



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 11:14 PM JST

PDB ID : 8ZOS / pdb_00008zos
EMDB ID : EMD-60317
Title : Cryo-EM structure of pyraclostrobin-bound porcine bc1 complex
Authors : Wang, Y.X.; Sun, J.Y.; Li, Z.W.; Cui, G.R.; Yang, G.F.
Deposited on : 2024-05-29
Resolution : 2.37 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

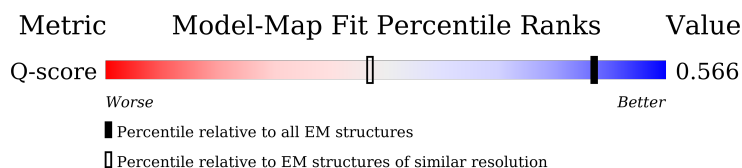
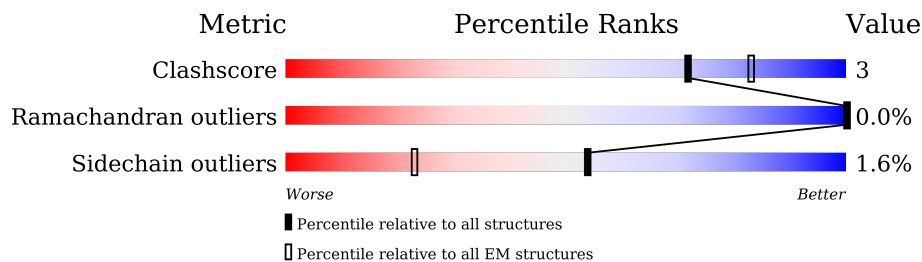
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.37 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	4742 (1.87 - 2.87)

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	378	
1	a	378	
2	B	241	
2	b	241	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	196	86% 84% 15% ..
3	c	196	89% 82% 18%
4	D	446	95% .
4	d	446	96% .
5	E	418	94% 6%
5	e	418	93% 7%
6	F	64	48% 84% 12% ..
6	f	64	50% 86% 11% ..
7	G	106	8% 98%
7	g	106	8% 97%
8	H	79	8% 90% 10%
8	h	79	15% 91% 9%
9	I	62	68% 71% 24% 5%
9	i	62	69% 65% 29% 6%
10	J	52	94% 75% 19% 6%
10	j	52	98% 83% 15%
11	K	57	33% 79% 16% 5%
11	k	57	35% 75% 19% 5%

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
15	HEC	b	401	X	-	-	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 33531 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	378	Total	C	N	O	S	0	0
			3017	2026	470	501	20		
1	a	378	Total	C	N	O	S	0	0
			3017	2026	470	501	20		

- Molecule 2 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	241	Total	C	N	O	S	0	0
			1920	1225	330	349	16		
2	b	239	Total	C	N	O	S	0	0
			1904	1214	327	347	16		

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	194	Total	C	N	O	S	0	0
			1502	946	261	288	7		
3	c	196	Total	C	N	O	S	0	0
			1517	954	265	291	7		

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	445	Total	C	N	O	S	0	0
			3452	2157	604	672	19		
4	d	446	Total	C	N	O	S	0	0
			3459	2161	605	674	19		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	418	Total	C	N	O	S	0	0
			3134	1962	556	607	9		
5	e	418	Total	C	N	O	S	0	0
			3134	1962	556	607	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	64	Total	C	N	O	S	0	0
			528	320	97	106	5		
6	f	64	Total	C	N	O	S	0	0
			528	320	97	106	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	106	Total	C	N	O	S	0	0
			921	589	162	168	2		
7	g	106	Total	C	N	O	S	0	0
			921	589	162	168	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	71	Total	C	N	O	S	0	0
			608	399	112	95	2		
8	h	79	Total	C	N	O	S	0	0
			666	434	122	108	2		

- Molecule 9 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	62	Total	C	N	O	0	0
			507	331	90	86		
9	i	62	Total	C	N	O	0	0
			507	331	90	86		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	49	Total	C	N	O	S	0	0
			405	269	71	63	2		

Continued on next page...

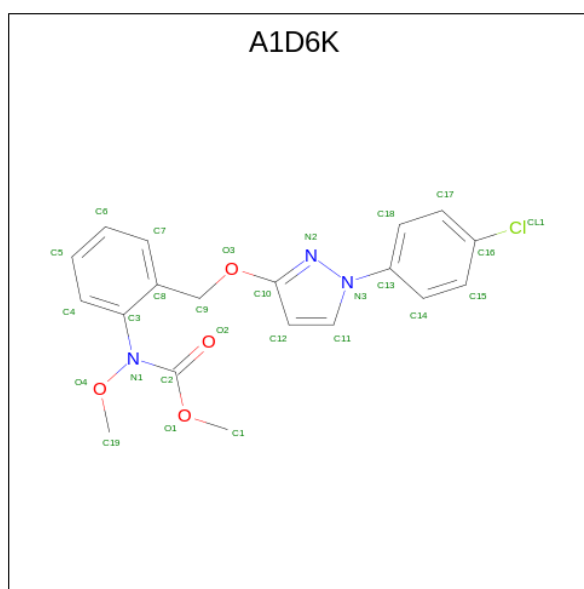
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

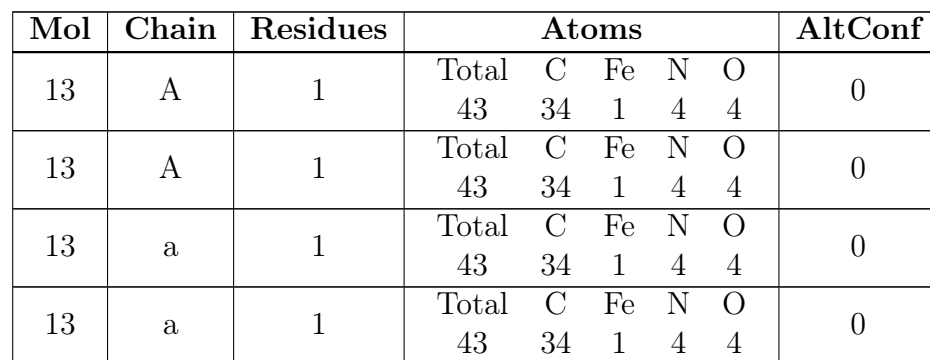
Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	57	Total	C	N	O	S	0	0
			404	252	74	76	2		
11	k	57	Total	C	N	O	S	0	0
			404	252	74	76	2		

- Molecule 12 is methyl {N}-[2-[[1-(4-chlorophenyl)pyrazol-3-yl]oxymethyl]phenyl]- {N}-methoxy-carbamate (CCD ID: A1D6K) (formula: C₁₉H₁₈ClN₃O₄) (labeled as "Ligand of Interest" by depositor).

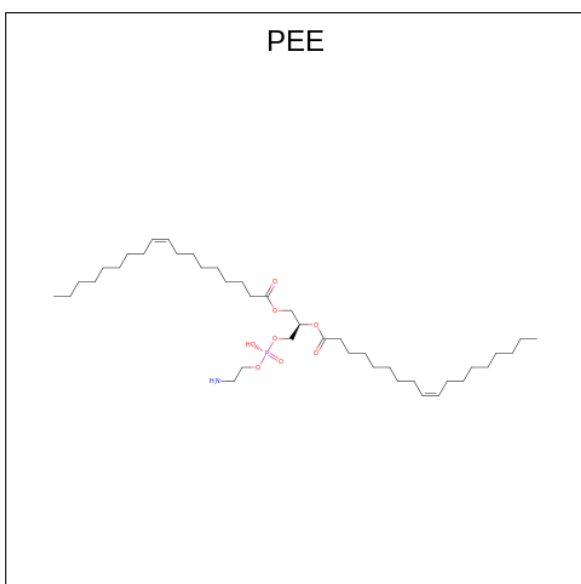


Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	Cl	N	O	0
			27	19	1	3	4	
12	a	1	Total	C	Cl	N	O	0
			27	19	1	3	4	

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).

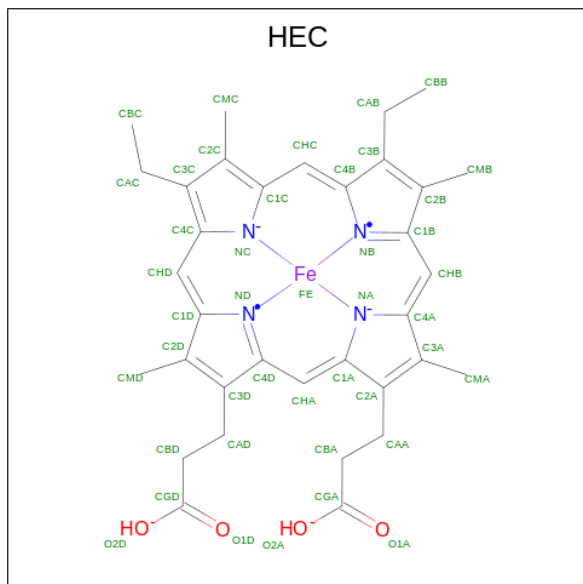


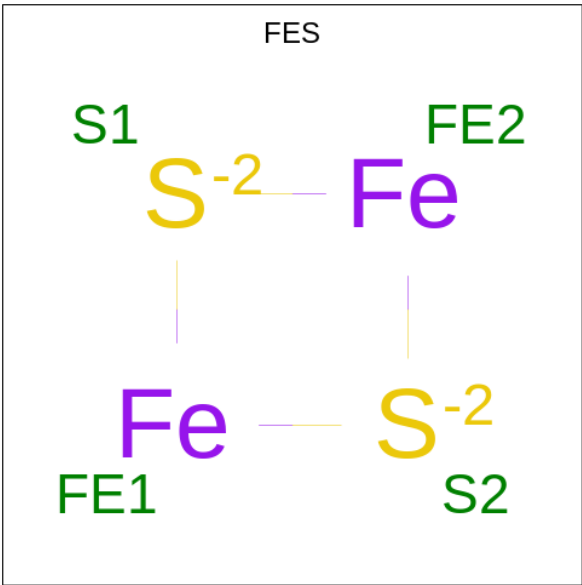
- Molecule 14 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $\text{C}_{41}\text{H}_{78}\text{NO}_8\text{P}$).



Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
14	D	1	Total	C	N	O	P	0
			49	39	1	8	1	
14	a	1	Total	C	N	O	P	0
			49	39	1	8	1	

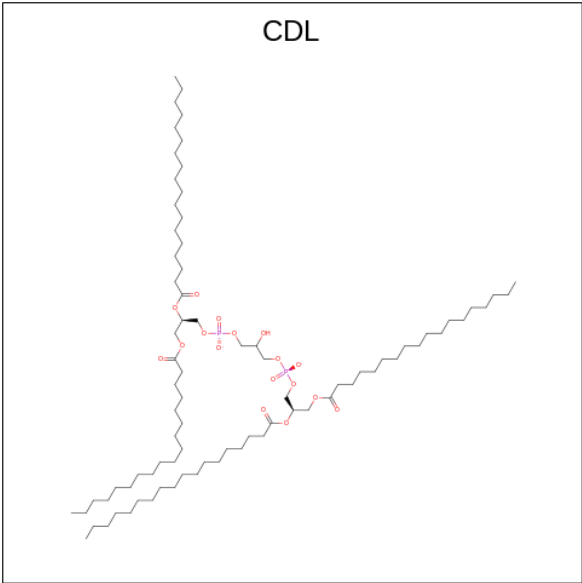
- Molecule 15 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).





Mol	Chain	Residues	Atoms			AltConf
16	a	1	Total	Fe	S	0
			4	2	2	
16	c	1	Total	Fe	S	0
			4	2	2	

- Molecule 17 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
17	a	1	Total	C	O	P	0
			64	45	17	2	
17	a	1	Total	C	O	P	0
			64	45	17	2	

Continued on next page...

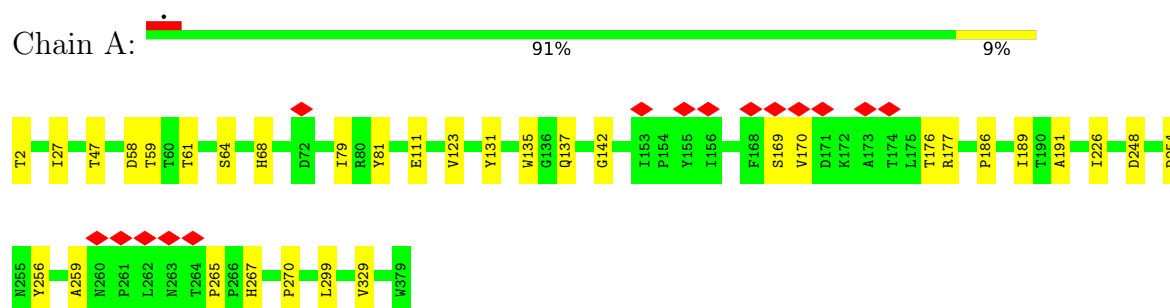
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
17	g	1	64	45	17	2	0

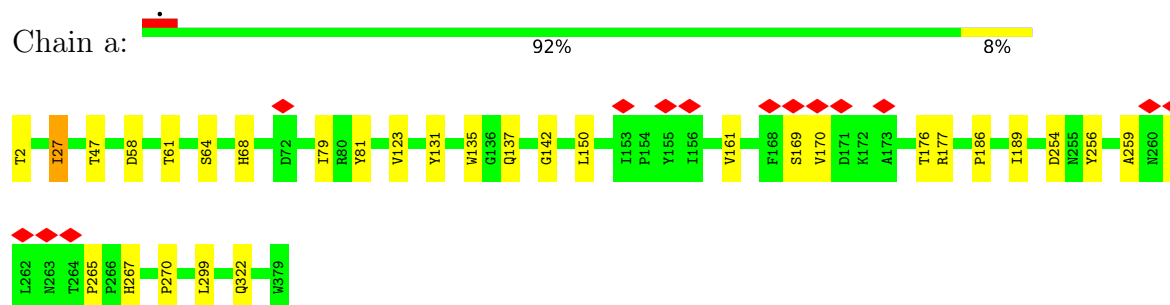
3 Residue-property plots [i](#)

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

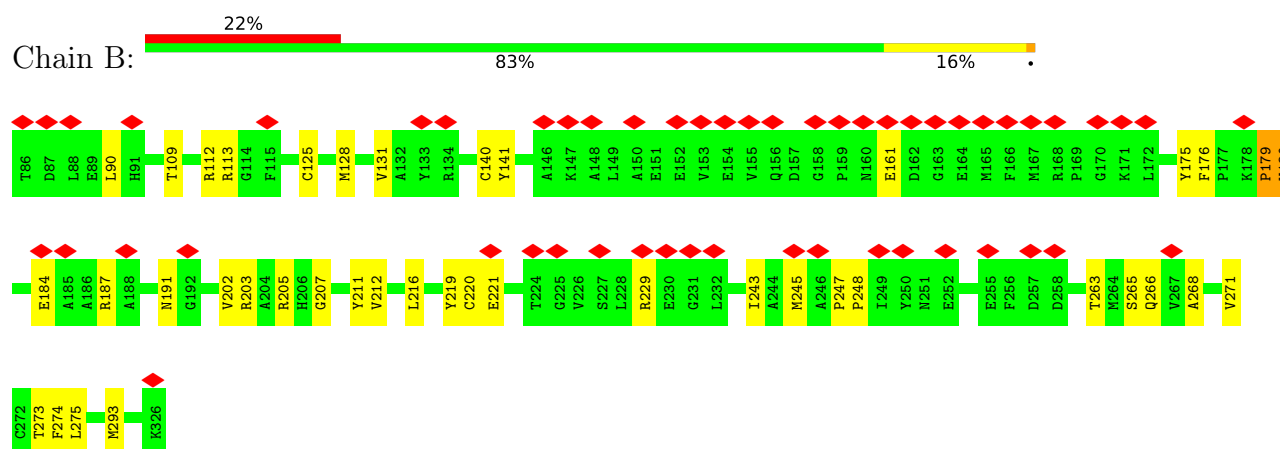
- Molecule 1: Cytochrome b



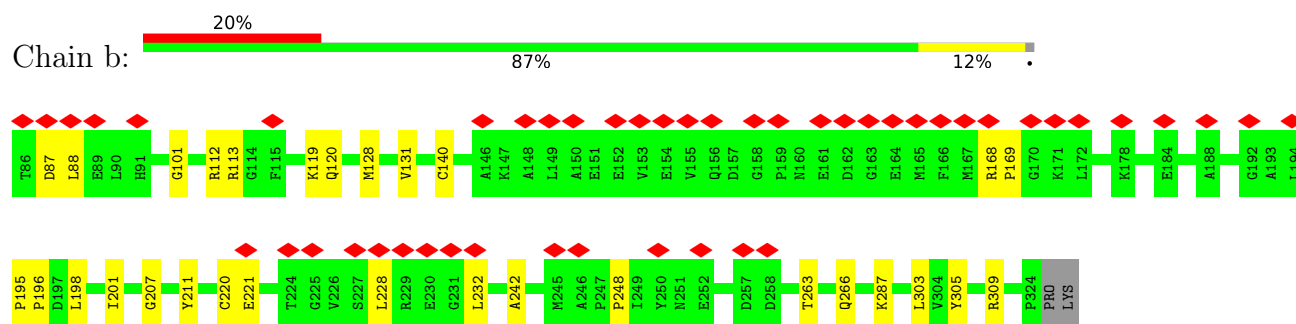
- Molecule 1: Cytochrome b



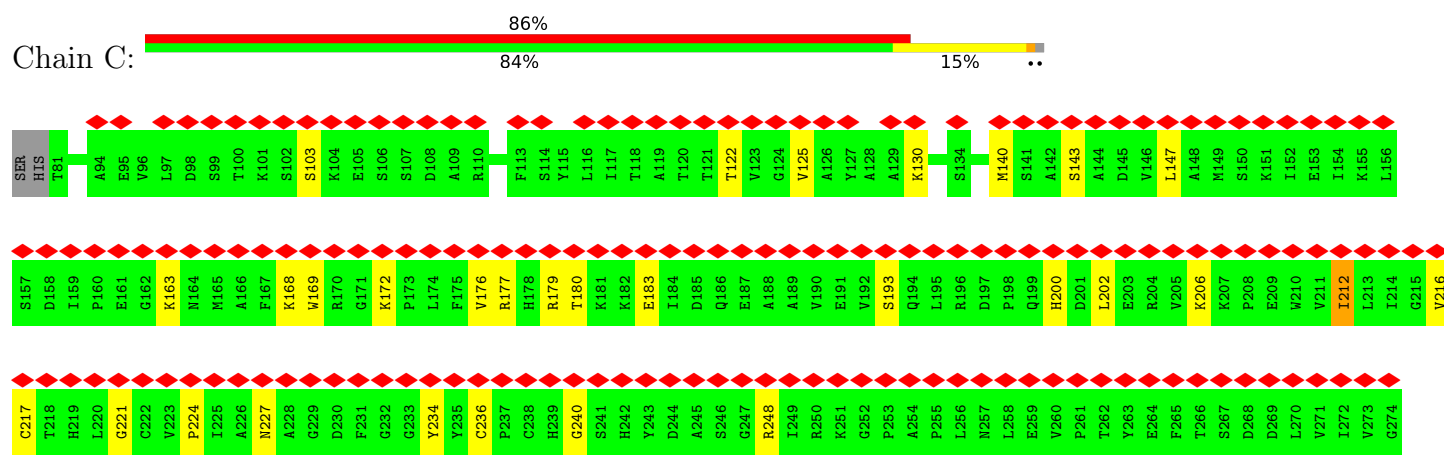
- Molecule 2: Cytochrome c1, heme protein, mitochondrial



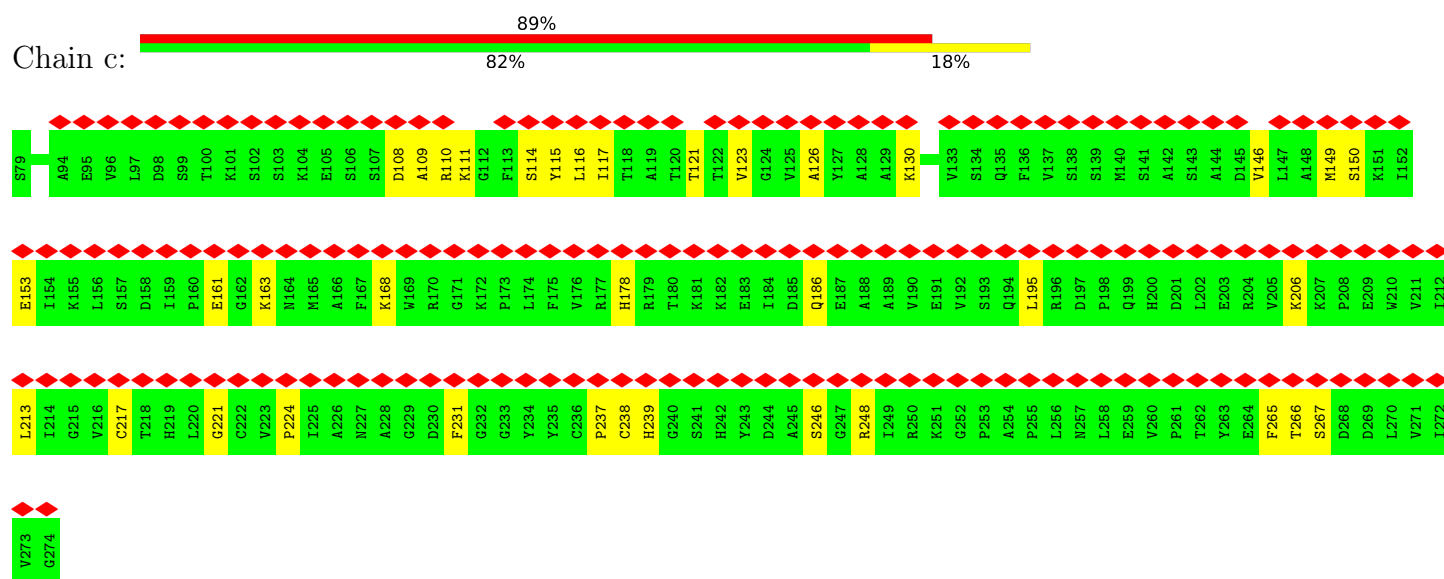
- Molecule 2: Cytochrome c1, heme protein, mitochondrial



- Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 4: Cytochrome b-c1 complex subunit 1, mitochondrial





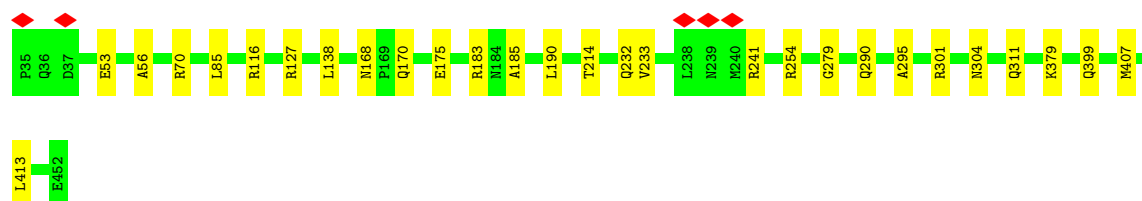
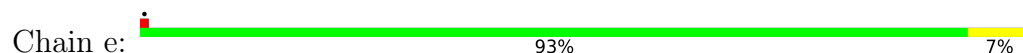
- Molecule 4: Cytochrome b-c1 complex subunit 1, mitochondrial



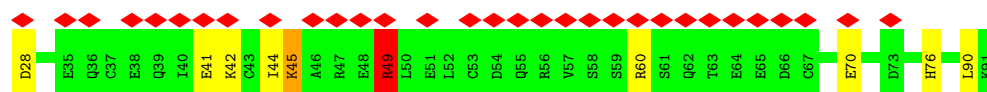
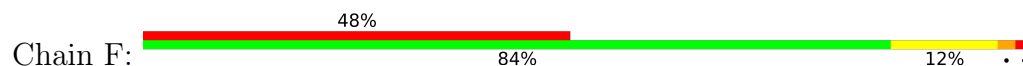
- Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial



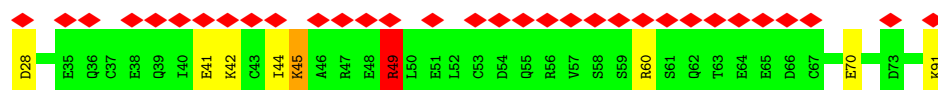
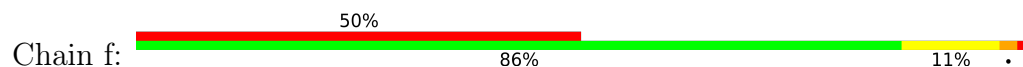
- Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial



- Molecule 6: Cytochrome b-c1 complex subunit 6

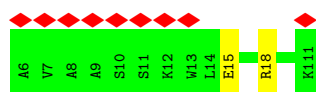


- Molecule 6: Cytochrome b-c1 complex subunit 6

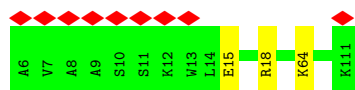


- Molecule 7: Cytochrome b-c1 complex subunit 7

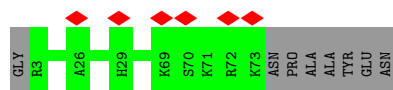
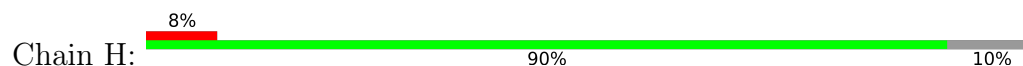




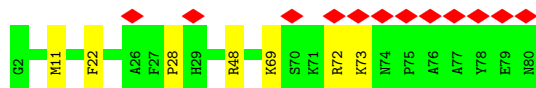
- Molecule 7: Cytochrome b-c1 complex subunit 7



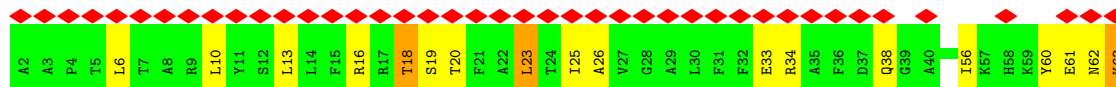
- Molecule 8: Cytochrome b-c1 complex subunit 8



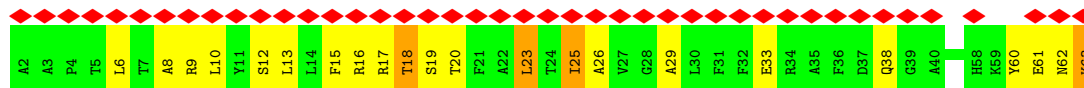
- Molecule 8: Cytochrome b-c1 complex subunit 8



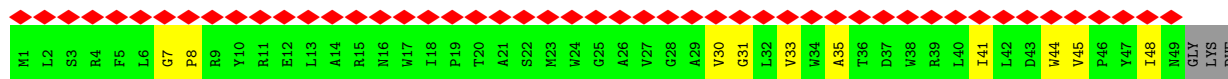
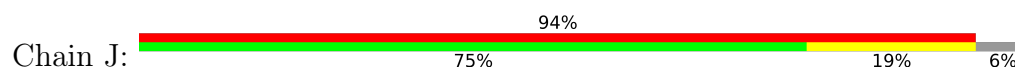
- Molecule 9: Complex III subunit 9



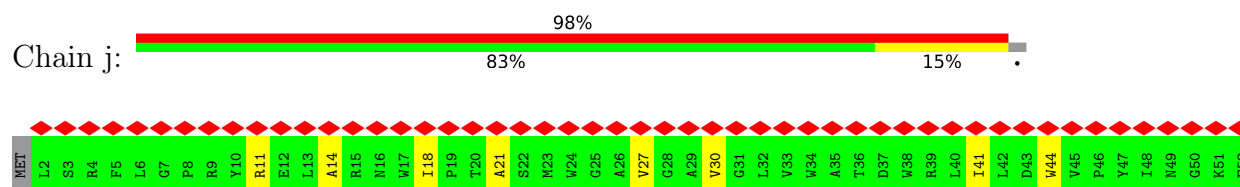
- Molecule 9: Complex III subunit 9



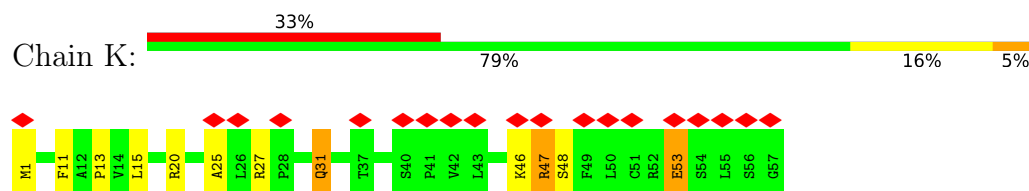
- Molecule 10: Cytochrome b-c1 complex subunit 10



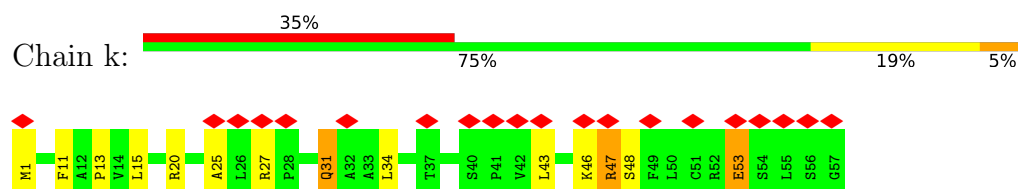
- Molecule 10: Cytochrome b-c1 complex subunit 10



- Molecule 11: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 11: Cytochrome b-c1 complex subunit Rieske, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	588793	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 ($e^-/\text{\AA}^2$)	51.68	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	5.756	Depositor
Minimum map value	-3.095	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.146	Depositor
Recommended contour level	0.543	Depositor
Map size ($\text{\AA}$)	304.0, 304.0, 304.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.95, 0.95, 0.95	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1D6K, CDL, HEC, FES, HEM, PEE

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	0.28	0/3115	0.55	0/4259
1	a	0.28	0/3115	0.55	0/4259
2	B	0.28	0/1978	0.73	7/2684 (0.3%)
2	b	0.25	0/1961	0.58	0/2661
3	C	0.30	0/1534	0.77	3/2075 (0.1%)
3	c	0.29	0/1549	0.71	1/2095 (0.0%)
4	D	0.26	0/3524	0.52	2/4783 (0.0%)
4	d	0.26	0/3531	0.54	0/4793
5	E	0.26	0/3187	0.52	0/4314
5	e	0.26	0/3187	0.52	0/4314
6	F	0.26	0/534	0.69	2/714 (0.3%)
6	f	0.26	0/534	0.69	2/714 (0.3%)
7	G	0.24	0/941	0.47	0/1262
7	g	0.24	0/941	0.46	0/1262
8	H	0.31	0/628	0.60	0/848
8	h	0.39	0/688	0.67	0/931
9	I	0.31	0/520	0.77	1/701 (0.1%)
9	i	0.31	0/520	0.77	1/701 (0.1%)
10	J	0.34	0/420	0.73	1/576 (0.2%)
10	j	0.25	0/437	0.63	0/598
11	K	0.37	0/410	0.91	1/556 (0.2%)
11	k	0.36	0/410	0.91	1/556 (0.2%)
All	All	0.28	0/33664	0.60	22/45656 (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
2	B	0	4

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	2
3	c	0	1
4	d	0	2
11	K	0	1
11	k	0	1
All	All	0	11

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	180	TYR	O-C-N	-11.42	108.18	121.32
3	c	267	SER	N-CA-C	8.46	119.42	108.34
3	C	248	ARG	CA-CB-CG	6.72	127.54	114.10
6	F	49	ARG	CG-CD-NE	5.92	125.02	112.00
6	f	49	ARG	CG-CD-NE	5.92	125.02	112.00
11	k	53	GLU	CB-CG-CD	5.88	122.60	112.60
11	K	53	GLU	CB-CG-CD	5.86	122.57	112.60
9	I	38	GLN	CA-CB-CG	5.44	124.99	114.10
9	i	38	GLN	CA-CB-CG	5.42	124.94	114.10
3	C	169	TRP	CA-C-N	5.31	130.11	122.35
3	C	169	TRP	C-N-CA	5.31	130.11	122.35
2	B	179	PRO	CA-C-N	5.24	134.60	121.80
2	B	179	PRO	C-N-CA	5.24	134.60	121.80
10	J	30	VAL	N-CA-C	-5.22	107.74	112.12
2	B	180	TYR	CA-C-N	5.17	126.30	119.84
2	B	180	TYR	C-N-CA	5.17	126.30	119.84
6	f	49	ARG	CD-NE-CZ	5.05	131.47	124.40
6	F	49	ARG	CD-NE-CZ	5.04	131.46	124.40
2	B	161	GLU	CA-C-N	5.01	131.10	121.54
2	B	161	GLU	C-N-CA	5.01	131.10	121.54
4	D	259	GLU	CA-C-N	5.01	129.52	122.46
4	D	259	GLU	C-N-CA	5.01	129.52	122.46

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	141	TYR	Peptide
2	B	175	TYR	Peptide
2	B	176	PHE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	B	273	THR	Peptide
3	C	200	HIS	Peptide
3	C	206	LYS	Peptide
11	K	31	GLN	Peptide
3	c	266	THR	Peptide
4	d	449	PHE	Peptide
4	d	64	SER	Peptide
11	k	31	GLN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3017	0	3078	23	0
1	a	3017	0	3078	23	0
2	B	1920	0	1869	27	0
2	b	1904	0	1849	19	0
3	C	1502	0	1490	16	0
3	c	1517	0	1498	23	0
4	D	3452	0	3343	14	0
4	d	3459	0	3350	12	0
5	E	3134	0	3112	17	0
5	e	3134	0	3112	17	0
6	F	528	0	510	8	0
6	f	528	0	510	6	0
7	G	921	0	917	1	0
7	g	921	0	917	2	0
8	H	608	0	616	0	0
8	h	666	0	663	6	0
9	I	507	0	509	7	0
9	i	507	0	509	12	0
10	J	405	0	405	6	0
10	j	421	0	418	4	0
11	K	404	0	425	14	0
11	k	404	0	425	14	0
12	A	27	0	0	6	0
12	a	27	0	0	7	0
13	A	86	0	60	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	a	86	0	60	0	0
14	A	45	0	67	1	0
14	D	49	0	75	5	0
14	a	49	0	75	0	0
15	B	43	0	32	4	0
15	b	43	0	32	1	0
16	a	4	0	0	0	0
16	c	4	0	0	0	0
17	a	128	0	144	4	0
17	g	64	0	72	2	0
All	All	33531	0	33220	228	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 3.

All (228) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:263:THR:HG1	6:f:28:ASP:N	1.66	0.91
2:B:263:THR:HG1	6:F:28:ASP:N	1.71	0.88
1:a:142:GLY:HA3	12:a:401:A1D6K:C5	2.20	0.72
1:A:142:GLY:HA3	12:A:401:A1D6K:C5	2.22	0.69
2:B:268:ALA:HA	2:B:271:VAL:HG12	1.76	0.68
3:c:111:LYS:HG2	8:h:22:PHE:HB3	1.80	0.64
9:I:26:ALA:HB1	10:J:31:GLY:HA3	1.79	0.64
4:d:318:TYR:OH	11:k:20:ARG:NH2	2.32	0.63
1:a:186:PRO:HA	1:a:189:ILE:HD12	1.79	0.63
1:A:186:PRO:HA	1:A:189:ILE:HD12	1.79	0.63
2:B:263:THR:OG1	6:F:28:ASP:N	2.30	0.63
7:g:64:LYS:HD2	8:h:11:MET:HE1	1.81	0.63
5:E:214:THR:HA	5:E:241:ARG:HB3	1.82	0.62
4:D:318:TYR:OH	11:K:20:ARG:NH2	2.32	0.62
5:e:214:THR:HA	5:e:241:ARG:HB3	1.82	0.62
4:d:317:THR:HG23	11:k:47:ARG:HH11	1.65	0.61
4:D:317:THR:HG23	11:K:47:ARG:HH11	1.64	0.61
3:c:217:CYS:HB3	3:c:221:GLY:H	1.66	0.61
3:C:224:PRO:HB2	3:C:234:TYR:HB3	1.83	0.60
5:e:138:LEU:HD11	5:e:233:VAL:HG13	1.83	0.60
1:A:248:ASP:OD2	2:B:203:ARG:NH1	2.36	0.59
5:E:138:LEU:HD11	5:E:233:VAL:HG13	1.83	0.59
5:E:279:GLY:HA2	11:K:1:MET:HG3	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:18:THR:O	9:i:18:THR:OG1	2.21	0.58
5:E:85:LEU:HA	11:K:15:LEU:HD22	1.85	0.57
3:c:110:ARG:NH1	8:h:22:PHE:O	2.37	0.57
5:e:168:ASN:OD1	5:e:170:GLN:NE2	2.38	0.57
5:E:399:GLN:HE22	5:E:407:MET:H	1.53	0.57
2:b:88:LEU:HG	8:h:72:ARG:HB3	1.85	0.57
4:D:446:SER:O	9:I:16:ARG:NH1	2.37	0.57
5:e:85:LEU:HA	11:k:15:LEU:HD22	1.85	0.57
5:E:168:ASN:OD1	5:E:170:GLN:NE2	2.38	0.57
2:b:119:LYS:HG2	2:b:120:GLN:HG3	1.86	0.57
2:b:168:ARG:HH11	2:b:169:PRO:HD2	1.70	0.56
5:e:399:GLN:HE22	5:e:407:MET:H	1.53	0.56
2:b:87:ASP:OD1	2:b:87:ASP:N	2.38	0.56
1:a:58:ASP:OD1	1:a:58:ASP:N	2.37	0.56
5:e:279:GLY:HA2	11:k:1:MET:HG3	1.88	0.56
4:d:274:GLU:HG3	4:d:456:VAL:HB	1.86	0.56
9:I:18:THR:O	9:I:18:THR:OG1	2.21	0.55
9:I:23:LEU:HD23	9:I:26:ALA:HB3	1.88	0.55
2:B:205:ARG:NH1	15:B:401:HEC:O1A	2.37	0.55
4:D:359:VAL:HG11	11:K:46:LYS:HD3	1.87	0.55
1:A:58:ASP:OD1	1:A:58:ASP:N	2.37	0.55
1:A:270:PRO:HB2	12:A:401:A1D6K:O2	2.07	0.55
9:i:23:LEU:HD23	9:i:26:ALA:HB3	1.88	0.55
5:e:116:ARG:NH1	5:e:175:GLU:OE2	2.40	0.54
11:K:20:ARG:HE	11:K:48:SER:HB2	1.71	0.54
11:k:20:ARG:HE	11:k:48:SER:HB2	1.71	0.54
5:E:190:LEU:HD13	11:K:13:PRO:HD3	1.89	0.54
7:g:15:GLU:OE2	7:g:18:ARG:NH1	2.41	0.54
3:c:161:GLU:HB2	3:c:178:HIS:HB2	1.89	0.54
3:C:236:CYS:HB2	3:C:240:GLY:HA2	1.90	0.54
7:G:15:GLU:OE2	7:G:18:ARG:NH1	2.41	0.54
10:J:41:ILE:HA	10:J:44:TRP:HD1	1.73	0.53
3:c:161:GLU:O	3:c:163:LYS:NZ	2.42	0.53
9:i:60:TYR:HA	9:i:63:LYS:HD3	1.90	0.53
2:b:303:LEU:HB3	3:c:121:THR:OG1	2.07	0.53
5:e:56:ALA:O	5:e:127:ARG:NH1	2.42	0.53
4:D:378:ARG:NH2	4:D:387:GLU:OE2	2.40	0.53
4:d:359:VAL:HG11	11:k:46:LYS:HD3	1.91	0.53
1:A:270:PRO:HB3	12:A:401:A1D6K:C8	2.39	0.53
1:a:47:THR:HG23	1:a:79:ILE:HG23	1.91	0.53
5:E:56:ALA:O	5:E:127:ARG:NH1	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:123:VAL:HG23	9:i:29:ALA:HA	1.90	0.52
9:I:60:TYR:HA	9:I:63:LYS:HD3	1.90	0.52
3:c:115:TYR:HE2	9:i:15:PHE:HB3	1.74	0.52
5:e:190:LEU:HD13	11:k:13:PRO:HD3	1.91	0.52
3:c:213:LEU:HD21	3:c:246:SER:HA	1.90	0.52
1:A:47:THR:HG23	1:A:79:ILE:HG23	1.92	0.52
6:f:41:GLU:HA	6:f:44:ILE:HG12	1.93	0.51
2:b:305:TYR:OH	2:b:309:ARG:NH1	2.41	0.51
1:A:191:ALA:HB1	17:a:407:CDL:H762	1.92	0.51
4:d:295:GLY:O	4:d:301:ASN:ND2	2.38	0.51
1:a:270:PRO:HB2	12:a:401:A1D6K:O2	2.10	0.50
1:A:59:THR:HG21	3:c:168:LYS:HZ1	1.76	0.50
6:F:41:GLU:HA	6:F:44:ILE:HG12	1.93	0.50
2:b:112:ARG:HB2	2:b:140:CYS:HB2	1.92	0.50
2:b:228:LEU:HB3	2:b:232:LEU:HB2	1.92	0.50
3:c:116:LEU:HB3	9:i:9:ARG:CZ	2.41	0.50
3:C:130:LYS:HE3	10:J:35:ALA:HA	1.93	0.50
2:B:216:LEU:HD21	15:B:401:HEC:HBB3	1.94	0.50
2:b:232:LEU:HD13	2:b:242:ALA:HB1	1.94	0.50
3:c:195:LEU:HD21	3:c:248:ARG:HD2	1.93	0.50
4:D:295:GLY:O	4:D:301:ASN:ND2	2.39	0.49
2:B:125:CYS:HG	2:B:180:TYR:HH	1.61	0.49
10:J:33:VAL:HG11	10:J:41:ILE:HG12	1.95	0.49
2:B:219:TYR:OH	2:B:245:MET:SD	2.57	0.49
2:B:248:PRO:HB3	15:B:401:HEC:HMC2	1.93	0.49
1:A:270:PRO:HB3	12:A:401:A1D6K:C3	2.42	0.49
3:c:109:ALA:HA	9:i:8:ALA:HB2	1.94	0.49
5:E:116:ARG:NH1	5:E:175:GLU:OE2	2.40	0.49
1:a:270:PRO:HB3	12:a:401:A1D6K:C8	2.42	0.49
4:d:452:GLN:HE21	9:i:16:ARG:HH11	1.60	0.49
3:c:146:VAL:HG22	3:c:149:MET:HA	1.94	0.49
2:B:191:ASN:HB3	2:B:229:ARG:HH22	1.77	0.48
2:B:113:ARG:NH1	2:B:266:GLN:OE1	2.46	0.48
1:A:254:ASP:OD1	1:A:267:HIS:NE2	2.44	0.48
2:B:220:CYS:SG	2:B:221:GLU:N	2.87	0.48
2:B:248:PRO:HG2	15:B:401:HEC:HBB2	1.95	0.48
3:C:177:ARG:HH22	3:C:183:GLU:HG2	1.77	0.48
3:C:163:LYS:HG2	3:C:227:ASN:HD21	1.79	0.48
2:B:184:GLU:O	2:B:187:ARG:NH2	2.46	0.48
1:a:270:PRO:HB3	12:a:401:A1D6K:C3	2.44	0.48
3:C:143:SER:HA	3:C:147:LEU:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:195:PRO:HA	2:b:196:PRO:HD3	1.80	0.47
4:d:450:TYR:CE2	9:i:17:ARG:HA	2.49	0.47
9:I:34:ARG:HG3	10:J:48:ILE:HG23	1.96	0.47
6:f:45:LYS:HB2	6:f:45:LYS:HE2	1.55	0.47
2:B:243:ILE:HG12	2:B:245:MET:H	1.78	0.47
1:a:81:TYR:OH	1:a:256:TYR:OH	2.33	0.47
1:A:64:SER:O	1:A:68:HIS:ND1	2.48	0.47
1:a:131:TYR:HB2	12:a:401:A1D6K:C1	2.45	0.47
10:j:27:VAL:HA	10:j:30:VAL:HG22	1.96	0.47
1:a:64:SER:O	1:a:68:HIS:ND1	2.48	0.46
3:c:186:GLN:HE22	3:c:231:PHE:HE2	1.63	0.46
3:C:176:VAL:HG12	3:C:212:ILE:HD12	1.97	0.46
10:j:11:ARG:HA	10:j:14:ALA:HB3	1.96	0.46
17:a:406:CDL:H711	17:a:406:CDL:H742	1.67	0.46
4:D:474:GLY:HA2	14:D:501:PEE:H49	1.98	0.46
5:E:304:ASN:O	5:E:311:GLN:NE2	2.49	0.46
11:K:11:PHE:HB3	11:K:27:ARG:HD2	1.97	0.46
2:B:112:ARG:HB2	2:B:140:CYS:HB2	1.97	0.46
1:a:254:ASP:OD1	1:a:267:HIS:NE2	2.44	0.46
5:E:170:GLN:NE2	11:K:27:ARG:O	2.49	0.45
2:b:128:MET:HE2	2:b:131:VAL:HG11	1.97	0.45
3:C:179:ARG:HD3	3:C:183:GLU:HB3	1.98	0.45
11:k:11:PHE:HB3	11:k:27:ARG:HD2	1.97	0.45
1:A:131:TYR:HB2	12:A:401:A1D6K:C1	2.45	0.45
2:b:113:ARG:HH22	6:f:91:LYS:HD3	1.82	0.45
1:A:111:GLU:HG3	17:a:407:CDL:H562	1.99	0.45
2:B:265:SER:HB3	6:F:90:LEU:HD11	1.98	0.45
6:F:45:LYS:HE2	6:F:45:LYS:HB2	1.55	0.45
1:A:2:THR:HB	4:D:371:PHE:HZ	1.82	0.45
3:c:126:ALA:HB1	3:c:130:LYS:HE2	1.99	0.45
2:B:109:THR:HG23	9:I:56:ILE:HD13	1.99	0.45
3:c:108:ASP:OD2	9:i:12:SER:OG	2.35	0.45
17:g:201:CDL:H162	17:g:201:CDL:H111	1.99	0.45
1:A:270:PRO:CB	12:A:401:A1D6K:O2	2.64	0.44
11:k:25:ALA:H	11:k:27:ARG:NH1	2.15	0.44
3:c:224:PRO:HG3	3:c:237:PRO:HD3	1.99	0.44
5:e:304:ASN:O	5:e:311:GLN:NE2	2.49	0.44
3:c:206:LYS:HD2	3:c:265:PHE:HB2	1.99	0.44
3:C:217:CYS:H	3:C:221:GLY:HA2	1.83	0.44
2:b:220:CYS:SG	2:b:221:GLU:N	2.90	0.44
3:c:238:CYS:SG	3:c:239:HIS:N	2.86	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:25:ILE:H	9:i:25:ILE:HG12	1.53	0.44
11:K:25:ALA:H	11:K:27:ARG:NH1	2.15	0.44
3:c:116:LEU:HD13	9:i:9:ARG:HD3	1.99	0.44
4:d:63:GLN:NE2	4:d:238:GLU:OE2	2.51	0.44
1:a:176:THR:OG1	1:a:177:ARG:NH2	2.51	0.44
17:g:201:CDL:H522	17:g:201:CDL:H551	1.87	0.44
5:e:170:GLN:NE2	11:k:27:ARG:O	2.51	0.44
3:C:103:SER:HB3	4:D:269:ARG:HA	2.01	0.43
2:B:247:PRO:HA	2:B:248:PRO:HD3	1.77	0.43
14:D:501:PEE:H28	14:D:501:PEE:H41	1.99	0.43
1:a:2:THR:HB	4:d:371:PHE:HZ	1.82	0.43
1:a:27:ILE:HD13	1:a:27:ILE:HA	1.85	0.43
3:C:140:MET:HA	1:a:177:ARG:HH11	1.83	0.43
4:d:276:ARG:NH2	4:d:466:PRO:O	2.40	0.43
4:D:339:GLN:OE1	11:K:47:ARG:NH2	2.52	0.43
5:e:290:GLN:HG2	5:e:295:ALA:HB2	2.00	0.43
1:A:135:TRP:CD1	1:A:259:ALA:HB3	2.54	0.43
5:E:290:GLN:HG2	5:E:295:ALA:HB2	2.00	0.43
1:a:137:GLN:HE21	1:a:265:PRO:HB3	1.84	0.43
3:c:114:SER:HA	3:c:117:ILE:HG13	2.00	0.43
5:e:183:ARG:HG3	5:e:254:ARG:HB2	2.01	0.43
1:A:81:TYR:OH	1:A:256:TYR:OH	2.33	0.43
14:D:501:PEE:H60	14:D:501:PEE:H67	1.78	0.43
1:A:176:THR:OG1	1:A:177:ARG:NH2	2.51	0.43
3:C:193:SER:O	3:C:193:SER:OG	2.33	0.43
1:a:270:PRO:CB	12:a:401:A1D6K:O2	2.67	0.43
1:a:135:TRP:CD1	1:a:259:ALA:HB3	2.54	0.42
5:e:70:ARG:HB2	5:e:185:ALA:O	2.20	0.42
4:d:339:GLN:OE1	11:k:47:ARG:NH2	2.52	0.42
1:A:329:VAL:HG13	14:A:404:PEE:H33	2.01	0.42
5:E:53:GLU:OE2	5:E:127:ARG:NH2	2.53	0.42
2:b:113:ARG:HH21	2:b:266:GLN:HE22	1.66	0.42
1:A:123:VAL:HG12	1:A:189:ILE:HD13	2.01	0.42
2:B:202:VAL:HG12	2:B:212:VAL:HG21	2.01	0.42
5:E:183:ARG:HG3	5:E:254:ARG:HB2	2.01	0.42
10:J:7:GLY:HA2	10:J:8:PRO:HD3	1.86	0.42
17:a:406:CDL:HB31	17:a:406:CDL:H531	2.01	0.42
2:B:125:CYS:SG	2:B:180:TYR:OH	2.73	0.42
1:A:137:GLN:HE21	1:A:265:PRO:HB3	1.84	0.42
2:B:274:PHE:HD2	2:B:275:LEU:HD12	1.85	0.42
5:E:70:ARG:HB2	5:E:185:ALA:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:123:VAL:HG12	1:a:189:ILE:HD13	2.01	0.42
2:b:101:GLY:O	2:b:287:LYS:NZ	2.53	0.42
6:F:49:ARG:HG3	6:F:49:ARG:HH11	1.85	0.41
5:e:379:LYS:HG2	5:e:413:LEU:HG	2.02	0.41
11:k:46:LYS:HE2	11:k:46:LYS:HB2	1.83	0.41
6:f:49:ARG:HG3	6:f:49:ARG:HH11	1.85	0.41
2:B:207:GLY:HA3	2:B:211:TYR:HB2	2.02	0.41
5:e:53:GLU:OE2	5:e:127:ARG:NH2	2.53	0.41
4:D:110:GLU:HG3	5:E:299:VAL:HG21	2.02	0.41
4:D:276:ARG:NH2	4:D:466:PRO:O	2.42	0.41
11:K:46:LYS:HE2	11:K:46:LYS:HB2	1.83	0.41
2:B:263:THR:HG23	2:B:266:GLN:H	1.84	0.41
3:C:168:LYS:HE2	1:a:261:PRO:HG2	2.03	0.41
4:D:257:TYR:H	4:D:260:ASP:HB3	1.84	0.41
1:a:142:GLY:HA3	12:a:401:A1D6K:C6	2.51	0.41
2:b:207:GLY:HA3	2:b:211:TYR:HB2	2.02	0.41
8:h:69:LYS:HA	8:h:73:LYS:HB2	2.01	0.41
14:D:501:PEE:H40	14:D:501:PEE:H46	1.83	0.41
5:e:301:ARG:HB3	11:k:34:LEU:HD13	2.01	0.41
2:B:90:LEU:HD11	6:F:76:HIS:HB2	2.03	0.41
3:C:172:LYS:HD2	3:C:216:VAL:HG21	2.02	0.41
6:F:49:ARG:NH1	6:F:70:GLU:OE1	2.53	0.41
2:b:248:PRO:HB3	15:b:401:HEC:HMC2	2.03	0.41
5:E:85:LEU:HD22	11:K:15:LEU:HD13	2.01	0.41
10:j:41:ILE:HG22	10:j:44:TRP:HB2	2.03	0.41
2:B:128:MET:HE2	2:B:131:VAL:HG11	2.03	0.40
11:k:43:LEU:HB2	11:k:46:LYS:HB3	2.03	0.40
2:B:293:MET:HE3	2:B:293:MET:HB3	2.01	0.40
1:a:150:LEU:HD23	1:a:161:VAL:HG12	2.03	0.40
2:b:198:LEU:HA	2:b:201:ILE:HB	2.03	0.40
3:C:122:THR:HA	3:C:125:VAL:HG12	2.03	0.40
4:D:214:ALA:O	4:D:218:GLU:HG3	2.22	0.40
3:c:150:SER:O	3:c:153:GLU:HB3	2.21	0.40
6:f:49:ARG:NH1	6:f:70:GLU:OE1	2.54	0.40
10:j:18:ILE:HD12	10:j:21:ALA:HB3	2.03	0.40
1:A:226:ILE:HD12	1:A:226:ILE:HA	1.97	0.40
14:D:501:PEE:H14	14:D:501:PEE:H1	1.83	0.40
1:a:322:GLN:HE21	8:h:48:ARG:HG2	1.87	0.40
4:d:335:ARG:HE	4:d:335:ARG:HB3	1.77	0.40
3:C:202:LEU:HD12	3:C:202:LEU:HA	1.91	0.40
11:K:20:ARG:NE	11:K:48:SER:HB2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	376/378 (100%)	362 (96%)	14 (4%)	0	100	100
1	a	376/378 (100%)	362 (96%)	14 (4%)	0	100	100
2	B	239/241 (99%)	210 (88%)	28 (12%)	1 (0%)	30	40
2	b	237/241 (98%)	211 (89%)	26 (11%)	0	100	100
3	C	192/196 (98%)	158 (82%)	34 (18%)	0	100	100
3	c	194/196 (99%)	158 (81%)	36 (19%)	0	100	100
4	D	443/446 (99%)	430 (97%)	13 (3%)	0	100	100
4	d	444/446 (100%)	428 (96%)	16 (4%)	0	100	100
5	E	416/418 (100%)	403 (97%)	13 (3%)	0	100	100
5	e	416/418 (100%)	403 (97%)	13 (3%)	0	100	100
6	F	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
6	f	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
7	G	104/106 (98%)	100 (96%)	4 (4%)	0	100	100
7	g	104/106 (98%)	100 (96%)	4 (4%)	0	100	100
8	H	69/79 (87%)	65 (94%)	4 (6%)	0	100	100
8	h	77/79 (98%)	70 (91%)	6 (8%)	1 (1%)	9	12
9	I	60/62 (97%)	50 (83%)	10 (17%)	0	100	100
9	i	60/62 (97%)	50 (83%)	10 (17%)	0	100	100
10	J	47/52 (90%)	41 (87%)	6 (13%)	0	100	100
10	j	49/52 (94%)	43 (88%)	6 (12%)	0	100	100
11	K	55/57 (96%)	49 (89%)	6 (11%)	0	100	100
11	k	55/57 (96%)	49 (89%)	6 (11%)	0	100	100
All	All	4137/4198 (98%)	3864 (93%)	271 (7%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	179	PRO
8	h	28	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/331 (100%)	326 (98%)	5 (2%)	57	75
1	a	331/331 (100%)	326 (98%)	5 (2%)	57	75
2	B	206/206 (100%)	206 (100%)	0	100	100
2	b	204/206 (99%)	204 (100%)	0	100	100
3	C	164/166 (99%)	162 (99%)	2 (1%)	63	79
3	c	165/166 (99%)	165 (100%)	0	100	100
4	D	371/372 (100%)	371 (100%)	0	100	100
4	d	372/372 (100%)	370 (100%)	2 (0%)	81	90
5	E	327/328 (100%)	326 (100%)	1 (0%)	86	93
5	e	327/328 (100%)	326 (100%)	1 (0%)	86	93
6	F	61/61 (100%)	57 (93%)	4 (7%)	15	24
6	f	61/61 (100%)	57 (93%)	4 (7%)	15	24
7	G	95/95 (100%)	95 (100%)	0	100	100
7	g	95/95 (100%)	95 (100%)	0	100	100
8	H	65/70 (93%)	65 (100%)	0	100	100
8	h	70/70 (100%)	70 (100%)	0	100	100
9	I	50/50 (100%)	38 (76%)	12 (24%)	1	1
9	i	50/50 (100%)	38 (76%)	12 (24%)	1	1
10	J	40/42 (95%)	39 (98%)	1 (2%)	42	61
10	j	41/42 (98%)	41 (100%)	0	100	100
11	K	44/44 (100%)	41 (93%)	3 (7%)	14	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	k	44/44 (100%)	41 (93%)	3 (7%)	14	23
All	All	3514/3530 (100%)	3459 (98%)	55 (2%)	54	74

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ILE
1	A	61	THR
1	A	169	SER
1	A	170	VAL
1	A	299	LEU
3	C	180	THR
3	C	212	ILE
5	E	232	GLN
6	F	42	LYS
6	F	45	LYS
6	F	49	ARG
6	F	60	ARG
9	I	6	LEU
9	I	10	LEU
9	I	13	LEU
9	I	18	THR
9	I	19	SER
9	I	20	THR
9	I	23	LEU
9	I	25	ILE
9	I	33	GLU
9	I	61	GLU
9	I	62	ASN
9	I	63	LYS
10	J	45	VAL
11	K	31	GLN
11	K	47	ARG
11	K	53	GLU
1	a	27	ILE
1	a	61	THR
1	a	169	SER
1	a	170	VAL
1	a	299	LEU
4	d	256	THR
4	d	262	VAL
5	e	232	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	f	42	LYS
6	f	45	LYS
6	f	49	ARG
6	f	60	ARG
9	i	6	LEU
9	i	10	LEU
9	i	13	LEU
9	i	18	THR
9	i	19	SER
9	i	20	THR
9	i	23	LEU
9	i	25	ILE
9	i	33	GLU
9	i	61	GLU
9	i	62	ASN
9	i	63	LYS
11	k	31	GLN
11	k	47	ARG
11	k	53	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	74	ASN
1	A	137	GLN
1	A	148	ASN
1	A	322	GLN
1	A	341	GLN
2	B	190	ASN
2	B	206	HIS
3	C	164	ASN
3	C	186	GLN
3	C	227	ASN
3	C	257	ASN
4	D	63	GLN
4	D	87	ASN
4	D	128	HIS
4	D	160	GLN
4	D	170	GLN
4	D	223	HIS
4	D	249	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	305	GLN
4	D	323	HIS
4	D	345	ASN
4	D	375	GLN
5	E	75	ASN
5	E	155	GLN
5	E	290	GLN
5	E	304	ASN
5	E	365	ASN
5	E	399	GLN
5	E	408	GLN
5	E	415	GLN
8	H	65	GLN
9	I	49	GLN
10	J	16	ASN
10	J	49	ASN
1	a	74	ASN
1	a	137	GLN
1	a	148	ASN
1	a	322	GLN
1	a	341	GLN
2	b	91	HIS
2	b	116	GLN
2	b	190	ASN
2	b	206	HIS
2	b	251	ASN
2	b	310	HIS
3	c	186	GLN
3	c	227	ASN
4	d	40	GLN
4	d	49	GLN
4	d	55	ASN
4	d	160	GLN
4	d	207	ASN
4	d	222	GLN
4	d	223	HIS
4	d	286	HIS
4	d	323	HIS
4	d	345	ASN
4	d	452	GLN
4	d	464	GLN
4	d	469	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	e	75	ASN
5	e	155	GLN
5	e	290	GLN
5	e	304	ASN
5	e	365	ASN
5	e	399	GLN
5	e	408	GLN
5	e	415	GLN
8	h	65	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	FES	a	404	-	0,4,4	-	-	-		
16	FES	c	301	-	0,4,4	-	-	-		
12	A1D6K	A	401	-	27,29,29	0.80	1 (3%)	29,39,39	1.35	2 (6%)
14	PEE	D	501	-	48,48,50	1.55	7 (14%)	51,53,55	1.22	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	HEM	a	402	1	50,50,50	1.33	6 (12%)	66,82,82	1.41	9 (13%)
13	HEM	A	402	1	50,50,50	1.47	6 (12%)	66,82,82	1.27	7 (10%)
17	CDL	a	406	-	63,63,99	1.09	8 (12%)	69,75,111	1.12	4 (5%)
13	HEM	a	403	1	50,50,50	1.47	6 (12%)	66,82,82	1.27	7 (10%)
17	CDL	g	201	-	63,63,99	1.07	6 (9%)	69,75,111	1.20	5 (7%)
13	HEM	A	403	1	50,50,50	1.39	7 (14%)	66,82,82	1.78	14 (21%)
15	HEC	B	401	-	50,50,50	1.78	5 (10%)	68,82,82	1.41	7 (10%)
14	PEE	A	404	-	44,44,50	1.56	5 (11%)	46,49,55	1.13	3 (6%)
17	CDL	a	407	-	63,63,99	1.08	8 (12%)	69,75,111	1.10	4 (5%)
14	PEE	a	405	-	48,48,50	1.49	5 (10%)	51,53,55	1.20	3 (5%)
12	A1D6K	a	401	-	27,29,29	0.80	1 (3%)	29,39,39	1.35	2 (6%)
15	HEC	b	401	-	50,50,50	1.81	6 (12%)	68,82,82	1.42	9 (13%)

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
16	FES	a	404	-	-	-	0/1/1/1
16	FES	c	301	-	-	-	0/1/1/1
12	A1D6K	A	401	-	-	0/18/21/21	0/3/3/3
14	PEE	D	501	-	-	32/52/52/54	-
13	HEM	A	402	1	-	2/14/54/54	-
13	HEM	a	402	1	-	2/14/54/54	-
17	CDL	a	406	-	-	43/74/74/110	-
13	HEM	a	403	1	-	2/14/54/54	-
17	CDL	g	201	-	-	46/74/74/110	-
13	HEM	A	403	1	-	4/14/54/54	-
15	HEC	B	401	-	-	3/14/54/54	-
14	PEE	A	404	-	-	19/48/48/54	-
17	CDL	a	407	-	-	40/74/74/110	-
14	PEE	a	405	-	-	21/52/52/54	-
12	A1D6K	a	401	-	-	0/18/21/21	0/3/3/3
15	HEC	b	401	-	1/1/3/7	0/14/54/54	-

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	401	HEC	C3D-C2D	8.20	1.54	1.36
15	b	401	HEC	C3D-C2D	7.90	1.53	1.36
15	b	401	HEC	FE-ND	5.41	2.11	1.94
13	A	402	HEM	FE-ND	4.67	2.09	1.94
15	B	401	HEC	FE-ND	4.66	2.09	1.94
13	a	403	HEM	FE-ND	4.63	2.09	1.94
14	a	405	PEE	C39-C38	4.38	1.57	1.31
14	D	501	PEE	C39-C38	4.37	1.57	1.31
14	A	404	PEE	C39-C38	4.36	1.57	1.31
14	A	404	PEE	C18-C19	4.21	1.56	1.31
14	D	501	PEE	C18-C19	4.18	1.56	1.31
14	a	405	PEE	C18-C19	4.13	1.55	1.31
13	A	403	HEM	FE-NB	3.83	2.06	1.94
15	b	401	HEC	FE-NB	3.61	2.06	1.94
14	D	501	PEE	O3-C30	3.59	1.43	1.33
12	a	401	A1D6K	C12-C10	-3.58	1.36	1.44
12	A	401	A1D6K	C12-C10	-3.57	1.36	1.44
14	A	404	PEE	O3-C30	3.54	1.43	1.33
13	a	402	HEM	FE-NB	3.51	2.05	1.94
15	B	401	HEC	FE-NA	3.51	2.07	1.95
13	A	403	HEM	FE-ND	3.50	2.05	1.94
14	D	501	PEE	O2-C10	3.49	1.44	1.34
15	b	401	HEC	FE-NA	3.30	2.06	1.95
13	a	403	HEM	CAB-C3B	3.25	1.56	1.47
14	a	405	PEE	O3-C30	3.24	1.42	1.33
13	a	402	HEM	CAC-C3C	3.24	1.56	1.47
13	A	402	HEM	CAB-C3B	3.24	1.56	1.47
13	A	403	HEM	CAC-C3C	3.23	1.56	1.47
13	A	402	HEM	FE-NA	3.20	2.06	1.95
13	a	403	HEM	FE-NA	3.20	2.06	1.95
13	a	402	HEM	CAB-C3B	3.18	1.56	1.47
13	A	403	HEM	CAB-C3B	3.18	1.56	1.47
14	A	404	PEE	O2-C10	3.07	1.43	1.34
14	a	405	PEE	O2-C10	3.04	1.42	1.34
13	a	403	HEM	FE-NC	3.02	2.05	1.95
13	a	402	HEM	FE-ND	3.01	2.04	1.94
13	A	402	HEM	CAC-C3C	3.01	1.55	1.47
13	a	403	HEM	CAC-C3C	3.01	1.55	1.47
13	A	402	HEM	FE-NC	2.95	2.05	1.95
17	g	201	CDL	OA6-CA4	-2.94	1.39	1.46
17	a	406	CDL	OA6-CA4	-2.65	1.40	1.46
14	A	404	PEE	O2-C2	-2.63	1.40	1.46
14	a	405	PEE	O2-C2	-2.61	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	401	HEC	FE-NC	2.57	2.03	1.95
15	B	401	HEC	FE-NB	2.54	2.02	1.94
17	a	407	CDL	OA6-CA4	-2.53	1.40	1.46
17	a	407	CDL	OB6-CB4	-2.51	1.40	1.46
15	b	401	HEC	FE-NC	2.47	2.03	1.95
17	g	201	CDL	OB8-CB7	2.47	1.40	1.33
14	D	501	PEE	C11-C10	2.44	1.57	1.50
17	a	406	CDL	OB6-CB4	-2.41	1.40	1.46
17	a	406	CDL	OB8-CB7	2.40	1.40	1.33
17	a	407	CDL	OA8-CA7	2.37	1.40	1.33
17	g	201	CDL	OB6-CB5	2.32	1.40	1.34
17	g	201	CDL	OA8-CA6	-2.32	1.39	1.45
17	a	406	CDL	OA8-CA7	2.31	1.40	1.33
17	a	407	CDL	OB8-CB6	-2.30	1.39	1.45
17	a	407	CDL	OB8-CB7	2.27	1.40	1.33
14	D	501	PEE	O2-C2	-2.24	1.41	1.46
13	A	403	HEM	CAD-C3D	2.24	1.57	1.51
17	a	406	CDL	OB6-CB5	2.21	1.40	1.34
17	a	406	CDL	OA6-CA5	2.20	1.40	1.34
17	a	407	CDL	OA6-CA5	2.20	1.40	1.34
17	a	406	CDL	OB8-CB6	-2.20	1.40	1.45
17	g	201	CDL	OA8-CA7	2.19	1.39	1.33
17	a	407	CDL	OB6-CB5	2.19	1.40	1.34
17	a	406	CDL	OA8-CA6	-2.11	1.40	1.45
13	a	403	HEM	CMB-C2B	2.09	1.55	1.50
17	a	407	CDL	OA8-CA6	-2.08	1.40	1.45
14	D	501	PEE	P-O3P	2.05	1.67	1.59
17	g	201	CDL	OB8-CB6	-2.05	1.40	1.45
13	A	402	HEM	CMB-C2B	2.05	1.55	1.50
13	A	403	HEM	CMC-C2C	2.05	1.55	1.50
15	b	401	HEC	CMB-C2B	2.04	1.55	1.50
13	a	402	HEM	CMB-C2B	2.03	1.55	1.50
13	A	403	HEM	CMB-C2B	2.03	1.55	1.50
13	a	402	HEM	CMC-C2C	2.01	1.55	1.50

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	401	HEC	C1D-ND-C4D	6.86	112.16	105.07
15	b	401	HEC	C1D-ND-C4D	6.24	111.52	105.07
12	A	401	A1D6K	C19-O4-N1	5.21	115.63	109.99
12	a	401	A1D6K	C19-O4-N1	5.17	115.59	109.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	403	HEM	CAD-C3D-C4D	5.00	133.40	124.66
14	D	501	PEE	O2-C10-C11	4.92	122.09	111.50
17	g	201	CDL	OB6-CB5-C51	4.48	121.15	111.50
13	A	403	HEM	C4D-ND-C1D	4.40	109.62	105.07
13	A	403	HEM	CAD-C3D-C2D	-4.24	119.98	127.88
17	a	406	CDL	OB6-CB5-C51	4.15	120.45	111.50
17	a	407	CDL	OB6-CB5-C51	3.76	119.61	111.50
13	A	403	HEM	CHA-C4D-C3D	3.72	132.30	125.33
13	a	402	HEM	C4D-ND-C1D	3.69	108.89	105.07
14	a	405	PEE	O2-C10-C11	3.60	119.25	111.50
17	a	407	CDL	OA6-CA5-C11	3.55	119.14	111.50
13	A	403	HEM	C4A-NA-C1A	3.52	108.80	105.35
13	a	402	HEM	C4A-NA-C1A	3.52	108.79	105.35
14	A	404	PEE	O2-C10-C11	3.50	119.05	111.50
17	a	406	CDL	OA6-CA5-C11	3.48	119.01	111.50
17	g	201	CDL	OA6-CA5-C11	3.46	118.95	111.50
12	a	401	A1D6K	C9-C8-C3	-3.43	120.00	123.63
12	A	401	A1D6K	C9-C8-C3	-3.36	120.08	123.63
13	A	403	HEM	CHA-C4D-ND	-3.28	120.33	124.37
13	a	403	HEM	C1B-NB-C4B	3.28	108.46	105.07
13	A	402	HEM	C4D-ND-C1D	3.28	108.46	105.07
13	A	402	HEM	C1B-NB-C4B	3.27	108.45	105.07
13	a	403	HEM	C4D-ND-C1D	3.21	108.39	105.07
13	a	402	HEM	C1B-NB-C4B	3.15	108.33	105.07
13	A	403	HEM	C1B-NB-C4B	3.11	108.29	105.07
13	a	403	HEM	C4A-NA-C1A	3.05	108.33	105.35
13	A	402	HEM	C4A-NA-C1A	3.01	108.29	105.35
13	A	402	HEM	C4C-NC-C1C	2.95	108.24	105.35
13	a	403	HEM	C4C-NC-C1C	2.90	108.19	105.35
13	A	403	HEM	C4C-NC-C1C	2.88	108.17	105.35
14	a	405	PEE	O3-C30-C31	2.85	120.85	111.91
15	B	401	HEC	C4A-NA-C1A	2.81	108.10	105.35
13	A	403	HEM	CBD-CAD-C3D	2.69	120.11	112.63
13	a	402	HEM	C4C-NC-C1C	2.69	107.98	105.35
17	g	201	CDL	OB8-CB7-C71	2.68	120.32	111.91
17	a	406	CDL	OA8-CA7-C31	2.67	120.30	111.91
13	a	402	HEM	C2A-C1A-NA	-2.67	107.16	110.15
13	A	403	HEM	C2D-C1D-ND	-2.65	106.71	109.88
15	B	401	HEC	C2A-C1A-NA	-2.64	107.76	110.32
13	A	403	HEM	CHD-C1D-C2D	2.63	129.09	124.98
17	a	406	CDL	OB8-CB7-C71	2.61	120.08	111.91
13	A	403	HEM	C1D-C2D-C3D	2.59	109.68	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	407	CDL	OB8-CB7-C71	2.58	120.02	111.91
17	a	407	CDL	OA8-CA7-C31	2.58	120.00	111.91
13	A	403	HEM	C2A-C1A-NA	-2.58	107.27	110.15
17	g	201	CDL	OA8-CA7-C31	2.52	119.81	111.91
13	A	403	HEM	C3D-C4D-ND	-2.51	107.37	110.17
15	b	401	HEC	C4C-NC-C1C	2.51	107.80	105.35
13	A	402	HEM	CMB-C2B-C1B	-2.50	121.23	125.04
13	a	403	HEM	CMB-C2B-C1B	-2.49	121.24	125.04
14	A	404	PEE	O3-C30-C31	2.47	119.66	111.91
14	D	501	PEE	O3-C30-C31	2.44	119.58	111.91
15	b	401	HEC	C2A-C1A-NA	-2.41	107.98	110.32
15	b	401	HEC	C4A-NA-C1A	2.40	107.70	105.35
15	b	401	HEC	C4B-NB-C1B	2.34	107.49	105.07
15	b	401	HEC	C3C-C4C-NC	-2.33	107.54	110.15
13	a	402	HEM	C3D-C4D-ND	-2.31	107.59	110.17
15	B	401	HEC	CAA-CBA-CGA	-2.30	108.66	113.60
13	a	402	HEM	CHD-C1D-C2D	2.29	128.56	124.98
13	a	402	HEM	C2D-C1D-ND	-2.27	107.16	109.88
14	D	501	PEE	O2-C10-O4	-2.19	118.41	123.70
15	B	401	HEC	CHB-C1B-NB	2.16	126.76	124.42
15	b	401	HEC	CAA-CBA-CGA	-2.15	108.97	113.60
15	B	401	HEC	C4B-NB-C1B	2.15	107.30	105.07
15	b	401	HEC	CMD-C2D-C1D	2.13	128.28	125.04
13	A	402	HEM	C2A-C1A-NA	-2.12	107.78	110.15
15	B	401	HEC	CAD-C3D-C4D	2.11	128.35	124.66
13	a	403	HEM	C2A-C1A-NA	-2.10	107.79	110.15
17	g	201	CDL	CA4-OA6-CA5	-2.10	112.61	117.79
15	b	401	HEC	CHB-C1B-NB	2.10	126.70	124.42
14	A	404	PEE	C37-C38-C39	-2.10	108.64	124.73
13	a	403	HEM	C3B-C2B-C1B	2.08	108.03	106.49
14	a	405	PEE	C37-C38-C39	-2.04	109.06	124.73
13	A	402	HEM	C3B-C2B-C1B	2.04	108.00	106.49
13	a	402	HEM	CAD-CBD-CGD	-2.03	109.23	113.60
14	D	501	PEE	C37-C38-C39	-2.00	109.35	124.73

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	b	401	HEC	NA

All (214) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	403	HEM	C2D-C3D-CAD-CBD
13	A	403	HEM	C4D-C3D-CAD-CBD
14	A	404	PEE	C1-O3P-P-O1P
14	A	404	PEE	C4-O4P-P-O3P
14	A	404	PEE	C4-O4P-P-O2P
14	A	404	PEE	C4-O4P-P-O1P
14	D	501	PEE	C11-C10-O2-C2
14	D	501	PEE	O4-C10-O2-C2
14	D	501	PEE	O3P-C1-C2-O2
14	D	501	PEE	O2-C2-C3-O3
14	D	501	PEE	C1-O3P-P-O2P
14	D	501	PEE	C1-O3P-P-O1P
14	D	501	PEE	C4-O4P-P-O2P
14	D	501	PEE	C4-O4P-P-O1P
14	a	405	PEE	C4-O4P-P-O2P
14	a	405	PEE	C4-O4P-P-O1P
17	a	406	CDL	CA2-OA2-PA1-OA3
17	a	406	CDL	CA3-OA5-PA1-OA2
17	a	406	CDL	CA3-OA5-PA1-OA3
17	a	406	CDL	CA3-OA5-PA1-OA4
17	a	406	CDL	OB6-CB4-CB6-OB8
17	a	406	CDL	C51-CB5-OB6-CB4
17	a	407	CDL	CA2-OA2-PA1-OA3
17	a	407	CDL	CA3-OA5-PA1-OA2
17	a	407	CDL	OA5-CA3-CA4-OA6
17	a	407	CDL	CB3-OB5-PB2-OB3
17	a	407	CDL	CB3-OB5-PB2-OB4
17	g	201	CDL	CA2-OA2-PA1-OA3
17	g	201	CDL	CA3-OA5-PA1-OA2
17	g	201	CDL	CA3-OA5-PA1-OA3
17	g	201	CDL	CA3-OA5-PA1-OA4
17	g	201	CDL	OA6-CA4-CA6-OA8
17	g	201	CDL	CB2-OB2-PB2-OB3
17	g	201	CDL	CB2-OB2-PB2-OB4
17	g	201	CDL	CB3-OB5-PB2-OB2
17	g	201	CDL	CB3-OB5-PB2-OB4
17	g	201	CDL	C51-CB5-OB6-CB4
17	g	201	CDL	OB9-CB7-OB8-CB6
17	a	406	CDL	OB7-CB5-OB6-CB4
17	g	201	CDL	OB7-CB5-OB6-CB4
17	g	201	CDL	C71-CB7-OB8-CB6
14	a	405	PEE	C37-C38-C39-C40
17	a	407	CDL	O1-C1-CB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	a	406	CDL	CA2-C1-CB2-OB2
17	g	201	CDL	OA5-CA3-CA4-OA6
17	a	406	CDL	O1-C1-CB2-OB2
17	a	407	CDL	OA6-CA4-CA6-OA8
14	a	405	PEE	C10-C11-C12-C13
17	g	201	CDL	CB5-C51-C52-C53
14	A	404	PEE	C10-C11-C12-C13
17	a	406	CDL	CA7-C31-C32-C33
17	a	406	CDL	CB5-C51-C52-C53
17	a	407	CDL	CA5-C11-C12-C13
17	a	407	CDL	CA7-C31-C32-C33
17	a	407	CDL	CB7-C71-C72-C73
17	g	201	CDL	CA5-C11-C12-C13
17	a	406	CDL	C31-CA7-OA8-CA6
17	a	406	CDL	CA5-C11-C12-C13
14	D	501	PEE	C17-C18-C19-C20
14	D	501	PEE	C1-O3P-P-O4P
14	D	501	PEE	C4-O4P-P-O3P
14	a	405	PEE	C4-O4P-P-O3P
17	a	406	CDL	CA2-OA2-PA1-OA5
17	a	407	CDL	CB2-OB2-PB2-OB5
17	a	407	CDL	CB3-OB5-PB2-OB2
17	g	201	CDL	CB2-OB2-PB2-OB5
17	a	407	CDL	CA2-C1-CB2-OB2
17	a	406	CDL	C71-CB7-OB8-CB6
17	a	406	CDL	C31-C32-C33-C34
14	D	501	PEE	C11-C12-C13-C14
17	a	406	CDL	C53-C54-C55-C56
17	a	407	CDL	C13-C14-C15-C16
17	g	201	CDL	CB3-CB4-OB6-CB5
14	D	501	PEE	C37-C38-C39-C40
14	a	405	PEE	C17-C18-C19-C20
14	a	405	PEE	C22-C23-C24-C25
17	a	407	CDL	C74-C75-C76-C77
13	a	402	HEM	C3D-CAD-CBD-CGD
14	D	501	PEE	C21-C22-C23-C24
14	a	405	PEE	C12-C13-C14-C15
17	a	406	CDL	C14-C15-C16-C17
17	a	406	CDL	OA9-CA7-OA8-CA6
17	g	201	CDL	C14-C15-C16-C17
14	a	405	PEE	C30-C31-C32-C33
14	D	501	PEE	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	a	407	CDL	CB5-C51-C52-C53
17	a	406	CDL	OB9-CB7-OB8-CB6
17	g	201	CDL	C72-C73-C74-C75
17	a	407	CDL	C71-C72-C73-C74
17	g	201	CDL	C11-CA5-OA6-CA4
17	a	406	CDL	C12-C13-C14-C15
17	a	406	CDL	C13-C14-C15-C16
17	a	407	CDL	C11-C12-C13-C14
14	A	404	PEE	C35-C36-C37-C38
14	D	501	PEE	C40-C41-C42-C43
17	g	201	CDL	OA7-CA5-OA6-CA4
17	a	407	CDL	C52-C53-C54-C55
17	g	201	CDL	C74-C75-C76-C77
17	a	406	CDL	C73-C74-C75-C76
17	a	407	CDL	C31-CA7-OA8-CA6
17	g	201	CDL	C13-C14-C15-C16
14	D	501	PEE	C35-C36-C37-C38
14	a	405	PEE	C35-C36-C37-C38
17	g	201	CDL	C31-CA7-OA8-CA6
17	a	407	CDL	C73-C74-C75-C76
14	a	405	PEE	C34-C35-C36-C37
17	a	407	CDL	OA9-CA7-OA8-CA6
17	g	201	CDL	CA2-OA2-PA1-OA5
17	a	406	CDL	OA5-CA3-CA4-CA6
17	a	407	CDL	OA5-CA3-CA4-CA6
17	g	201	CDL	OA5-CA3-CA4-CA6
14	D	501	PEE	C13-C14-C15-C16
14	D	501	PEE	C30-C31-C32-C33
17	g	201	CDL	C73-C74-C75-C76
14	D	501	PEE	C19-C20-C21-C22
14	D	501	PEE	C1-C2-C3-O3
17	a	407	CDL	CA3-CA4-CA6-OA8
14	D	501	PEE	C22-C23-C24-C25
14	A	404	PEE	C30-C31-C32-C33
17	g	201	CDL	OA9-CA7-OA8-CA6
17	a	406	CDL	C15-C16-C17-C18
14	D	501	PEE	C23-C24-C25-C26
17	g	201	CDL	C15-C16-C17-C18
17	a	407	CDL	C71-CB7-OB8-CB6
17	a	406	CDL	OB5-CB3-CB4-OB6
17	g	201	CDL	C12-C13-C14-C15
17	a	406	CDL	OA6-CA4-CA6-OA8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	g	201	CDL	C53-C54-C55-C56
17	a	407	CDL	C14-C15-C16-C17
17	a	407	CDL	C35-C36-C37-C38
17	g	201	CDL	C54-C55-C56-C57
14	D	501	PEE	C2-C1-O3P-P
17	a	406	CDL	CA4-CA3-OA5-PA1
17	a	407	CDL	C15-C16-C17-C18
17	a	407	CDL	C12-C11-CA5-OA6
14	a	405	PEE	C31-C30-O3-C3
17	g	201	CDL	CA3-CA4-CA6-OA8
14	A	404	PEE	C17-C18-C19-C20
14	A	404	PEE	C21-C22-C23-C24
14	D	501	PEE	C10-C11-C12-C13
17	a	407	CDL	OB9-CB7-OB8-CB6
17	a	406	CDL	C74-C75-C76-C77
17	g	201	CDL	C71-C72-C73-C74
14	A	404	PEE	C38-C39-C40-C41
14	D	501	PEE	O3P-C1-C2-C3
17	a	407	CDL	OB5-CB3-CB4-CB6
14	a	405	PEE	C1-C2-C3-O3
17	a	406	CDL	CB3-CB4-CB6-OB8
17	a	407	CDL	OB5-CB3-CB4-OB6
17	a	406	CDL	C55-C56-C57-C58
17	a	406	CDL	C72-C73-C74-C75
14	a	405	PEE	O5-C30-O3-C3
17	a	406	CDL	C33-C34-C35-C36
14	A	404	PEE	C20-C21-C22-C23
17	a	407	CDL	C31-C32-C33-C34
17	a	407	CDL	CA2-OA2-PA1-OA5
17	a	406	CDL	C1-CB2-OB2-PB2
17	a	407	CDL	CB2-OB2-PB2-OB3
17	a	407	CDL	CB2-OB2-PB2-OB4
17	g	201	CDL	CA2-OA2-PA1-OA4
17	g	201	CDL	CB3-OB5-PB2-OB3
17	a	406	CDL	OB5-CB3-CB4-CB6
14	a	405	PEE	O2-C2-C3-O3
17	g	201	CDL	C33-C34-C35-C36
17	g	201	CDL	C32-C33-C34-C35
17	a	406	CDL	CB4-CB3-OB5-PB2
17	a	407	CDL	C1-CB2-OB2-PB2
17	g	201	CDL	C1-CA2-OA2-PA1
17	a	406	CDL	OA5-CA3-CA4-OA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	a	406	CDL	CB3-OB5-PB2-OB2
17	a	406	CDL	CB7-C71-C72-C73
17	a	406	CDL	CA3-CA4-CA6-OA8
17	g	201	CDL	C52-C53-C54-C55
14	D	501	PEE	C12-C13-C14-C15
14	a	405	PEE	C19-C20-C21-C22
15	B	401	HEC	C3D-CAD-CBD-CGD
14	A	404	PEE	O2-C2-C3-O3
14	A	404	PEE	C23-C24-C25-C26
17	a	406	CDL	C71-C72-C73-C74
14	A	404	PEE	C36-C37-C38-C39
14	a	405	PEE	C32-C33-C34-C35
14	D	501	PEE	O3-C30-C31-C32
13	a	403	HEM	CAA-CBA-CGA-O2A
14	A	404	PEE	C16-C17-C18-C19
13	A	402	HEM	CAA-CBA-CGA-O1A
14	A	404	PEE	C31-C32-C33-C34
13	A	402	HEM	CAA-CBA-CGA-O2A
13	a	403	HEM	CAA-CBA-CGA-O1A
17	a	406	CDL	C52-C51-CB5-OB6
17	g	201	CDL	OB6-CB4-CB6-OB8
17	a	407	CDL	OB7-CB5-OB6-CB4
17	g	201	CDL	C75-C76-C77-C78
15	B	401	HEC	CAD-CBD-CGD-O2D
14	D	501	PEE	C36-C37-C38-C39
14	A	404	PEE	C1-O3P-P-O4P
17	a	407	CDL	C12-C11-CA5-OA7
14	A	404	PEE	C18-C19-C20-C21
15	B	401	HEC	CAD-CBD-CGD-O1D
17	g	201	CDL	C55-C56-C57-C58
17	a	407	CDL	C51-CB5-OB6-CB4
14	A	404	PEE	C1-C2-C3-O3
14	D	501	PEE	C20-C21-C22-C23
17	a	406	CDL	CB3-OB5-PB2-OB3
14	a	405	PEE	O4P-C4-C5-N
14	D	501	PEE	O2-C10-C11-C12
14	a	405	PEE	O2-C10-C11-C12
13	A	403	HEM	CAA-CBA-CGA-O2A
13	a	402	HEM	CAA-CBA-CGA-O2A
14	a	405	PEE	C38-C39-C40-C41
14	a	405	PEE	O4-C10-C11-C12
14	D	501	PEE	O4-C10-C11-C12

Continued on next page...

Continued from previous page...

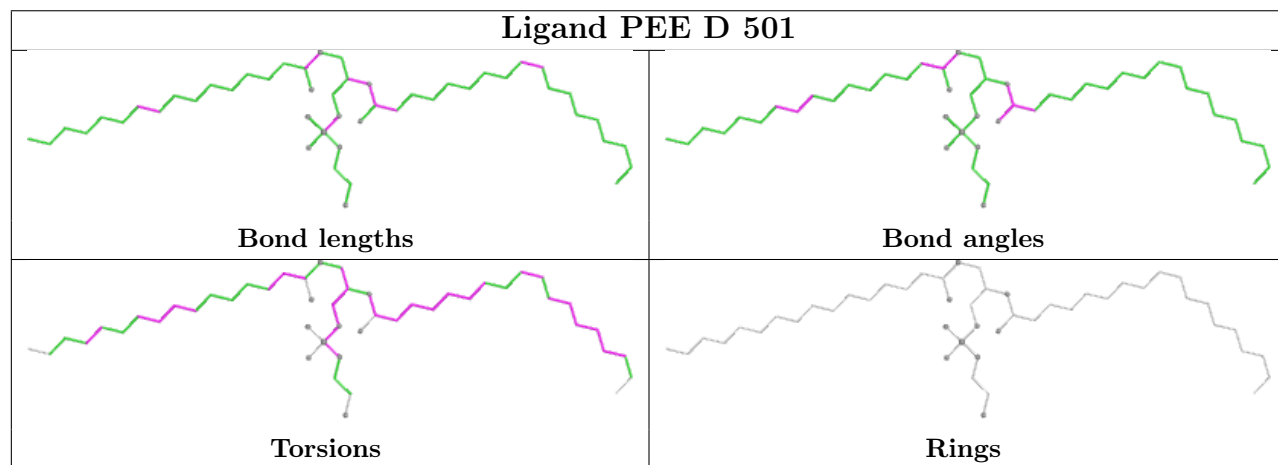
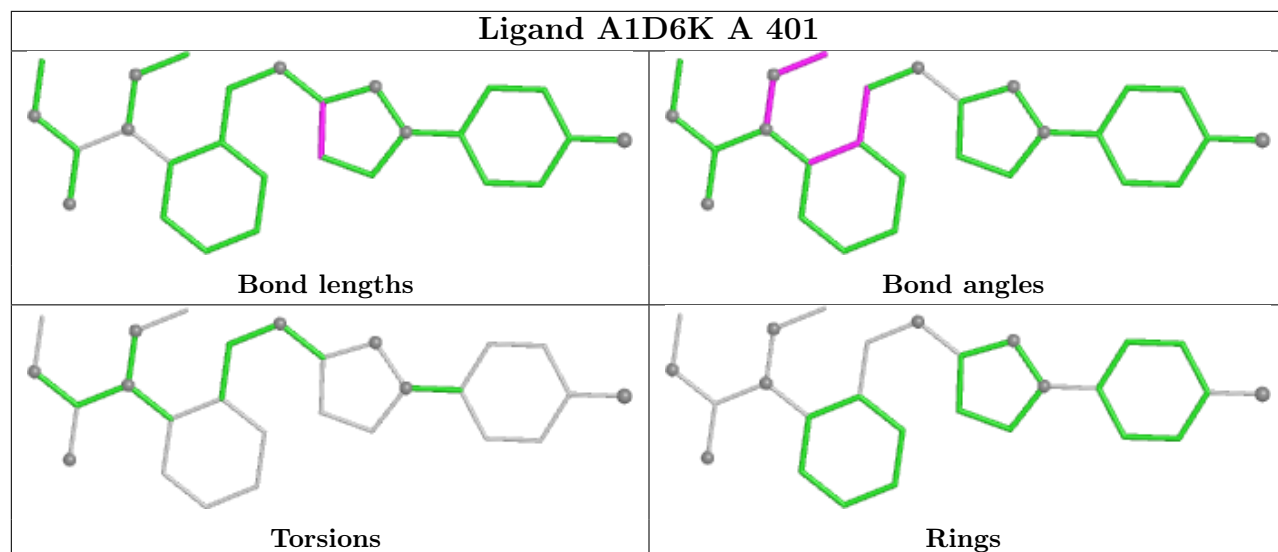
Mol	Chain	Res	Type	Atoms
17	g	201	CDL	C12-C11-CA5-OA6
17	g	201	CDL	C72-C71-CB7-OB8
13	A	403	HEM	CAA-CBA-CGA-O1A

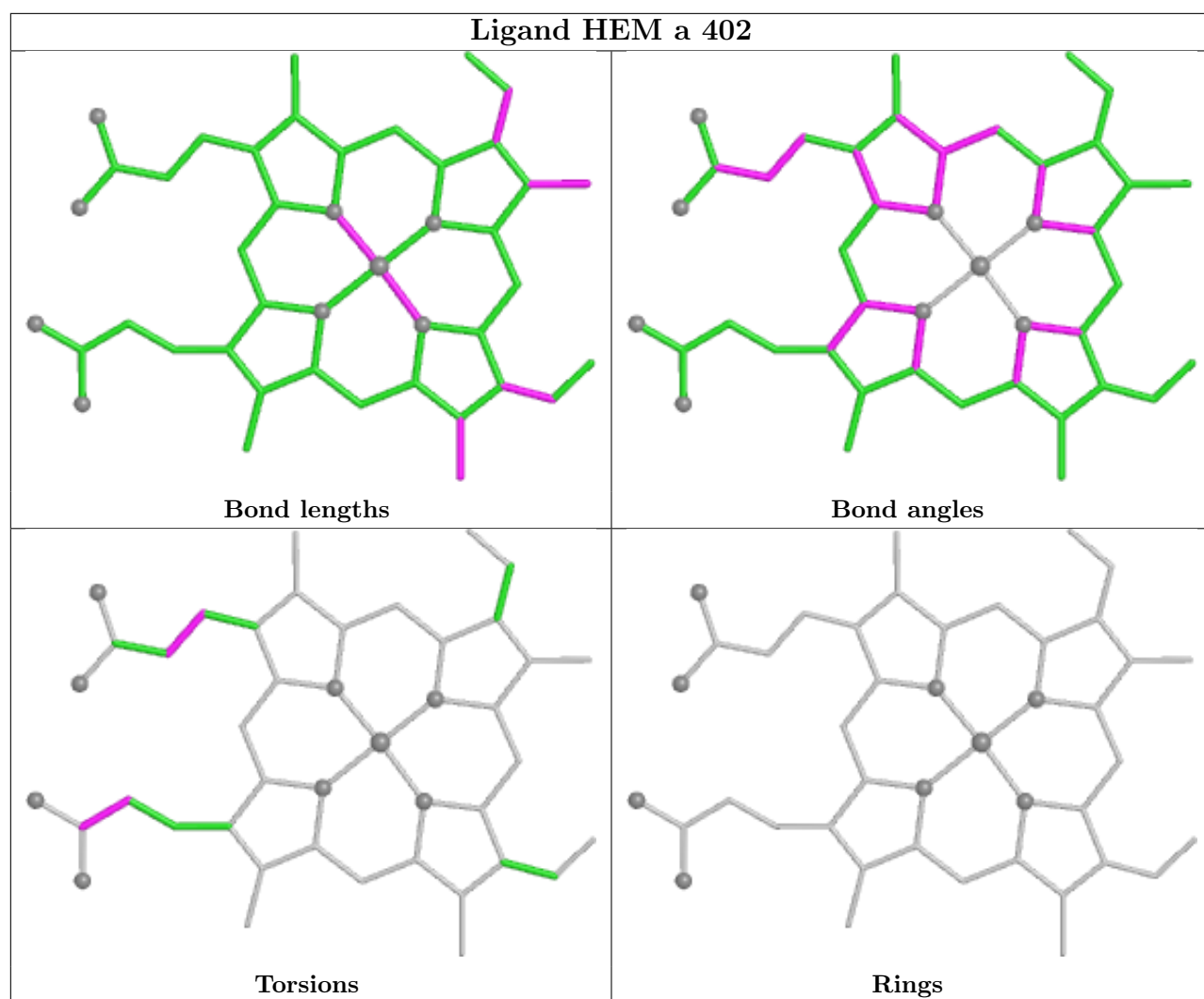
There are no ring outliers.

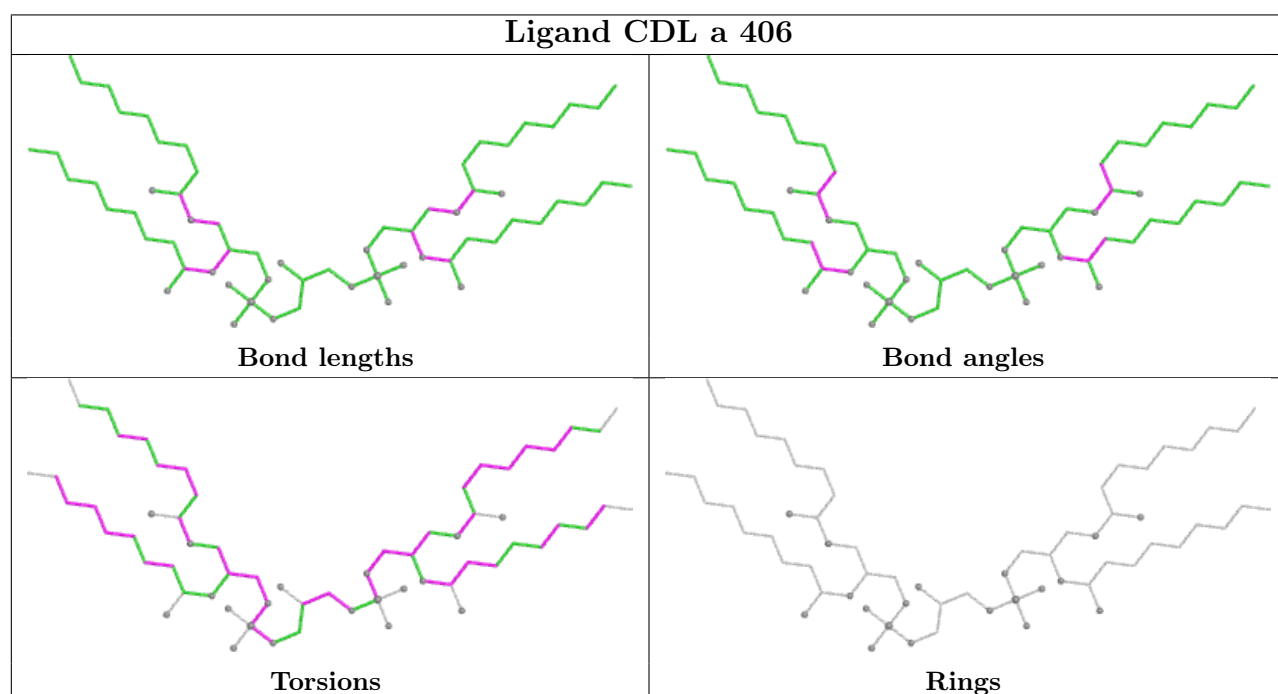
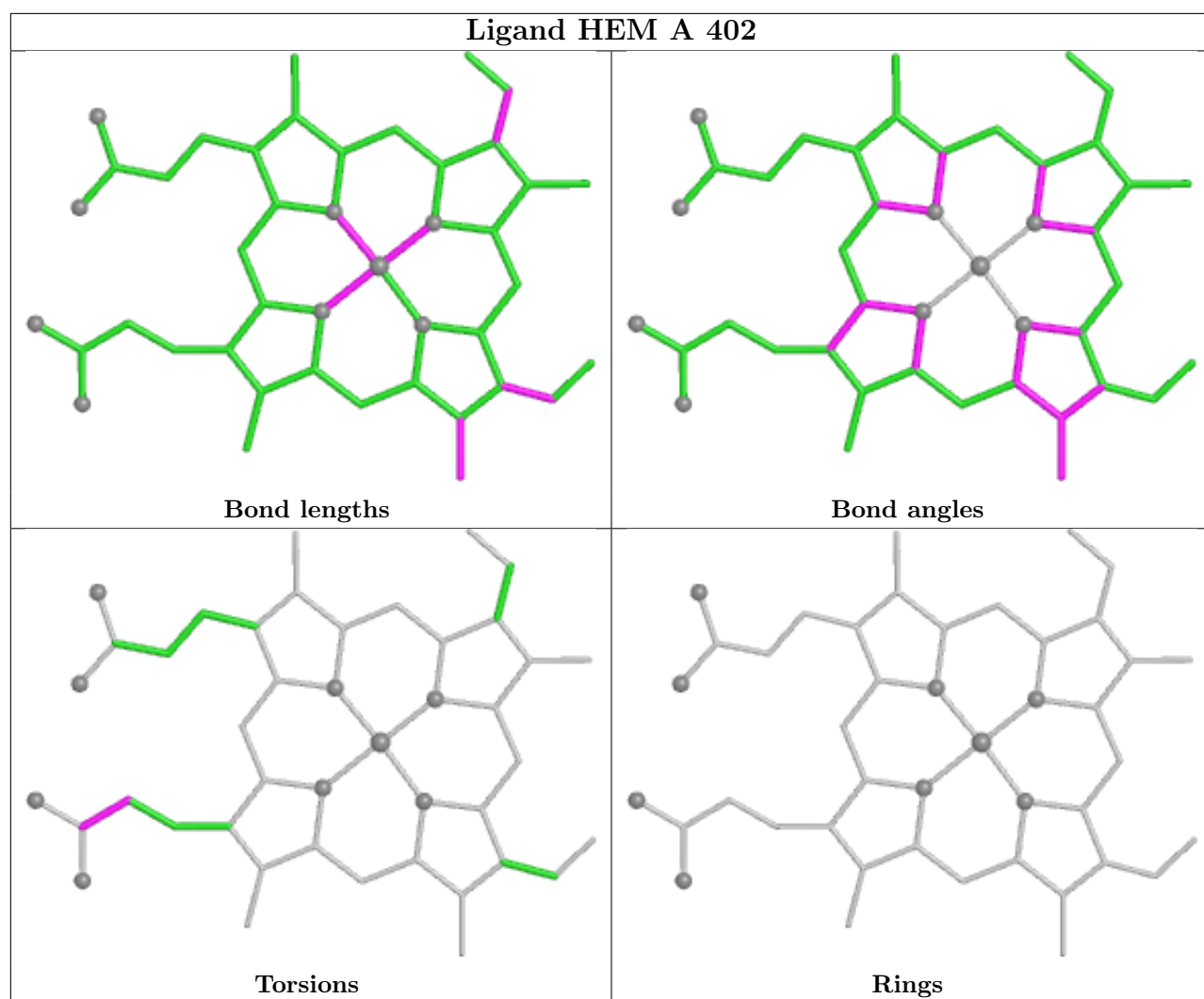
9 monomers are involved in 30 short contacts:

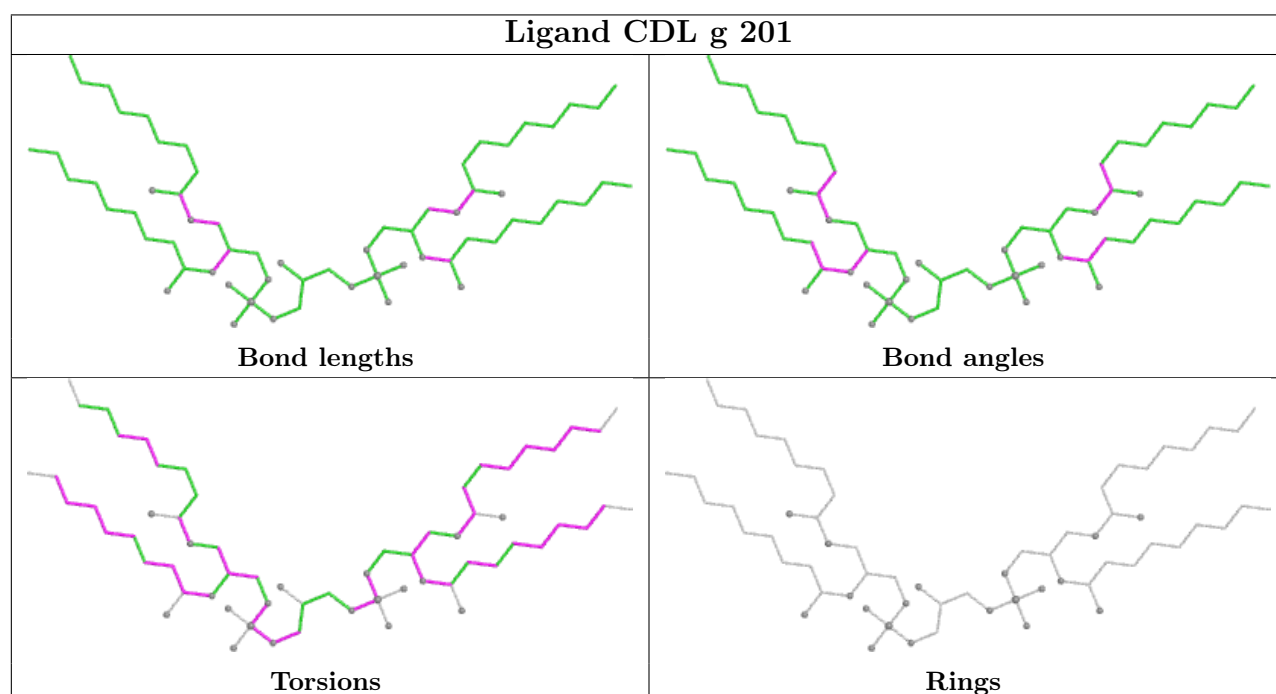
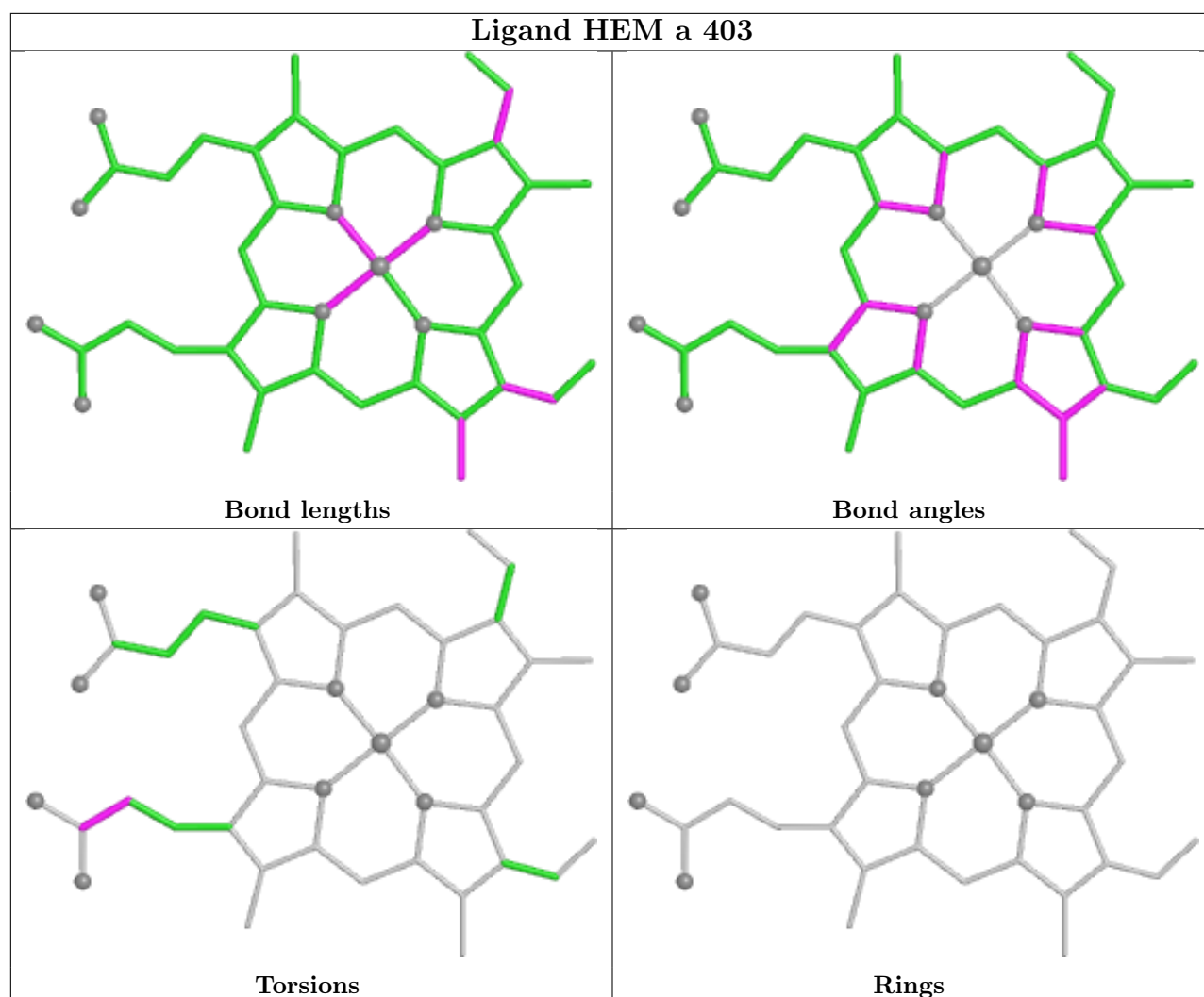
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	401	A1D6K	6	0
14	D	501	PEE	5	0
17	a	406	CDL	2	0
17	g	201	CDL	2	0
15	B	401	HEC	4	0
14	A	404	PEE	1	0
17	a	407	CDL	2	0
12	a	401	A1D6K	7	0
15	b	401	HEC	1	0

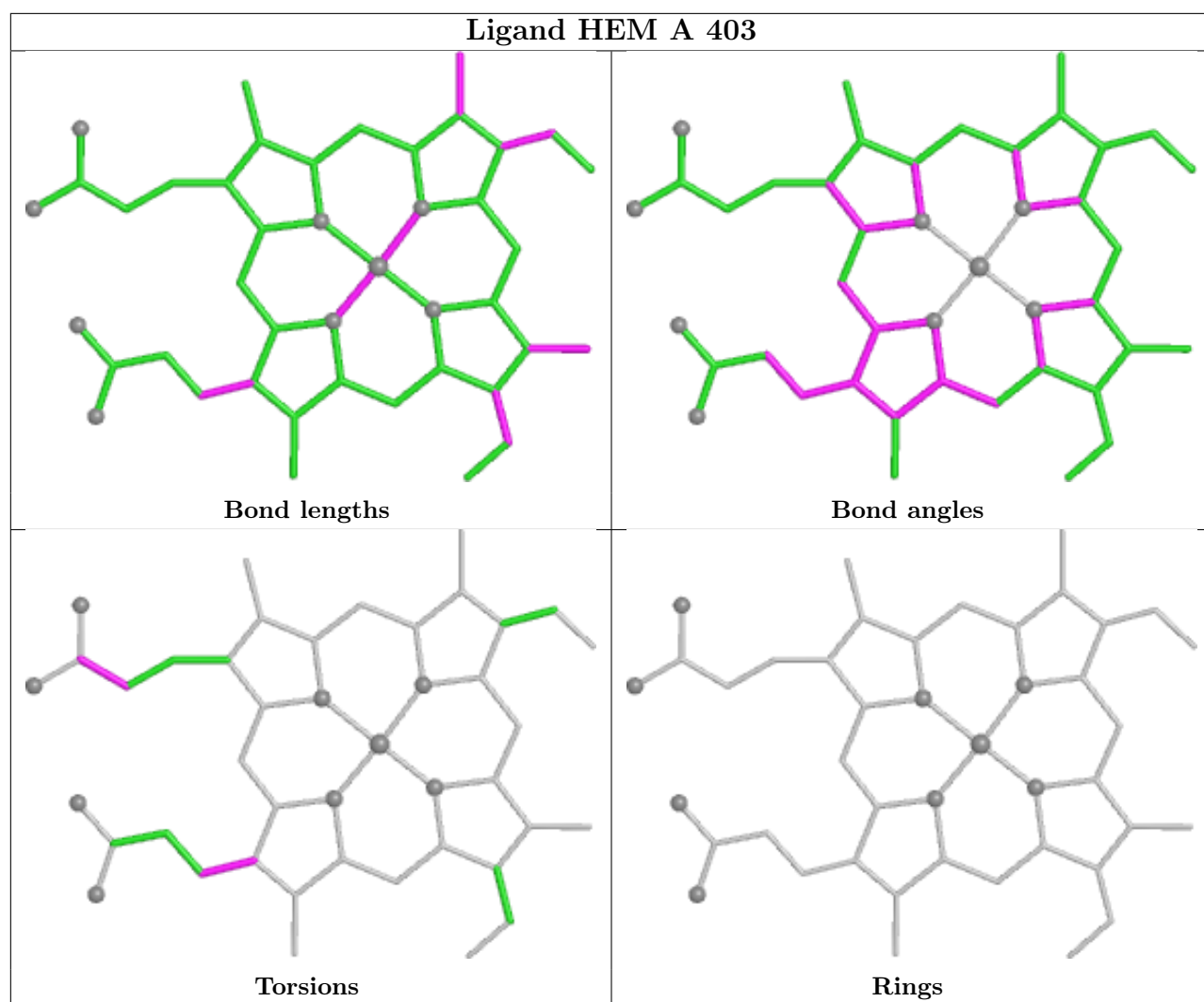
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



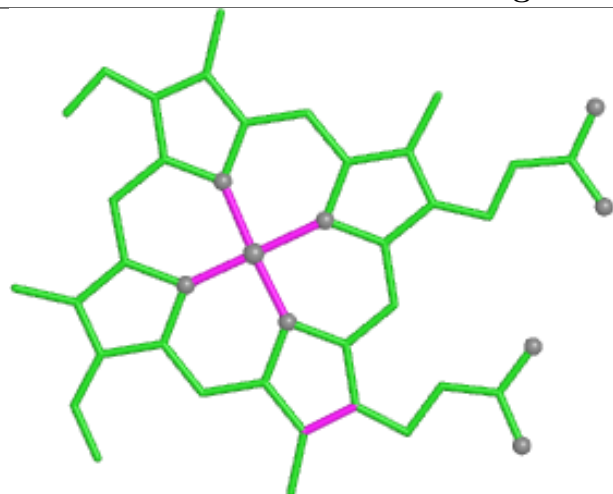




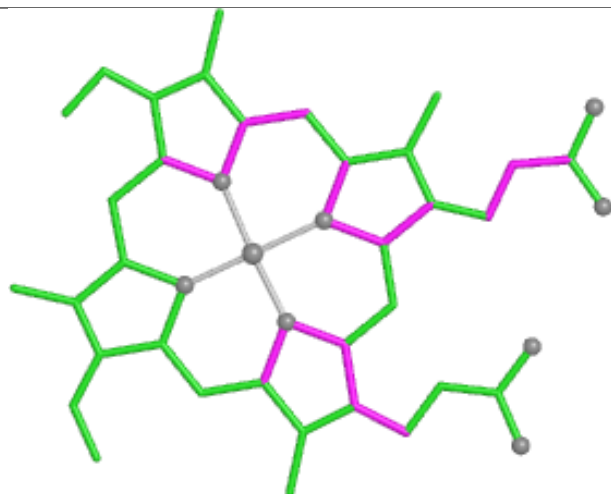




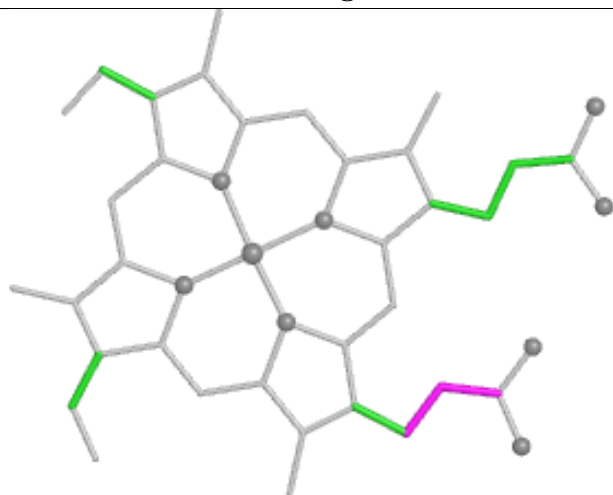
Ligand HEC B 401



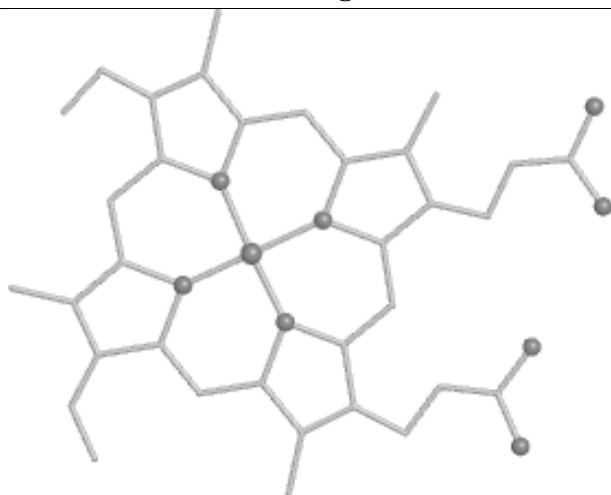
Bond lengths



Bond angles

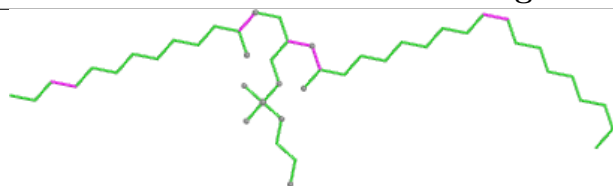


Torsions

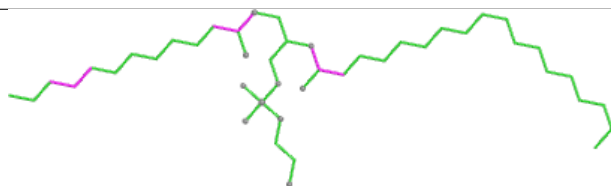


Rings

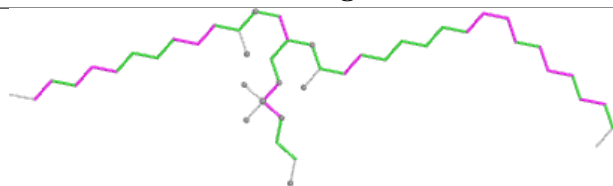
Ligand PEE A 404



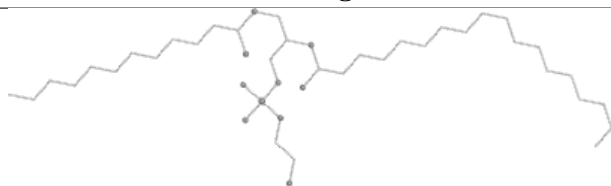
Bond lengths



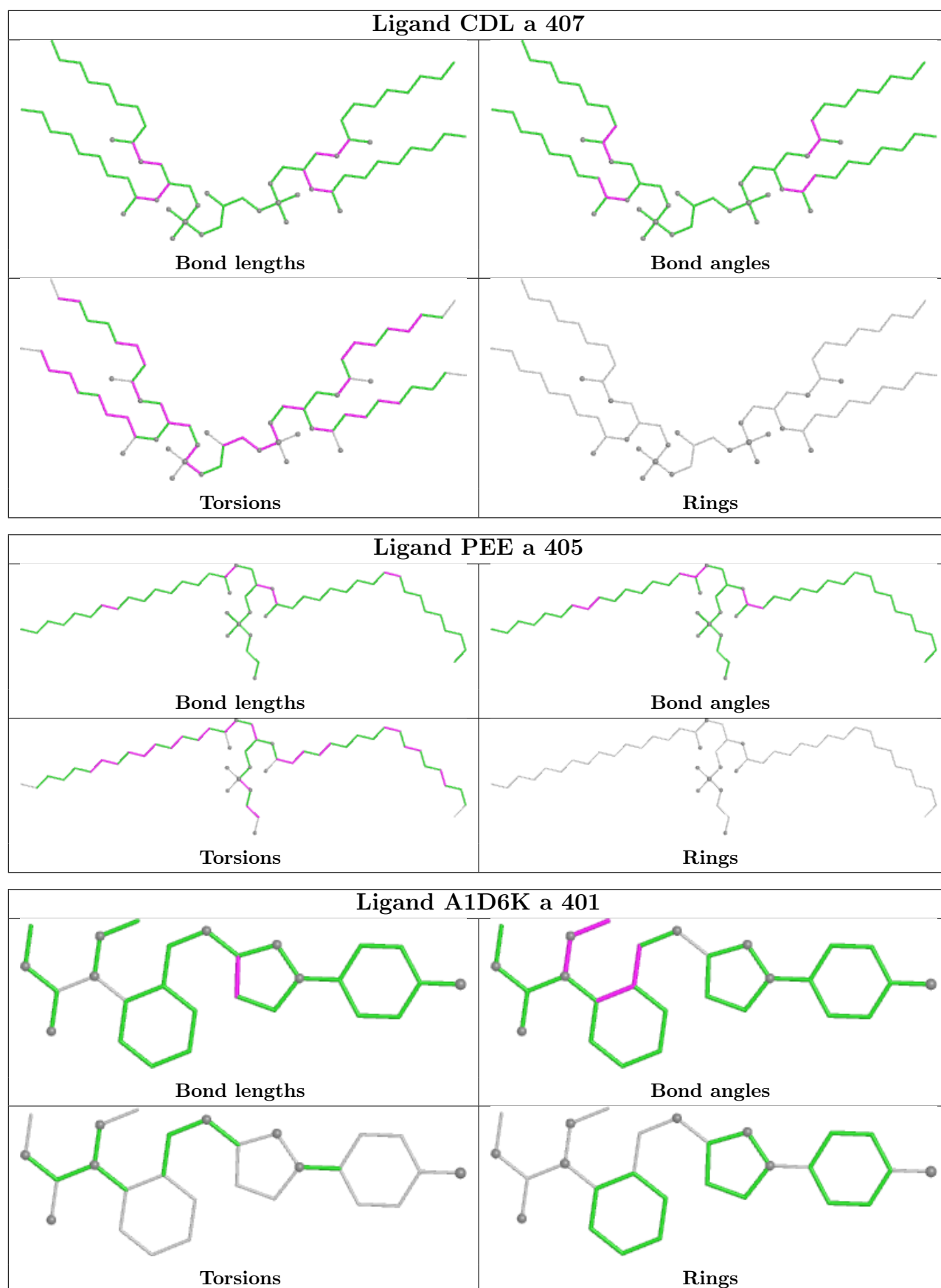
Bond angles

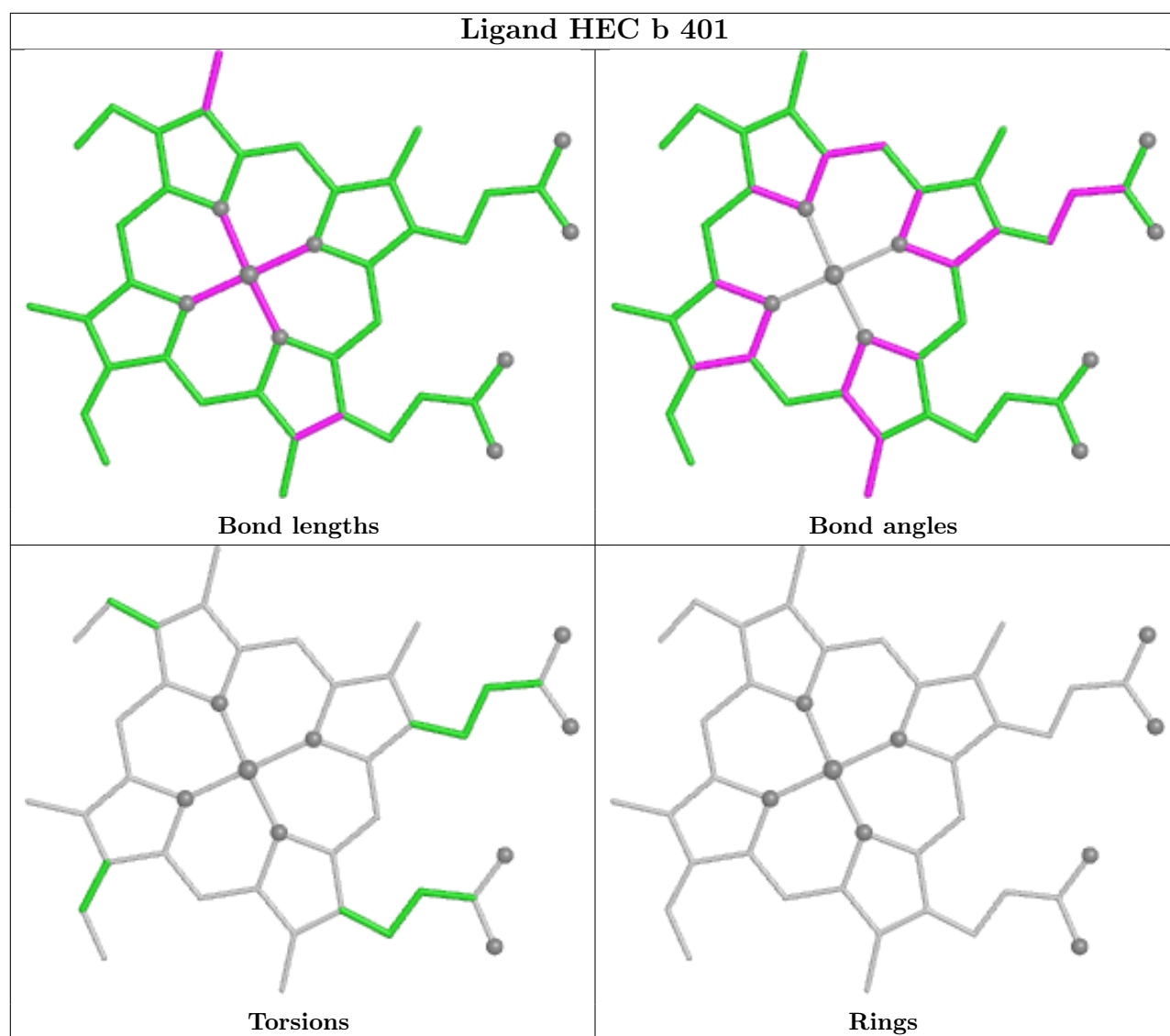


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

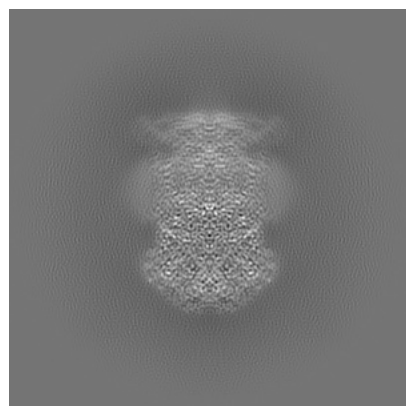
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60317. These allow visual inspection of the internal detail of the map and identification of artifacts.

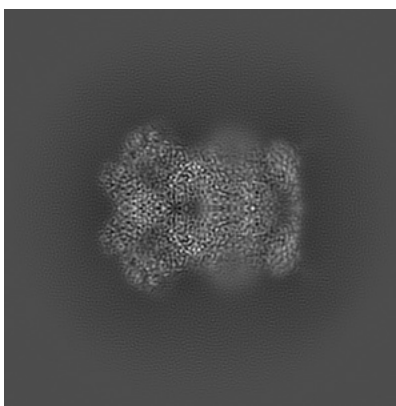
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

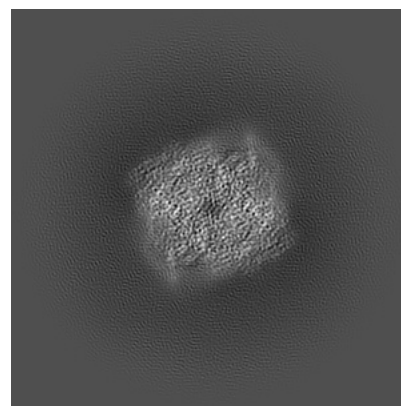
6.1.1 Primary map



X

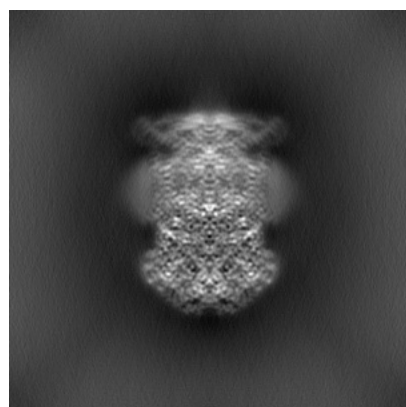


Y

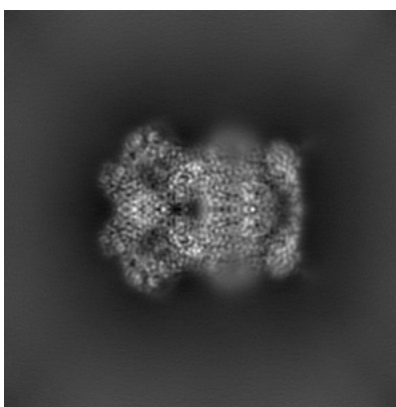


Z

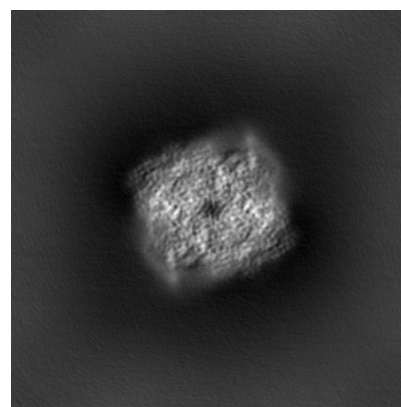
6.1.2 Raw map



X



Y

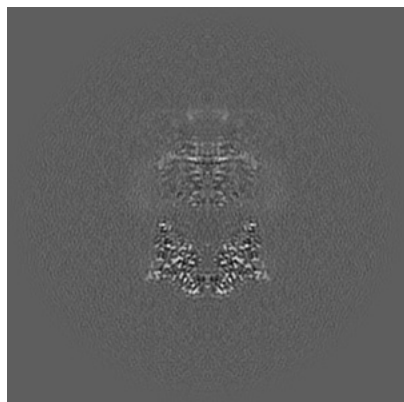


Z

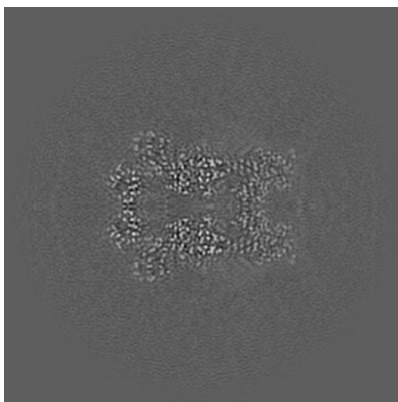
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

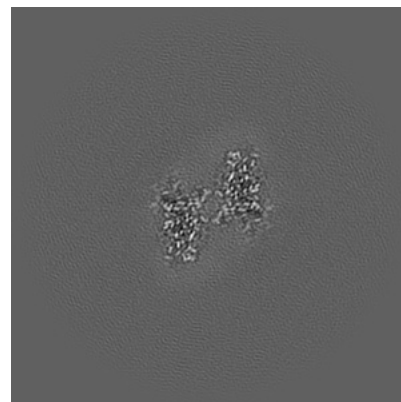
6.2.1 Primary map



X Index: 160

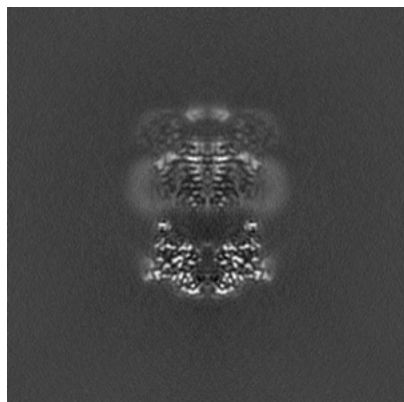


Y Index: 160

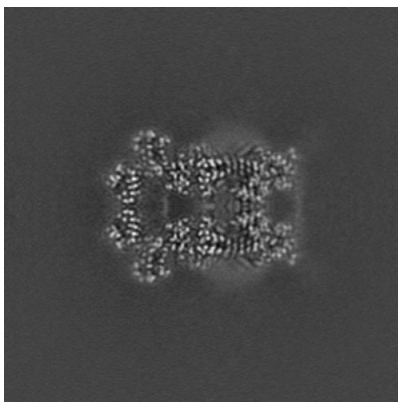


Z Index: 160

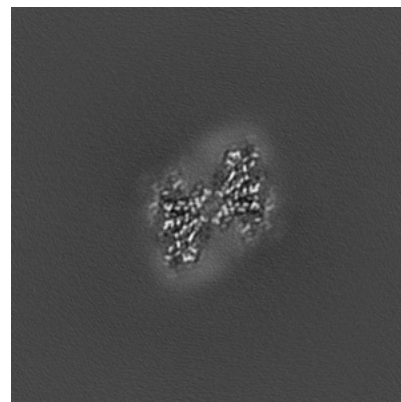
6.2.2 Raw map



X Index: 160



Y Index: 160

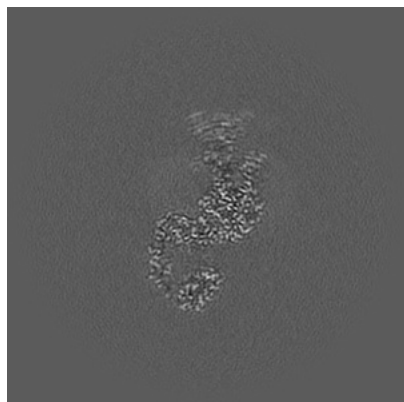


Z Index: 160

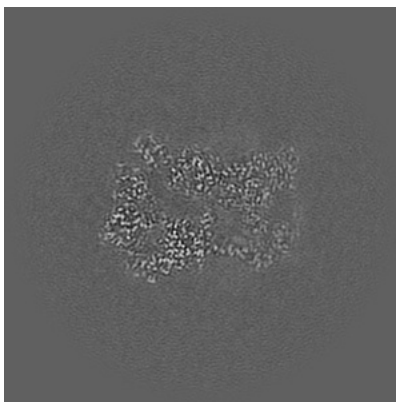
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

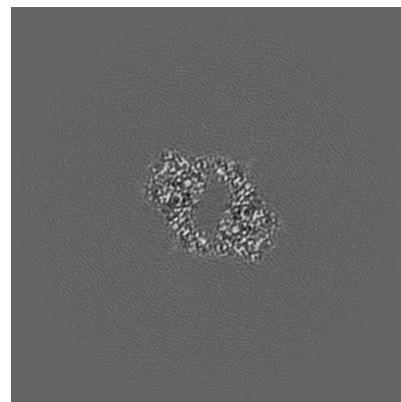
6.3.1 Primary map



X Index: 182

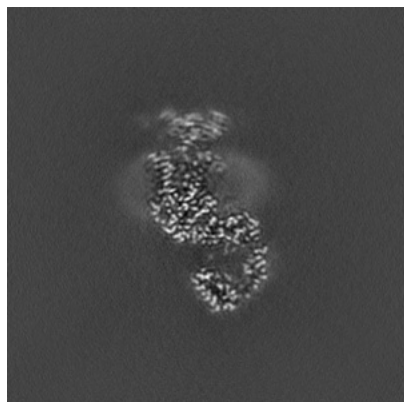


Y Index: 165

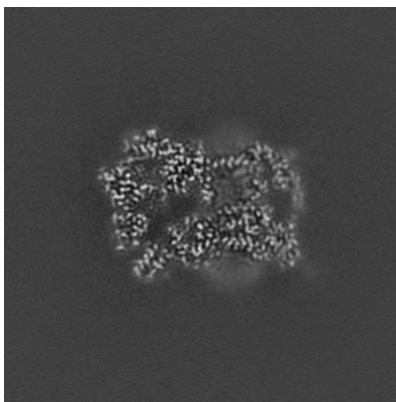


Z Index: 138

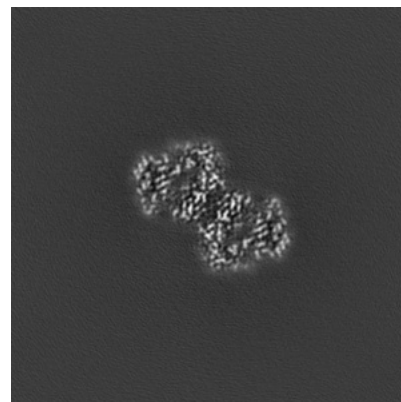
6.3.2 Raw map



X Index: 138



Y Index: 155

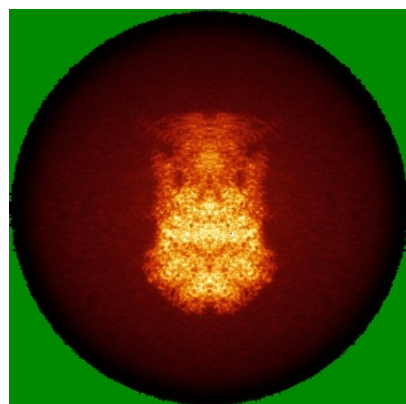


Z Index: 105

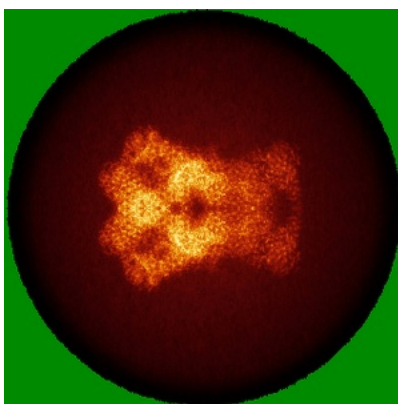
The images above show the largest variance slices of the map in three orthogonal directions.

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

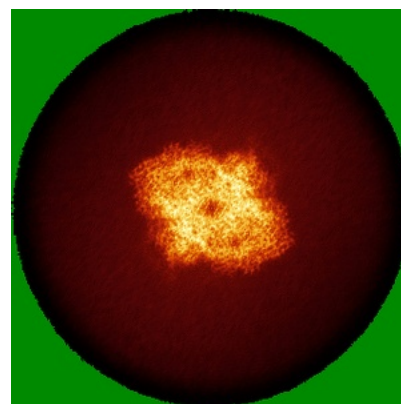
6.4.1 Primary map



X

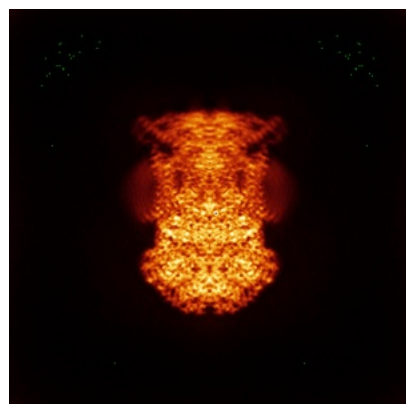


Y

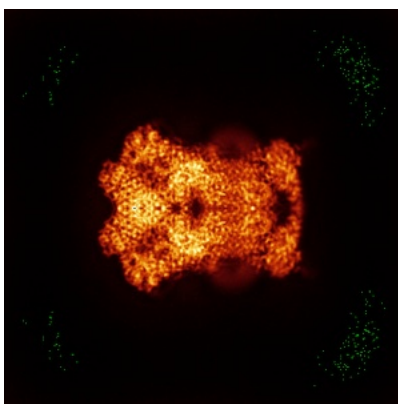


Z

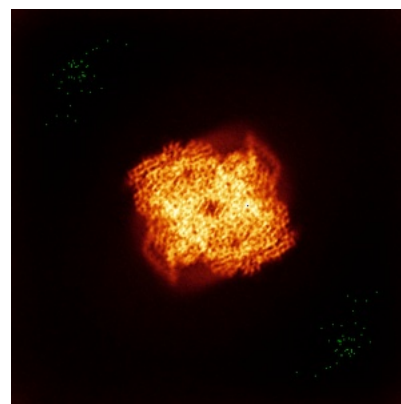
6.4.2 Raw map



X



Y



Z

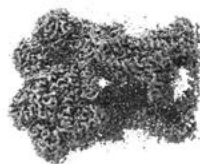
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



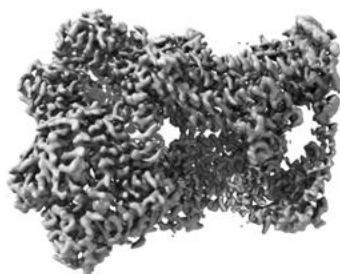
Z

The images above show the 3D surface view of the map at the recommended contour level 0.543. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

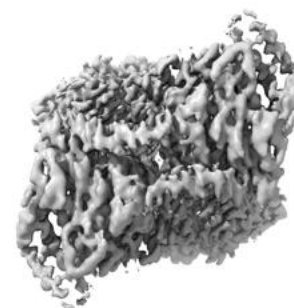
6.5.2 Raw map



X



Y



Z

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

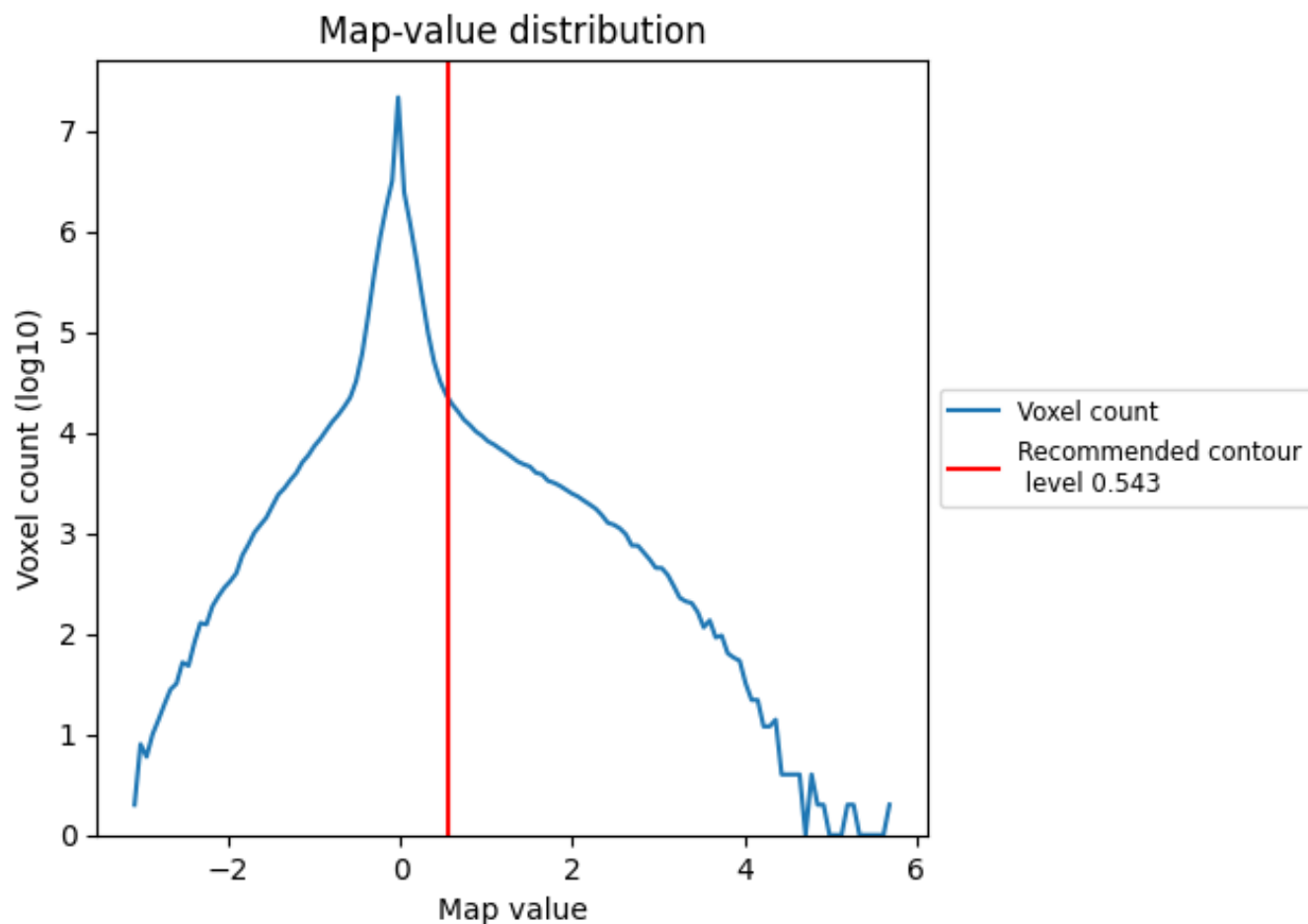
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

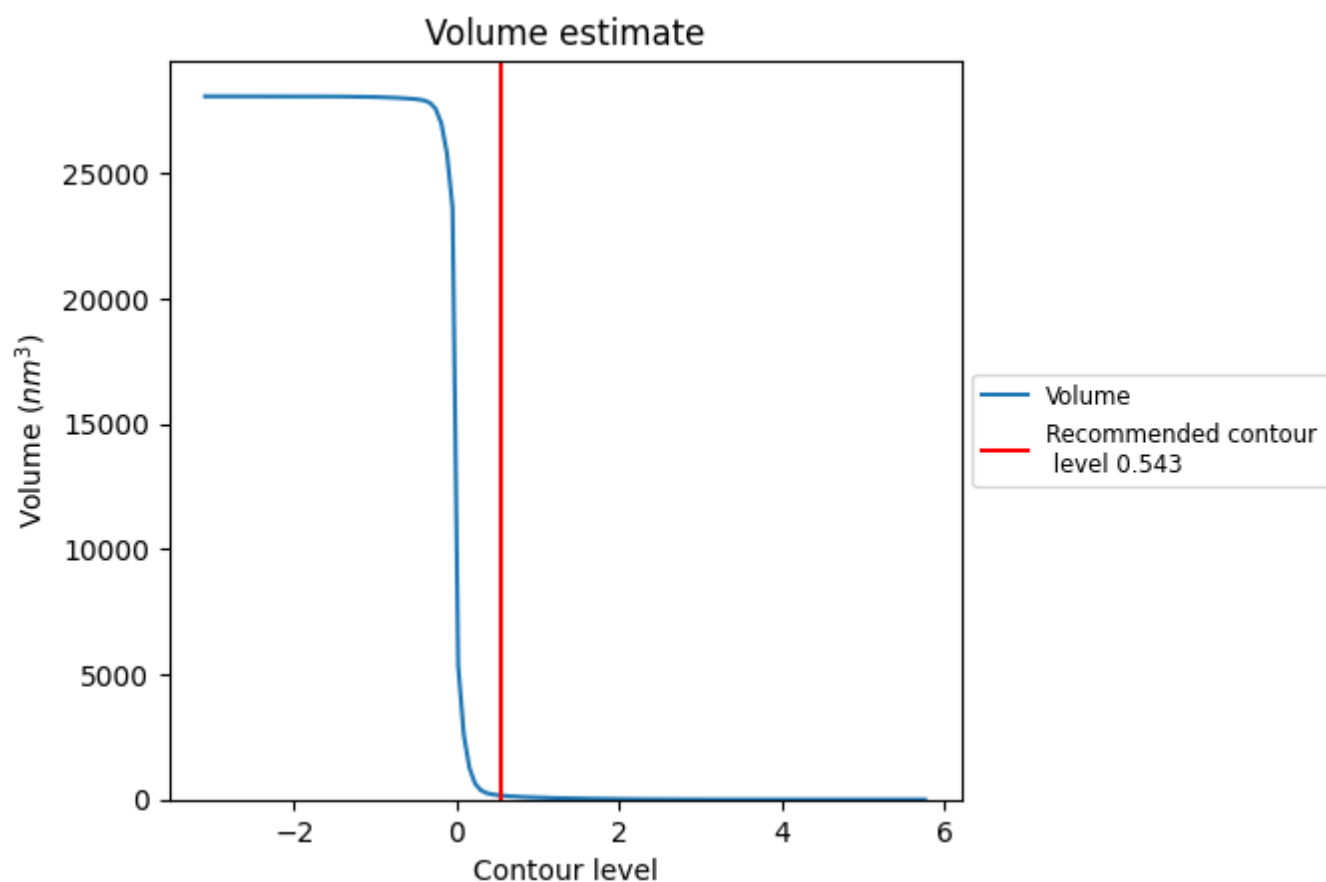
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

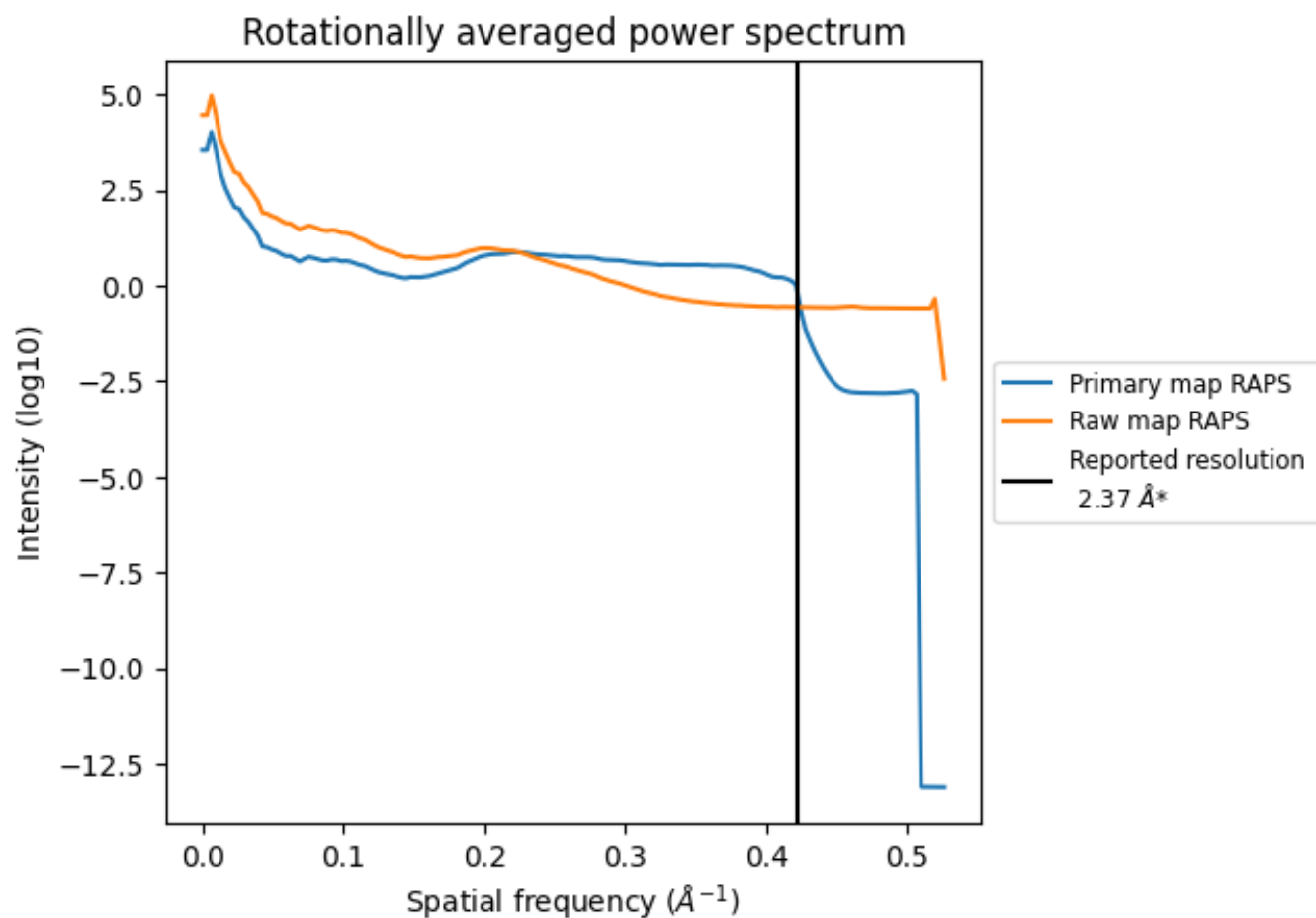
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 164 nm³; this corresponds to an approximate mass of 148 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 ⓘ

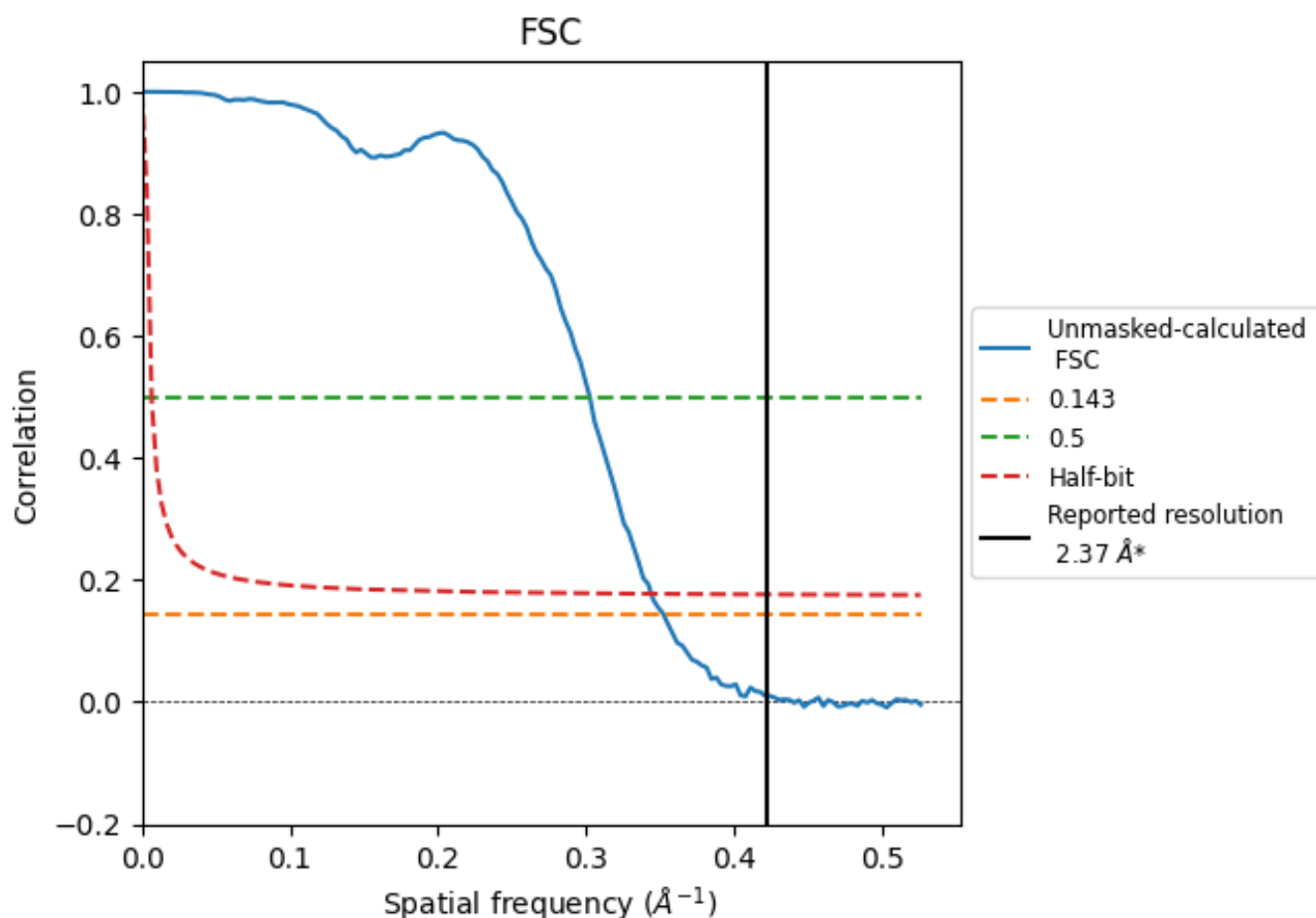


*Reported resolution corresponds to spatial frequency of 0.422 Å⁻¹

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 0.422 Å⁻¹

8.2 Resolution estimates [i](#)

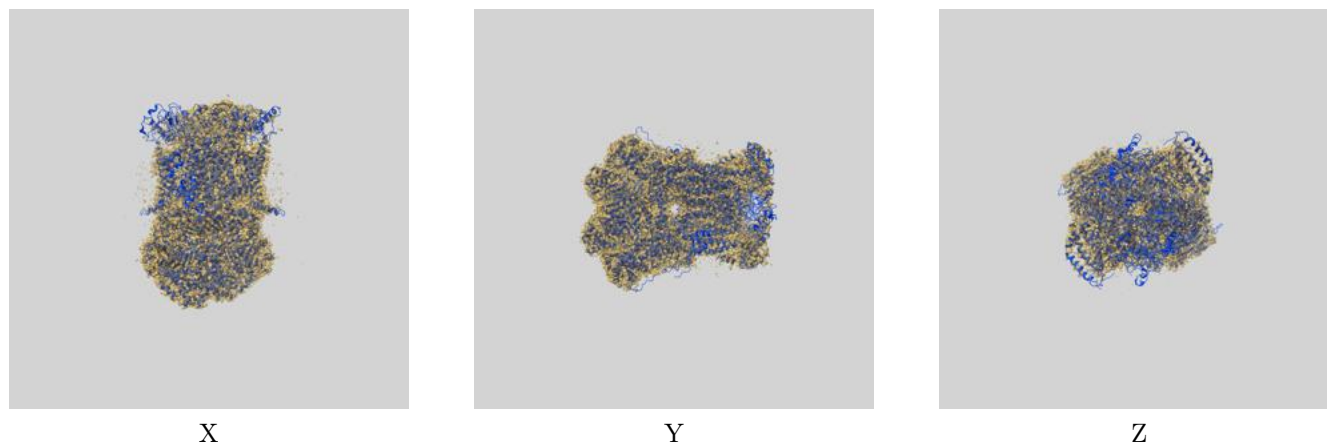
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.37	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.84	3.30	2.91

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.84 differs from the reported value 2.37 by more than 10 %

9 Map-model fit [i](#)

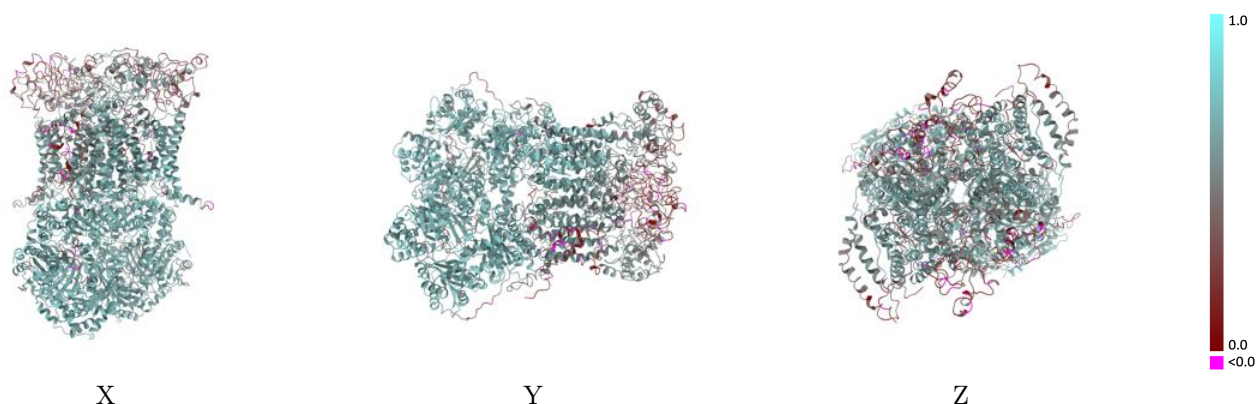
This section contains information regarding the fit between EMDB map EMD-60317 and PDB model 8ZOS. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



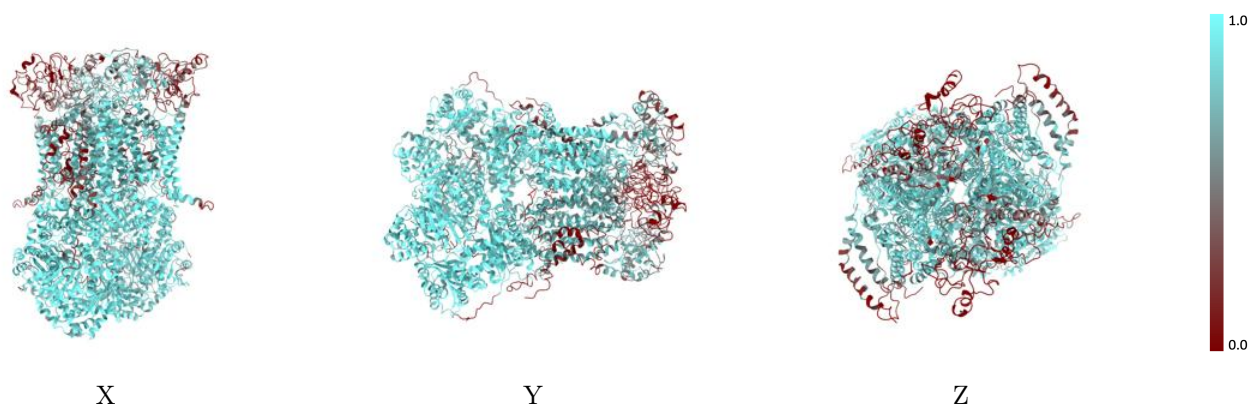
The images above show the 3D surface view of the map at the recommended contour level 0.543 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



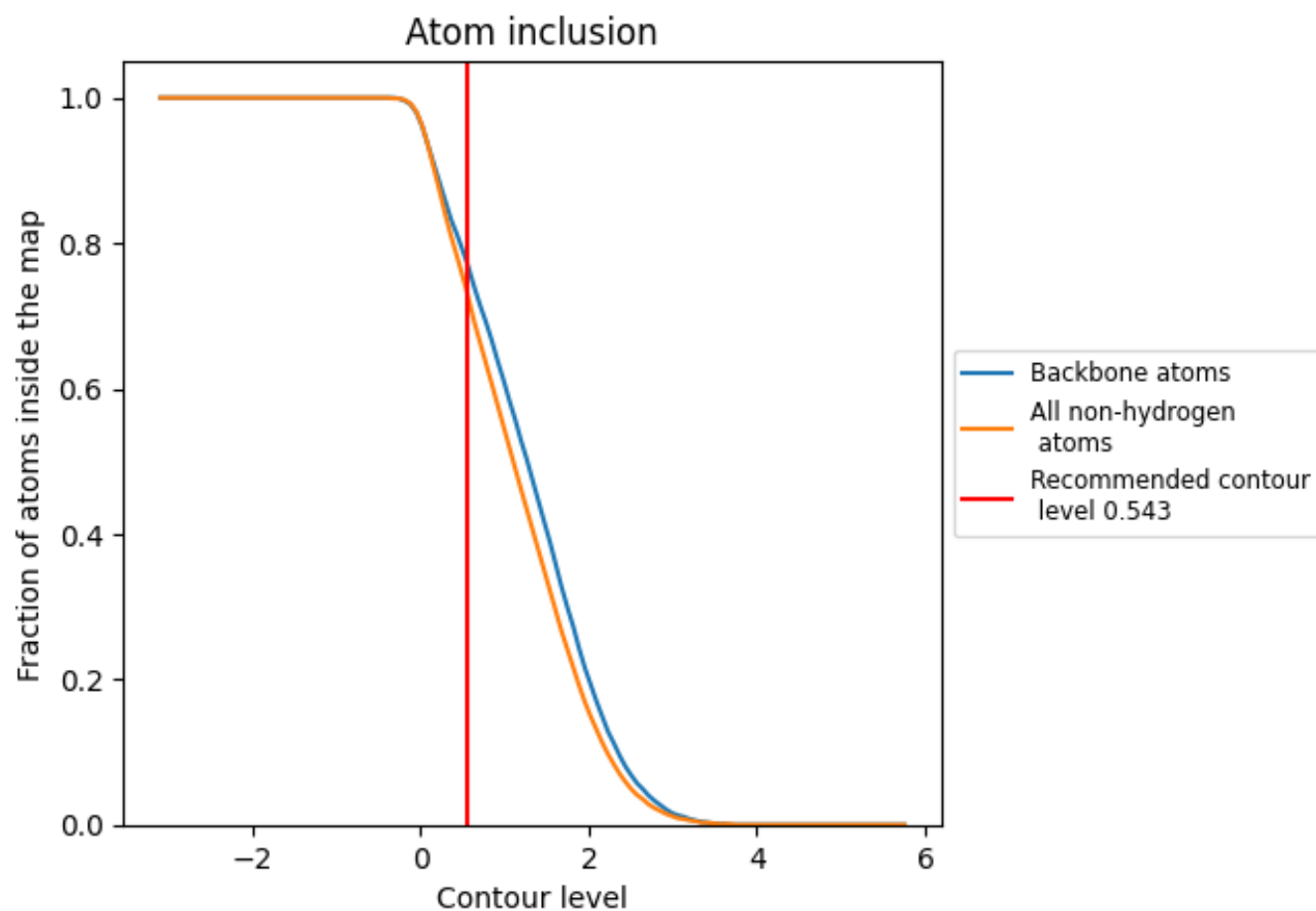
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.543).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 74% 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 (0.543) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7360	 0.5660
A	 0.8760	 0.6200
B	 0.6490	 0.4920
C	 0.1370	 0.3050
D	 0.9080	 0.6570
E	 0.9370	 0.6720
F	 0.4190	 0.4470
G	 0.8810	 0.6570
H	 0.8430	 0.6290
I	 0.2910	 0.3000
J	 0.0030	 0.2290
K	 0.5230	 0.4590
a	 0.8490	 0.6120
b	 0.6800	 0.5050
c	 0.1210	 0.2890
d	 0.9180	 0.6600
e	 0.9360	 0.6730
f	 0.4170	 0.4470
g	 0.8610	 0.6480
h	 0.7740	 0.5910
i	 0.2810	 0.2860
j	 0.0070	 0.1920
k	 0.5200	 0.4590

