



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 04:33 AM UTC

PDB ID : 7SSS / pdb_00007sss
EMDB ID : EMD-25413
Title : Structure of the NADH-bound human COQ7:COQ9 complex by single-particle electron cryo-microscopy
Authors : Aydin, H.; Frost, A.
Deposited on : 2021-11-11
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

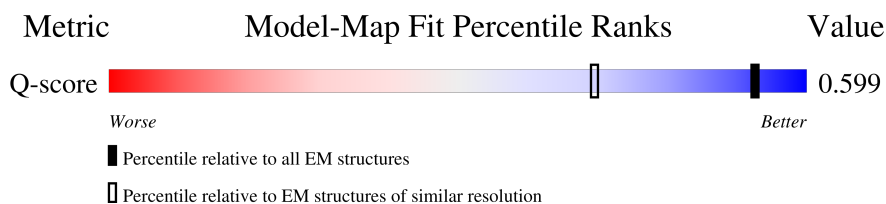
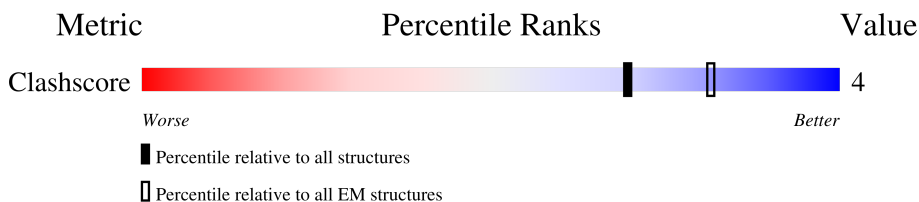
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

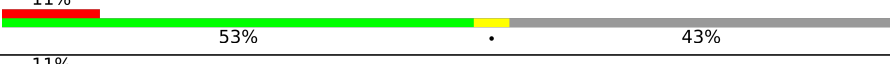
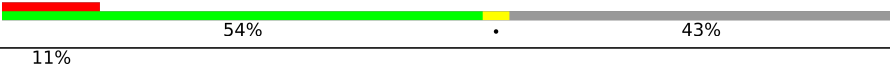
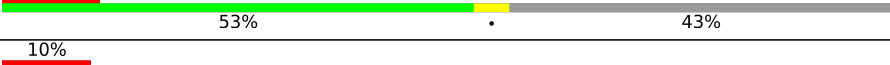
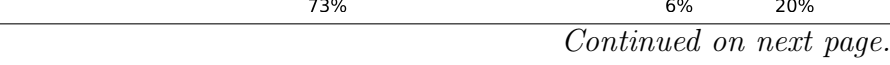
The reported resolution of this entry is 2.40 Å.

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	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	318	
1	B	318	
1	C	318	
1	D	318	
2	E	217	
2	F	217	

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Mol	Chain	Length	Quality of chain
2	G	217	
2	H	217	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12190 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.

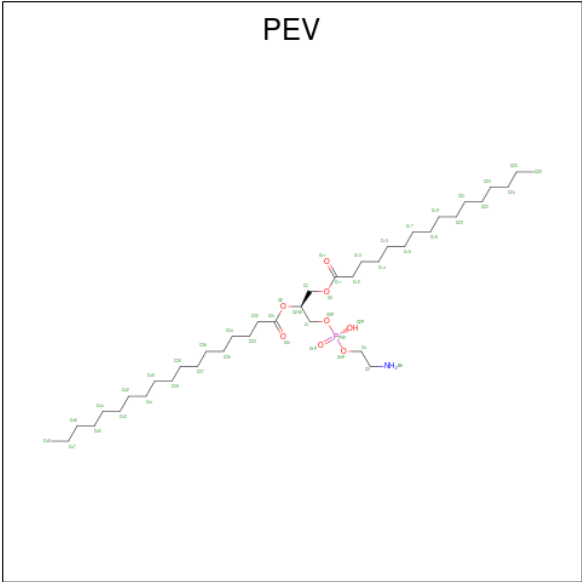
- Molecule 1 is a protein called Ubiquinone biosynthesis protein COQ9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	181	Total	C	N	O	S	1	0
			1446	909	251	276	10		
1	B	181	Total	C	N	O	S	2	0
			1461	917	256	278	10		
1	C	181	Total	C	N	O	S	1	0
			1449	910	252	277	10		
1	D	181	Total	C	N	O	S	2	0
			1457	915	256	276	10		

- Molecule 2 is a protein called 5-demethoxyubiquinone hydroxylase, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	173	Total	C	N	O	S	1	0
			1350	861	244	237	8		
2	F	173	Total	C	N	O	S	1	0
			1354	862	244	240	8		
2	G	173	Total	C	N	O	S	1	0
			1354	862	244	240	8		
2	H	173	Total	C	N	O	S	1	0
			1354	862	244	240	8		

- Molecule 3 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY]-1-[(PALMITOYL)OXY]METHYL]ETHYL STEARATE (CCD ID: PEV) (formula: C₃₉H₇₈NO₈P) (labeled as "Ligand of Interest" by depositor).



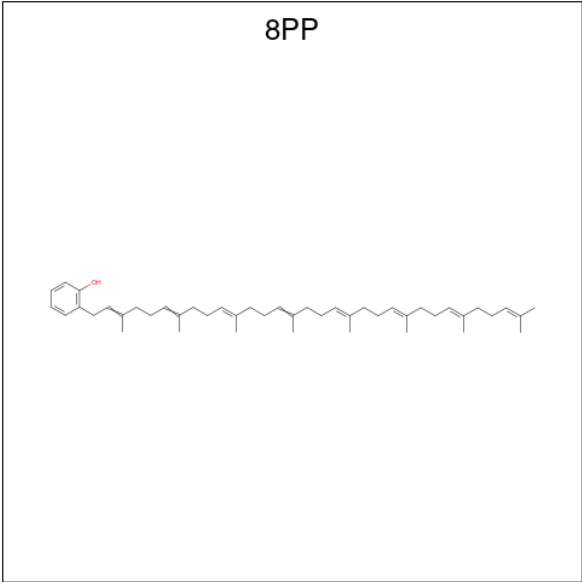
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C				0
			9	9				
3	A	1	Total	C	O	P		0
			24	15	8	1		
3	A	1	Total	C				0
			10	10				
3	B	1	Total	C				0
			8	8				
3	B	1	Total	C	O	P		0
			23	14	8	1		
3	C	1	Total	C	N	O	P	0
			26	16	1	8	1	
3	C	1	Total	C				0
			9	9				
3	C	1	Total	C	O	P		0
			23	14	8	1		
3	C	1	Total	C				0
			10	10				
3	C	1	Total	C	O	P		0
			28	19	8	1		
3	D	1	Total	C				0
			8	8				
3	D	1	Total	C	O	P		0
			24	15	8	1		
3	D	1	Total	C				0
			11	11				
3	D	1	Total	C				0
			14	14				

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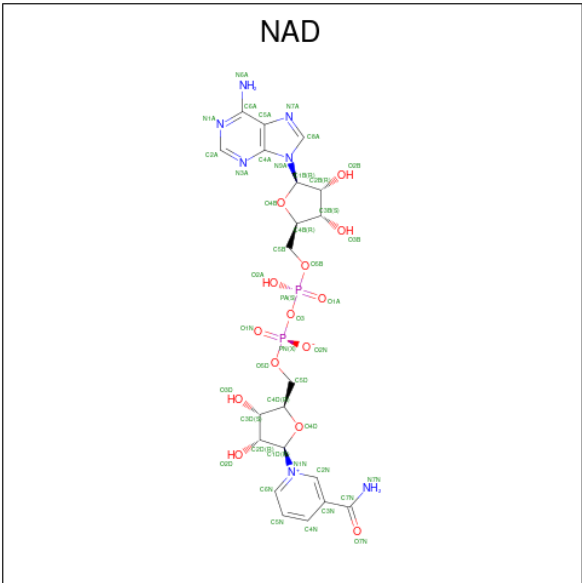
Mol	Chain	Residues	Atoms				AltConf
3	E	1	Total	C	O	P	0
			24	15	8	1	
3	E	1	Total	C	N	O	P
			27	17	1	8	1
3	E	1	Total	C	O	P	0
			28	19	8	1	
3	E	1	Total	C			0
			8	8			
3	F	1	Total	C	N	O	P
			27	17	1	8	1
3	F	1	Total	C	O	P	0
			25	16	8	1	
3	F	1	Total	C			0
			8	8			
3	F	1	Total	C			0
			13	13			
3	F	1	Total	C			0
			8	8			
3	G	1	Total	C	O	P	0
			25	16	8	1	
3	G	1	Total	C	O	P	0
			27	18	8	1	
3	G	1	Total	C			0
			14	14			
3	G	1	Total	C			0
			7	7			
3	H	1	Total	C	O	P	0
			25	16	8	1	
3	H	1	Total	C	N	O	P
			26	16	1	8	1
3	H	1	Total	C	O	P	0
			28	19	8	1	
3	H	1	Total	C			0
			7	7			
3	H	1	Total	C			0
			13	13			

- Molecule 4 is 2-[(2E,6E,10E,14E,18E,22E,26E)-3,7,11,15,19,23,27,31-OCTAMETHYLD OTRIACONTA-2,6,10,14,18,22,26,30-OCTAENYL]PHENOL (CCD ID: 8PP) (formula: C₄₆H₇₀O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
4	B	1	Total	C	O	0
			37	36	1	
4	E	1	Total	C	O	0
			35	34	1	
4	G	1	Total	C	O	0
			34	33	1	
4	H	1	Total	C	O	0
			34	33	1	

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					AltConf
5	E	1	Total	C	N	O	P	0
			44	21	7	14	2	
5	F	1	Total	C	N	O	P	0
			44	21	7	14	2	

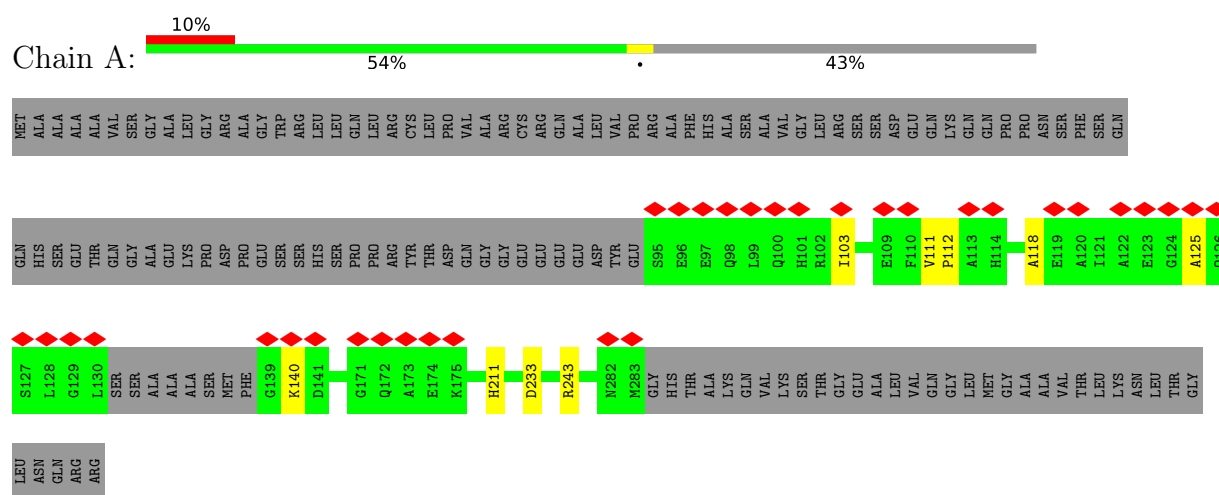
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	26	Total	O	0
			26	26	
6	B	19	Total	O	0
			19	19	
6	C	30	Total	O	0
			30	30	
6	D	31	Total	O	0
			31	31	
6	E	19	Total	O	0
			19	19	
6	F	15	Total	O	0
			15	15	
6	G	14	Total	O	0
			14	14	
6	H	16	Total	O	0
			16	16	

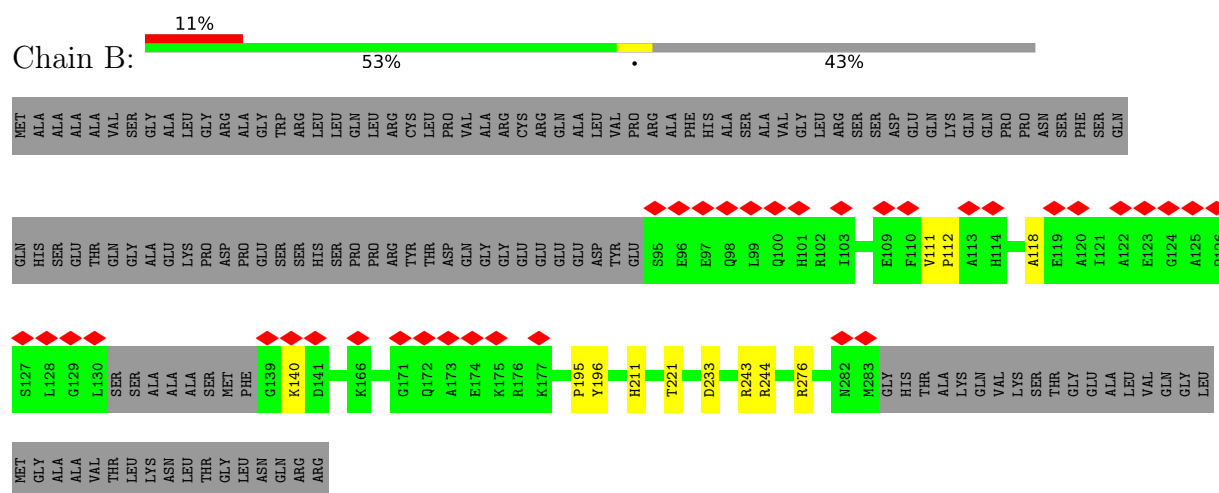
3 Residue-property plots

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.

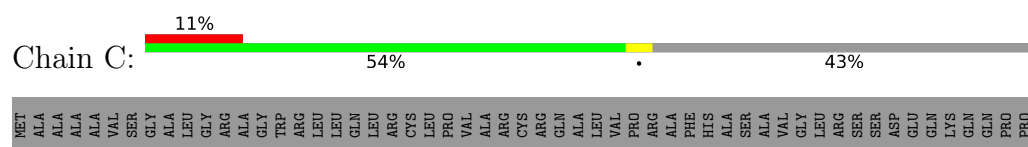
- Molecule 1: Ubiquinone biosynthesis protein COQ9, mitochondrial



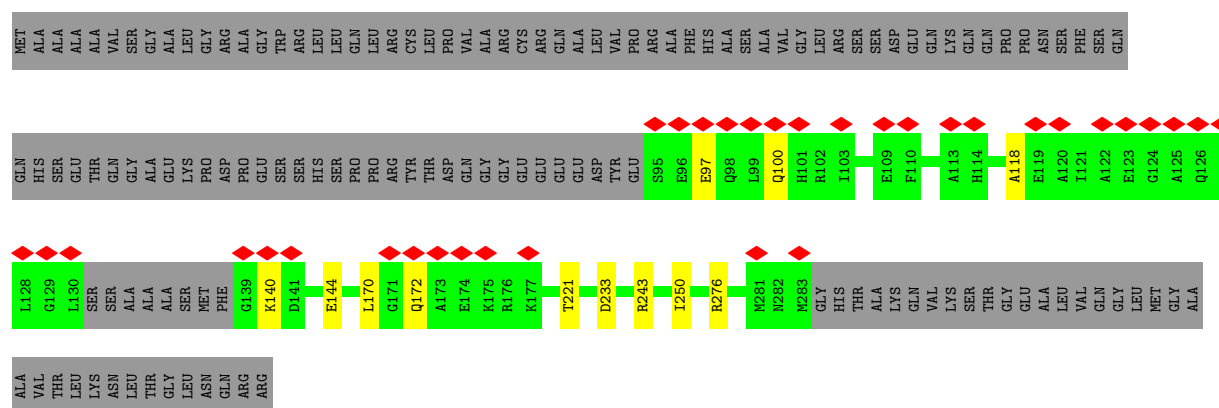
- Molecule 1: Ubiquinone biosynthesis protein COQ9, mitochondrial



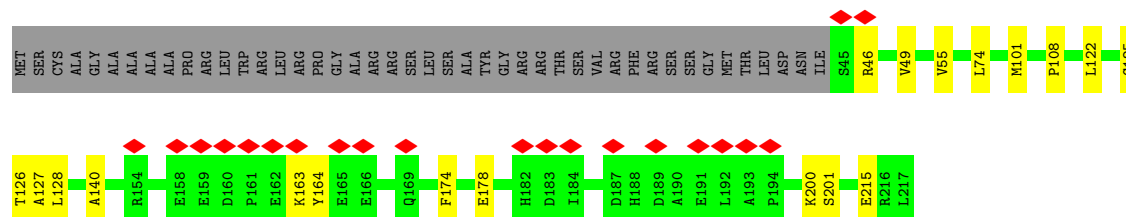
- Molecule 1: Ubiquinone biosynthesis protein COQ9, mitochondrial



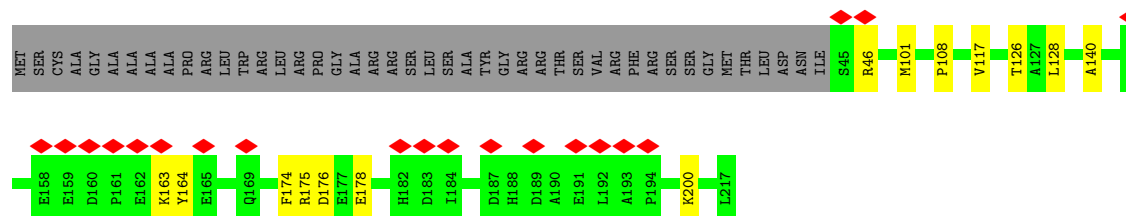
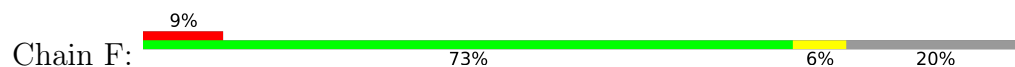
- Molecule 1: Ubiquinone biosynthesis protein COQ9, mitochondrial



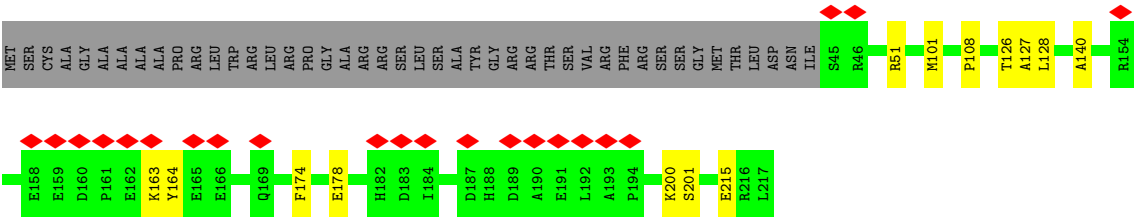
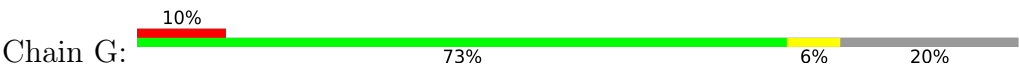
- Molecule 2: 5-demethoxyubiquinone hydroxylase, mitochondrial



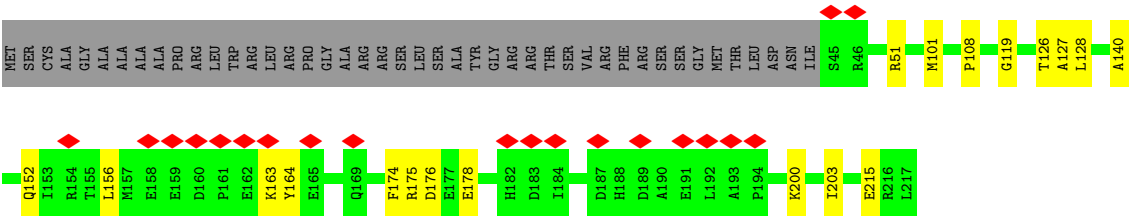
- Molecule 2: 5-demethoxyubiquinone hydroxylase, mitochondrial



- Molecule 2: 5-demethoxyubiquinone hydroxylase, mitochondrial



● Molecule 2: 5-demethoxyubiquinone hydroxylase, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	372917	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 ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.219	Depositor
Minimum map value	-0.128	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.035	Depositor
Map size ($\text{\AA}$)	213.248, 213.248, 213.248	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.833, 0.833, 0.833	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEV, NAD, 8PP

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	0.19	0/1476	0.32	0/2004
1	B	0.15	0/1491	0.27	0/2023
1	C	0.16	0/1478	0.27	0/2006
1	D	0.16	0/1487	0.27	0/2018
2	E	0.16	0/1375	0.29	0/1858
2	F	0.16	0/1379	0.29	0/1863
2	G	0.16	0/1379	0.29	0/1863
2	H	0.16	0/1379	0.29	0/1863
All	All	0.16	0/11444	0.29	0/15498

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1446	0	1378	5	0
1	B	1461	0	1396	9	0
1	C	1449	0	1378	7	0
1	D	1457	0	1392	8	0
2	E	1350	0	1359	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1354	0	1364	8	0
2	G	1354	0	1364	8	0
2	H	1354	0	1364	12	0
3	A	43	0	51	1	0
3	B	31	0	31	0	0
3	C	96	0	109	2	0
3	D	57	0	81	2	0
3	E	87	0	89	5	0
3	F	81	0	96	4	0
3	G	73	0	87	1	0
3	H	99	0	109	7	0
4	B	37	0	51	1	0
4	E	35	0	48	2	0
4	G	34	0	46	1	0
4	H	34	0	47	5	0
5	E	44	0	26	1	0
5	F	44	0	26	0	0
6	A	26	0	0	0	0
6	B	19	0	0	0	0
6	C	30	0	0	0	0
6	D	31	0	0	0	0
6	E	19	0	0	0	0
6	F	15	0	0	0	0
6	G	14	0	0	0	0
6	H	16	0	0	0	0
All	All	12190	0	11892	86	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 4.

All (86) 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:F:117:VAL:HG22	3:F:302:PEV:H122	1.69	0.74
1:C:214:PRO:HG2	3:C:405:PEV:H32	1.74	0.68
2:E:122:LEU:HD22	4:E:303:8PP:H112	1.84	0.59
1:C:233:ASP:OD1	1:C:243:ARG:NH1	2.37	0.57
2:E:101:MET:HE1	2:E:108:PRO:HA	1.85	0.57
2:H:101:MET:HE1	2:H:108:PRO:HA	1.86	0.57
2:G:101:MET:HE1	2:G:108:PRO:HA	1.86	0.56
1:B:221:THR:HG21	3:H:302:PEV:H31	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:101:MET:HE1	2:F:108:PRO:HA	1.87	0.55
2:H:175:ARG:NH1	2:H:176:ASP:OD1	2.39	0.55
2:F:175:ARG:NH1	2:F:176:ASP:OD1	2.39	0.55
1:A:233:ASP:OD1	1:A:243:ARG:NH1	2.37	0.55
2:F:140:ALA:HB2	2:F:200:LYS:HG3	1.89	0.55
2:G:140:ALA:HB2	2:G:200:LYS:HG3	1.89	0.54
1:D:97:GLU:O	1:D:100:GLN:NE2	2.41	0.53
2:E:140:ALA:HB2	2:E:200:LYS:HG3	1.90	0.53
1:A:118:ALA:HB2	1:A:140:LYS:HA	1.89	0.53
2:H:51:ARG:HG3	2:H:215:GLU:HB2	1.90	0.53
1:D:221:THR:HG21	3:E:302:PEV:H31	1.91	0.53
1:D:250:ILE:HG12	1:D:276[A]:ARG:HG3	1.91	0.53
1:C:249:ALA:HB2	3:E:301:PEV:H122	1.92	0.52
1:C:118:ALA:HB2	1:C:140:LYS:HA	1.90	0.52
2:G:51:ARG:HG3	2:G:215:GLU:HB2	1.91	0.52
2:H:140:ALA:HB2	2:H:200:LYS:HG3	1.90	0.52
1:B:118:ALA:HB2	1:B:140:LYS:HA	1.91	0.51
2:H:203:ILE:HG12	4:H:303:8PP:H18	1.93	0.50
1:D:118:ALA:HB2	1:D:140:LYS:HA	1.94	0.49
1:B:233:ASP:OD1	1:B:243:ARG:NH1	2.42	0.49
4:B:403:8PP:H172	4:B:403:8PP:H151	1.53	0.48
3:A:401:PEV:H161	3:H:305:PEV:H212	1.95	0.48
4:G:302:8PP:H172	4:G:302:8PP:H151	1.50	0.47
3:D:402:PEV:H122	3:E:302:PEV:H2	1.97	0.47
5:E:306:NAD:H6N	5:E:306:NAD:H2D	1.74	0.47
3:H:306:PEV:H151	3:H:306:PEV:H181	1.50	0.47
2:E:125:GLY:HA3	4:E:303:8PP:H271	1.96	0.47
3:F:302:PEV:H121	3:F:302:PEV:H151	1.51	0.46
3:C:404:PEV:H221	3:C:404:PEV:H251	1.48	0.46
1:A:103:ILE:HG23	1:A:125:ALA:HB2	1.97	0.46
3:D:404:PEV:H171	3:D:404:PEV:H141	1.74	0.45
4:H:303:8PP:H201	4:H:303:8PP:H222	1.69	0.45
2:E:46:ARG:HA	2:E:49:VAL:HG12	1.99	0.44
2:F:174:PHE:O	2:F:178:GLU:HG2	2.17	0.44
1:B:276[B]:ARG:HD3	1:B:276[B]:ARG:HA	1.78	0.44
2:G:174:PHE:O	2:G:178:GLU:HG2	2.17	0.44
2:H:119:GLY:HA2	4:H:303:8PP:H102	1.99	0.44
3:E:304:PEV:H321	3:E:304:PEV:H352	1.31	0.44
1:C:249:ALA:HB2	3:E:301:PEV:H141	2.00	0.44
3:F:305:PEV:H202	3:F:305:PEV:H172	1.42	0.43
1:D:144:GLU:CD	1:D:144:GLU:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:SER:HB3	2:E:128:LEU:HB3	2.01	0.43
4:H:303:8PP:H172	4:H:303:8PP:H151	1.56	0.43
2:E:174:PHE:O	2:E:178:GLU:HG2	2.19	0.43
3:H:302:PEV:H121	3:H:302:PEV:H151	1.74	0.43
3:H:306:PEV:H182	3:H:306:PEV:H212	1.75	0.43
1:B:111:VAL:N	1:B:112:PRO:HD2	2.34	0.43
1:C:111:VAL:N	1:C:112:PRO:HD2	2.34	0.43
3:H:304:PEV:H351	3:H:304:PEV:H382	1.59	0.42
2:H:174:PHE:O	2:H:178:GLU:HG2	2.18	0.42
1:B:211:HIS:ND1	2:E:201:SER:OG	2.32	0.42
1:A:211:HIS:ND1	2:G:201:SER:OG	2.33	0.42
1:D:233:ASP:OD1	1:D:243:ARG:NH1	2.42	0.42
1:D:276[B]:ARG:HA	1:D:276[B]:ARG:HD3	1.78	0.42
1:B:211:HIS:HD1	2:E:201:SER:HG	1.63	0.42
2:E:74:LEU:HG	2:E:127:ALA:HB1	2.01	0.42
2:E:55:VAL:HB	2:E:215:GLU:HB3	2.01	0.42
2:E:163:LYS:HE3	2:E:164:TYR:CZ	2.55	0.42
2:H:163:LYS:HE3	2:H:164:TYR:CZ	2.55	0.42
1:A:111:VAL:N	1:A:112:PRO:HD2	2.35	0.41
2:H:156:LEU:HD12	2:H:156:LEU:HA	1.93	0.41
2:F:126:THR:C	2:F:128:LEU:H	2.29	0.41
2:G:163:LYS:HE3	2:G:164:TYR:CZ	2.55	0.41
2:H:152:GLN:O	2:H:156:LEU:HB2	2.20	0.41
1:B:244:ARG:HB3	3:H:302:PEV:H152	2.02	0.41
2:F:46:ARG:HA	2:F:46:ARG:HD3	1.88	0.41
3:F:303:PEV:H202	3:F:305:PEV:H162	2.03	0.41
3:G:303:PEV:H151	3:G:303:PEV:H121	1.62	0.41
2:G:126:THR:C	2:G:128:LEU:H	2.29	0.40
4:H:303:8PP:H322	4:H:303:8PP:H28	1.70	0.40
2:G:126:THR:O	2:G:127:ALA:HB3	2.22	0.40
1:B:195:PRO:HG2	1:B:196:TYR:CE2	2.57	0.40
2:E:126:THR:C	2:E:128:LEU:H	2.30	0.40
2:H:126:THR:C	2:H:128:LEU:H	2.30	0.40
2:H:126:THR:O	2:H:127:ALA:HB3	2.22	0.40
1:D:170:LEU:HB2	1:D:172:GLN:OE1	2.20	0.40
2:E:126:THR:O	2:E:127:ALA:HB3	2.21	0.40
2:F:163:LYS:HE3	2:F:164:TYR:CZ	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

38 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	$\# Z > 2$
3	PEV	C	404	-	9,9,48	0.11	0	8,8,53	0.08	0
3	PEV	F	305	-	7,7,48	0.13	0	6,6,53	0.10	0
3	PEV	C	402	-	8,8,48	0.13	0	7,7,53	0.10	0
3	PEV	E	301	-	23,23,48	0.52	0	26,28,53	0.64	1 (3%)
3	PEV	E	302	-	26,26,48	0.37	0	29,31,53	0.38	0
4	8PP	B	403	-	37,37,47	0.27	0	45,45,57	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEV	C	403	-	22,22,48	0.52	0	25,27,53	0.65	1 (4%)
3	PEV	G	304	-	13,13,48	0.13	0	12,12,53	0.07	0
3	PEV	F	302	-	24,24,48	0.50	0	27,29,53	0.64	1 (3%)
3	PEV	E	304	-	27,27,48	0.47	0	30,32,53	0.58	1 (3%)
4	8PP	H	303	-	34,34,47	0.25	0	40,41,57	0.25	0
3	PEV	D	401	-	7,7,48	0.11	0	6,6,53	0.10	0
3	PEV	D	404	-	13,13,48	0.14	0	12,12,53	0.09	0
3	PEV	F	304	-	12,12,48	0.12	0	11,11,53	0.08	0
3	PEV	D	403	-	10,10,48	0.11	0	9,9,53	0.08	0
3	PEV	G	301	-	24,24,48	0.50	0	27,29,53	0.69	1 (3%)
3	PEV	C	405	-	27,27,48	0.47	0	30,32,53	0.60	1 (3%)
3	PEV	H	306	-	12,12,48	0.12	0	11,11,53	0.09	0
3	PEV	A	403	-	9,9,48	0.10	0	8,8,53	0.09	0
3	PEV	C	401	-	25,25,48	0.38	0	28,30,53	0.49	0
3	PEV	B	402	-	22,22,48	0.51	0	25,27,53	0.68	1 (4%)
4	8PP	E	303	-	35,35,47	0.30	0	42,42,57	0.24	0
3	PEV	F	301	-	26,26,48	0.37	0	29,31,53	0.41	0
3	PEV	G	303	-	26,26,48	0.48	0	29,31,53	0.58	1 (3%)
3	PEV	H	302	-	25,25,48	0.36	0	28,30,53	0.44	0
3	PEV	H	305	-	6,6,48	0.12	0	5,5,53	0.13	0
3	PEV	H	304	-	27,27,48	0.48	0	30,32,53	0.59	1 (3%)
3	PEV	H	301	-	24,24,48	0.50	0	27,29,53	0.61	1 (3%)
3	PEV	F	303	-	7,7,48	0.11	0	6,6,53	0.10	0
3	PEV	G	305	-	6,6,48	0.12	0	5,5,53	0.11	0
4	8PP	G	302	-	34,34,47	0.24	0	40,41,57	0.22	0
3	PEV	A	402	-	23,23,48	0.51	0	26,28,53	0.64	1 (3%)
3	PEV	B	401	-	7,7,48	0.11	0	6,6,53	0.10	0
5	NAD	E	306	-	46,48,48	0.58	1 (2%)	64,73,73	0.57	1 (1%)
3	PEV	D	402	-	23,23,48	0.50	0	26,28,53	0.66	1 (3%)
3	PEV	A	401	-	8,8,48	0.13	0	7,7,53	0.14	0
5	NAD	F	306	-	46,48,48	0.62	1 (2%)	64,73,73	0.54	1 (1%)
3	PEV	E	305	-	7,7,48	0.13	0	6,6,53	0.11	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEV	C	404	-	-	6/7/7/52	-
3	PEV	F	305	-	-	4/5/5/52	-
3	PEV	C	402	-	-	6/6/6/52	-
3	PEV	E	301	-	-	12/25/25/52	-
3	PEV	E	302	-	-	14/30/30/52	-
4	8PP	B	403	-	-	19/35/35/47	0/1/1/1
3	PEV	C	403	-	-	13/24/24/52	-
3	PEV	G	304	-	-	8/11/11/52	-
3	PEV	F	302	-	-	13/26/26/52	-
3	PEV	E	304	-	-	14/29/29/52	-
4	8PP	H	303	-	-	12/32/32/47	0/1/1/1
3	PEV	D	401	-	-	2/5/5/52	-
3	PEV	D	404	-	-	5/11/11/52	-
3	PEV	F	304	-	-	3/10/10/52	-
3	PEV	D	403	-	-	4/8/8/52	-
3	PEV	G	301	-	-	8/26/26/52	-
3	PEV	C	405	-	-	16/29/29/52	-
3	PEV	H	306	-	-	7/10/10/52	-
3	PEV	A	403	-	-	5/7/7/52	-
3	PEV	C	401	-	-	22/29/29/52	-
3	PEV	B	402	-	-	15/24/24/52	-
4	8PP	E	303	-	-	17/33/33/47	0/1/1/1
3	PEV	F	301	-	-	10/30/30/52	-
3	PEV	G	303	-	-	13/28/28/52	-
3	PEV	H	302	-	-	12/29/29/52	-
3	PEV	H	305	-	-	3/4/4/52	-
3	PEV	H	304	-	-	12/29/29/52	-
3	PEV	H	301	-	-	15/26/26/52	-
3	PEV	F	303	-	-	2/5/5/52	-
3	PEV	G	305	-	-	4/4/4/52	-
4	8PP	G	302	-	-	16/32/32/47	0/1/1/1
3	PEV	A	402	-	-	14/25/25/52	-
3	PEV	B	401	-	-	2/5/5/52	-
5	NAD	E	306	-	-	12/30/62/62	0/5/5/5
3	PEV	D	402	-	-	16/25/25/52	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEV	A	401	-	-	4/6/6/52	-
5	NAD	F	306	-	-	10/30/62/62	0/5/5/5
3	PEV	E	305	-	-	3/5/5/52	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	306	NAD	C2N-N1N	2.52	1.37	1.35
5	E	306	NAD	C2N-N1N	2.45	1.37	1.35

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	306	NAD	C6N-N1N-C2N	-2.80	119.50	121.88
5	F	306	NAD	C6N-N1N-C2N	-2.70	119.58	121.88
3	F	302	PEV	O2P-P-O1P	2.41	120.24	110.83
3	E	301	PEV	O2P-P-O1P	2.41	120.21	110.83
3	H	301	PEV	O2P-P-O1P	2.39	120.14	110.83
3	E	304	PEV	O2P-P-O1P	2.39	120.13	110.83
3	D	402	PEV	O2P-P-O1P	2.38	120.10	110.83
3	C	403	PEV	O2P-P-O1P	2.37	120.06	110.83
3	B	402	PEV	O2P-P-O1P	2.36	120.05	110.83
3	C	405	PEV	O2P-P-O1P	2.34	119.95	110.83
3	A	402	PEV	O2P-P-O1P	2.34	119.93	110.83
3	G	301	PEV	O2P-P-O1P	2.33	119.93	110.83
3	H	304	PEV	O2P-P-O1P	2.32	119.87	110.83
3	G	303	PEV	O2P-P-O1P	2.32	119.86	110.83

There are no chirality outliers.

All (373) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	PEV	O31-C31-O2-C2
3	A	402	PEV	C1-O3P-P-O1P
3	A	402	PEV	C1-O3P-P-O2P
3	A	402	PEV	C1-O3P-P-O4P
3	B	402	PEV	C32-C31-O2-C2
3	B	402	PEV	O3P-C1-C2-O2
3	B	402	PEV	C1-O3P-P-O1P
3	B	402	PEV	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
3	B	402	PEV	C1-O3P-P-O4P
3	C	401	PEV	C4-O4P-P-O3P
3	C	401	PEV	C4-O4P-P-O1P
3	C	401	PEV	C4-O4P-P-O2P
3	C	401	PEV	O4P-C4-C5-N6
3	C	403	PEV	C1-O3P-P-O1P
3	C	403	PEV	C1-O3P-P-O2P
3	D	402	PEV	C32-C31-O2-C2
3	D	402	PEV	C1-O3P-P-O1P
3	D	402	PEV	C1-O3P-P-O2P
3	D	402	PEV	C1-O3P-P-O4P
3	E	301	PEV	C1-O3P-P-O1P
3	E	301	PEV	C1-O3P-P-O2P
3	E	301	PEV	C1-O3P-P-O4P
3	E	302	PEV	C4-O4P-P-O3P
3	E	302	PEV	C4-O4P-P-O1P
3	E	302	PEV	C4-O4P-P-O2P
3	E	304	PEV	C1-O3P-P-O1P
3	F	301	PEV	C1-O3P-P-O1P
3	F	301	PEV	C1-O3P-P-O2P
3	F	301	PEV	C1-O3P-P-O4P
3	F	302	PEV	C1-O3P-P-O1P
3	F	302	PEV	C1-O3P-P-O2P
3	F	302	PEV	C1-O3P-P-O4P
3	G	301	PEV	O11-C11-O3-C3
3	G	301	PEV	C12-C11-O3-C3
3	G	303	PEV	C32-C31-O2-C2
3	G	303	PEV	C1-O3P-P-O2P
3	G	303	PEV	C1-O3P-P-O4P
3	G	303	PEV	C12-C11-O3-C3
3	H	301	PEV	C32-C31-O2-C2
3	H	301	PEV	C1-O3P-P-O1P
3	H	301	PEV	C1-O3P-P-O2P
3	H	301	PEV	C1-O3P-P-O4P
3	H	301	PEV	O11-C11-O3-C3
3	H	301	PEV	C12-C11-O3-C3
3	H	302	PEV	O4P-C4-C5-N6
3	H	304	PEV	C1-O3P-P-O2P
3	H	304	PEV	C1-O3P-P-O4P
4	B	403	8PP	C7-C8-C9-C10
4	B	403	8PP	C7-C8-C9-C11
4	B	403	8PP	C9-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
4	B	403	8PP	C17-C18-C19-C20
4	B	403	8PP	C18-C19-C21-C22
4	B	403	8PP	C20-C19-C21-C22
4	B	403	8PP	C27-C28-C29-C30
4	B	403	8PP	C27-C28-C29-C31
4	B	403	8PP	C32-C33-C34-C36
4	E	303	8PP	C12-C13-C14-C15
4	E	303	8PP	C12-C13-C14-C16
4	E	303	8PP	C22-C23-C24-C25
4	E	303	8PP	C22-C23-C24-C26
4	E	303	8PP	C24-C26-C27-C28
4	E	303	8PP	C27-C28-C29-C30
4	E	303	8PP	C27-C28-C29-C31
4	E	303	8PP	C29-C31-C32-C33
4	G	302	8PP	C7-C8-C9-C10
4	G	302	8PP	C7-C8-C9-C11
4	G	302	8PP	C9-C11-C12-C13
4	G	302	8PP	C17-C18-C19-C20
4	G	302	8PP	C17-C18-C19-C21
4	G	302	8PP	C22-C23-C24-C25
4	G	302	8PP	C22-C23-C24-C26
4	G	302	8PP	C27-C28-C29-C30
4	G	302	8PP	C27-C28-C29-C31
4	H	303	8PP	C7-C8-C9-C10
4	H	303	8PP	C7-C8-C9-C11
4	H	303	8PP	C20-C19-C21-C22
4	H	303	8PP	C19-C21-C22-C23
5	E	306	NAD	C5B-O5B-PA-O3
5	E	306	NAD	O4D-C1D-N1N-C2N
5	E	306	NAD	O4D-C1D-N1N-C6N
5	E	306	NAD	C2D-C1D-N1N-C2N
5	E	306	NAD	C2N-C3N-C7N-O7N
5	E	306	NAD	C2N-C3N-C7N-N7N
5	F	306	NAD	C5B-O5B-PA-O1A
5	F	306	NAD	C5B-O5B-PA-O2A
5	F	306	NAD	C5B-O5B-PA-O3
5	F	306	NAD	C2B-C1B-N9A-C8A
5	F	306	NAD	C2B-C1B-N9A-C4A
3	C	401	PEV	O11-C11-O3-C3
3	F	302	PEV	O11-C11-O3-C3
3	G	303	PEV	O11-C11-O3-C3
5	E	306	NAD	C4N-C3N-C7N-O7N

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Mol	Chain	Res	Type	Atoms
5	E	306	NAD	C4N-C3N-C7N-N7N
4	B	403	8PP	C32-C33-C34-C35
3	C	401	PEV	C12-C11-O3-C3
3	F	302	PEV	C12-C11-O3-C3
3	B	402	PEV	O11-C11-O3-C3
3	C	403	PEV	O11-C11-O3-C3
3	H	302	PEV	O11-C11-O3-C3
3	B	402	PEV	O31-C31-O2-C2
3	D	402	PEV	O31-C31-O2-C2
3	G	303	PEV	O31-C31-O2-C2
3	H	301	PEV	O31-C31-O2-C2
3	B	402	PEV	C12-C11-O3-C3
3	H	302	PEV	C12-C11-O3-C3
3	A	402	PEV	C32-C31-O2-C2
4	B	403	8PP	C15-C14-C16-C17
4	E	303	8PP	C15-C14-C16-C17
4	G	302	8PP	C15-C14-C16-C17
4	G	302	8PP	C20-C19-C21-C22
4	B	403	8PP	C13-C14-C16-C17
4	E	303	8PP	C13-C14-C16-C17
4	G	302	8PP	C13-C14-C16-C17
4	G	302	8PP	C18-C19-C21-C22
4	H	303	8PP	C18-C19-C21-C22
3	C	403	PEV	C12-C11-O3-C3
4	B	403	8PP	C22-C23-C24-C25
4	H	303	8PP	C22-C23-C24-C25
4	B	403	8PP	C17-C18-C19-C21
4	B	403	8PP	C22-C23-C24-C26
4	H	303	8PP	C22-C23-C24-C26
3	D	402	PEV	O11-C11-O3-C3
3	E	301	PEV	O31-C31-O2-C2
3	H	306	PEV	C15-C16-C17-C18
3	G	304	PEV	C21-C22-C23-C24
3	A	402	PEV	C12-C11-O3-C3
3	E	302	PEV	C12-C11-O3-C3
3	D	404	PEV	C16-C17-C18-C19
3	E	301	PEV	C32-C31-O2-C2
3	G	301	PEV	C32-C31-O2-C2
3	H	302	PEV	C32-C31-O2-C2
3	D	402	PEV	C12-C11-O3-C3
3	A	402	PEV	O11-C11-O3-C3
4	H	303	8PP	C24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
3	E	302	PEV	O11-C11-O3-C3
3	E	304	PEV	C32-C33-C34-C35
3	F	305	PEV	C17-C18-C19-C20
3	C	404	PEV	C22-C23-C24-C25
3	D	403	PEV	C21-C22-C23-C24
3	G	303	PEV	C12-C13-C14-C15
3	G	304	PEV	C18-C19-C20-C21
3	G	301	PEV	O31-C31-O2-C2
3	H	302	PEV	O31-C31-O2-C2
3	C	405	PEV	C12-C11-O3-C3
3	F	302	PEV	C12-C13-C14-C15
3	C	405	PEV	C34-C35-C36-C37
3	D	404	PEV	C14-C15-C16-C17
3	F	304	PEV	C16-C17-C18-C19
4	H	303	8PP	C15-C14-C16-C17
4	H	303	8PP	C13-C14-C16-C17
3	H	306	PEV	C18-C19-C20-C21
3	A	402	PEV	C32-C33-C34-C35
4	H	303	8PP	C29-C31-C32-C33
3	C	403	PEV	C32-C33-C34-C35
3	E	305	PEV	C17-C18-C19-C20
3	B	402	PEV	C11-C12-C13-C14
3	D	402	PEV	C31-C32-C33-C34
3	H	302	PEV	C31-C32-C33-C34
4	B	403	8PP	C29-C31-C32-C33
4	G	302	8PP	C24-C26-C27-C28
3	G	303	PEV	C11-C12-C13-C14
3	F	302	PEV	C32-C31-O2-C2
3	C	401	PEV	C11-C12-C13-C14
3	C	405	PEV	C31-C32-C33-C34
3	E	302	PEV	C11-C12-C13-C14
3	E	304	PEV	C31-C32-C33-C34
3	C	405	PEV	O11-C11-O3-C3
3	H	304	PEV	C35-C36-C37-C38
3	F	302	PEV	O31-C31-O2-C2
3	A	403	PEV	C19-C20-C21-C22
3	F	301	PEV	C11-C12-C13-C14
3	H	304	PEV	C31-C32-C33-C34
3	G	301	PEV	C12-C13-C14-C15
3	F	301	PEV	C31-C32-C33-C34
3	G	305	PEV	C19-C20-C21-C22
3	H	304	PEV	C32-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
3	F	303	PEV	C15-C16-C17-C18
3	C	405	PEV	C11-C12-C13-C14
5	F	306	NAD	O4D-C4D-C5D-O5D
3	B	402	PEV	C12-C13-C14-C15
3	G	304	PEV	C20-C21-C22-C23
3	H	301	PEV	C32-C33-C34-C35
3	H	306	PEV	C19-C20-C21-C22
3	F	301	PEV	C33-C34-C35-C36
3	F	304	PEV	C19-C20-C21-C22
3	G	304	PEV	C15-C16-C17-C18
3	C	401	PEV	C31-C32-C33-C34
3	D	402	PEV	C11-C12-C13-C14
3	G	303	PEV	C32-C33-C34-C35
3	E	304	PEV	C36-C37-C38-C39
3	A	402	PEV	C12-C13-C14-C15
3	A	401	PEV	C16-C17-C18-C19
3	C	403	PEV	C12-C13-C14-C15
3	B	401	PEV	C18-C19-C20-C21
3	F	302	PEV	C32-C33-C34-C35
3	H	304	PEV	O31-C31-O2-C2
3	C	402	PEV	C19-C20-C21-C22
3	E	302	PEV	C33-C34-C35-C36
3	E	304	PEV	C12-C13-C14-C15
3	F	303	PEV	C18-C19-C20-C21
3	C	401	PEV	C32-C31-O2-C2
3	C	405	PEV	C32-C31-O2-C2
3	E	304	PEV	C32-C31-O2-C2
3	F	301	PEV	C32-C31-O2-C2
3	G	304	PEV	C17-C18-C19-C20
3	F	301	PEV	O31-C31-O2-C2
3	F	302	PEV	C33-C34-C35-C36
3	F	304	PEV	C13-C14-C15-C16
3	G	303	PEV	C14-C15-C16-C17
5	F	306	NAD	C3D-C4D-C5D-O5D
3	C	401	PEV	O31-C31-O2-C2
3	C	402	PEV	C20-C21-C22-C23
3	E	302	PEV	C32-C33-C34-C35
3	B	401	PEV	C16-C17-C18-C19
3	C	405	PEV	O31-C31-O2-C2
3	E	304	PEV	O31-C31-O2-C2
3	C	402	PEV	C23-C24-C25-C26
3	C	401	PEV	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
3	B	402	PEV	O3P-C1-C2-C3
3	C	403	PEV	O3P-C1-C2-C3
3	C	405	PEV	O3P-C1-C2-C3
3	G	303	PEV	O3P-C1-C2-C3
4	E	303	8PP	C30-C29-C31-C32
4	E	303	8PP	C28-C29-C31-C32
3	E	304	PEV	C33-C34-C35-C36
3	H	306	PEV	C13-C14-C15-C16
3	C	403	PEV	C31-C32-C33-C34
3	H	305	PEV	C19-C20-C21-C22
3	H	304	PEV	C12-C13-C14-C15
3	B	402	PEV	C1-C2-C3-O3
4	G	302	8PP	C19-C21-C22-C23
3	F	305	PEV	C15-C16-C17-C18
3	A	401	PEV	C13-C14-C15-C16
3	C	405	PEV	C1-O3P-P-O1P
3	H	304	PEV	C1-O3P-P-O1P
3	D	401	PEV	C17-C18-C19-C20
3	A	402	PEV	O3P-C1-C2-O2
3	C	405	PEV	C36-C37-C38-C39
3	E	305	PEV	C19-C20-C21-C22
3	H	301	PEV	C13-C14-C15-C16
3	H	304	PEV	O2-C2-C3-O3
3	C	405	PEV	C13-C14-C15-C16
3	H	304	PEV	C14-C15-C16-C17
3	C	402	PEV	C21-C22-C23-C24
3	E	302	PEV	C32-C31-O2-C2
3	D	401	PEV	C20-C21-C22-C23
3	D	402	PEV	C33-C34-C35-C36
3	E	302	PEV	C31-C32-C33-C34
3	H	302	PEV	C13-C14-C15-C16
3	G	305	PEV	C21-C22-C23-C24
3	D	402	PEV	C32-C33-C34-C35
3	E	301	PEV	C12-C11-O3-C3
3	C	404	PEV	C21-C22-C23-C24
3	F	302	PEV	C13-C14-C15-C16
3	A	401	PEV	C12-C13-C14-C15
3	A	402	PEV	C13-C14-C15-C16
3	H	301	PEV	O3P-C1-C2-C3
3	A	403	PEV	C21-C22-C23-C24
3	A	401	PEV	C11-C12-C13-C14
3	C	405	PEV	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
3	D	403	PEV	C23-C24-C25-C26
3	C	403	PEV	C1-C2-C3-O3
3	H	304	PEV	C34-C35-C36-C37
3	D	403	PEV	C19-C20-C21-C22
3	F	305	PEV	C16-C17-C18-C19
3	C	405	PEV	O3P-C1-C2-O2
3	E	302	PEV	O3P-C1-C2-O2
3	G	303	PEV	O3P-C1-C2-O2
3	H	302	PEV	O3P-C1-C2-O2
3	C	405	PEV	C12-C13-C14-C15
3	B	402	PEV	O2-C2-C3-O3
3	H	305	PEV	C17-C18-C19-C20
3	C	404	PEV	C20-C21-C22-C23
3	H	306	PEV	C14-C15-C16-C17
3	D	402	PEV	O3P-C1-C2-C3
3	E	301	PEV	O11-C11-O3-C3
3	C	405	PEV	C1-O3P-P-O4P
3	E	304	PEV	C1-O3P-P-O4P
3	D	403	PEV	C18-C19-C20-C21
3	G	301	PEV	C3-C2-O2-C31
3	E	302	PEV	O31-C31-O2-C2
3	C	401	PEV	O3P-C1-C2-O2
3	D	402	PEV	O3P-C1-C2-O2
3	H	301	PEV	O3P-C1-C2-O2
3	C	401	PEV	C12-C13-C14-C15
3	C	404	PEV	C17-C18-C19-C20
3	E	301	PEV	C12-C13-C14-C15
3	D	402	PEV	O2-C2-C3-O3
3	E	304	PEV	O2-C2-C3-O3
3	H	302	PEV	O2-C2-C3-O3
5	F	306	NAD	C4B-C5B-O5B-PA
3	F	305	PEV	C18-C19-C20-C21
4	E	303	8PP	C25-C24-C26-C27
3	H	302	PEV	C12-C13-C14-C15
3	H	305	PEV	C18-C19-C20-C21
3	A	402	PEV	O3P-C1-C2-C3
3	C	401	PEV	O3P-C1-C2-C3
3	E	302	PEV	O3P-C1-C2-C3
3	F	301	PEV	O3P-C1-C2-C3
3	G	304	PEV	C19-C20-C21-C22
4	E	303	8PP	C20-C19-C21-C22
3	E	304	PEV	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
3	C	403	PEV	O3P-C1-C2-O2
3	F	301	PEV	O3P-C1-C2-O2
3	G	303	PEV	C33-C34-C35-C36
3	C	401	PEV	O2-C2-C3-O3
3	F	302	PEV	O2-C2-C3-O3
3	H	301	PEV	O2-C2-C3-O3
3	D	402	PEV	C1-C2-C3-O3
3	H	301	PEV	C1-C2-C3-O3
3	H	304	PEV	C1-C2-C3-O3
4	B	403	8PP	C25-C24-C26-C27
3	A	403	PEV	C18-C19-C20-C21
3	G	304	PEV	C16-C17-C18-C19
3	E	301	PEV	C32-C33-C34-C35
5	E	306	NAD	C5B-O5B-PA-O1A
3	B	402	PEV	C2-C1-O3P-P
5	E	306	NAD	C4D-C5D-O5D-PN
3	H	306	PEV	C12-C13-C14-C15
4	E	303	8PP	C18-C19-C21-C22
3	E	305	PEV	C18-C19-C20-C21
3	D	404	PEV	C13-C14-C15-C16
5	E	306	NAD	C4B-C5B-O5B-PA
3	C	401	PEV	C1-C2-C3-O3
3	F	302	PEV	C1-C2-C3-O3
3	G	301	PEV	C1-C2-C3-O3
5	F	306	NAD	PA-O3-PN-O1N
5	F	306	NAD	PA-O3-PN-O2N
3	A	403	PEV	C16-C17-C18-C19
3	D	404	PEV	C22-C23-C24-C25
3	G	305	PEV	C18-C19-C20-C21
5	E	306	NAD	C2D-C1D-N1N-C6N
3	C	401	PEV	C2-C1-O3P-P
4	B	403	8PP	C23-C24-C26-C27
3	H	302	PEV	C1-C2-C3-O3
4	H	303	8PP	C9-C11-C12-C13
3	C	402	PEV	C22-C23-C24-C25
4	E	303	8PP	C2-C7-C8-C9
3	H	301	PEV	C31-C32-C33-C34
3	E	302	PEV	C12-C13-C14-C15
3	G	304	PEV	C23-C24-C25-C26
3	D	404	PEV	C19-C20-C21-C22
3	C	404	PEV	C19-C20-C21-C22
3	H	301	PEV	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
3	H	306	PEV	C16-C17-C18-C19
3	H	302	PEV	O3P-C1-C2-C3
3	C	403	PEV	O2-C2-C3-O3
3	G	305	PEV	C20-C21-C22-C23
3	C	403	PEV	C1-O3P-P-O4P
4	E	303	8PP	C23-C24-C26-C27
3	A	403	PEV	C20-C21-C22-C23
3	E	304	PEV	O2-C31-C32-C33
3	A	402	PEV	O2-C2-C3-O3
3	E	304	PEV	O3P-C1-C2-C3
3	C	401	PEV	O3-C11-C12-C13
3	C	405	PEV	C14-C15-C16-C17
3	C	404	PEV	C23-C24-C25-C26
3	B	402	PEV	C32-C33-C34-C35
3	C	402	PEV	C18-C19-C20-C21
3	A	402	PEV	C1-C2-C3-O3
3	E	304	PEV	C1-C2-C3-O3
3	C	401	PEV	O2-C31-C32-C33
3	E	301	PEV	O3-C11-C12-C13
3	D	402	PEV	C2-C3-O3-C11
3	C	401	PEV	C33-C34-C35-C36
3	E	301	PEV	O11-C11-C12-C13
3	C	401	PEV	O31-C31-C32-C33
3	C	401	PEV	O11-C11-C12-C13
4	B	403	8PP	C2-C7-C8-C9
4	G	302	8PP	C2-C7-C8-C9
3	C	403	PEV	O2-C31-C32-C33
3	G	301	PEV	C33-C34-C35-C36
3	E	301	PEV	O2-C31-C32-C33

There are no ring outliers.

21 monomers are involved in 30 short contacts:

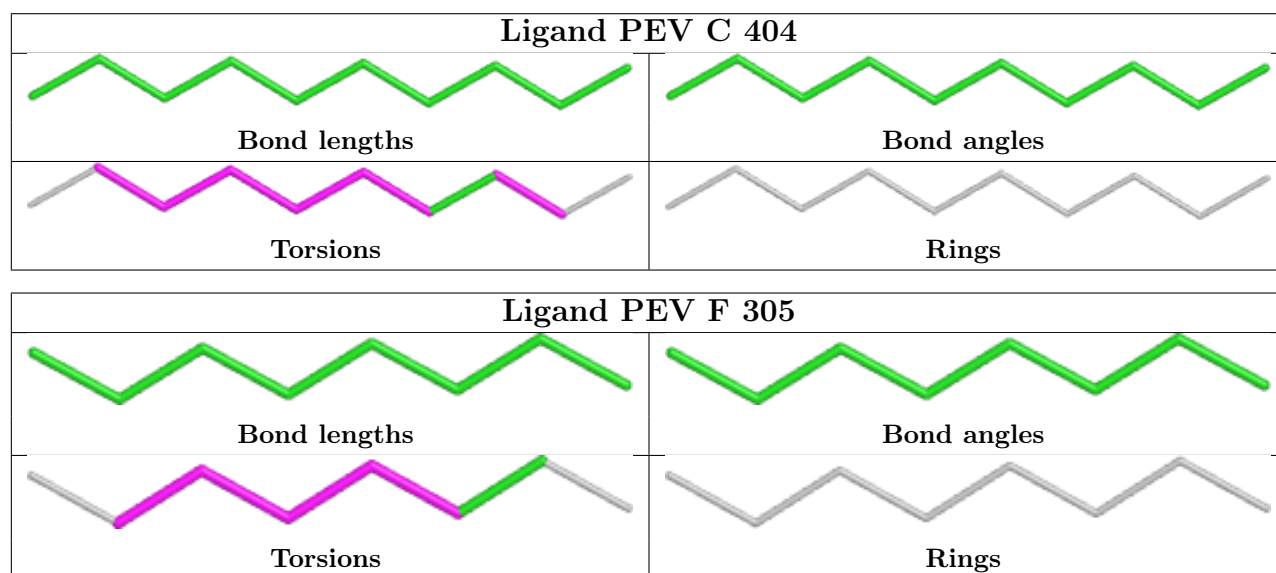
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	404	PEV	1	0
3	F	305	PEV	2	0
3	E	301	PEV	2	0
3	E	302	PEV	2	0
4	B	403	8PP	1	0
3	F	302	PEV	2	0
3	E	304	PEV	1	0
4	H	303	8PP	5	0

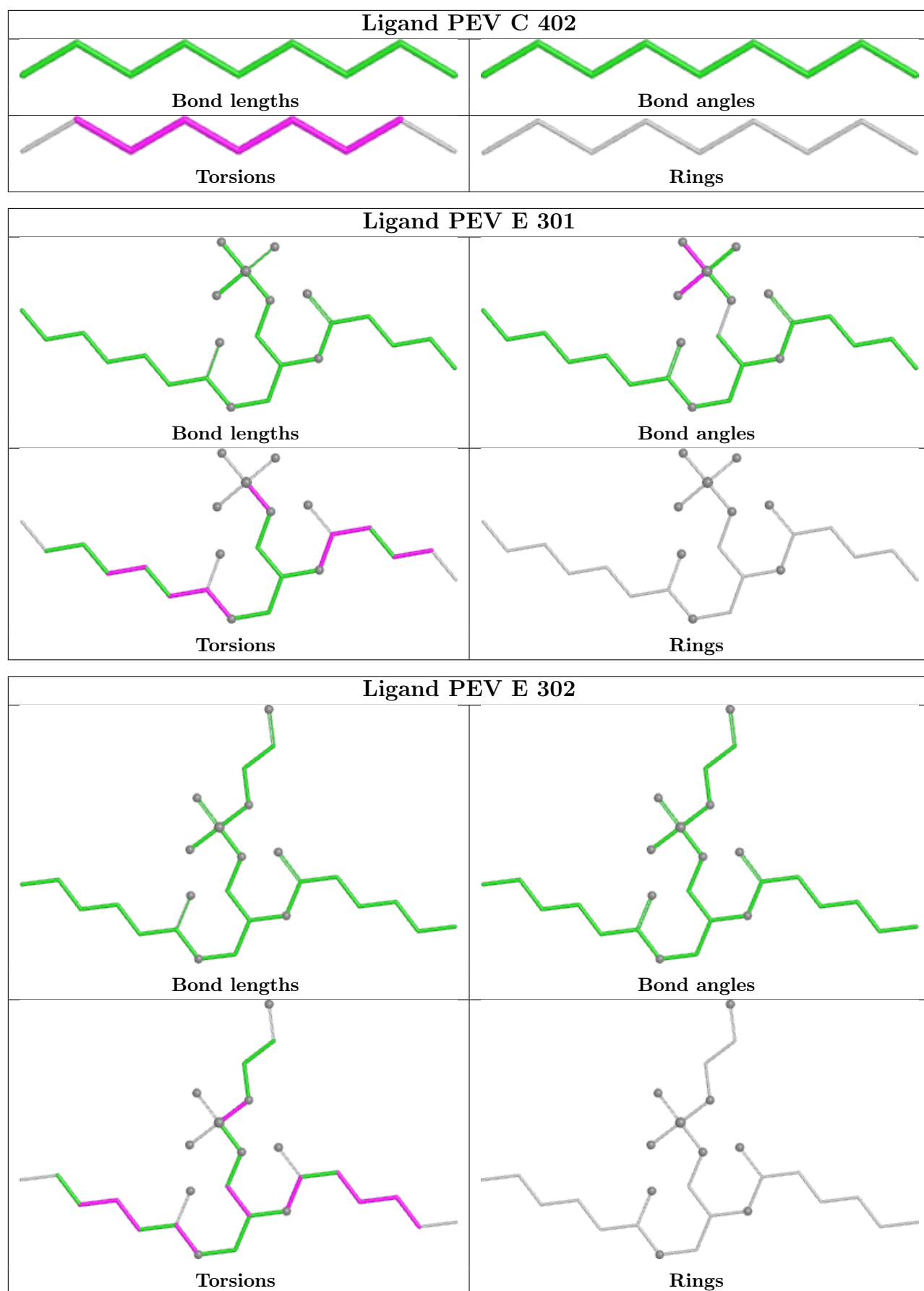
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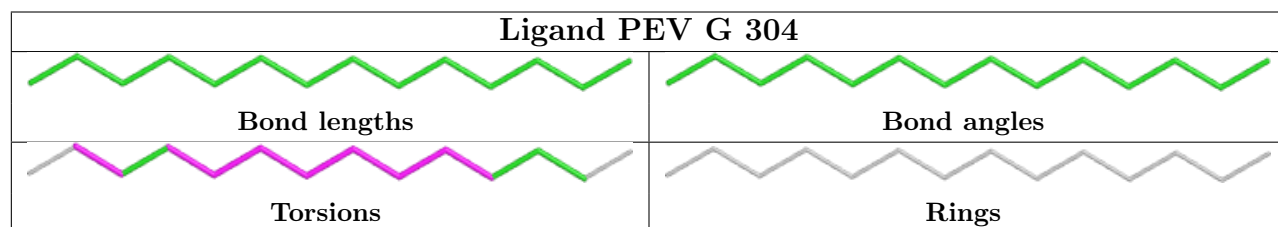
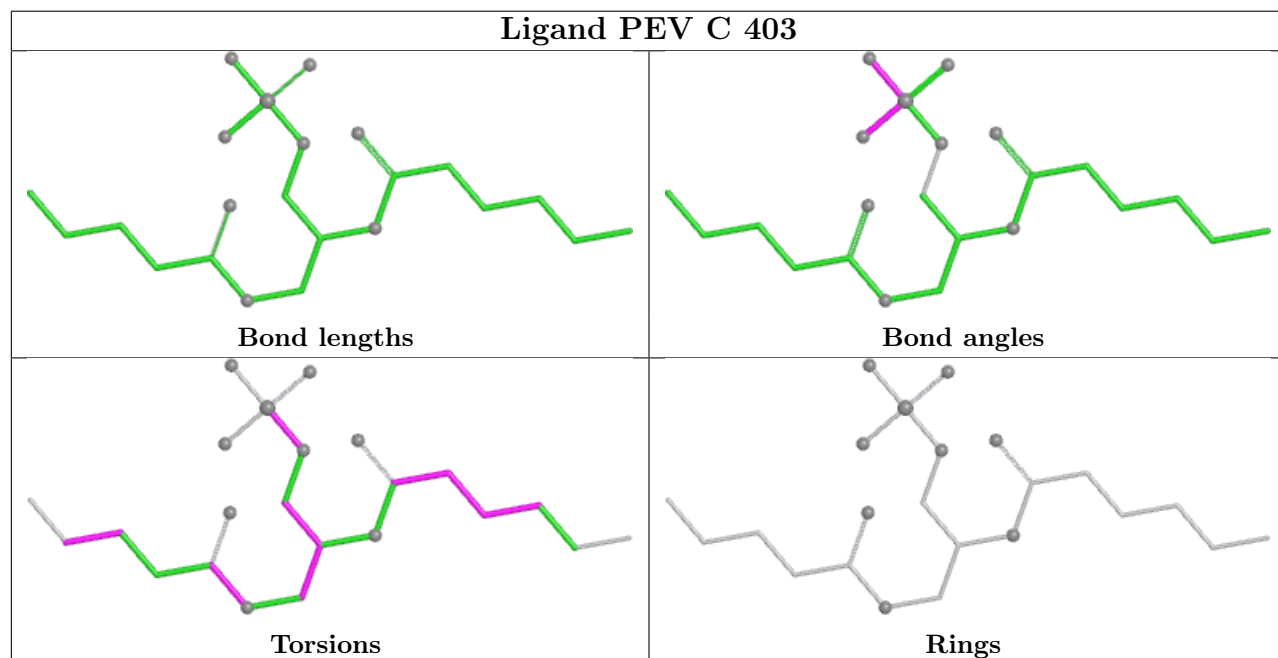
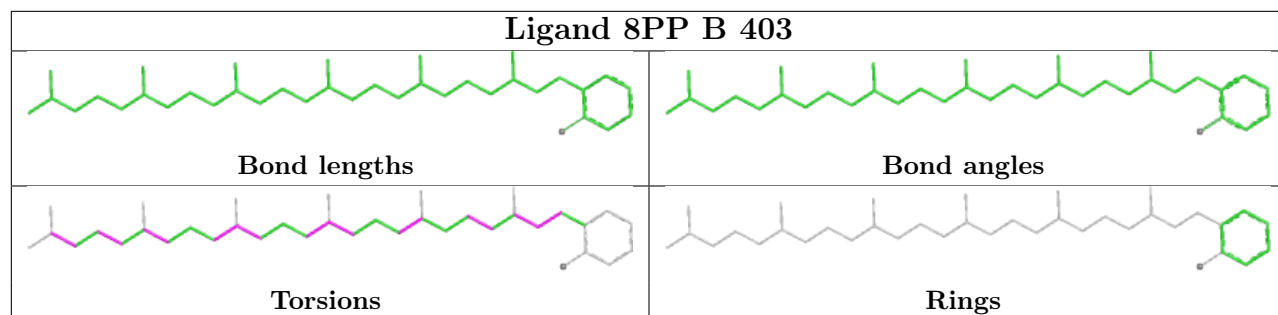
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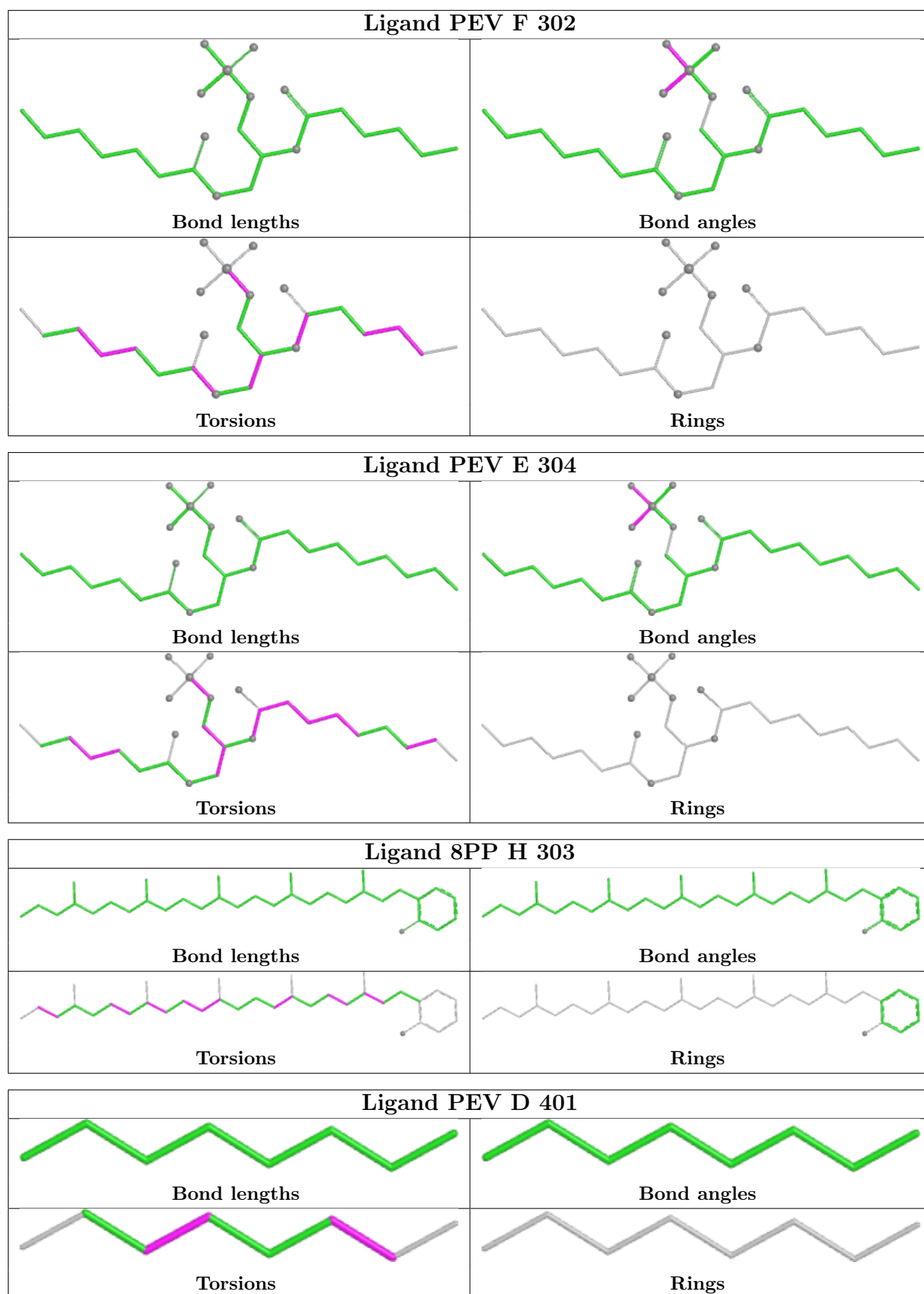
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	404	PEV	1	0
3	C	405	PEV	1	0
3	H	306	PEV	2	0
4	E	303	8PP	2	0
3	G	303	PEV	1	0
3	H	302	PEV	3	0
3	H	305	PEV	1	0
3	H	304	PEV	1	0
3	F	303	PEV	1	0
4	G	302	8PP	1	0
5	E	306	NAD	1	0
3	D	402	PEV	1	0
3	A	401	PEV	1	0

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.





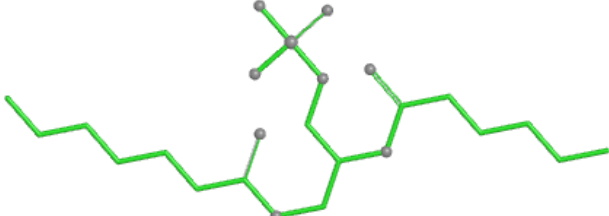
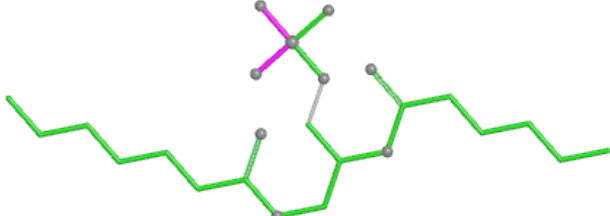
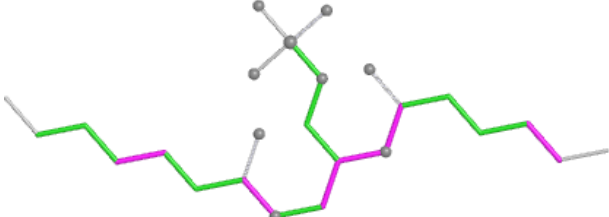
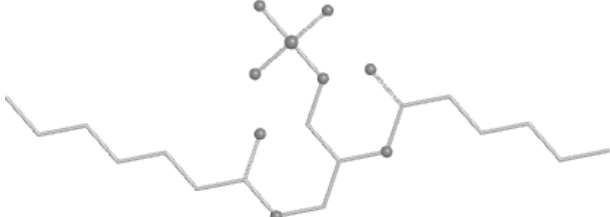


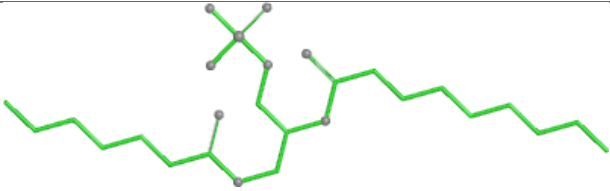
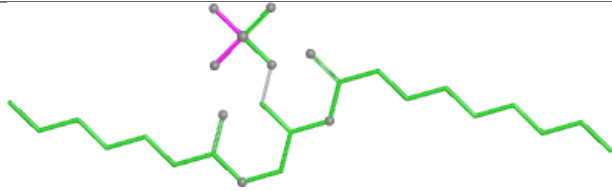
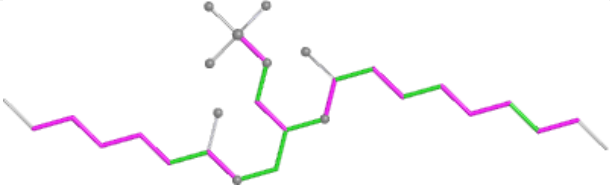
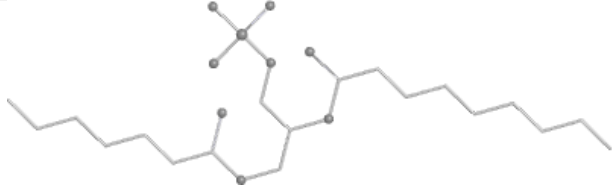


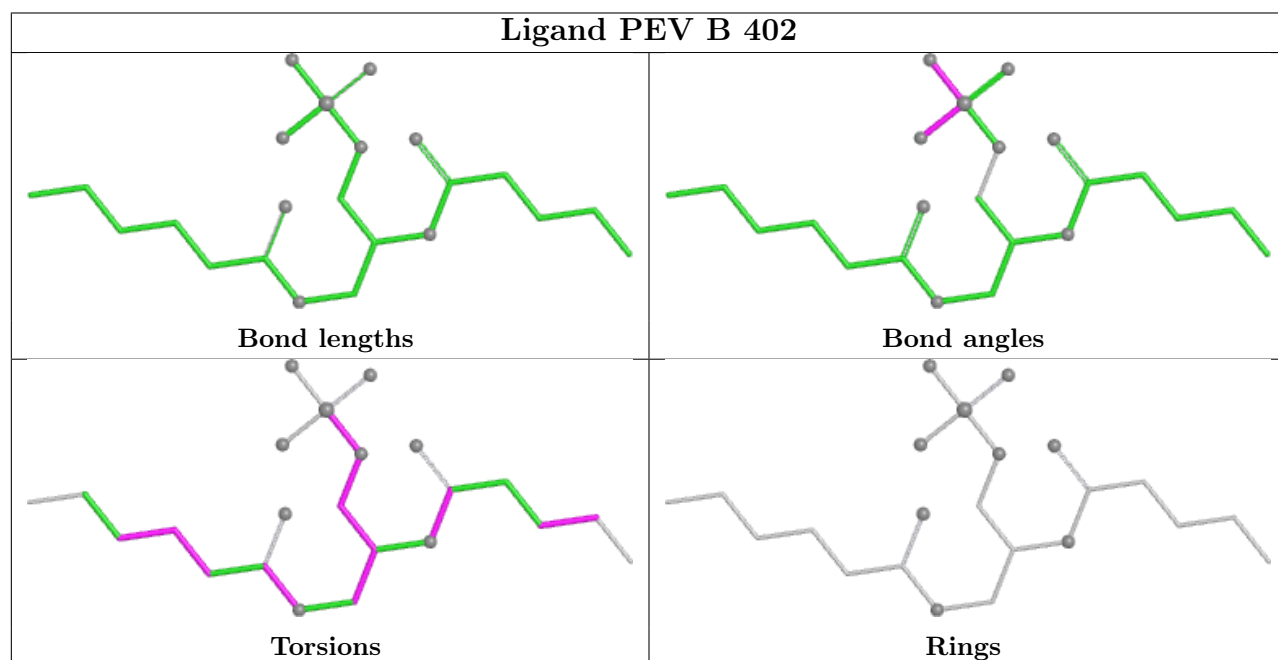
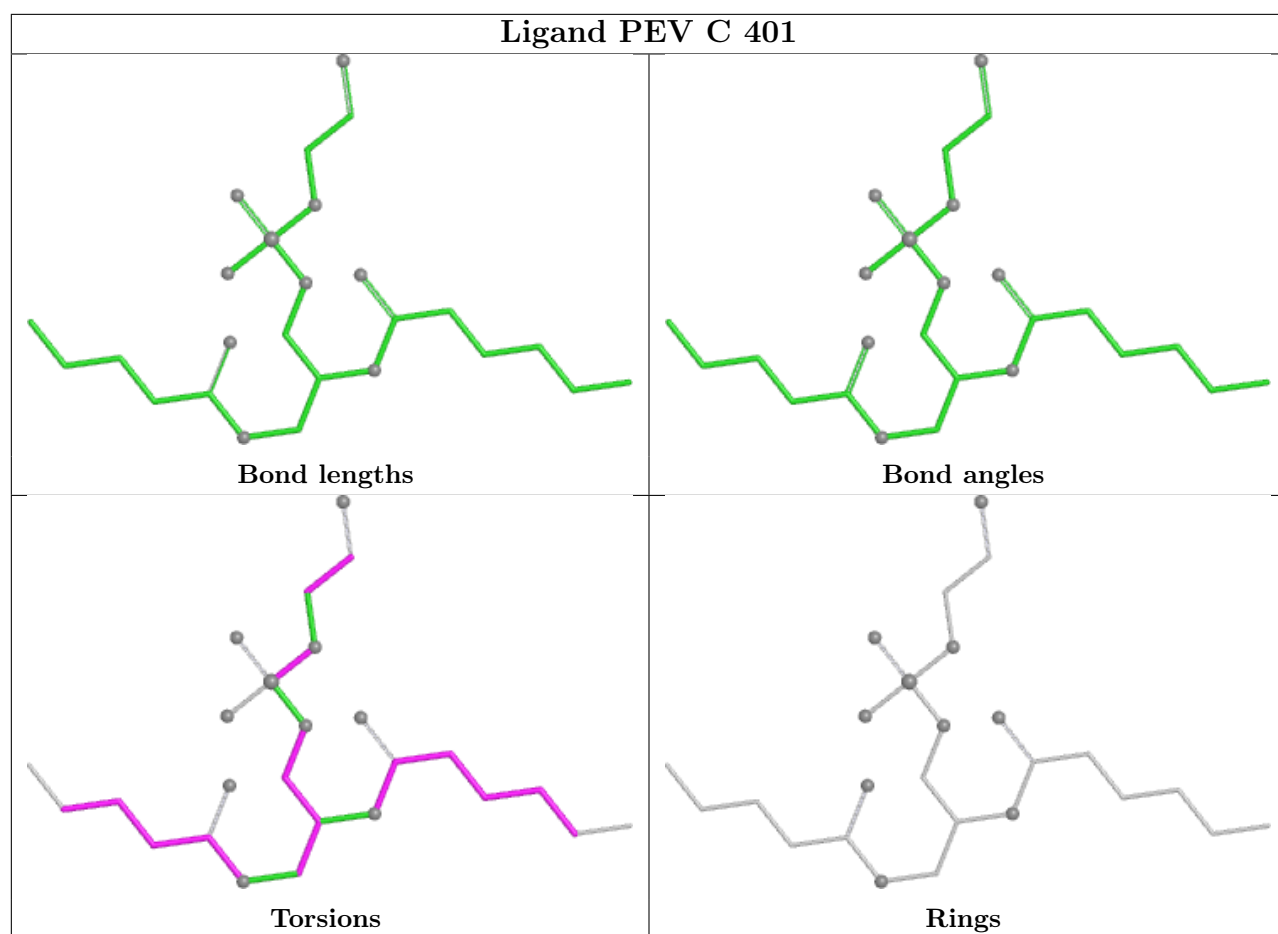
Ligand PEV D 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

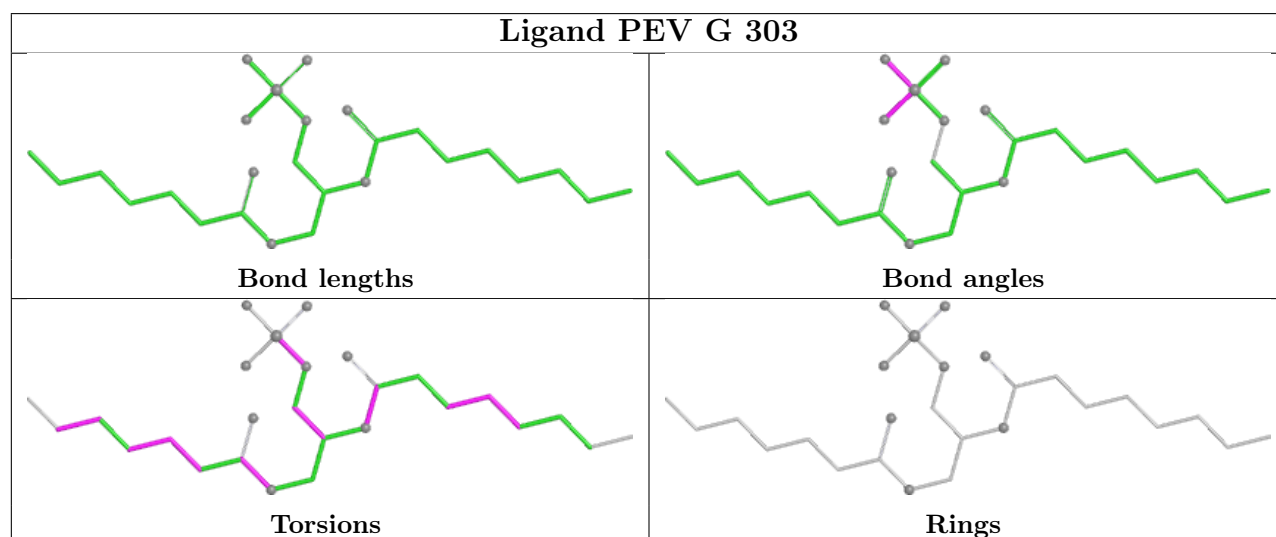
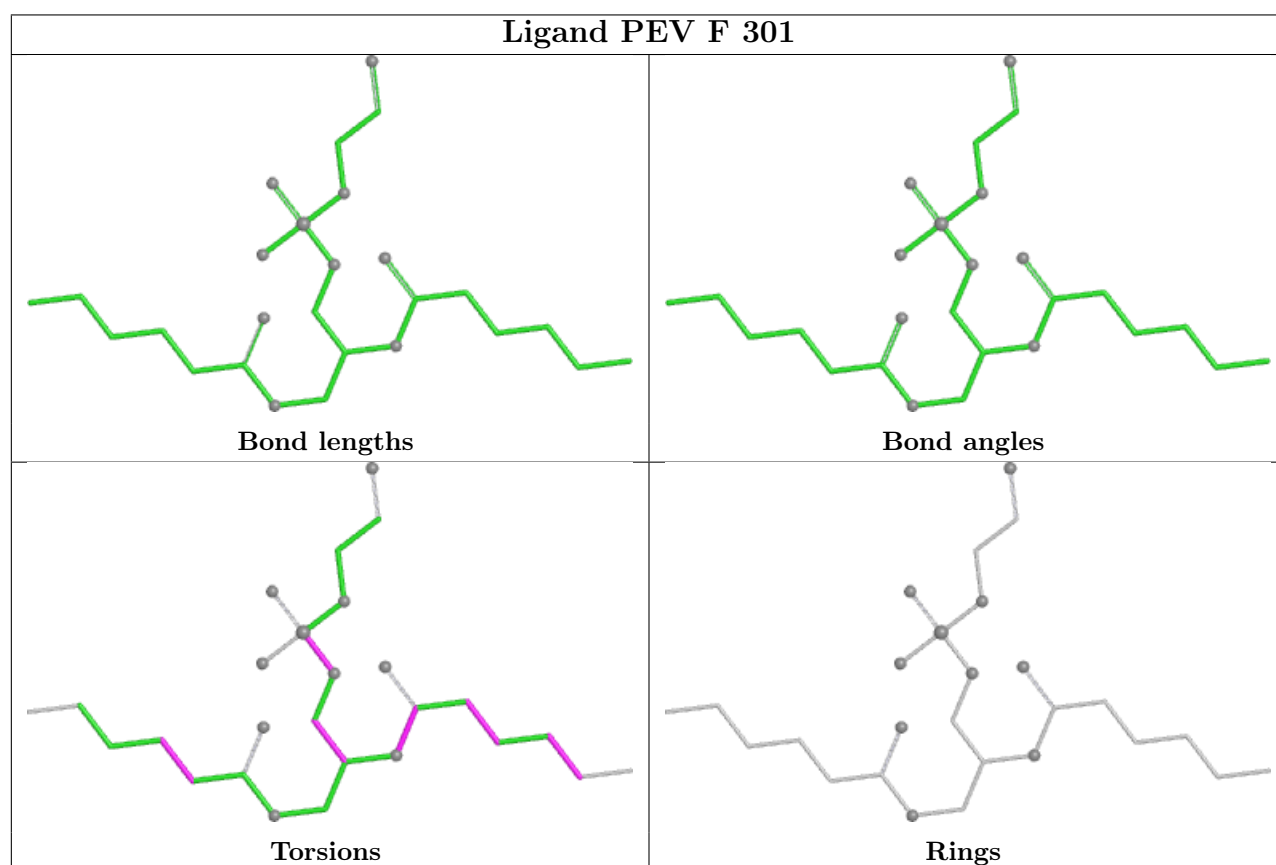
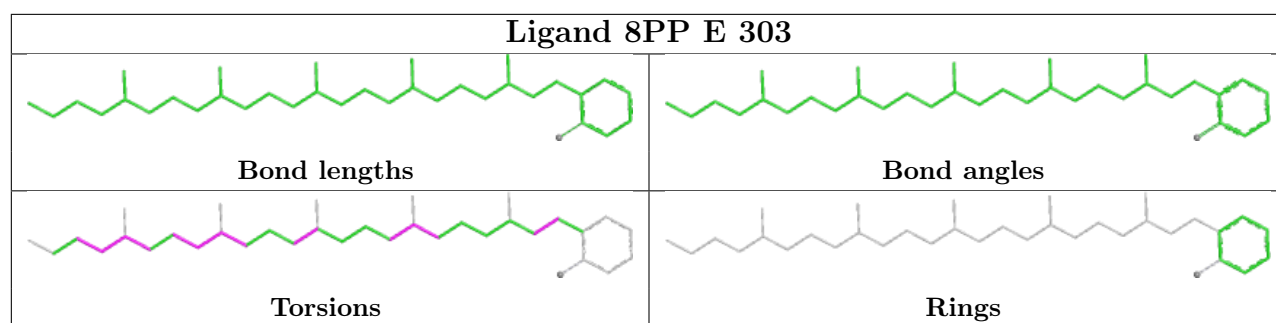
Ligand PEV F 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

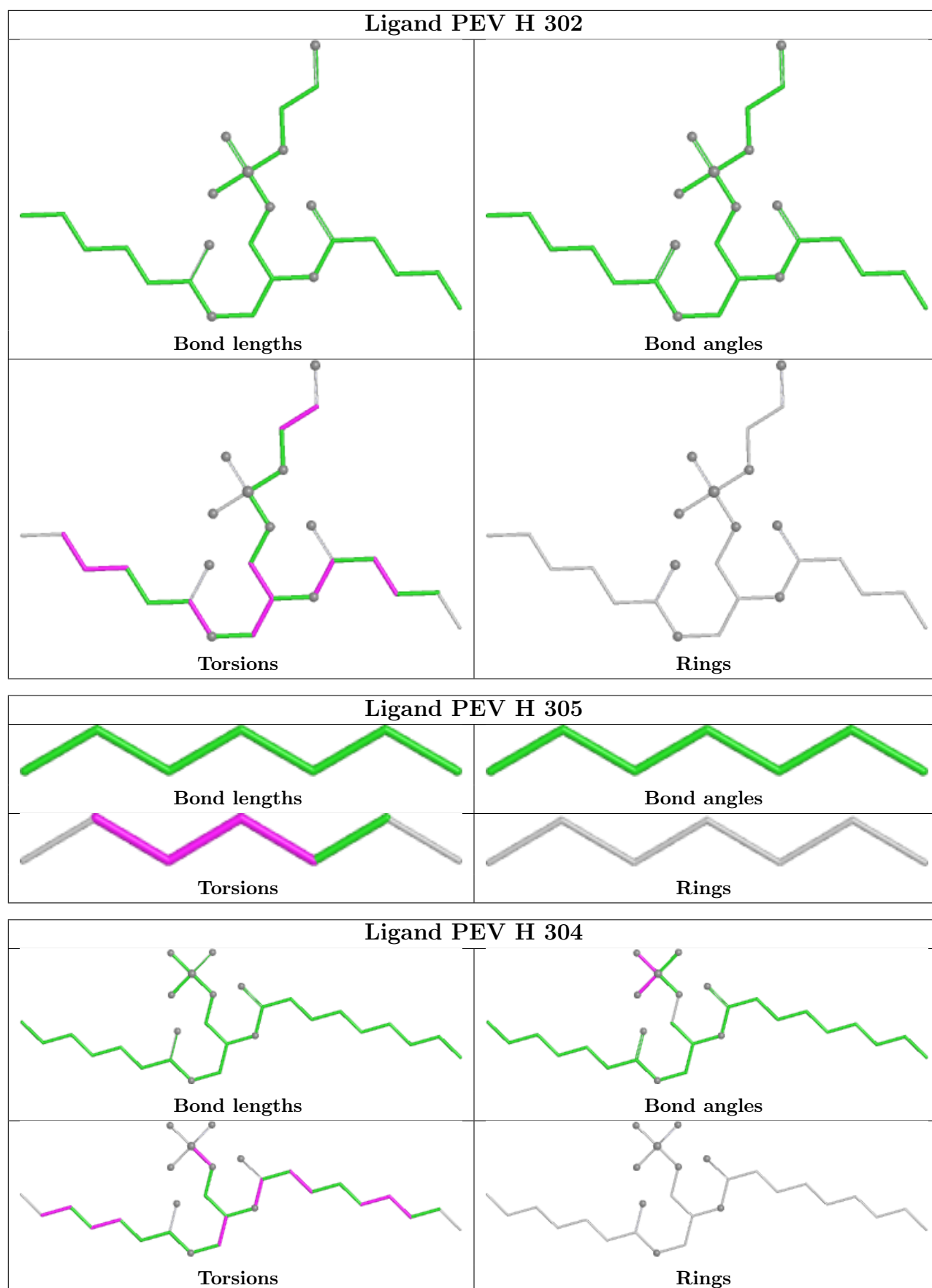
Ligand PEV D 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

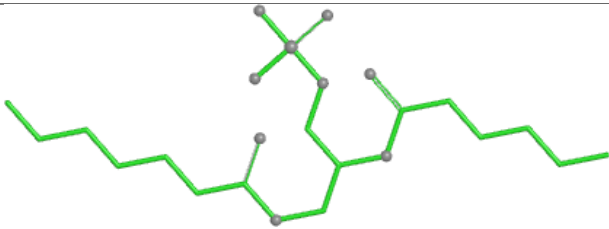
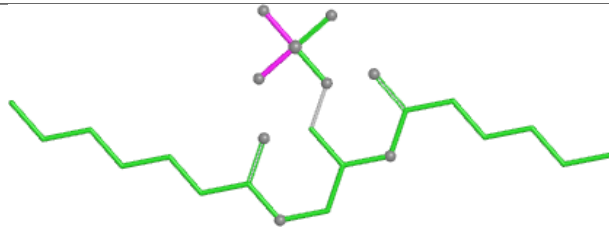
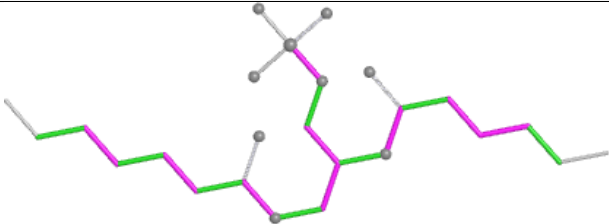
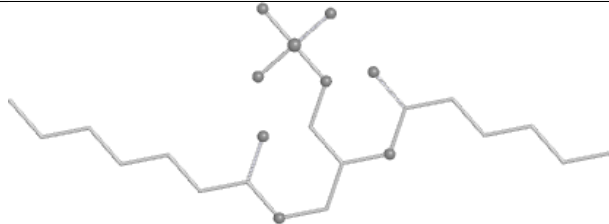
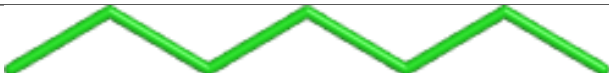
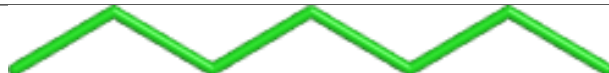
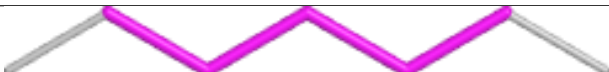
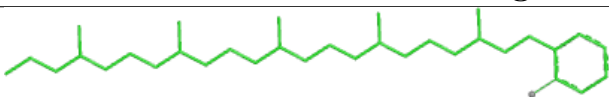
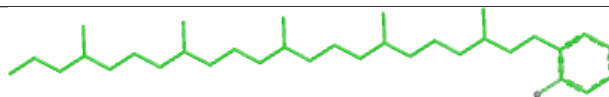
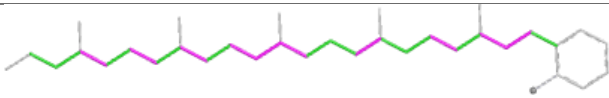
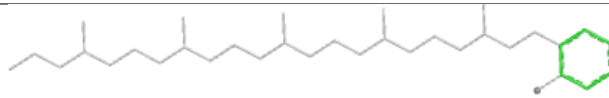
Ligand PEV G 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

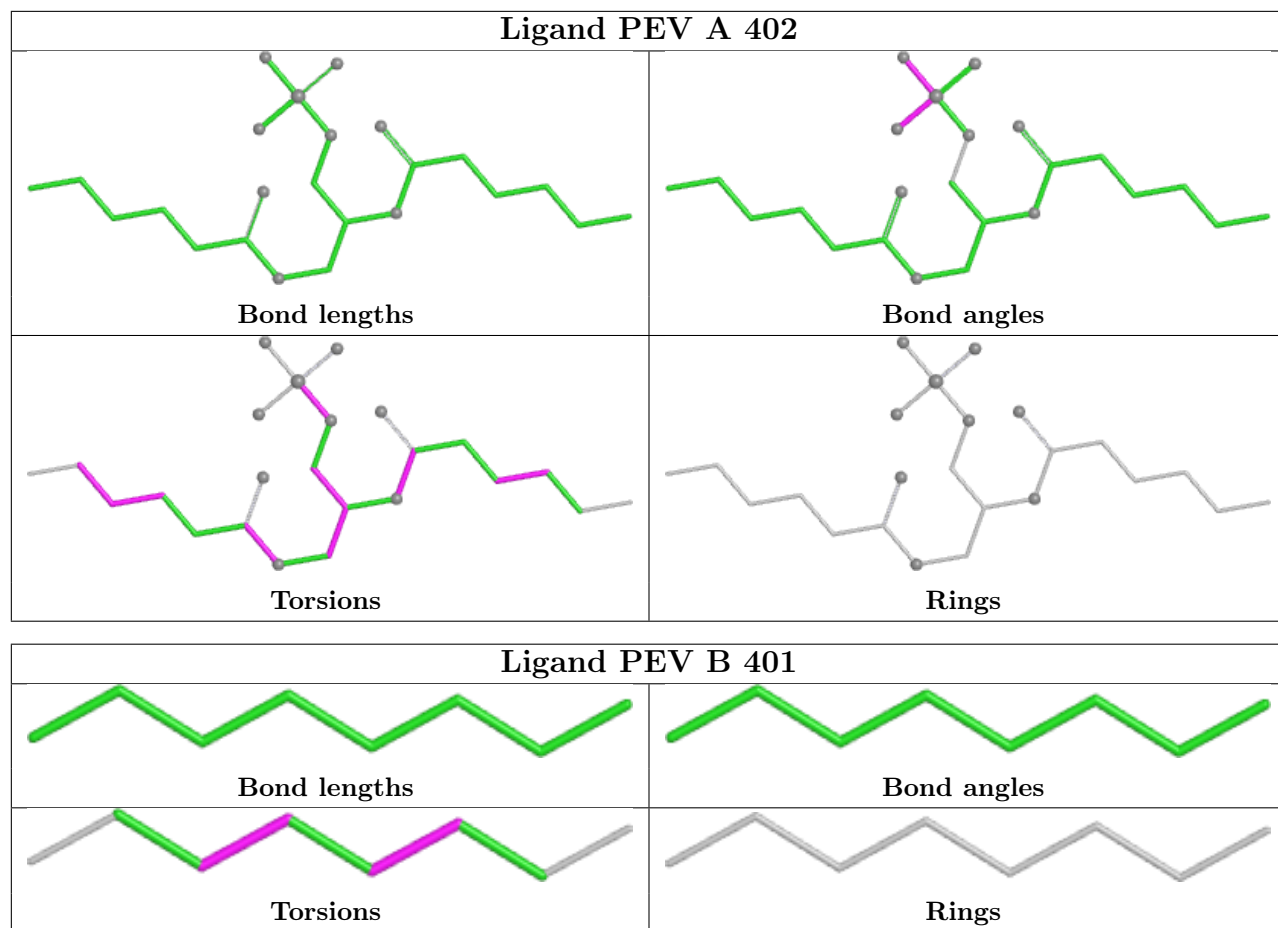
Ligand PEV C 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEV H 306	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEV A 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

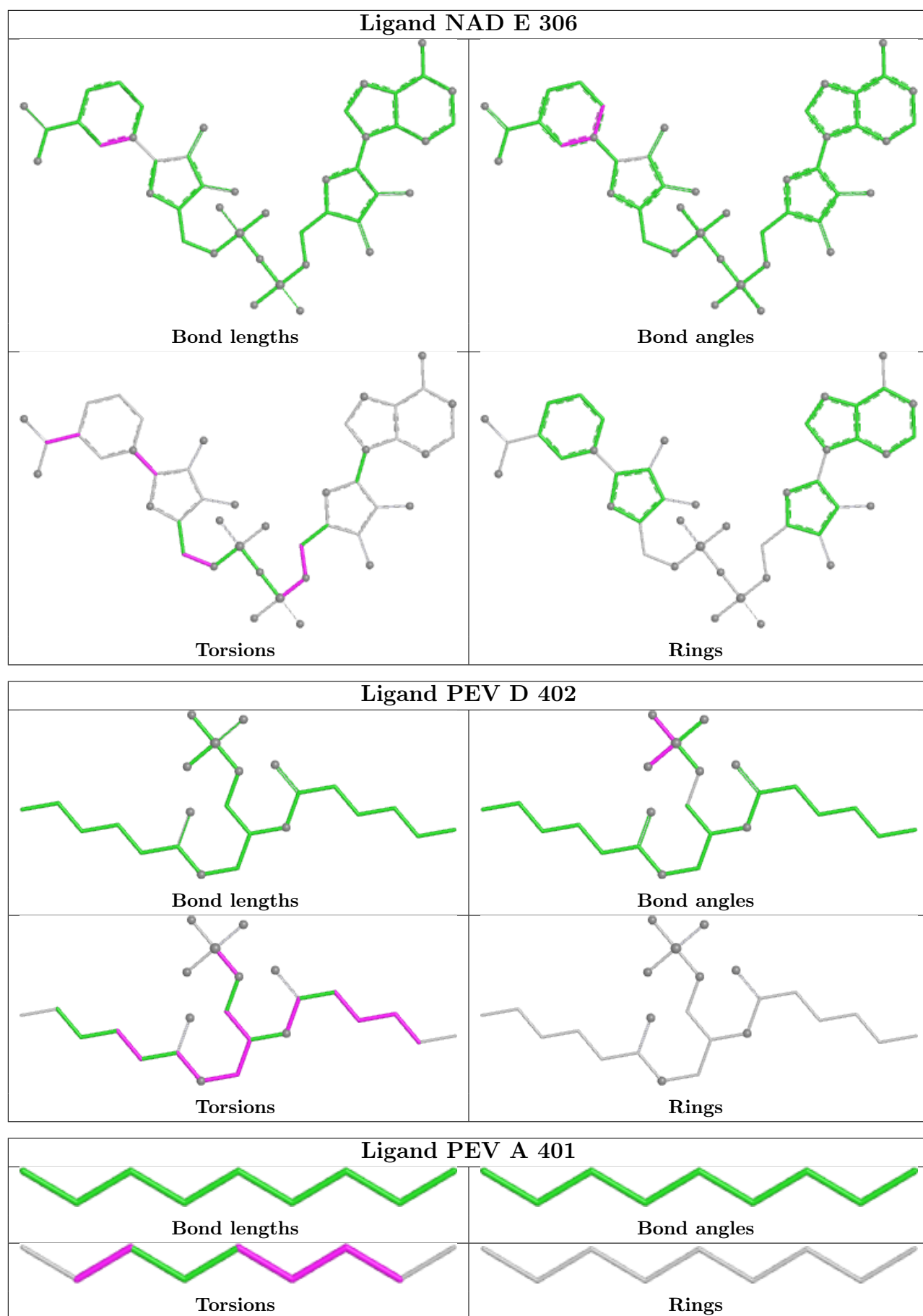


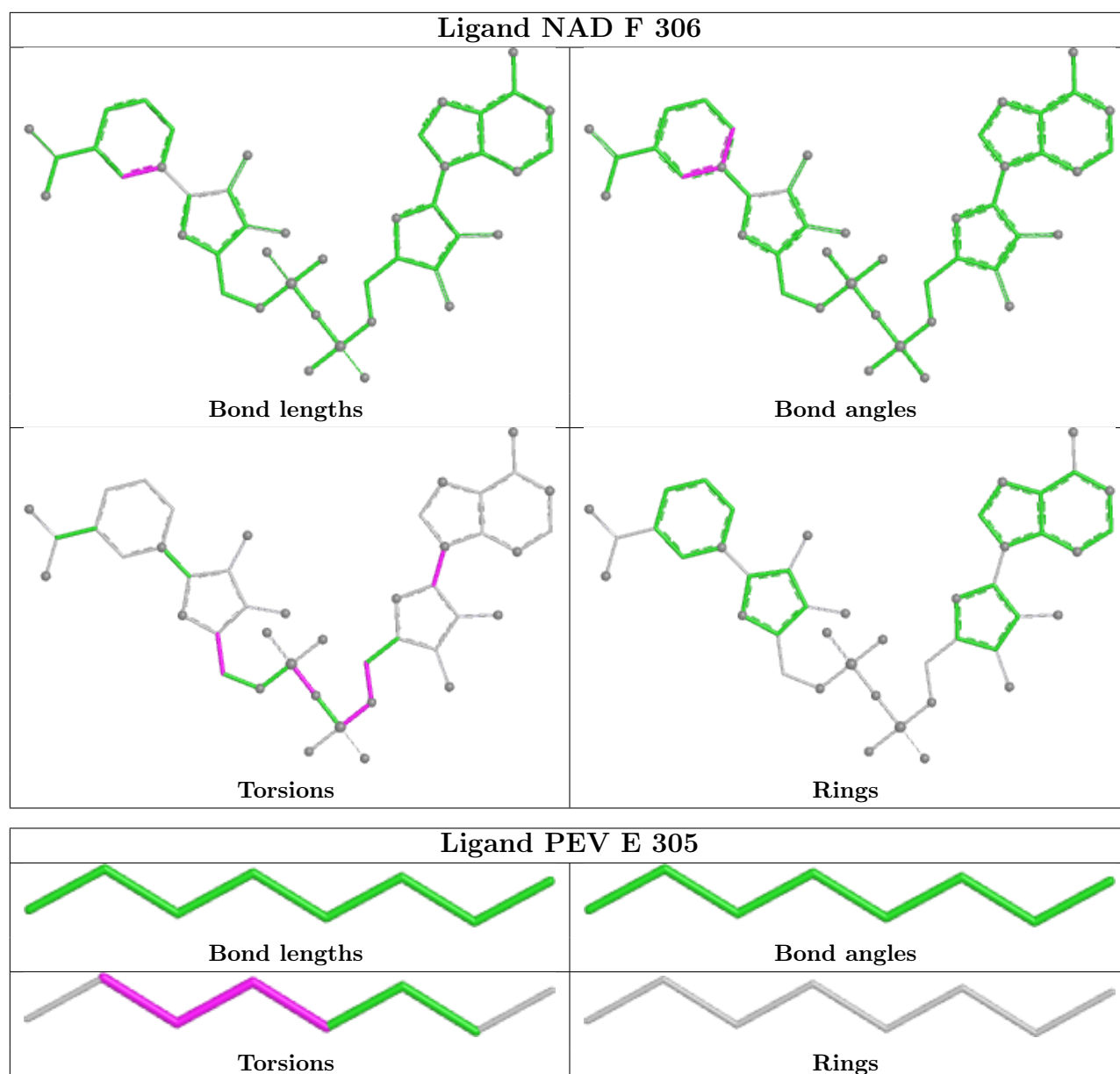




Ligand PEV H 301	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEV F 303	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEV G 305	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand 8PP G 302	
 Bond lengths	 Bond angles
 Torsions	 Rings







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.

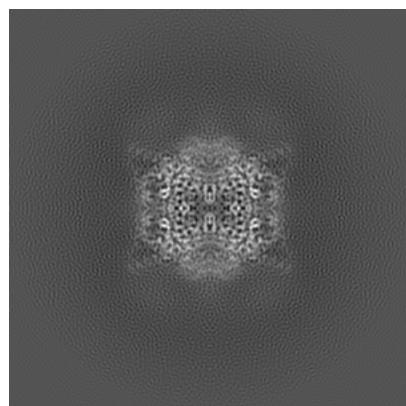
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25413. These allow visual inspection of the internal detail of the map and identification of artifacts.

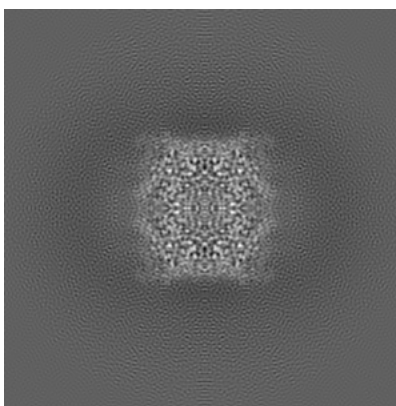
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

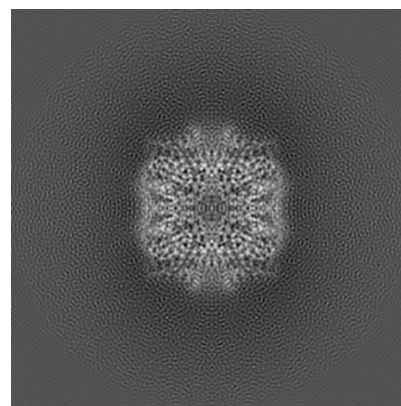
6.1.1 Primary map



X

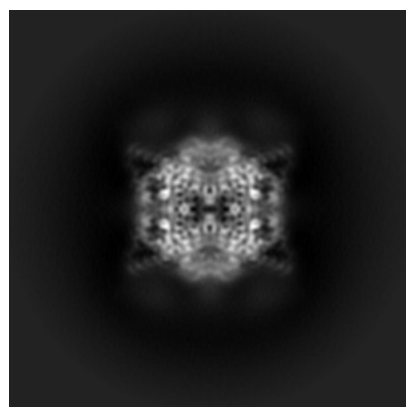


Y

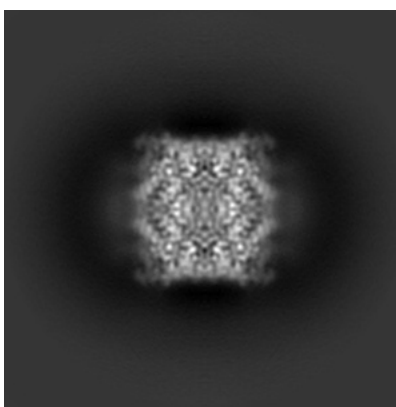


Z

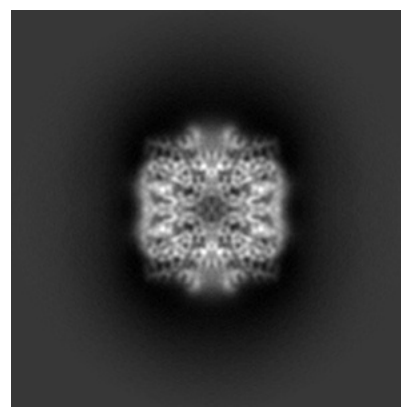
6.1.2 Raw map



X



Y

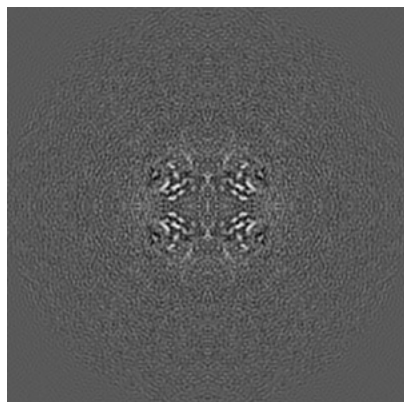


Z

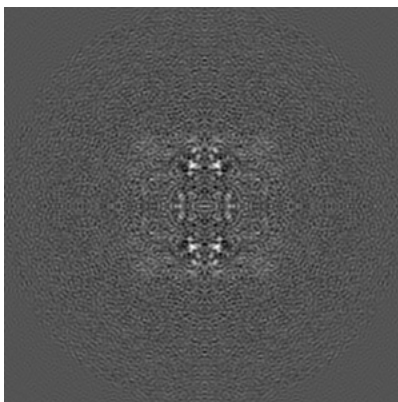
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

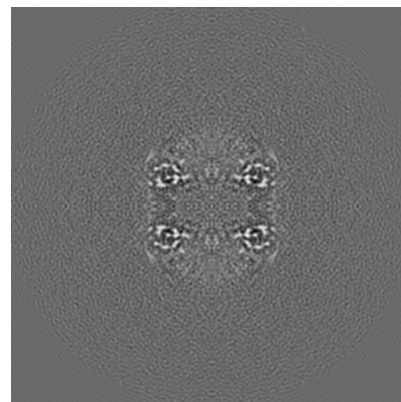
6.2.1 Primary map



X Index: 128

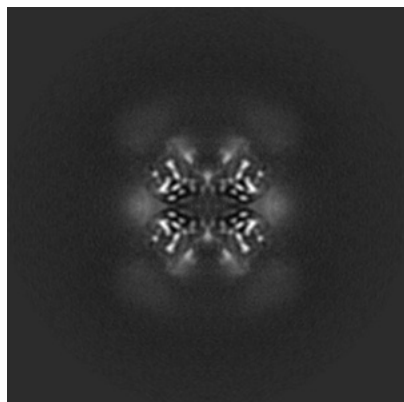


Y Index: 128

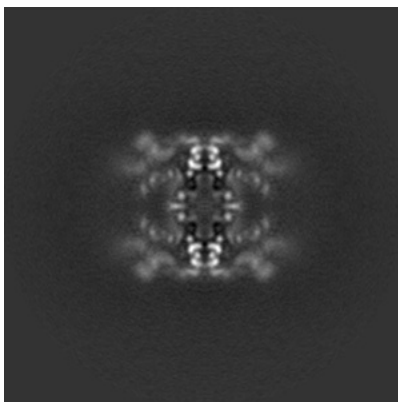


Z Index: 128

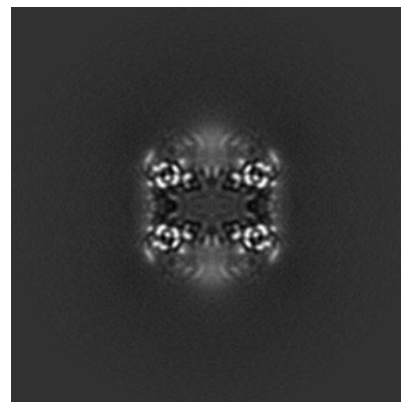
6.2.2 Raw map



X Index: 128



Y Index: 128

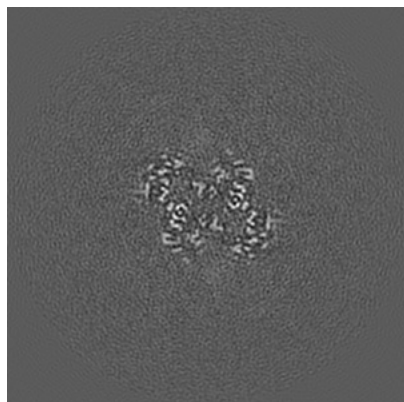


Z Index: 128

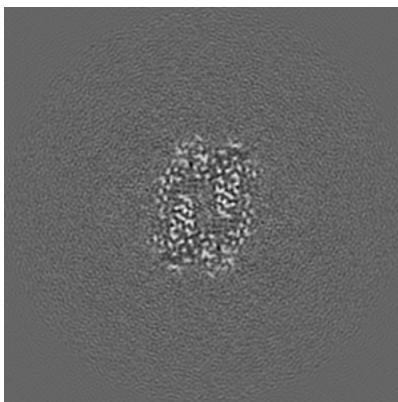
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

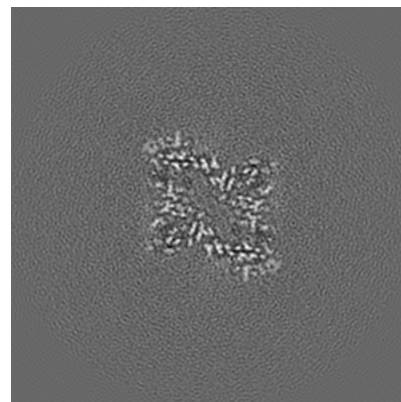
6.3.1 Primary map



X Index: 105

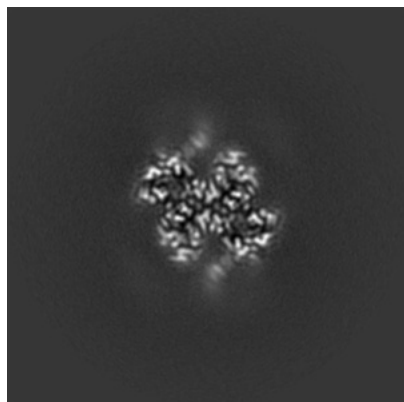


Y Index: 154

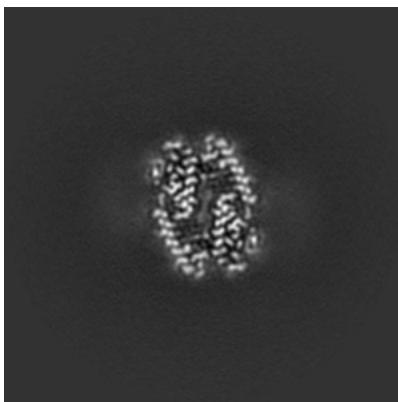


Z Index: 119

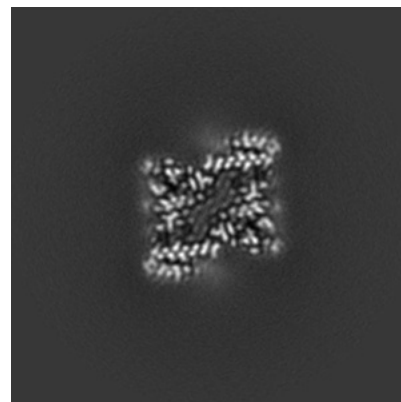
6.3.2 Raw map



X Index: 103



Y Index: 101

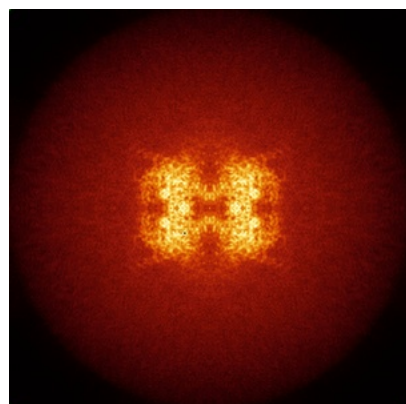


Z Index: 137

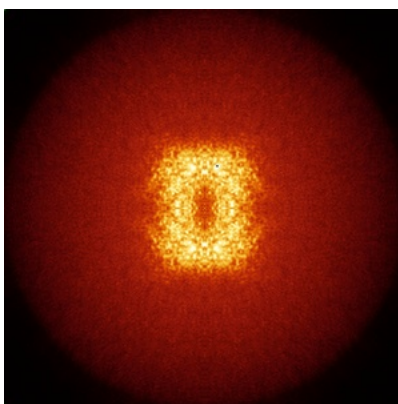
The images above show the largest variance slices of the map in three orthogonal directions.

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

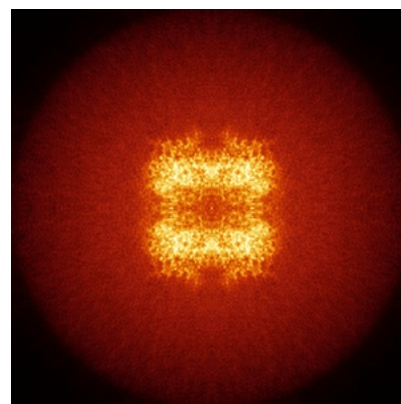
6.4.1 Primary map



X

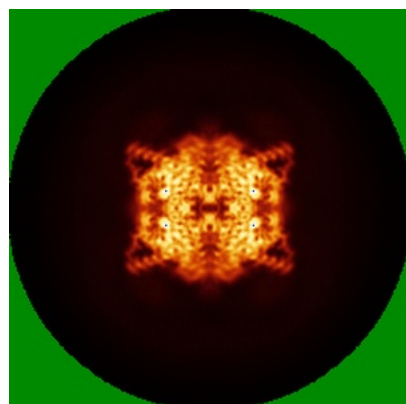


Y

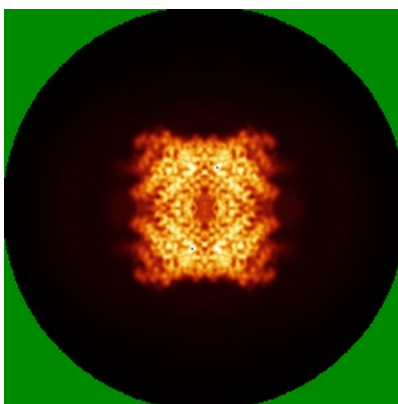


Z

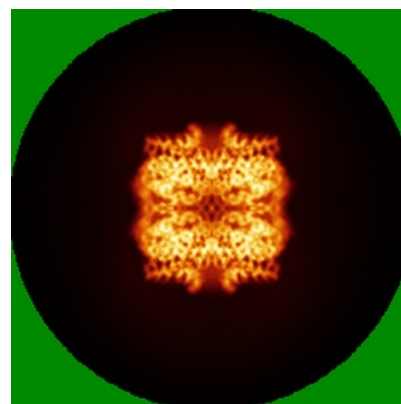
6.4.2 Raw map



X



Y

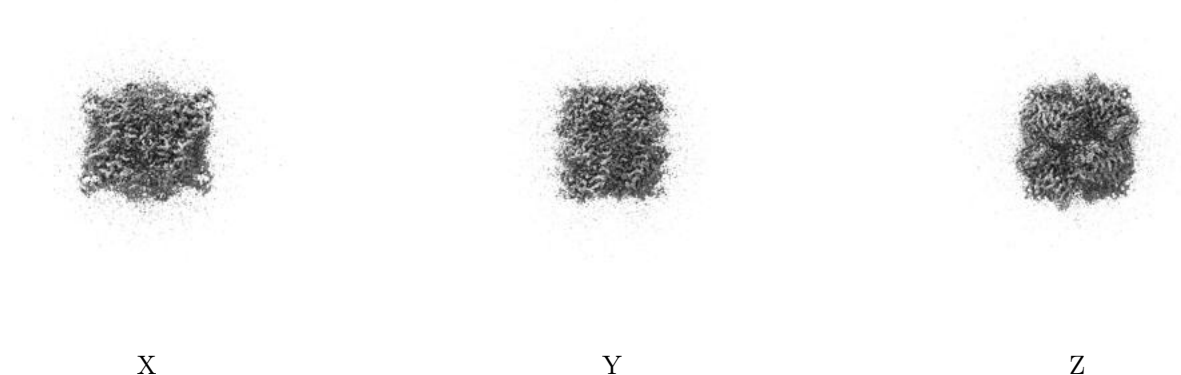


Z

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.

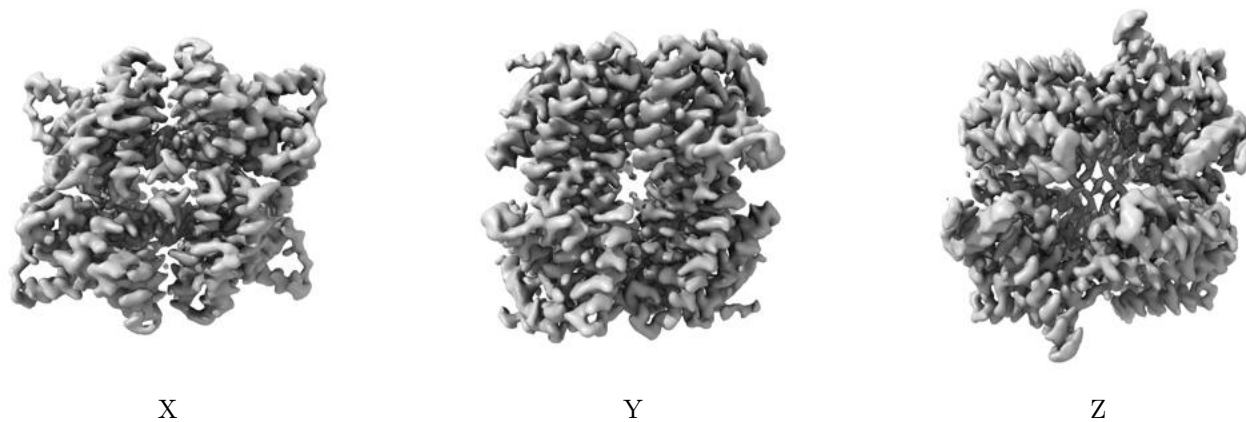
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. 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.

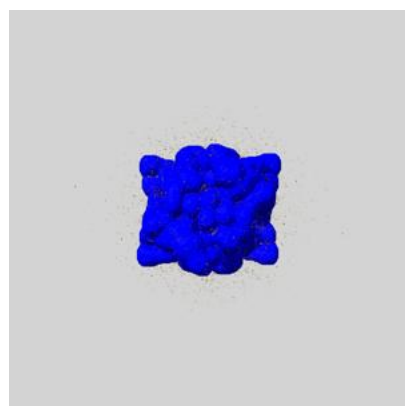
6.6 Mask visualisation [i](#)

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

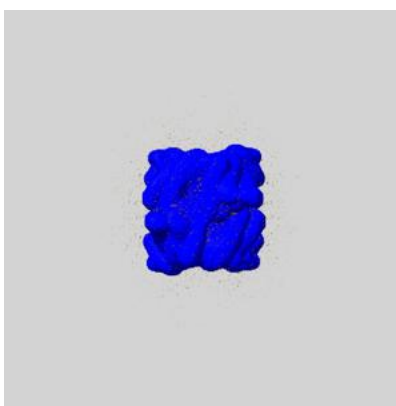
A mask typically either:

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

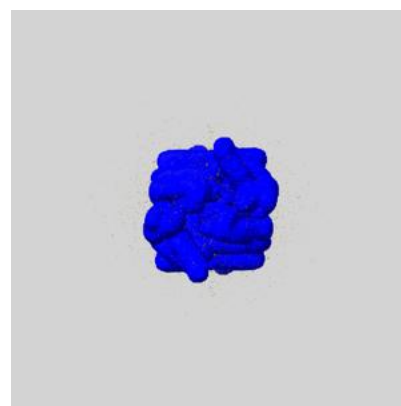
6.6.1 emd_25413_msk_1.map [i](#)



X



Y

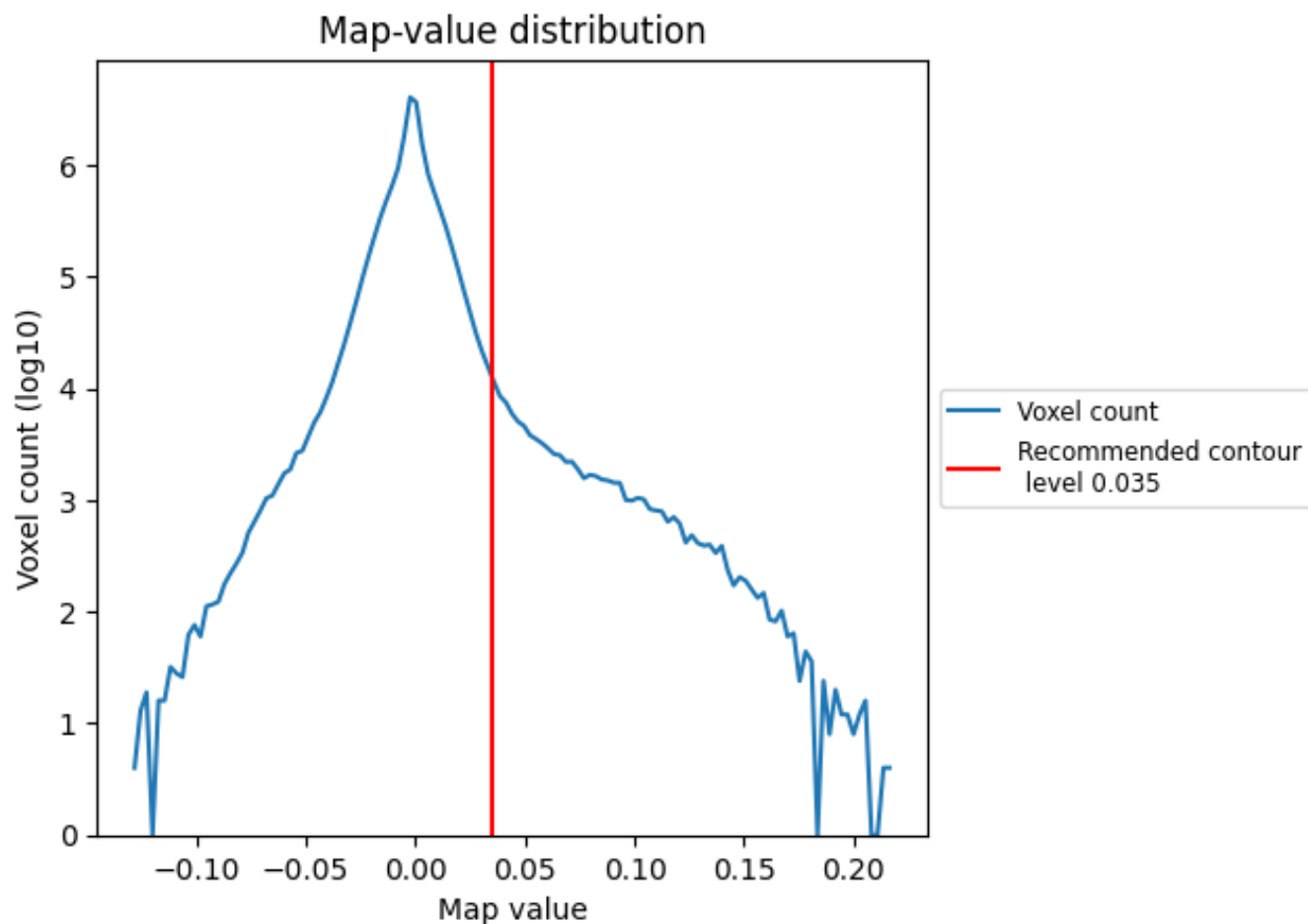


Z

7 Map analysis [i](#)

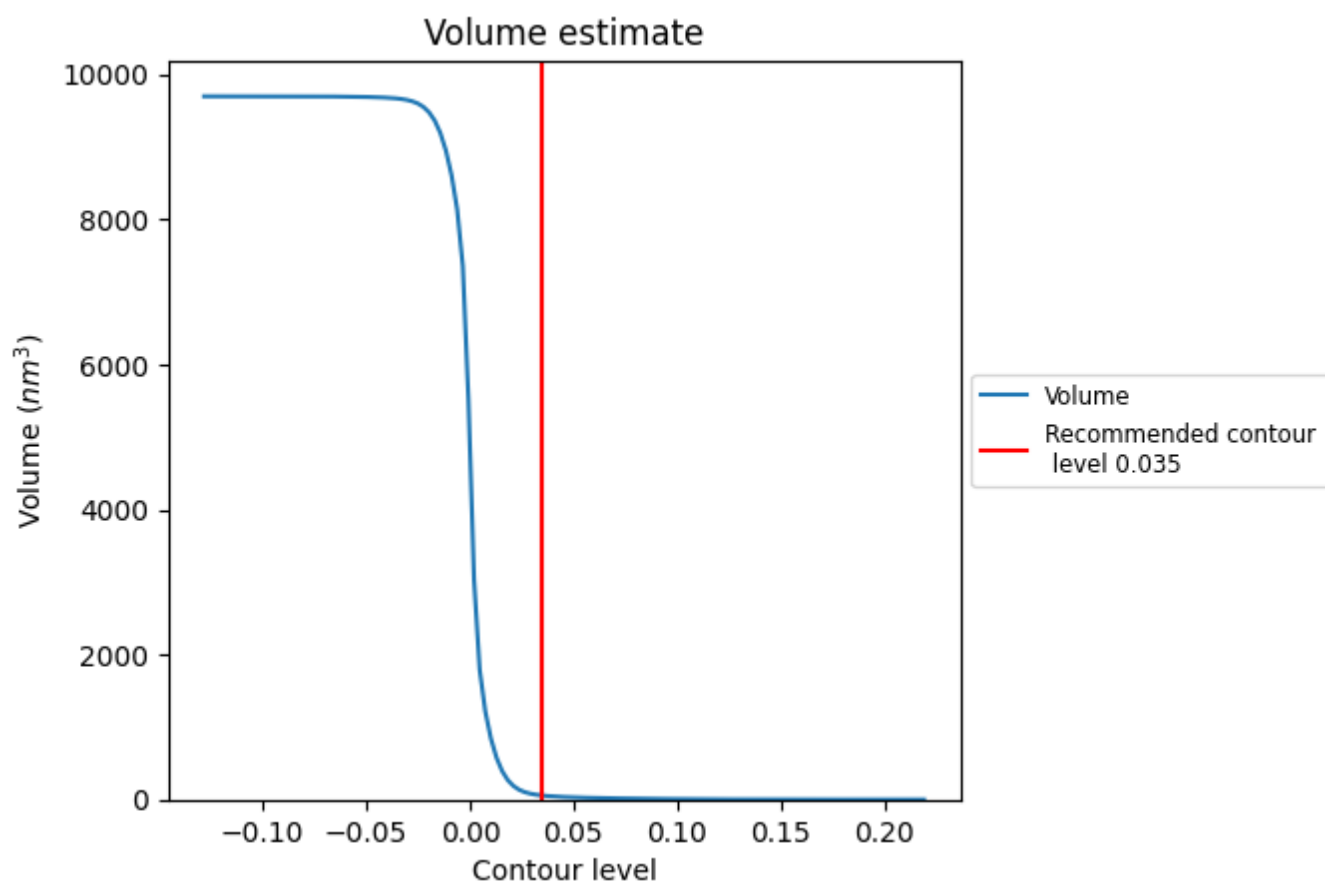
This section contains the results of statistical analysis of the map.

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.

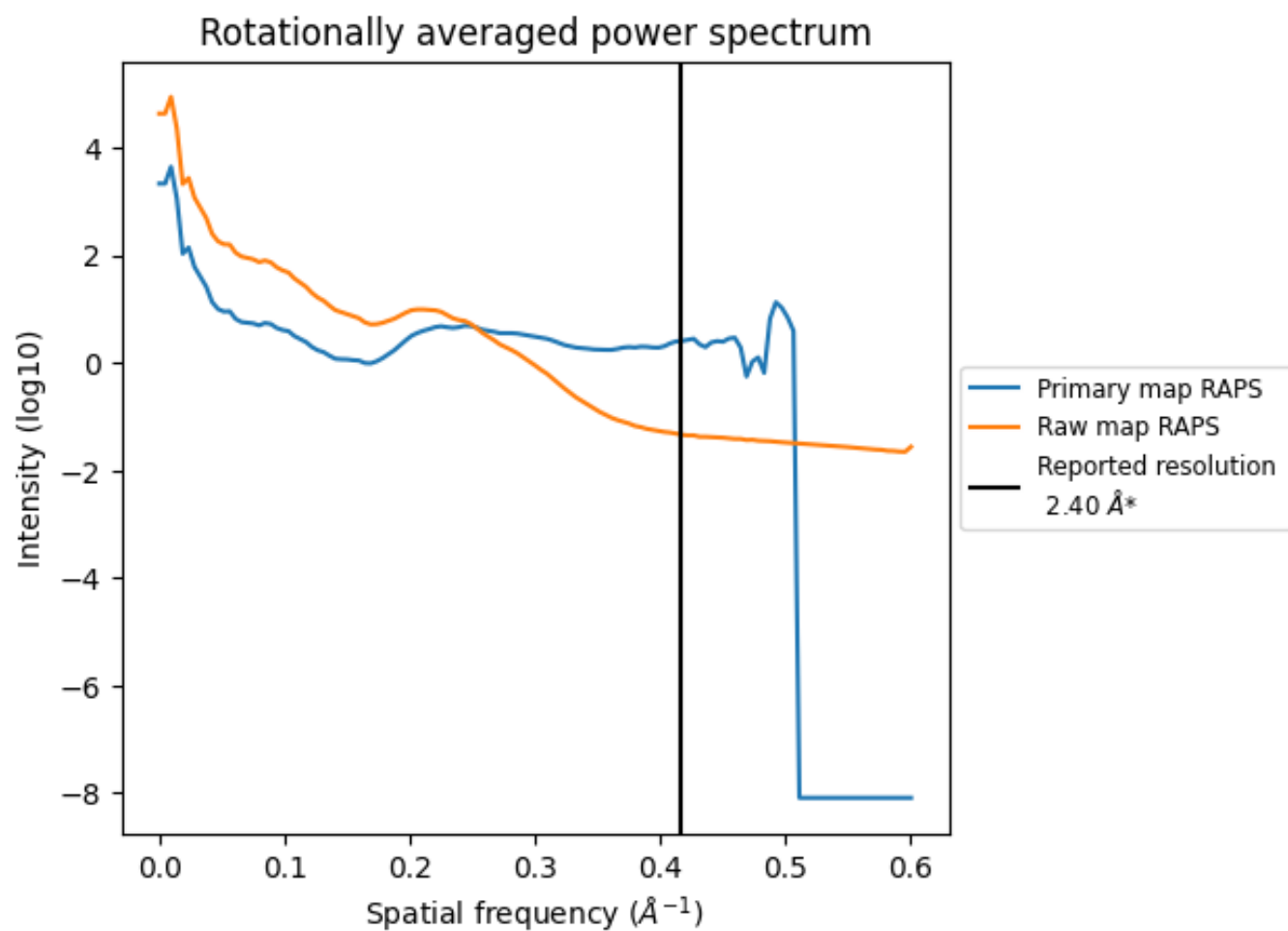
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 56 nm³; this corresponds to an approximate mass of 50 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 ⓘ

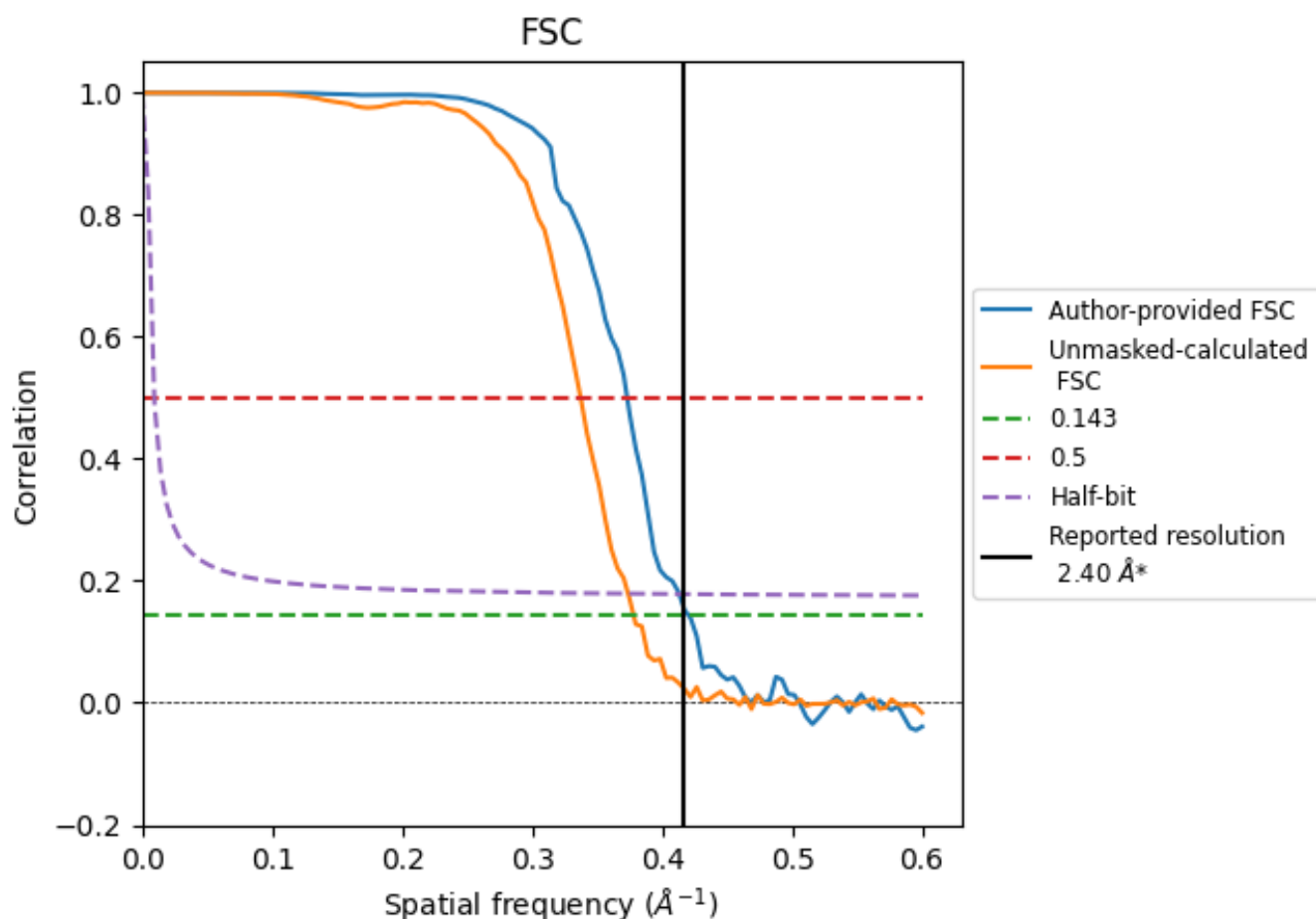


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

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 0.417 $\text{\AA}^{-1}$

8.2 Resolution estimates

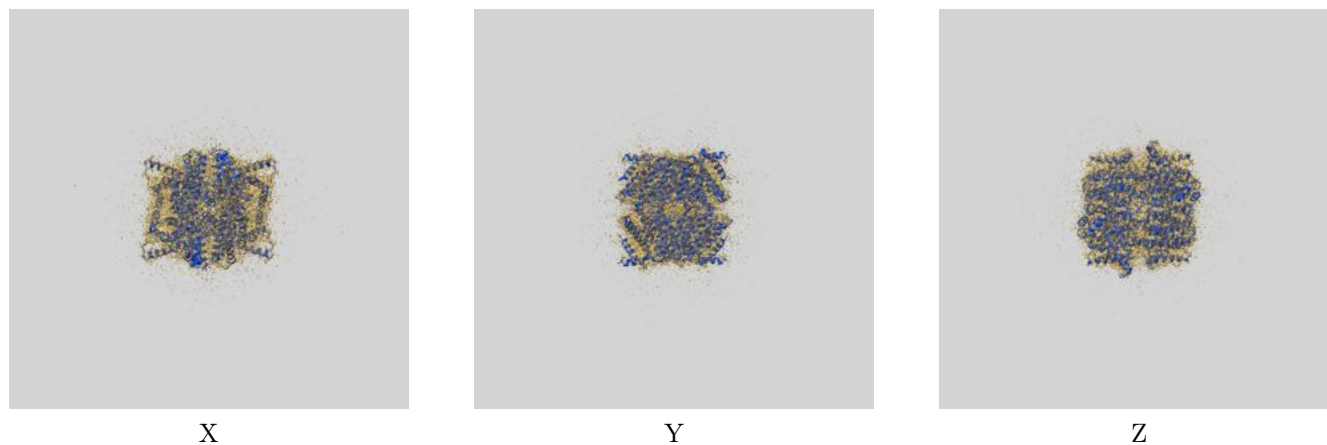
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.38	2.68	2.42
Unmasked-calculated*	2.64	2.96	2.67

*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 2.64 differs from the reported value 2.4 by more than 10 %

9 Map-model fit [i](#)

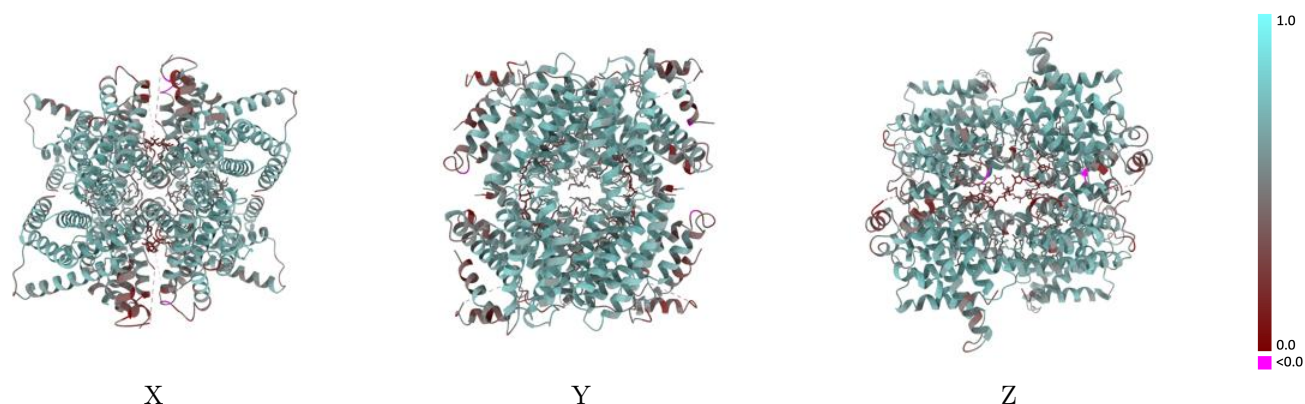
This section contains information regarding the fit between EMDB map EMD-25413 and PDB model 7SSS. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



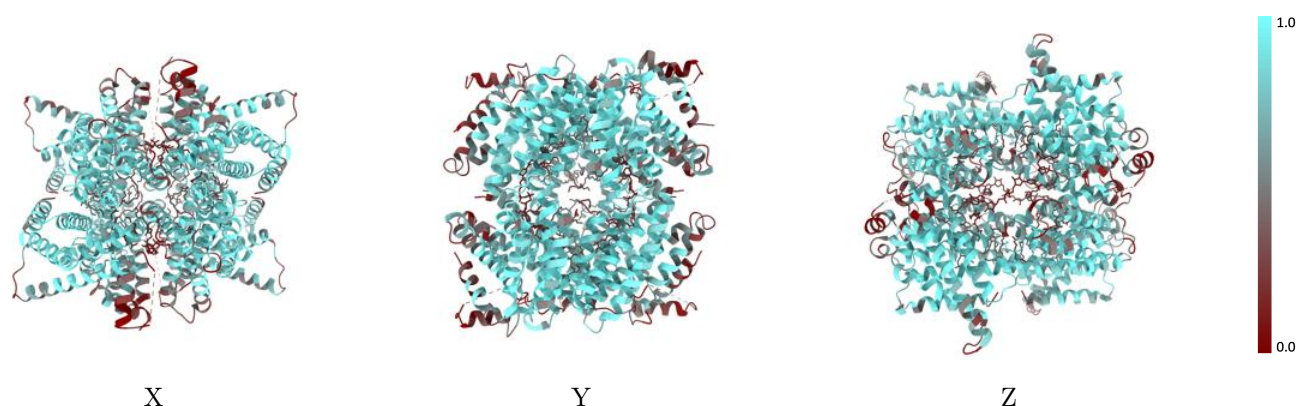
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



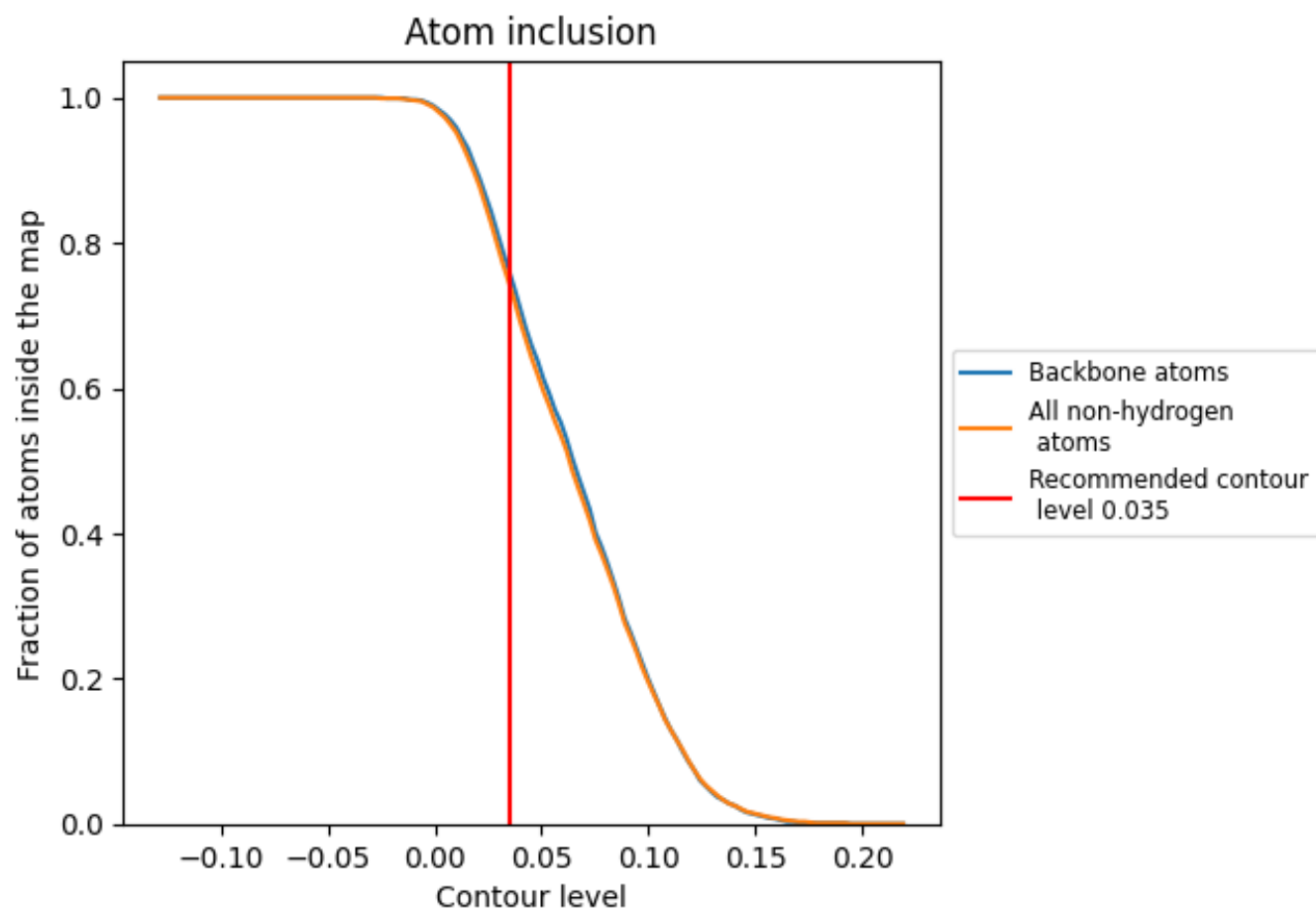
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7430	0.5990
A	0.7500	0.6040
B	0.7390	0.6000
C	0.7320	0.5970
D	0.7470	0.6050
E	0.7390	0.5880
F	0.7490	0.5920
G	0.7600	0.6030
H	0.7550	0.6020

1.0

0.0

<0.0