



Full wwPDB EM Validation Report ⓘ

Jun 4, 2026 – 12:25 pm BST

PDB ID : 9RZV / pdb_00009rzv
EMDB ID : EMD-54414
Title : E. coli cytochrome bd-I dimer bound to menaquinone
Authors : van der Velden, T.T.; Kayastha, K.; Bruenle, S.; Jeuken, L.J.C.
Deposited on : 2025-07-16
Resolution : 2.23 Å (reported)
Based on initial model : .

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:

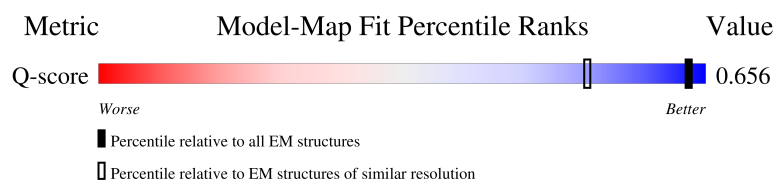
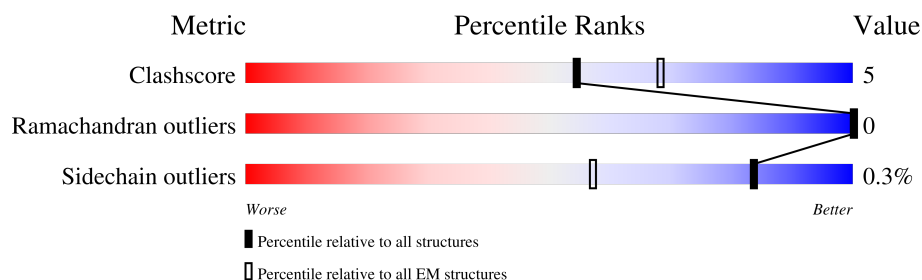
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 2.23 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	3335 (1.73 - 2.73)

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	522	
1	a	522	
2	B	379	
2	b	379	

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Mol	Chain	Length	Quality of chain
3	H	29	 90% 10%
3	h	29	 83% 17%
4	X	37	 68% 14% 19%
4	x	37	 68% 14% 19%

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
6	A1JN4	A	602	X	-	-	-
6	A1JN4	a	605	X	-	-	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 32907 atoms, of which 16596 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	513	Total	C	H	N	O	S	0	0
			8108	2663	4068	648	705	24		
1	a	513	Total	C	H	N	O	S	0	0
			8108	2663	4068	648	705	24		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	379	Total	C	H	N	O	S	0	0
			6021	1986	3025	483	505	22		
2	b	379	Total	C	H	N	O	S	0	0
			6021	1986	3025	483	505	22		

- Molecule 3 is a protein called Cytochrome bd-I ubiquinol oxidase CydH (Uncharacterized protein YnhF).

Mol	Chain	Residues	Atoms						AltConf	Trace
3	H	29	Total	C	H	N	O	S	0	0
			432	139	222	32	38	1		
3	h	29	Total	C	H	N	O	S	0	0
			432	139	222	32	38	1		

- Molecule 4 is a protein called Cytochrome bd-I ubiquinol oxidase subunit X.

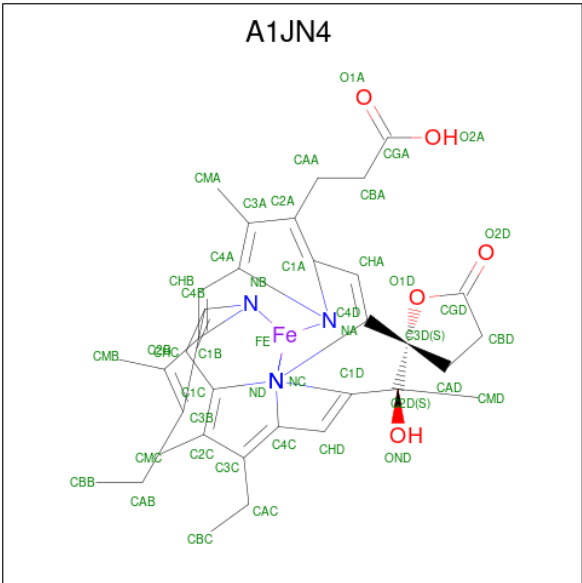
Mol	Chain	Residues	Atoms						AltConf	Trace
4	X	30	Total	C	H	N	O	S	0	0
			451	157	219	34	39	2		
4	x	30	Total	C	H	N	O	S	0	0
			451	157	219	34	39	2		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



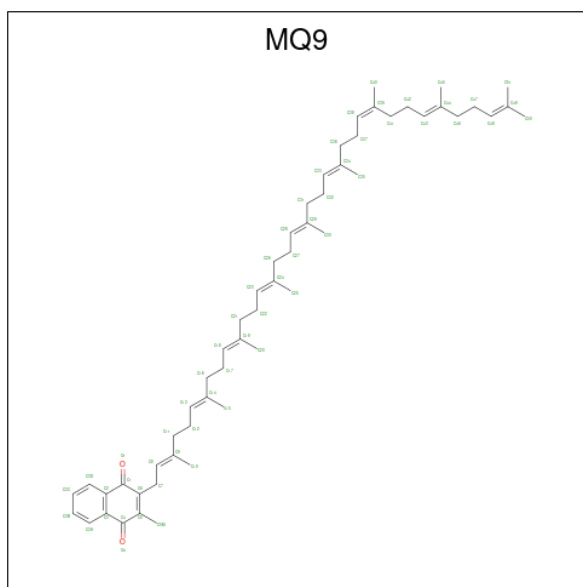
Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
5	A	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
5	a	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
5	a	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 6 is TRANS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: A1JN4) (formula: $C_{34}H_{36}FeN_4O_5$).



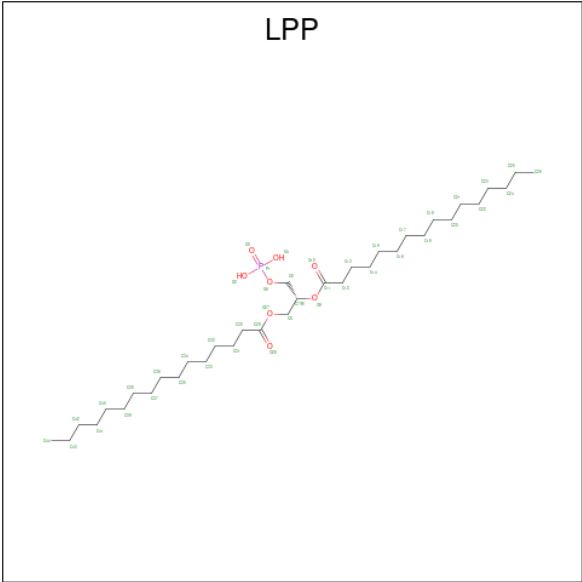
Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	Fe	H	N	O	0
			75	34	1	31	4	5	
6	a	1	Total	C	Fe	H	N	O	0
			75	34	1	31	4	5	

- Molecule 7 is MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



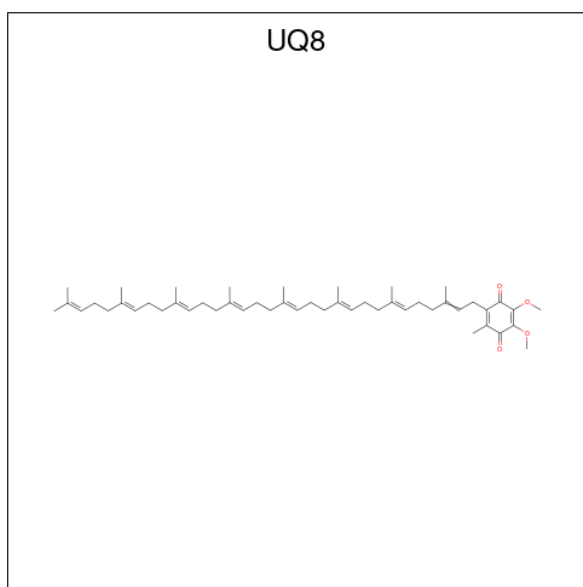
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	H	O	0
			138	56	80	2	
7	B	1	Total	C	H	O	0
			138	56	80	2	
7	a	1	Total	C	H	O	0
			138	56	80	2	
7	b	1	Total	C	H	O	0
			138	56	80	2	

- Molecule 8 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: $C_{35}H_{69}O_8P$).



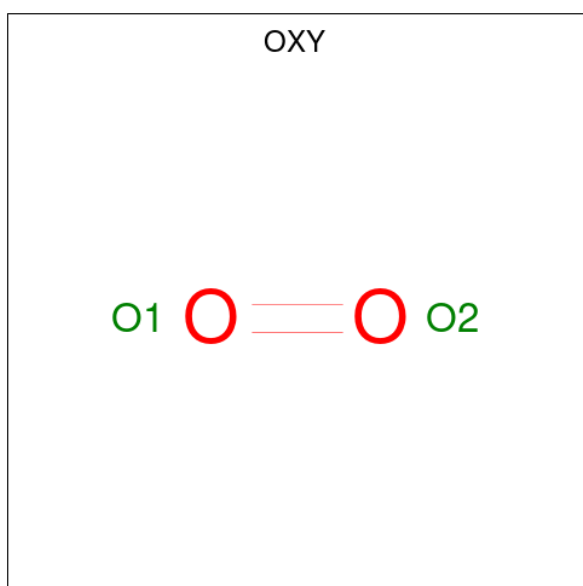
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	H	O	P	0
			111	35	67	8	1	
8	B	1	Total	C	H	O	P	0
			111	35	67	8	1	
8	B	1	Total	C	H	O	P	0
			111	35	67	8	1	
8	a	1	Total	C	H	O	P	0
			111	35	67	8	1	
8	b	1	Total	C	H	O	P	0
			111	35	67	8	1	
8	b	1	Total	C	H	O	P	0
			111	35	67	8	1	

- Molecule 9 is Ubiquinone-8 (CCD ID: UQ8) (formula: C₄₉H₇₄O₄).



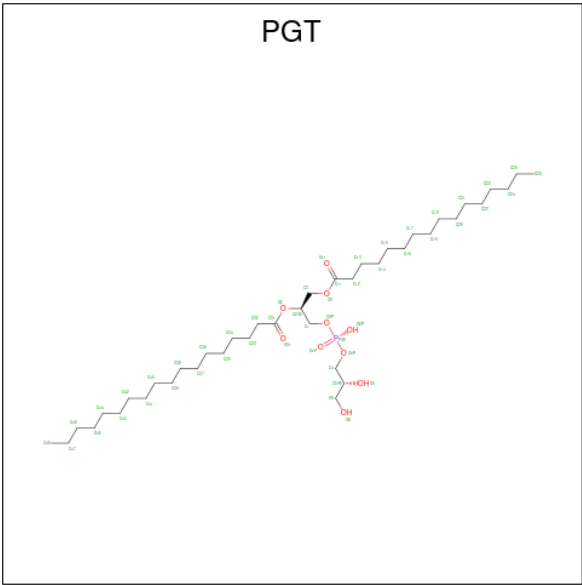
Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	H	O	0
			127	49	74	4	
9	a	1	Total	C	H	O	0
			127	49	74	4	

- Molecule 10 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



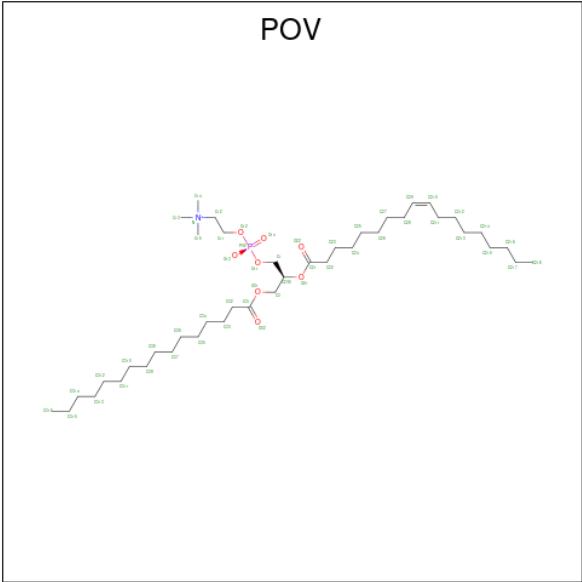
Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	O	0
			2	2	
10	a	1	Total	O	0
			2	2	

- Molecule 11 is (1S)-2-{{[[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	H	O	P	0
			129	40	78	10	1	
11	X	1	Total	C	H	O	P	0
			129	40	78	10	1	
11	a	1	Total	C	H	O	P	0
			129	40	78	10	1	
11	x	1	Total	C	H	O	P	0
			129	40	78	10	1	

- Molecule 12 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms						AltConf
12	B	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
12	B	1	Total	C	N	O	P		0
			52	42	1	8	1		
12	b	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
12	b	1	Total	C	N	O	P		0
			52	42	1	8	1		

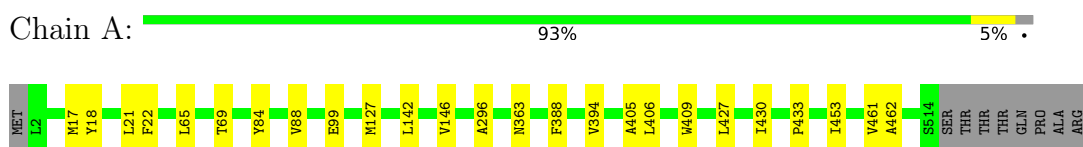
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		AltConf
13	A	29	Total	O	0
			29	29	
13	B	9	Total	O	0
			9	9	
13	a	29	Total	O	0
			29	29	
13	b	10	Total	O	0
			10	10	

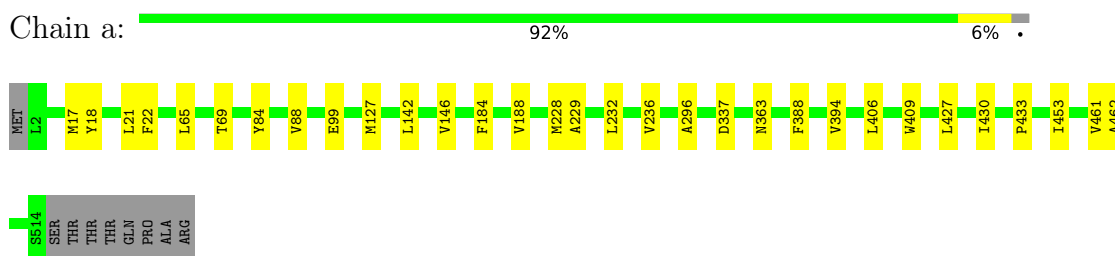
3 Residue-property plots

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

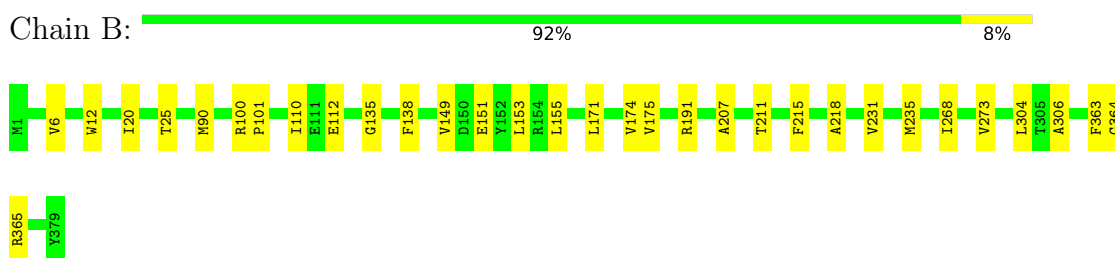
- Molecule 1: Cytochrome bd-I ubiquinol oxidase subunit 1



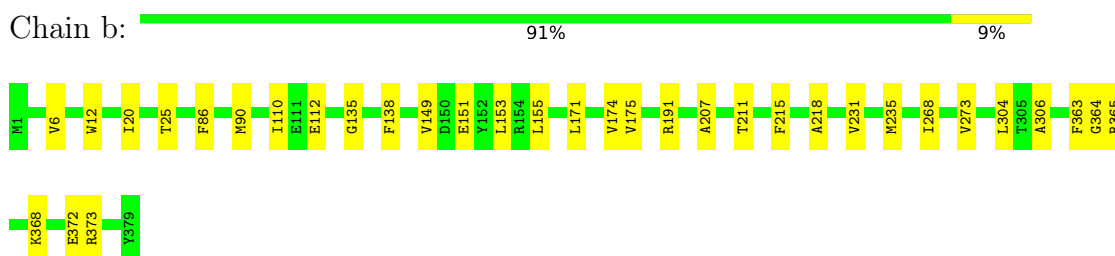
- Molecule 1: Cytochrome bd-I ubiquinol oxidase subunit 1



- Molecule 2: Cytochrome bd-I ubiquinol oxidase subunit 2

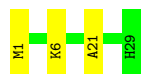


- Molecule 2: Cytochrome bd-I ubiquinol oxidase subunit 2



- Molecule 3: Cytochrome bd-I ubiquinol oxidase CydH (Uncharacterized protein YnhF)

Chain H:  90% 10%



- Molecule 3: Cytochrome bd-I ubiquinol oxidase CydH (Uncharacterized protein YnhF)

Chain h:  83% 17%



- Molecule 4: Cytochrome bd-I ubiquinol oxidase subunit X

Chain X:  68% 14% 19%



- Molecule 4: Cytochrome bd-I ubiquinol oxidase subunit X

Chain x:  68% 14% 19%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	530094	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.425	Depositor
Minimum map value	-0.200	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0364	Depositor
Map size (Å)	300.96002, 300.96002, 300.96002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8360001, 0.8360001, 0.8360001	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, LPP, PGT, UQ8, POV, MQ9, OXY, A1JN4

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	0.18	0/4146	0.29	0/5624
1	a	0.18	0/4146	0.29	0/5624
2	B	0.16	0/3083	0.33	2/4212 (0.0%)
2	b	0.16	0/3083	0.33	2/4212 (0.0%)
3	H	0.14	0/211	0.19	0/286
3	h	0.14	0/211	0.19	0/286
4	X	0.18	0/239	0.35	0/326
4	x	0.18	0/239	0.31	0/326
All	All	0.17	0/15358	0.31	4/20896 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	174	VAL	CA-C-N	7.51	130.02	120.56
2	B	174	VAL	C-N-CA	7.51	130.02	120.56
2	b	174	VAL	CA-C-N	7.47	129.98	120.56
2	b	174	VAL	C-N-CA	7.47	129.98	120.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4040	4068	4066	18	0
1	a	4040	4068	4066	25	0
2	B	2996	3025	3025	32	0
2	b	2996	3025	3025	35	0
3	H	210	222	238	3	0
3	h	210	222	238	3	0
4	X	232	219	230	3	0
4	x	232	219	230	3	0
5	A	86	60	60	9	0
5	a	86	60	60	9	0
6	A	44	31	0	0	0
6	a	44	31	0	0	0
7	A	58	80	80	5	0
7	B	58	80	80	16	0
7	a	58	80	80	5	0
7	b	58	80	80	16	0
8	A	44	67	67	4	0
8	B	88	134	134	1	0
8	a	44	67	67	4	0
8	b	88	134	134	1	0
9	A	53	74	74	7	0
9	a	53	74	74	10	0
10	A	2	0	0	1	0
10	a	2	0	0	1	0
11	A	51	78	78	1	0
11	X	51	78	78	0	0
11	a	51	78	78	1	0
11	x	51	78	78	0	0
12	B	104	82	163	14	0
12	b	104	82	163	14	0
13	A	29	0	0	0	0
13	B	9	0	0	0	0
13	a	29	0	0	0	0
13	b	10	0	0	0	0
All	All	16311	16596	16746	169	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 5.

All (169) 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)
5:A:605:HEM:HBB2	5:A:605:HEM:HHC	1.59	0.82
7:b:401:MQ9:H103	7:b:401:MQ9:H13	1.64	0.79
7:B:405:MQ9:H103	7:B:405:MQ9:H13	1.64	0.79
5:A:605:HEM:HBC2	5:A:605:HEM:HHD	1.64	0.79
9:a:601:UQ8:H25	9:a:601:UQ8:H20A	1.66	0.77
5:a:603:HEM:HBC2	5:a:603:HEM:HHD	1.64	0.77
5:A:601:HEM:HHD	5:A:601:HEM:HBC2	1.69	0.75
5:a:603:HEM:HBB2	5:a:603:HEM:HHC	1.70	0.72
5:a:606:HEM:HBC2	5:a:606:HEM:HHD	1.69	0.72
2:B:365:ARG:NH1	12:B:404:POV:H1	2.09	0.68
2:B:364:GLY:HA2	12:B:404:POV:H12	1.77	0.66
2:b:365:ARG:NH1	12:b:403:POV:H1	2.10	0.66
7:b:401:MQ9:H103	7:b:401:MQ9:C13	2.25	0.66
2:b:364:GLY:HA2	12:b:403:POV:H12	1.77	0.65
7:B:405:MQ9:H103	7:B:405:MQ9:C13	2.26	0.65
2:B:20:ILE:HD11	2:B:304:LEU:CD1	2.27	0.64
1:A:17:MET:HG2	5:A:605:HEM:HBC1	1.80	0.64
2:b:20:ILE:HD11	2:b:304:LEU:CD1	2.27	0.64
1:a:17:MET:HG2	5:a:603:HEM:HBC1	1.81	0.63
5:A:605:HEM:HHA	5:A:605:HEM:HBA1	1.81	0.62
2:b:215:PHE:CE1	7:b:401:MQ9:H451	2.37	0.60
2:B:215:PHE:CE1	7:B:405:MQ9:H451	2.37	0.60
1:a:388:PHE:CD1	7:a:602:MQ9:H352	2.38	0.58
8:A:604:LPP:H443	8:A:604:LPP:H261	1.84	0.58
2:b:20:ILE:HD11	2:b:304:LEU:HD13	1.86	0.58
7:b:401:MQ9:H43	7:b:401:MQ9:H403	1.86	0.58
2:B:20:ILE:HD11	2:B:304:LEU:HD13	1.85	0.58
8:a:604:LPP:H443	8:a:604:LPP:H261	1.84	0.58
1:A:388:PHE:CD1	7:A:603:MQ9:H352	2.39	0.58
9:A:606:UQ8:H45B	9:A:606:UQ8:H30A	1.86	0.58
7:B:405:MQ9:H403	7:B:405:MQ9:H43	1.86	0.57
4:X:25:GLU:OE1	4:X:25:GLU:HA	2.06	0.56
1:A:406:LEU:HD23	9:A:606:UQ8:H45	1.88	0.55
2:b:365:ARG:HG3	12:b:403:POV:H12A	1.89	0.54
2:B:138:PHE:HE2	7:B:405:MQ9:H5M2	1.73	0.54
2:b:138:PHE:HE2	7:b:401:MQ9:H5M2	1.72	0.53
1:a:427:LEU:HD21	8:a:604:LPP:HC82	1.92	0.52
2:B:171:LEU:O	2:B:175:VAL:HG23	2.09	0.52
1:a:394:VAL:HG11	7:a:602:MQ9:H18	1.92	0.52
2:b:12:TRP:O	7:b:401:MQ9:H3D	2.10	0.52
4:x:25:GLU:HA	4:x:25:GLU:OE2	2.09	0.52
2:b:191:ARG:HD2	12:b:403:POV:H22A	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:LEU:HD21	8:A:604:LPP:HC82	1.92	0.51
2:b:151:GLU:H	2:b:151:GLU:CD	2.18	0.51
2:B:151:GLU:CD	2:B:151:GLU:H	2.18	0.51
2:B:363:PHE:HD2	12:B:404:POV:H23	1.76	0.51
2:b:135:GLY:HA2	7:b:401:MQ9:H351	1.93	0.51
2:b:171:LEU:O	2:b:175:VAL:HG23	2.10	0.51
2:B:12:TRP:O	7:B:405:MQ9:H3D	2.10	0.51
2:B:365:ARG:HG3	12:B:404:POV:H12A	1.91	0.51
1:a:88:VAL:HG11	1:a:453:ILE:HG13	1.93	0.51
2:B:207:ALA:O	2:B:211:THR:HG23	2.11	0.51
1:a:461:VAL:HG12	1:a:461:VAL:O	2.11	0.51
1:A:394:VAL:HG11	7:A:603:MQ9:H18	1.93	0.50
1:a:84:TYR:HB2	1:a:462:ALA:HB1	1.93	0.50
2:b:207:ALA:O	2:b:211:THR:HG23	2.10	0.50
2:B:363:PHE:CE1	12:B:404:POV:H11A	2.45	0.50
1:A:461:VAL:HG12	1:A:461:VAL:O	2.11	0.50
2:B:191:ARG:HD2	12:B:404:POV:H22A	1.93	0.50
2:B:306:ALA:HB2	7:B:405:MQ9:C40	2.42	0.50
1:a:22:PHE:CZ	1:a:65:LEU:HD13	2.47	0.50
2:b:306:ALA:HB2	7:b:401:MQ9:C40	2.42	0.50
9:A:606:UQ8:H45B	9:A:606:UQ8:C29	2.41	0.50
1:A:22:PHE:CZ	1:A:65:LEU:HD13	2.47	0.50
1:A:88:VAL:HG11	1:A:453:ILE:HG13	1.93	0.50
1:A:84:TYR:HB2	1:A:462:ALA:HB1	1.93	0.50
2:b:363:PHE:HD2	12:b:403:POV:H23	1.77	0.49
2:B:135:GLY:HA2	7:B:405:MQ9:H351	1.94	0.49
5:a:606:HEM:HBB2	5:a:606:HEM:HMB2	1.94	0.49
2:B:306:ALA:HB2	7:B:405:MQ9:H402	1.95	0.49
2:b:306:ALA:HB2	7:b:401:MQ9:H402	1.93	0.49
4:X:4:PHE:O	4:X:7:ILE:HG22	2.13	0.49
1:A:21:LEU:HB3	8:A:604:LPP:H263	1.95	0.48
9:A:606:UQ8:H45B	9:A:606:UQ8:C30	2.43	0.48
1:a:21:LEU:HB3	8:a:604:LPP:H263	1.95	0.48
5:A:601:HEM:HBB2	5:A:601:HEM:HMB2	1.94	0.48
2:b:363:PHE:CE1	12:b:403:POV:H11A	2.49	0.48
2:B:363:PHE:CD2	12:B:404:POV:H23	2.49	0.47
7:B:405:MQ9:H403	7:B:405:MQ9:C43	2.44	0.47
7:a:602:MQ9:H122	7:a:602:MQ9:H103	1.64	0.47
11:a:608:PGT:H442	11:a:608:PGT:H482	1.97	0.47
1:a:337:ASP:OD1	1:a:337:ASP:C	2.58	0.47
7:b:401:MQ9:H403	7:b:401:MQ9:C43	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:a:606:HEM:HBB2	5:a:606:HEM:CMB	2.45	0.47
1:A:296:ALA:HA	7:A:603:MQ9:H102	1.96	0.47
1:a:296:ALA:HA	7:a:602:MQ9:H102	1.96	0.47
2:b:373:ARG:HG3	2:b:373:ARG:HH11	1.80	0.47
2:b:363:PHE:CD2	12:b:403:POV:H23	2.50	0.47
2:B:231:VAL:HG11	2:B:235:MET:HG3	1.98	0.46
11:A:608:PGT:H442	11:A:608:PGT:H482	1.97	0.46
1:a:228:MET:HE1	9:a:601:UQ8:H25A	1.97	0.46
2:b:149:VAL:HG13	2:b:153:LEU:HA	1.97	0.46
2:B:149:VAL:HG13	2:B:153:LEU:HA	1.97	0.46
5:A:601:HEM:HBB2	5:A:601:HEM:CMB	2.45	0.46
12:B:404:POV:H24A	12:B:404:POV:O22	2.16	0.46
2:b:218:ALA:HB3	7:b:401:MQ9:H452	1.98	0.46
2:B:218:ALA:HB3	7:B:405:MQ9:H452	1.98	0.46
2:B:364:GLY:H	12:B:404:POV:H22	1.81	0.45
2:B:365:ARG:H	12:B:404:POV:H14A	1.80	0.45
7:b:401:MQ9:H453	7:b:401:MQ9:H48	1.99	0.45
7:A:603:MQ9:H103	7:A:603:MQ9:H122	1.64	0.45
2:b:364:GLY:H	12:b:403:POV:H22	1.81	0.45
7:B:405:MQ9:H453	7:B:405:MQ9:H48	1.99	0.45
2:B:6:VAL:HG22	8:B:403:LPP:H142	1.98	0.45
2:b:365:ARG:H	12:b:403:POV:H14A	1.81	0.45
2:b:6:VAL:HG22	8:b:404:LPP:H142	1.98	0.45
2:b:110:ILE:HG22	2:b:112:GLU:H	1.82	0.45
2:B:110:ILE:HG22	2:B:112:GLU:H	1.82	0.45
2:B:138:PHE:CE2	7:B:405:MQ9:H5M2	2.52	0.44
3:h:1:MET:HE3	3:h:6:LYS:HG3	1.98	0.44
1:A:99:GLU:OE1	10:A:607:OXY:O1	2.36	0.44
5:A:601:HEM:HHA	5:A:601:HEM:HBA1	2.00	0.44
1:a:406:LEU:HD21	9:a:601:UQ8:H33	2.00	0.44
2:b:231:VAL:HG11	2:b:235:MET:HG3	1.98	0.44
7:b:401:MQ9:H321	7:b:401:MQ9:H303	1.85	0.44
12:b:403:POV:O22	12:b:403:POV:H24A	2.17	0.44
8:A:604:LPP:H443	8:A:604:LPP:C26	2.47	0.44
7:B:405:MQ9:C35	7:B:405:MQ9:C38	2.95	0.44
1:a:229:ALA:O	9:a:601:UQ8:H10A	2.18	0.44
8:a:604:LPP:H443	8:a:604:LPP:C26	2.47	0.44
5:a:606:HEM:HHA	5:a:606:HEM:HBA1	1.99	0.44
7:A:603:MQ9:H511	3:H:21:ALA:HB1	1.99	0.44
7:b:401:MQ9:C35	7:b:401:MQ9:C38	2.95	0.44
4:x:1:MET:O	4:x:2:TRP:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:99:GLU:OE1	10:a:607:OXY:O1	2.36	0.43
7:B:405:MQ9:H321	7:B:405:MQ9:H303	1.85	0.43
2:b:138:PHE:CE2	7:b:401:MQ9:H5M2	2.52	0.43
1:a:127:MET:HE2	1:a:127:MET:HB3	1.94	0.43
1:A:18:TYR:CD2	1:A:69:THR:HG21	2.54	0.43
9:a:601:UQ8:H45	9:a:601:UQ8:H31A	1.99	0.43
1:a:18:TYR:CD2	1:a:69:THR:HG21	2.54	0.43
2:b:273:VAL:O	2:b:273:VAL:HG12	2.19	0.43
5:a:603:HEM:HHC	5:a:603:HEM:CBB	2.45	0.43
1:A:142:LEU:O	1:A:146:VAL:HG23	2.19	0.43
1:a:228:MET:CE	9:a:601:UQ8:H25A	2.49	0.43
2:B:25:THR:CG2	12:B:404:POV:H21D	2.49	0.42
4:X:1:MET:O	4:X:2:TRP:HB2	2.19	0.42
2:B:273:VAL:HG12	2:B:273:VAL:O	2.19	0.42
1:A:127:MET:HE2	1:A:127:MET:HB3	1.94	0.42
2:B:191:ARG:CD	12:B:404:POV:H22A	2.50	0.42
1:a:142:LEU:O	1:a:146:VAL:HG23	2.19	0.42
2:b:25:THR:CG2	12:b:403:POV:H21D	2.50	0.42
12:B:404:POV:O22	12:B:404:POV:H3A	2.19	0.42
2:b:191:ARG:CD	12:b:403:POV:H22A	2.50	0.42
4:x:24:LEU:O	4:x:28:GLU:HG3	2.20	0.42
1:A:409:TRP:CD1	9:A:606:UQ8:H40B	2.55	0.41
7:a:602:MQ9:H511	3:h:21:ALA:HB1	2.02	0.41
1:A:430:ILE:O	1:A:433:PRO:HD2	2.21	0.41
3:h:18:LEU:O	3:h:22:VAL:HG23	2.21	0.41
9:A:606:UQ8:H30A	9:A:606:UQ8:C45	2.49	0.41
1:a:430:ILE:O	1:a:433:PRO:HD2	2.21	0.41
1:A:405:ALA:C	9:A:606:UQ8:H45A	2.46	0.41
2:b:363:PHE:CE2	12:b:403:POV:H3A	2.56	0.41
1:a:236:VAL:HG21	9:a:601:UQ8:H16	2.02	0.41
1:a:409:TRP:CE3	9:a:601:UQ8:H46B	2.56	0.41
5:a:603:HEM:HBC2	5:a:603:HEM:CHD	2.38	0.41
2:b:268:ILE:HD11	12:b:402:POV:H21C	2.03	0.41
2:B:100:ARG:HB2	2:B:101:PRO:HD3	2.03	0.41
2:B:268:ILE:HD11	12:B:402:POV:H21C	2.03	0.41
1:a:406:LEU:HD22	9:a:601:UQ8:H40B	2.03	0.41
3:H:1:MET:HE3	3:H:6:LYS:HG3	2.02	0.41
2:b:86:PHE:O	2:b:90:MET:HG2	2.21	0.41
3:H:1:MET:HE3	3:H:1:MET:HB3	1.93	0.40
1:a:184:PHE:O	1:a:188:VAL:HG22	2.21	0.40
2:b:368:LYS:O	2:b:372:GLU:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:90:MET:HE1	7:b:401:MQ9:H201	2.03	0.40
5:A:605:HEM:HHA	5:A:605:HEM:CBA	2.48	0.40
1:a:232:LEU:HB3	9:a:601:UQ8:H16A	2.03	0.40
2:B:90:MET:HE1	7:B:405:MQ9:H201	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	511/522 (98%)	509 (100%)	2 (0%)	0	100	100
1	a	511/522 (98%)	508 (99%)	3 (1%)	0	100	100
2	B	377/379 (100%)	373 (99%)	4 (1%)	0	100	100
2	b	377/379 (100%)	373 (99%)	4 (1%)	0	100	100
3	H	27/29 (93%)	27 (100%)	0	0	100	100
3	h	27/29 (93%)	27 (100%)	0	0	100	100
4	X	28/37 (76%)	27 (96%)	1 (4%)	0	100	100
4	x	28/37 (76%)	27 (96%)	1 (4%)	0	100	100
All	All	1886/1934 (98%)	1871 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	418/426 (98%)	417 (100%)	1 (0%)	87	92
1	a	418/426 (98%)	417 (100%)	1 (0%)	87	92
2	B	313/313 (100%)	312 (100%)	1 (0%)	86	90
2	b	313/313 (100%)	312 (100%)	1 (0%)	86	90
3	H	24/24 (100%)	24 (100%)	0	100	100
3	h	24/24 (100%)	24 (100%)	0	100	100
4	X	23/28 (82%)	23 (100%)	0	100	100
4	x	23/28 (82%)	23 (100%)	0	100	100
All	All	1556/1582 (98%)	1552 (100%)	4 (0%)	84	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	363	ASN
2	B	155	LEU
1	a	363	ASN
2	b	155	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	56	HIS
2	B	143	GLN
2	B	163	GLN
2	B	205	GLN
1	a	330	GLN
2	b	56	HIS
2	b	143	GLN
2	b	163	GLN
2	b	205	GLN
3	h	29	HIS

5.3.3 RNA ⓘ

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](#)

28 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$
6	A1JN4	A	602	1	46,52,52	2.90	17 (36%)	62,89,89	4.58	38 (61%)
9	UQ8	a	601	-	53,53,53	0.64	2 (3%)	64,67,67	0.76	1 (1%)
5	HEM	a	603	1	50,50,50	1.50	9 (18%)	66,82,82	1.43	9 (13%)
8	LPP	a	604	-	43,43,43	1.07	2 (4%)	47,48,48	1.11	2 (4%)
12	POV	b	402	-	51,51,51	1.08	3 (5%)	57,59,59	1.12	3 (5%)
7	MQ9	B	405	-	59,59,59	0.32	0	72,75,75	0.72	3 (4%)
12	POV	b	403	-	51,51,51	1.08	3 (5%)	57,59,59	1.17	3 (5%)
8	LPP	B	403	-	43,43,43	1.10	2 (4%)	47,48,48	1.05	2 (4%)
10	OXY	a	607	-	1,1,1	0.16	0	-	-	-
8	LPP	b	404	-	43,43,43	1.09	2 (4%)	47,48,48	1.05	2 (4%)
11	PGT	X	101	-	50,50,50	1.12	4 (8%)	53,56,56	1.06	2 (3%)
11	PGT	A	608	-	50,50,50	1.10	4 (8%)	53,56,56	1.05	2 (3%)
7	MQ9	b	401	-	59,59,59	0.33	0	72,75,75	0.71	2 (2%)
12	POV	B	404	-	51,51,51	1.08	3 (5%)	57,59,59	1.17	3 (5%)
9	UQ8	A	606	-	53,53,53	0.68	2 (3%)	64,67,67	0.56	0
6	A1JN4	a	605	1	46,52,52	2.91	16 (34%)	62,89,89	4.56	35 (56%)
8	LPP	A	604	-	43,43,43	1.06	2 (4%)	47,48,48	1.11	2 (4%)
5	HEM	a	606	1	50,50,50	1.51	8 (16%)	66,82,82	1.48	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	PGT	a	608	-	50,50,50	1.10	4 (8%)	53,56,56	1.05	2 (3%)
8	LPP	b	405	-	43,43,43	1.09	2 (4%)	47,48,48	1.12	2 (4%)
11	PGT	x	101	-	50,50,50	1.11	4 (8%)	53,56,56	1.08	2 (3%)
5	HEM	A	605	1	50,50,50	1.54	9 (18%)	66,82,82	1.52	11 (16%)
10	OXY	A	607	-	1,1,1	0.16	0	-		
7	MQ9	a	602	-	59,59,59	0.33	0	72,75,75	0.64	1 (1%)
8	LPP	B	401	-	43,43,43	1.09	2 (4%)	47,48,48	1.12	2 (4%)
5	HEM	A	601	1	50,50,50	1.51	8 (16%)	66,82,82	1.47	8 (12%)
7	MQ9	A	603	-	59,59,59	0.33	0	72,75,75	0.63	1 (1%)
12	POV	B	402	-	51,51,51	1.08	3 (5%)	57,59,59	1.11	3 (5%)

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
6	A1JN4	A	602	1	1/1/12/12	5/9/89/89	0/1/9/9
9	UQ8	a	601	-	-	18/51/75/75	0/1/1/1
5	HEM	a	603	1	-	6/14/54/54	-
8	LPP	a	604	-	-	21/45/45/45	-
12	POV	b	402	-	-	26/55/55/55	-
7	MQ9	B	405	-	-	18/53/73/73	0/2/2/2
12	POV	b	403	-	-	32/55/55/55	-
8	LPP	B	403	-	-	19/45/45/45	-
8	LPP	b	404	-	-	19/45/45/45	-
11	PGT	X	101	-	-	29/55/55/55	-
11	PGT	A	608	-	-	18/55/55/55	-
7	MQ9	b	401	-	-	18/53/73/73	0/2/2/2
12	POV	B	404	-	-	32/55/55/55	-
9	UQ8	A	606	-	-	12/51/75/75	0/1/1/1
6	A1JN4	a	605	1	1/1/12/12	4/9/89/89	0/1/9/9
8	LPP	A	604	-	-	21/45/45/45	-
5	HEM	a	606	1	-	3/14/54/54	-
11	PGT	a	608	-	-	18/55/55/55	-
8	LPP	b	405	-	-	23/45/45/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PGT	x	101	-	-	25/55/55/55	-
5	HEM	A	605	1	-	6/14/54/54	-
7	MQ9	a	602	-	-	10/53/73/73	0/2/2/2
8	LPP	B	401	-	-	23/45/45/45	-
5	HEM	A	601	1	-	3/14/54/54	-
7	MQ9	A	603	-	-	10/53/73/73	0/2/2/2
12	POV	B	402	-	-	26/55/55/55	-

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	a	605	A1JN4	C3D-C2D	-11.62	1.26	1.55
6	A	602	A1JN4	C3D-C2D	-11.59	1.26	1.55
6	a	605	A1JN4	O1D-C3D	6.61	1.57	1.46
6	A	602	A1JN4	O1D-C3D	6.56	1.57	1.46
6	A	602	A1JN4	CBB-CAB	-5.73	1.25	1.51
6	a	605	A1JN4	CBB-CAB	-5.70	1.26	1.51
6	a	605	A1JN4	CBC-CAC	-5.56	1.26	1.51
6	A	602	A1JN4	CBC-CAC	-5.54	1.26	1.51
5	A	601	HEM	FE-NA	4.59	2.10	1.95
5	a	606	HEM	FE-NA	4.57	2.10	1.95
6	a	605	A1JN4	OND-C2D	4.50	1.51	1.42
6	A	602	A1JN4	OND-C2D	4.47	1.51	1.42
5	A	605	HEM	FE-NB	4.25	2.08	1.94
5	a	603	HEM	FE-NB	4.20	2.07	1.94
5	A	605	HEM	FE-NA	4.14	2.09	1.95
5	a	603	HEM	FE-NA	4.06	2.08	1.95
6	a	605	A1JN4	CBD-CGD	-3.61	1.42	1.50
6	a	605	A1JN4	CAD-C3D	3.58	1.60	1.53
6	A	602	A1JN4	CBD-CGD	-3.54	1.42	1.50
6	a	605	A1JN4	O1D-CGD	-3.54	1.30	1.35
6	A	602	A1JN4	CAD-C3D	3.51	1.59	1.53
5	A	605	HEM	FE-NC	3.48	2.06	1.95
5	A	601	HEM	FE-ND	3.47	2.05	1.94
5	a	606	HEM	FE-ND	3.47	2.05	1.94
6	A	602	A1JN4	O1D-CGD	-3.42	1.30	1.35
5	a	606	HEM	FE-NC	3.40	2.06	1.95
5	A	601	HEM	FE-NC	3.37	2.06	1.95
8	B	403	LPP	O27-C29	3.33	1.43	1.33
5	a	603	HEM	FE-NC	3.30	2.06	1.95
8	b	404	LPP	O27-C29	3.29	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	608	PGT	O3-C11	3.24	1.42	1.33
11	A	608	PGT	O3-C11	3.22	1.42	1.33
11	x	101	PGT	O3-C11	3.22	1.42	1.33
8	B	401	LPP	O27-C29	3.22	1.42	1.33
8	b	405	LPP	O27-C29	3.22	1.42	1.33
11	X	101	PGT	O3-C11	3.21	1.42	1.33
8	b	405	LPP	O9-C11	3.09	1.43	1.34
8	a	604	LPP	O9-C11	3.04	1.42	1.34
8	B	401	LPP	O9-C11	3.03	1.42	1.34
8	A	604	LPP	O9-C11	3.02	1.42	1.34
8	A	604	LPP	O27-C29	2.98	1.42	1.33
8	a	604	LPP	O27-C29	2.98	1.42	1.33
8	B	403	LPP	O9-C11	2.98	1.42	1.34
8	b	404	LPP	O9-C11	2.94	1.42	1.34
6	A	602	A1JN4	C1B-NB	-2.93	1.34	1.39
6	a	605	A1JN4	C1B-NB	-2.92	1.34	1.39
9	A	606	UQ8	C3-C2	-2.92	1.40	1.48
5	A	601	HEM	FE-NB	2.92	2.03	1.94
5	a	606	HEM	FE-NB	2.92	2.03	1.94
5	a	603	HEM	FE-ND	2.88	2.03	1.94
12	b	403	POV	O31-C31	2.88	1.41	1.33
12	B	404	POV	O31-C31	2.86	1.41	1.33
12	b	402	POV	O31-C31	2.84	1.41	1.33
12	B	402	POV	O31-C31	2.83	1.41	1.33
11	A	608	PGT	O2-C31	2.81	1.42	1.34
11	a	608	PGT	O2-C31	2.80	1.42	1.34
5	A	601	HEM	CAC-C3C	2.78	1.55	1.47
11	X	101	PGT	O2-C2	-2.78	1.39	1.46
11	x	101	PGT	O2-C2	-2.77	1.39	1.46
11	X	101	PGT	O2-C31	2.77	1.42	1.34
5	a	606	HEM	CAC-C3C	2.77	1.55	1.47
11	x	101	PGT	O2-C31	2.77	1.42	1.34
11	A	608	PGT	O2-C2	-2.71	1.39	1.46
11	a	608	PGT	O2-C2	-2.71	1.39	1.46
5	A	601	HEM	CAB-C3B	2.70	1.54	1.47
12	B	404	POV	O21-C21	2.70	1.41	1.34
12	B	402	POV	O21-C21	2.70	1.41	1.34
12	b	403	POV	O21-C21	2.69	1.41	1.34
5	a	606	HEM	CAB-C3B	2.68	1.54	1.47
12	b	402	POV	O21-C21	2.67	1.41	1.34
9	a	601	UQ8	C3-C2	-2.63	1.41	1.48
5	A	605	HEM	FE-ND	2.62	2.02	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	606	UQ8	C4-C5	-2.59	1.41	1.48
5	a	603	HEM	CAB-C3B	2.58	1.54	1.47
5	A	605	HEM	CAB-C3B	2.55	1.54	1.47
6	a	605	A1JN4	CMB-C2B	2.50	1.56	1.50
6	A	602	A1JN4	CMC-C2C	2.49	1.56	1.50
12	B	402	POV	O21-C2	-2.49	1.40	1.46
6	A	602	A1JN4	CBA-CAA	2.48	1.59	1.52
12	b	402	POV	O21-C2	-2.46	1.40	1.46
6	a	605	A1JN4	CBA-CAA	2.45	1.59	1.52
6	A	602	A1JN4	CMB-C2B	2.44	1.56	1.50
5	A	605	HEM	CAC-C3C	2.41	1.54	1.47
6	a	605	A1JN4	CMC-C2C	2.41	1.55	1.50
5	a	603	HEM	CAC-C3C	2.40	1.54	1.47
9	a	601	UQ8	C4-C5	-2.37	1.42	1.48
12	b	403	POV	O21-C2	-2.35	1.40	1.46
12	B	404	POV	O21-C2	-2.35	1.40	1.46
6	a	605	A1JN4	C4A-C3A	2.33	1.48	1.43
6	A	602	A1JN4	C4A-C3A	2.31	1.48	1.43
6	a	605	A1JN4	C4C-NC	-2.23	1.35	1.39
5	A	605	HEM	C2A-C3A	-2.23	1.32	1.38
5	A	605	HEM	C3B-C2B	-2.22	1.32	1.37
6	A	602	A1JN4	C4C-NC	-2.20	1.35	1.39
6	a	605	A1JN4	C2A-C3A	-2.20	1.33	1.38
11	X	101	PGT	P-O3P	2.19	1.68	1.59
5	A	605	HEM	C3C-C2C	-2.19	1.32	1.37
11	x	101	PGT	P-O3P	2.18	1.68	1.59
6	a	605	A1JN4	CBA-CGA	2.15	1.55	1.50
5	a	606	HEM	CMC-C2C	2.15	1.55	1.50
6	A	602	A1JN4	CBA-CGA	2.15	1.55	1.50
5	a	603	HEM	C3B-C2B	-2.14	1.32	1.37
5	a	603	HEM	C3C-C2C	-2.14	1.32	1.37
11	a	608	PGT	P-O3P	2.13	1.67	1.59
6	A	602	A1JN4	C2A-C3A	-2.13	1.33	1.38
11	A	608	PGT	P-O3P	2.12	1.67	1.59
5	A	601	HEM	CMC-C2C	2.08	1.55	1.50
6	A	602	A1JN4	CMD-C2D	2.07	1.56	1.53
5	A	601	HEM	CMB-C2B	2.07	1.55	1.50
5	a	606	HEM	CMB-C2B	2.07	1.55	1.50
5	a	603	HEM	C2A-C3A	-2.01	1.33	1.38

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	a	605	A1JN4	O1D-C3D-C4D	-13.33	81.17	108.25
6	A	602	A1JN4	O1D-C3D-C4D	-13.13	81.58	108.25
6	A	602	A1JN4	C3B-C4B-NB	-10.28	100.32	110.32
6	a	605	A1JN4	C3B-C4B-NB	-10.26	100.34	110.32
6	a	605	A1JN4	CHD-C1D-ND	9.87	138.67	124.20
6	A	602	A1JN4	CHD-C1D-ND	9.86	138.66	124.20
6	A	602	A1JN4	O1D-C3D-CAD	-9.28	85.56	103.01
6	A	602	A1JN4	C4B-NB-C1B	8.96	114.12	105.35
6	a	605	A1JN4	O1D-C3D-CAD	-8.92	86.23	103.01
6	a	605	A1JN4	C4B-NB-C1B	8.89	114.06	105.35
6	a	605	A1JN4	C4C-NC-C1C	8.65	113.82	105.35
6	A	602	A1JN4	C4C-NC-C1C	8.42	113.59	105.35
6	a	605	A1JN4	CHC-C4B-NB	7.24	132.27	124.44
6	A	602	A1JN4	CHC-C4B-NB	7.03	132.04	124.44
6	A	602	A1JN4	C4B-C3B-C2B	6.74	115.91	107.13
6	a	605	A1JN4	C4B-C3B-C2B	6.74	115.91	107.13
6	a	605	A1JN4	C3C-C4C-NC	-6.63	102.74	110.15
6	A	602	A1JN4	C2A-C1A-NA	-6.50	102.88	110.15
6	A	602	A1JN4	CAC-C3C-C4C	-6.50	115.89	124.92
6	A	602	A1JN4	C3C-C4C-NC	-6.47	102.91	110.15
6	a	605	A1JN4	C2A-C1A-NA	-6.40	102.99	110.15
6	A	602	A1JN4	CAB-C3B-C4B	-6.39	114.61	124.68
6	A	602	A1JN4	OND-C2D-CMD	-6.39	97.82	109.59
6	a	605	A1JN4	CAC-C3C-C4C	-6.29	116.19	124.92
6	a	605	A1JN4	OND-C2D-CMD	-6.25	98.09	109.59
6	A	602	A1JN4	C4A-NA-C1A	5.89	111.11	105.35
6	a	605	A1JN4	CAB-C3B-C4B	-5.88	115.42	124.68
6	a	605	A1JN4	C4A-NA-C1A	5.74	110.97	105.35
6	a	605	A1JN4	CHB-C1B-NB	5.53	130.42	124.44
6	A	602	A1JN4	CHB-C1B-NB	5.53	130.42	124.44
6	A	602	A1JN4	C1A-C2A-C3A	5.23	115.13	106.89
6	a	605	A1JN4	C1A-C2A-C3A	5.15	115.00	106.89
6	a	605	A1JN4	O1D-CGD-CBD	-4.98	105.17	110.19
6	A	602	A1JN4	O1D-CGD-CBD	-4.96	105.19	110.19
6	a	605	A1JN4	O1A-CGA-CBA	-4.94	107.20	123.08
6	A	602	A1JN4	O1A-CGA-CBA	-4.91	107.30	123.08
6	a	605	A1JN4	C2D-C1D-CHD	-4.74	116.45	124.28
6	A	602	A1JN4	C2D-C1D-CHD	-4.74	116.45	124.28
11	X	101	PGT	O2-C31-C32	4.61	121.44	111.50
11	x	101	PGT	O2-C31-C32	4.55	121.32	111.50
6	a	605	A1JN4	O2A-CGA-O1A	4.40	134.27	123.30
6	a	605	A1JN4	CHD-C4C-NC	4.39	131.93	123.85
6	A	602	A1JN4	O2A-CGA-O1A	4.37	134.18	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	602	A1JN4	CHD-C4C-NC	4.29	131.75	123.85
6	a	605	A1JN4	CHA-C4D-ND	-4.23	118.00	124.20
12	b	402	POV	O21-C21-C22	4.21	120.58	111.50
6	A	602	A1JN4	CHA-C4D-ND	-4.21	118.03	124.20
12	B	402	POV	O21-C21-C22	4.18	120.52	111.50
12	b	403	POV	O21-C21-C22	4.08	120.30	111.50
12	B	404	POV	O21-C21-C22	4.08	120.29	111.50
6	A	602	A1JN4	C4A-C3A-C2A	-4.00	102.15	106.83
11	A	608	PGT	O2-C31-C32	3.93	119.98	111.50
11	a	608	PGT	O2-C31-C32	3.92	119.95	111.50
8	A	604	LPP	O9-C11-C12	3.90	119.90	111.50
8	B	401	LPP	O9-C11-C12	3.89	119.89	111.50
8	a	604	LPP	O9-C11-C12	3.88	119.86	111.50
8	b	405	LPP	O9-C11-C12	3.86	119.83	111.50
6	a	605	A1JN4	C4A-C3A-C2A	-3.85	102.32	106.83
12	b	402	POV	C28-C29-C210	3.75	153.47	124.73
12	B	402	POV	C28-C29-C210	3.74	153.45	124.73
5	a	606	HEM	C4A-NA-C1A	3.73	109.00	105.35
6	a	605	A1JN4	C3D-C4D-CHA	3.71	135.36	124.34
6	A	602	A1JN4	C3D-C4D-CHA	3.70	135.32	124.34
5	A	601	HEM	C4A-NA-C1A	3.70	108.97	105.35
5	a	606	HEM	C4D-ND-C1D	3.60	108.80	105.07
12	B	404	POV	C28-C29-C210	3.59	152.26	124.73
12	b	403	POV	C28-C29-C210	3.58	152.23	124.73
5	A	601	HEM	C4D-ND-C1D	3.58	108.77	105.07
9	a	601	UQ8	C7-C6-C5	3.54	122.74	118.48
6	A	602	A1JN4	C1B-C2B-C3B	-3.49	101.85	106.94
6	A	602	A1JN4	CAC-C3C-C2C	3.47	132.42	126.86
5	A	605	HEM	CAA-C2A-C1A	3.43	131.64	124.89
6	a	605	A1JN4	C1B-C2B-C3B	-3.41	101.96	106.94
8	B	403	LPP	O9-C11-C12	3.40	118.84	111.50
8	b	404	LPP	O9-C11-C12	3.40	118.82	111.50
5	a	603	HEM	C4D-ND-C1D	3.39	108.58	105.07
6	a	605	A1JN4	CAC-C3C-C2C	3.30	132.15	126.86
5	A	605	HEM	C4D-ND-C1D	3.29	108.47	105.07
5	a	606	HEM	C4C-NC-C1C	3.14	108.42	105.35
5	A	601	HEM	C4C-NC-C1C	3.13	108.42	105.35
5	a	603	HEM	C4C-NC-C1C	3.11	108.40	105.35
5	A	605	HEM	C4C-NC-C1C	3.11	108.40	105.35
6	a	605	A1JN4	CAA-CBA-CGA	-3.09	106.95	113.60
5	A	601	HEM	C1B-NB-C4B	3.08	108.25	105.07
6	A	602	A1JN4	CBB-CAB-C3B	3.06	120.88	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	a	606	HEM	C1B-NB-C4B	3.05	108.22	105.07
6	A	602	A1JN4	C4C-C3C-C2C	3.05	111.68	106.89
6	a	605	A1JN4	C4C-C3C-C2C	3.03	111.66	106.89
6	a	605	A1JN4	CBB-CAB-C3B	2.97	120.63	112.43
6	A	602	A1JN4	CAA-CBA-CGA	-2.96	107.23	113.60
5	a	603	HEM	C1B-NB-C4B	2.95	108.12	105.07
5	A	605	HEM	CAA-C2A-C3A	-2.86	120.51	127.07
5	A	601	HEM	C3D-C4D-ND	-2.85	106.99	110.17
5	a	606	HEM	C3D-C4D-ND	-2.85	106.99	110.17
6	A	602	A1JN4	CAA-C2A-C1A	-2.84	119.30	124.89
6	a	605	A1JN4	C1C-CHC-C4B	-2.83	116.00	124.74
12	b	403	POV	O31-C31-C32	2.80	120.69	111.91
12	B	404	POV	O31-C31-C32	2.79	120.67	111.91
5	A	605	HEM	C4A-NA-C1A	2.78	108.07	105.35
8	b	404	LPP	O27-C29-C30	2.75	120.52	111.91
6	A	602	A1JN4	C1C-CHC-C4B	-2.74	116.26	124.74
8	B	403	LPP	O27-C29-C30	2.73	120.47	111.91
6	a	605	A1JN4	CHC-C1C-NC	2.72	128.86	123.85
5	A	605	HEM	C1B-NB-C4B	2.71	107.87	105.07
5	A	601	HEM	C2A-C1A-NA	-2.70	107.13	110.15
6	a	605	A1JN4	CAA-C2A-C1A	-2.69	119.59	124.89
5	a	606	HEM	C2A-C1A-NA	-2.68	107.15	110.15
11	A	608	PGT	O3-C11-C12	2.66	120.25	111.91
6	a	605	A1JN4	OND-C2D-C3D	-2.66	103.84	110.45
11	a	608	PGT	O3-C11-C12	2.65	120.21	111.91
6	A	602	A1JN4	OND-C2D-C3D	-2.56	104.09	110.45
11	x	101	PGT	O3-C11-C12	2.55	119.91	111.91
8	a	604	LPP	O27-C29-C30	2.53	119.85	111.91
11	X	101	PGT	O3-C11-C12	2.52	119.83	111.91
8	A	604	LPP	O27-C29-C30	2.51	119.80	111.91
5	A	605	HEM	C2A-C1A-NA	-2.51	107.34	110.15
6	A	602	A1JN4	CHC-C1C-NC	2.49	128.42	123.85
5	a	606	HEM	CAA-C2A-C1A	2.46	129.72	124.89
5	a	603	HEM	C4A-NA-C1A	2.45	107.75	105.35
8	b	405	LPP	O27-C29-C30	2.45	119.59	111.91
8	B	401	LPP	O27-C29-C30	2.45	119.58	111.91
6	a	605	A1JN4	C2C-C1C-NC	-2.44	106.36	110.08
5	A	601	HEM	CAA-C2A-C1A	2.44	129.69	124.89
7	a	602	MQ9	C7-C6-C1	-2.39	115.94	118.50
5	A	605	HEM	C3D-C4D-ND	-2.38	107.51	110.17
5	A	605	HEM	CHA-C4D-ND	2.38	127.30	124.37
6	A	602	A1JN4	CHA-C1A-C2A	2.35	130.50	125.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	b	401	MQ9	C8-C7-C6	-2.33	105.77	112.05
5	a	603	HEM	C3D-C4D-ND	-2.32	107.59	110.17
6	A	602	A1JN4	C2C-C1C-NC	-2.32	106.55	110.08
7	B	405	MQ9	C8-C7-C6	-2.32	105.80	112.05
12	B	402	POV	O31-C31-C32	2.31	119.16	111.91
12	b	402	POV	O31-C31-C32	2.31	119.15	111.91
7	A	603	MQ9	C7-C6-C1	-2.30	116.04	118.50
6	a	605	A1JN4	CHA-C1A-C2A	2.30	130.38	125.36
5	a	603	HEM	CHA-C4D-ND	2.26	127.17	124.37
5	A	601	HEM	CHC-C4B-NB	2.26	126.87	124.42
5	a	606	HEM	CHC-C4B-NB	2.19	126.80	124.42
7	B	405	MQ9	C7-C6-C1	-2.18	116.16	118.50
5	A	605	HEM	C2D-C1D-ND	-2.16	107.29	109.88
5	a	603	HEM	C2D-C1D-ND	-2.16	107.30	109.88
7	b	401	MQ9	C7-C6-C1	-2.15	116.20	118.50
5	a	603	HEM	C4C-C3C-C2C	2.13	108.50	106.75
5	A	605	HEM	C4C-C3C-C2C	2.12	108.49	106.75
7	B	405	MQ9	C41-C39-C38	2.05	125.26	121.12
6	A	602	A1JN4	CBA-CAA-C2A	-2.04	106.96	112.63
6	A	602	A1JN4	CBC-CAC-C3C	2.03	118.02	112.43
6	A	602	A1JN4	CMA-C3A-C2A	2.01	129.97	125.61
5	a	603	HEM	C4B-C3B-C2B	2.01	108.71	107.11

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	602	A1JN4	NB
6	a	605	A1JN4	NB

All (445) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	HEM	C1A-C2A-CAA-CBA
5	A	601	HEM	C3A-C2A-CAA-CBA
5	a	606	HEM	C1A-C2A-CAA-CBA
5	a	606	HEM	C3A-C2A-CAA-CBA
7	A	603	MQ9	C29-C31-C32-C33
7	A	603	MQ9	C34-C36-C37-C38
7	B	405	MQ9	C23-C24-C26-C27
7	B	405	MQ9	C25-C24-C26-C27
7	a	602	MQ9	C29-C31-C32-C33
7	a	602	MQ9	C34-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
7	b	401	MQ9	C23-C24-C26-C27
7	b	401	MQ9	C25-C24-C26-C27
8	B	401	LPP	C12-C11-O9-C7
8	B	403	LPP	C6-O5-P1-O2
8	B	403	LPP	C6-O5-P1-O3
8	B	403	LPP	C6-O5-P1-O4
8	b	404	LPP	C6-O5-P1-O2
8	b	404	LPP	C6-O5-P1-O3
8	b	404	LPP	C6-O5-P1-O4
8	b	405	LPP	C12-C11-O9-C7
9	A	606	UQ8	C42-C43-C44-C45
9	A	606	UQ8	C37-C38-C39-C40
9	A	606	UQ8	C29-C31-C32-C33
9	A	606	UQ8	C1-C6-C7-C8
9	A	606	UQ8	C5-C6-C7-C8
9	a	601	UQ8	C42-C43-C44-C46
9	a	601	UQ8	C22-C23-C24-C26
9	a	601	UQ8	C22-C23-C24-C25
9	a	601	UQ8	C12-C13-C14-C16
9	a	601	UQ8	C1-C6-C7-C8
9	a	601	UQ8	C5-C6-C7-C8
11	A	608	PGT	O31-C31-O2-C2
11	A	608	PGT	C4-O4P-P-O1P
11	X	101	PGT	O31-C31-O2-C2
11	X	101	PGT	O2-C2-C3-O3
11	a	608	PGT	O31-C31-O2-C2
11	a	608	PGT	C4-O4P-P-O1P
11	x	101	PGT	O31-C31-O2-C2
11	x	101	PGT	O2-C2-C3-O3
12	B	402	POV	C11-O12-P-O13
12	B	402	POV	C11-O12-P-O14
12	B	402	POV	O22-C21-O21-C2
12	B	404	POV	C1-O11-P-O13
12	B	404	POV	C1-O11-P-O14
12	B	404	POV	C12-C11-O12-P
12	B	404	POV	C32-C31-O31-C3
12	b	402	POV	C11-O12-P-O13
12	b	402	POV	C11-O12-P-O14
12	b	402	POV	O22-C21-O21-C2
12	b	403	POV	C1-O11-P-O13
12	b	403	POV	C1-O11-P-O14
6	A	602	A1JN4	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
6	a	605	A1JN4	C4C-C3C-CAC-CBC
8	A	604	LPP	O28-C29-O27-C8
8	a	604	LPP	O28-C29-O27-C8
12	B	404	POV	O32-C31-O31-C3
12	b	403	POV	O32-C31-O31-C3
6	A	602	A1JN4	C2C-C3C-CAC-CBC
6	a	605	A1JN4	C2C-C3C-CAC-CBC
12	b	403	POV	C32-C31-O31-C3
9	a	601	UQ8	C42-C43-C44-C45
8	B	401	LPP	O28-C29-O27-C8
8	b	405	LPP	O28-C29-O27-C8
8	A	604	LPP	O10-C11-O9-C7
8	B	401	LPP	O10-C11-O9-C7
8	a	604	LPP	O10-C11-O9-C7
8	b	405	LPP	O10-C11-O9-C7
8	A	604	LPP	C30-C29-O27-C8
8	a	604	LPP	C30-C29-O27-C8
8	A	604	LPP	C12-C11-O9-C7
8	a	604	LPP	C12-C11-O9-C7
11	A	608	PGT	C32-C31-O2-C2
11	X	101	PGT	C32-C31-O2-C2
11	a	608	PGT	C32-C31-O2-C2
11	x	101	PGT	C32-C31-O2-C2
12	B	402	POV	C22-C21-O21-C2
12	b	402	POV	C22-C21-O21-C2
9	A	606	UQ8	C42-C43-C44-C46
7	A	603	MQ9	C12-C11-C9-C10
8	B	401	LPP	C30-C29-O27-C8
8	b	405	LPP	C30-C29-O27-C8
9	A	606	UQ8	C7-C8-C9-C10
9	a	601	UQ8	C32-C33-C34-C35
9	a	601	UQ8	C12-C13-C14-C15
9	a	601	UQ8	C7-C8-C9-C10
9	A	606	UQ8	C37-C38-C39-C41
9	A	606	UQ8	C7-C8-C9-C11
9	a	601	UQ8	C32-C33-C34-C36
9	a	601	UQ8	C7-C8-C9-C11
5	A	605	HEM	C1A-C2A-CAA-CBA
8	B	401	LPP	C7-C6-O5-P1
8	b	405	LPP	C7-C6-O5-P1
7	a	602	MQ9	C12-C11-C9-C10
7	A	603	MQ9	C12-C11-C9-C8

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Mol	Chain	Res	Type	Atoms
7	a	602	MQ9	C12-C11-C9-C8
9	a	601	UQ8	C24-C26-C27-C28
12	B	404	POV	C11-C12-N-C13
12	b	403	POV	C11-C12-N-C13
5	A	605	HEM	C3A-C2A-CAA-CBA
12	B	402	POV	C21-C22-C23-C24
12	b	402	POV	C21-C22-C23-C24
12	B	404	POV	C31-C32-C33-C34
12	b	403	POV	C31-C32-C33-C34
6	A	602	A1JN4	C2B-C3B-CAB-CBB
7	A	603	MQ9	C9-C11-C12-C13
7	A	603	MQ9	C19-C21-C22-C23
7	A	603	MQ9	C24-C26-C27-C28
7	B	405	MQ9	C14-C16-C17-C18
7	a	602	MQ9	C9-C11-C12-C13
7	a	602	MQ9	C19-C21-C22-C23
7	a	602	MQ9	C24-C26-C27-C28
7	b	401	MQ9	C14-C16-C17-C18
11	A	608	PGT	C4-O4P-P-O3P
11	X	101	PGT	C1-O3P-P-O4P
11	a	608	PGT	C4-O4P-P-O3P
11	x	101	PGT	C1-O3P-P-O4P
12	B	402	POV	C1-O11-P-O12
12	B	402	POV	C11-O12-P-O11
12	B	404	POV	C1-O11-P-O12
12	b	402	POV	C1-O11-P-O12
12	b	402	POV	C11-O12-P-O11
12	b	403	POV	C1-O11-P-O12
8	A	604	LPP	C29-C30-C31-C32
8	a	604	LPP	C29-C30-C31-C32
11	A	608	PGT	C31-C32-C33-C34
11	a	608	PGT	C31-C32-C33-C34
12	B	404	POV	C11-C12-N-C14
12	B	404	POV	C11-C12-N-C15
12	b	403	POV	C11-C12-N-C14
12	b	403	POV	C11-C12-N-C15
8	B	401	LPP	C34-C35-C36-C37
8	B	403	LPP	C30-C31-C32-C33
8	b	404	LPP	C30-C31-C32-C33
8	b	405	LPP	C34-C35-C36-C37
12	B	404	POV	C310-C311-C312-C313
12	b	403	POV	C310-C311-C312-C313

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Mol	Chain	Res	Type	Atoms
11	X	101	PGT	C17-C18-C19-C20
12	B	404	POV	C36-C37-C38-C39
12	b	403	POV	C36-C37-C38-C39
8	a	604	LPP	C34-C35-C36-C37
8	A	604	LPP	C34-C35-C36-C37
11	x	101	PGT	C33-C34-C35-C36
11	x	101	PGT	C17-C18-C19-C20
11	X	101	PGT	C43-C44-C45-C46
12	B	404	POV	C211-C212-C213-C214
8	B	403	LPP	C13-C14-C15-C16
8	b	404	LPP	C13-C14-C15-C16
12	B	402	POV	C33-C34-C35-C36
12	b	402	POV	C33-C34-C35-C36
12	b	403	POV	C211-C212-C213-C214
8	B	403	LPP	C12-C11-O9-C7
8	b	404	LPP	C12-C11-O9-C7
8	A	604	LPP	C39-C40-C41-C42
8	a	604	LPP	C39-C40-C41-C42
12	B	402	POV	C312-C313-C314-C315
12	B	404	POV	C213-C214-C215-C216
12	b	402	POV	C312-C313-C314-C315
12	b	403	POV	C213-C214-C215-C216
8	B	401	LPP	C37-C38-C39-C40
8	b	405	LPP	C37-C38-C39-C40
8	A	604	LPP	C31-C32-C33-C34
12	B	404	POV	C39-C310-C311-C312
12	b	403	POV	C39-C310-C311-C312
8	a	604	LPP	C31-C32-C33-C34
8	B	401	LPP	C20-C21-C22-C23
8	b	405	LPP	C20-C21-C22-C23
8	A	604	LPP	C12-C13-C14-C15
11	x	101	PGT	C43-C44-C45-C46
8	A	604	LPP	C37-C38-C39-C40
8	a	604	LPP	C12-C13-C14-C15
8	B	403	LPP	O10-C11-O9-C7
8	b	404	LPP	O10-C11-O9-C7
8	a	604	LPP	C37-C38-C39-C40
8	B	403	LPP	C15-C16-C17-C18
8	b	404	LPP	C15-C16-C17-C18
12	B	402	POV	C36-C37-C38-C39
12	b	402	POV	C36-C37-C38-C39
12	B	404	POV	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
12	b	403	POV	C33-C34-C35-C36
12	B	404	POV	C24-C25-C26-C27
12	b	403	POV	C24-C25-C26-C27
12	B	402	POV	C26-C27-C28-C29
12	b	402	POV	C26-C27-C28-C29
12	b	402	POV	C39-C310-C311-C312
12	B	402	POV	C39-C310-C311-C312
8	B	401	LPP	C30-C31-C32-C33
8	b	405	LPP	C30-C31-C32-C33
8	a	604	LPP	C16-C17-C18-C19
8	A	604	LPP	C16-C17-C18-C19
5	A	601	HEM	C4C-C3C-CAC-CBC
5	a	606	HEM	C4C-C3C-CAC-CBC
7	B	405	MQ9	C30-C29-C31-C32
11	A	608	PGT	C39-C40-C41-C42
11	a	608	PGT	C39-C40-C41-C42
12	B	402	POV	O11-C1-C2-C3
12	b	402	POV	O11-C1-C2-C3
6	A	602	A1JN4	C4B-C3B-CAB-CBB
11	A	608	PGT	C16-C17-C18-C19
7	b	401	MQ9	C30-C29-C31-C32
12	b	403	POV	C35-C36-C37-C38
12	B	404	POV	C35-C36-C37-C38
12	b	403	POV	C312-C313-C314-C315
7	B	405	MQ9	C19-C21-C22-C23
7	b	401	MQ9	C19-C21-C22-C23
11	a	608	PGT	C16-C17-C18-C19
8	A	604	LPP	C17-C18-C19-C20
8	a	604	LPP	C17-C18-C19-C20
8	b	404	LPP	C23-C24-C25-C26
8	B	403	LPP	C23-C24-C25-C26
8	b	404	LPP	C17-C18-C19-C20
11	x	101	PGT	C37-C38-C39-C40
8	B	403	LPP	C17-C18-C19-C20
8	A	604	LPP	C8-C7-O9-C11
8	a	604	LPP	C8-C7-O9-C11
8	a	604	LPP	C20-C21-C22-C23
11	A	608	PGT	C44-C45-C46-C47
11	X	101	PGT	C22-C23-C24-C25
8	A	604	LPP	C20-C21-C22-C23
12	B	404	POV	C312-C313-C314-C315
8	B	403	LPP	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
8	b	404	LPP	C11-C12-C13-C14
8	B	403	LPP	O9-C7-C8-O27
8	b	404	LPP	O9-C7-C8-O27
11	a	608	PGT	C44-C45-C46-C47
11	x	101	PGT	C16-C17-C18-C19
12	B	404	POV	C34-C35-C36-C37
12	b	403	POV	C34-C35-C36-C37
11	x	101	PGT	C22-C23-C24-C25
8	B	401	LPP	C12-C13-C14-C15
8	b	405	LPP	C12-C13-C14-C15
11	x	101	PGT	C21-C22-C23-C24
11	X	101	PGT	C21-C22-C23-C24
8	a	604	LPP	C23-C24-C25-C26
11	X	101	PGT	O3P-C1-C2-C3
11	x	101	PGT	O3P-C1-C2-C3
7	b	401	MQ9	C24-C26-C27-C28
11	x	101	PGT	C20-C21-C22-C23
8	A	604	LPP	C23-C24-C25-C26
7	B	405	MQ9	C15-C14-C16-C17
7	b	401	MQ9	C15-C14-C16-C17
7	B	405	MQ9	C13-C14-C16-C17
7	B	405	MQ9	C28-C29-C31-C32
7	b	401	MQ9	C13-C14-C16-C17
8	A	604	LPP	C30-C31-C32-C33
8	a	604	LPP	C30-C31-C32-C33
11	X	101	PGT	C13-C14-C15-C16
8	B	403	LPP	C6-C7-C8-O27
8	b	404	LPP	C6-C7-C8-O27
11	x	101	PGT	C1-C2-C3-O3
12	B	402	POV	C313-C314-C315-C316
12	b	402	POV	C313-C314-C315-C316
12	B	404	POV	C11-O12-P-O11
12	b	403	POV	C11-O12-P-O11
11	X	101	PGT	O3P-C1-C2-O2
11	x	101	PGT	O3P-C1-C2-O2
11	a	608	PGT	C13-C14-C15-C16
11	x	101	PGT	C38-C39-C40-C41
11	X	101	PGT	C2-C1-O3P-P
12	B	404	POV	C27-C28-C29-C210
12	b	403	POV	C27-C28-C29-C210
11	A	608	PGT	C13-C14-C15-C16
12	b	403	POV	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
11	X	101	PGT	C16-C17-C18-C19
11	x	101	PGT	C39-C40-C41-C42
9	A	606	UQ8	C17-C18-C19-C20
8	b	404	LPP	C34-C35-C36-C37
8	B	403	LPP	C34-C35-C36-C37
8	A	604	LPP	C7-C6-O5-P1
8	a	604	LPP	C7-C6-O5-P1
11	X	101	PGT	C1-C2-C3-O3
11	x	101	PGT	C42-C43-C44-C45
12	B	404	POV	O11-C1-C2-O21
5	A	605	HEM	C4B-C3B-CAB-CBB
5	A	605	HEM	C4C-C3C-CAC-CBC
5	a	603	HEM	C4C-C3C-CAC-CBC
11	X	101	PGT	C12-C13-C14-C15
11	A	608	PGT	C12-C13-C14-C15
12	B	404	POV	O21-C2-C3-O31
11	a	608	PGT	C12-C13-C14-C15
7	b	401	MQ9	C28-C29-C31-C32
11	X	101	PGT	C36-C37-C38-C39
8	B	401	LPP	C32-C33-C34-C35
8	b	405	LPP	C32-C33-C34-C35
8	B	403	LPP	C38-C39-C40-C41
8	b	404	LPP	C38-C39-C40-C41
11	x	101	PGT	C2-C1-O3P-P
7	A	603	MQ9	C6-C7-C8-C9
7	a	602	MQ9	C6-C7-C8-C9
9	a	601	UQ8	C6-C7-C8-C9
11	X	101	PGT	C1-O3P-P-O1P
11	X	101	PGT	C1-O3P-P-O2P
11	x	101	PGT	C1-O3P-P-O1P
11	x	101	PGT	C1-O3P-P-O2P
12	B	402	POV	C1-O11-P-O13
12	B	404	POV	C11-O12-P-O13
12	b	402	POV	C1-O11-P-O13
12	b	403	POV	C11-O12-P-O13
11	X	101	PGT	C33-C34-C35-C36
8	B	401	LPP	O5-C6-C7-C8
8	b	405	LPP	O5-C6-C7-C8
7	B	405	MQ9	C24-C26-C27-C28
7	b	401	MQ9	C29-C31-C32-C33
11	X	101	PGT	C39-C40-C41-C42
12	b	403	POV	C12-C11-O12-P

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Mol	Chain	Res	Type	Atoms
8	B	403	LPP	C33-C34-C35-C36
8	b	404	LPP	C33-C34-C35-C36
8	B	401	LPP	O5-C6-C7-O9
8	b	405	LPP	O5-C6-C7-O9
12	B	402	POV	O11-C1-C2-O21
12	b	402	POV	O11-C1-C2-O21
12	b	403	POV	O11-C1-C2-O21
12	B	402	POV	O12-C11-C12-N
12	B	402	POV	C32-C33-C34-C35
12	b	402	POV	O12-C11-C12-N
12	b	402	POV	C32-C33-C34-C35
12	b	403	POV	O21-C2-C3-O31
8	B	401	LPP	C16-C17-C18-C19
7	B	405	MQ9	C29-C31-C32-C33
9	A	606	UQ8	C9-C11-C12-C13
8	b	405	LPP	C16-C17-C18-C19
12	B	404	POV	C210-C211-C212-C213
12	b	403	POV	C210-C211-C212-C213
12	b	402	POV	C22-C23-C24-C25
8	B	401	LPP	C33-C34-C35-C36
8	b	405	LPP	C33-C34-C35-C36
12	B	402	POV	C22-C23-C24-C25
12	B	404	POV	O11-C1-C2-C3
11	a	608	PGT	C21-C22-C23-C24
11	A	608	PGT	C32-C33-C34-C35
11	a	608	PGT	C32-C33-C34-C35
11	X	101	PGT	C38-C39-C40-C41
9	A	606	UQ8	C21-C22-C23-C24
8	a	604	LPP	C38-C39-C40-C41
8	A	604	LPP	C38-C39-C40-C41
11	X	101	PGT	C20-C21-C22-C23
12	b	402	POV	C27-C28-C29-C210
11	X	101	PGT	C19-C20-C21-C22
7	B	405	MQ9	C34-C36-C37-C38
11	X	101	PGT	C42-C43-C44-C45
7	B	405	MQ9	C12-C11-C9-C10
7	b	401	MQ9	C12-C11-C9-C10
12	B	402	POV	C27-C28-C29-C210
8	a	604	LPP	C19-C20-C21-C22
11	a	608	PGT	C20-C21-C22-C23
11	A	608	PGT	C21-C22-C23-C24
8	A	604	LPP	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
12	b	403	POV	C1-C2-C3-O31
5	a	603	HEM	CAA-CBA-CGA-O1A
5	a	603	HEM	CAD-CBD-CGD-O2D
5	A	605	HEM	CAD-CBD-CGD-O1D
7	B	405	MQ9	C44-C46-C47-C48
7	b	401	MQ9	C34-C36-C37-C38
7	b	401	MQ9	C44-C46-C47-C48
12	B	404	POV	C3-C2-O21-C21
12	b	403	POV	C3-C2-O21-C21
11	X	101	PGT	C35-C36-C37-C38
5	a	603	HEM	CAA-CBA-CGA-O2A
5	a	603	HEM	CAD-CBD-CGD-O1D
9	a	601	UQ8	C15-C14-C16-C17
11	X	101	PGT	C41-C42-C43-C44
12	B	402	POV	C212-C213-C214-C215
12	b	402	POV	C212-C213-C214-C215
11	A	608	PGT	O2-C2-C3-O3
11	a	608	PGT	O2-C2-C3-O3
6	a	605	A1JN4	CAA-CBA-CGA-O1A
5	A	605	HEM	CAD-CBD-CGD-O2D
8	b	405	LPP	C14-C15-C16-C17
8	B	401	LPP	C14-C15-C16-C17
12	B	404	POV	C32-C33-C34-C35
12	b	403	POV	C32-C33-C34-C35
8	b	405	LPP	C15-C16-C17-C18
8	B	401	LPP	C17-C18-C19-C20
8	B	401	LPP	C15-C16-C17-C18
8	b	405	LPP	C17-C18-C19-C20
11	x	101	PGT	O3-C11-C12-C13
11	A	608	PGT	C20-C21-C22-C23
7	B	405	MQ9	C20-C19-C21-C22
7	b	401	MQ9	C20-C19-C21-C22
5	a	603	HEM	C2A-CAA-CBA-CGA
8	b	405	LPP	C23-C24-C25-C26
11	a	608	PGT	C45-C46-C47-C48
8	B	401	LPP	C23-C24-C25-C26
7	B	405	MQ9	C9-C11-C12-C13
7	b	401	MQ9	C9-C11-C12-C13
9	a	601	UQ8	C19-C21-C22-C23
7	B	405	MQ9	C18-C19-C21-C22
7	b	401	MQ9	C18-C19-C21-C22
9	a	601	UQ8	C13-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
11	x	101	PGT	C45-C46-C47-C48
11	A	608	PGT	C45-C46-C47-C48
8	B	401	LPP	C6-O5-P1-O2
8	b	405	LPP	C6-O5-P1-O2
8	B	401	LPP	C18-C19-C20-C21
11	X	101	PGT	C32-C33-C34-C35
8	b	405	LPP	C18-C19-C20-C21
7	A	603	MQ9	C1-C6-C7-C8
7	a	602	MQ9	C1-C6-C7-C8
11	X	101	PGT	O2-C31-C32-C33
12	B	404	POV	C1-C2-O21-C21
8	A	604	LPP	O27-C29-C30-C31
8	a	604	LPP	O27-C29-C30-C31
12	B	404	POV	C311-C312-C313-C314
12	b	403	POV	C311-C312-C313-C314
8	B	401	LPP	C13-C14-C15-C16
12	B	402	POV	C37-C38-C39-C310
12	b	402	POV	C37-C38-C39-C310
12	B	404	POV	C1-C2-C3-O31
8	b	405	LPP	C13-C14-C15-C16
12	B	402	POV	C23-C24-C25-C26
12	b	402	POV	C23-C24-C25-C26
11	A	608	PGT	C15-C16-C17-C18
12	b	402	POV	C25-C26-C27-C28
12	B	402	POV	C25-C26-C27-C28
12	B	402	POV	C214-C215-C216-C217
9	a	601	UQ8	C5-C4-O4-C4M
12	b	402	POV	C214-C215-C216-C217
11	x	101	PGT	O2-C31-C32-C33
11	X	101	PGT	O31-C31-C32-C33
8	B	403	LPP	C32-C33-C34-C35
8	b	404	LPP	C32-C33-C34-C35
11	A	608	PGT	C1-O3P-P-O1P
11	a	608	PGT	C1-O3P-P-O1P
12	B	402	POV	C1-O11-P-O14
12	b	402	POV	C1-O11-P-O14
7	b	401	MQ9	C26-C27-C28-C29
8	A	604	LPP	O28-C29-C30-C31
8	B	403	LPP	C35-C36-C37-C38
8	b	404	LPP	C35-C36-C37-C38
8	b	405	LPP	O27-C29-C30-C31
6	a	605	A1JN4	CAA-CBA-CGA-O2A

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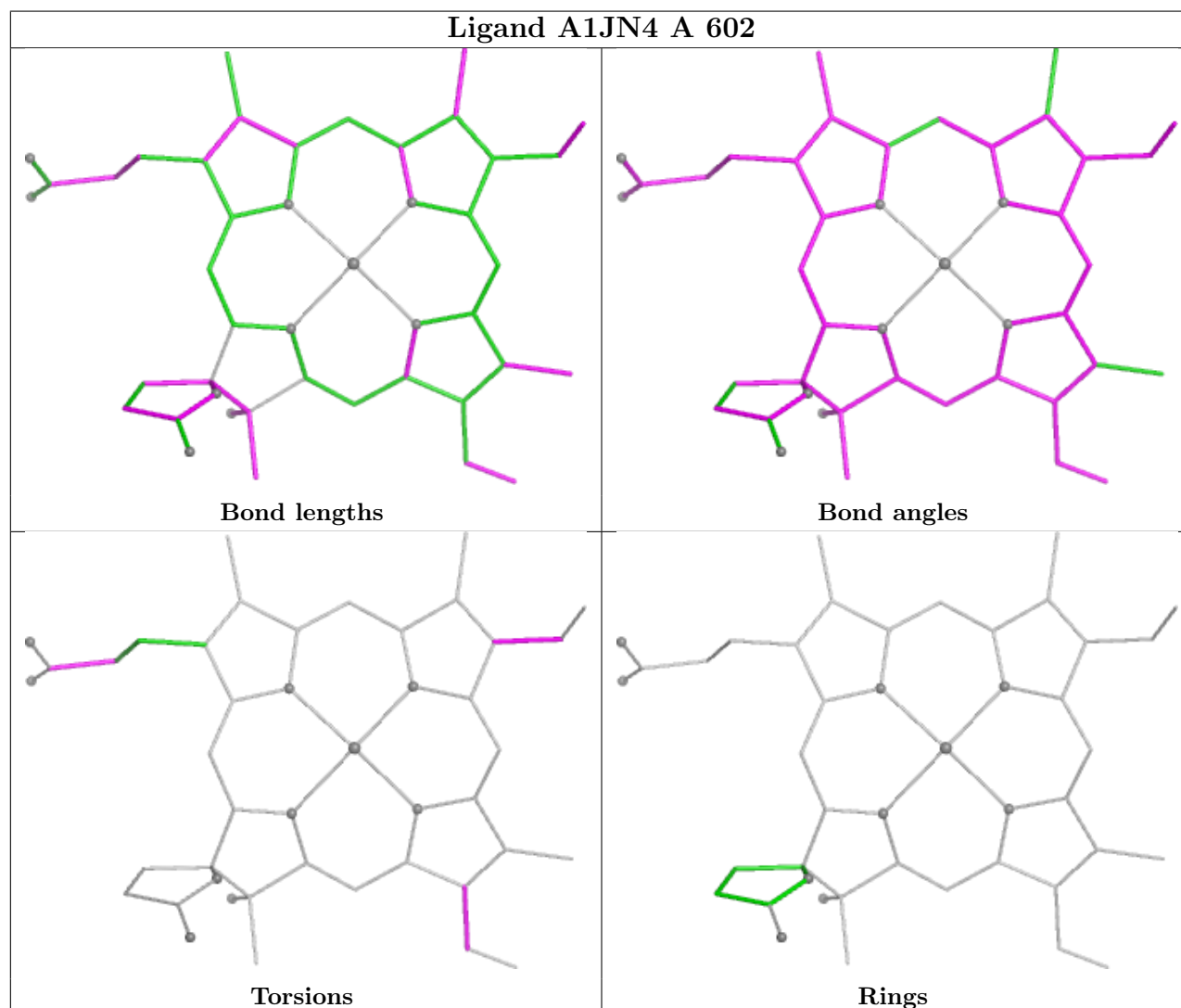
Mol	Chain	Res	Type	Atoms
8	a	604	LPP	O28-C29-C30-C31
8	B	401	LPP	O27-C29-C30-C31
7	A	603	MQ9	C16-C17-C18-C19
7	B	405	MQ9	C26-C27-C28-C29
12	b	403	POV	C1-C2-O21-C21
6	A	602	A1JN4	CAA-CBA-CGA-O1A
11	A	608	PGT	O2-C31-C32-C33
11	a	608	PGT	O2-C31-C32-C33
7	B	405	MQ9	C12-C11-C9-C8
7	b	401	MQ9	C12-C11-C9-C8
8	B	403	LPP	O5-C6-C7-O9
8	b	404	LPP	O5-C6-C7-O9
11	a	608	PGT	C15-C16-C17-C18
7	a	602	MQ9	C16-C17-C18-C19
11	x	101	PGT	O31-C31-C32-C33

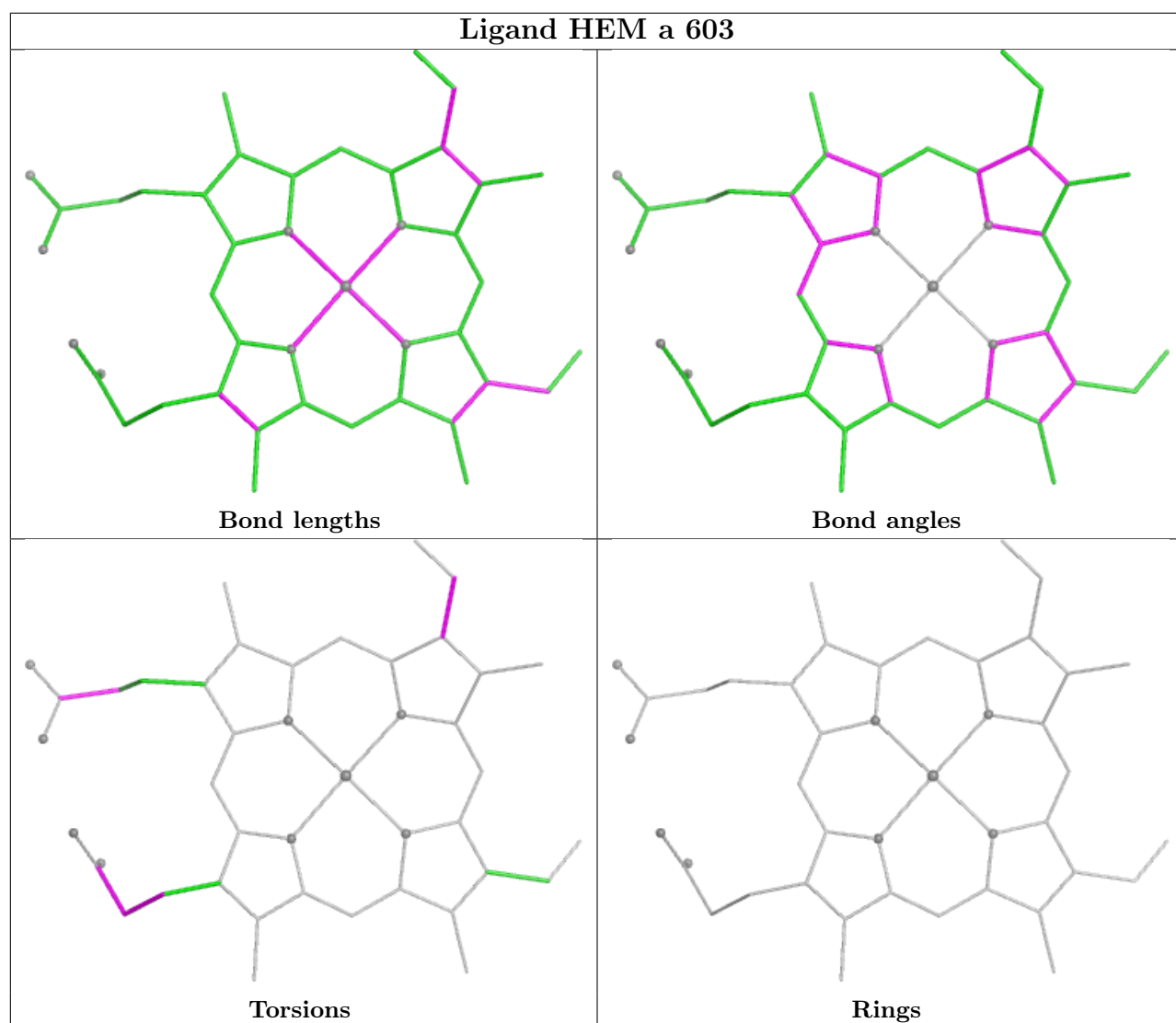
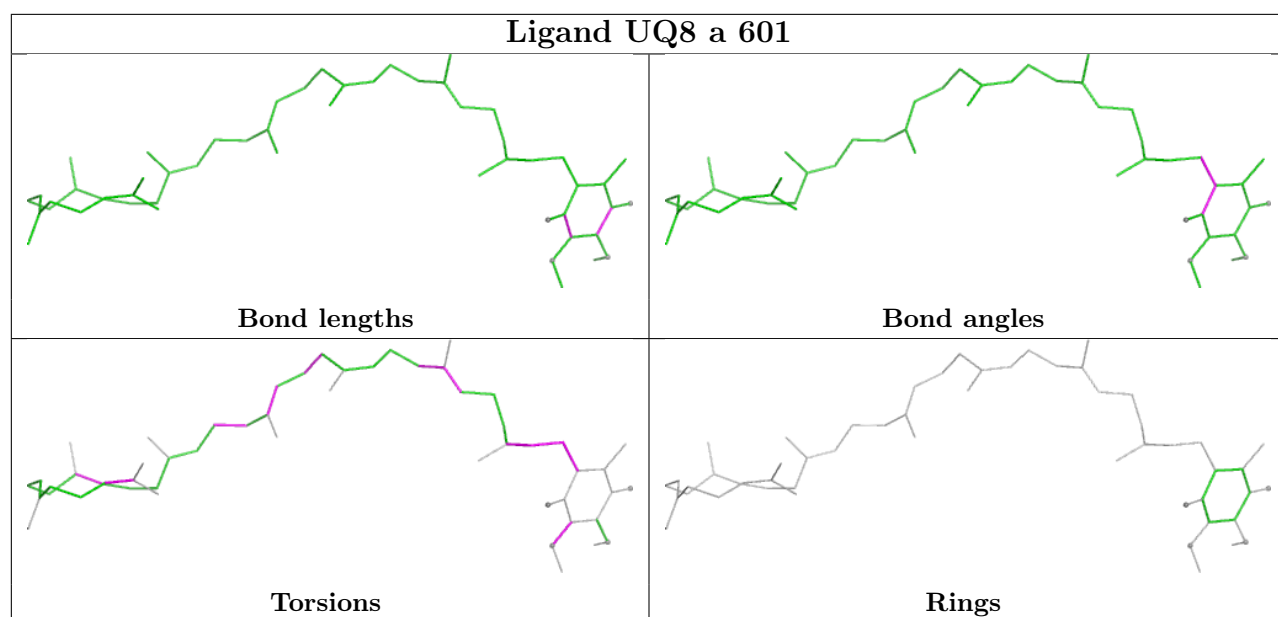
There are no ring outliers.

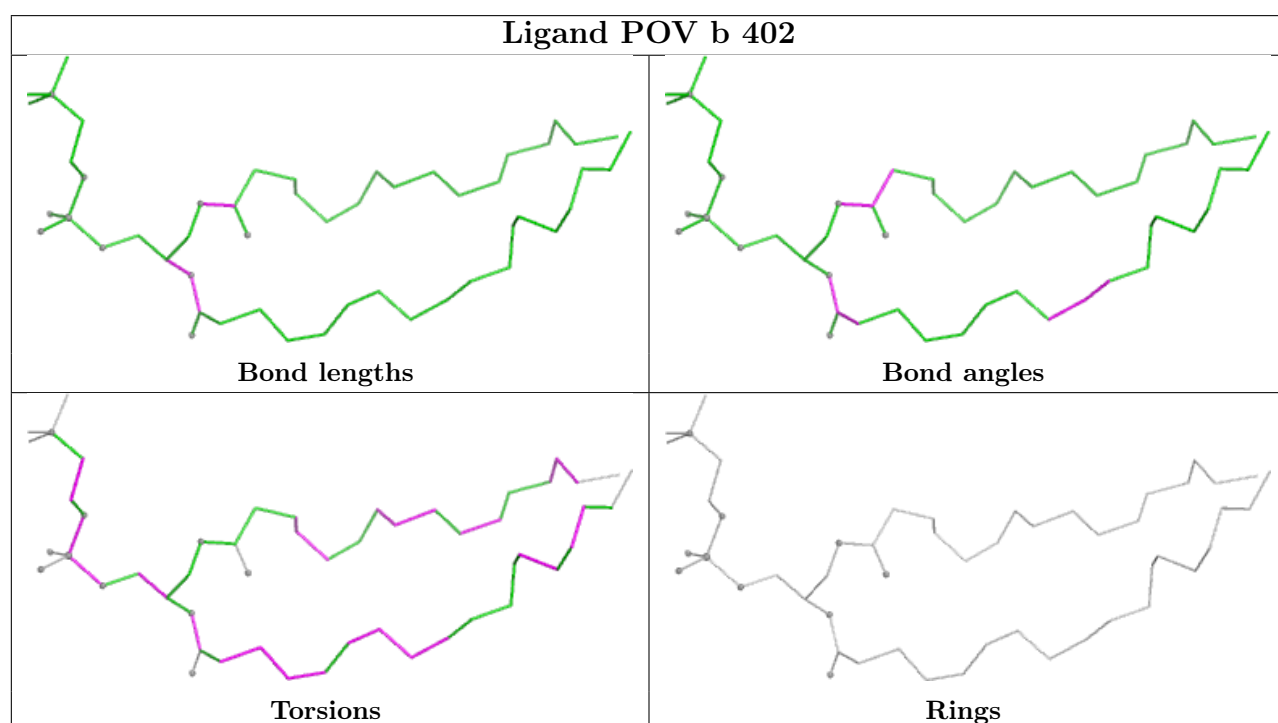
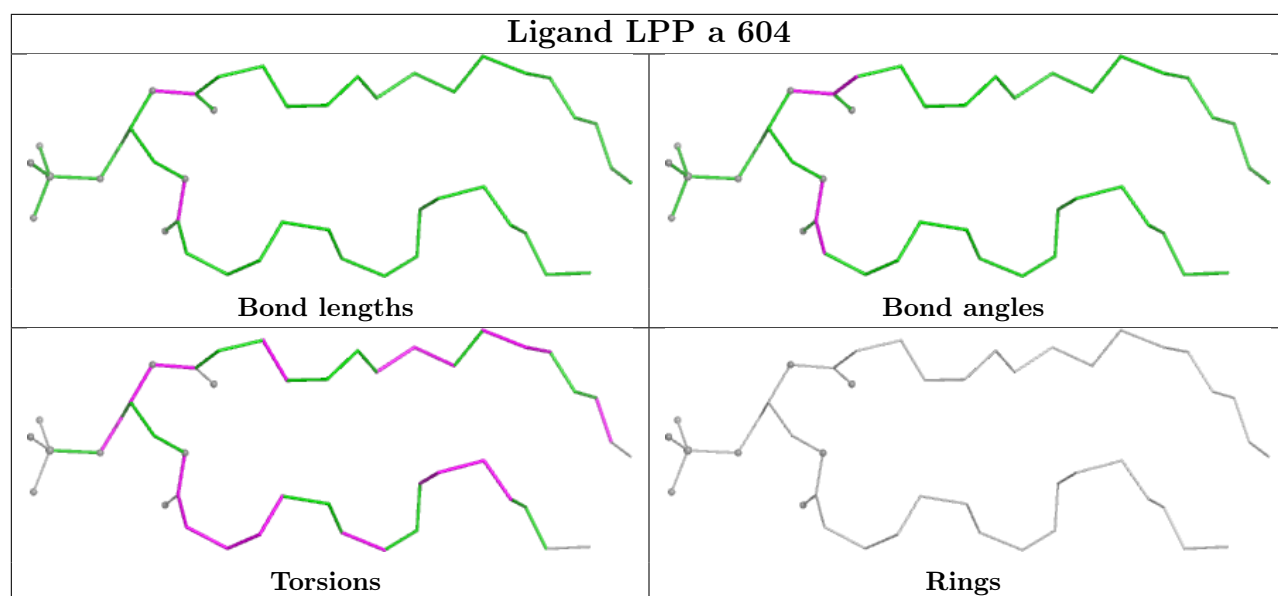
22 monomers are involved in 119 short contacts:

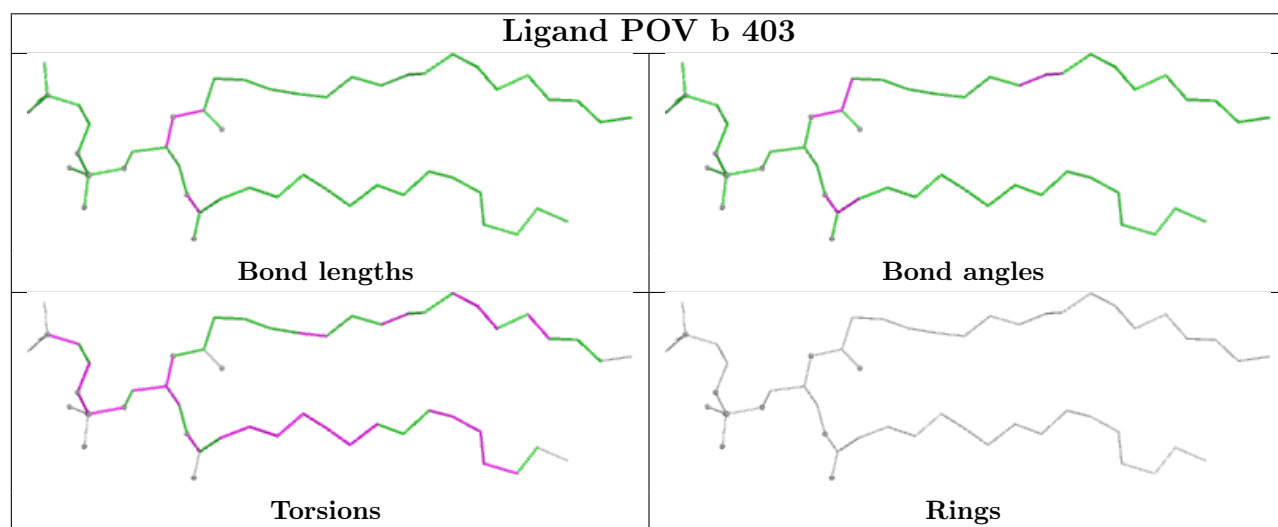
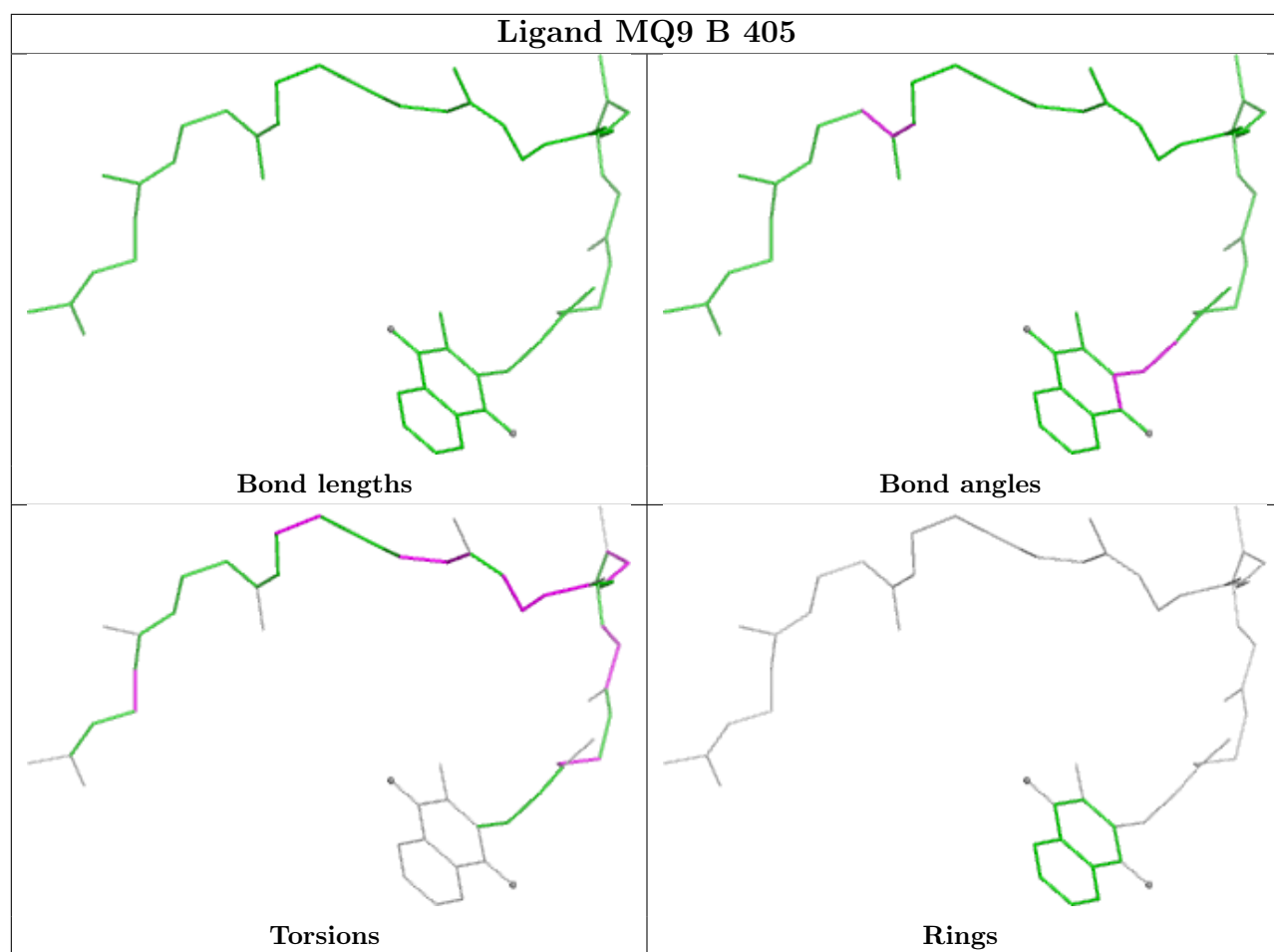
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	a	601	UQ8	10	0
5	a	603	HEM	5	0
8	a	604	LPP	4	0
12	b	402	POV	1	0
7	B	405	MQ9	16	0
12	b	403	POV	13	0
8	B	403	LPP	1	0
10	a	607	OXY	1	0
8	b	404	LPP	1	0
11	A	608	PGT	1	0
7	b	401	MQ9	16	0
12	B	404	POV	13	0
9	A	606	UQ8	7	0
8	A	604	LPP	4	0
5	a	606	HEM	4	0
11	a	608	PGT	1	0
5	A	605	HEM	5	0
10	A	607	OXY	1	0
7	a	602	MQ9	5	0
5	A	601	HEM	4	0
7	A	603	MQ9	5	0
12	B	402	POV	1	0

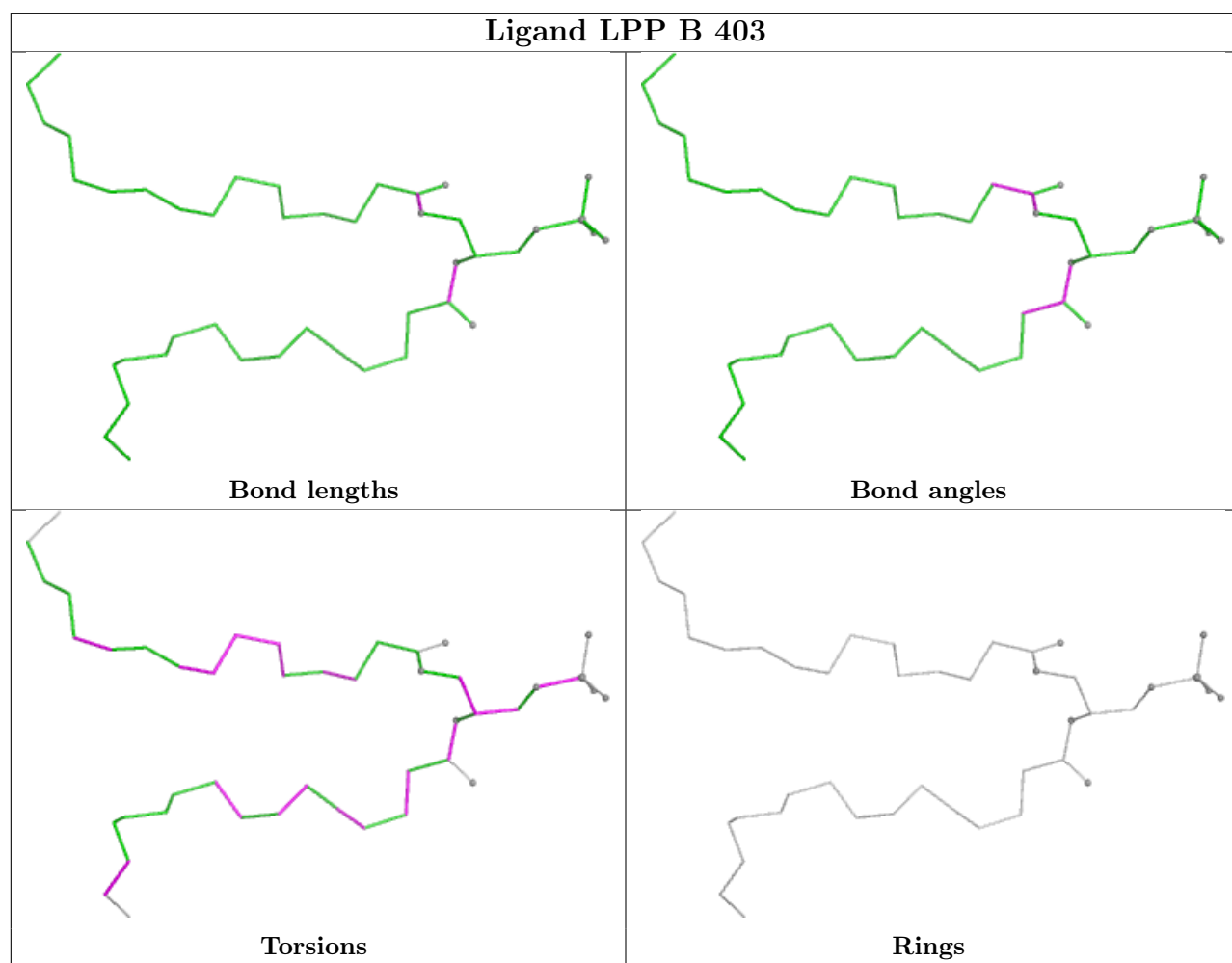
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

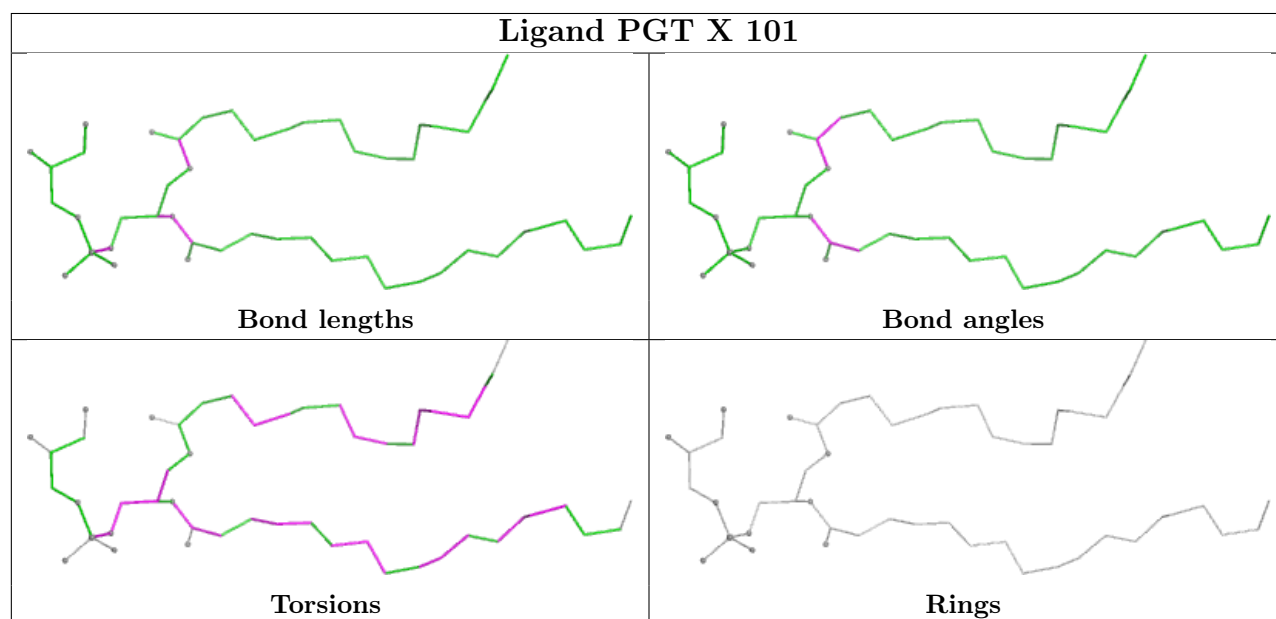
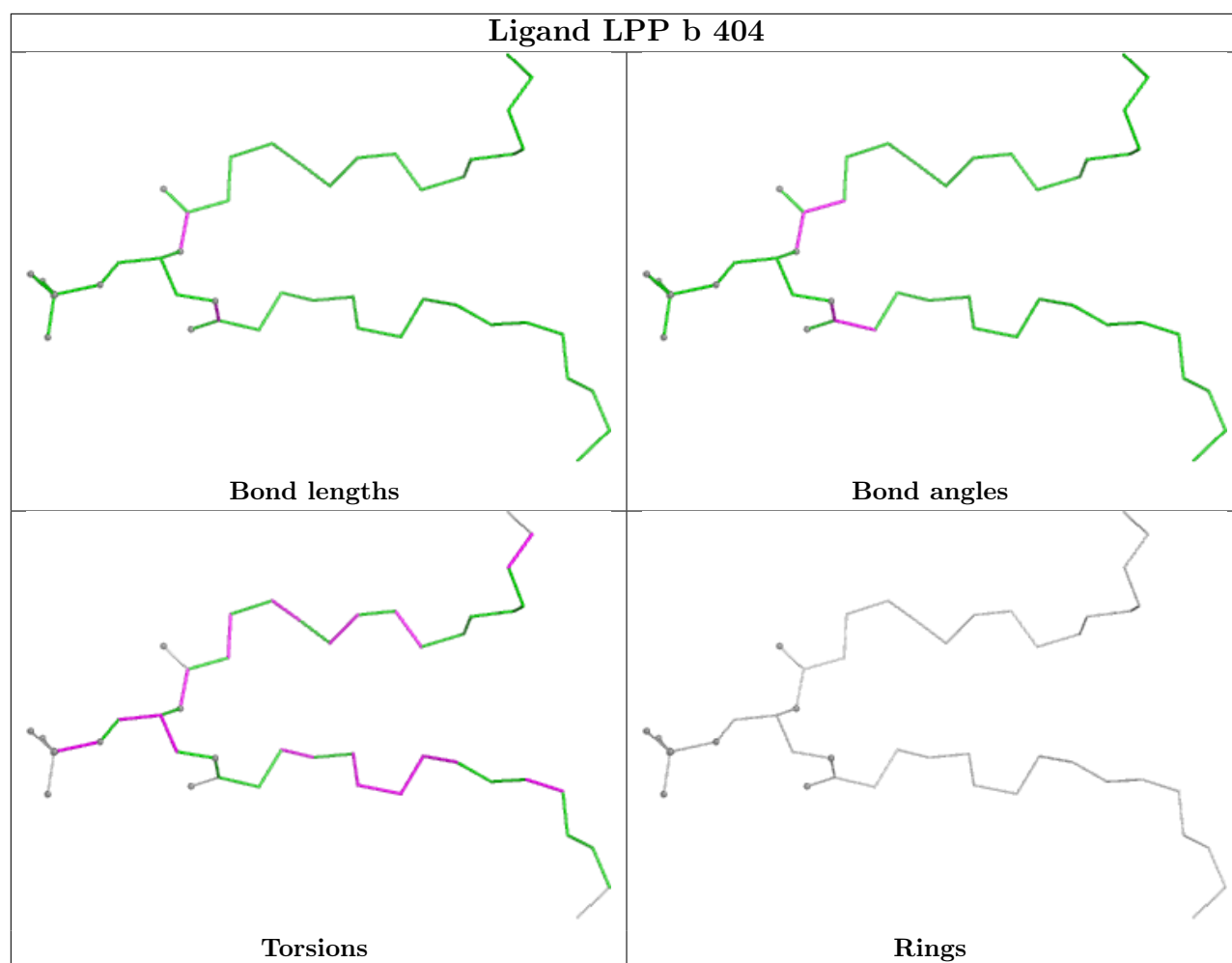


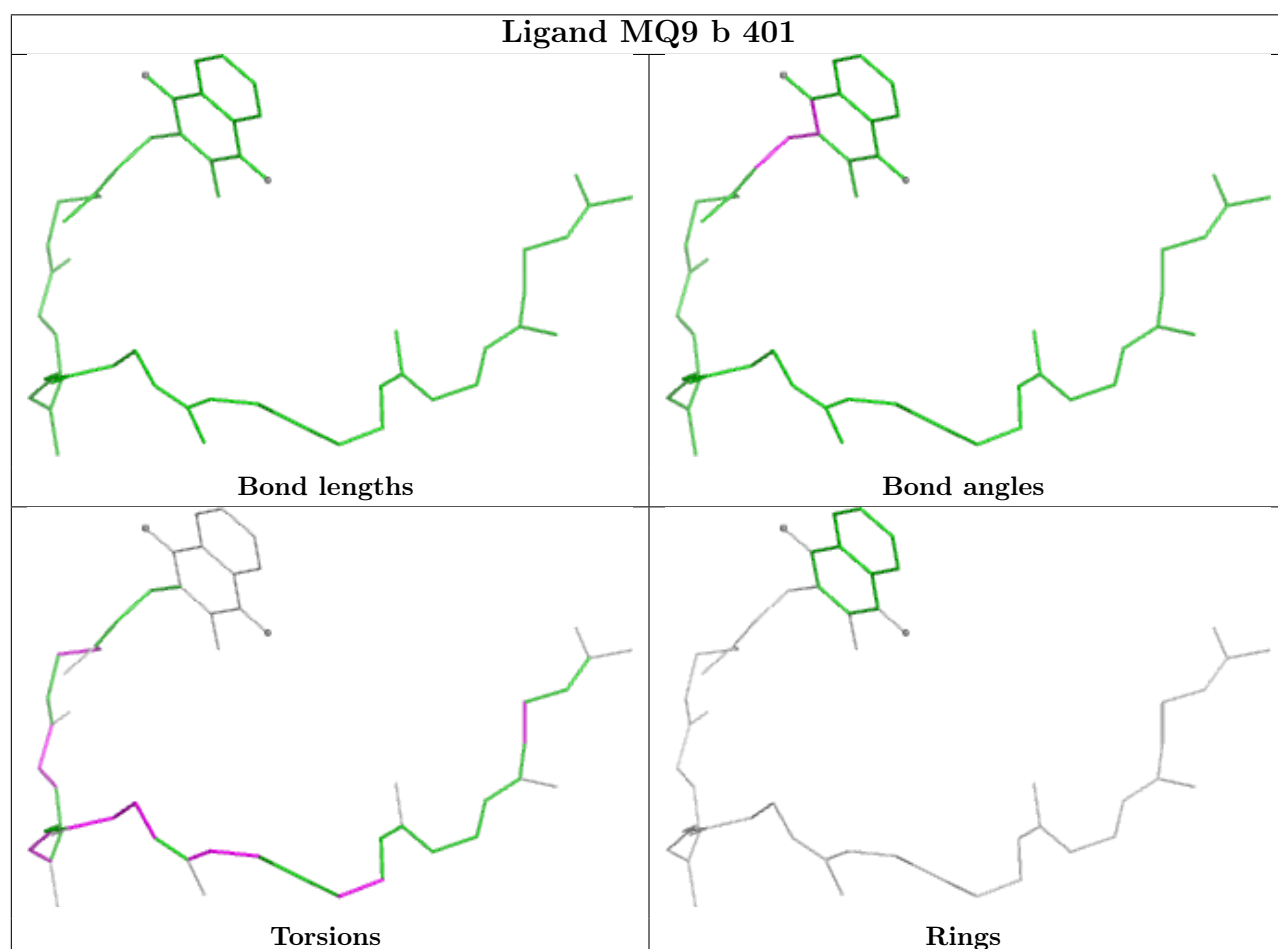
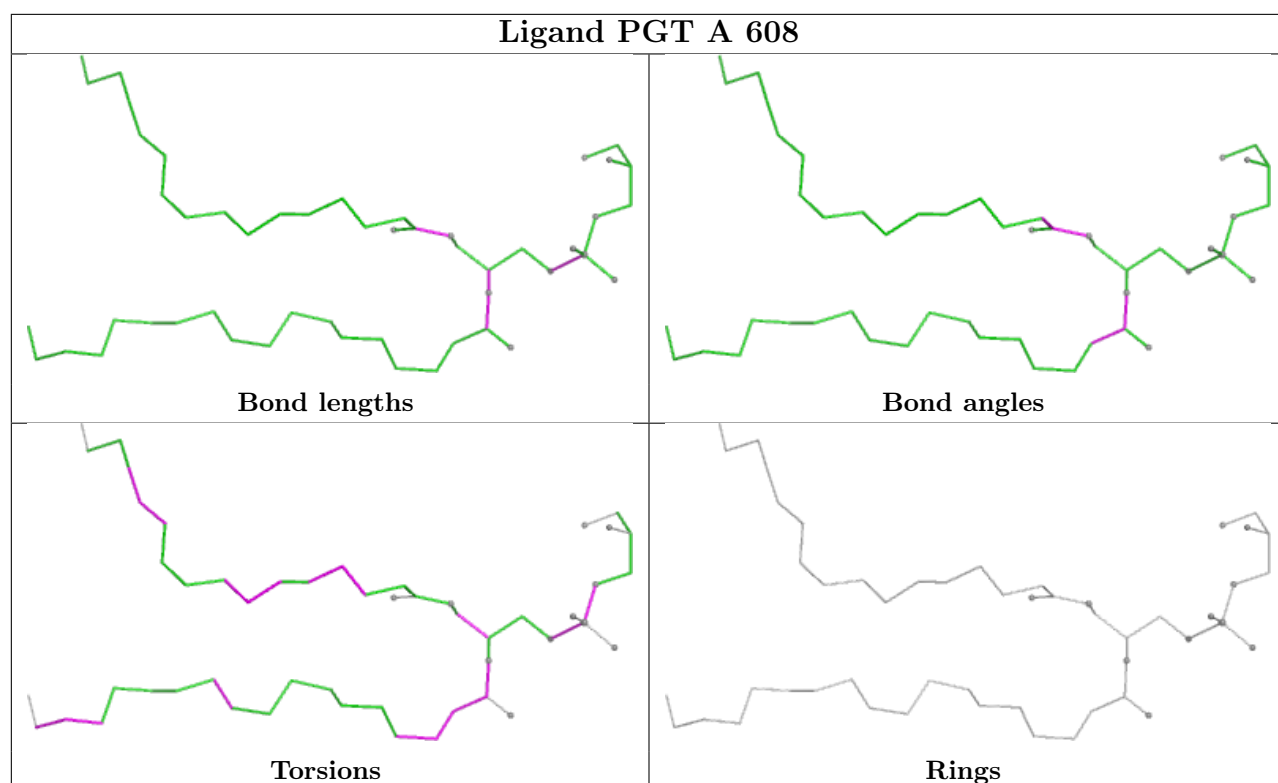


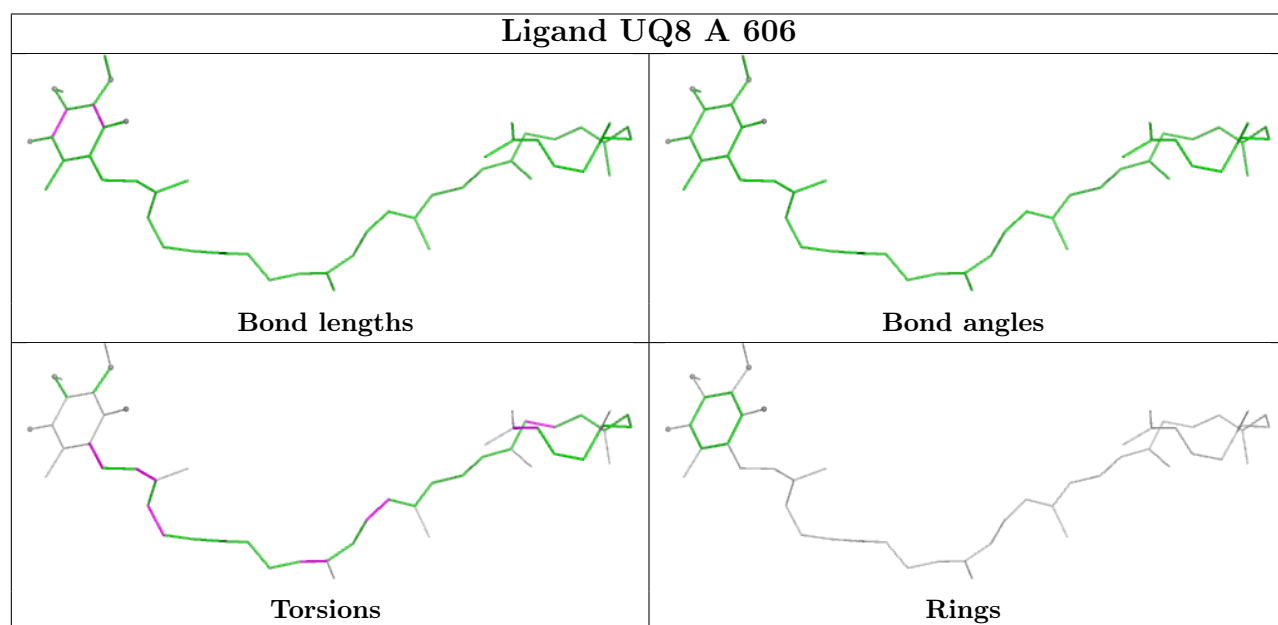
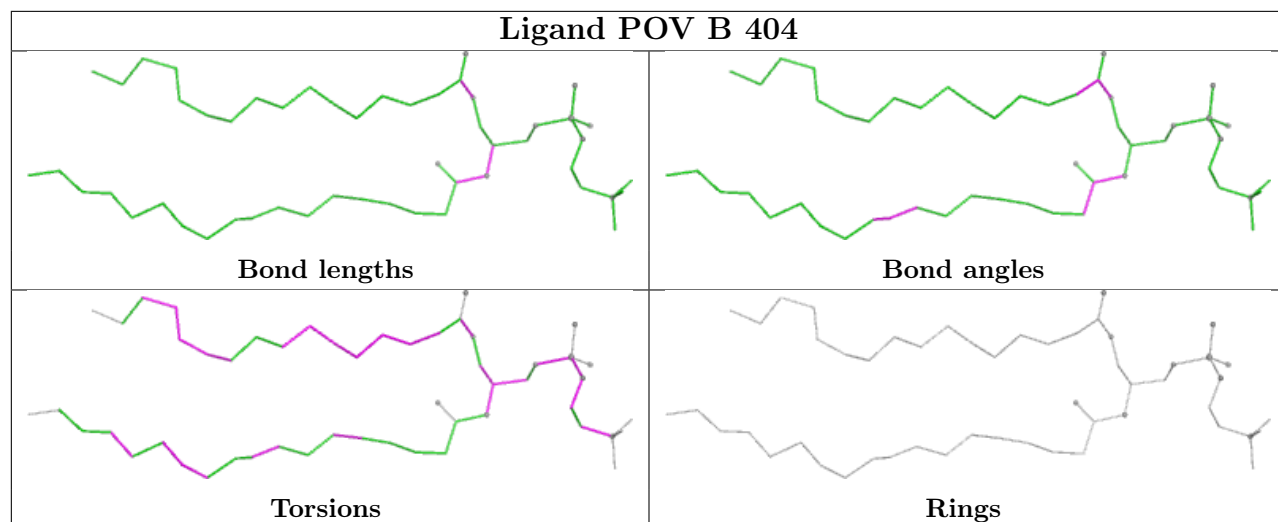




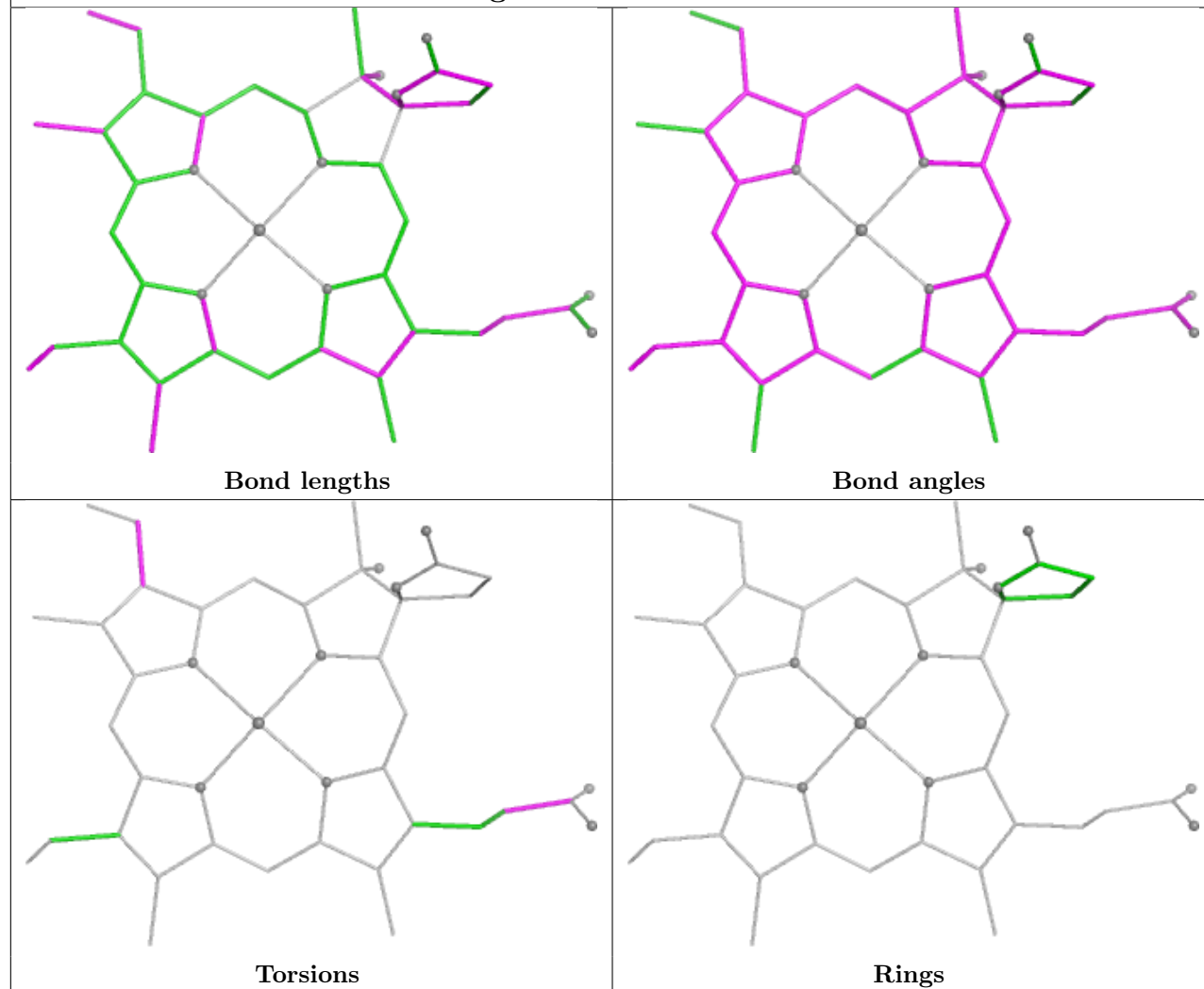




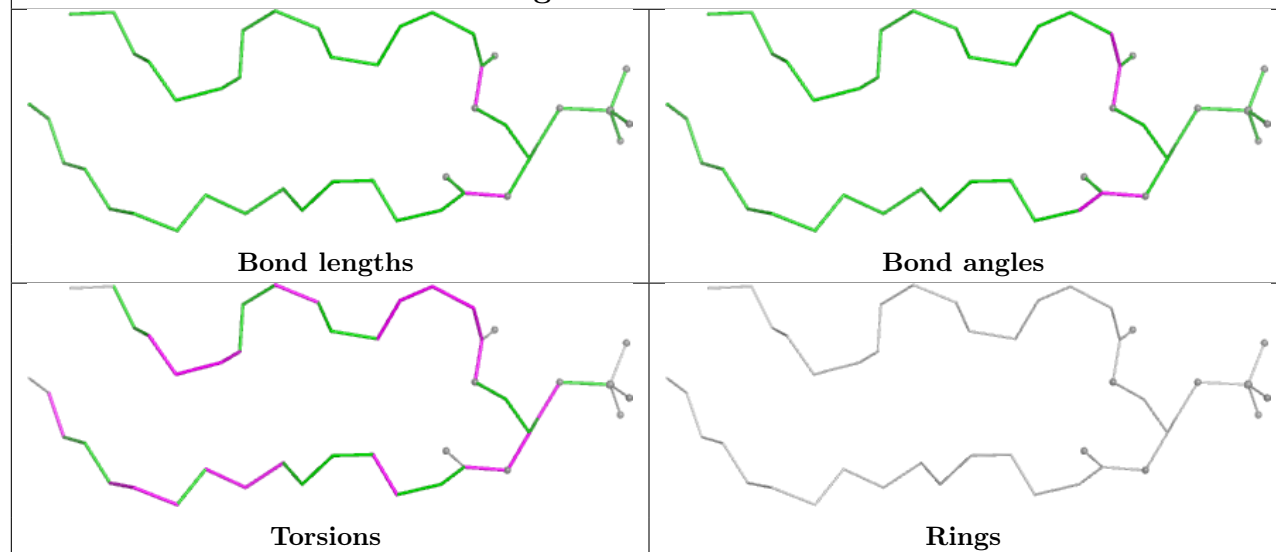


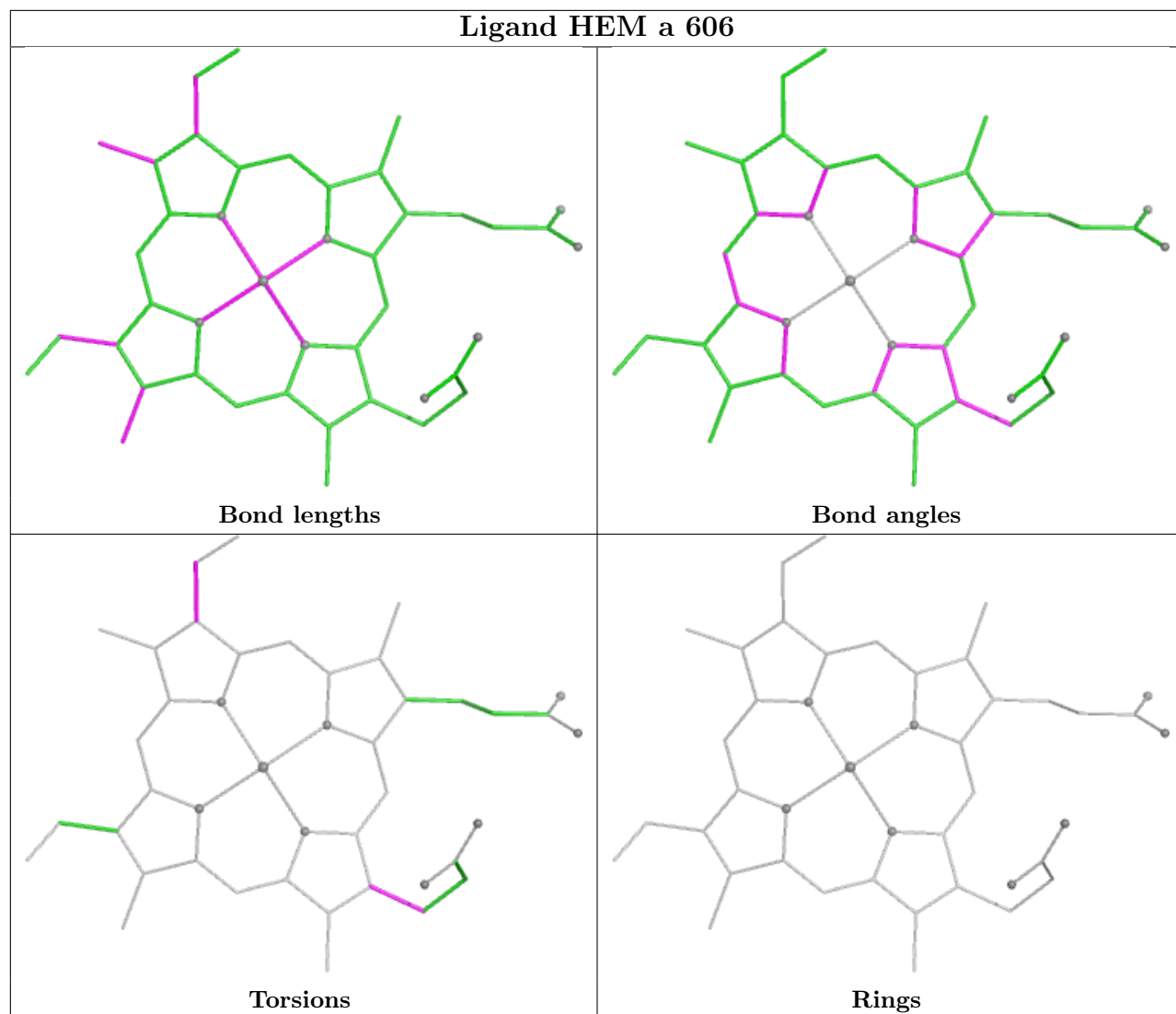


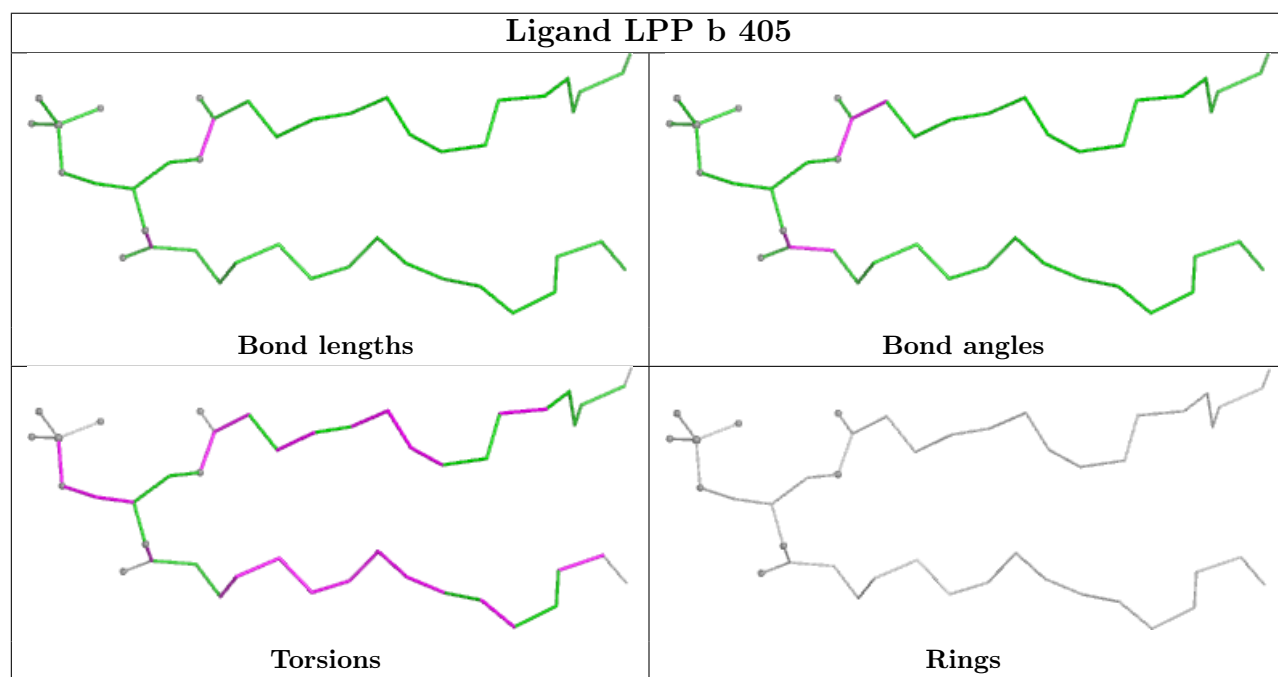
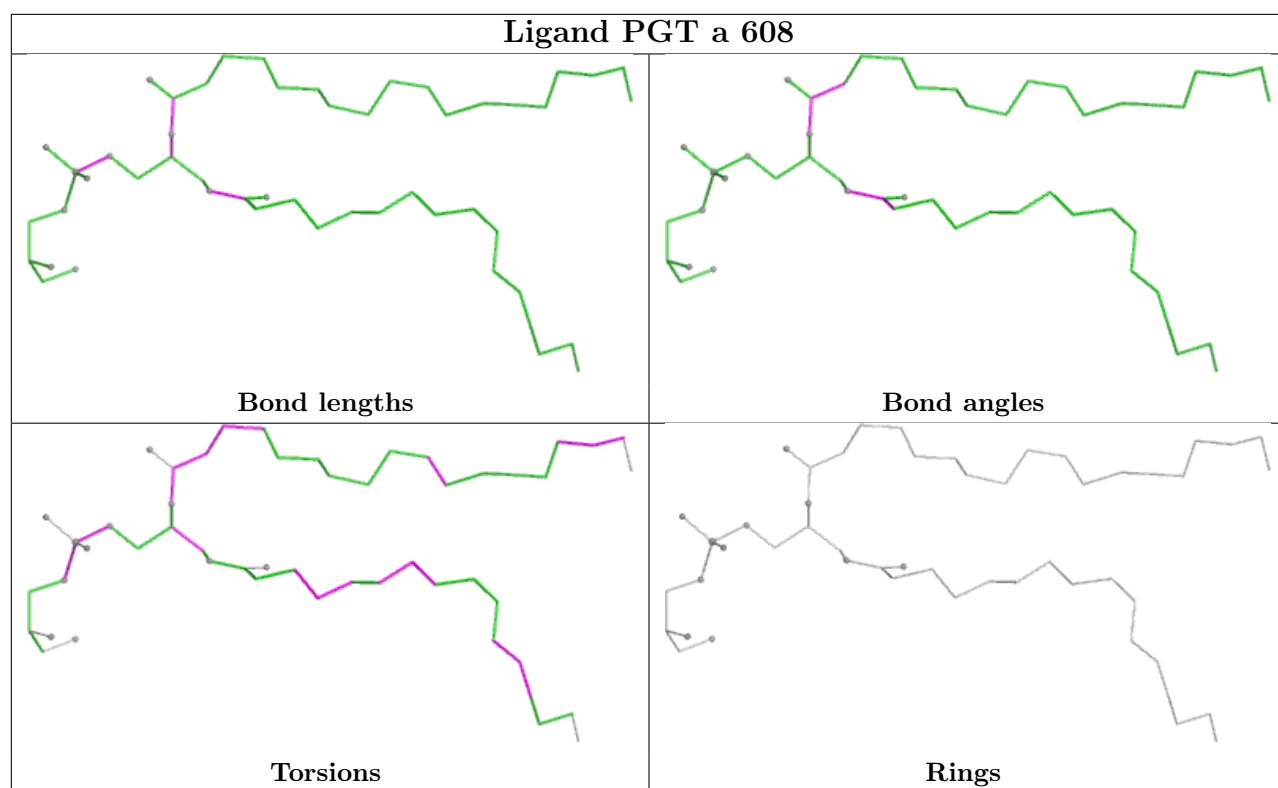
Ligand A1JN4 a 605

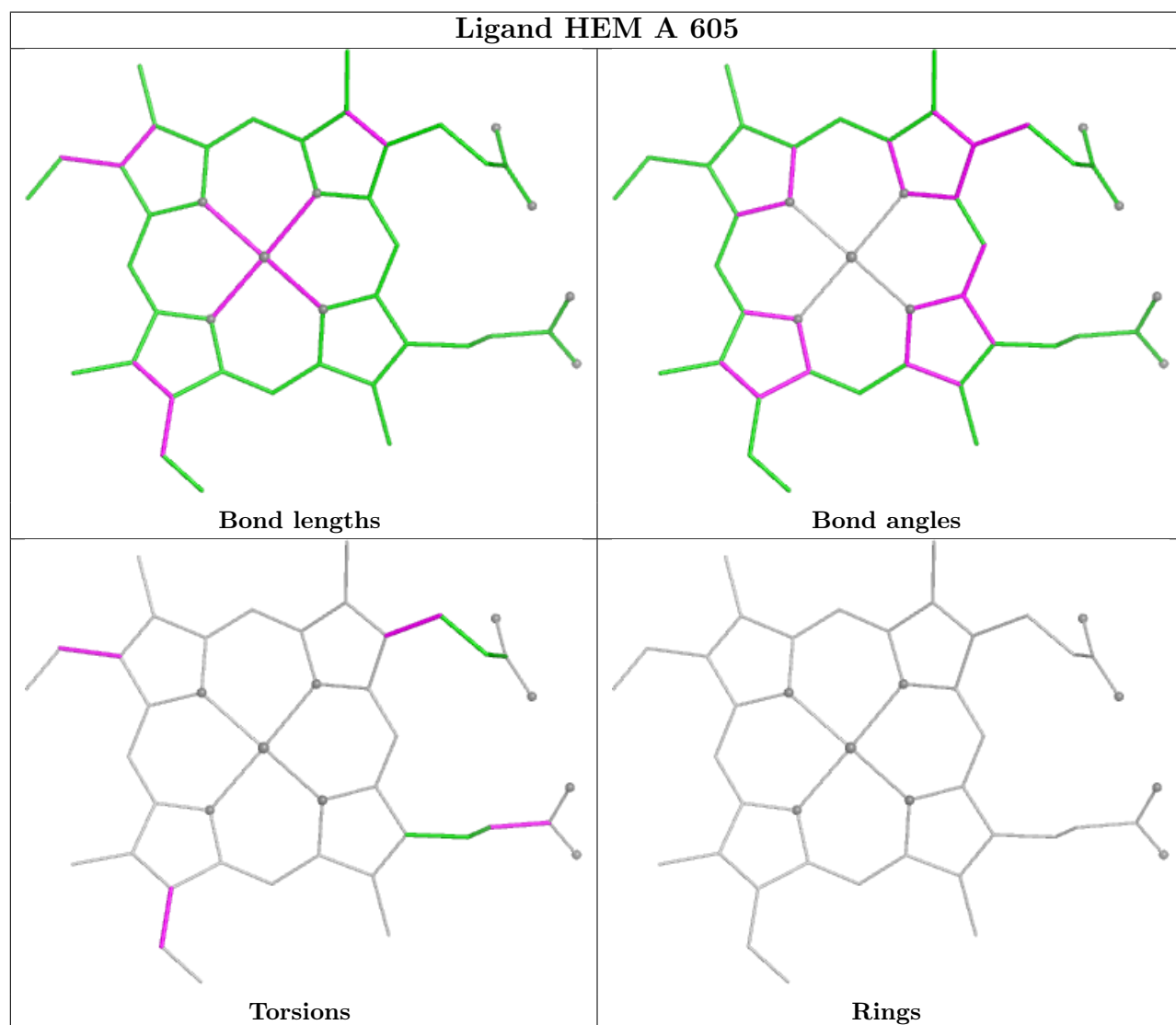
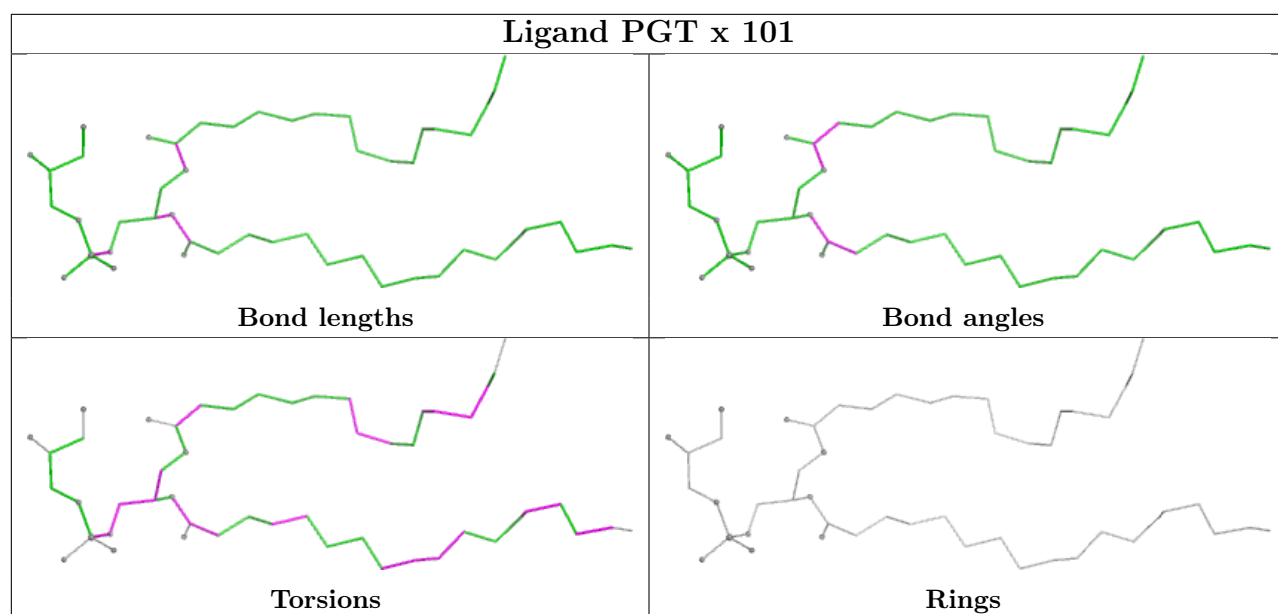


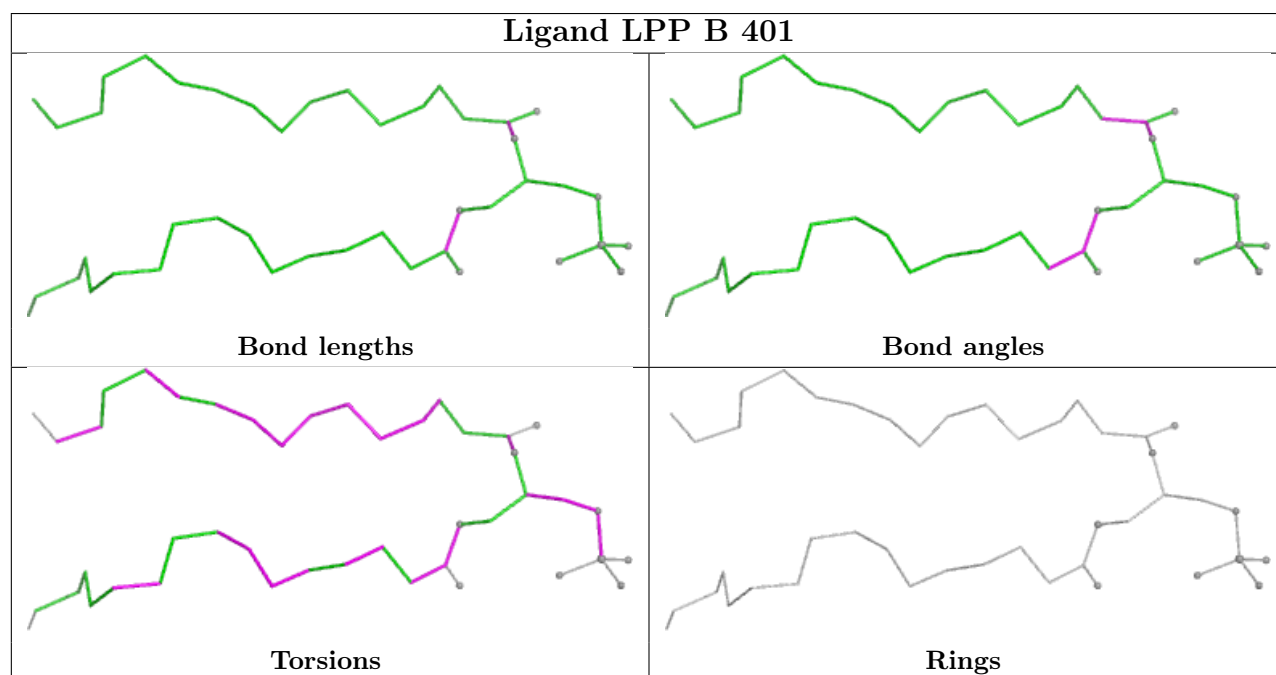
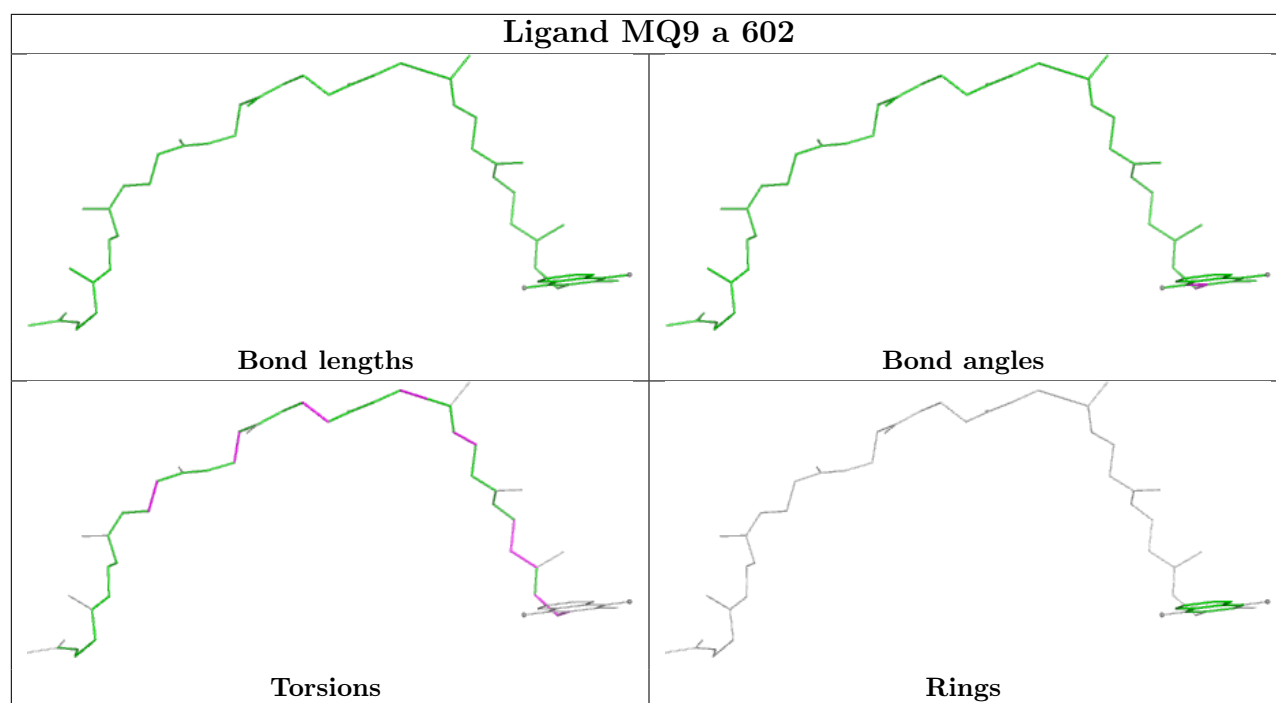
Ligand LPP A 604

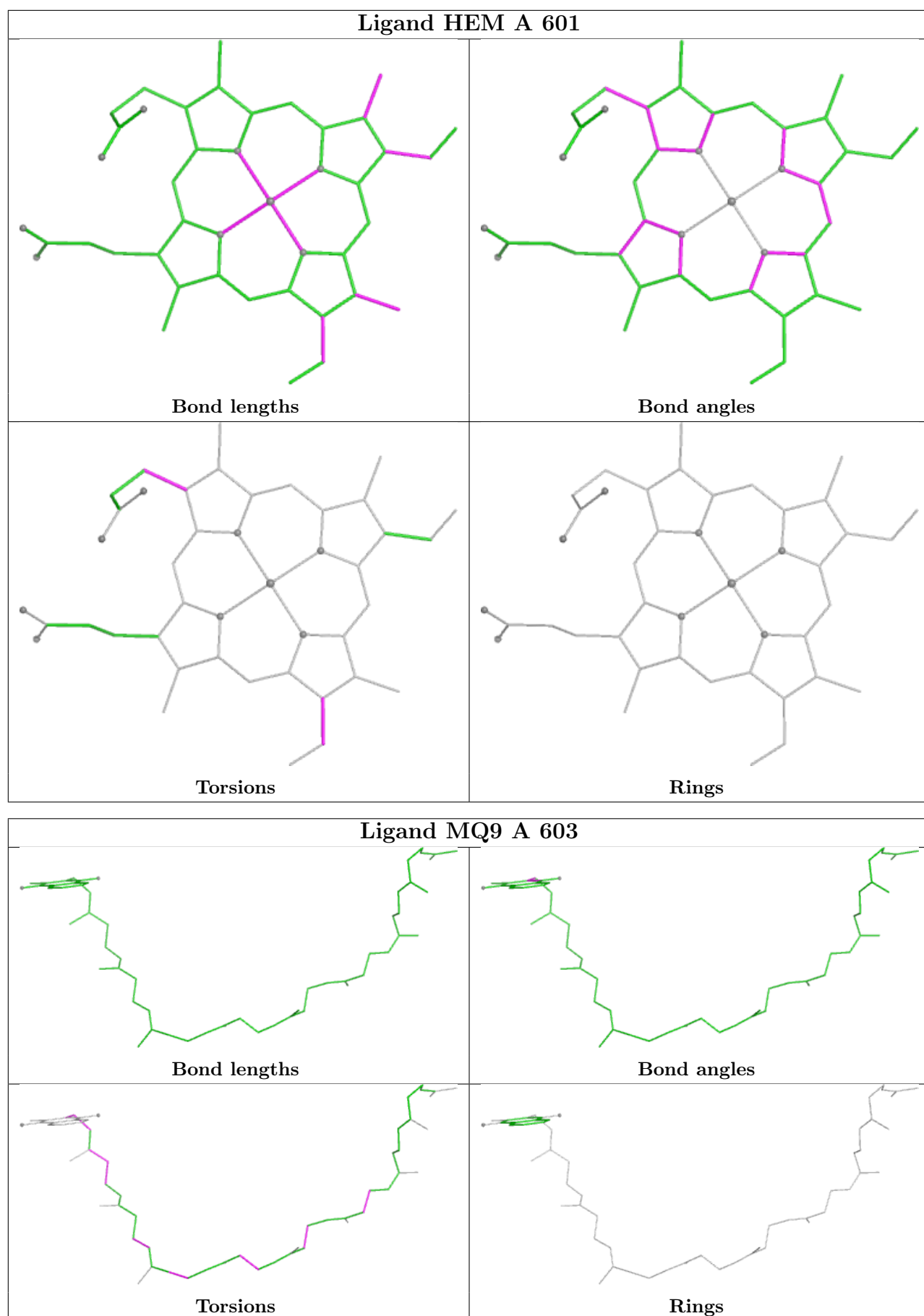


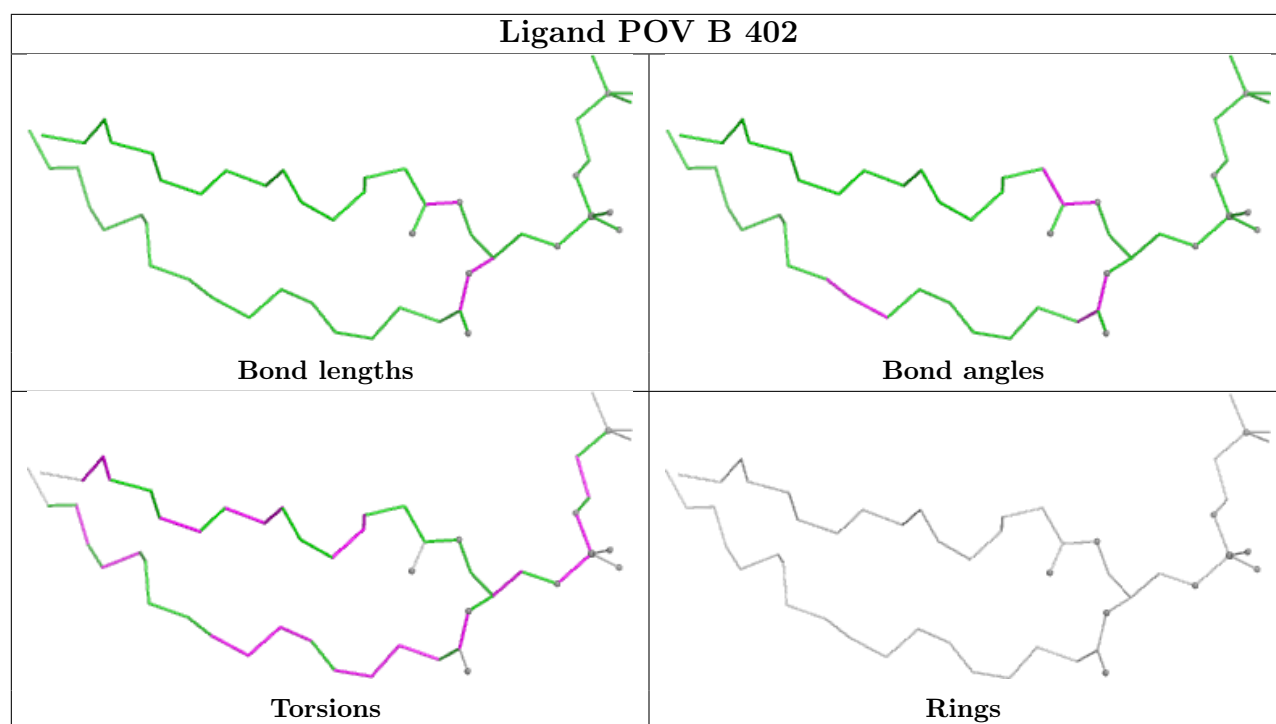












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

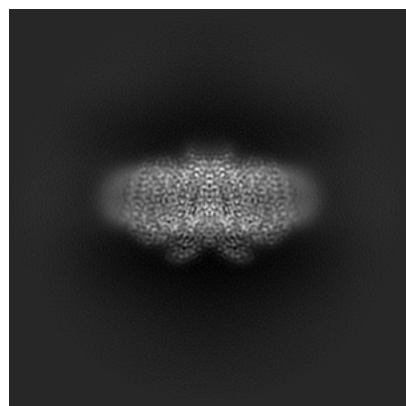
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54414. These allow visual inspection of the internal detail of the map and identification of artifacts.

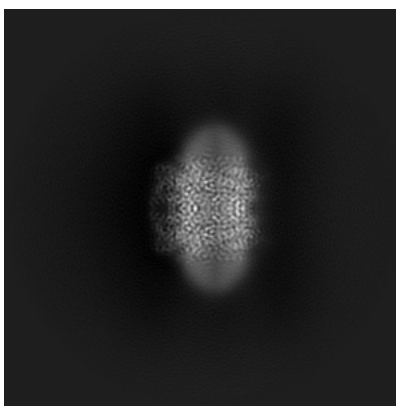
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

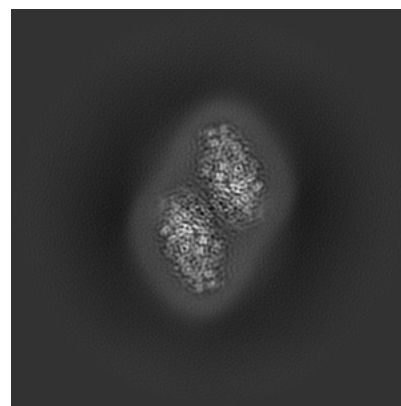
6.1.1 Primary map



X

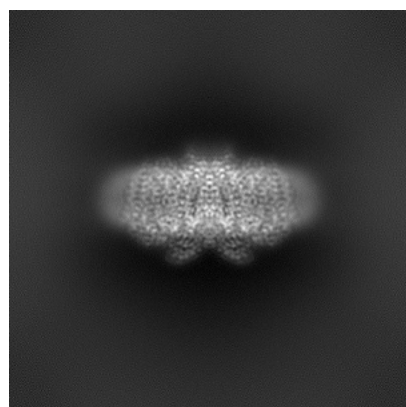


Y

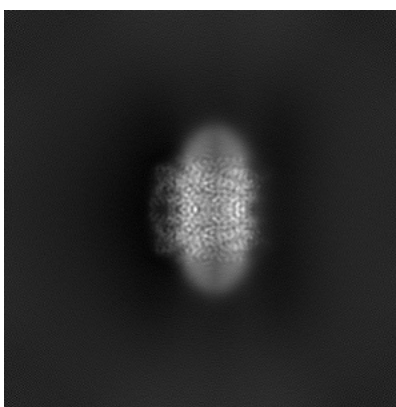


Z

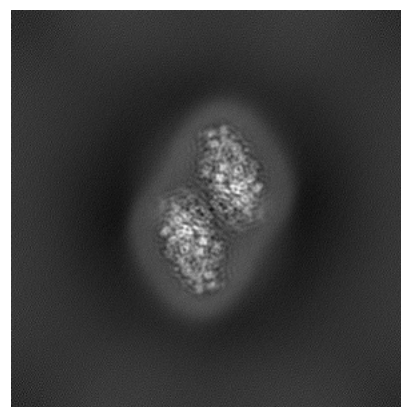
6.1.2 Raw map



X



Y

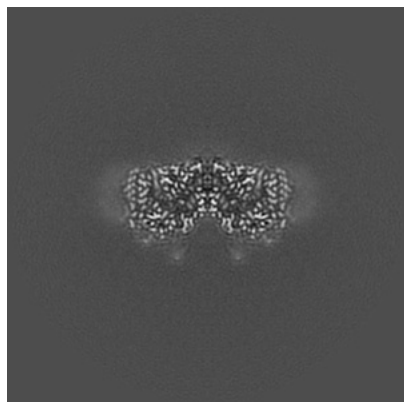


Z

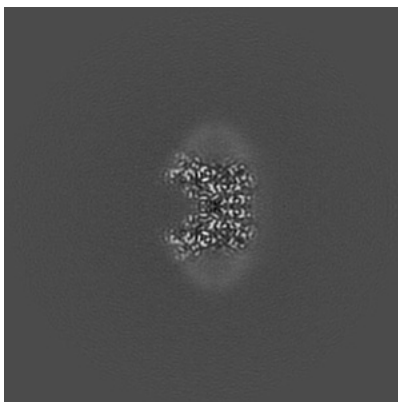
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

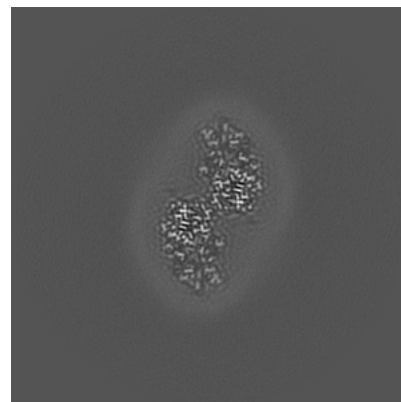
6.2.1 Primary map



X Index: 180

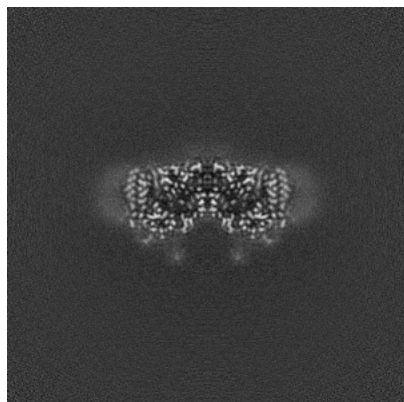


Y Index: 180

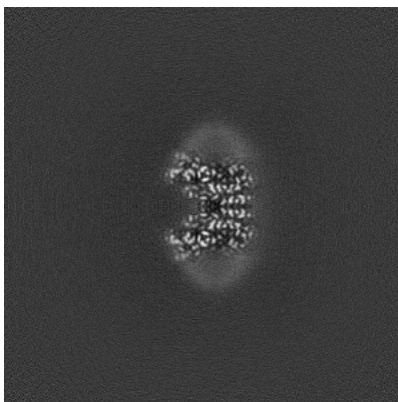


Z Index: 180

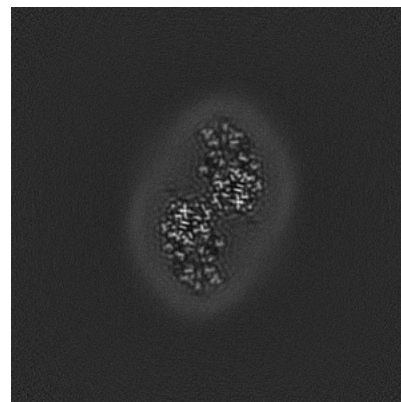
6.2.2 Raw map



X Index: 180



Y Index: 180

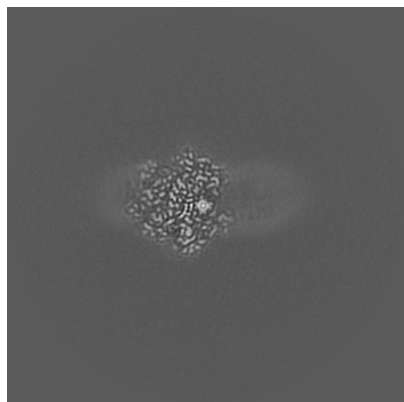


Z Index: 180

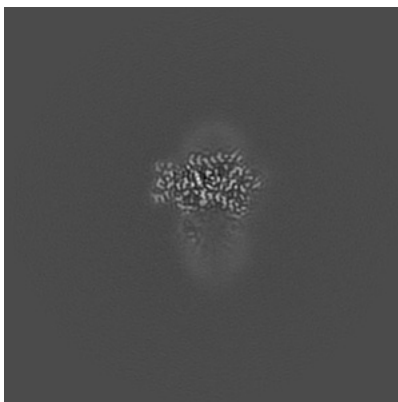
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

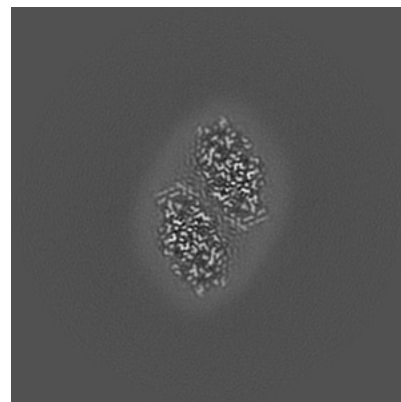
6.3.1 Primary map



X Index: 156

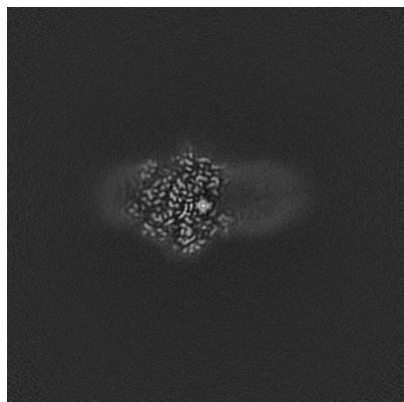


Y Index: 201

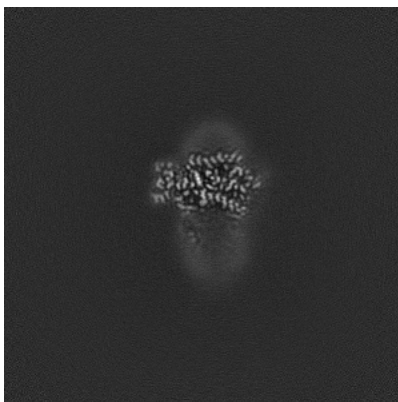


Z Index: 170

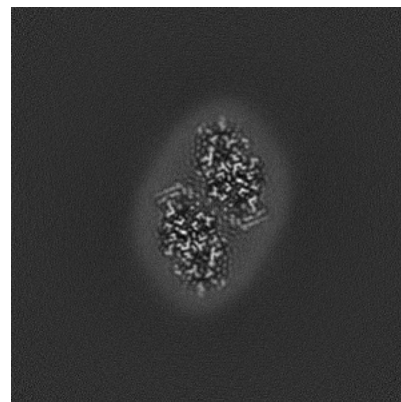
6.3.2 Raw map



X Index: 156



Y Index: 201

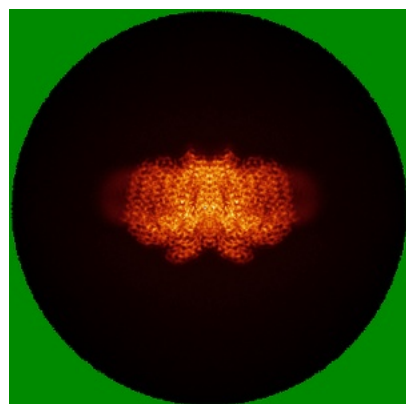


Z Index: 171

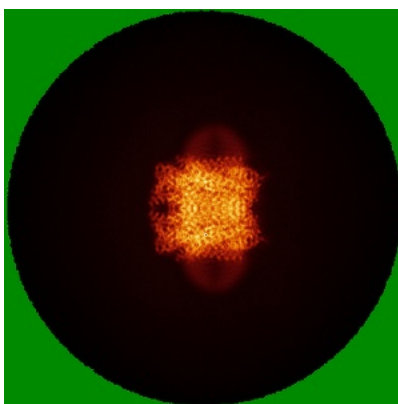
The images above show the largest variance slices of the map in three orthogonal directions.

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

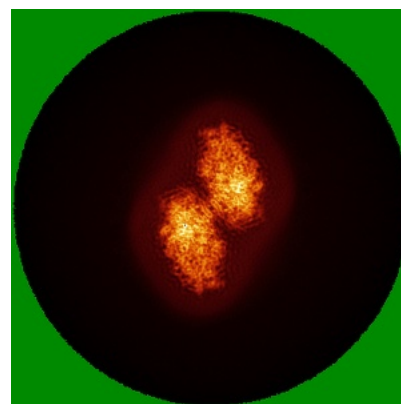
6.4.1 Primary map



X

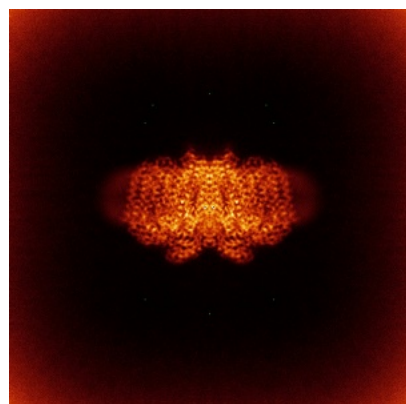


Y

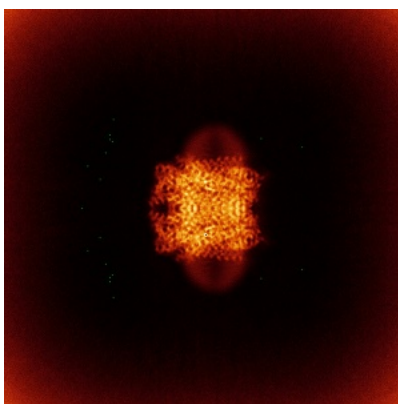


Z

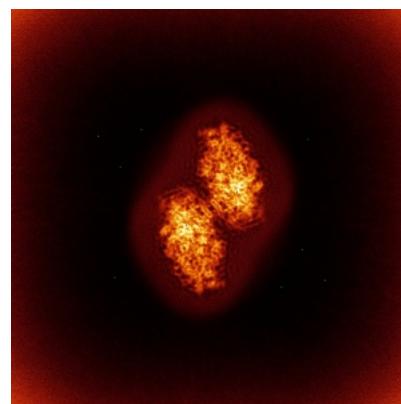
6.4.2 Raw map



X



Y

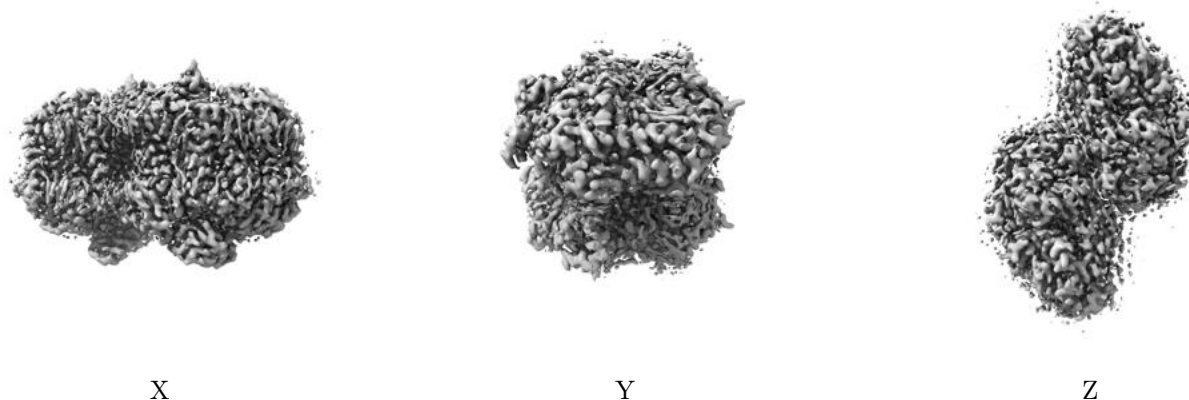


Z

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

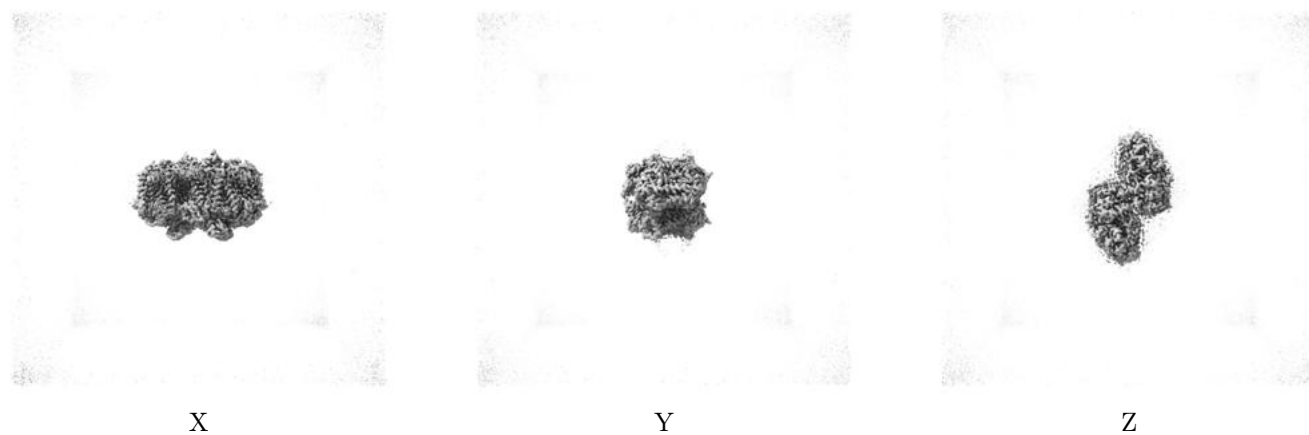
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0364. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

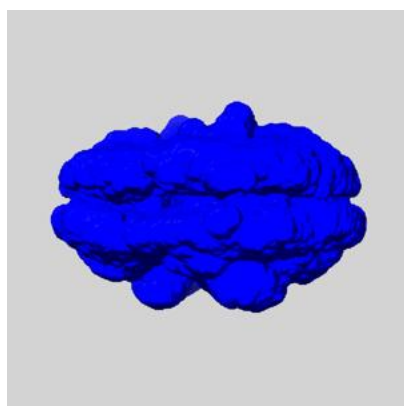
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

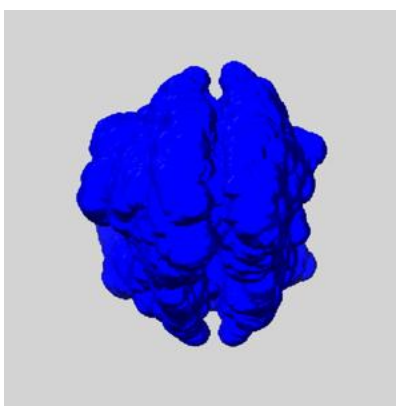
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

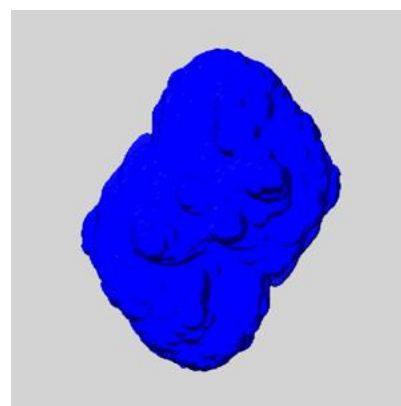
6.6.1 emd_54414_msk_1.map [i](#)



X



Y

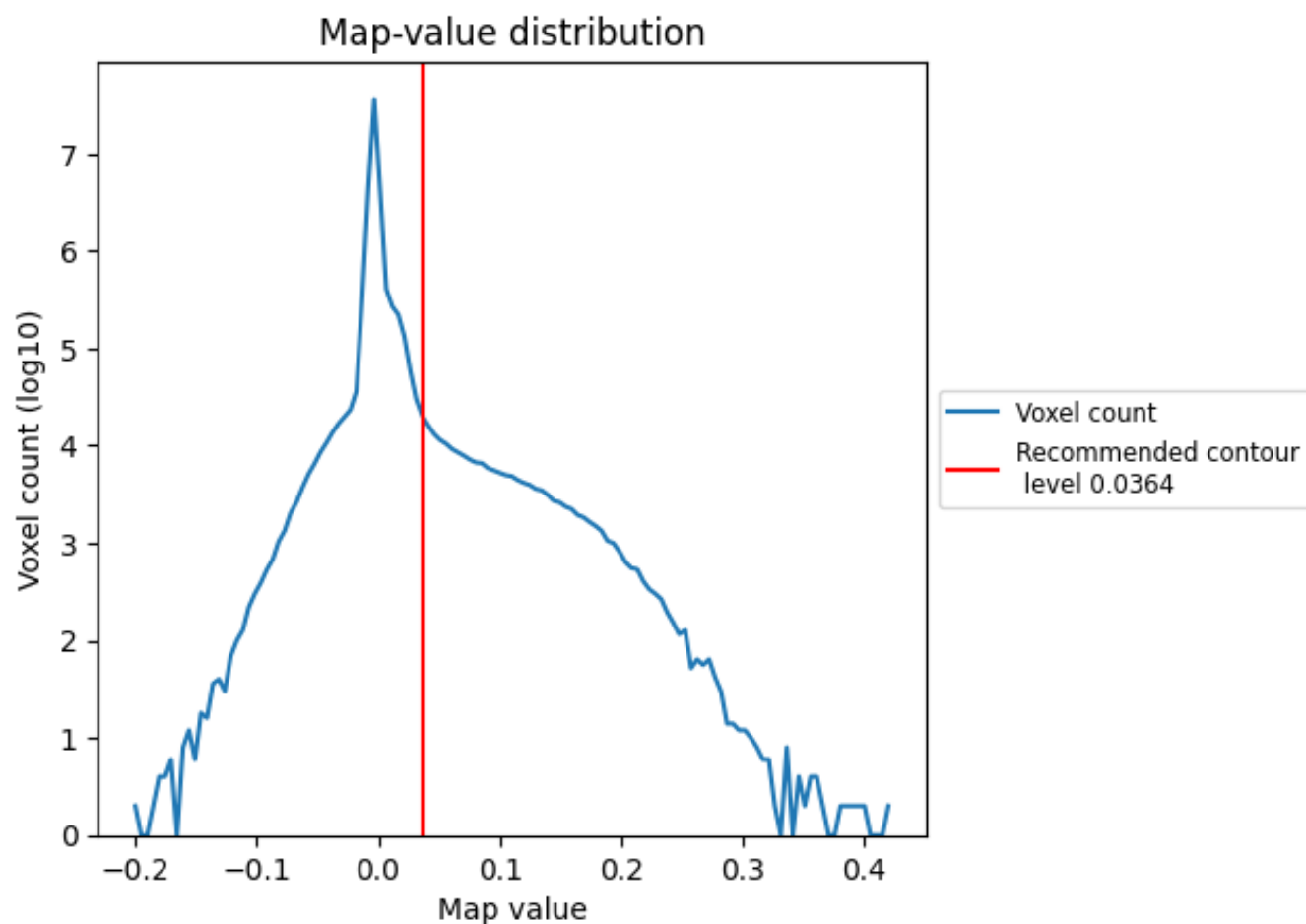


Z

7 Map analysis [i](#)

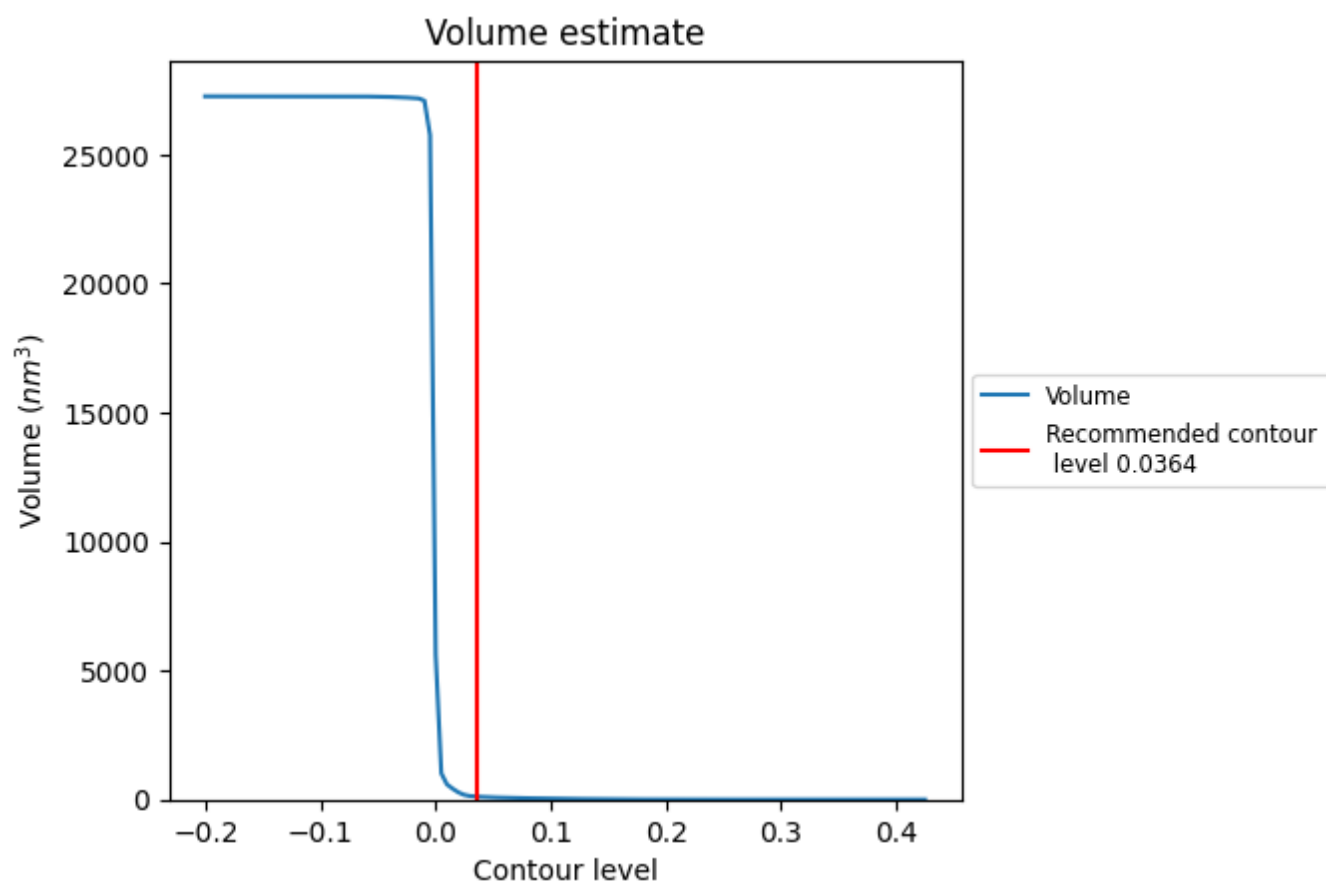
This section contains the results of statistical analysis of the map.

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.

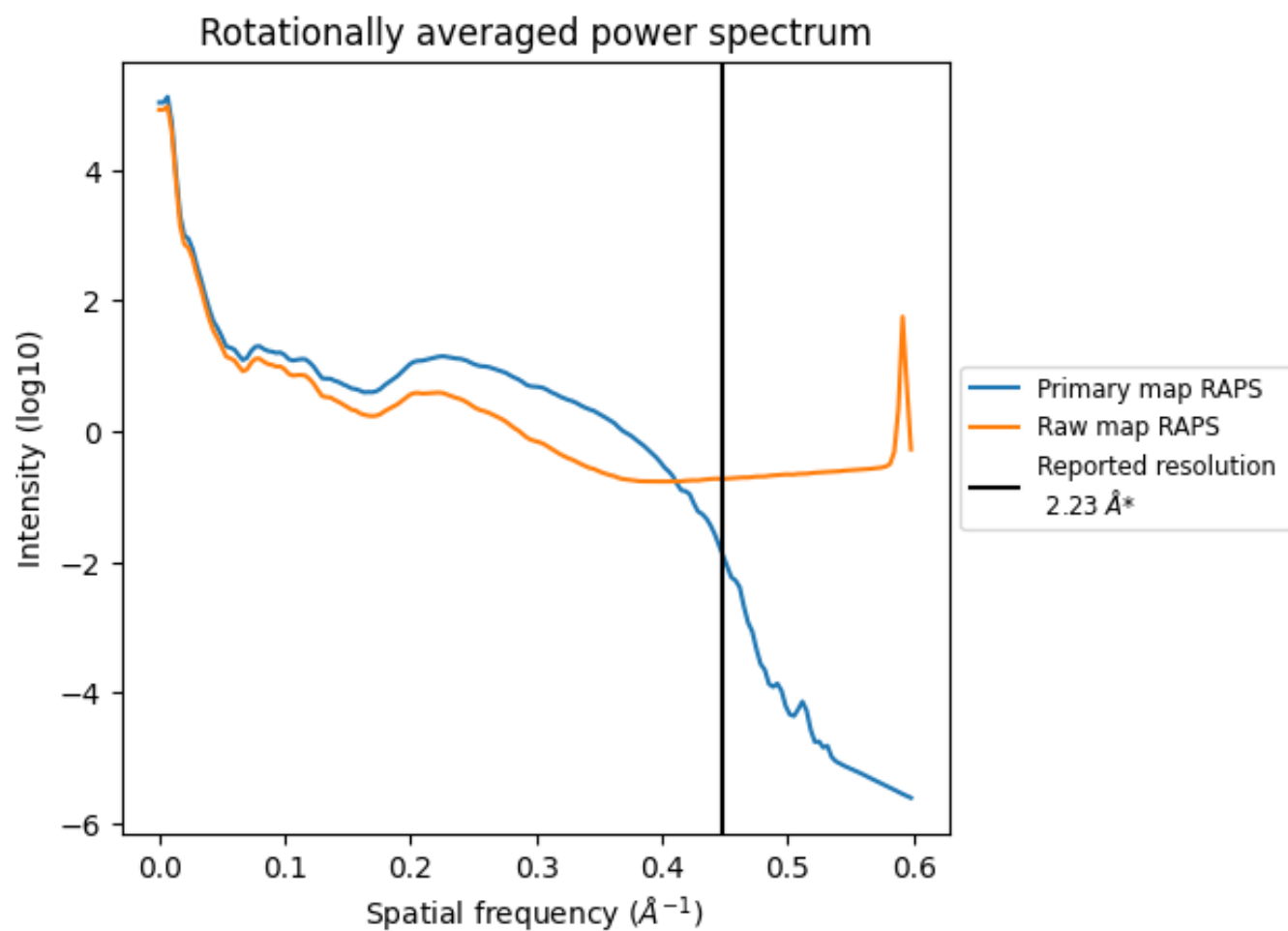
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 113 nm³; this corresponds to an approximate mass of 102 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 ⓘ

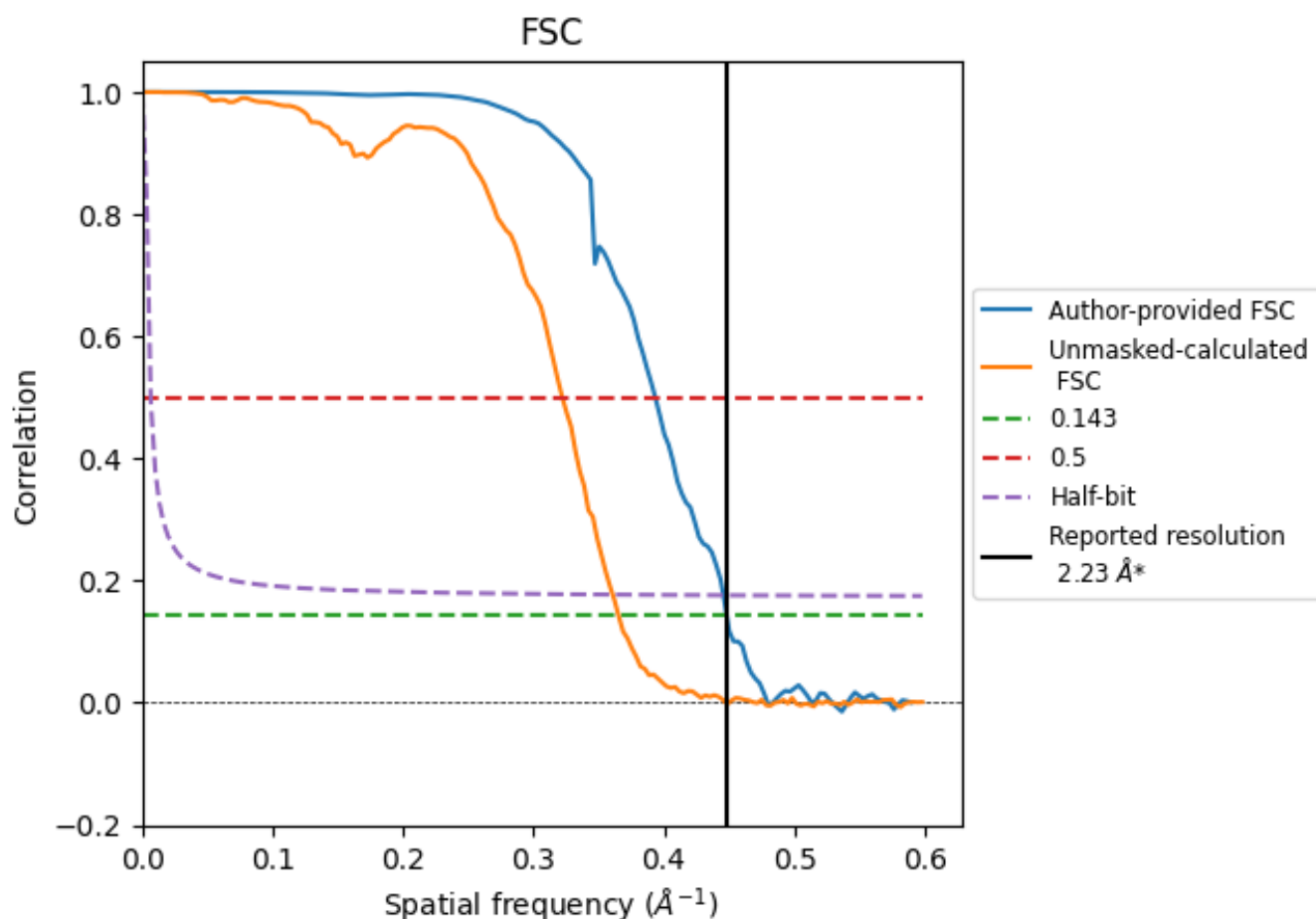


*Reported resolution corresponds to spatial frequency of 0.448 Å⁻¹

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 0.448 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

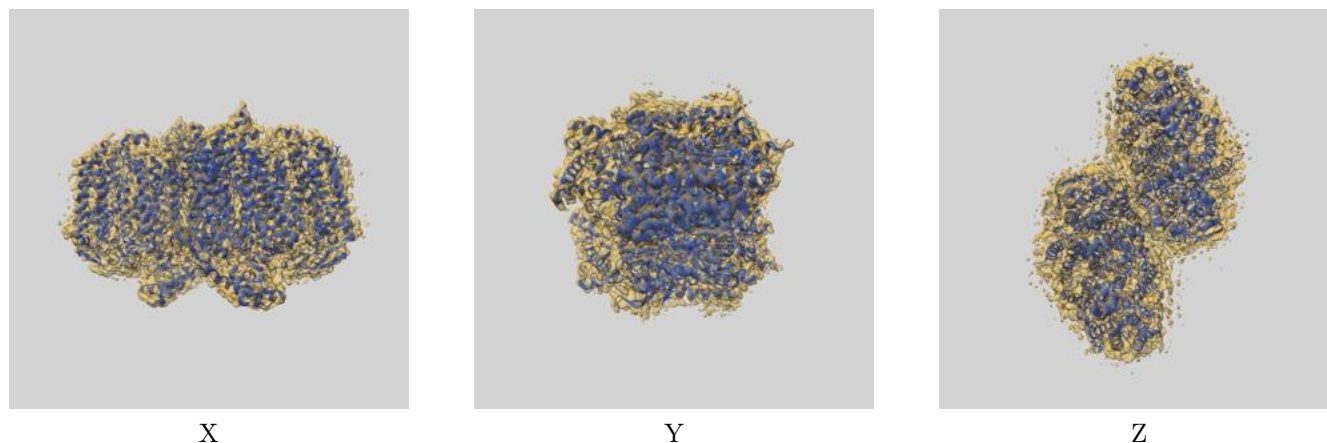
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.23	-	-
Author-provided FSC curve	2.23	2.54	2.24
Unmasked-calculated*	2.74	3.10	2.77

*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 2.74 differs from the reported value 2.23 by more than 10 %

9 Map-model fit [i](#)

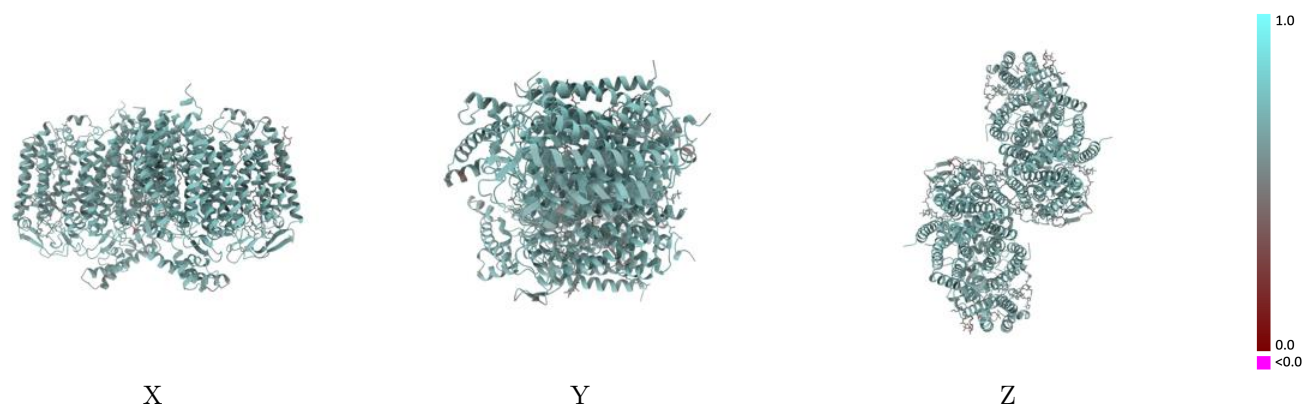
This section contains information regarding the fit between EMDB map EMD-54414 and PDB model 9RZV. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



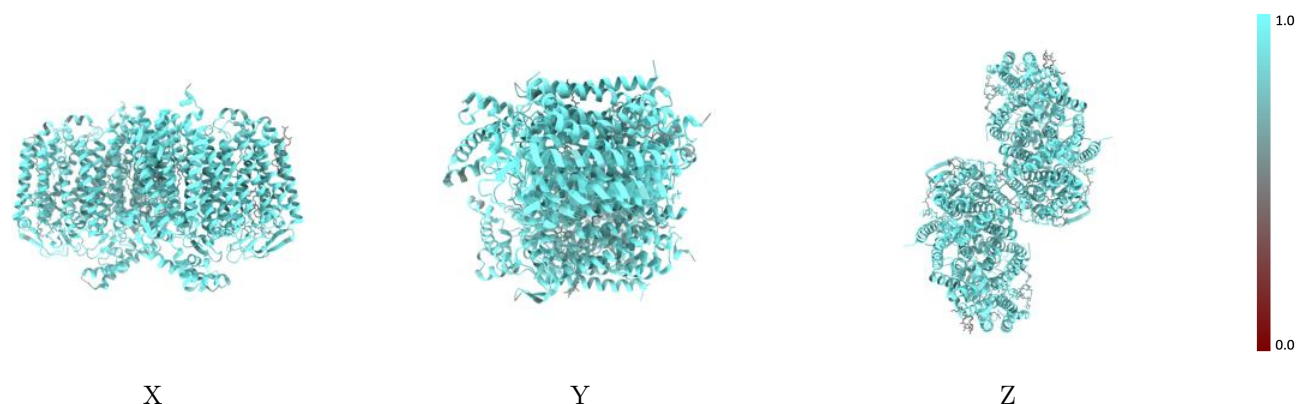
The images above show the 3D surface view of the map at the recommended contour level 0.0364 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



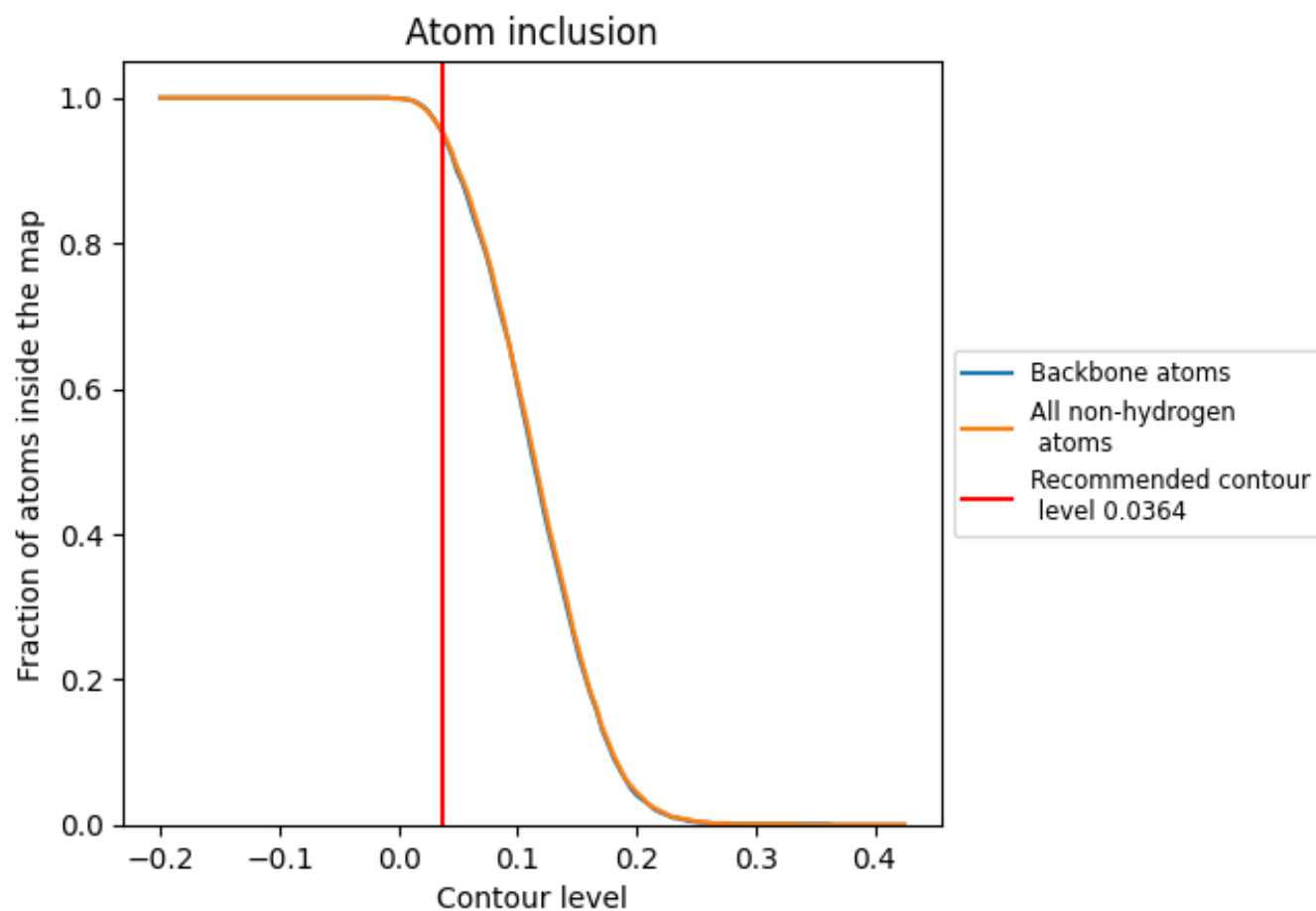
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0364).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0364) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9540	0.6560
A	0.9600	0.6630
B	0.9520	0.6450
H	0.9810	0.6560
X	0.9430	0.6550
a	0.9590	0.6630
b	0.9530	0.6450
h	0.9910	0.6630
x	0.9500	0.6590

1.0

0.0

<0.0