
34	HEA	a	602	11	-	18/36/76/76	-
28	7PH	P	301	-	-	16/39/39/39	-
31	9PE	N	401	-	-	17/43/43/43	-
24	HEC	O	401	4	-	4/14/54/54	-
24	HEC	N	403	3	-	5/14/54/54	-
27	UQ6	N	405	-	-	8/39/39/39	0/1/1/1

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	403	HEC	CAB-C3B	6.13	1.54	1.35
24	C	402	HEC	CAB-C3B	6.12	1.54	1.35
24	C	402	HEC	CAC-C3C	5.92	1.54	1.35
24	N	403	HEC	CAC-C3C	5.92	1.54	1.35
24	D	401	HEC	CBB-CAB	-4.91	1.31	1.49
24	O	401	HEC	CBB-CAB	-4.85	1.31	1.49
24	C	403	HEC	CBC-CAC	-4.75	1.31	1.49
24	C	403	HEC	CBB-CAB	-4.72	1.32	1.49
24	O	401	HEC	CBC-CAC	-4.51	1.32	1.49
24	N	403	HEC	CBC-CAC	-4.37	1.33	1.49
24	N	404	HEC	CBC-CAC	-4.37	1.33	1.49
24	C	402	HEC	CBC-CAC	-4.35	1.33	1.49
24	D	401	HEC	CBC-CAC	-4.34	1.33	1.49
24	N	404	HEC	CBB-CAB	-4.31	1.33	1.49
24	N	403	HEC	CBB-CAB	-4.17	1.34	1.49
24	C	402	HEC	CBB-CAB	-4.17	1.34	1.49
24	C	403	HEC	C3C-C4C	-4.07	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	401	HEC	C4D-ND	-4.05	1.32	1.39
24	C	403	HEC	C1B-NB	-3.99	1.32	1.39
34	a	602	HEA	CMA-C3A	-3.97	1.36	1.45
24	N	404	HEC	CAB-C3B	3.96	1.47	1.35
34	a	603	HEA	CMA-C3A	-3.95	1.36	1.45
24	N	404	HEC	CAC-C3C	3.93	1.47	1.35
24	C	403	HEC	C1D-ND	-3.77	1.32	1.39
24	C	403	HEC	C4D-ND	-3.62	1.32	1.39
24	C	403	HEC	C4B-NB	-3.61	1.32	1.39
24	C	403	HEC	C4A-C3A	-3.60	1.38	1.45
24	D	401	HEC	CAC-C3C	3.48	1.46	1.35
24	O	401	HEC	C1D-ND	-3.43	1.33	1.39
24	O	401	HEC	C1B-NB	-3.35	1.33	1.39
24	O	401	HEC	C4B-NB	-3.35	1.33	1.39
24	O	401	HEC	C4D-ND	-3.31	1.33	1.39
24	O	401	HEC	CAC-C3C	3.29	1.45	1.35
24	D	401	HEC	C4B-NB	-3.24	1.33	1.39
24	O	401	HEC	C3C-C4C	-3.24	1.40	1.46
24	C	403	HEC	CAB-C3B	3.17	1.45	1.35
24	D	401	HEC	CAB-C3B	3.17	1.45	1.35
24	D	401	HEC	C1B-NB	-3.09	1.33	1.39
24	C	403	HEC	C1A-C2A	-2.97	1.40	1.45
24	C	403	HEC	CAC-C3C	2.97	1.44	1.35
24	O	401	HEC	CAB-C3B	2.96	1.44	1.35
24	O	401	HEC	C1A-C2A	-2.96	1.40	1.45
34	a	603	HEA	C4C-NC	-2.96	1.34	1.39
24	D	401	HEC	C1D-ND	-2.93	1.34	1.39
24	C	402	HEC	C3C-C2C	-2.90	1.31	1.41
34	a	602	HEA	C4C-NC	-2.89	1.34	1.39
24	N	403	HEC	C3C-C2C	-2.88	1.31	1.41
34	a	602	HEA	CHC-C1C	-2.83	1.33	1.39
24	D	401	HEC	C4A-C3A	-2.78	1.39	1.45
24	D	401	HEC	C3C-C4C	-2.76	1.41	1.46
24	N	404	HEC	C1B-NB	-2.75	1.34	1.39
34	a	603	HEA	CHC-C1C	-2.72	1.33	1.39
24	C	403	HEC	C1C-NC	-2.67	1.34	1.39
26	C	405	CN5	P'-O1'	2.65	1.69	1.59
24	O	401	HEC	C4A-C3A	-2.60	1.40	1.45
26	C	405	CN5	P-O11	2.56	1.69	1.59
24	D	401	HEC	C3D-C2D	-2.55	1.32	1.38
24	O	401	HEC	C1C-NC	-2.55	1.34	1.39
34	a	602	HEA	C1D-C2D	2.54	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	603	HEA	CMD-C2D	2.51	1.55	1.50
24	N	404	HEC	C1D-ND	-2.49	1.34	1.39
24	N	404	HEC	C4D-ND	-2.49	1.34	1.39
24	O	401	HEC	C3D-C2D	-2.48	1.32	1.38
24	C	403	HEC	C4C-NC	-2.46	1.35	1.39
24	C	402	HEC	C3D-C2D	-2.46	1.32	1.38
24	N	403	HEC	C3D-C2D	-2.45	1.32	1.38
34	a	602	HEA	C3C-C2C	-2.39	1.33	1.41
34	a	603	HEA	C1D-ND	-2.37	1.36	1.40
24	C	403	HEC	C4A-NA	-2.37	1.35	1.39
24	N	404	HEC	C4B-NB	-2.36	1.35	1.39
34	a	602	HEA	C1D-ND	-2.33	1.36	1.40
24	C	403	HEC	C1C-C2C	-2.32	1.37	1.43
24	D	401	HEC	C1C-NC	-2.31	1.35	1.39
24	N	404	HEC	C1A-C2A	-2.24	1.41	1.45
24	O	401	HEC	C3B-C2B	-2.24	1.33	1.41
27	N	405	UQ6	C5-C6	-2.23	1.36	1.40
24	O	401	HEC	C4C-NC	-2.21	1.35	1.39
24	D	401	HEC	C3B-C2B	-2.21	1.33	1.41
24	C	403	HEC	C3B-C2B	-2.21	1.33	1.41
24	D	401	HEC	C4C-NC	-2.19	1.35	1.39
24	C	403	HEC	C3D-C2D	-2.18	1.33	1.38
24	N	403	HEC	C2A-C3A	-2.12	1.32	1.36
24	C	402	HEC	C2A-C3A	-2.11	1.32	1.36
24	D	401	HEC	O2D-CGD	-2.09	1.23	1.30
34	a	603	HEA	FE-NC	2.09	2.02	1.95
24	O	401	HEC	O2D-CGD	-2.07	1.24	1.30
24	N	404	HEC	C4A-C3A	-2.07	1.41	1.45
24	D	401	HEC	C1A-C2A	-2.06	1.41	1.45
34	a	602	HEA	CHA-C1A	-2.05	1.34	1.38
24	C	403	HEC	C1A-NA	-2.05	1.35	1.39
34	a	603	HEA	C1D-C2D	2.02	1.48	1.44
34	a	602	HEA	FE-NC	2.02	2.01	1.95
24	N	403	HEC	CMB-C2B	2.01	1.54	1.50
24	O	401	HEC	O2A-CGA	-2.01	1.24	1.30
24	C	402	HEC	CMB-C2B	2.01	1.54	1.50
24	C	403	HEC	O2A-CGA	-2.00	1.24	1.30

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	O	401	HEC	CBB-CAB-C3B	-7.19	113.06	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	401	HEC	CBC-CAC-C3C	-6.96	113.52	127.43
24	C	403	HEC	CBC-CAC-C3C	-6.00	115.43	127.43
24	C	403	HEC	CHC-C4B-NB	5.87	130.85	124.45
27	N	405	UQ6	C7-C8-C9	-5.71	119.24	127.42
34	a	602	HEA	CMD-C2D-C1D	5.69	133.93	125.03
24	D	401	HEC	CBB-CAB-C3B	-5.59	116.25	127.43
24	O	401	HEC	CHC-C4B-NB	5.59	130.54	124.45
24	O	401	HEC	CBC-CAC-C3C	-5.28	116.88	127.43
24	C	403	HEC	CBB-CAB-C3B	-5.28	116.89	127.43
27	C	406	UQ6	C7-C8-C9	-5.28	119.86	127.42
24	D	401	HEC	CHC-C4B-NB	5.07	129.98	124.45
24	N	404	HEC	CHC-C4B-NB	4.79	129.67	124.45
34	a	602	HEA	CHB-C4A-NA	-4.56	119.49	124.45
27	C	406	UQ6	C6-C7-C8	4.46	119.67	112.06
32	N	408	CN3	O51-C51-C52	4.44	121.08	111.48
32	N	408	CN3	O21-C21-C22	4.18	120.52	111.48
25	N	406	8PE	O21-C21-C22	4.17	120.51	111.48
24	N	404	HEC	CBB-CAB-C3B	-4.15	119.15	127.43
25	C	404	8PE	O21-C21-C22	4.12	120.39	111.48
24	N	404	HEC	CBC-CAC-C3C	-3.98	119.47	127.43
31	N	401	9PE	O21-C21-C22	3.87	119.84	111.48
34	a	603	HEA	CHB-C4A-NA	-3.86	120.25	124.45
34	a	603	HEA	CAD-C3D-C2D	3.80	134.98	127.87
31	N	407	9PE	O21-C21-C22	3.74	119.56	111.48
34	a	603	HEA	CAD-C3D-C4D	-3.72	118.21	124.70
24	C	403	HEC	CHD-C1D-ND	3.67	130.52	123.86
24	D	401	HEC	CHD-C4C-NC	3.64	128.41	124.45
23	C	401	6PH	O21-C21-C22	3.64	119.35	111.48
23	N	402	6PH	O21-C21-C22	3.63	119.34	111.48
24	C	403	HEC	CHD-C4C-NC	3.57	128.34	124.45
34	a	603	HEA	C3C-C4C-NC	3.57	112.81	109.80
28	D	402	7PH	O21-C21-C22	3.49	119.03	111.48
28	P	301	7PH	O21-C21-C22	3.49	119.03	111.48
27	C	406	UQ6	C30-C29-C31	3.47	121.26	115.23
24	O	401	HEC	CHD-C4C-NC	3.33	128.08	124.45
34	a	603	HEA	CMB-C2B-C3B	-3.29	123.92	130.28
32	N	408	CN3	O41-C41-C42	3.28	121.85	111.83
24	C	403	HEC	CHB-C4A-NA	3.27	128.01	124.45
34	a	602	HEA	C2A-C1A-NA	3.14	113.36	110.32
24	C	403	HEC	CHB-C1B-NB	3.10	129.49	123.86
34	a	603	HEA	C1D-C2D-C3D	-3.10	103.72	106.98
24	O	401	HEC	CHA-C4D-ND	3.09	129.47	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	603	HEA	C20-C19-C18	-3.08	114.25	121.17
24	D	401	HEC	CAA-C2A-C3A	-3.00	122.24	127.87
24	O	401	HEC	CHD-C1D-ND	2.99	129.29	123.86
24	N	404	HEC	CHA-C1A-NA	2.95	127.67	124.45
34	a	603	HEA	C3D-C4D-ND	2.93	113.18	110.35
27	N	405	UQ6	C25-C24-C26	2.90	120.26	115.23
24	O	401	HEC	CHB-C1B-NB	2.89	129.09	123.86
31	N	401	9PE	O31-C31-C32	2.87	120.58	111.83
32	N	408	CN3	O31-C31-C32	2.86	119.84	111.15
25	C	404	8PE	O31-C31-C32	2.86	120.56	111.83
34	a	602	HEA	CHD-C1D-ND	-2.85	120.85	124.37
24	N	404	HEC	CHD-C1D-ND	2.84	129.01	123.86
24	D	401	HEC	CHA-C4D-ND	2.83	128.99	123.86
24	C	402	HEC	CMB-C2B-C1B	-2.81	121.13	125.42
24	N	403	HEC	CMB-C2B-C1B	-2.81	121.14	125.42
24	C	403	HEC	CHD-C1D-C2D	-2.78	119.34	127.43
34	a	603	HEA	CMC-C2C-C3C	2.78	133.09	126.55
24	C	403	HEC	C2A-C1A-NA	-2.74	107.67	110.32
31	N	407	9PE	O31-C31-C32	2.74	120.18	111.83
25	N	406	8PE	O31-C31-C32	2.71	120.09	111.83
34	a	603	HEA	OMA-CMA-C3A	-2.68	119.56	125.62
23	C	401	6PH	O31-C31-C32	2.67	119.99	111.83
34	a	602	HEA	CHB-C4A-C3A	2.67	129.71	125.21
23	N	402	6PH	O31-C31-C32	2.66	119.96	111.83
34	a	602	HEA	O1D-CGD-CBD	-2.66	114.67	123.09
27	N	405	UQ6	C4M-O4-C4	-2.63	107.59	114.74
24	D	401	HEC	CHA-C4D-C3D	-2.62	119.57	125.30
24	D	401	HEC	CAA-C2A-C1A	2.61	130.16	124.85
24	C	403	HEC	CHB-C1B-C2B	-2.61	119.86	127.43
24	C	403	HEC	CAA-CBA-CGA	-2.60	106.76	113.67
24	C	403	HEC	CHA-C1A-NA	2.60	127.28	124.45
34	a	603	HEA	CMC-C2C-C1C	-2.60	121.47	125.42
24	C	403	HEC	CHA-C4D-ND	2.59	128.56	123.86
28	D	402	7PH	O31-C31-C32	2.59	119.72	111.83
28	P	301	7PH	O31-C31-C32	2.58	119.70	111.83
27	N	405	UQ6	C15-C14-C16	2.56	119.67	115.23
24	C	403	HEC	CAA-C2A-C3A	-2.53	123.12	127.87
24	C	403	HEC	O2D-CGD-CBD	2.50	121.91	114.00
27	C	406	UQ6	C20-C19-C21	2.49	119.55	115.23
34	a	602	HEA	C12-C11-C3B	2.48	115.99	112.12
24	D	401	HEC	CHB-C1B-NB	2.48	128.35	123.86
34	a	603	HEA	CHA-C4D-C3D	-2.47	121.17	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	603	HEA	C26-C15-C14	-2.47	117.29	123.63
24	N	404	HEC	CHA-C4D-ND	2.47	128.33	123.86
24	D	401	HEC	O2A-CGA-CBA	2.46	121.78	114.00
27	N	405	UQ6	C12-C13-C14	-2.45	122.01	127.62
27	N	405	UQ6	C30-C29-C31	2.45	119.48	115.23
34	a	603	HEA	C2A-C1A-NA	2.45	112.69	110.32
34	a	603	HEA	CBD-CAD-C3D	2.43	119.25	112.53
34	a	603	HEA	C2D-C1D-ND	2.42	112.62	109.84
27	C	406	UQ6	C22-C23-C24	-2.39	122.15	127.62
24	D	401	HEC	C4C-NC-C1C	2.39	109.71	105.82
34	a	602	HEA	C1D-C2D-C3D	-2.39	104.47	106.98
24	D	401	HEC	CHB-C1B-C2B	-2.38	120.52	127.43
27	N	405	UQ6	C30-C29-C28	-2.38	117.52	123.63
27	N	405	UQ6	C22-C23-C24	-2.36	122.23	127.62
26	C	405	CN5	O4'-P'-O2'	2.36	123.40	112.44
34	a	603	HEA	CBA-CAA-C2A	2.34	119.00	112.53
27	N	405	UQ6	C17-C18-C19	-2.33	122.28	127.62
26	C	405	CN5	O12-P-O14	2.33	123.29	112.44
24	C	403	HEC	CAD-CBD-CGD	-2.33	107.48	113.67
34	a	602	HEA	C3D-C4D-ND	2.32	112.59	110.35
24	O	401	HEC	CHD-C1D-C2D	-2.30	120.74	127.43
27	C	406	UQ6	C12-C13-C14	-2.29	122.38	127.62
34	a	603	HEA	CHB-C4A-C3A	2.28	129.05	125.21
24	N	404	HEC	CHB-C1B-NB	2.26	127.96	123.86
24	O	401	HEC	CHA-C1A-NA	2.26	126.91	124.45
24	O	401	HEC	CHA-C4D-C3D	-2.25	120.36	125.30
34	a	602	HEA	CMB-C2B-C3B	-2.22	125.97	130.28
24	D	401	HEC	CMD-C2D-C1D	2.22	128.80	125.42
24	O	401	HEC	CAD-CBD-CGD	-2.22	107.78	113.67
24	N	404	HEC	CHD-C1D-C2D	-2.21	121.01	127.43
24	D	401	HEC	CHB-C4A-NA	2.19	126.84	124.45
27	N	405	UQ6	C7-C6-C5	-2.19	117.39	120.85
27	C	406	UQ6	C25-C24-C26	2.19	119.02	115.23
24	D	401	HEC	CMB-C2B-C1B	2.18	128.74	125.42
27	C	406	UQ6	C20-C19-C18	-2.18	118.04	123.63
34	a	602	HEA	C3C-C4C-NC	2.16	111.62	109.80
34	a	603	HEA	O1D-CGD-CBD	-2.16	116.25	123.09
27	N	405	UQ6	C20-C19-C21	2.15	118.97	115.23
27	C	406	UQ6	C4M-O4-C4	-2.14	108.92	114.74
24	N	404	HEC	CHD-C4C-NC	2.13	126.77	124.45
24	N	403	HEC	CMB-C2B-C3B	2.12	131.54	126.55
24	C	402	HEC	CMB-C2B-C3B	2.12	131.54	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	O	401	HEC	O2D-CGD-CBD	2.12	120.70	114.00
24	O	401	HEC	CHB-C1B-C2B	-2.11	121.31	127.43
34	a	603	HEA	CAD-CBD-CGD	-2.09	108.12	113.67
34	a	602	HEA	C3B-C4B-NB	2.09	112.24	109.84
24	D	401	HEC	O2A-CGA-O1A	-2.08	117.98	123.33
34	a	602	HEA	C26-C15-C14	-2.06	118.33	123.63
24	C	402	HEC	CHA-C1A-NA	2.06	126.69	124.45
27	N	405	UQ6	C3M-O3-C3	-2.05	109.18	114.74
24	N	404	HEC	CHB-C1B-C2B	-2.04	121.49	127.43
24	N	403	HEC	CMC-C2C-C1C	2.04	128.52	125.42
24	D	401	HEC	CBD-CAD-C3D	-2.04	106.90	112.53
24	D	401	HEC	CHA-C1A-NA	2.03	126.67	124.45
24	N	403	HEC	CHA-C1A-NA	2.03	126.67	124.45
27	C	406	UQ6	C15-C14-C16	2.01	118.71	115.23
32	N	408	CN3	O41-C41-O42	-2.01	118.61	123.63
24	C	402	HEC	CMC-C2C-C1C	2.00	128.47	125.42

There are no chirality outliers.

All (295) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	C	401	6PH	C1-O11-P-O12
23	C	401	6PH	C1-O11-P-O14
23	C	401	6PH	O21-C2-C3-O31
23	N	402	6PH	C1-O11-P-O12
23	N	402	6PH	C1-O11-P-O14
23	N	402	6PH	O21-C2-C3-O31
24	C	402	HEC	C2B-C3B-CAB-CBB
24	C	402	HEC	C4B-C3B-CAB-CBB
24	C	403	HEC	C2B-C3B-CAB-CBB
24	C	403	HEC	C4B-C3B-CAB-CBB
24	C	403	HEC	C2C-C3C-CAC-CBC
24	C	403	HEC	C4C-C3C-CAC-CBC
24	D	401	HEC	C2B-C3B-CAB-CBB
24	D	401	HEC	C4B-C3B-CAB-CBB
24	D	401	HEC	C2C-C3C-CAC-CBC
24	N	403	HEC	C2B-C3B-CAB-CBB
24	N	403	HEC	C4B-C3B-CAB-CBB
24	N	404	HEC	C2B-C3B-CAB-CBB
24	N	404	HEC	C4B-C3B-CAB-CBB
24	N	404	HEC	C2C-C3C-CAC-CBC
24	N	404	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
24	O	401	HEC	C2B-C3B-CAB-CBB
24	O	401	HEC	C4B-C3B-CAB-CBB
25	C	404	8PE	C1-O11-P-O12
25	C	404	8PE	C1-O11-P-O13
25	C	404	8PE	C1-O11-P-O14
25	C	404	8PE	C11-O13-P-O11
25	C	404	8PE	C11-O13-P-O14
25	N	406	8PE	C1-O11-P-O13
25	N	406	8PE	C1-O11-P-O14
25	N	406	8PE	O13-C11-C12-N
26	C	405	CN5	CC-O13-P-O12
26	C	405	CN5	CB-CC-O13-P
26	C	405	CN5	CA-CB-CC-O13
27	N	405	UQ6	C9-C11-C12-C13
28	D	402	7PH	C1-O11-P-O12
28	P	301	7PH	C1-O11-P-O12
30	I	101	PCF	C11-O13-P-O11
30	I	101	PCF	C11-O13-P-O12
30	I	101	PCF	C11-O13-P-O14
30	I	101	PCF	O21-C2-C3-O31
30	T	101	PCF	C11-O13-P-O11
30	T	101	PCF	C11-O13-P-O12
30	T	101	PCF	C11-O13-P-O14
30	T	101	PCF	O21-C2-C3-O31
31	N	401	9PE	C1-O11-P-O12
31	N	401	9PE	C1-O11-P-O13
31	N	401	9PE	C11-O13-P-O11
31	N	401	9PE	C11-O13-P-O14
31	N	401	9PE	O13-C11-C12-N
31	N	407	9PE	C1-O11-P-O12
31	N	407	9PE	C1-O11-P-O13
31	N	407	9PE	O13-C11-C12-N
32	N	408	CN3	CC-O13-P-O11
32	N	408	CN3	CC-O13-P-O12
32	N	408	CN3	CC-O13-P-O14
32	N	408	CN3	O11-C1-C2-O21
32	N	408	CN3	O22-C21-O21-C2
32	N	408	CN3	C1'-O1'-P'-O2'
32	N	408	CN3	C1'-O1'-P'-O3'
32	N	408	CN3	C1'-O1'-P'-O4'
32	N	408	CN3	CA-O3'-P'-O1'
32	N	408	CN3	CA-O3'-P'-O2'

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Mol	Chain	Res	Type	Atoms
32	N	408	CN3	CA-O3'-P'-O4'
32	N	408	CN3	O52-C51-O51-C2'
32	N	408	CN3	C52-C51-O51-C2'
34	a	602	HEA	C2A-C3A-CMA-OMA
34	a	602	HEA	C4C-C3C-CAC-CBC
34	a	602	HEA	C13-C14-C15-C26
34	a	602	HEA	C20-C21-C22-C23
34	a	602	HEA	C21-C22-C23-C24
34	a	602	HEA	C21-C22-C23-C25
34	a	603	HEA	C2A-C3A-CMA-OMA
34	a	603	HEA	C4A-C3A-CMA-OMA
34	a	603	HEA	C2D-C3D-CAD-CBD
34	a	603	HEA	C4D-C3D-CAD-CBD
34	a	603	HEA	C21-C22-C23-C25
32	N	408	CN3	C22-C21-O21-C2
34	a	602	HEA	C14-C15-C16-C17
26	C	405	CN5	OA-CB-CC-O13
27	C	406	UQ6	C30-C29-C31-C32
27	C	406	UQ6	C28-C29-C31-C32
27	C	406	UQ6	C14-C16-C17-C18
27	C	406	UQ6	C19-C21-C22-C23
27	N	405	UQ6	C19-C21-C22-C23
34	a	603	HEA	C3D-CAD-CBD-CGD
27	N	405	UQ6	C25-C24-C26-C27
31	N	407	9PE	C21-C22-C23-C24
26	C	405	CN5	C32-C31-O31-C3
25	N	406	8PE	C31-C32-C33-C34
27	C	406	UQ6	C24-C26-C27-C28
27	N	405	UQ6	C29-C31-C32-C33
26	C	405	CN5	C31-C32-C33-C34
31	N	401	9PE	C21-C22-C23-C24
28	D	402	7PH	C32-C31-O31-C3
28	P	301	7PH	C32-C31-O31-C3
23	N	402	6PH	C31-C32-C33-C34
23	C	401	6PH	C31-C32-C33-C34
27	N	405	UQ6	C23-C24-C26-C27
32	N	408	CN3	O3'-CA-CB-OA
26	C	405	CN5	O32-C31-O31-C3
24	D	401	HEC	C1A-C2A-CAA-CBA
28	D	402	7PH	O32-C31-O31-C3
28	P	301	7PH	O32-C31-O31-C3
28	D	402	7PH	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
28	P	301	7PH	C27-C28-C29-C2A
28	D	402	7PH	C36-C37-C38-C39
25	N	406	8PE	C39-C3A-C3B-C3C
28	P	301	7PH	C36-C37-C38-C39
25	N	406	8PE	C32-C31-O31-C3
25	N	406	8PE	C37-C38-C39-C3A
31	N	401	9PE	C25-C26-C27-C28
31	N	407	9PE	C2B-C2C-C2D-C2E
23	N	402	6PH	C37-C38-C39-C3A
26	C	405	CN5	C3A-C3B-C3C-C3D
23	C	401	6PH	C37-C38-C39-C3A
34	a	602	HEA	C2C-C3C-CAC-CBC
25	C	404	8PE	C22-C21-O21-C2
31	N	401	9PE	C22-C21-O21-C2
26	C	405	CN5	C1-C2-C3-O31
28	D	402	7PH	C26-C27-C28-C29
28	P	301	7PH	C26-C27-C28-C29
24	D	401	HEC	C3A-C2A-CAA-CBA
26	C	405	CN5	C3B-C3C-C3D-C3E
32	N	408	CN3	C46-C47-C48-C49
23	C	401	6PH	C2A-C2B-C2C-C2D
23	N	402	6PH	C2A-C2B-C2C-C2D
25	N	406	8PE	C22-C21-O21-C2
25	N	406	8PE	O32-C31-O31-C3
31	N	401	9PE	C2D-C2E-C2F-C2G
25	C	404	8PE	C36-C37-C38-C39
31	N	401	9PE	C23-C24-C25-C26
34	a	602	HEA	C2A-CAA-CBA-CGA
32	N	408	CN3	C51-C52-C53-C54
34	a	602	HEA	C18-C19-C20-C21
25	N	406	8PE	O22-C21-O21-C2
31	N	407	9PE	C2D-C2E-C2F-C2G
28	D	402	7PH	C22-C23-C24-C25
28	P	301	7PH	C22-C23-C24-C25
25	C	404	8PE	O22-C21-O21-C2
26	C	405	CN5	C38-C39-C3A-C3B
31	N	407	9PE	C23-C24-C25-C26
34	a	602	HEA	C17-C18-C19-C27
31	N	401	9PE	O22-C21-O21-C2
23	C	401	6PH	C1-C2-C3-O31
23	N	402	6PH	C1-C2-C3-O31
27	C	406	UQ6	C9-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
30	I	101	PCF	C1-C2-C3-O31
30	T	101	PCF	C1-C2-C3-O31
26	C	405	CN5	C32-C33-C34-C35
34	a	602	HEA	C27-C19-C20-C21
34	a	603	HEA	C2A-CAA-CBA-CGA
28	D	402	7PH	C1-O11-P-O14
28	P	301	7PH	C1-O11-P-O14
31	N	407	9PE	C25-C26-C27-C28
25	C	404	8PE	C28-C29-C2A-C2B
34	a	603	HEA	C1A-C2A-CAA-CBA
26	C	405	CN5	C33-C34-C35-C36
34	a	603	HEA	C3B-C11-C12-C13
25	N	406	8PE	C3F-C3G-C3H-C3I
25	C	404	8PE	C32-C31-O31-C3
32	N	408	CN3	C42-C41-O41-C3'
25	C	404	8PE	C25-C26-C27-C28
34	a	603	HEA	C27-C19-C20-C21
31	N	407	9PE	C2C-C2D-C2E-C2F
31	N	401	9PE	O11-C1-C2-C3
31	N	401	9PE	C24-C25-C26-C27
32	N	408	CN3	O3'-CA-CB-CC
34	a	603	HEA	C21-C22-C23-C24
34	a	603	HEA	C3A-C2A-CAA-CBA
25	N	406	8PE	C23-C24-C25-C26
23	C	401	6PH	C22-C23-C24-C25
23	N	402	6PH	C22-C23-C24-C25
28	D	402	7PH	O11-C1-C2-C3
28	P	301	7PH	O11-C1-C2-C3
32	N	408	CN3	O11-C1-C2-C3
31	N	407	9PE	C22-C23-C24-C25
23	C	401	6PH	C32-C31-O31-C3
23	N	402	6PH	C32-C31-O31-C3
28	D	402	7PH	C1-O11-P-O13
28	P	301	7PH	C1-O11-P-O13
25	C	404	8PE	O32-C31-O31-C3
32	N	408	CN3	O42-C41-O41-C3'
28	D	402	7PH	O11-C1-C2-O21
28	P	301	7PH	O11-C1-C2-O21
32	N	408	CN3	C1-C2-C3-O31
32	N	408	CN3	C1'-C2'-C3'-O41
32	N	408	CN3	O21-C2-C3-O31
28	P	301	7PH	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
25	C	404	8PE	C33-C34-C35-C36
28	D	402	7PH	C23-C24-C25-C26
30	I	101	PCF	O13-C11-C12-N
30	T	101	PCF	O13-C11-C12-N
27	C	406	UQ6	C20-C19-C21-C22
27	N	405	UQ6	C30-C29-C31-C32
25	N	406	8PE	C36-C37-C38-C39
31	N	401	9PE	O31-C31-C32-C33
25	C	404	8PE	C3F-C3G-C3H-C3I
24	D	401	HEC	C4C-C3C-CAC-CBC
31	N	401	9PE	O11-C1-C2-O21
24	C	403	HEC	C3D-CAD-CBD-CGD
28	P	301	7PH	C34-C35-C36-C37
28	D	402	7PH	C34-C35-C36-C37
32	N	408	CN3	C53-C54-C55-C56
25	N	406	8PE	C3D-C3E-C3F-C3G
25	C	404	8PE	C38-C39-C3A-C3B
34	a	602	HEA	C4A-C3A-CMA-OMA
23	C	401	6PH	O32-C31-O31-C3
23	N	402	6PH	O32-C31-O31-C3
32	N	408	CN3	O51-C2'-C3'-O41
25	N	406	8PE	C2B-C2C-C2D-C2E
26	C	405	CN5	O1'-C1'-C2'-C3'
26	C	405	CN5	C39-C3A-C3B-C3C
28	P	301	7PH	C28-C29-C2A-C2B
28	D	402	7PH	C28-C29-C2A-C2B
24	O	401	HEC	C2C-C3C-CAC-CBC
25	C	404	8PE	C11-O13-P-O12
25	N	406	8PE	C1-O11-P-O12
25	N	406	8PE	C11-O13-P-O12
26	C	405	CN5	CC-O13-P-O11
30	I	101	PCF	C1-O11-P-O12
30	I	101	PCF	C1-O11-P-O13
30	I	101	PCF	C1-O11-P-O14
30	T	101	PCF	C1-O11-P-O12
30	T	101	PCF	C1-O11-P-O13
30	T	101	PCF	C1-O11-P-O14
34	a	602	HEA	C11-C12-C13-C14
28	D	402	7PH	C25-C26-C27-C28
32	N	408	CN3	C45-C46-C47-C48
28	P	301	7PH	C25-C26-C27-C28
25	N	406	8PE	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
25	C	404	8PE	C31-C32-C33-C34
25	C	404	8PE	C3D-C3E-C3F-C3G
27	C	406	UQ6	C25-C24-C26-C27
25	N	406	8PE	C38-C39-C3A-C3B
31	N	407	9PE	C32-C33-C34-C35
32	N	408	CN3	O1'-C1'-C2'-O51
30	I	101	PCF	C36-C37-C38-C39
30	T	101	PCF	C36-C37-C38-C39
28	D	402	7PH	C32-C33-C34-C35
28	P	301	7PH	C32-C33-C34-C35
24	C	403	HEC	CAD-CBD-CGD-O2D
32	N	408	CN3	C55-C56-C57-C58
32	N	408	CN3	C43-C44-C45-C46
30	T	101	PCF	C33-C34-C35-C36
30	I	101	PCF	C33-C34-C35-C36
31	N	401	9PE	C33-C34-C35-C36
34	a	603	HEA	C18-C19-C20-C21
27	N	405	UQ6	C20-C19-C21-C22
25	N	406	8PE	C35-C36-C37-C38
24	C	402	HEC	CAA-CBA-CGA-O1A
24	N	403	HEC	CAA-CBA-CGA-O1A
27	C	406	UQ6	C18-C19-C21-C22
27	N	405	UQ6	C28-C29-C31-C32
34	a	602	HEA	CAA-CBA-CGA-O1A
26	C	405	CN5	CB-CA-O3'-P'
25	C	404	8PE	C34-C35-C36-C37
24	C	402	HEC	CAA-CBA-CGA-O2A
24	N	403	HEC	CAA-CBA-CGA-O2A
24	C	403	HEC	CAD-CBD-CGD-O1D
34	a	603	HEA	CAD-CBD-CGD-O2D
34	a	602	HEA	CAA-CBA-CGA-O2A
34	a	602	HEA	C13-C14-C15-C16
31	N	407	9PE	O11-C1-C2-C3
27	C	406	UQ6	C23-C24-C26-C27
31	N	407	9PE	O31-C31-C32-C33
31	N	407	9PE	O11-C1-C2-O21
24	N	404	HEC	CAA-CBA-CGA-O1A
24	N	404	HEC	C2D-C3D-CAD-CBD
25	N	406	8PE	O11-C1-C2-C3
24	C	402	HEC	C3D-CAD-CBD-CGD
25	N	406	8PE	C22-C23-C24-C25
25	C	404	8PE	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
30	I	101	PCF	O31-C31-C32-C33
30	T	101	PCF	O31-C31-C32-C33
34	a	602	HEA	C16-C17-C18-C19
24	N	403	HEC	C3D-CAD-CBD-CGD
32	N	408	CN3	O51-C51-C52-C53
32	N	408	CN3	O1'-C1'-C2'-C3'
25	N	406	8PE	C3A-C3B-C3C-C3D
24	N	404	HEC	CAA-CBA-CGA-O2A
25	N	406	8PE	C33-C34-C35-C36
25	N	406	8PE	C28-C29-C2A-C2B
31	N	407	9PE	O22-C21-O21-C2
24	O	401	HEC	C4C-C3C-CAC-CBC
32	N	408	CN3	C21-C22-C23-C24
30	T	101	PCF	O32-C31-C32-C33
34	a	603	HEA	O11-C11-C12-C13
30	I	101	PCF	O32-C31-C32-C33
32	N	408	CN3	O52-C51-C52-C53
31	N	401	9PE	O32-C31-C32-C33
27	C	406	UQ6	C6-C7-C8-C9
31	N	407	9PE	C22-C21-O21-C2
30	I	101	PCF	O22-C21-C22-C23
30	T	101	PCF	O22-C21-C22-C23

There are no ring outliers.

20 monomers are involved in 84 short contacts:

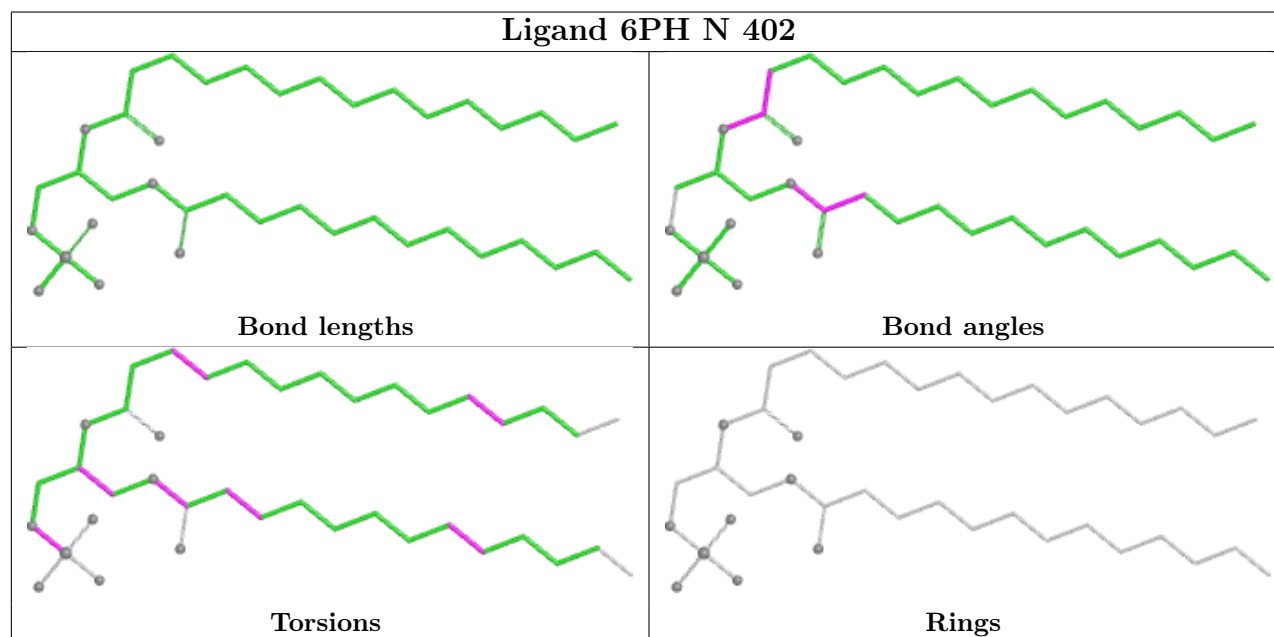
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	P	302	FES	2	0
23	N	402	6PH	5	0
28	D	402	7PH	3	0
26	C	405	CN5	3	0
34	a	603	HEA	4	0
29	E	301	FES	2	0
23	C	401	6PH	1	0
30	T	101	PCF	1	0
24	C	403	HEC	10	0
27	C	406	UQ6	1	0
24	D	401	HEC	17	0
25	N	406	8PE	1	0
24	C	402	HEC	1	0
24	N	404	HEC	12	0
32	N	408	CN3	3	0

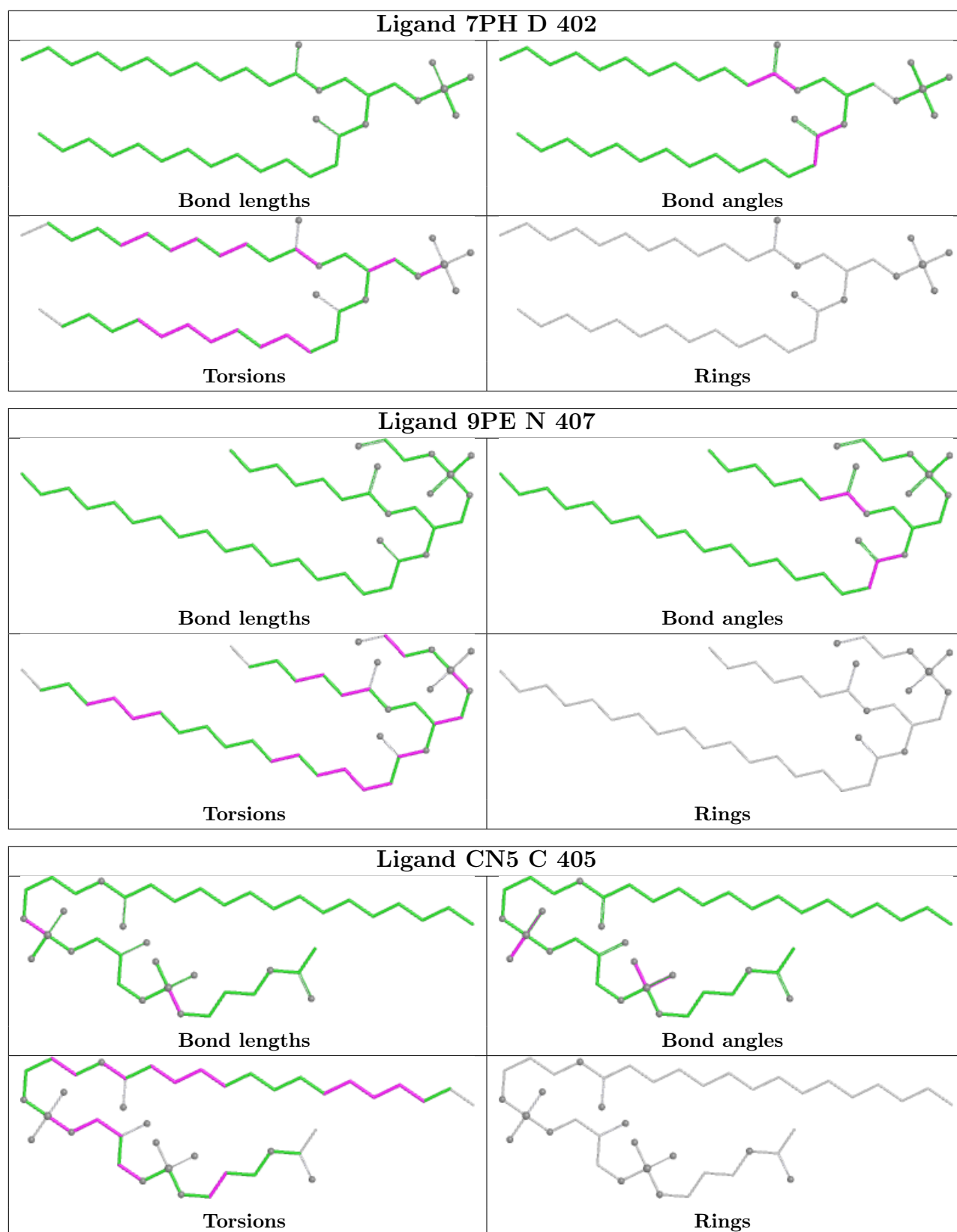
Continued on next page...

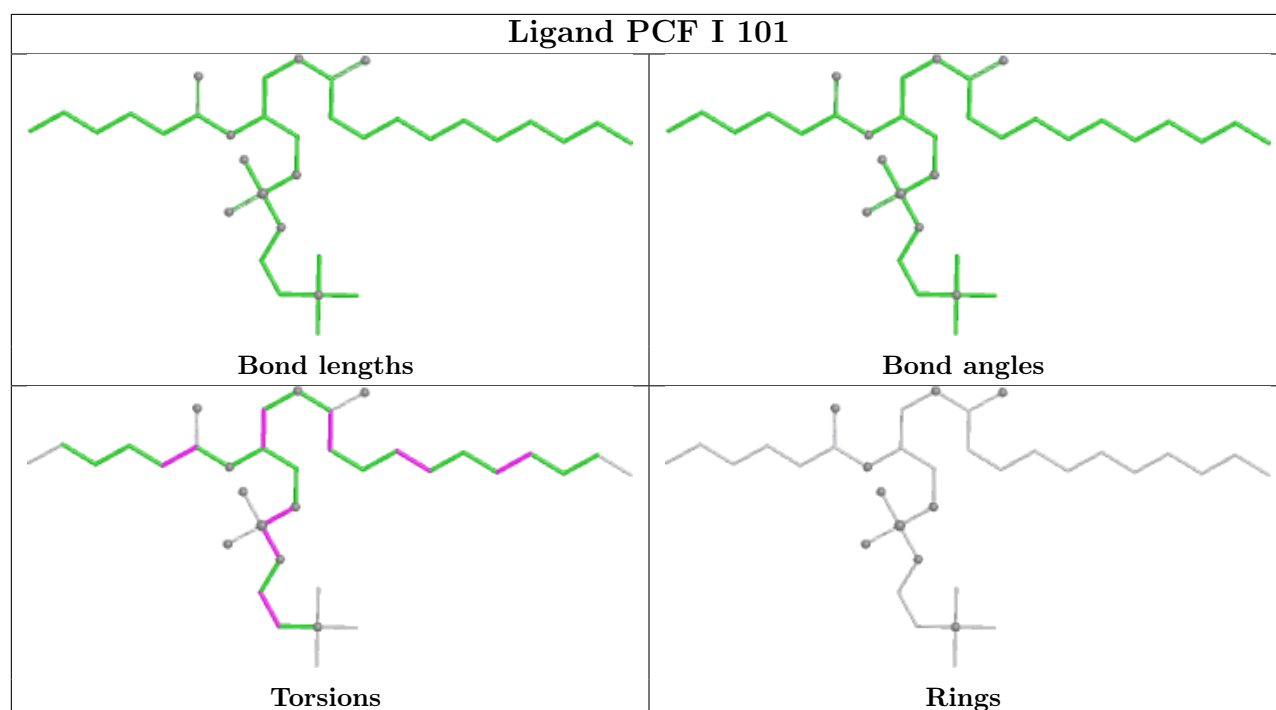
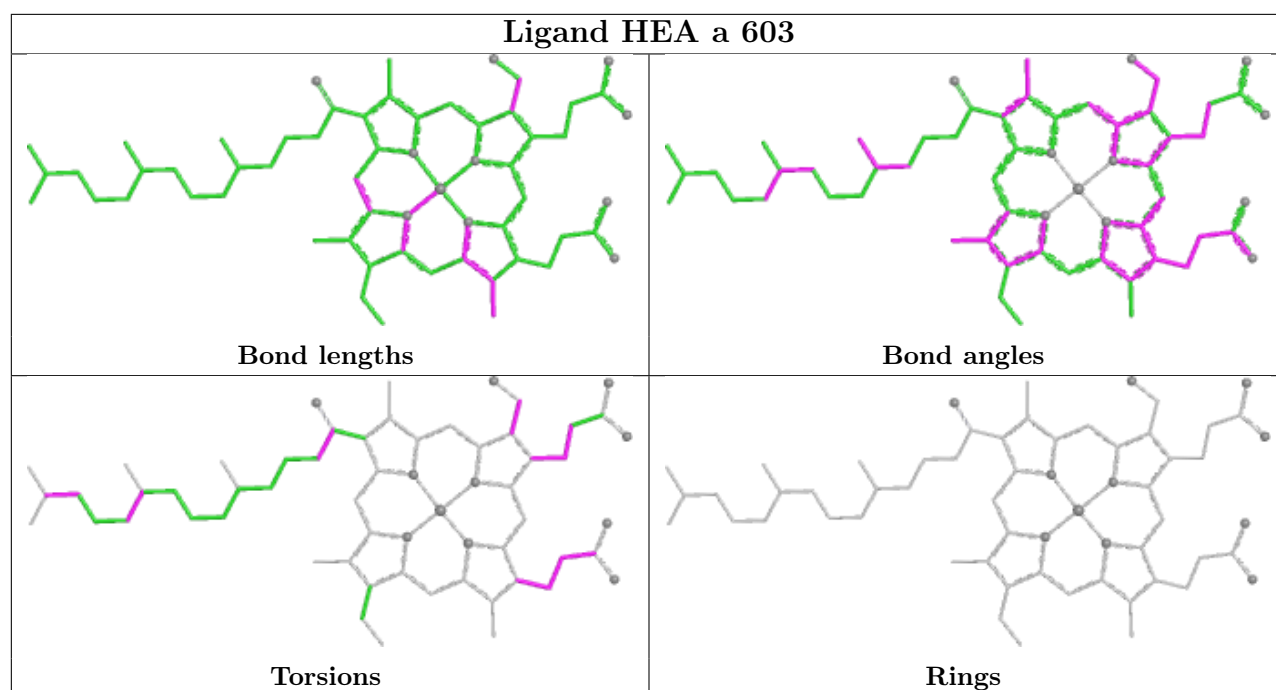
Continued from previous page...

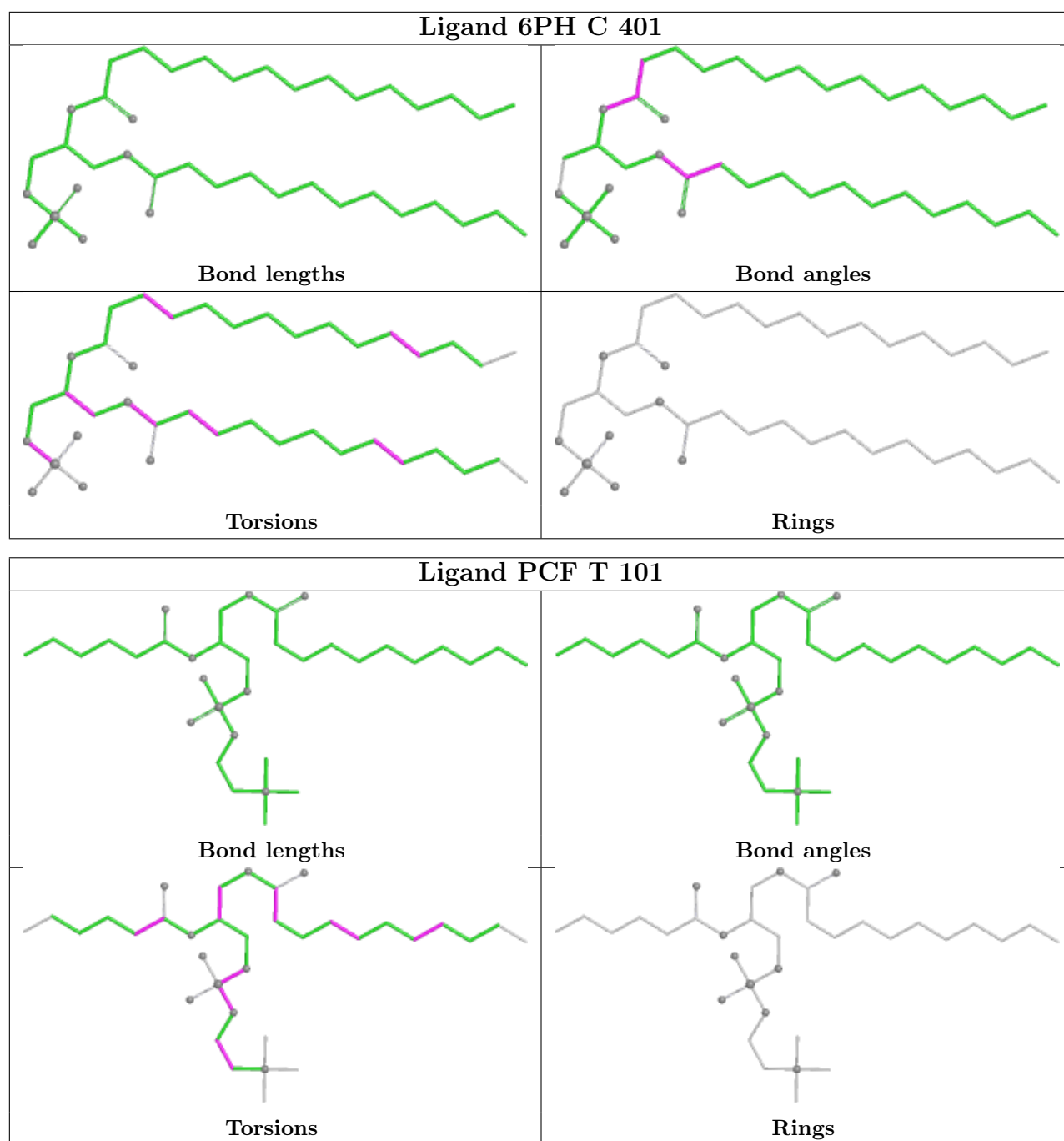
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	a	602	HEA	5	0
28	P	301	7PH	4	0
24	O	401	HEC	8	0
24	N	403	HEC	1	0
27	N	405	UQ6	3	0

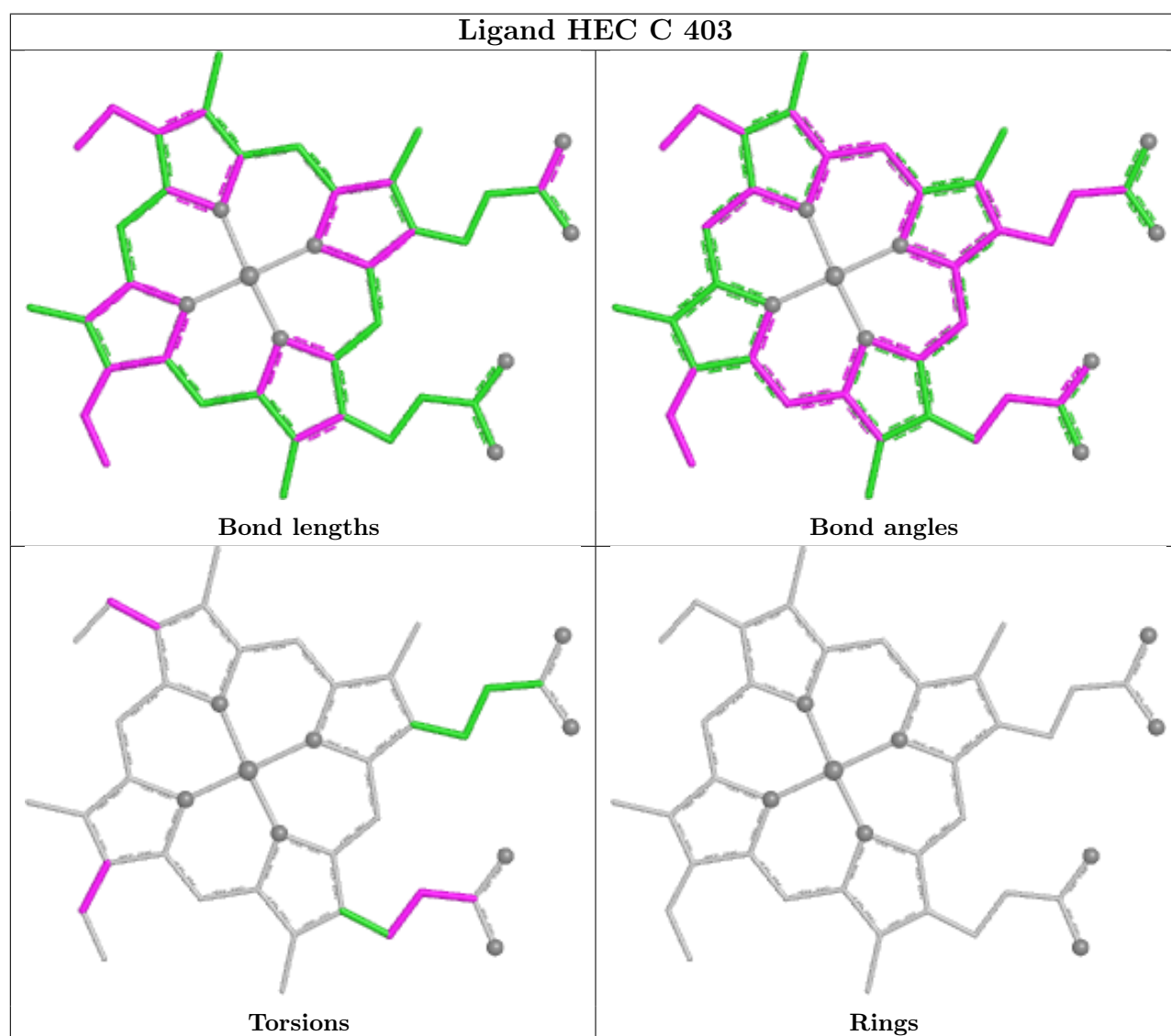
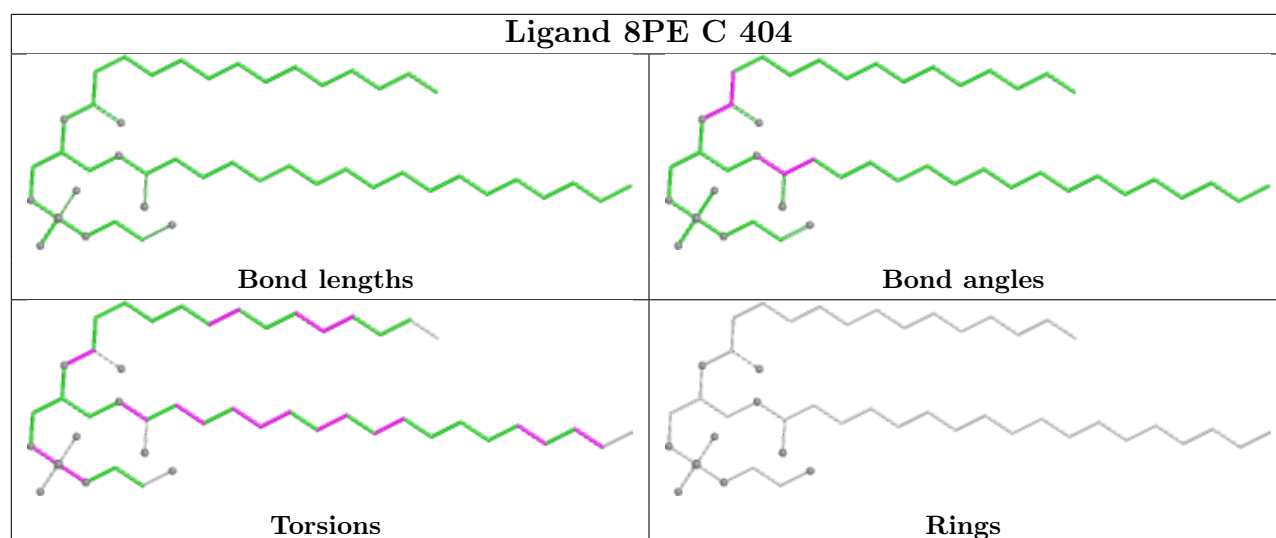
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

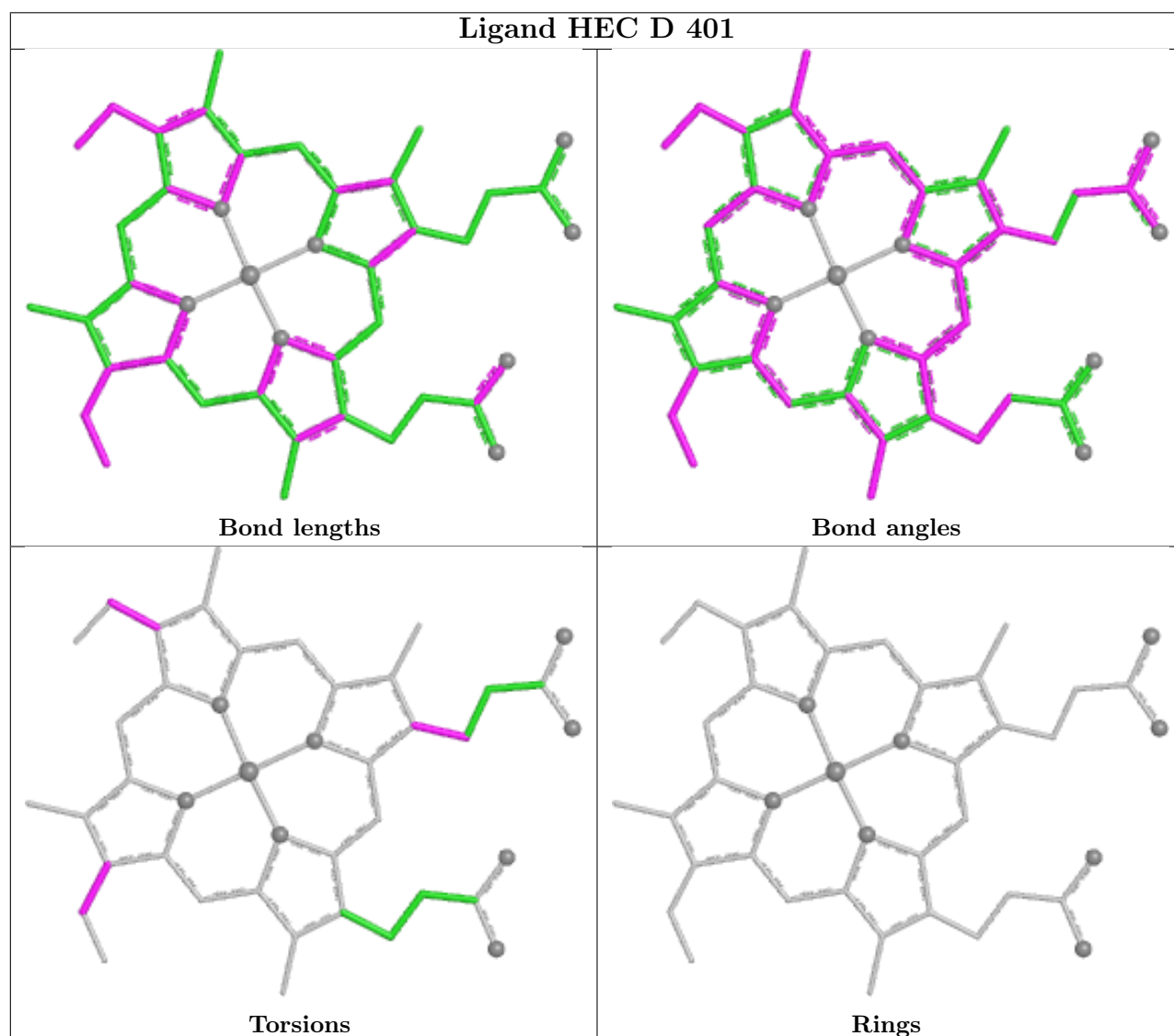
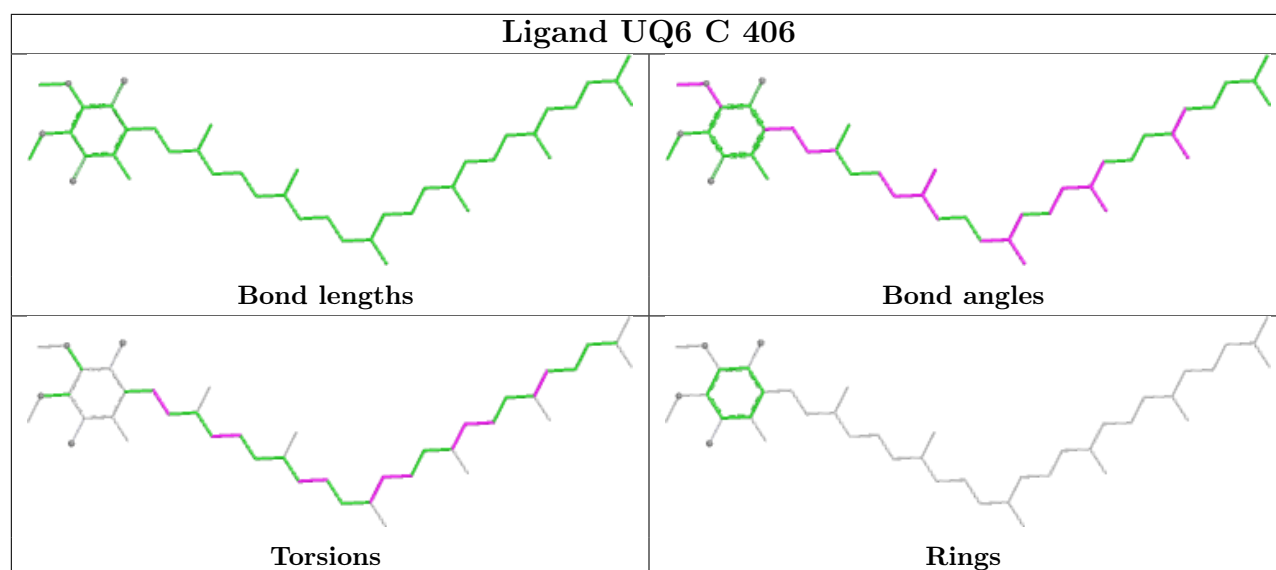


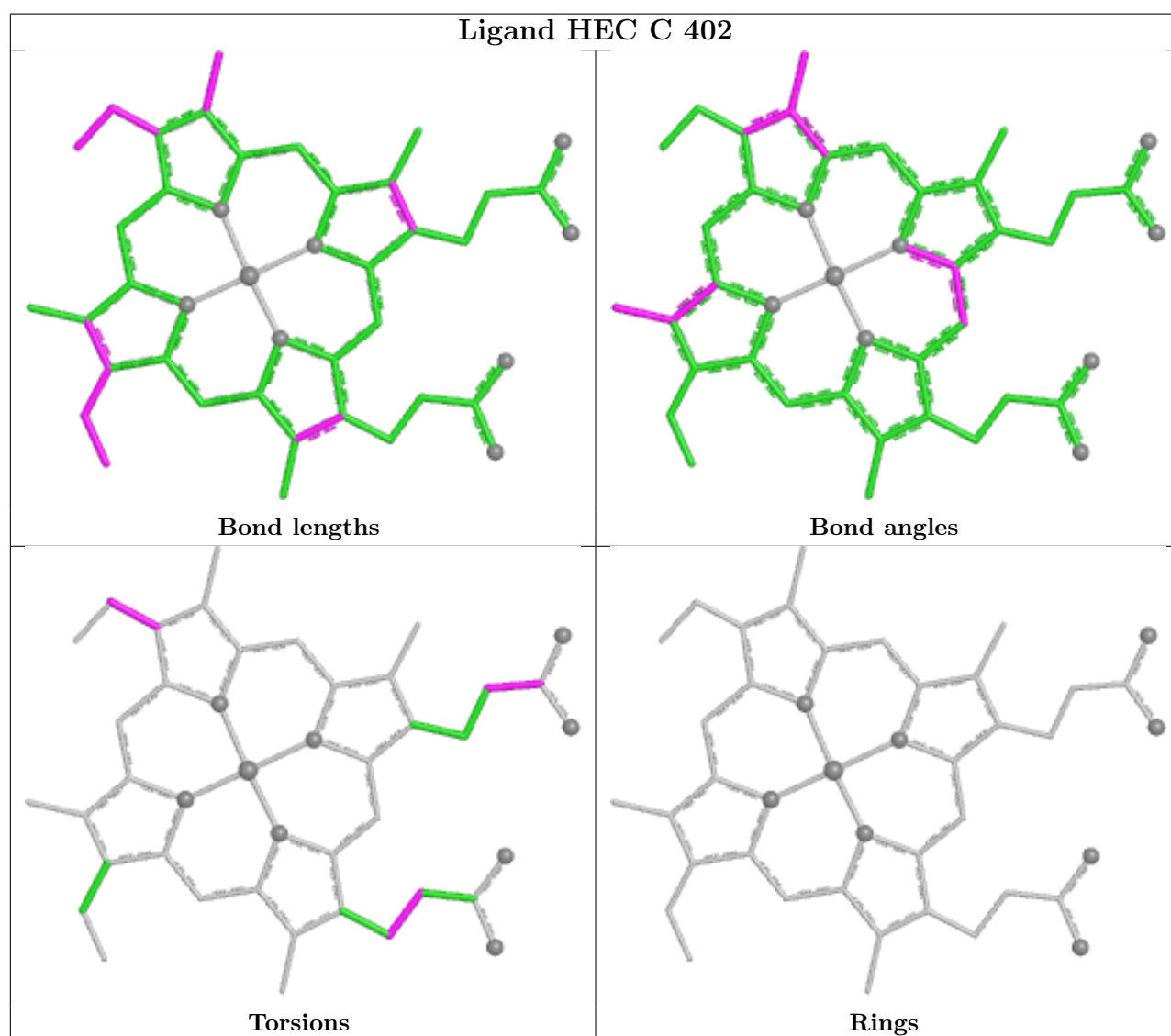
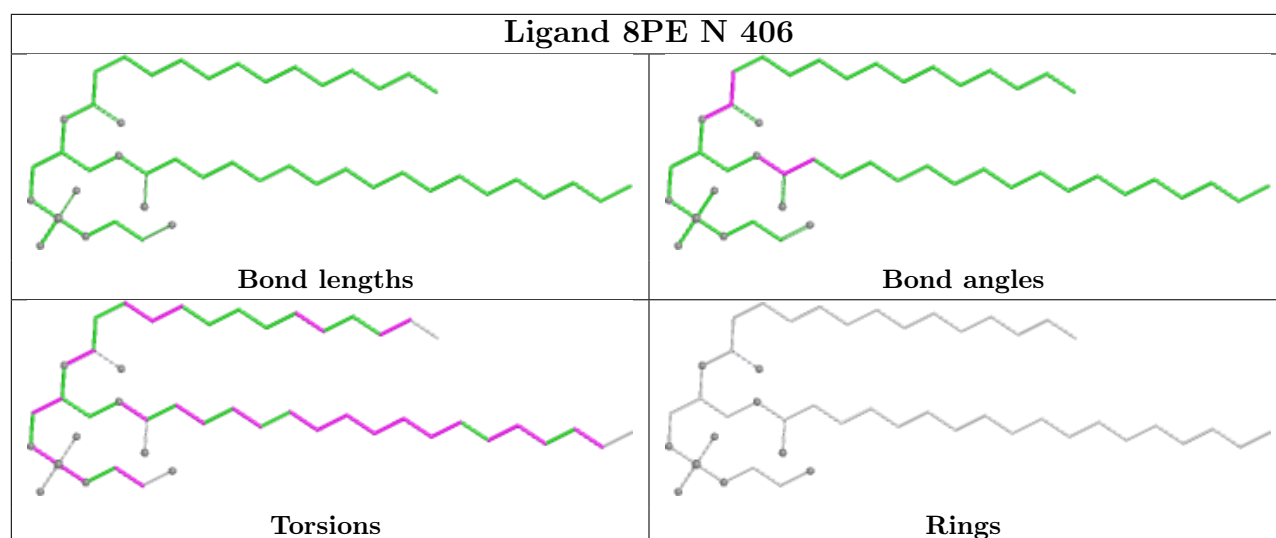


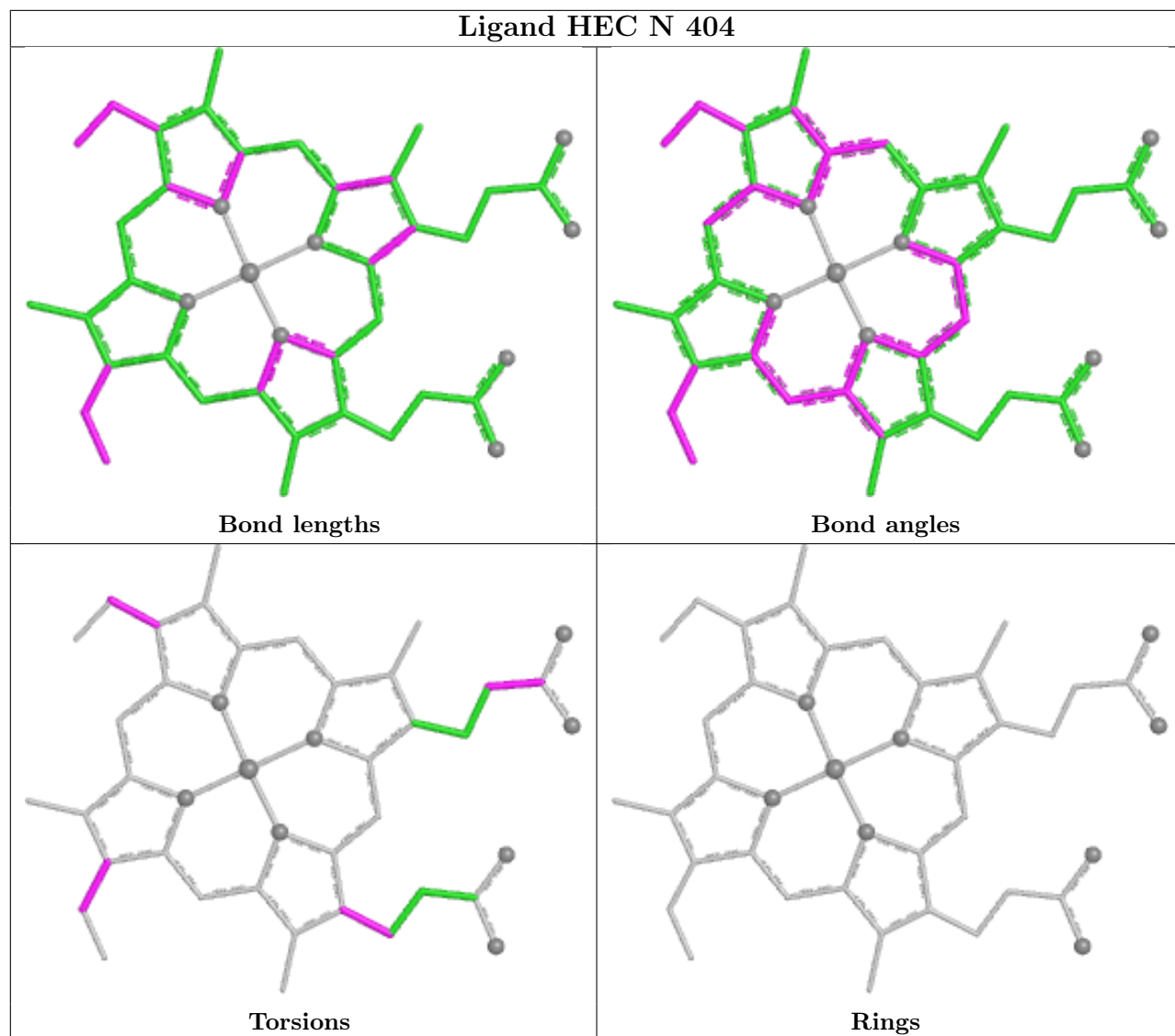


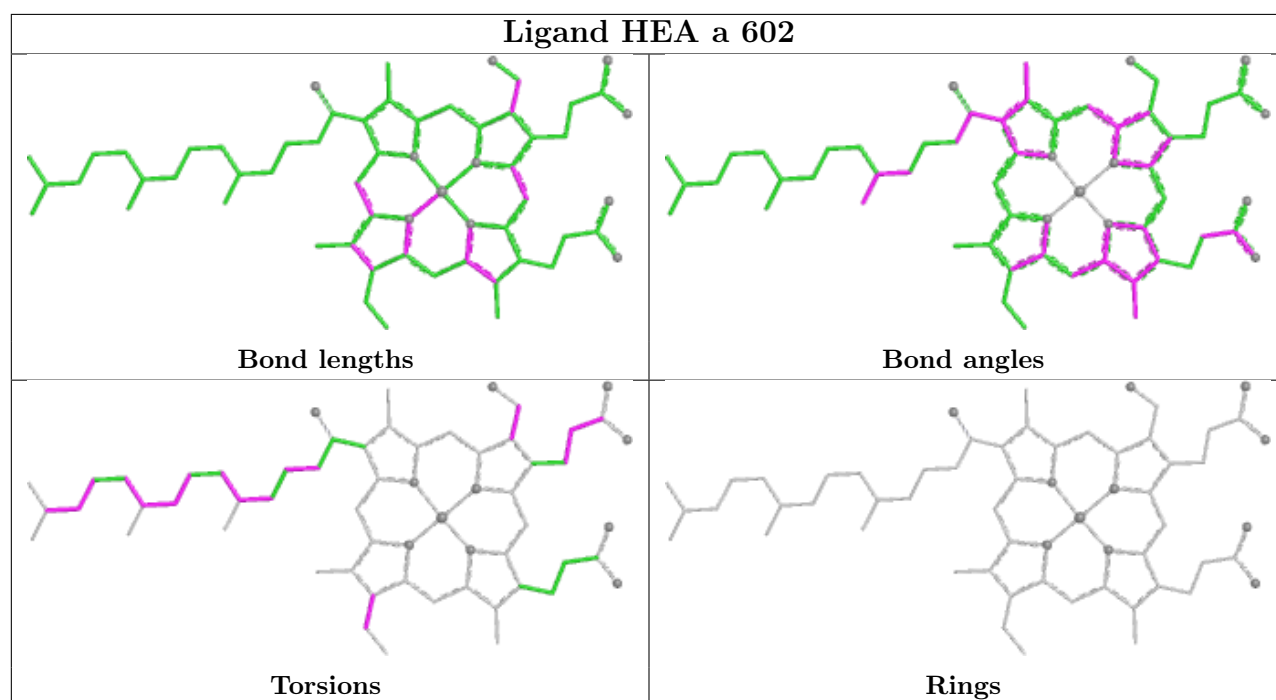
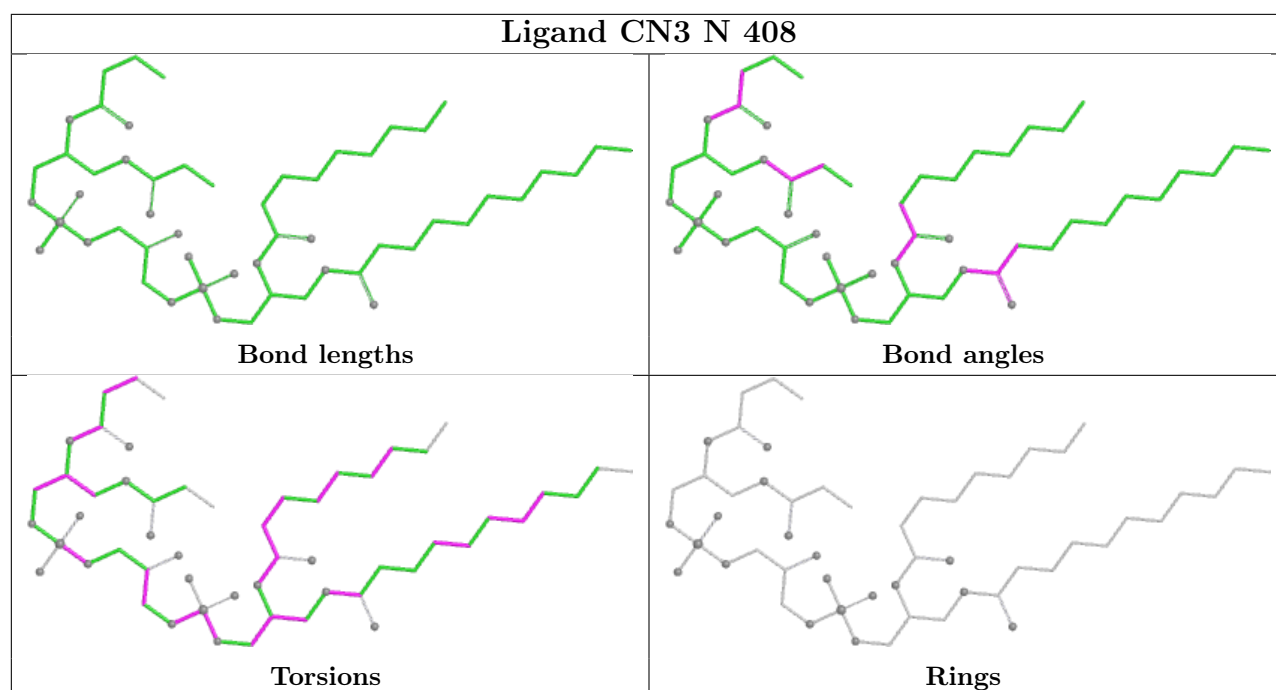


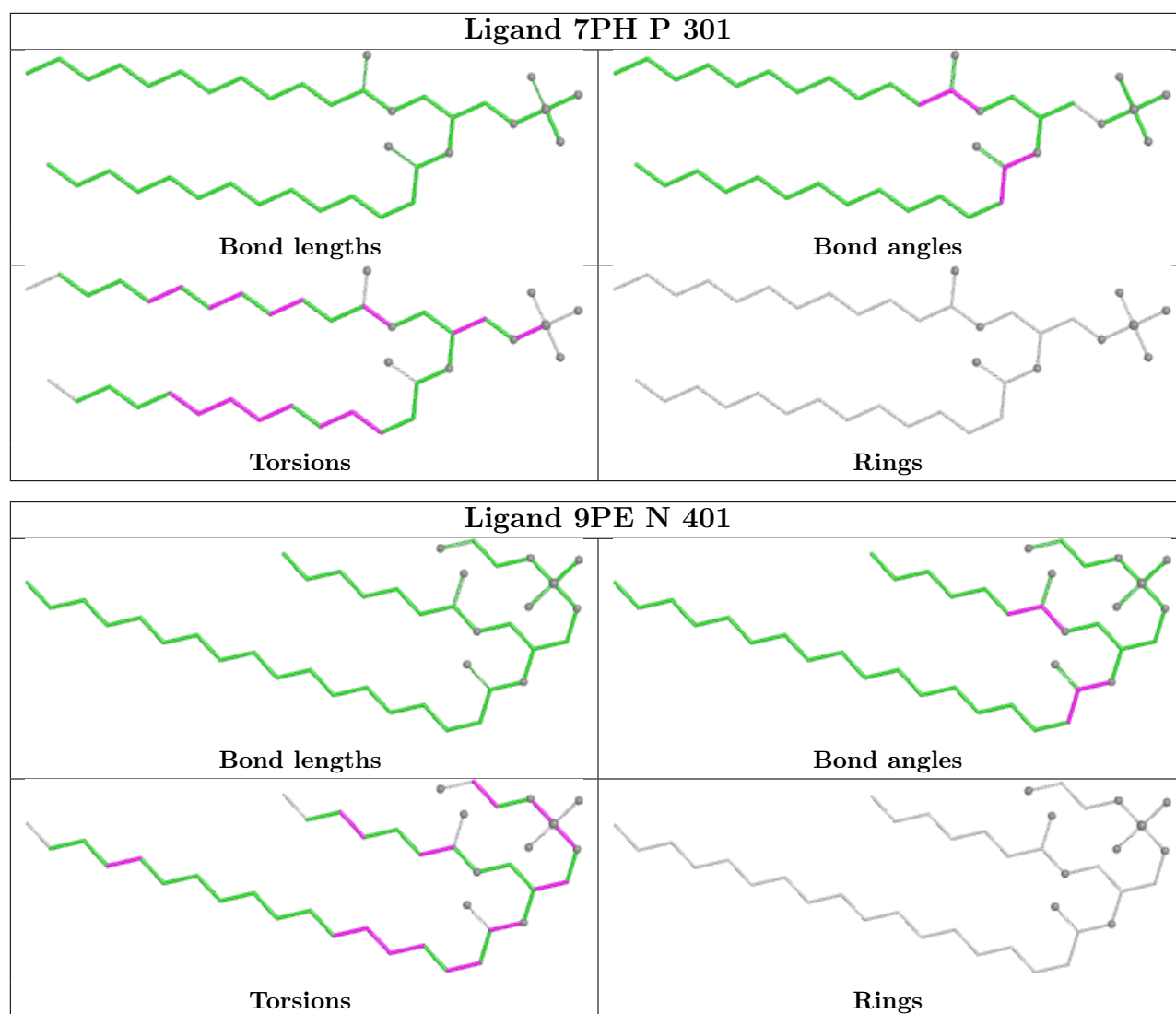


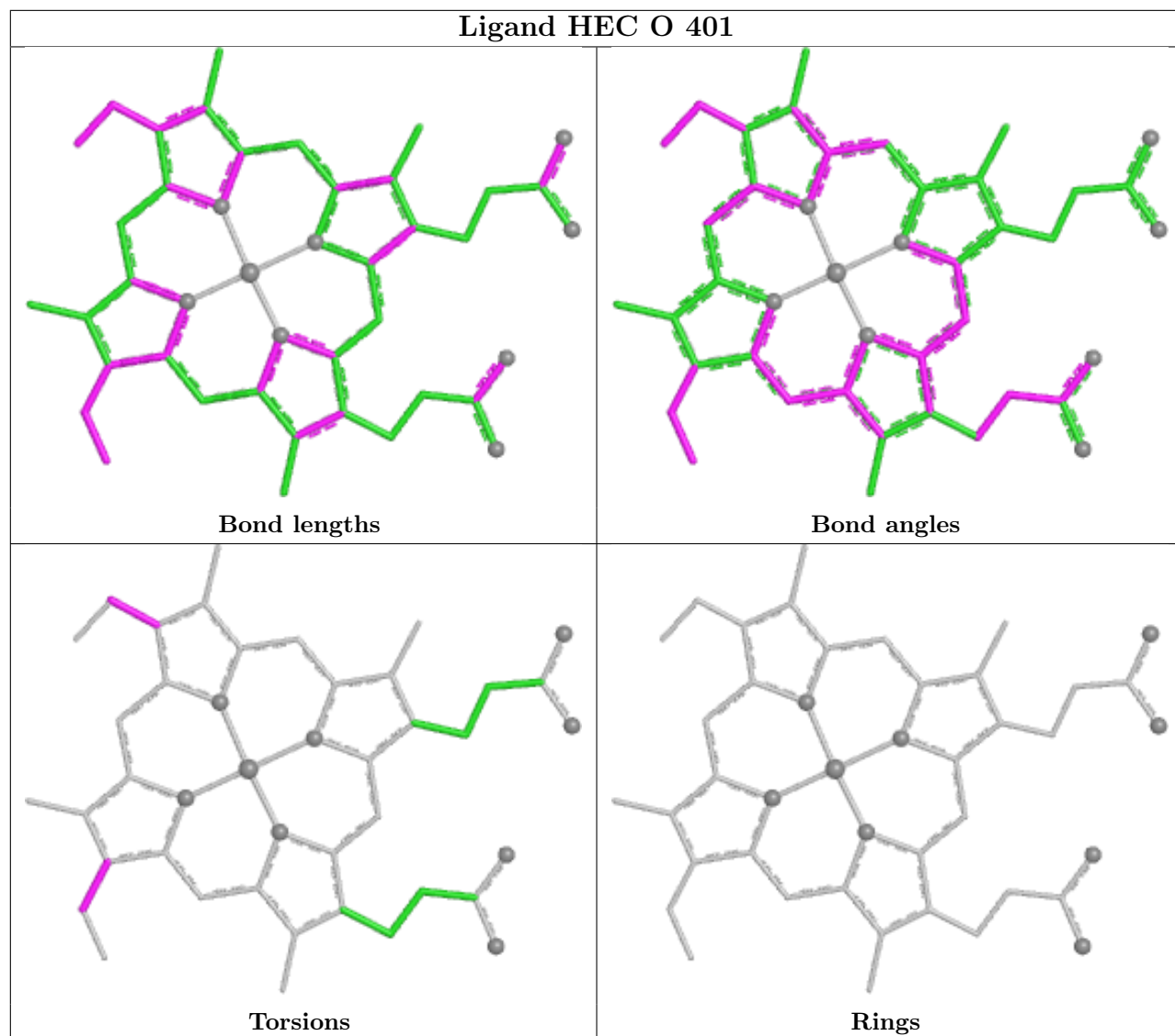


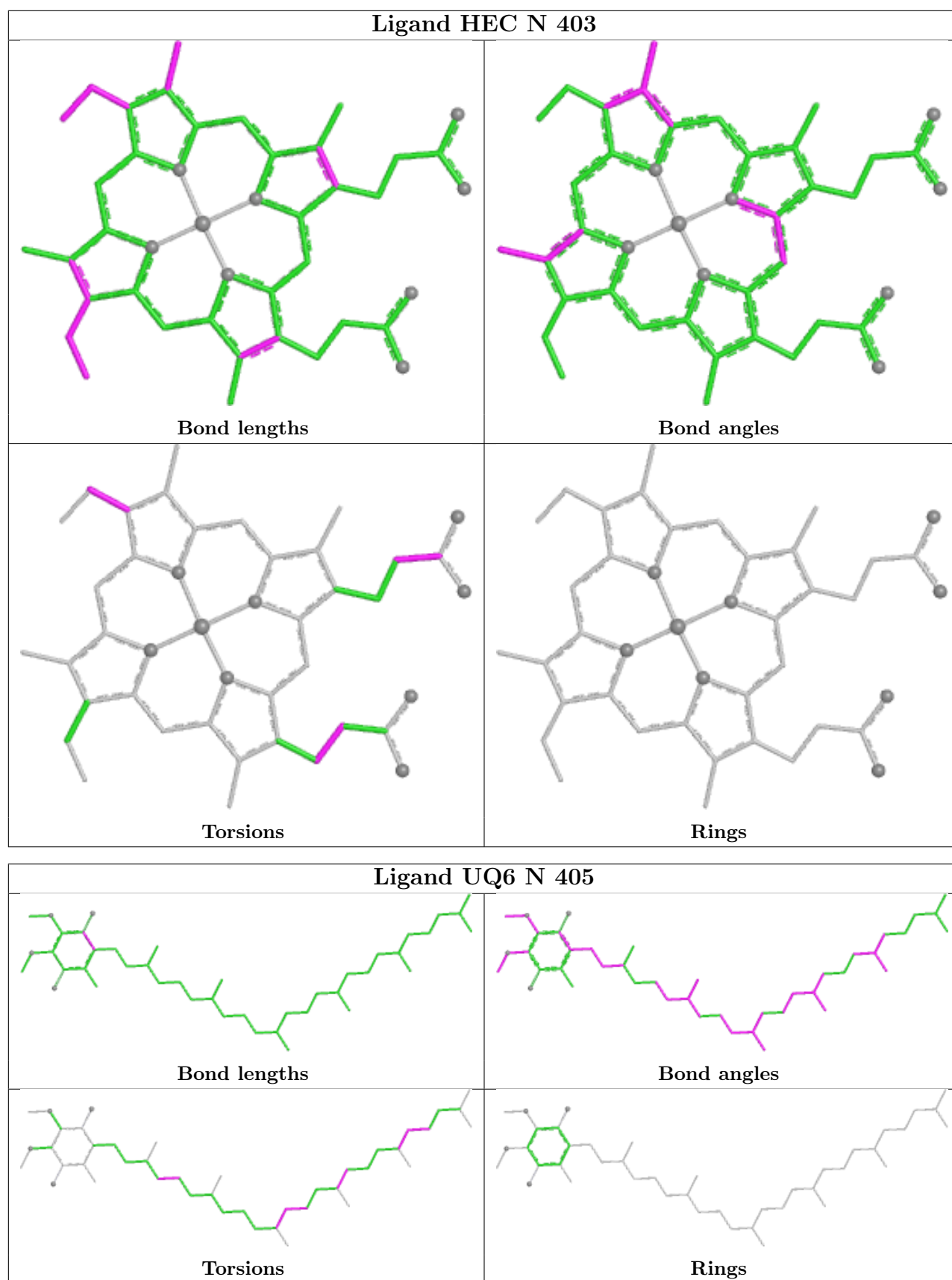












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

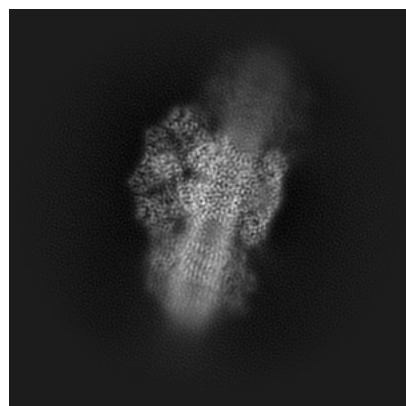
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0004. These allow visual inspection of the internal detail of the map and identification of artifacts.

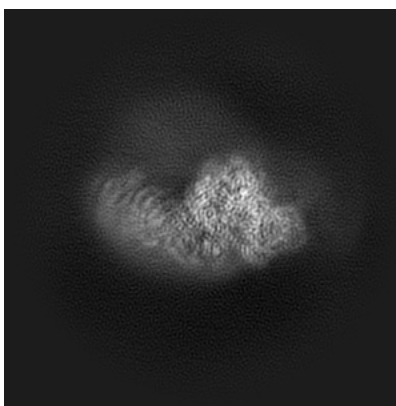
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

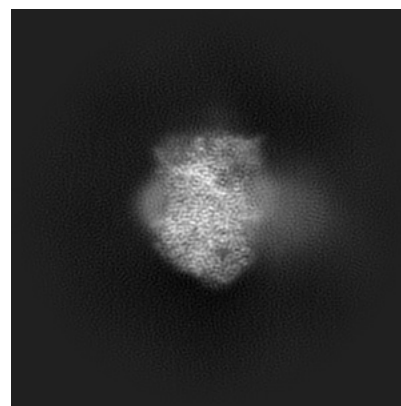
6.1.1 Primary map



X

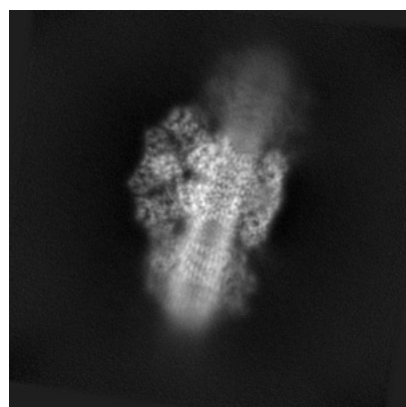


Y

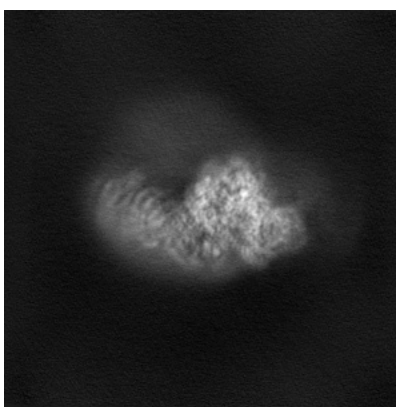


Z

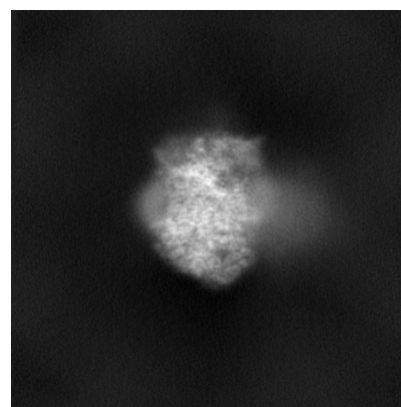
6.1.2 Raw map



X



Y

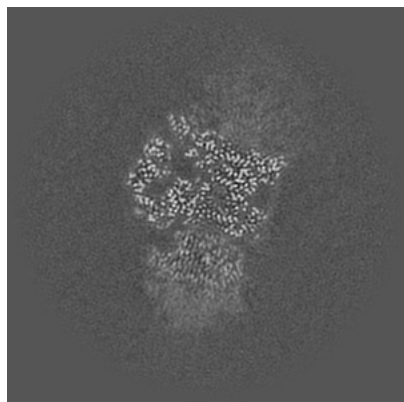


Z

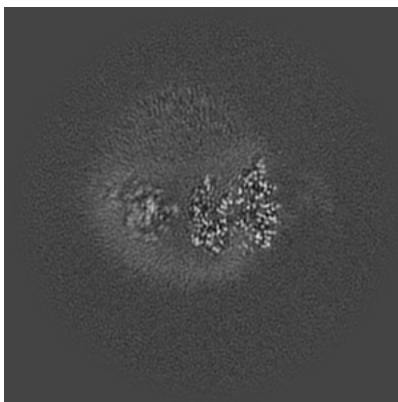
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

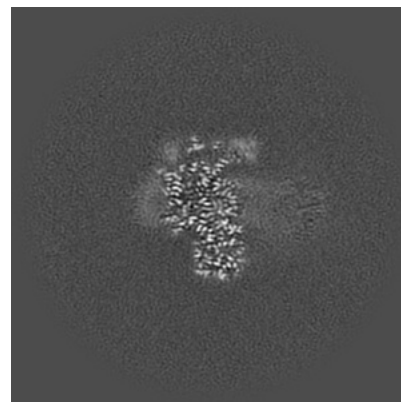
6.2.1 Primary map



X Index: 185

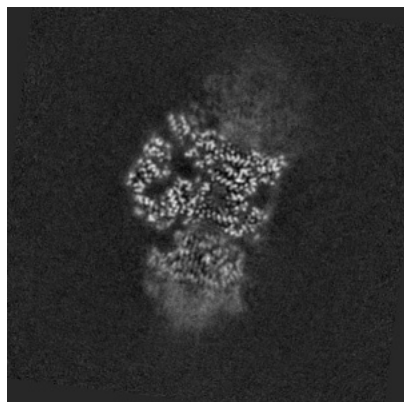


Y Index: 185

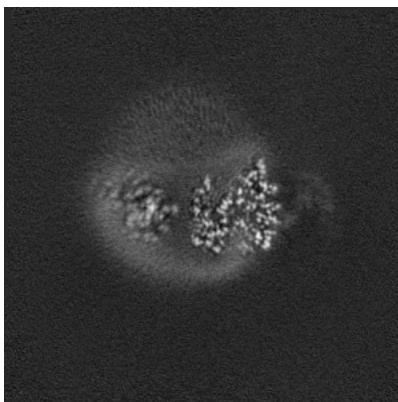


Z Index: 185

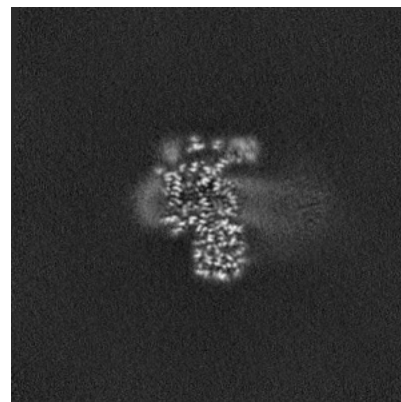
6.2.2 Raw map



X Index: 185



Y Index: 185

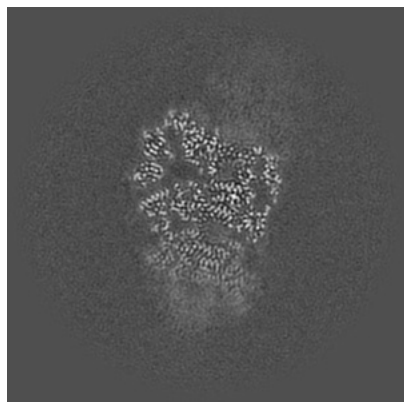


Z Index: 185

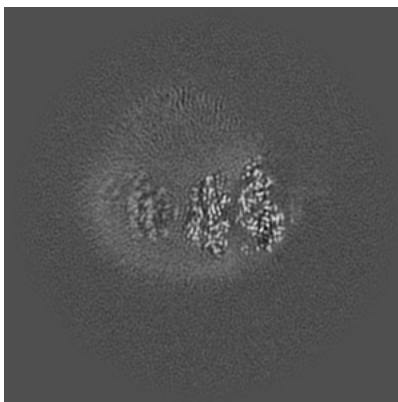
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

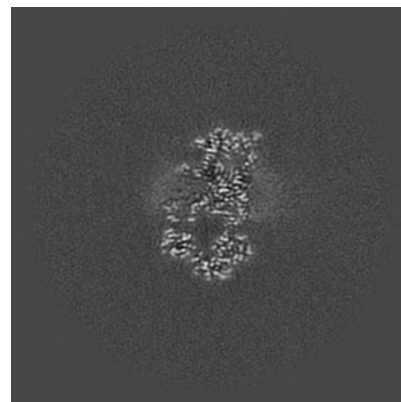
6.3.1 Primary map



X Index: 176

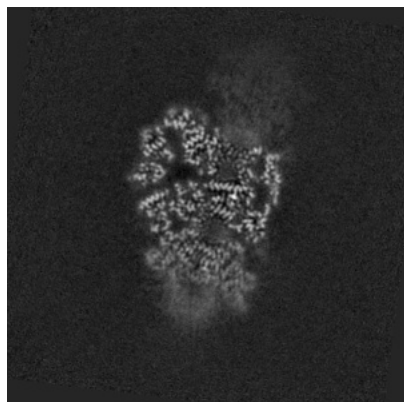


Y Index: 180

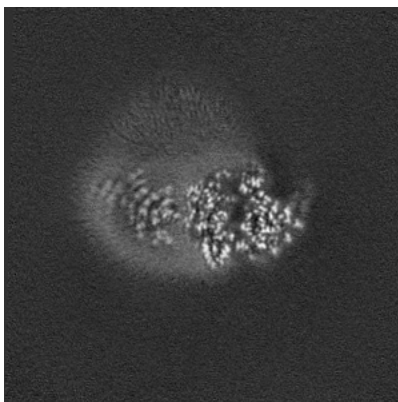


Z Index: 221

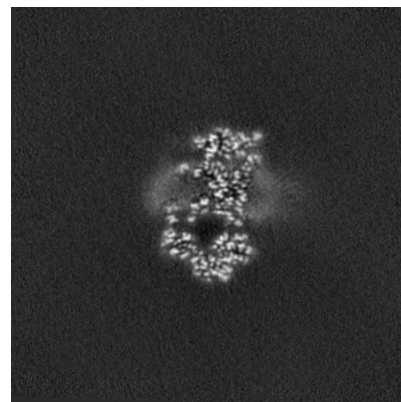
6.3.2 Raw map



X Index: 175



Y Index: 173

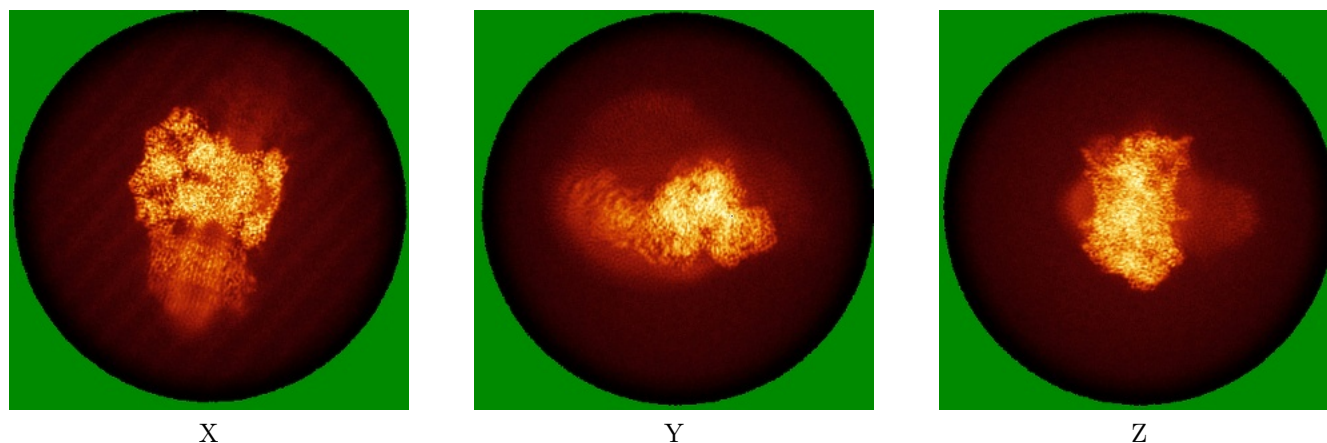


Z Index: 220

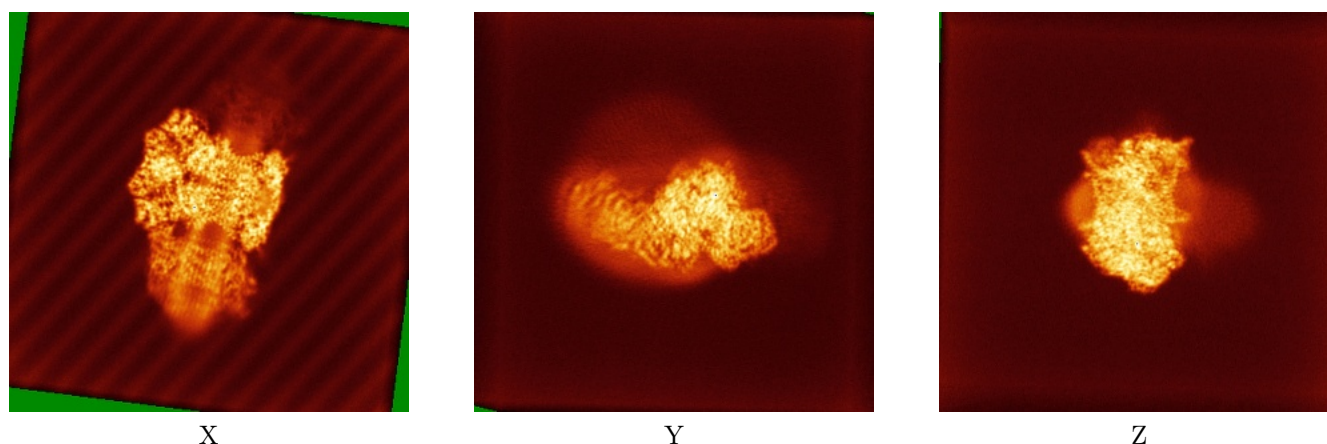
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

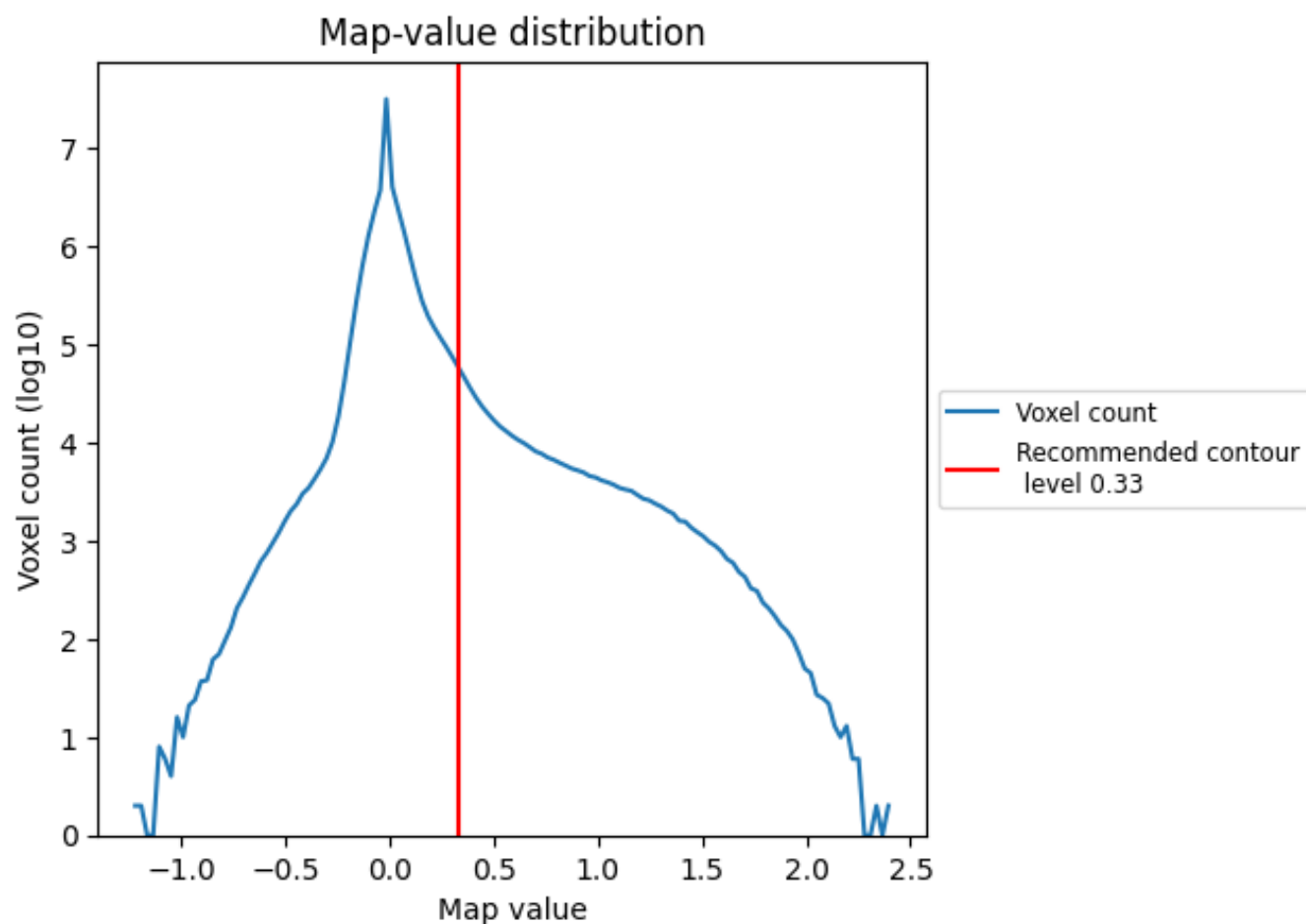
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

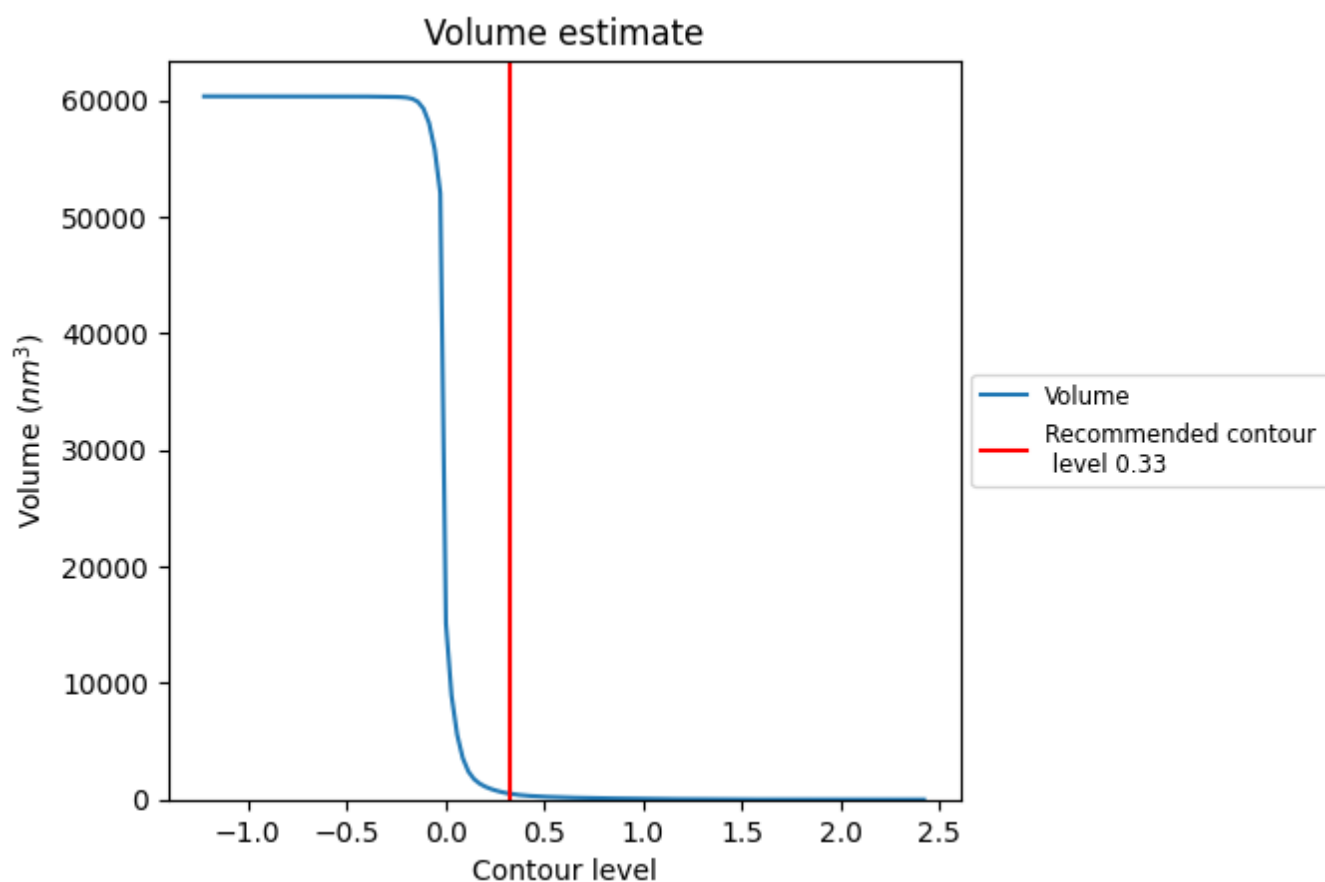
This section contains the results of statistical analysis of the map.

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.

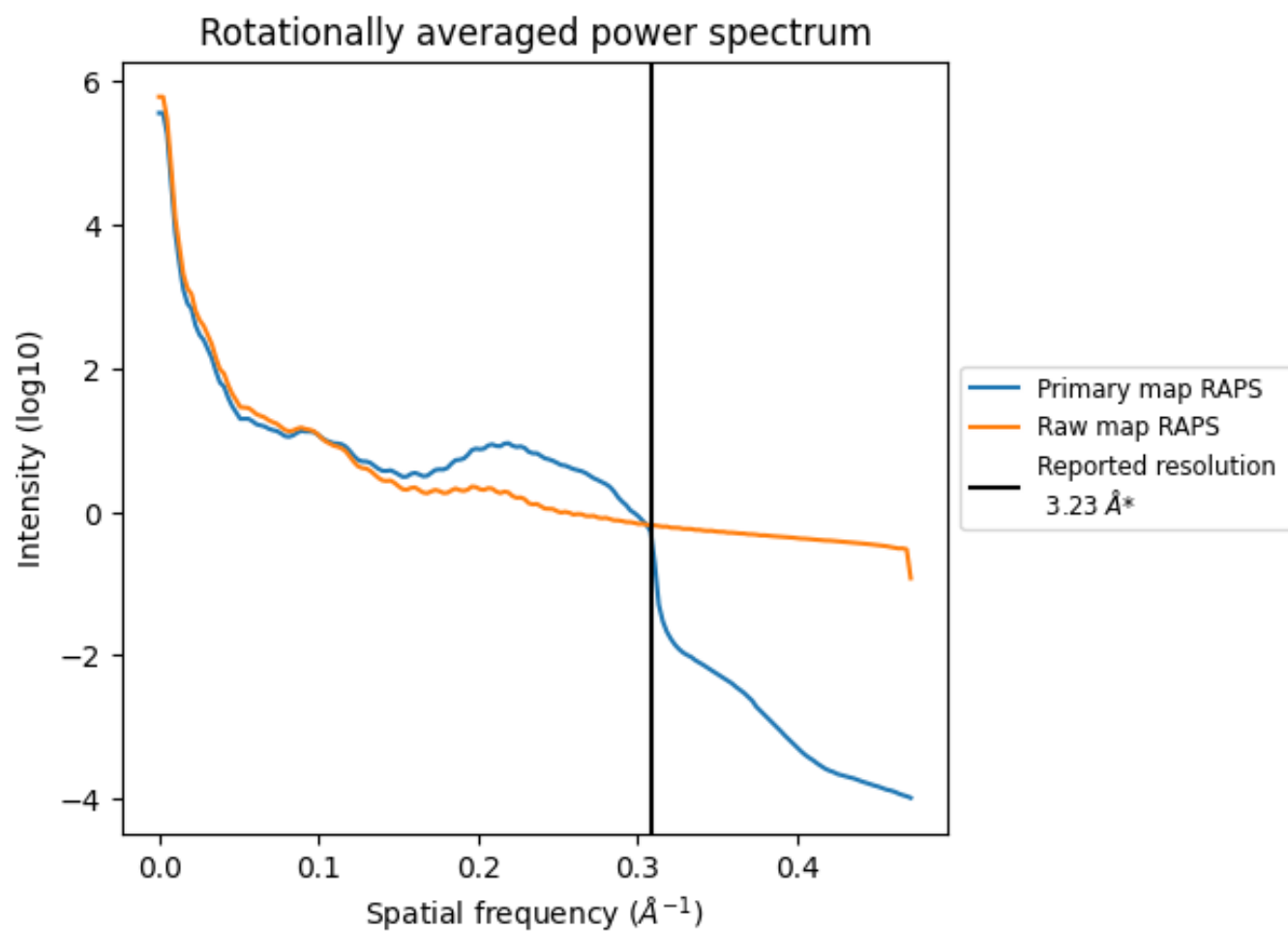
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 495 nm³; this corresponds to an approximate mass of 447 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 ⓘ

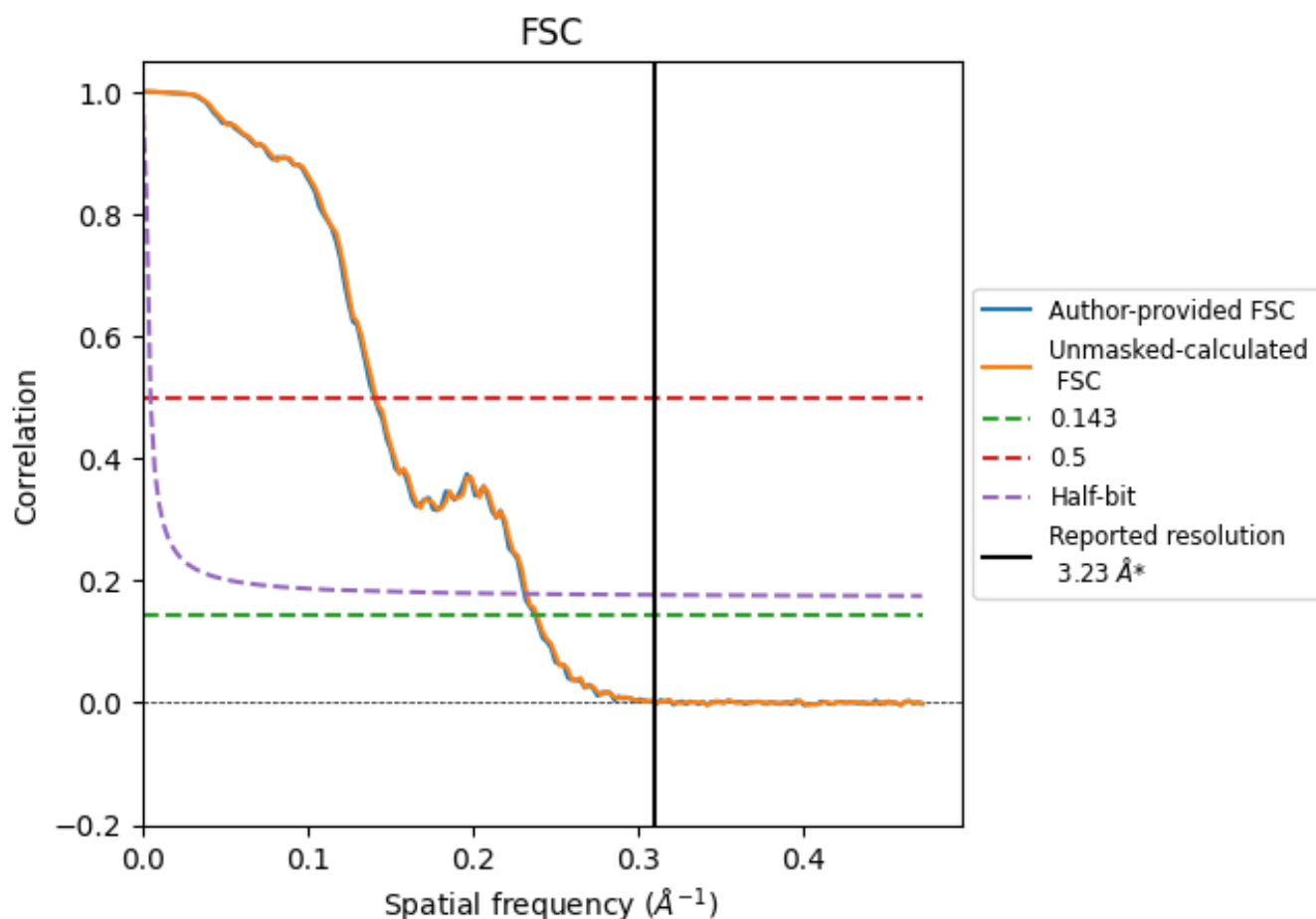


*Reported resolution corresponds to spatial frequency of 0.310 Å⁻¹

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 0.310 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.23	-	-
Author-provided FSC curve	4.21	7.12	4.33
Unmasked-calculated*	4.19	7.07	4.30

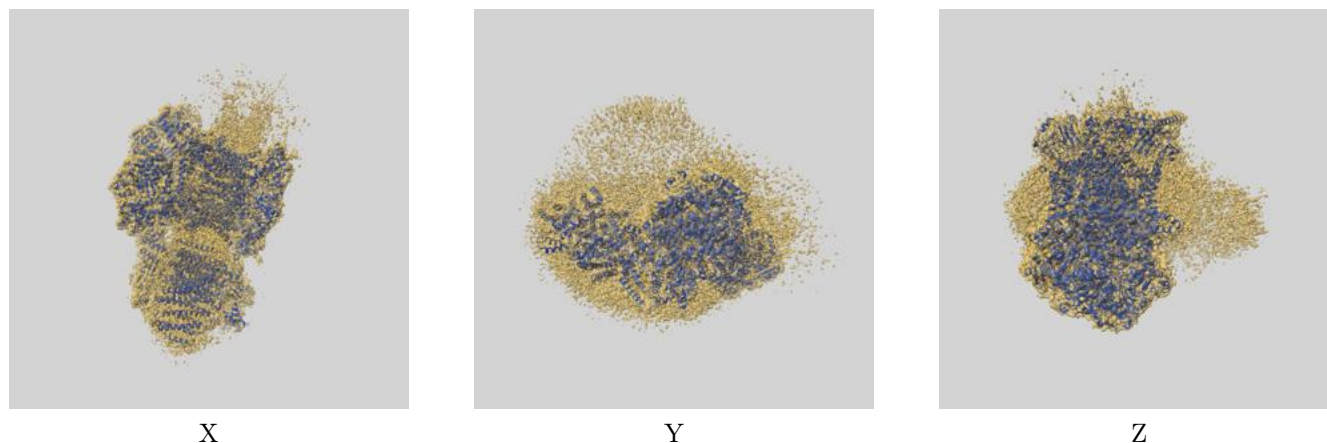
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.21 differs from the reported value 3.23 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.19 differs from the reported value 3.23 by more than 10 %

9 Map-model fit [i](#)

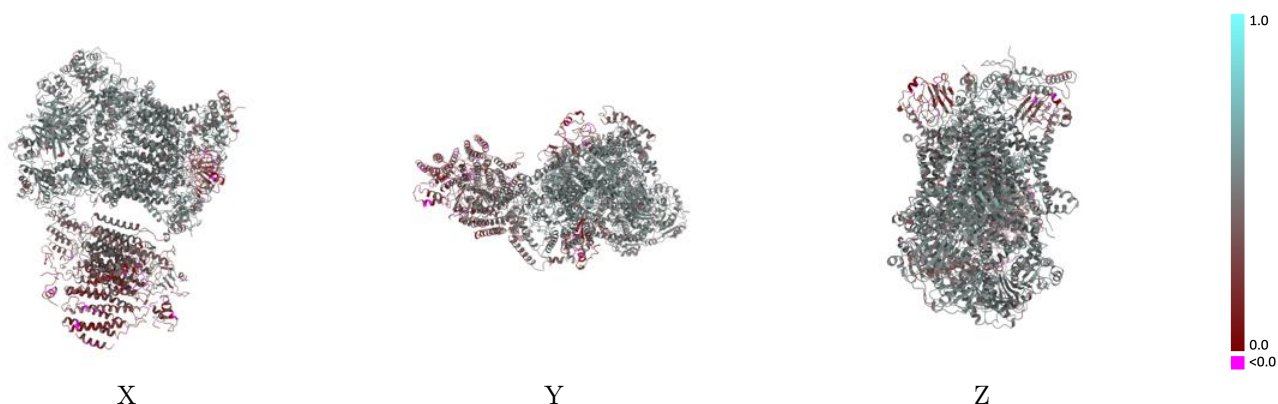
This section contains information regarding the fit between EMDB map EMD-0004 and PDB model 6GIQ. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.33 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](#)

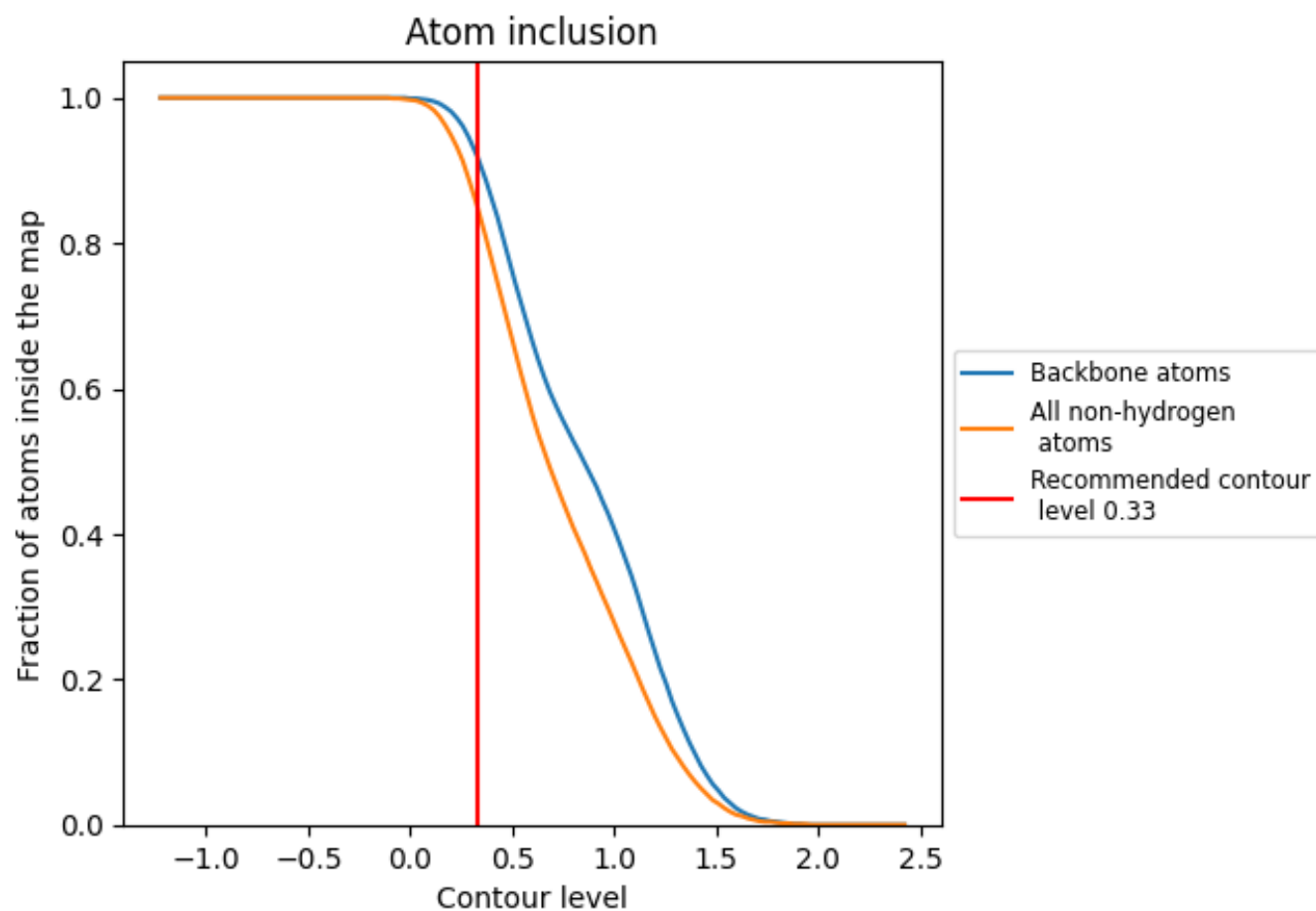


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 85% 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 (0.33) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8500	 0.4440
A	 0.9180	 0.5070
B	 0.9200	 0.5090
C	 0.9180	 0.5240
D	 0.9310	 0.5160
E	 0.7290	 0.3060
F	 0.8620	 0.4360
G	 0.9020	 0.5000
H	 0.9280	 0.4940
I	 0.8870	 0.4960
L	 0.9220	 0.5040
M	 0.9080	 0.4980
N	 0.9230	 0.5280
O	 0.9310	 0.5190
P	 0.6720	 0.3010
Q	 0.8730	 0.4270
R	 0.9120	 0.5020
S	 0.9160	 0.4850
T	 0.9300	 0.5000
U	 0.8650	 0.4190
V	 0.8740	 0.4780
a	 0.7680	 0.3770
b	 0.7460	 0.3430
c	 0.6450	 0.2390
d	 0.6000	 0.2070
e	 0.8170	 0.4110
f	 0.7820	 0.3300
g	 0.5830	 0.2190
h	 0.6740	 0.3180
i	 0.7110	 0.2840
j	 0.4480	 0.2090
k	 0.4890	 0.2230
m	 0.9290	 0.4090

