



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:54 AM UTC

PDB ID : 9FQ8 / pdb_00009fq8
EMDB ID : EMD-50363
Title : Perkinsus marinus Respiratory complex CIV
Authors : Wu, F.; Amunts, A.
Deposited on : 2024-06-14
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

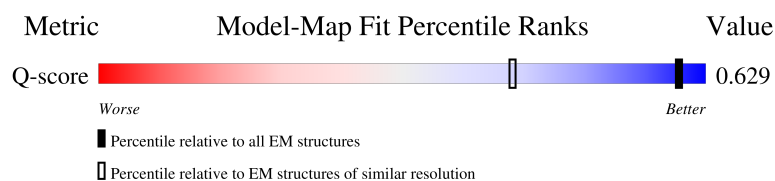
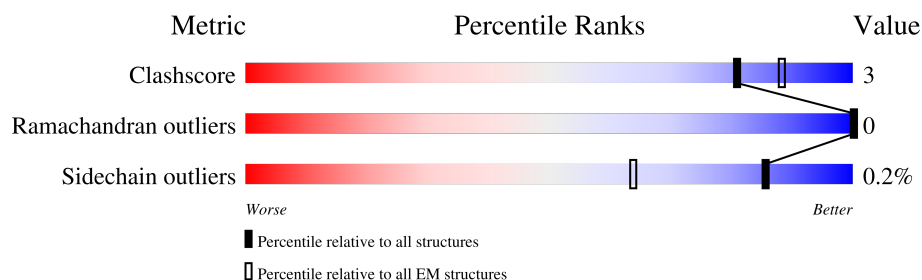
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 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.



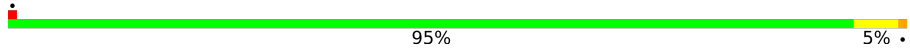
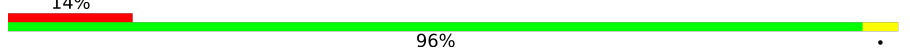
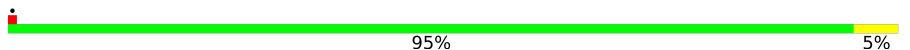
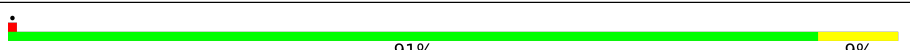
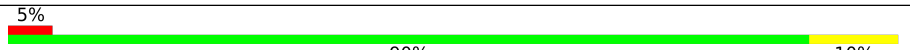
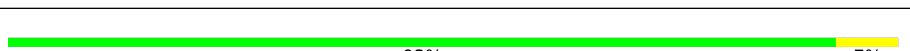
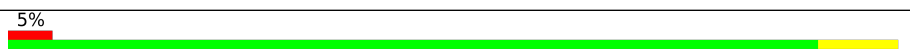
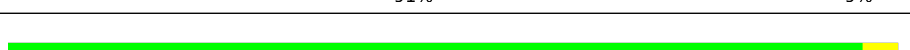
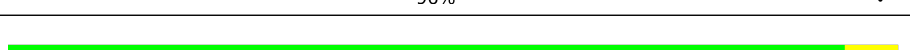
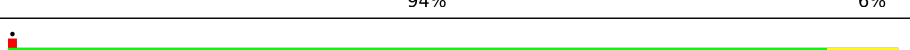
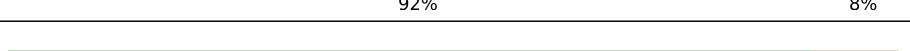
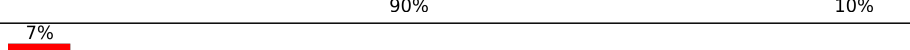
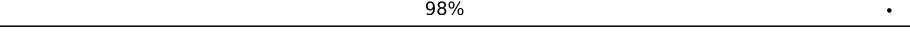
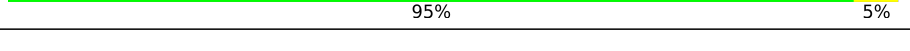
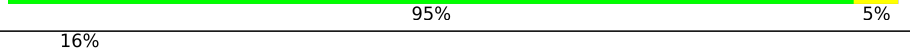
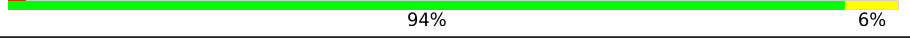
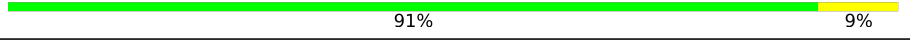
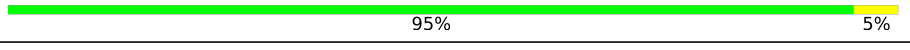
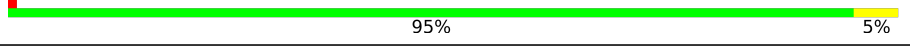
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3184 (1.71 - 2.70)

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	4A	100	
2	4B	93	
3	4C	75	
4	4D	90	

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Mol	Chain	Length	Quality of chain
5	4E	152	
6	4F	80	
7	4G	100	
8	4H	141	
9	4I	196	
10	4J	186	
11	4K	93	
12	4L	122	
13	4M	99	
14	4N	131	
15	4O	47	
16	4P	180	
17	4Q	459	
18	4R	103	
19	4S	65	
20	4T	121	
21	4U	91	
22	4V	185	
23	4W	141	
24	4X	226	
25	4Y	107	
26	4Z	186	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 31410 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome c oxidase subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	4A	100	Total	C	N	O	S	0	0
			841	518	157	157	9		

- Molecule 2 is a protein called Peptidase M14 carboxypeptidase A domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4B	93	Total	C	N	O	S	0	0
			732	479	116	129	8		

- Molecule 3 is a protein called Cytochrome c oxidase subunit 40.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4C	75	Total	C	N	O	S	0	0
			626	414	95	113	4		

- Molecule 4 is a protein called Cytochrome c oxidase subunit 34.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4D	90	Total	C	N	O	S	0	0
			787	525	128	131	3		

- Molecule 5 is a protein called Merozoite surface protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4E	152	Total	C	N	O	S	0	0
			1313	840	229	229	15		

- Molecule 6 is a protein called Ubiquitin, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4F	80	Total	C	N	O	S	0	0
			669	438	119	110	2		

- Molecule 7 is a protein called Cytochrome c oxidase subunit 33.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	4G	100	Total	C	N	O	S	0	0
			854	550	156	144	4		

- Molecule 8 is a protein called Cytochrome c oxidase subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	4H	141	Total	C	N	O	S	0	0
			1125	711	195	217	2		

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	4I	196	Total	C	N	O	S	0	0
			1695	1105	276	305	9		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	4J	186	Total	C	N	O	S	0	0
			1517	990	268	253	6		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 37.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	4K	93	Total	C	N	O	S	0	0
			722	473	129	118	2		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 7A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	4L	122	Total	C	N	O	S	0	0
			1083	715	192	168	8		

- Molecule 13 is a protein called Cytochrome c oxidase subunit 35.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	4M	99	Total	C	N	O	S	0	0
			778	501	148	128	1		

- Molecule 14 is a protein called Cytochrome c oxidase polypeptide II.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	4N	131	Total	C	N	O	S	0	0
			1025	661	173	184	7		

- Molecule 15 is a protein called GINS subunit domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	4O	47	Total	C	N	O	S	0	0
			383	257	60	63	3		

- Molecule 16 is a protein called Cytochrome oxidase subunit II copper A binding domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4P	180	Total	C	N	O	S	0	0
			1504	977	246	276	5		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	4Q	459	Total	C	N	O	S	0	0
			3687	2519	545	612	11		

- Molecule 18 is a protein called Cytochrome c oxidase subunit 32.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	4R	103	Total	C	N	O	S	0	0
			916	609	156	145	6		

- Molecule 19 is a protein called Cytochrome c oxidase subunit 7C.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	4S	65	Total	C	N	O	S	0	0
			541	350	85	100	6		

- Molecule 20 is a protein called Cytochrome c oxidase 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	4T	121	Total	C	N	O	S	0	0
			983	634	170	167	12		

- Molecule 21 is a protein called Amino acid transporter transmembrane domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	4U	91	Total	C	N	O	S	0	0
			758	503	125	127	3		

- Molecule 22 is a protein called Cg8 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	4V	185	Total	C	N	O	S	0	0
			1539	1003	270	260	6		

- Molecule 23 is a protein called Cytochrome c oxidase subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	4W	141	Total	C	N	O	S	0	0
			1193	782	206	198	7		

- Molecule 24 is a protein called Cytochrome Coxidase subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	4X	226	Total	C	N	O	S	0	0
			1860	1186	313	344	17		

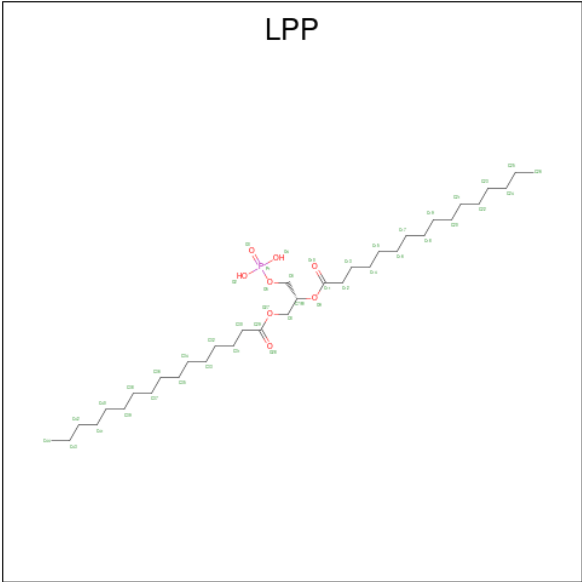
- Molecule 25 is a protein called Cytochrome c oxidase subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	4Y	107	Total	C	N	O	S	0	0
			905	567	153	179	6		

- Molecule 26 is a protein called Cytochrome c oxidase subunit 31.

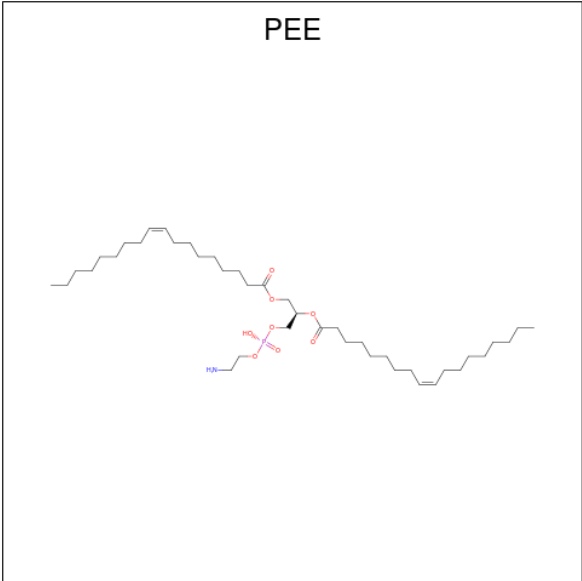
Mol	Chain	Residues	Atoms					AltConf	Trace
26	4Z	186	Total	C	N	O	S	0	0
			1582	1041	270	266	5		

- Molecule 27 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: C₃₅H₆₉O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
27	4C	1	Total	C	O	P	0
			44	35	8	1	
27	4Z	1	Total	C	O	P	0
			44	35	8	1	

- Molecule 28 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P) (labeled as "Ligand of Interest" by depositor).



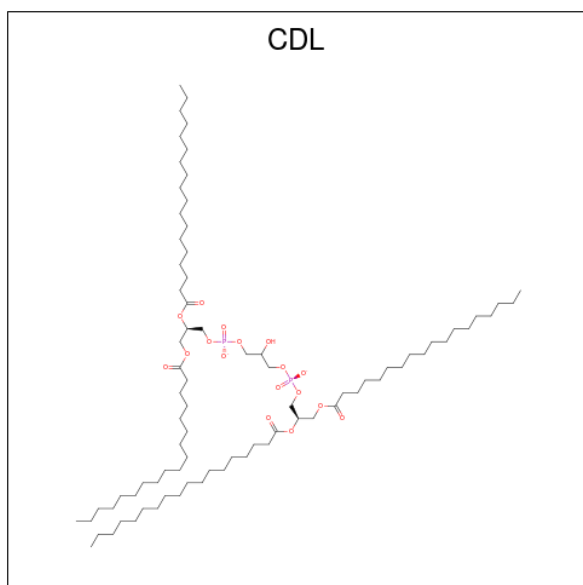
Mol	Chain	Residues	Atoms					AltConf
28	4D	1	Total	C	N	O	P	0
			40	30	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
28	4E	1	Total	C	N	O	P	0
			31	21	1	8	1	
28	4G	1	Total	C	N	O	P	0
			45	35	1	8	1	
28	4L	1	Total	C	N	O	P	0
			35	25	1	8	1	
28	4Q	1	Total	C	N	O	P	0
			36	26	1	8	1	
28	4Q	1	Total	C	N	O	P	0
			47	37	1	8	1	
28	4R	1	Total	C	N	O	P	0
			43	33	1	8	1	
28	4S	1	Total	C	N	O	P	0
			27	17	1	8	1	
28	4W	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	4Z	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 29 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



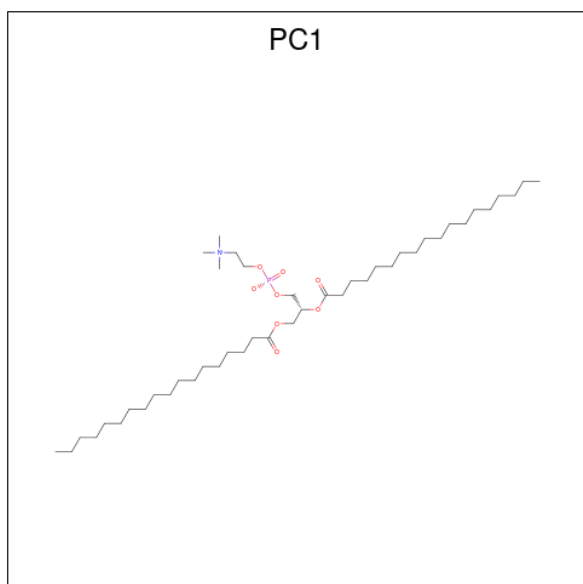
Mol	Chain	Residues	Atoms				AltConf
29	4E	1	Total	C	O	P	0
			89	70	17	2	
29	4E	1	Total	C	O	P	0
			46	27	17	2	

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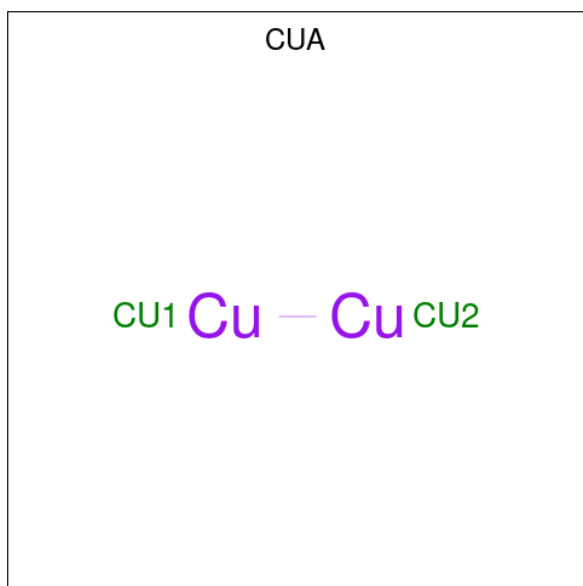
Mol	Chain	Residues	Atoms				AltConf
29	4F	1	Total	C	O	P	0
			100	81	17	2	
29	4J	1	Total	C	O	P	0
			59	40	17	2	
29	4K	1	Total	C	O	P	0
			90	71	17	2	
29	4L	1	Total	C	O	P	0
			94	75	17	2	
29	4M	1	Total	C	O	P	0
			75	56	17	2	
29	4O	1	Total	C	O	P	0
			97	78	17	2	
29	4Q	1	Total	C	O	P	0
			95	76	17	2	
29	4Q	1	Total	C	O	P	0
			75	56	17	2	
29	4S	1	Total	C	O	P	0
			100	81	17	2	
29	4U	1	Total	C	O	P	0
			72	53	17	2	
29	4W	1	Total	C	O	P	0
			73	54	17	2	
29	4Z	1	Total	C	O	P	0
			48	29	17	2	

- Molecule 30 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
30	4F	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 31 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
31	4N	1	Total	Cu	0
			2	2	

- Molecule 32 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

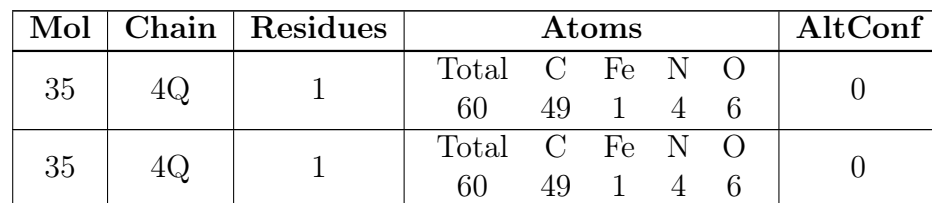
Mol	Chain	Residues	Atoms		AltConf
32	4Q	1	Total	K	0
			1	1	

- Molecule 33 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

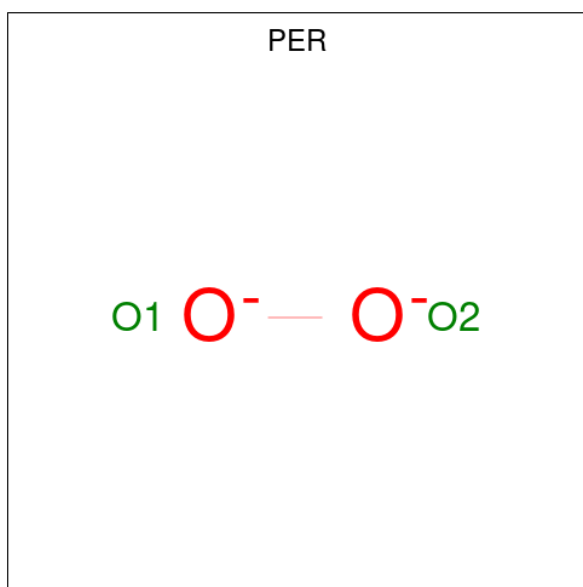
Mol	Chain	Residues	Atoms		AltConf
33	4Q	1	Total	Cu	0
			1	1	

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

- Molecule 35 is HEME-A (CCD ID: HEA) (formula: $\text{C}_{49}\text{H}_{56}\text{FeN}_4\text{O}_6$) (labeled as "Ligand of Interest" by depositor).



- Molecule 36 is PEROXIDE ION (CCD ID: PER) (formula: O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
36	4Q	1	Total	O	0
			2	2	

- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
37	4T	2	Total	Zn	0
			2	2	
37	4X	1	Total	Zn	0
			1	1	

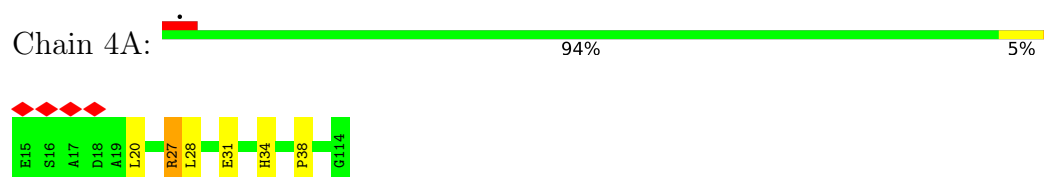
- Molecule 38 is water.

Mol	Chain	Residues	Atoms		AltConf
38	4Q	1	Total	O	0
			1	1	

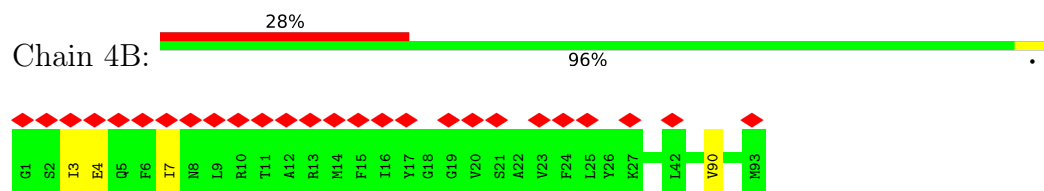
3 Residue-property plots [i](#)

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

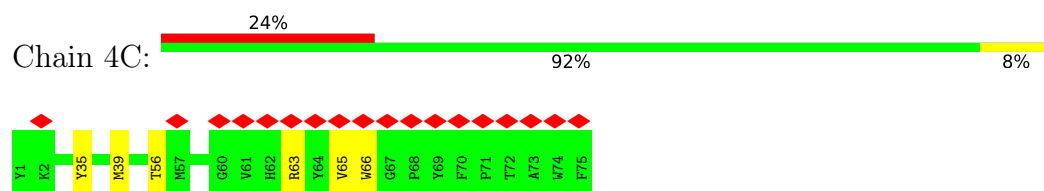
- Molecule 1: Cytochrome c oxidase subunit 6B



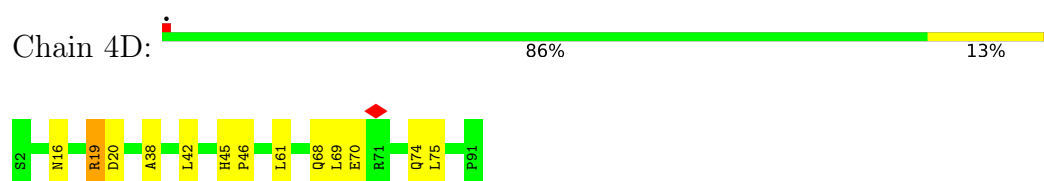
- Molecule 2: Peptidase M14 carboxypeptidase A domain-containing protein



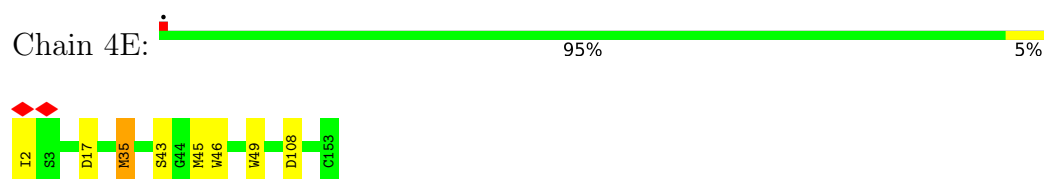
- Molecule 3: Cytochrome c oxidase subunit 40



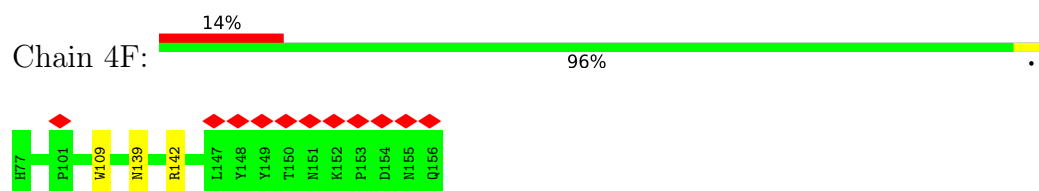
- Molecule 4: Cytochrome c oxidase subunit 34



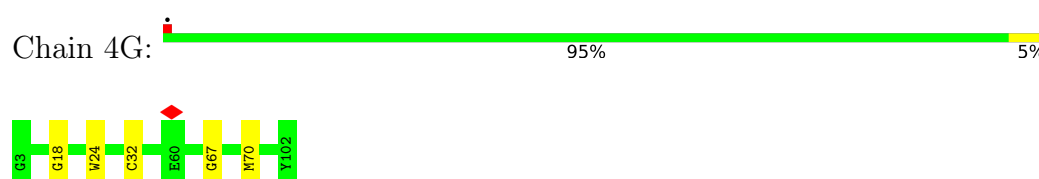
- Molecule 5: Merozoite surface protein, putative



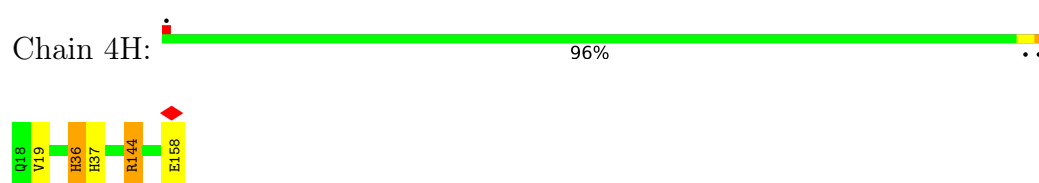
- Molecule 6: Ubiquitin, putative



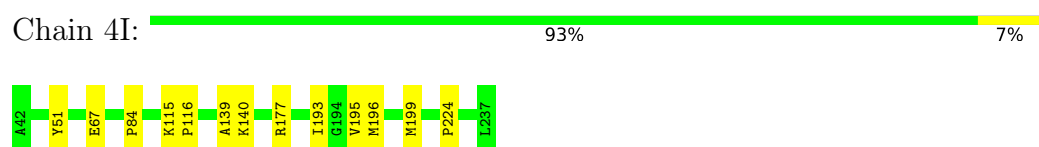
- Molecule 7: Cytochrome c oxidase subunit 33



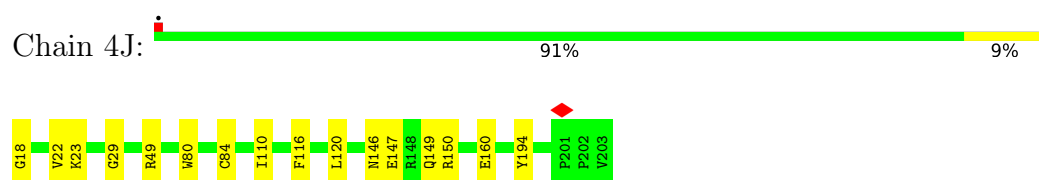
- Molecule 8: Cytochrome c oxidase subunit 30



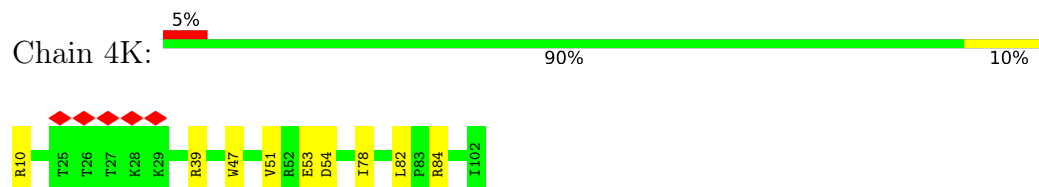
- Molecule 9: Cytochrome c oxidase subunit 6C



- Molecule 10: Cytochrome c oxidase subunit 24



- Molecule 11: Cytochrome c oxidase subunit 37

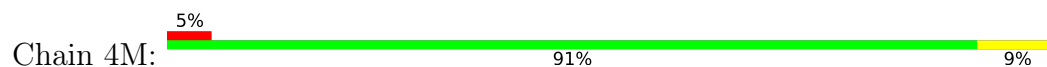


- Molecule 12: Cytochrome c oxidase subunit 7A





- Molecule 13: Cytochrome c oxidase subunit 35



- Molecule 14: Cytochrome c oxidase polypeptide II



- Molecule 15: GINS subunit domain-containing protein



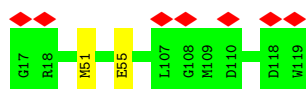
- Molecule 16: Cytochrome oxidase subunit II copper A binding domain-containing protein



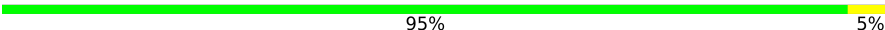
- Molecule 17: Cytochrome c oxidase subunit 1

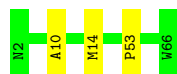


- Molecule 18: Cytochrome c oxidase subunit 32

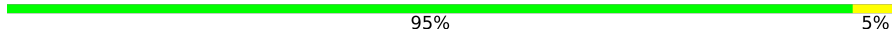


- Molecule 19: Cytochrome c oxidase subunit 7C

Chain 4S:  95% 5%



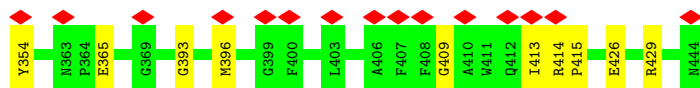
- Molecule 20: Cytochrome c oxidase 13

Chain 4T:  95% 5%

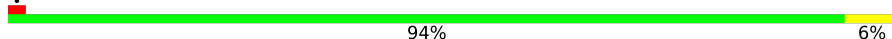


- Molecule 21: Amino acid transporter transmembrane domain-containing protein

Chain 4U:  16% 89% 11%

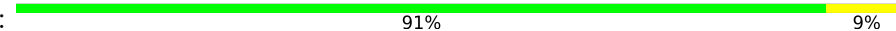


- Molecule 22: Cg8 protein

Chain 4V:  94% 6%

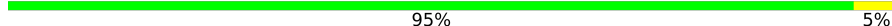


- Molecule 23: Cytochrome c oxidase subunit 19

Chain 4W:  91% 9%

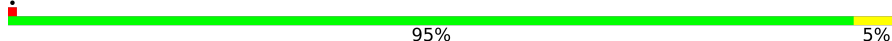


- Molecule 24: Cytochrome Coxidase subunit, putative

Chain 4X:  95% 5%

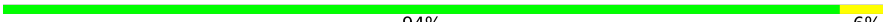


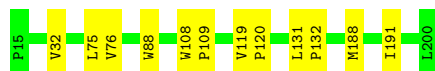
- Molecule 25: Cytochrome c oxidase subunit 18

Chain 4Y:  95% 5%



- Molecule 26: Cytochrome c oxidase subunit 31

Chain 4Z:  94% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	296890	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.207	Depositor
Minimum map value	-0.075	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	423.2, 423.2, 423.2	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8464, 0.8464, 0.8464	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEA, LPP, PER, CDL, CU, K, PC1, PEE, ZN, MG, CUA

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	4A	0.16	0/863	0.32	0/1166
2	4B	0.17	0/751	0.30	0/1013
3	4C	0.16	0/653	0.30	0/891
4	4D	0.16	0/819	0.31	0/1110
5	4E	0.17	0/1353	0.34	0/1824
6	4F	0.21	0/695	0.34	0/948
7	4G	0.16	0/883	0.26	0/1199
8	4H	0.14	0/1149	0.26	0/1565
9	4I	0.22	0/1757	0.28	0/2386
10	4J	0.22	0/1573	0.33	0/2131
11	4K	0.21	0/745	0.34	0/1017
12	4L	0.17	0/1131	0.27	0/1537
13	4M	0.17	0/805	0.30	0/1104
14	4N	0.18	0/1055	0.32	0/1436
15	4O	0.29	0/400	0.36	0/549
16	4P	0.17	0/1551	0.30	0/2106
17	4Q	0.24	0/3774	0.36	0/5155
18	4R	0.14	0/958	0.25	0/1301
19	4S	0.15	0/560	0.23	0/760
20	4T	0.18	0/1024	0.27	0/1391
21	4U	0.14	0/790	0.34	0/1073
22	4V	0.23	0/1600	0.32	0/2183
23	4W	0.17	0/1240	0.33	0/1686
24	4X	0.18	0/1912	0.32	0/2592
25	4Y	0.17	0/929	0.27	0/1261
26	4Z	0.18	0/1639	0.32	0/2233
All	All	0.19	0/30609	0.31	0/41617

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	4A	0	1
3	4C	0	1
4	4D	0	1
6	4F	0	1
8	4H	0	1
10	4J	0	1
11	4K	0	2
22	4V	0	1
24	4X	0	1
All	All	0	10

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	4A	27	ARG	Sidechain
3	4C	63	ARG	Sidechain
4	4D	19	ARG	Sidechain
6	4F	142	ARG	Sidechain
8	4H	144	ARG	Sidechain
10	4J	49	ARG	Sidechain
11	4K	10	ARG	Sidechain
11	4K	84	ARG	Sidechain
22	4V	127	ARG	Sidechain
24	4X	38	ARG	Sidechain

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	4A	841	0	766	6	0
2	4B	732	0	746	3	0
3	4C	626	0	575	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	4D	787	0	745	8	0
5	4E	1313	0	1269	8	0
6	4F	669	0	642	3	0
7	4G	854	0	811	3	0
8	4H	1125	0	1112	4	0
9	4I	1695	0	1593	11	0
10	4J	1517	0	1435	9	0
11	4K	722	0	760	4	0
12	4L	1083	0	1027	8	0
13	4M	778	0	802	8	0
14	4N	1025	0	1018	6	0
15	4O	383	0	368	3	0
16	4P	1504	0	1461	12	0
17	4Q	3687	0	3956	45	0
18	4R	916	0	854	1	0
19	4S	541	0	489	2	0
20	4T	983	0	902	4	0
21	4U	758	0	713	8	0
22	4V	1539	0	1482	10	0
23	4W	1193	0	1164	9	0
24	4X	1860	0	1764	7	0
25	4Y	905	0	835	5	0
26	4Z	1582	0	1548	8	0
27	4C	44	0	67	1	0
27	4Z	44	0	67	0	0
28	4D	40	0	57	0	0
28	4E	31	0	36	1	0
28	4G	45	0	67	0	0
28	4L	35	0	44	0	0
28	4Q	83	0	117	0	0
28	4R	43	0	63	0	0
28	4S	27	0	28	0	0
28	4W	51	0	82	0	0
28	4Z	51	0	82	2	0
29	4E	135	0	167	2	0
29	4F	100	0	156	0	0
29	4J	59	0	64	0	0
29	4K	90	0	133	0	0
29	4L	94	0	141	0	0
29	4M	75	0	100	1	0
29	4O	97	0	147	0	0
29	4Q	170	0	243	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	4S	100	0	156	0	0
29	4U	72	0	88	0	0
29	4W	73	0	93	0	0
29	4Z	48	0	40	1	0
30	4F	54	0	88	2	0
31	4N	2	0	0	0	0
32	4Q	1	0	0	0	0
33	4Q	1	0	0	0	0
34	4Q	1	0	0	0	0
35	4Q	120	0	108	10	0
36	4Q	2	0	0	0	0
37	4T	2	0	0	0	0
37	4X	1	0	0	0	0
38	4Q	1	0	0	0	0
All	All	31410	0	31271	163	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (163) 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)
17:4Q:632:HIS:NE2	17:4Q:636:TYR:HE2	1.60	0.97
17:4Q:762:HIS:CD2	17:4Q:763:ASP:OD2	2.38	0.76
17:4Q:468:MET:HE3	35:4Q:908:HEA:HMC2	1.70	0.74
17:4Q:632:HIS:HE2	17:4Q:636:TYR:HE2	1.36	0.73
17:4Q:632:HIS:NE2	17:4Q:636:TYR:CE2	2.52	0.70
1:4A:20:LEU:HD11	1:4A:31:GLU:HG3	1.77	0.66
22:4V:89:MET:HA	22:4V:89:MET:HE2	1.79	0.65
14:4N:134:CYS:SG	14:4N:138:HIS:HA	2.37	0.64
1:4A:20:LEU:HD12	1:4A:28:LEU:HA	1.79	0.64
1:4A:20:LEU:HD11	1:4A:31:GLU:CG	2.28	0.64
17:4Q:632:HIS:O	17:4Q:635:VAL:HG22	2.01	0.61
17:4Q:636:TYR:HA	17:4Q:639:ILE:HG22	1.82	0.60
1:4A:34:HIS:O	16:4P:184:THR:OG1	2.19	0.60
17:4Q:767:ILE:HD12	35:4Q:909:HEA:HBA1	1.85	0.58
3:4C:65:VAL:HG22	3:4C:66:TRP:HD1	1.69	0.58
16:4P:133:PRO:HB2	22:4V:38:MET:HE2	1.87	0.57
5:4E:46:TRP:O	9:4I:84:PRO:CD	2.54	0.56
8:4H:144:ARG:HG2	8:4H:144:ARG:HH11	1.69	0.56
17:4Q:468:MET:CE	35:4Q:908:HEA:HMC2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:4J:116:PHE:CZ	10:4J:120:LEU:HD11	2.41	0.56
6:4F:109:TRP:HB2	30:4F:201:PC1:H222	1.88	0.55
21:4U:393:GLY:O	21:4U:396:MET:HE2	2.07	0.55
17:4Q:468:MET:HB3	35:4Q:908:HEA:CAC	2.37	0.54
5:4E:17:ASP:O	12:4L:35:ARG:NH1	2.42	0.53
28:4Z:302:PEE:H54	28:4Z:302:PEE:H63	1.91	0.53
17:4Q:670:MET:HA	17:4Q:670:MET:HE2	1.90	0.52
4:4D:70:GLU:HG2	4:4D:75:LEU:HD23	1.92	0.52
24:4X:252:GLU:HA	24:4X:255:THR:HG22	1.93	0.51
13:4M:71:GLN:HG3	20:4T:149:VAL:HG21	1.92	0.51
17:4Q:835:LEU:H	17:4Q:835:LEU:HD23	1.76	0.51
21:4U:409:GLY:HA3	22:4V:140:LEU:HD11	1.92	0.51
13:4M:23:PRO:HA	29:4M:201:CDL:HB22	1.92	0.51
15:4O:377:MET:HG2	17:4Q:756:ILE:HG22	1.94	0.49
10:4J:22:VAL:HG21	10:4J:110:ILE:HA	1.93	0.49
17:4Q:670:MET:HE1	26:4Z:76:VAL:HB	1.94	0.49
4:4D:20:ASP:OD1	26:4Z:32:VAL:HG23	2.13	0.49
29:4Q:903:CDL:OB7	29:4Q:903:CDL:HB31	2.12	0.49
35:4Q:909:HEA:HHC	35:4Q:909:HEA:O11	2.13	0.49
21:4U:365:GLU:HA	21:4U:365:GLU:OE1	2.13	0.48
17:4Q:430:GLY:HA3	17:4Q:468:MET:SD	2.54	0.48
17:4Q:450:LYS:HD2	19:4S:53:PRO:HB3	1.95	0.48
22:4V:150:ARG:NH2	22:4V:151:ASN:HD21	2.12	0.48
9:4I:195:VAL:O	9:4I:199:MET:HG2	2.14	0.48
26:4Z:131:LEU:N	26:4Z:132:PRO:HD2	2.28	0.48
16:4P:42:THR:HG22	16:4P:43:GLN:HG2	1.95	0.48
8:4H:158:GLU:HB2	12:4L:19:ARG:HH22	1.79	0.48
23:4W:56:ARG:HB2	25:4Y:129:ASP:OD2	2.13	0.48
11:4K:78:ILE:HG23	11:4K:82:LEU:HD12	1.96	0.47
4:4D:68:GLN:CD	4:4D:68:GLN:C	2.81	0.47
16:4P:81:ASP:N	16:4P:81:ASP:OD1	2.44	0.47
4:4D:16:ASN:HA	4:4D:19:ARG:HG3	1.96	0.47
12:4L:123:ASP:OD1	12:4L:126:ASN:HB2	2.15	0.47
17:4Q:464:HIS:O	17:4Q:468:MET:HG2	2.15	0.47
17:4Q:474:MET:HB3	17:4Q:475:PRO:HD3	1.97	0.47
10:4J:160:GLU:OE1	10:4J:160:GLU:HA	2.12	0.47
17:4Q:702:ILE:HG23	26:4Z:75:LEU:HD11	1.97	0.47
17:4Q:771:PHE:HB2	35:4Q:909:HEA:HMD3	1.97	0.47
2:4B:3:ILE:HD12	2:4B:3:ILE:N	2.30	0.47
1:4A:28:LEU:HD23	1:4A:38:PRO:HD3	1.97	0.46
4:4D:61:LEU:HD22	29:4Z:303:CDL:C54	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:4K:39:ARG:HG3	11:4K:47:TRP:CZ3	2.50	0.46
12:4L:122:ASN:ND2	17:4Q:521:ILE:O	2.45	0.46
24:4X:153:THR:HG21	25:4Y:116:LEU:HD21	1.98	0.46
4:4D:45:HIS:O	4:4D:46:PRO:C	2.59	0.46
35:4Q:908:HEA:HHC	35:4Q:908:HEA:H11	1.79	0.46
24:4X:151:ALA:HB2	24:4X:165:TRP:CD2	2.51	0.46
12:4L:101:ARG:HD3	29:4Q:903:CDL:HA4	1.98	0.46
17:4Q:597:ASN:O	17:4Q:601:LEU:HG	2.15	0.46
6:4F:139:ASN:O	23:4W:134:MET:HG3	2.16	0.46
17:4Q:486:LEU:HD11	17:4Q:579:ILE:HG23	1.97	0.46
17:4Q:491:VAL:HG23	17:4Q:572:ASP:HB2	1.98	0.46
17:4Q:440:GLU:OE2	17:4Q:835:LEU:HD12	2.16	0.45
22:4V:170:GLU:HA	22:4V:170:GLU:OE1	2.16	0.45
4:4D:38:ALA:HB1	4:4D:42:LEU:HD12	1.99	0.45
25:4Y:40:ASP:OD1	25:4Y:40:ASP:N	2.49	0.45
10:4J:18:GLY:O	10:4J:23:LYS:NZ	2.50	0.45
17:4Q:814:ASN:HB3	17:4Q:855:THR:HG23	1.99	0.45
26:4Z:188:MET:HE2	26:4Z:191:ILE:HD12	1.99	0.45
2:4B:4:GLU:HA	2:4B:7:ILE:HD12	1.99	0.45
12:4L:89:GLY:N	12:4L:93:ASP:OD2	2.45	0.45
16:4P:174:ILE:HD12	17:4Q:756:ILE:HB	1.99	0.45
5:4E:49:TRP:CH2	23:4W:96:ILE:HD11	2.52	0.45
7:4G:67:GLY:HA2	7:4G:70:MET:HE2	1.98	0.44
6:4F:109:TRP:CD1	30:4F:201:PC1:H252	2.52	0.44
23:4W:14:PHE:CE2	23:4W:16:ASP:OD1	2.70	0.44
24:4X:56:LYS:HG3	24:4X:213:LEU:HD11	1.99	0.44
17:4Q:762:HIS:HA	35:4Q:909:HEA:O2A	2.17	0.44
10:4J:147:GLU:HG2	10:4J:150:ARG:HH12	1.82	0.44
13:4M:44:MET:HA	16:4P:136:PRO:HG3	1.98	0.44
14:4N:71:GLU:HA	14:4N:71:GLU:OE1	2.18	0.43
14:4N:134:CYS:H	14:4N:138:HIS:HB2	1.83	0.43
21:4U:413:ILE:HG23	22:4V:146:PHE:CZ	2.53	0.43
24:4X:176:CYS:HA	25:4Y:93:MET:HE1	1.99	0.43
26:4Z:88:TRP:CD1	28:4Z:302:PEE:H25	2.52	0.43
24:4X:138:PRO:HB3	24:4X:182:ILE:HG22	2.00	0.43
1:4A:20:LEU:HD13	1:4A:27:ARG:HG2	1.99	0.43
21:4U:426:GLU:OE1	21:4U:429:ARG:NH2	2.51	0.43
23:4W:87:PRO:HG2	23:4W:92:LEU:HD21	2.00	0.43
9:4I:193:ILE:HD13	9:4I:196:MET:CE	2.48	0.43
22:4V:89:MET:CE	22:4V:92:ILE:HD11	2.48	0.43
17:4Q:478:TYR:HA	17:4Q:482:PRO:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:4W:81:ARG:HG2	23:4W:82:PRO:HD2	2.00	0.43
9:4I:140:LYS:C	23:4W:69:MET:HE2	2.43	0.43
3:4C:35:TYR:CE1	3:4C:39:MET:HE3	2.54	0.42
28:4E:201:PEE:O4	28:4E:201:PEE:H7	2.18	0.42
9:4I:224:PRO:HA	13:4M:88:ARG:HG3	2.01	0.42
16:4P:149:VAL:HG12	16:4P:150:MET:HE2	2.01	0.42
14:4N:141:MET:HE2	16:4P:197:TRP:NE1	2.34	0.42
5:4E:108:ASP:OD1	5:4E:108:ASP:N	2.51	0.42
20:4T:37:ILE:HG13	20:4T:38:TRP:CD1	2.55	0.42
5:4E:35:MET:HE1	5:4E:43:SER:HB3	2.00	0.42
11:4K:53:GLU:HG3	11:4K:54:ASP:N	2.33	0.42
12:4L:123:ASP:O	12:4L:123:ASP:CG	2.62	0.42
17:4Q:656:LYS:HD3	17:4Q:717:LEU:O	2.19	0.42
17:4Q:828:ASN:N	17:4Q:829:VAL:HA	2.35	0.42
9:4I:177:ARG:CG	13:4M:27:VAL:HG11	2.49	0.42
17:4Q:424:ILE:HG13	35:4Q:908:HEA:H242	2.01	0.42
9:4I:196:MET:SD	13:4M:64:LEU:HD11	2.59	0.42
21:4U:414:ARG:N	21:4U:415:PRO:HD2	2.35	0.42
27:4C:101:LPP:H311	7:4G:18:GLY:HA3	2.02	0.42
8:4H:19:VAL:HG11	8:4H:37:HIS:NE2	2.35	0.42
17:4Q:768:VAL:HA	17:4Q:771:PHE:CE2	2.55	0.42
17:4Q:769:SER:HB3	17:4Q:822:GLN:HB2	2.02	0.41
23:4W:14:PHE:CE1	23:4W:20:ASP:HA	2.55	0.41
24:4X:151:ALA:HB2	24:4X:165:TRP:CE3	2.55	0.41
4:4D:69:LEU:HD22	4:4D:74:GLN:HB3	2.02	0.41
12:4L:123:ASP:OD1	12:4L:126:ASN:ND2	2.53	0.41
13:4M:21:ARG:HB3	13:4M:22:PRO:HD2	2.02	0.41
21:4U:354:TYR:O	21:4U:354:TYR:CG	2.72	0.41
26:4Z:119:VAL:N	26:4Z:120:PRO:HD2	2.34	0.41
16:4P:174:ILE:HB	17:4Q:756:ILE:HG13	2.02	0.41
8:4H:36:HIS:CE1	9:4I:139:ALA:HB2	2.55	0.41
14:4N:64:PRO:HA	22:4V:103:TRP:CD2	2.55	0.41
15:4O:376:LEU:O	15:4O:380:THR:HG23	2.20	0.41
17:4Q:578:TYR:CE2	17:4Q:582:ILE:HD11	2.54	0.41
5:4E:46:TRP:O	9:4I:84:PRO:HD2	2.21	0.41
17:4Q:474:MET:HB2	17:4Q:638:LEU:HD21	2.02	0.41
2:4B:90:VAL:HG21	10:4J:194:TYR:HB2	2.02	0.41
10:4J:146:ASN:O	10:4J:149:GLN:HG2	2.21	0.41
13:4M:41:HIS:CD2	25:4Y:46:GLU:HG2	2.56	0.41
17:4Q:774:ILE:HG21	35:4Q:909:HEA:HMC1	2.02	0.41
20:4T:98:GLU:OE1	22:4V:37:TYR:HE1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:4P:175:ASN:HB3	17:4Q:690:LEU:HD11	2.03	0.41
19:4S:10:ALA:O	19:4S:14:MET:HG2	2.21	0.41
21:4U:413:ILE:HG23	22:4V:146:PHE:CE2	2.56	0.41
9:4I:115:LYS:N	9:4I:116:PRO:HD2	2.37	0.40
10:4J:80:TRP:HB2	10:4J:84:CYS:SG	2.61	0.40
17:4Q:425:ILE:HA	17:4Q:428:ILE:HD12	2.02	0.40
26:4Z:108:TRP:N	26:4Z:109:PRO:HD2	2.36	0.40
3:4C:56:THR:HG23	7:4G:32:CYS:HA	2.02	0.40
5:4E:2:ILE:HA	29:4E:203:CDL:OB3	2.20	0.40
5:4E:45:MET:HE3	9:4I:51:TYR:CD2	2.56	0.40
10:4J:29:GLY:HA2	11:4K:51:VAL:HG22	2.03	0.40
17:4Q:486:LEU:HG	17:4Q:567:ILE:HD13	2.03	0.40
16:4P:194:GLN:HA	16:4P:195:TRP:HA	1.85	0.40
20:4T:106:CYS:SG	20:4T:109:LYS:N	2.89	0.40
29:4E:203:CDL:HB61	29:4E:203:CDL:OB7	2.22	0.40
14:4N:138:HIS:HD2	17:4Q:833:ARG:O	2.04	0.40
17:4Q:632:HIS:CD2	17:4Q:636:TYR:HE2	2.34	0.40
18:4R:51:MET:HA	18:4R:55:GLU:HG2	2.03	0.40
15:4O:377:MET:HE3	17:4Q:756:ILE:O	2.21	0.40
16:4P:176:PHE:HD1	17:4Q:690:LEU:HD21	1.87	0.40
23:4W:128:GLU:O	23:4W:143:GLU:HA	2.21	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	4A	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	4B	91/93 (98%)	89 (98%)	2 (2%)	0	100	100
3	4C	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
4	4D	88/90 (98%)	87 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	4E	150/152 (99%)	147 (98%)	3 (2%)	0	100	100
6	4F	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
7	4G	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
8	4H	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
9	4I	194/196 (99%)	193 (100%)	1 (0%)	0	100	100
10	4J	184/186 (99%)	179 (97%)	5 (3%)	0	100	100
11	4K	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
12	4L	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
13	4M	97/99 (98%)	97 (100%)	0	0	100	100
14	4N	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
15	4O	45/47 (96%)	45 (100%)	0	0	100	100
16	4P	178/180 (99%)	172 (97%)	6 (3%)	0	100	100
17	4Q	457/459 (100%)	441 (96%)	16 (4%)	0	100	100
18	4R	101/103 (98%)	101 (100%)	0	0	100	100
19	4S	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
20	4T	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
21	4U	89/91 (98%)	88 (99%)	1 (1%)	0	100	100
22	4V	183/185 (99%)	181 (99%)	2 (1%)	0	100	100
23	4W	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
24	4X	224/226 (99%)	220 (98%)	4 (2%)	0	100	100
25	4Y	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
26	4Z	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
All	All	3517/3569 (98%)	3440 (98%)	77 (2%)	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	4A	91/91 (100%)	91 (100%)	0	100	100
2	4B	77/77 (100%)	77 (100%)	0	100	100
3	4C	64/64 (100%)	64 (100%)	0	100	100
4	4D	81/81 (100%)	81 (100%)	0	100	100
5	4E	146/146 (100%)	145 (99%)	1 (1%)	76	87
6	4F	70/70 (100%)	70 (100%)	0	100	100
7	4G	83/83 (100%)	82 (99%)	1 (1%)	63	78
8	4H	124/124 (100%)	123 (99%)	1 (1%)	73	85
9	4I	180/180 (100%)	179 (99%)	1 (1%)	78	89
10	4J	148/148 (100%)	148 (100%)	0	100	100
11	4K	77/77 (100%)	77 (100%)	0	100	100
12	4L	108/108 (100%)	108 (100%)	0	100	100
13	4M	85/85 (100%)	85 (100%)	0	100	100
14	4N	112/112 (100%)	112 (100%)	0	100	100
15	4O	40/40 (100%)	40 (100%)	0	100	100
16	4P	163/163 (100%)	162 (99%)	1 (1%)	78	89
17	4Q	419/419 (100%)	419 (100%)	0	100	100
18	4R	92/92 (100%)	92 (100%)	0	100	100
19	4S	59/59 (100%)	59 (100%)	0	100	100
20	4T	102/102 (100%)	102 (100%)	0	100	100
21	4U	76/76 (100%)	76 (100%)	0	100	100
22	4V	156/156 (100%)	156 (100%)	0	100	100
23	4W	128/128 (100%)	128 (100%)	0	100	100
24	4X	198/198 (100%)	198 (100%)	0	100	100
25	4Y	100/100 (100%)	100 (100%)	0	100	100
26	4Z	167/167 (100%)	167 (100%)	0	100	100
All	All	3146/3146 (100%)	3141 (100%)	5 (0%)	85	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	4E	35	MET
7	4G	24	TRP
8	4H	36	HIS

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Mol	Chain	Res	Type
9	4I	67	GLU
16	4P	186	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	4A	56	GLN
4	4D	57	HIS
4	4D	74	GLN
5	4E	26	HIS
5	4E	42	ASN
6	4F	77	HIS
6	4F	125	GLN
8	4H	36	HIS
9	4I	50	HIS
9	4I	54	GLN
9	4I	89	GLN
10	4J	64	HIS
10	4J	79	HIS
10	4J	123	ASN
13	4M	99	HIS
15	4O	381	HIS
16	4P	88	HIS
16	4P	110	GLN
16	4P	178	GLN
17	4Q	443	ASN
17	4Q	502	ASN
17	4Q	654	ASN
18	4R	30	GLN
18	4R	97	ASN
19	4S	35	HIS
22	4V	143	HIS
23	4W	61	HIS
23	4W	83	GLN
23	4W	127	HIS
24	4X	35	HIS
24	4X	37	HIS
24	4X	104	GLN
25	4Y	108	HIS
26	4Z	125	GLN
26	4Z	187	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 37 ligands modelled in this entry, 6 are monoatomic - leaving 31 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
29	CDL	4W	202	-	72,72,99	0.33	0	78,84,111	0.40	0
27	LPP	4C	101	-	43,43,43	0.24	0	46,48,48	0.39	0
29	CDL	4K	201	-	89,89,99	0.30	0	95,101,111	0.39	0
28	PEE	4Q	901	-	35,35,50	0.85	2 (5%)	38,40,55	0.70	1 (2%)
31	CUA	4N	201	14	0,1,1	-	-	-	-	-
27	LPP	4Z	301	-	43,43,43	0.23	0	46,48,48	0.44	1 (2%)
28	PEE	4S	101	-	26,26,50	0.37	0	29,31,55	0.34	0
29	CDL	4M	201	-	74,74,99	0.32	0	80,86,111	0.43	0
29	CDL	4U	501	-	71,71,99	0.34	0	77,83,111	0.44	0
29	CDL	4E	202	-	88,88,99	0.30	0	94,100,111	0.37	0
36	PER	4Q	910	33,35	1,1,1	0.17	0	-	-	-
28	PEE	4L	201	-	34,34,50	0.67	1 (2%)	37,39,55	0.58	1 (2%)
29	CDL	4S	102	-	99,99,99	0.29	0	105,111,111	0.44	1 (0%)
29	CDL	4O	501	-	96,96,99	0.30	0	102,108,111	0.41	0
28	PEE	4Z	302	-	50,50,50	0.77	2 (4%)	53,55,55	0.56	0
29	CDL	4E	203	-	45,45,99	0.40	0	51,57,111	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PC1	4F	201	-	53,53,53	0.30	0	59,61,61	0.42	0
35	HEA	4Q	908	17	67,67,67	1.37	8 (11%)	81,103,103	2.36	28 (34%)
29	CDL	4Q	903	-	94,94,99	0.29	0	100,106,111	0.48	0
29	CDL	4F	202	-	99,99,99	0.29	0	105,111,111	0.43	0
29	CDL	4J	301	-	58,58,99	0.36	0	62,69,111	0.50	0
29	CDL	4Z	303	-	47,47,99	0.40	0	53,59,111	0.50	0
28	PEE	4G	201	-	44,44,50	0.80	2 (4%)	47,49,55	0.64	1 (2%)
28	PEE	4W	201	-	50,50,50	0.76	2 (4%)	53,55,55	0.56	0
28	PEE	4Q	902	-	46,46,50	0.82	2 (4%)	49,51,55	0.61	0
28	PEE	4R	201	-	42,42,50	0.85	2 (4%)	45,47,55	0.65	0
35	HEA	4Q	909	17,36	67,67,67	1.35	7 (10%)	81,103,103	2.28	29 (35%)
29	CDL	4Q	904	-	74,74,99	0.32	0	80,86,111	0.42	0
28	PEE	4E	201	-	30,30,50	0.31	0	33,35,55	0.51	0
29	CDL	4L	202	-	93,93,99	0.29	0	99,105,111	0.35	0
28	PEE	4D	101	-	39,39,50	0.67	1 (2%)	42,44,55	0.46	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
29	CDL	4W	202	-	-	19/83/83/110	-
27	LPP	4C	101	-	-	8/45/45/45	-
29	CDL	4K	201	-	-	25/100/100/110	-
28	PEE	4Q	901	-	-	13/39/39/54	-
27	LPP	4Z	301	-	-	5/45/45/45	-
28	PEE	4S	101	-	-	3/30/30/54	-
29	CDL	4M	201	-	-	22/85/85/110	-
29	CDL	4U	501	-	-	20/82/82/110	-
29	CDL	4E	202	-	-	10/99/99/110	-
28	PEE	4L	201	-	-	10/38/38/54	-
29	CDL	4S	102	-	-	16/110/110/110	-
29	CDL	4O	501	-	-	24/107/107/110	-
28	PEE	4Z	302	-	-	21/54/54/54	-
29	CDL	4E	203	-	-	11/55/55/110	-
30	PC1	4F	201	-	-	15/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HEA	4Q	908	17	-	6/36/76/76	-
29	CDL	4Q	903	-	-	30/105/105/110	-
29	CDL	4F	202	-	-	31/110/110/110	-
29	CDL	4J	301	-	-	20/68/68/110	-
29	CDL	4Z	303	-	-	16/58/58/110	-
28	PEE	4G	201	-	-	19/48/48/54	-
28	PEE	4W	201	-	-	9/54/54/54	-
28	PEE	4Q	902	-	-	15/50/50/54	-
28	PEE	4R	201	-	-	12/46/46/54	-
35	HEA	4Q	909	17,36	-	8/36/76/76	-
29	CDL	4Q	904	-	-	12/84/84/110	-
28	PEE	4E	201	-	-	6/34/34/54	-
29	CDL	4L	202	-	-	21/104/104/110	-
28	PEE	4D	101	-	-	4/43/43/54	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	4Q	909	HEA	C3B-C2B	4.56	1.45	1.34
35	4Q	908	HEA	C3B-C2B	4.46	1.44	1.34
35	4Q	908	HEA	C3D-C2D	3.78	1.44	1.36
28	4Z	302	PEE	C39-C38	3.66	1.52	1.31
28	4Q	902	PEE	C39-C38	3.66	1.52	1.31
28	4D	101	PEE	C18-C19	3.62	1.52	1.31
28	4Q	902	PEE	C18-C19	3.61	1.52	1.31
28	4R	201	PEE	C19-C18	3.58	1.52	1.29
28	4G	201	PEE	C39-C38	3.56	1.51	1.31
35	4Q	909	HEA	C3D-C2D	3.56	1.44	1.36
28	4R	201	PEE	C39-C38	3.55	1.51	1.31
35	4Q	909	HEA	C3A-C2A	3.55	1.45	1.37
28	4W	201	PEE	C39-C38	3.54	1.51	1.31
28	4Z	302	PEE	C18-C19	3.54	1.51	1.31
28	4L	201	PEE	C18-C19	3.52	1.51	1.31
28	4W	201	PEE	C18-C19	3.52	1.51	1.31
28	4Q	901	PEE	C19-C18	3.49	1.51	1.29
28	4G	201	PEE	C18-C19	3.48	1.51	1.31
35	4Q	908	HEA	C3A-C2A	3.37	1.44	1.37
28	4Q	901	PEE	C38-C39	3.09	1.52	1.29
35	4Q	908	HEA	C11-C3B	-3.03	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	4Q	909	HEA	C4B-C3B	2.80	1.49	1.44
35	4Q	908	HEA	C1D-ND	-2.64	1.35	1.40
35	4Q	909	HEA	C1D-ND	-2.30	1.36	1.40
35	4Q	909	HEA	C1C-C2C	2.21	1.48	1.43
35	4Q	908	HEA	C1C-C2C	2.20	1.48	1.43
35	4Q	908	HEA	C4A-NA	-2.16	1.35	1.39
35	4Q	908	HEA	C4B-NB	-2.07	1.36	1.40
35	4Q	909	HEA	C4D-C3D	2.02	1.48	1.45

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	4Q	908	HEA	C3A-C2A-C1A	-6.83	100.58	107.05
35	4Q	909	HEA	C3A-C2A-C1A	-6.72	100.68	107.05
35	4Q	909	HEA	C2A-C1A-NA	5.14	115.28	110.32
35	4Q	908	HEA	CMC-C2C-C3C	4.80	137.85	126.55
35	4Q	908	HEA	C2A-C1A-NA	4.60	114.76	110.32
35	4Q	909	HEA	CMC-C2C-C3C	4.58	137.31	126.55
35	4Q	909	HEA	C3D-C4D-ND	4.57	114.77	110.35
35	4Q	908	HEA	C3D-C4D-ND	4.54	114.74	110.35
35	4Q	909	HEA	C13-C12-C11	-4.22	107.65	114.39
35	4Q	908	HEA	CMC-C2C-C1C	-4.20	119.02	125.42
35	4Q	908	HEA	CAA-CBA-CGA	-4.19	102.56	113.67
35	4Q	909	HEA	CMC-C2C-C1C	-4.19	119.05	125.42
35	4Q	908	HEA	CMB-C2B-C1B	-4.15	118.55	125.03
35	4Q	909	HEA	CMB-C2B-C1B	-4.14	118.56	125.03
35	4Q	908	HEA	CMD-C2D-C1D	-4.13	118.58	125.03
35	4Q	908	HEA	OMA-CMA-C3A	-4.01	116.57	125.62
35	4Q	909	HEA	CHA-C1A-C2A	-3.98	118.58	124.86
35	4Q	908	HEA	CHA-C4D-C3D	-3.97	118.98	124.77
35	4Q	909	HEA	CHA-C4D-C3D	-3.84	119.17	124.77
35	4Q	908	HEA	CHA-C1A-C2A	-3.76	118.92	124.86
35	4Q	909	HEA	CMD-C2D-C1D	-3.70	119.26	125.03
35	4Q	909	HEA	CAD-CBD-CGD	-3.68	103.91	113.67
35	4Q	908	HEA	CMB-C2B-C3B	3.63	137.30	130.28
35	4Q	908	HEA	C4D-C3D-C2D	-3.59	101.67	106.89
35	4Q	909	HEA	C4D-C3D-C2D	-3.49	101.82	106.89
35	4Q	908	HEA	C3C-C2C-C1C	-3.43	103.13	107.17
35	4Q	909	HEA	CAA-CBA-CGA	-3.39	104.68	113.67
35	4Q	908	HEA	CMD-C2D-C3D	3.31	135.09	126.15
35	4Q	909	HEA	C17-C18-C19	-3.30	120.06	127.62
35	4Q	908	HEA	C13-C12-C11	-3.23	109.23	114.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	4Q	909	HEA	CMD-C2D-C3D	3.08	134.47	126.15
35	4Q	909	HEA	OMA-CMA-C3A	-3.07	118.69	125.62
35	4Q	908	HEA	C17-C18-C19	-3.05	120.65	127.62
35	4Q	909	HEA	CMB-C2B-C3B	3.04	136.15	130.28
35	4Q	909	HEA	C3C-C2C-C1C	-3.00	103.64	107.17
35	4Q	908	HEA	C13-C14-C15	-2.95	120.87	127.62
35	4Q	909	HEA	C26-C15-C16	2.79	120.08	115.23
35	4Q	909	HEA	CHB-C1B-C2B	-2.65	120.84	125.03
35	4Q	908	HEA	CHB-C1B-C2B	-2.62	120.89	125.03
35	4Q	909	HEA	C27-C19-C20	2.61	119.76	115.23
35	4Q	908	HEA	C26-C15-C16	2.61	119.76	115.23
35	4Q	908	HEA	CHB-C4A-NA	2.54	127.21	124.45
35	4Q	909	HEA	C13-C14-C15	-2.43	122.07	127.62
35	4Q	908	HEA	C25-C23-C24	2.42	120.17	114.59
35	4Q	908	HEA	C2B-C1B-NB	2.35	112.62	109.90
35	4Q	908	HEA	O11-C11-C3B	-2.34	106.97	111.26
35	4Q	908	HEA	C1B-C2B-C3B	-2.29	104.15	106.80
28	4L	201	PEE	C20-C19-C18	-2.27	112.75	126.42
35	4Q	909	HEA	C4B-C3B-C2B	-2.26	103.64	107.44
35	4Q	909	HEA	C21-C22-C23	-2.22	120.23	127.64
35	4Q	909	HEA	C2B-C1B-NB	2.22	112.47	109.90
35	4Q	908	HEA	C21-C22-C23	-2.22	120.26	127.64
28	4Q	901	PEE	C37-C38-C39	-2.19	113.89	130.48
28	4G	201	PEE	C20-C19-C18	-2.17	113.35	126.42
35	4Q	909	HEA	C3B-C4B-NB	2.16	112.32	109.84
35	4Q	909	HEA	C25-C23-C24	2.15	119.53	114.59
35	4Q	908	HEA	O1A-CGA-CBA	-2.11	116.39	123.09
35	4Q	909	HEA	CHB-C1B-NB	2.11	126.69	124.42
35	4Q	909	HEA	CHC-C1C-C2C	-2.02	121.55	127.43
35	4Q	908	HEA	CAA-C2A-C1A	2.02	128.97	124.85
29	4S	102	CDL	OB8-CB6-CB4	-2.02	102.58	108.40
27	4Z	301	LPP	O5-P1-O3	2.00	111.86	106.44

There are no chirality outliers.

All (431) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	4C	101	LPP	C6-O5-P1-O3
27	4C	101	LPP	C6-O5-P1-O4
27	4Z	301	LPP	C6-O5-P1-O2
27	4Z	301	LPP	C6-O5-P1-O4
28	4E	201	PEE	C3-C2-O2-C10

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Mol	Chain	Res	Type	Atoms
28	4E	201	PEE	O4P-C4-C5-N
28	4G	201	PEE	C1-O3P-P-O2P
28	4G	201	PEE	C1-O3P-P-O1P
28	4G	201	PEE	C1-O3P-P-O4P
28	4L	201	PEE	C1-O3P-P-O1P
28	4Q	901	PEE	O4P-C4-C5-N
28	4Q	901	PEE	C37-C38-C39-C40
28	4Q	902	PEE	C1-O3P-P-O2P
28	4Q	902	PEE	C1-O3P-P-O1P
28	4Q	902	PEE	C1-O3P-P-O4P
28	4Q	902	PEE	C4-O4P-P-O3P
28	4Q	902	PEE	C4-O4P-P-O2P
28	4Q	902	PEE	C4-O4P-P-O1P
28	4R	201	PEE	C1-O3P-P-O2P
28	4R	201	PEE	C1-O3P-P-O1P
28	4R	201	PEE	C1-O3P-P-O4P
28	4S	101	PEE	C4-O4P-P-O3P
28	4S	101	PEE	C4-O4P-P-O1P
28	4W	201	PEE	C1-O3P-P-O1P
28	4W	201	PEE	C1-O3P-P-O4P
28	4Z	302	PEE	C1-O3P-P-O2P
28	4Z	302	PEE	C1-O3P-P-O1P
28	4Z	302	PEE	C1-O3P-P-O4P
28	4Z	302	PEE	C4-O4P-P-O3P
28	4Z	302	PEE	C4-O4P-P-O2P
28	4Z	302	PEE	C4-O4P-P-O1P
29	4E	203	CDL	CA2-OA2-PA1-OA5
29	4E	203	CDL	CA3-OA5-PA1-OA2
29	4E	203	CDL	CA3-OA5-PA1-OA3
29	4F	202	CDL	CA2-OA2-PA1-OA4
29	4F	202	CDL	CA2-OA2-PA1-OA5
29	4F	202	CDL	CB2-OB2-PB2-OB3
29	4F	202	CDL	CB3-OB5-PB2-OB2
29	4J	301	CDL	CA3-OA5-PA1-OA2
29	4J	301	CDL	CA3-OA5-PA1-OA3
29	4J	301	CDL	CA3-OA5-PA1-OA4
29	4J	301	CDL	C11-CA5-OA6-CA4
29	4J	301	CDL	CB6-CB4-OB6-CB5
29	4K	201	CDL	O1-C1-CB2-OB2
29	4K	201	CDL	CA2-C1-CB2-OB2
29	4K	201	CDL	CA2-OA2-PA1-OA4
29	4K	201	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
29	4K	201	CDL	CA3-OA5-PA1-OA2
29	4K	201	CDL	CB2-OB2-PB2-OB5
29	4L	202	CDL	CA2-OA2-PA1-OA3
29	4L	202	CDL	CA2-OA2-PA1-OA5
29	4L	202	CDL	CB2-OB2-PB2-OB4
29	4L	202	CDL	CB2-OB2-PB2-OB5
29	4M	201	CDL	CA2-OA2-PA1-OA4
29	4M	201	CDL	CA2-OA2-PA1-OA5
29	4M	201	CDL	CA3-OA5-PA1-OA2
29	4M	201	CDL	CA3-OA5-PA1-OA4
29	4M	201	CDL	CB2-OB2-PB2-OB3
29	4M	201	CDL	CB2-OB2-PB2-OB4
29	4M	201	CDL	CB2-OB2-PB2-OB5
29	4M	201	CDL	CB3-OB5-PB2-OB3
29	4O	501	CDL	CA2-OA2-PA1-OA3
29	4O	501	CDL	CA2-OA2-PA1-OA4
29	4O	501	CDL	CA2-OA2-PA1-OA5
29	4O	501	CDL	CB2-OB2-PB2-OB4
29	4O	501	CDL	CB2-OB2-PB2-OB5
29	4O	501	CDL	CB3-OB5-PB2-OB2
29	4Q	903	CDL	O1-C1-CA2-OA2
29	4Q	903	CDL	CA2-OA2-PA1-OA3
29	4Q	903	CDL	CA2-OA2-PA1-OA4
29	4Q	903	CDL	CA2-OA2-PA1-OA5
29	4Q	903	CDL	CA3-OA5-PA1-OA2
29	4Q	903	CDL	C11-CA5-OA6-CA4
29	4Q	903	CDL	CB2-OB2-PB2-OB3
29	4Q	903	CDL	CB2-OB2-PB2-OB5
29	4Q	903	CDL	CB3-OB5-PB2-OB2
29	4Q	903	CDL	CB3-OB5-PB2-OB4
29	4Q	903	CDL	C51-CB5-OB6-CB4
29	4Q	904	CDL	O1-C1-CB2-OB2
29	4Q	904	CDL	CA2-C1-CB2-OB2
29	4Q	904	CDL	CA3-OA5-PA1-OA2
29	4Q	904	CDL	CA3-OA5-PA1-OA3
29	4Q	904	CDL	CA3-OA5-PA1-OA4
29	4S	102	CDL	CA2-OA2-PA1-OA5
29	4S	102	CDL	CA3-OA5-PA1-OA2
29	4S	102	CDL	CA3-OA5-PA1-OA3
29	4S	102	CDL	CB3-OB5-PB2-OB2
29	4U	501	CDL	O1-C1-CB2-OB2
29	4U	501	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
29	4U	501	CDL	CA2-OA2-PA1-OA5
29	4U	501	CDL	CA3-OA5-PA1-OA4
29	4U	501	CDL	CA4-CA3-OA5-PA1
29	4U	501	CDL	CB2-OB2-PB2-OB3
29	4W	202	CDL	O1-C1-CA2-OA2
29	4W	202	CDL	CB3-OB5-PB2-OB4
29	4Z	303	CDL	O1-C1-CA2-OA2
29	4Z	303	CDL	CA2-OA2-PA1-OA5
29	4Z	303	CDL	CA3-OA5-PA1-OA2
29	4Z	303	CDL	CB3-OB5-PB2-OB2
30	4F	201	PC1	C11-O13-P-O11
30	4F	201	PC1	C22-C21-O21-C2
35	4Q	908	HEA	C2A-C3A-CMA-OMA
35	4Q	908	HEA	C4A-C3A-CMA-OMA
35	4Q	909	HEA	C2A-C3A-CMA-OMA
35	4Q	909	HEA	C4A-C3A-CMA-OMA
29	4J	301	CDL	OA7-CA5-OA6-CA4
29	4Q	903	CDL	OA7-CA5-OA6-CA4
29	4Q	903	CDL	OB7-CB5-OB6-CB4
30	4F	201	PC1	O22-C21-O21-C2
29	4O	501	CDL	O1-C1-CB2-OB2
29	4K	201	CDL	C31-CA7-OA8-CA6
35	4Q	908	HEA	C15-C16-C17-C18
29	4F	202	CDL	CB4-CB3-OB5-PB2
29	4K	201	CDL	OA9-CA7-OA8-CA6
29	4Q	903	CDL	CB2-C1-CA2-OA2
29	4U	501	CDL	CA2-C1-CB2-OB2
29	4Z	303	CDL	CB2-C1-CA2-OA2
28	4Q	901	PEE	C31-C30-O3-C3
29	4W	202	CDL	OA6-CA4-CA6-OA8
28	4Q	901	PEE	O5-C30-O3-C3
29	4E	203	CDL	O1-C1-CB2-OB2
29	4F	202	CDL	O1-C1-CA2-OA2
29	4M	201	CDL	O1-C1-CA2-OA2
28	4G	201	PEE	O4-C10-O2-C2
29	4E	203	CDL	CA2-C1-CB2-OB2
29	4F	202	CDL	CB2-C1-CA2-OA2
29	4M	201	CDL	CB2-C1-CA2-OA2
29	4O	501	CDL	CA2-C1-CB2-OB2
29	4W	202	CDL	CB2-C1-CA2-OA2
28	4G	201	PEE	C11-C10-O2-C2
28	4D	101	PEE	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
29	4J	301	CDL	CA6-CA4-OA6-CA5
29	4F	202	CDL	C51-CB5-OB6-CB4
29	4J	301	CDL	O1-C1-CA2-OA2
28	4Q	902	PEE	C30-C31-C32-C33
29	4F	202	CDL	C51-C52-C53-C54
28	4Q	902	PEE	C11-C10-O2-C2
28	4Q	901	PEE	C11-C12-C13-C14
28	4E	201	PEE	C11-C10-O2-C2
28	4Z	302	PEE	C11-C10-O2-C2
29	4K	201	CDL	C11-CA5-OA6-CA4
29	4W	202	CDL	C11-CA5-OA6-CA4
29	4L	202	CDL	C82-C83-C84-C85
29	4Q	903	CDL	C21-C22-C23-C24
28	4G	201	PEE	C36-C37-C38-C39
28	4Q	902	PEE	C12-C13-C14-C15
29	4J	301	CDL	CB2-C1-CA2-OA2
29	4M	201	CDL	O1-C1-CB2-OB2
29	4K	201	CDL	CA4-CA6-OA8-CA7
29	4J	301	CDL	CB7-C71-C72-C73
28	4Z	302	PEE	C15-C16-C17-C18
28	4Z	302	PEE	O3P-C1-C2-C3
29	4E	203	CDL	OB5-CB3-CB4-CB6
29	4F	202	CDL	OB5-CB3-CB4-CB6
29	4L	202	CDL	OA5-CA3-CA4-CA6
29	4M	201	CDL	OA5-CA3-CA4-CA6
29	4Q	903	CDL	OB5-CB3-CB4-CB6
29	4S	102	CDL	OB5-CB3-CB4-CB6
29	4U	501	CDL	OA5-CA3-CA4-CA6
29	4U	501	CDL	OB5-CB3-CB4-CB6
28	4E	201	PEE	O4-C10-O2-C2
29	4F	202	CDL	OB7-CB5-OB6-CB4
29	4K	201	CDL	OA7-CA5-OA6-CA4
29	4U	501	CDL	C11-CA5-OA6-CA4
29	4K	201	CDL	C74-C75-C76-C77
29	4J	301	CDL	CB3-CB4-CB6-OB8
29	4W	202	CDL	CA3-CA4-CA6-OA8
29	4F	202	CDL	C71-CB7-OB8-CB6
29	4M	201	CDL	C12-C11-CA5-OA6
29	4W	202	CDL	OA7-CA5-OA6-CA4
27	4Z	301	LPP	C6-O5-P1-O3
29	4E	202	CDL	C31-CA7-OA8-CA6
29	4Q	903	CDL	CB3-CB4-OB6-CB5

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Mol	Chain	Res	Type	Atoms
28	4Q	901	PEE	C31-C32-C33-C34
29	4M	201	CDL	CA2-C1-CB2-OB2
29	4J	301	CDL	OB5-CB3-CB4-OB6
29	4O	501	CDL	OA5-CA3-CA4-OA6
29	4W	202	CDL	OB5-CB3-CB4-OB6
29	4K	201	CDL	C71-CB7-OB8-CB6
29	4M	201	CDL	C56-C57-C58-C59
29	4E	202	CDL	C75-C76-C77-C78
29	4Q	903	CDL	C52-C51-CB5-OB6
29	4L	202	CDL	C31-CA7-OA8-CA6
29	4E	202	CDL	C79-C80-C81-C82
28	4Q	902	PEE	O4-C10-O2-C2
29	4F	202	CDL	C37-C38-C39-C40
29	4F	202	CDL	C74-C75-C76-C77
29	4O	501	CDL	C32-C31-CA7-OA8
29	4K	201	CDL	CB3-CB4-CB6-OB8
28	4G	201	PEE	C12-C13-C14-C15
29	4J	301	CDL	C12-C11-CA5-OA6
29	4O	501	CDL	C19-C20-C21-C22
28	4Z	302	PEE	C14-C15-C16-C17
28	4Q	902	PEE	O3P-C1-C2-O2
28	4Z	302	PEE	O3P-C1-C2-O2
29	4Q	903	CDL	OB5-CB3-CB4-OB6
29	4S	102	CDL	OB5-CB3-CB4-OB6
29	4U	501	CDL	OA5-CA3-CA4-OA6
29	4L	202	CDL	C11-CA5-OA6-CA4
28	4G	201	PEE	O2-C2-C3-O3
29	4K	201	CDL	OB6-CB4-CB6-OB8
29	4F	202	CDL	C32-C33-C34-C35
28	4Q	901	PEE	C16-C17-C18-C19
30	4F	201	PC1	C11-C12-N-C14
28	4Q	901	PEE	C33-C34-C35-C36
28	4L	201	PEE	C18-C19-C20-C21
29	4Q	903	CDL	C71-CB7-OB8-CB6
28	4Q	902	PEE	O3P-C1-C2-C3
29	4J	301	CDL	OB5-CB3-CB4-CB6
29	4Q	903	CDL	OA5-CA3-CA4-CA6
29	4W	202	CDL	OB5-CB3-CB4-CB6
29	4Z	303	CDL	OB5-CB3-CB4-CB6
29	4F	202	CDL	C31-CA7-OA8-CA6
29	4K	201	CDL	C17-C18-C19-C20
29	4F	202	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
29	4L	202	CDL	OA7-CA5-OA6-CA4
29	4L	202	CDL	OA9-CA7-OA8-CA6
29	4Z	303	CDL	CB3-CB4-OB6-CB5
29	4E	202	CDL	OA9-CA7-OA8-CA6
28	4Z	302	PEE	C20-C21-C22-C23
28	4Z	302	PEE	O4-C10-O2-C2
29	4E	203	CDL	OB5-CB3-CB4-OB6
29	4M	201	CDL	OA5-CA3-CA4-OA6
29	4Q	903	CDL	OA5-CA3-CA4-OA6
29	4Z	303	CDL	OB5-CB3-CB4-OB6
30	4F	201	PC1	C1-C2-C3-O31
29	4W	202	CDL	C51-CB5-OB6-CB4
28	4R	201	PEE	C5-C4-O4P-P
28	4W	201	PEE	C5-C4-O4P-P
29	4O	501	CDL	C62-C63-C64-C65
30	4F	201	PC1	C11-C12-N-C13
29	4Z	303	CDL	C51-CB5-OB6-CB4
28	4L	201	PEE	C31-C30-O3-C3
29	4K	201	CDL	OB9-CB7-OB8-CB6
29	4L	202	CDL	C72-C73-C74-C75
28	4G	201	PEE	C11-C12-C13-C14
28	4W	201	PEE	C36-C37-C38-C39
28	4W	201	PEE	C38-C39-C40-C41
30	4F	201	PC1	C2-C1-O11-P
29	4Q	903	CDL	C76-C77-C78-C79
29	4L	202	CDL	OA5-CA3-CA4-OA6
29	4M	201	CDL	OB5-CB3-CB4-OB6
29	4U	501	CDL	OB5-CB3-CB4-OB6
28	4R	201	PEE	C16-C17-C18-C19
28	4W	201	PEE	C18-C19-C20-C21
29	4J	301	CDL	OB6-CB4-CB6-OB8
29	4O	501	CDL	C76-C77-C78-C79
28	4G	201	PEE	C1-C2-C3-O3
28	4G	201	PEE	C32-C33-C34-C35
28	4L	201	PEE	C16-C17-C18-C19
28	4Q	902	PEE	C38-C39-C40-C41
28	4Z	302	PEE	C36-C37-C38-C39
29	4Q	904	CDL	C76-C77-C78-C79
28	4G	201	PEE	C4-O4P-P-O3P
28	4L	201	PEE	C1-O3P-P-O4P
28	4S	101	PEE	C4-O4P-P-O2P
28	4W	201	PEE	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
29	4E	202	CDL	CA2-OA2-PA1-OA3
29	4E	203	CDL	CA2-OA2-PA1-OA3
29	4F	202	CDL	CA3-OA5-PA1-OA3
29	4F	202	CDL	CB2-OB2-PB2-OB4
29	4F	202	CDL	CB2-OB2-PB2-OB5
29	4F	202	CDL	CB3-OB5-PB2-OB3
29	4K	201	CDL	CA3-OA5-PA1-OA3
29	4K	201	CDL	CB2-OB2-PB2-OB3
29	4L	202	CDL	CA2-OA2-PA1-OA4
29	4M	201	CDL	CA2-OA2-PA1-OA3
29	4M	201	CDL	CA3-OA5-PA1-OA3
29	4M	201	CDL	CB3-OB5-PB2-OB2
29	4O	501	CDL	CB3-OB5-PB2-OB3
29	4Q	903	CDL	CA3-OA5-PA1-OA3
29	4Q	904	CDL	CA2-OA2-PA1-OA3
29	4S	102	CDL	CA2-OA2-PA1-OA3
29	4S	102	CDL	CB3-OB5-PB2-OB3
29	4U	501	CDL	CA2-OA2-PA1-OA4
29	4U	501	CDL	CA3-OA5-PA1-OA2
29	4U	501	CDL	CA3-OA5-PA1-OA3
29	4U	501	CDL	CB2-OB2-PB2-OB5
29	4W	202	CDL	CA2-OA2-PA1-OA3
29	4W	202	CDL	CB3-OB5-PB2-OB2
29	4W	202	CDL	CB3-OB5-PB2-OB3
29	4Z	303	CDL	CA3-OA5-PA1-OA3
29	4Z	303	CDL	CB3-OB5-PB2-OB3
30	4F	201	PC1	C11-O13-P-O14
30	4F	201	PC1	C11-C12-N-C15
29	4F	202	CDL	C1-CB2-OB2-PB2
29	4J	301	CDL	C1-CA2-OA2-PA1
29	4K	201	CDL	CA4-CA3-OA5-PA1
29	4U	501	CDL	OA7-CA5-OA6-CA4
27	4Z	301	LPP	C14-C15-C16-C17
29	4E	202	CDL	C72-C73-C74-C75
28	4Q	902	PEE	C36-C37-C38-C39
28	4G	201	PEE	C1-C2-O2-C10
29	4S	102	CDL	CB6-CB4-OB6-CB5
30	4F	201	PC1	C3-C2-O21-C21
27	4C	101	LPP	C36-C37-C38-C39
29	4F	202	CDL	OA9-CA7-OA8-CA6
28	4R	201	PEE	C38-C39-C40-C41
29	4F	202	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
29	4L	202	CDL	C78-C79-C80-C81
29	4J	301	CDL	C79-C80-C81-C82
28	4G	201	PEE	C18-C19-C20-C21
29	4K	201	CDL	C81-C82-C83-C84
29	4O	501	CDL	C53-C54-C55-C56
29	4L	202	CDL	OB7-CB5-OB6-CB4
28	4W	201	PEE	C16-C17-C18-C19
29	4L	202	CDL	C51-CB5-OB6-CB4
29	4E	203	CDL	C1-CA2-OA2-PA1
29	4K	201	CDL	C1-CB2-OB2-PB2
29	4L	202	CDL	C1-CB2-OB2-PB2
28	4D	101	PEE	C16-C17-C18-C19
35	4Q	908	HEA	C12-C11-C3B-C2B
29	4Q	903	CDL	OB9-CB7-OB8-CB6
29	4O	501	CDL	C32-C31-CA7-OA9
28	4Q	902	PEE	C18-C19-C20-C21
28	4R	201	PEE	C36-C37-C38-C39
28	4Z	302	PEE	C16-C17-C18-C19
29	4S	102	CDL	C22-C23-C24-C25
29	4U	501	CDL	CA5-C11-C12-C13
28	4G	201	PEE	C31-C32-C33-C34
29	4E	202	CDL	CA3-CA4-CA6-OA8
35	4Q	908	HEA	CAA-CBA-CGA-O1A
28	4L	201	PEE	O5-C30-O3-C3
29	4E	203	CDL	CB6-CB4-OB6-CB5
30	4F	201	PC1	C33-C34-C35-C36
29	4W	202	CDL	OB7-CB5-OB6-CB4
29	4F	202	CDL	C52-C53-C54-C55
28	4L	201	PEE	O3P-C1-C2-O2
28	4G	201	PEE	C2-C1-O3P-P
28	4R	201	PEE	C2-C1-O3P-P
29	4O	501	CDL	C1-CA2-OA2-PA1
29	4O	501	CDL	CB4-CB3-OB5-PB2
29	4Q	904	CDL	CB4-CB3-OB5-PB2
29	4S	102	CDL	CB4-CB3-OB5-PB2
35	4Q	909	HEA	CAD-CBD-CGD-O1D
35	4Q	909	HEA	C26-C15-C16-C17
29	4O	501	CDL	OA5-CA3-CA4-CA6
35	4Q	908	HEA	CAA-CBA-CGA-O2A
27	4C	101	LPP	O9-C7-C8-O27
28	4Q	901	PEE	O2-C2-C3-O3
30	4F	201	PC1	C3A-C3B-C3C-C3D

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Mol	Chain	Res	Type	Atoms
28	4R	201	PEE	C31-C30-O3-C3
29	4U	501	CDL	C1-CB2-OB2-PB2
29	4W	202	CDL	CB4-CB3-OB5-PB2
35	4Q	909	HEA	CAD-CBD-CGD-O2D
29	4Q	903	CDL	C52-C51-CB5-OB7
27	4C	101	LPP	C6-C7-C8-O27
29	4O	501	CDL	C31-C32-C33-C34
29	4F	202	CDL	C36-C37-C38-C39
29	4Z	303	CDL	OB7-CB5-OB6-CB4
28	4W	201	PEE	O3P-C1-C2-O2
28	4G	201	PEE	C38-C39-C40-C41
29	4O	501	CDL	CB2-C1-CA2-OA2
28	4G	201	PEE	C2-C3-O3-C30
30	4F	201	PC1	C39-C3A-C3B-C3C
29	4Z	303	CDL	CB4-CB3-OB5-PB2
29	4M	201	CDL	C12-C11-CA5-OA7
27	4C	101	LPP	C6-O5-P1-O2
29	4J	301	CDL	CB3-CB4-OB6-CB5
28	4Q	901	PEE	C36-C37-C38-C39
28	4Z	302	PEE	C38-C39-C40-C41
35	4Q	909	HEA	C1A-C2A-CAA-CBA
29	4L	202	CDL	C64-C65-C66-C67
35	4Q	909	HEA	C14-C15-C16-C17
29	4M	201	CDL	C55-C56-C57-C58
28	4D	101	PEE	C18-C19-C20-C21
29	4Q	904	CDL	CA4-CA3-OA5-PA1
29	4Q	904	CDL	C71-CB7-OB8-CB6
29	4Q	903	CDL	C51-C52-C53-C54
30	4F	201	PC1	C28-C29-C2A-C2B
29	4Q	903	CDL	C19-C20-C21-C22
29	4S	102	CDL	C12-C13-C14-C15
29	4E	202	CDL	OA6-CA4-CA6-OA8
29	4L	202	CDL	C58-C59-C60-C61
28	4G	201	PEE	C16-C17-C18-C19
27	4C	101	LPP	C30-C31-C32-C33
28	4L	201	PEE	O3P-C1-C2-C3
28	4R	201	PEE	O3P-C1-C2-C3
29	4F	202	CDL	OA5-CA3-CA4-CA6
29	4S	102	CDL	C53-C54-C55-C56
29	4Q	904	CDL	C51-CB5-OB6-CB4
28	4Z	302	PEE	C18-C19-C20-C21
29	4K	201	CDL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	4F	202	CDL	C76-C77-C78-C79
28	4Q	901	PEE	O3-C30-C31-C32
35	4Q	909	HEA	C4D-C3D-CAD-CBD
29	4O	501	CDL	C15-C16-C17-C18
29	4S	102	CDL	C52-C51-CB5-OB6
28	4E	201	PEE	O2-C10-C11-C12
29	4F	202	CDL	C12-C11-CA5-OA6
29	4O	501	CDL	C52-C51-CB5-OB6
28	4Z	302	PEE	C10-C11-C12-C13
29	4K	201	CDL	C12-C11-CA5-OA6
29	4Z	303	CDL	C32-C31-CA7-OA8
29	4E	202	CDL	C52-C51-CB5-OB6
29	4L	202	CDL	C84-C85-C86-C87
29	4E	203	CDL	CA3-CA4-OA6-CA5
29	4Z	303	CDL	C72-C71-CB7-OB8
28	4L	201	PEE	C11-C10-O2-C2
29	4F	202	CDL	C16-C17-C18-C19
29	4U	501	CDL	C52-C51-CB5-OB6
29	4S	102	CDL	C72-C73-C74-C75
28	4Q	901	PEE	O3P-C1-C2-O2
27	4C	101	LPP	C11-C12-C13-C14
27	4Z	301	LPP	C32-C33-C34-C35
28	4Z	302	PEE	O3-C30-C31-C32
29	4W	202	CDL	C32-C31-CA7-OA8
29	4L	202	CDL	C71-C72-C73-C74
29	4J	301	CDL	C12-C11-CA5-OA7
28	4D	101	PEE	C22-C23-C24-C25
29	4Q	903	CDL	C32-C31-CA7-OA8
29	4S	102	CDL	C19-C20-C21-C22
28	4R	201	PEE	O5-C30-O3-C3
30	4F	201	PC1	O21-C2-C3-O31
29	4Q	904	CDL	CB4-CB6-OB8-CB7
28	4Q	901	PEE	O5-C30-C31-C32
29	4W	202	CDL	C32-C31-CA7-OA9
28	4Z	302	PEE	C21-C22-C23-C24
29	4O	501	CDL	C52-C51-CB5-OB7
29	4Z	303	CDL	C72-C71-CB7-OB9
28	4Z	302	PEE	O5-C30-C31-C32
29	4K	201	CDL	C12-C11-CA5-OA7
28	4L	201	PEE	O2-C10-C11-C12
29	4Q	903	CDL	C12-C11-CA5-OA6
29	4W	202	CDL	C12-C11-CA5-OA6

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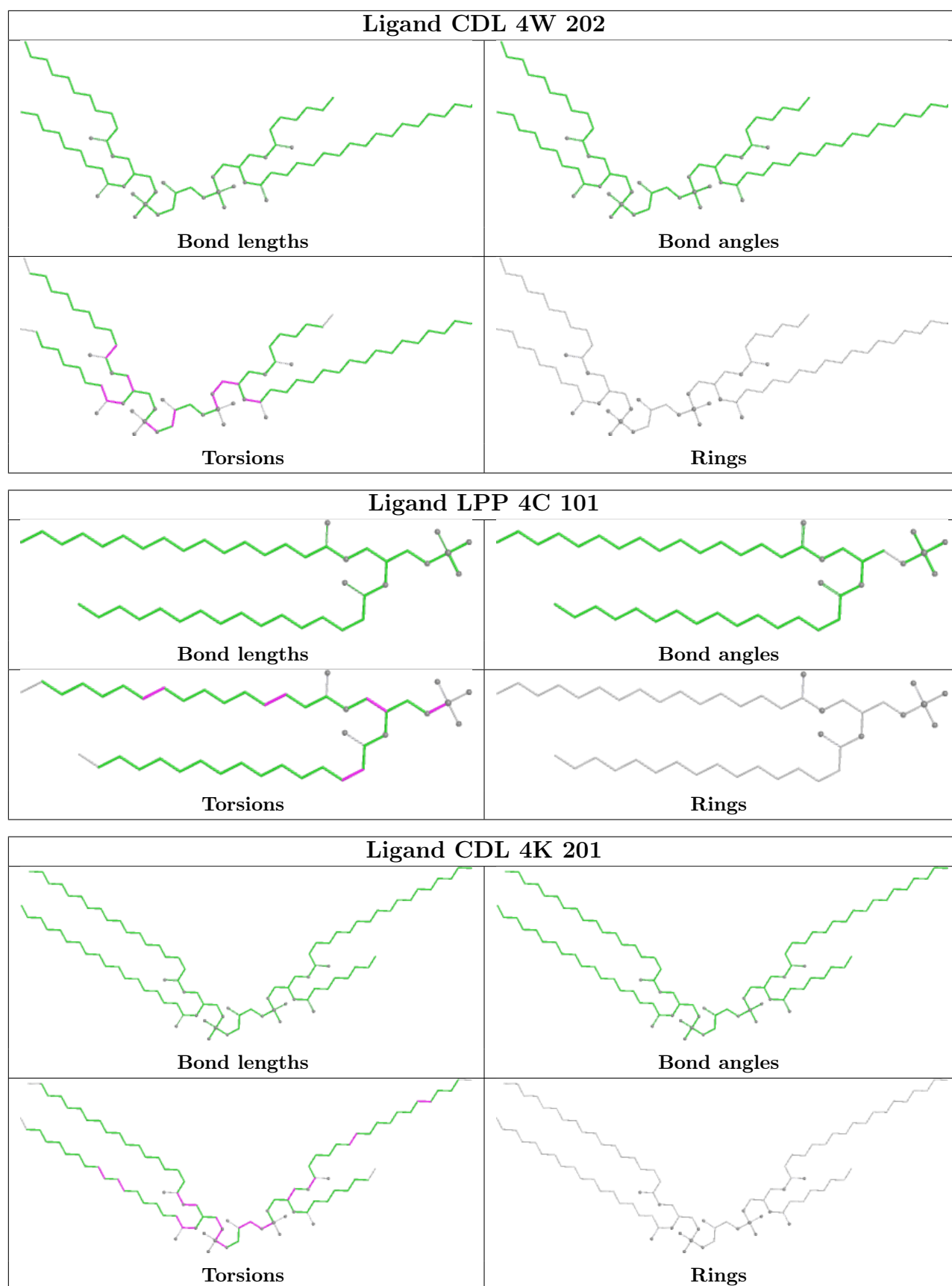
Mol	Chain	Res	Type	Atoms
29	4W	202	CDL	C12-C11-CA5-OA7
28	4R	201	PEE	O3-C30-C31-C32
29	4J	301	CDL	C72-C71-CB7-OB8
28	4E	201	PEE	O4-C10-C11-C12
29	4E	202	CDL	C52-C51-CB5-OB7
29	4F	202	CDL	C12-C11-CA5-OA7

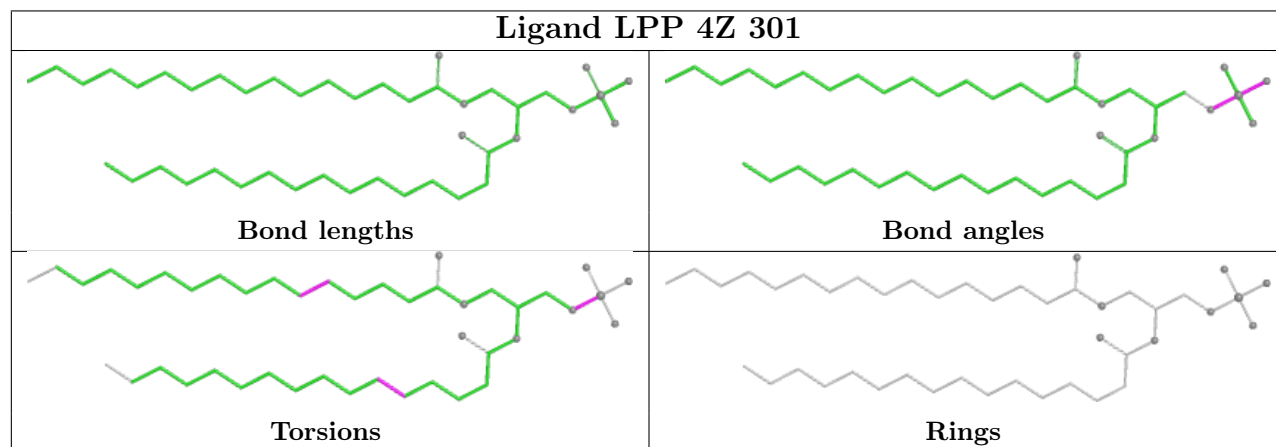
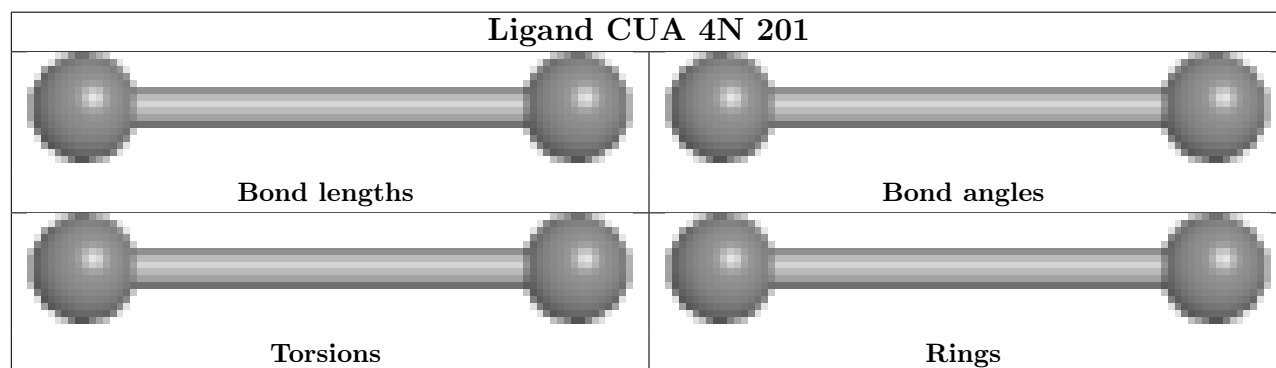
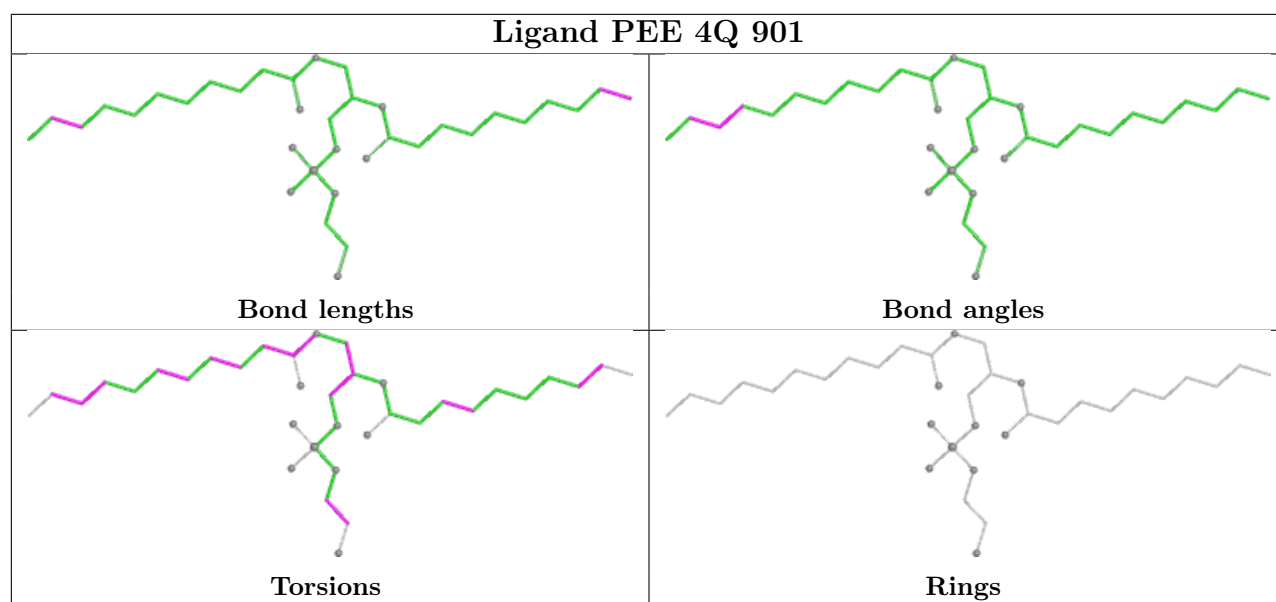
There are no ring outliers.

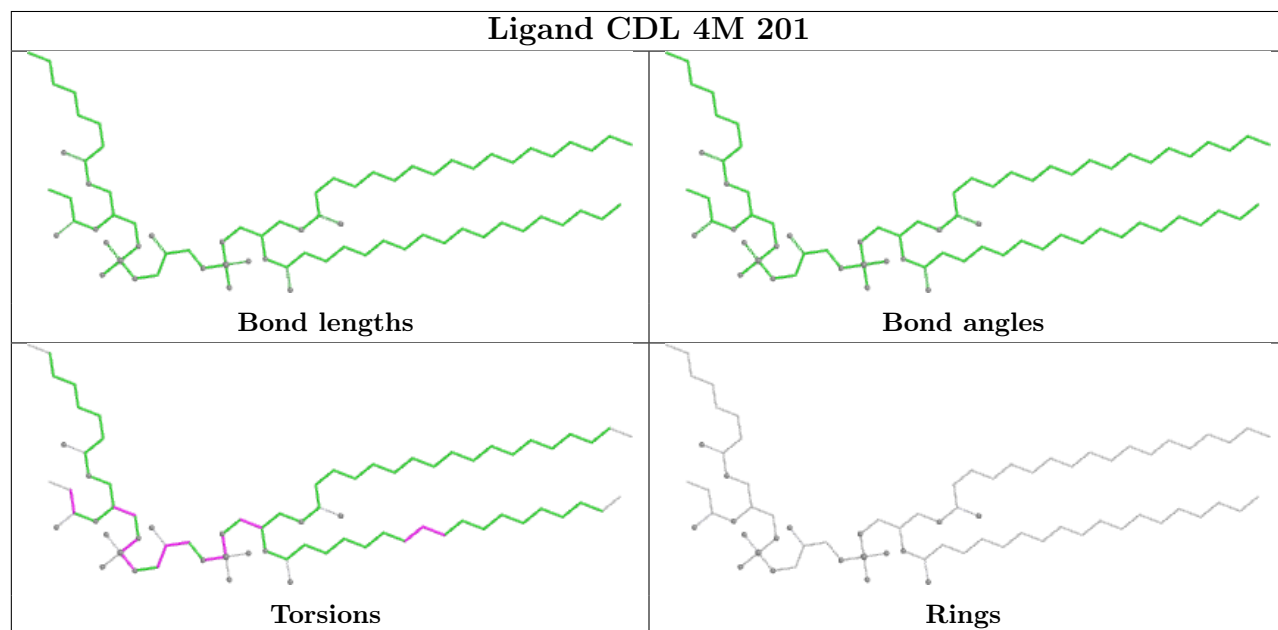
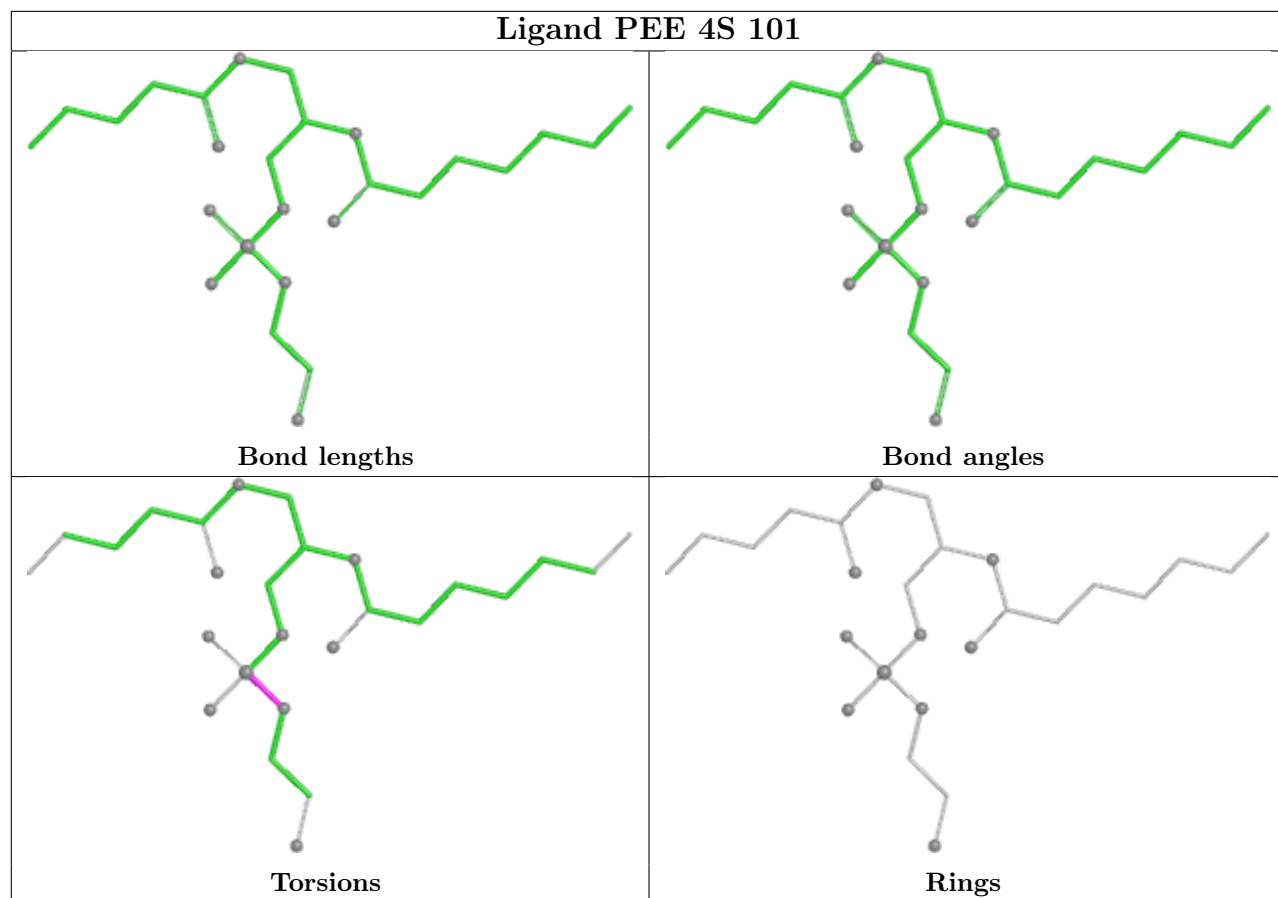
10 monomers are involved in 22 short contacts:

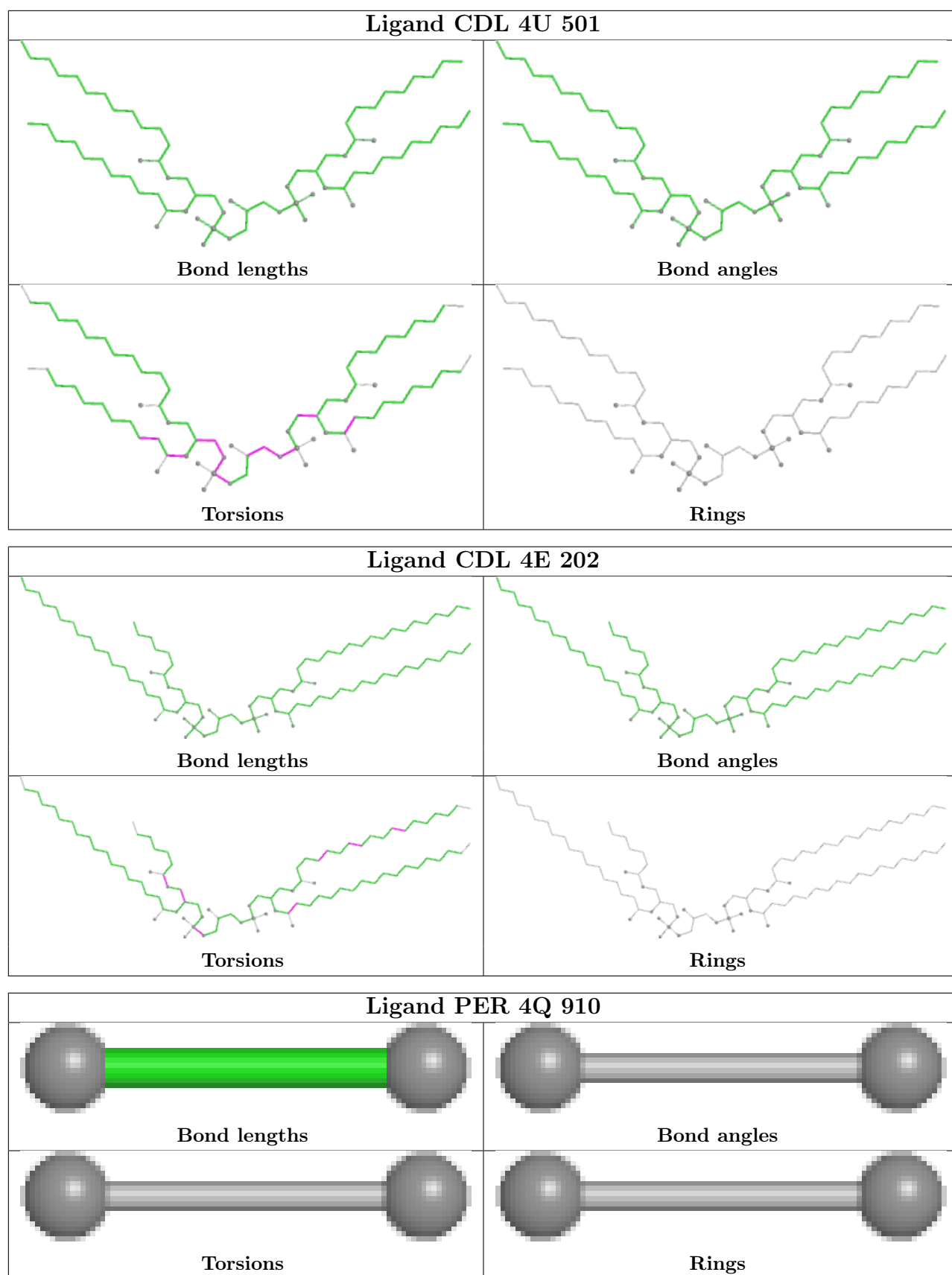
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	4C	101	LPP	1	0
29	4M	201	CDL	1	0
28	4Z	302	PEE	2	0
29	4E	203	CDL	2	0
30	4F	201	PC1	2	0
35	4Q	908	HEA	5	0
29	4Q	903	CDL	2	0
29	4Z	303	CDL	1	0
35	4Q	909	HEA	5	0
28	4E	201	PEE	1	0

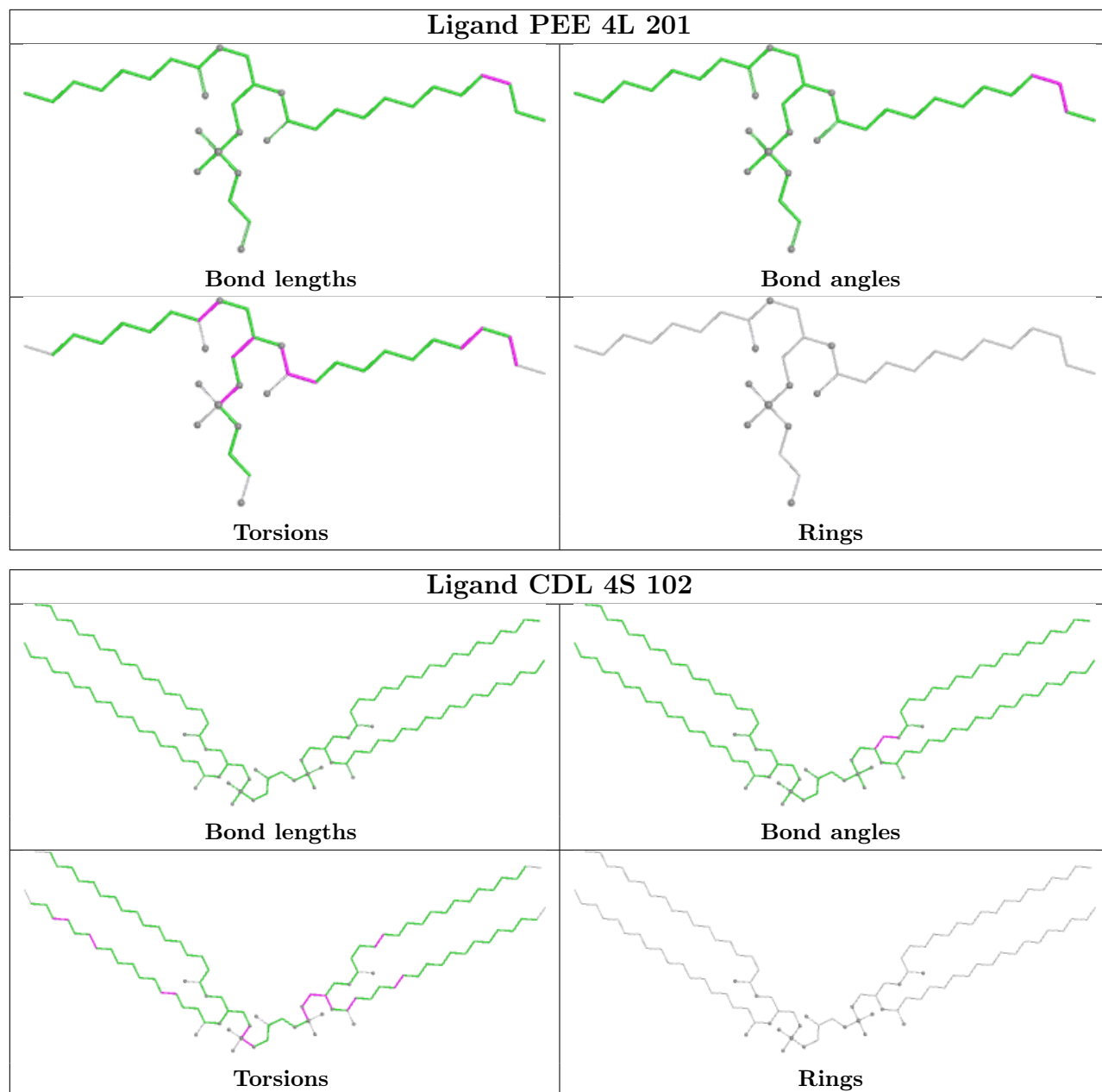
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

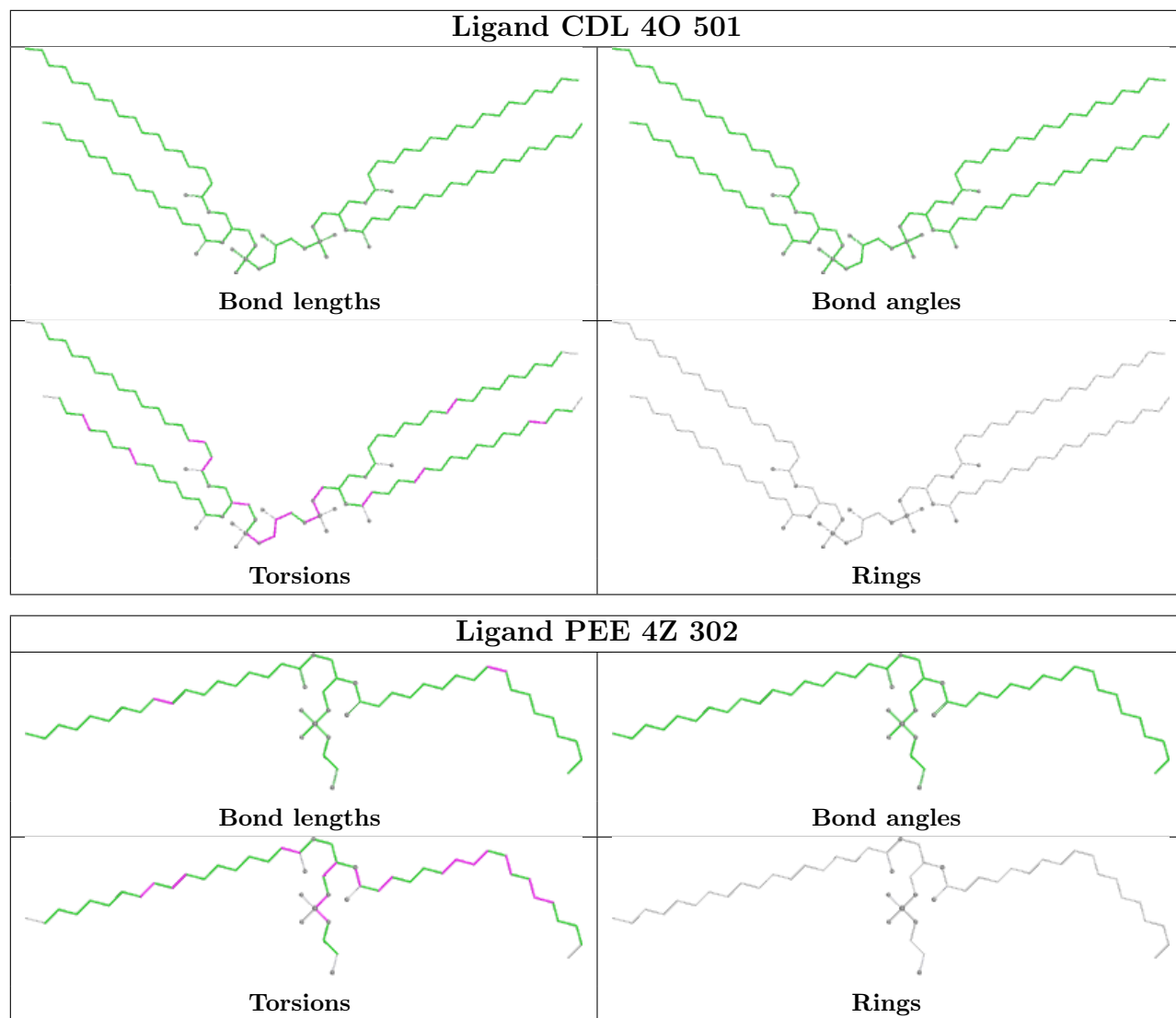


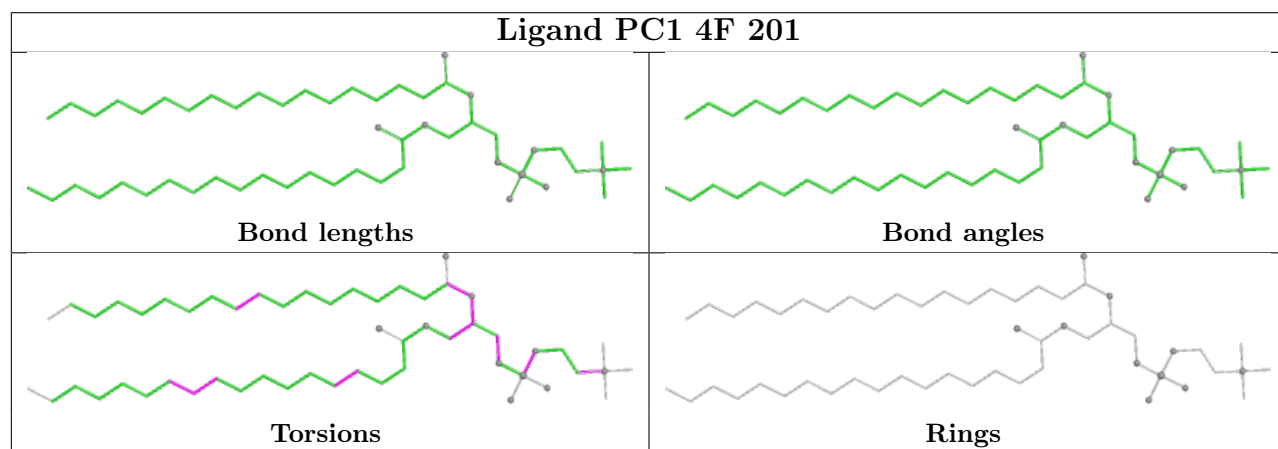
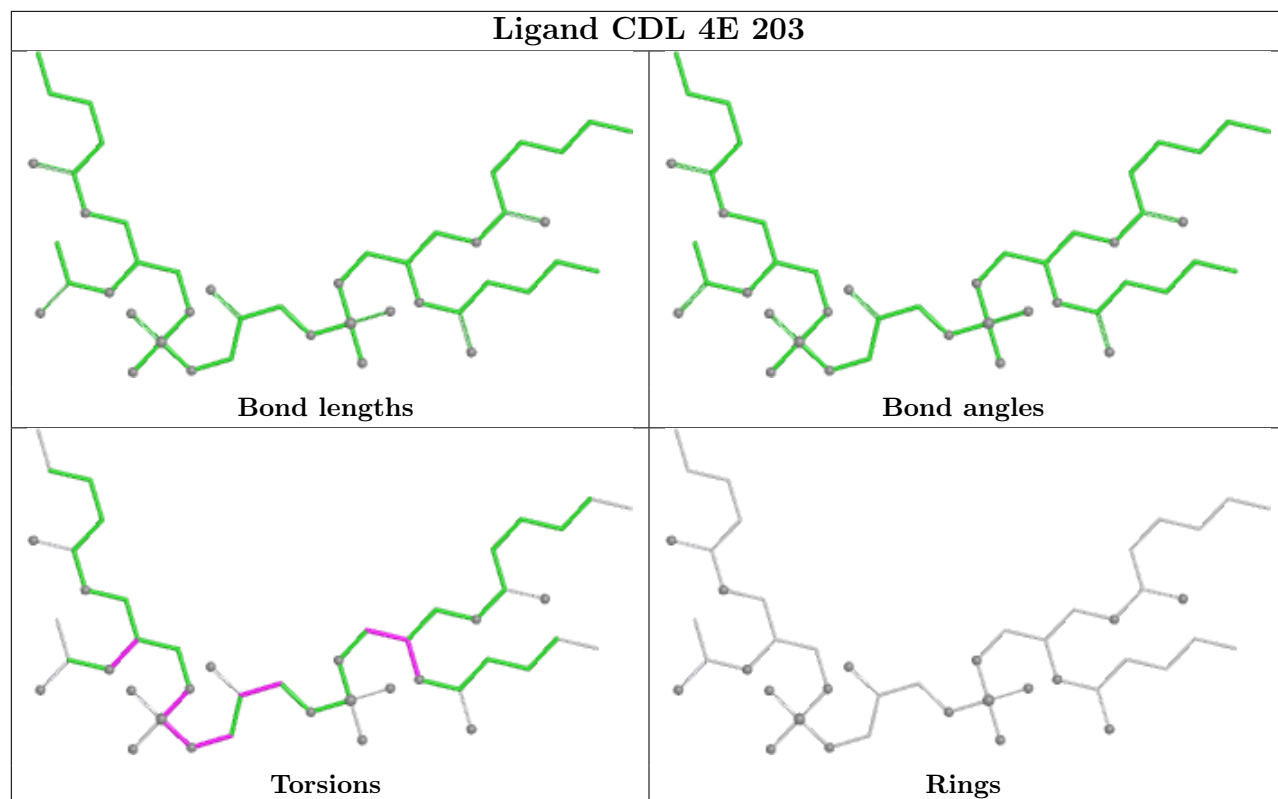


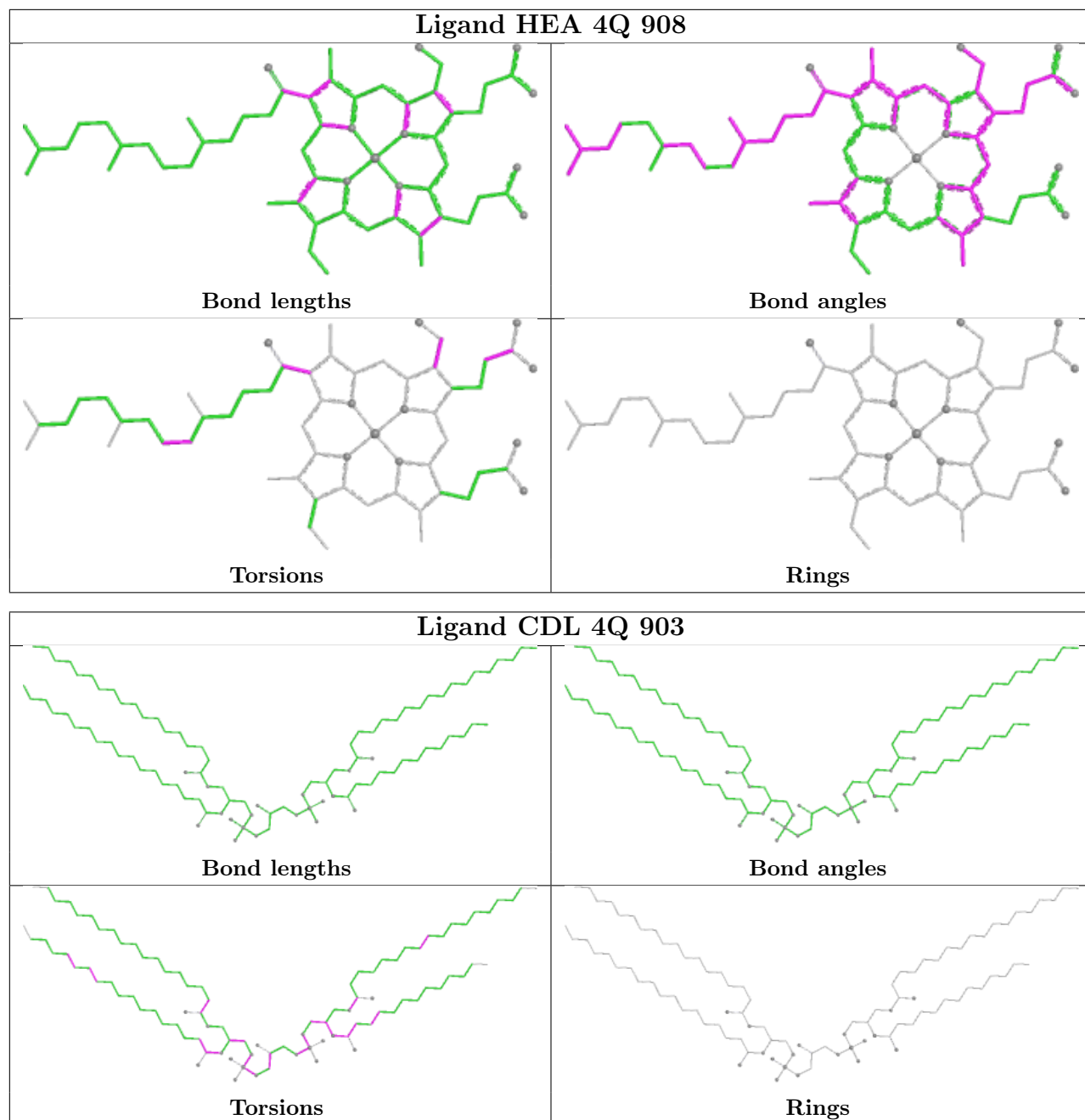


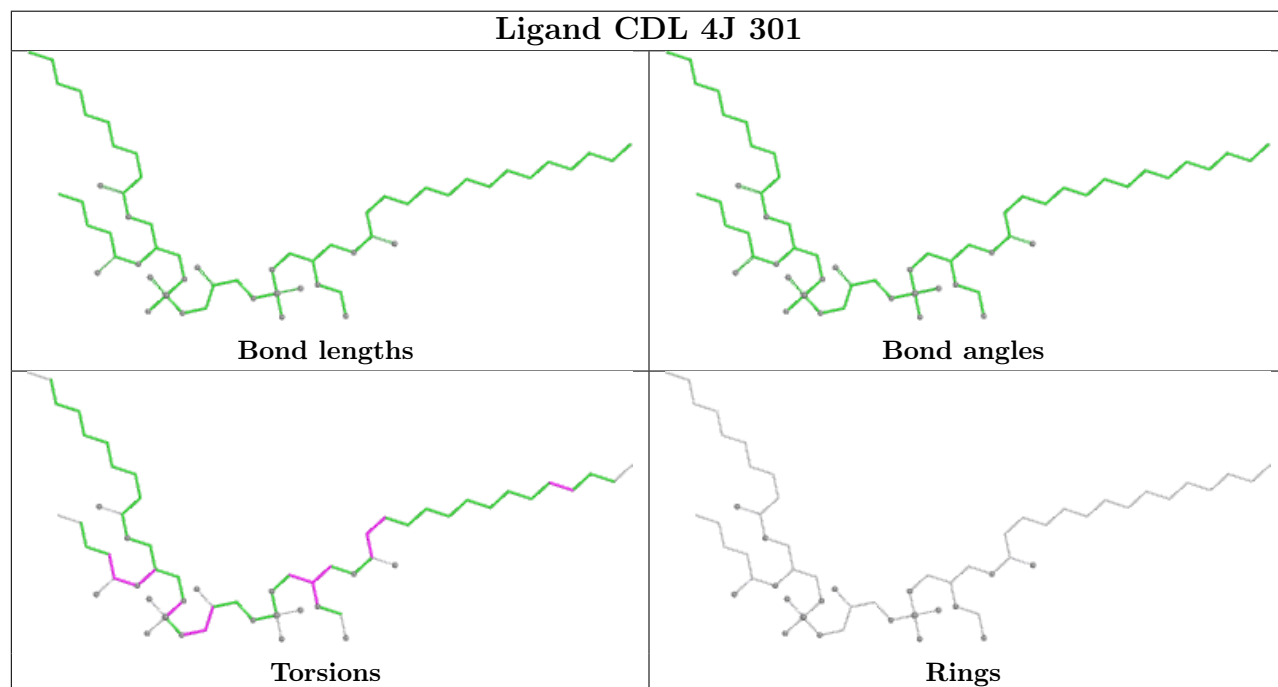
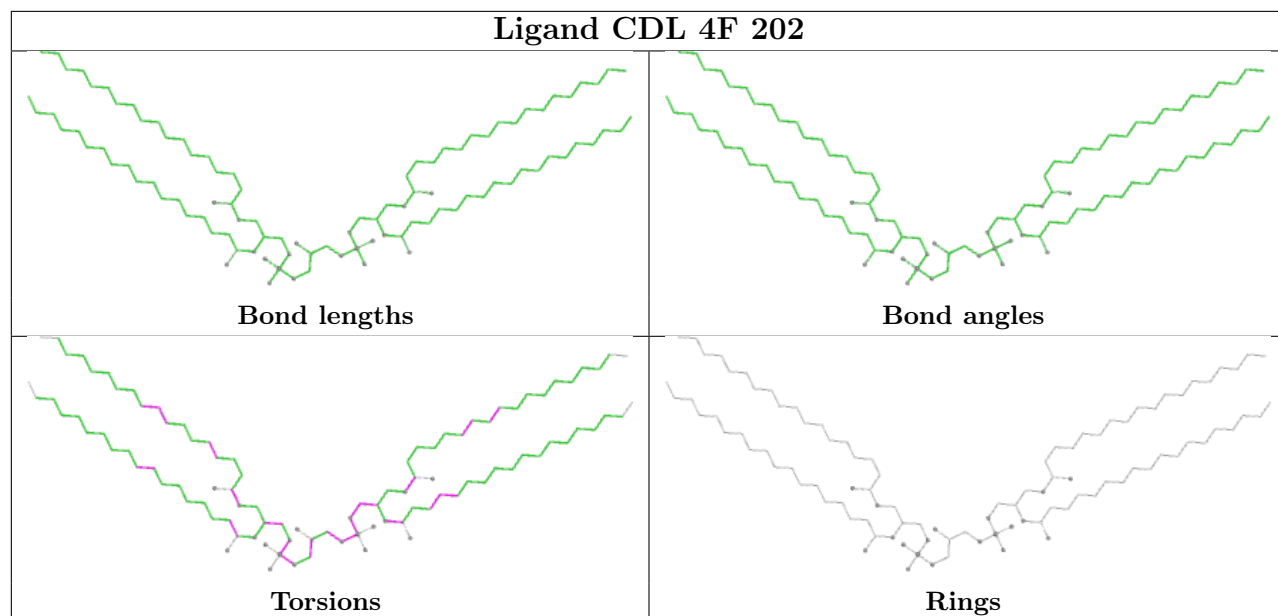


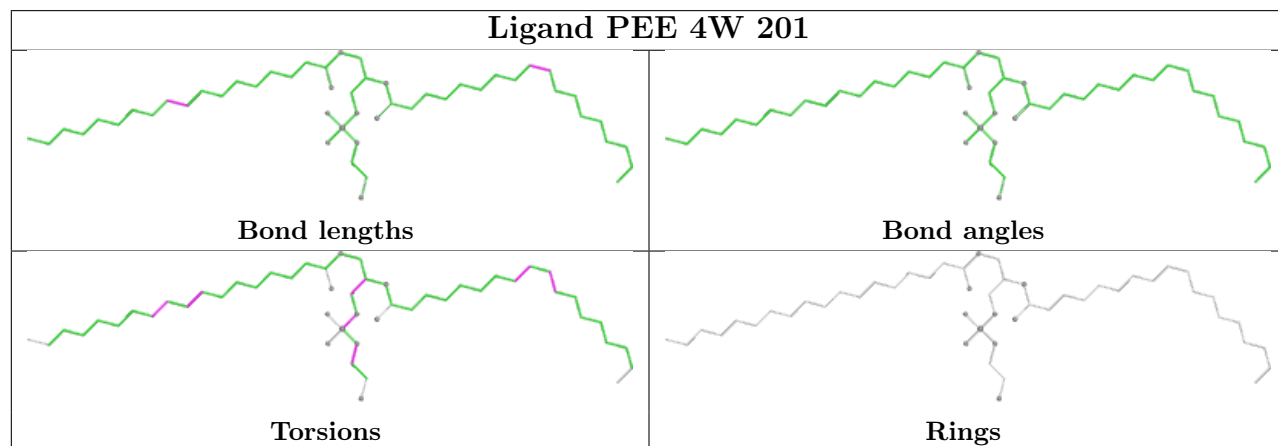
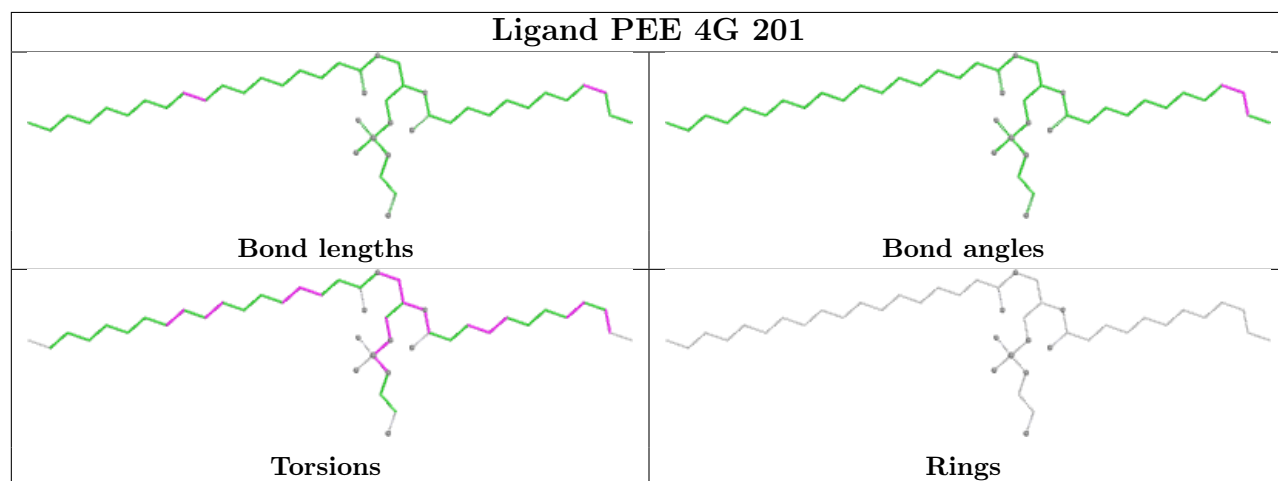
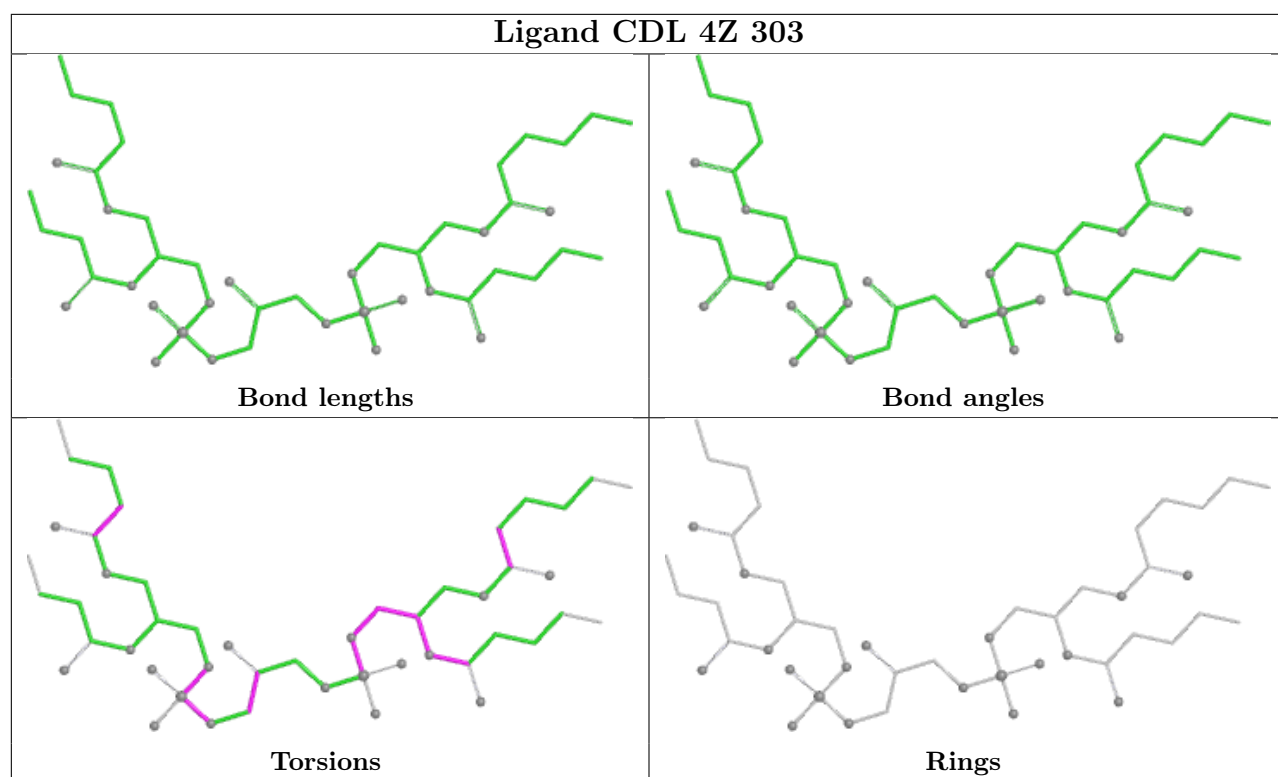


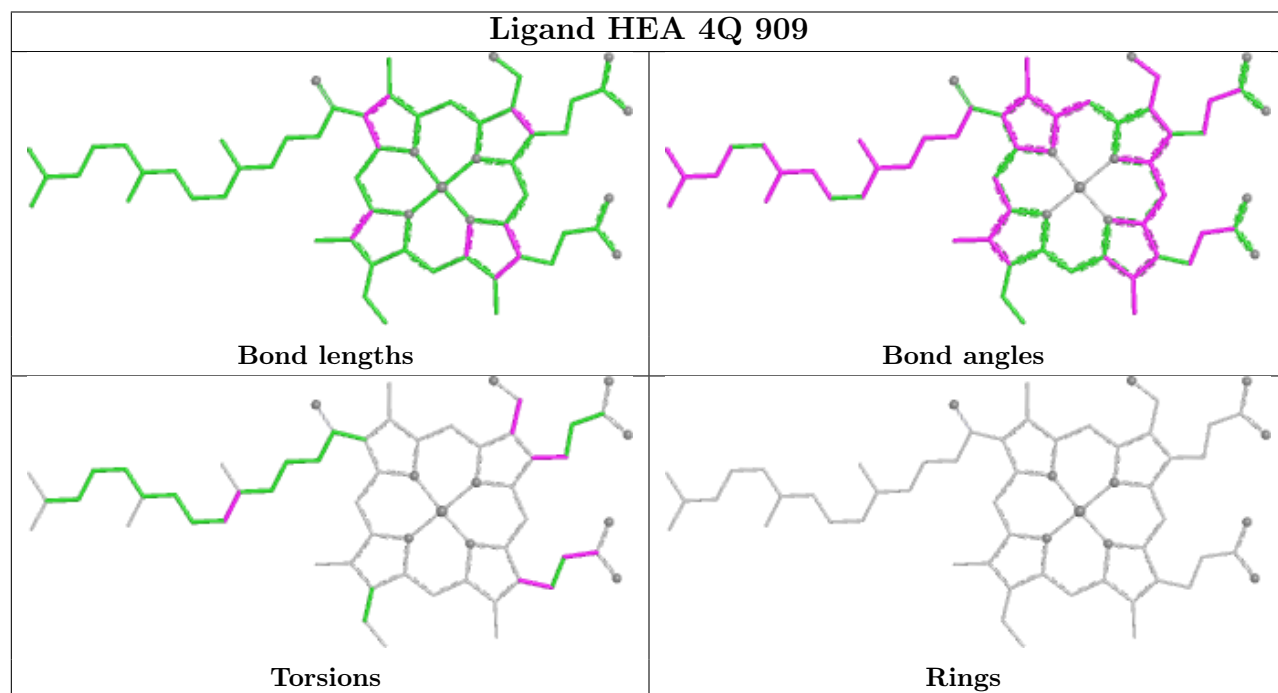
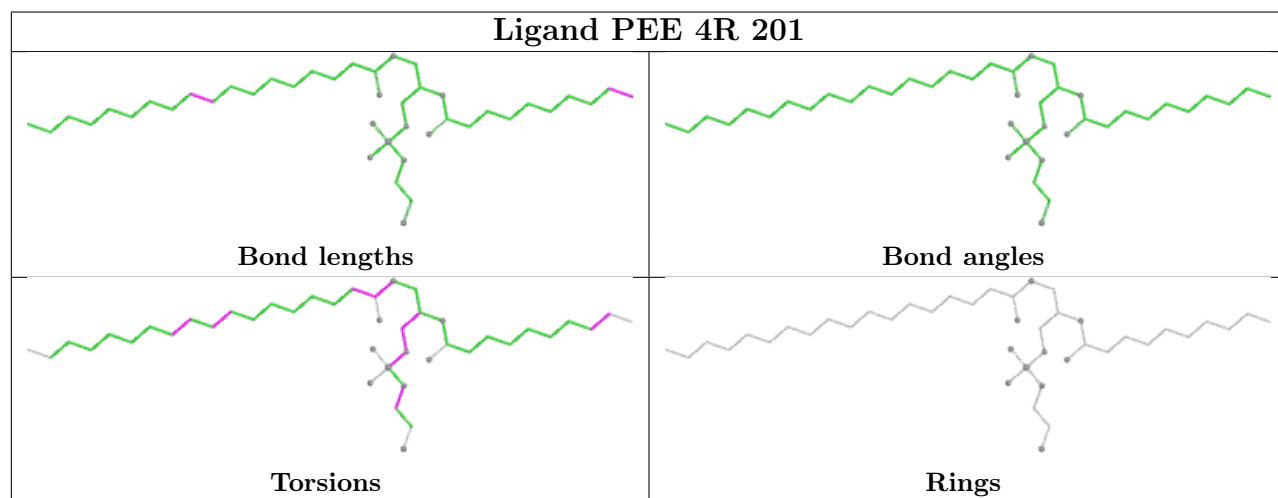
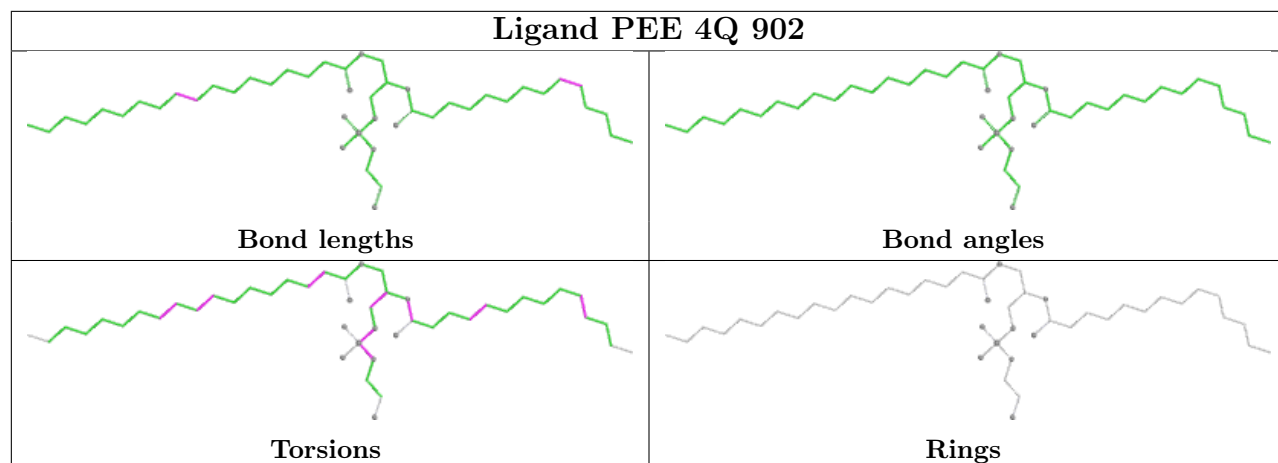


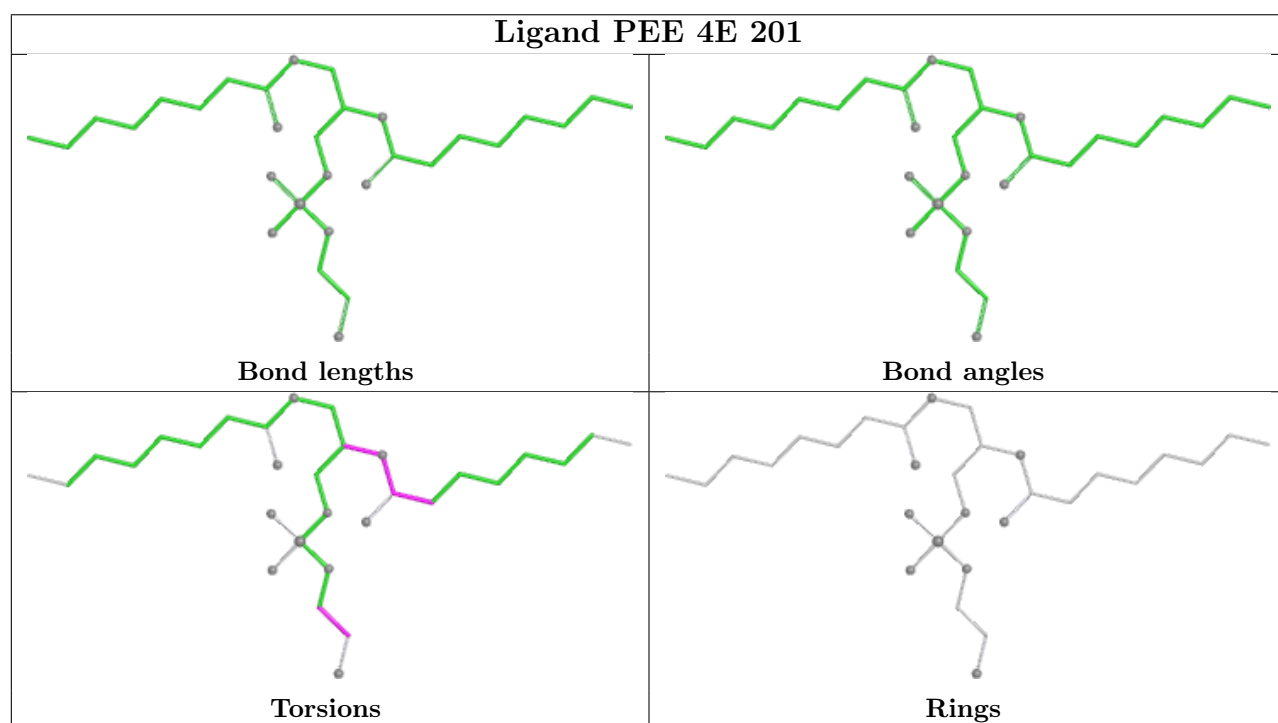
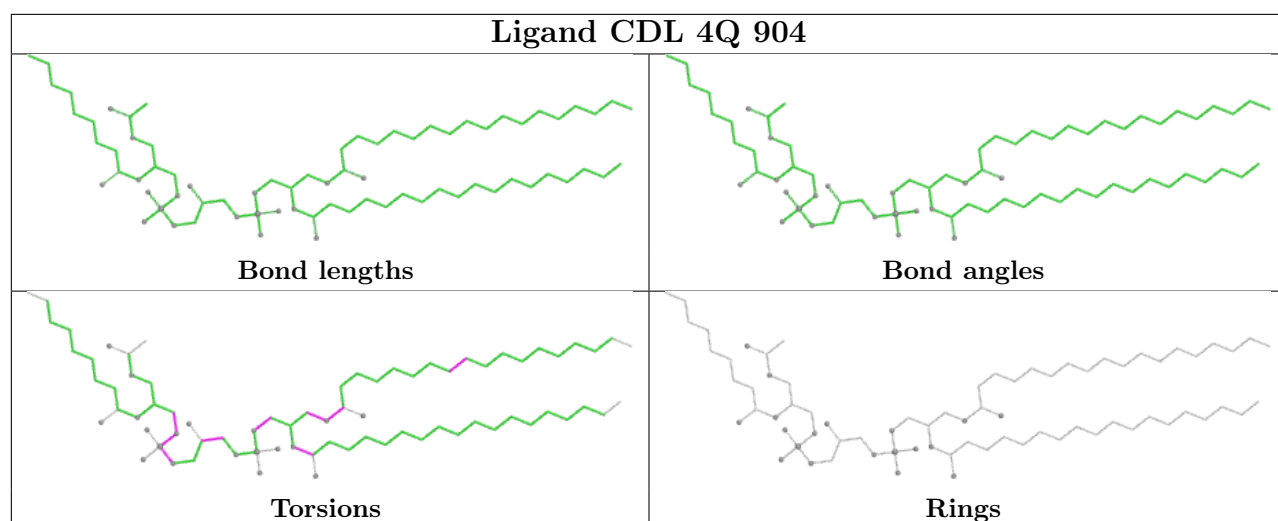


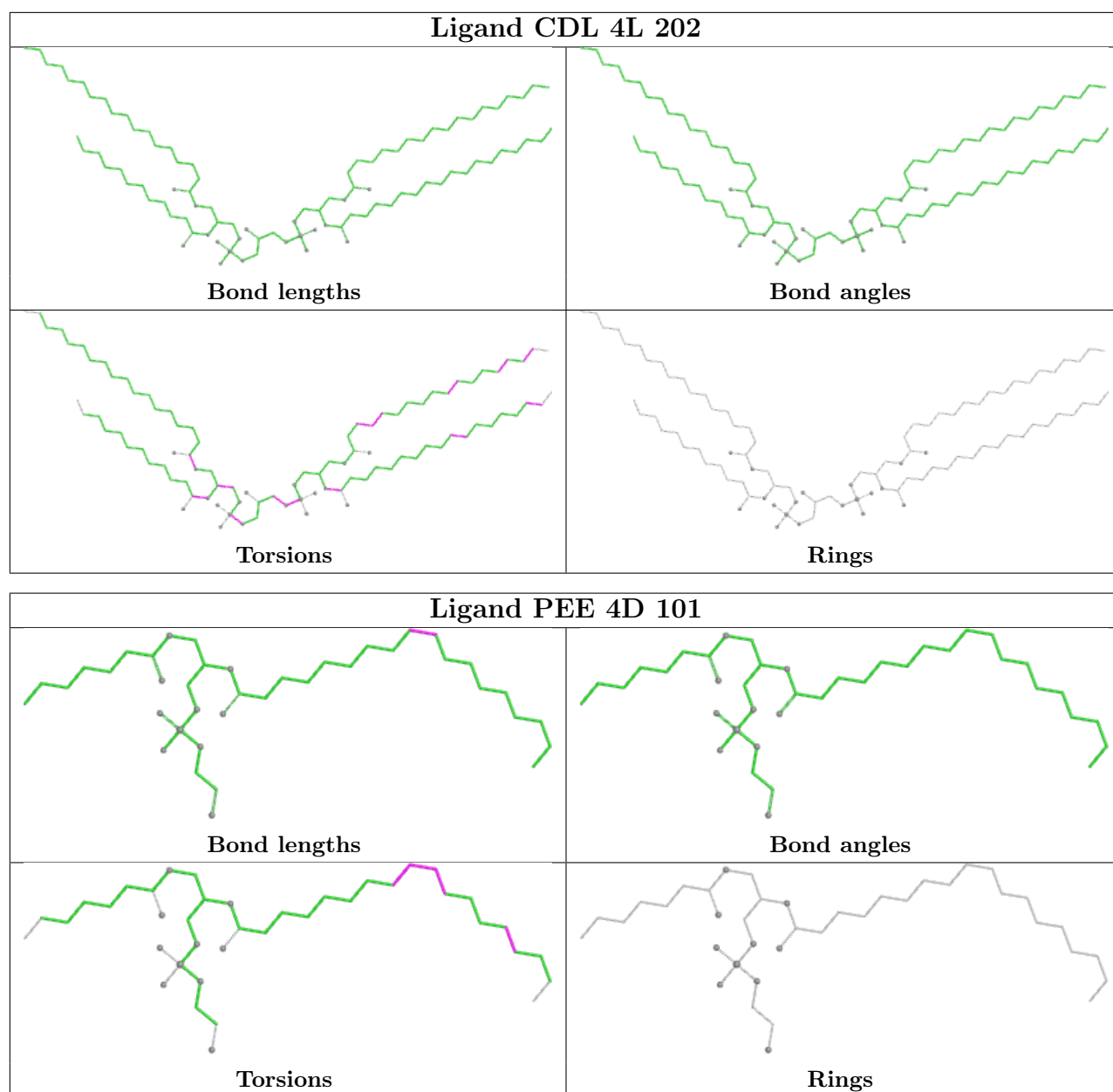












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

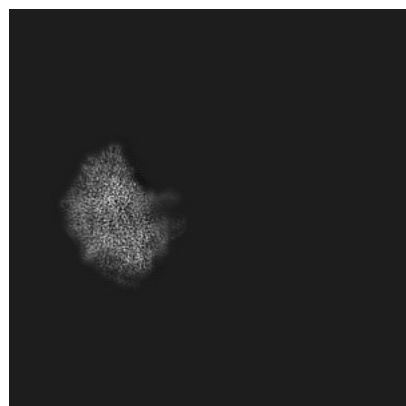
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50363. These allow visual inspection of the internal detail of the map and identification of artifacts.

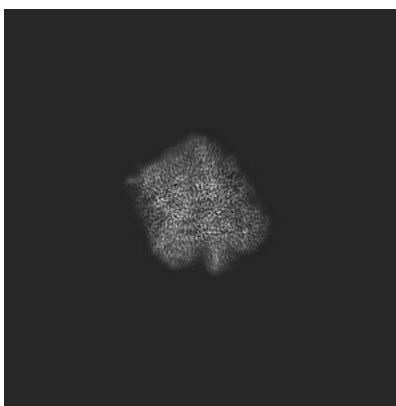
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

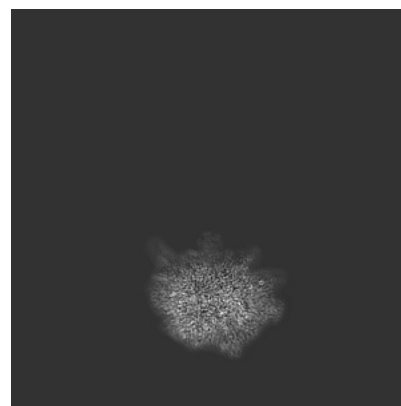
6.1.1 Primary map



X

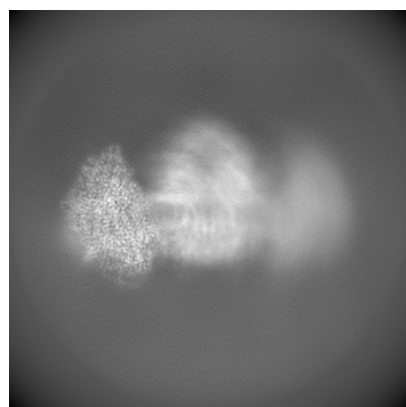


Y

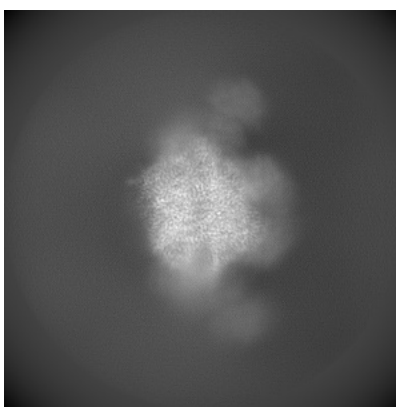


Z

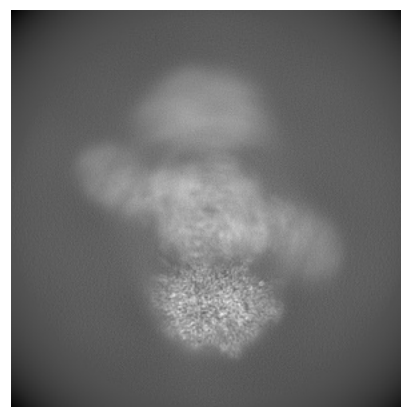
6.1.2 Raw map



X



Y

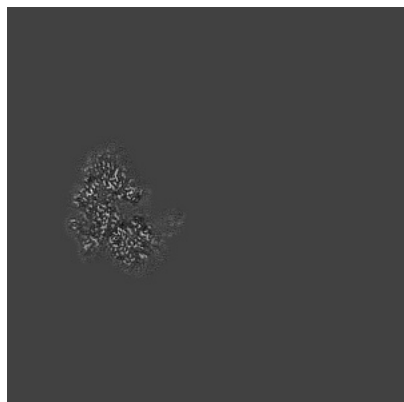


Z

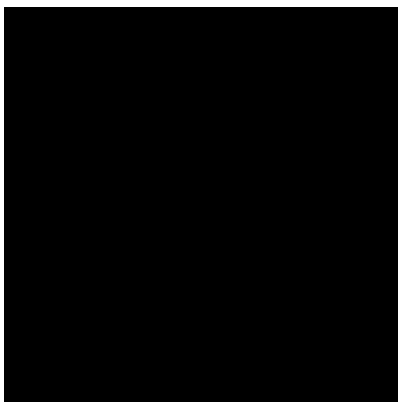
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 250

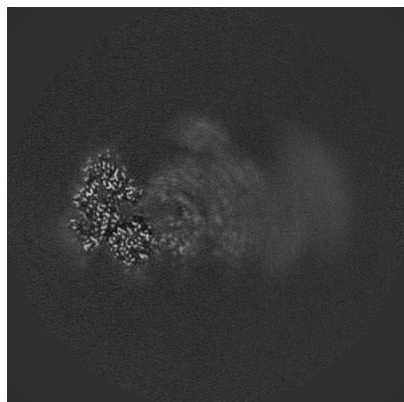


Y Index: 250

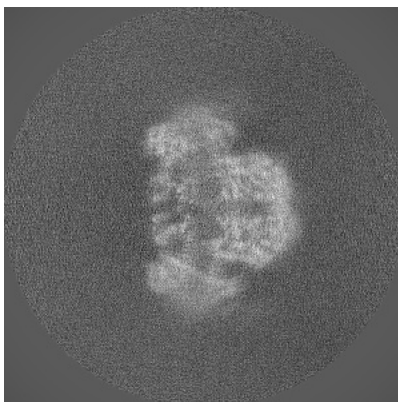


Z Index: 250

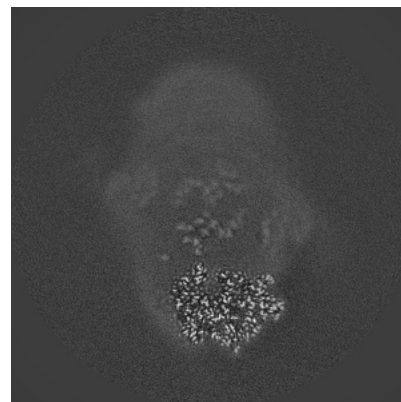
6.2.2 Raw map



X Index: 250



Y Index: 250

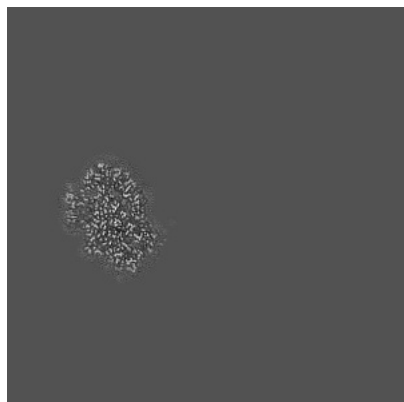


Z Index: 250

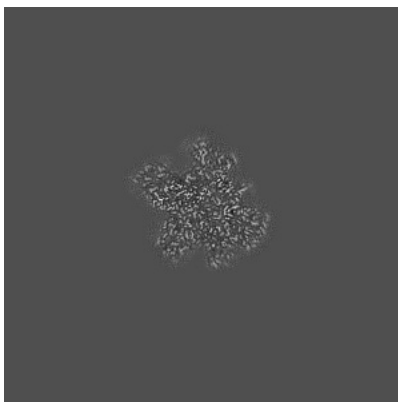
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

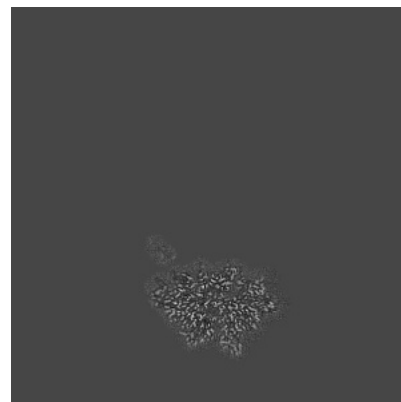
6.3.1 Primary map



X Index: 266

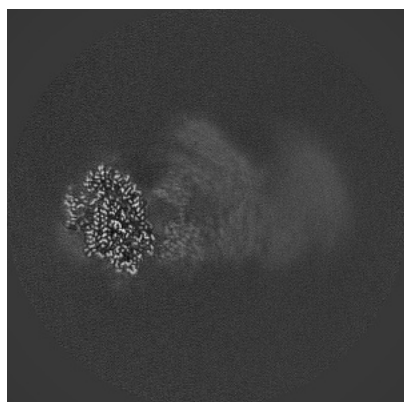


Y Index: 135

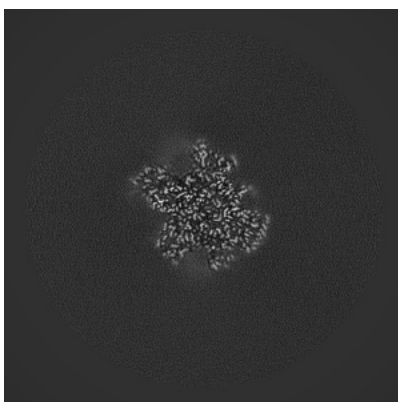


Z Index: 260

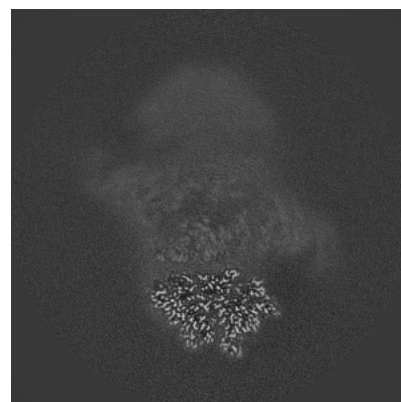
6.3.2 Raw map



X Index: 265



Y Index: 135

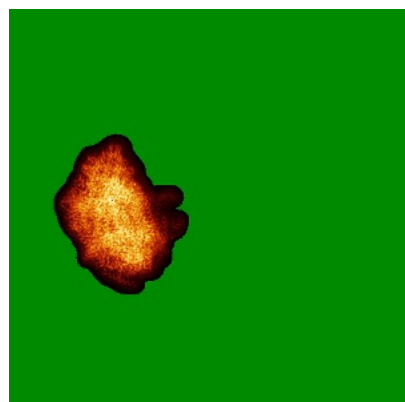


Z Index: 261

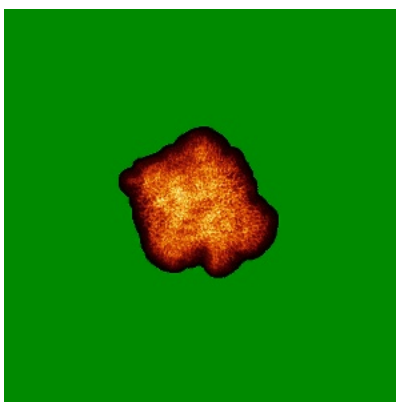
The images above show the largest variance slices of the map in three orthogonal directions.

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

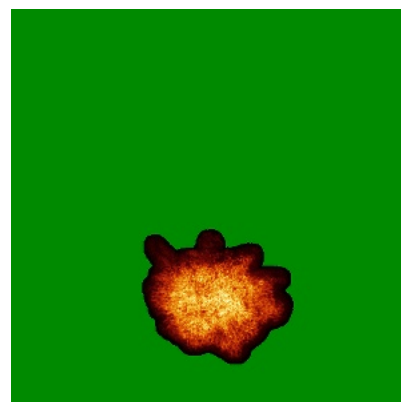
6.4.1 Primary map



X

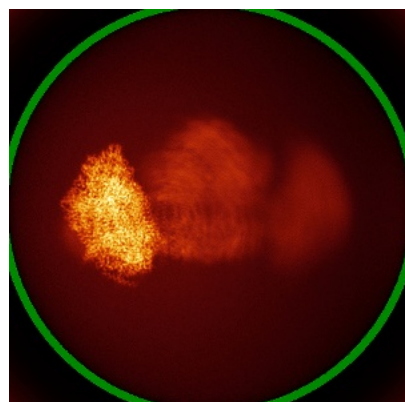


Y

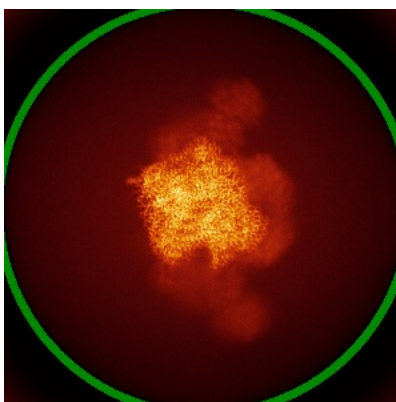


Z

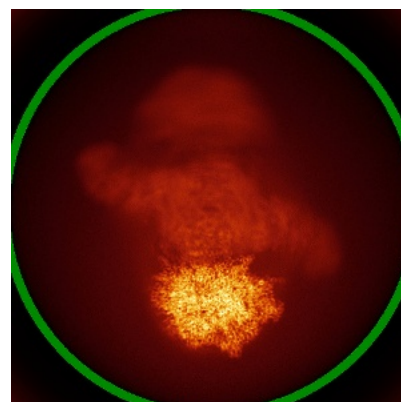
6.4.2 Raw map



X



Y



Z

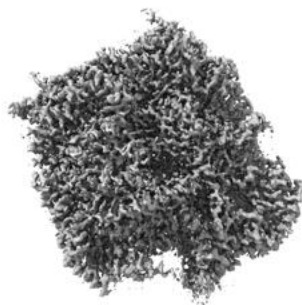
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



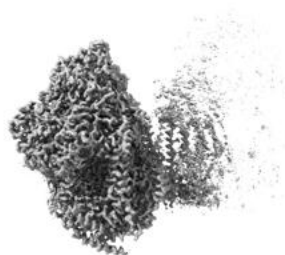
Y



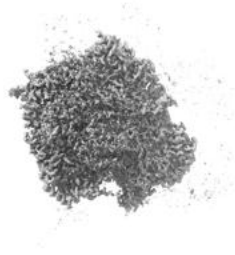
Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

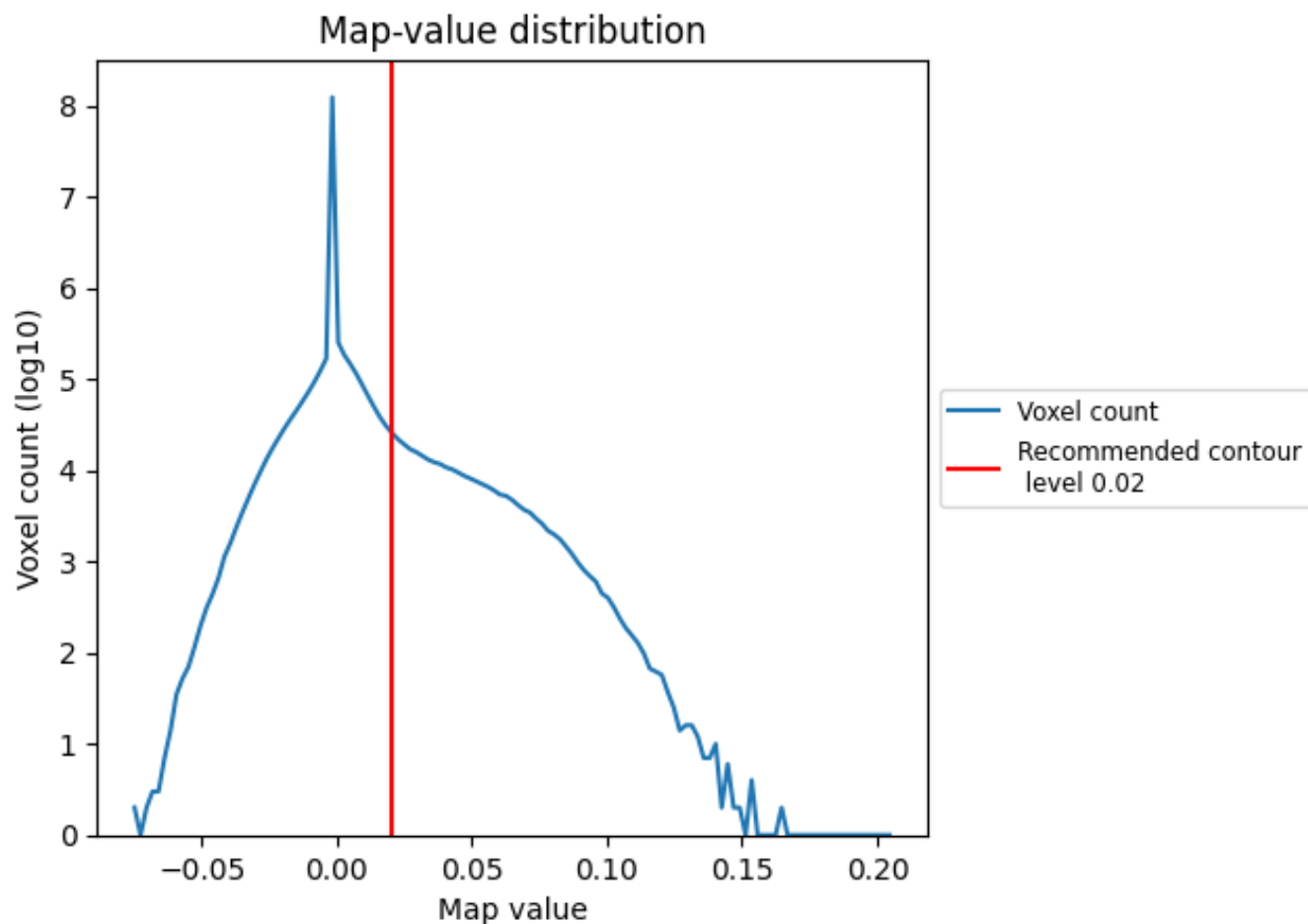
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

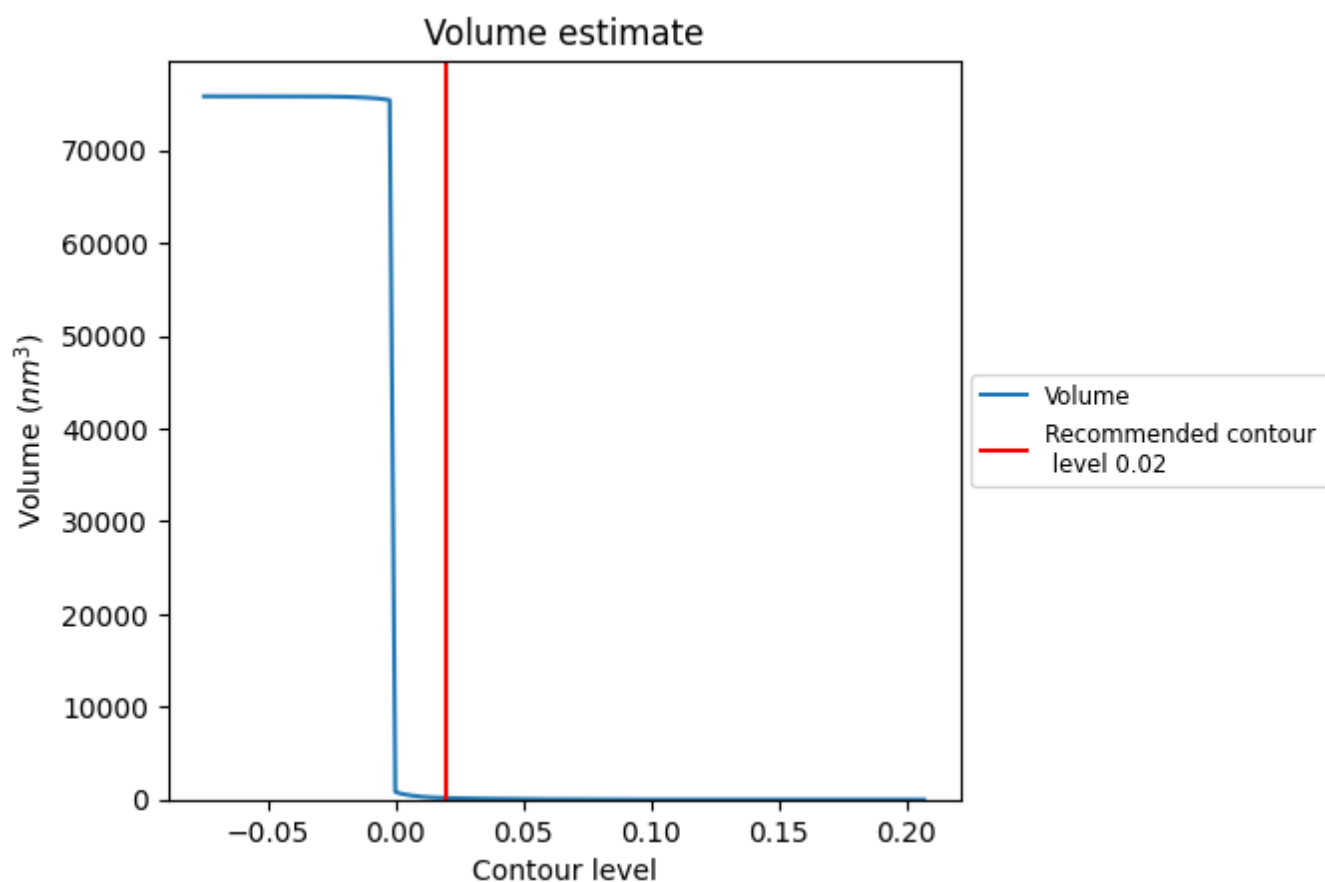
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

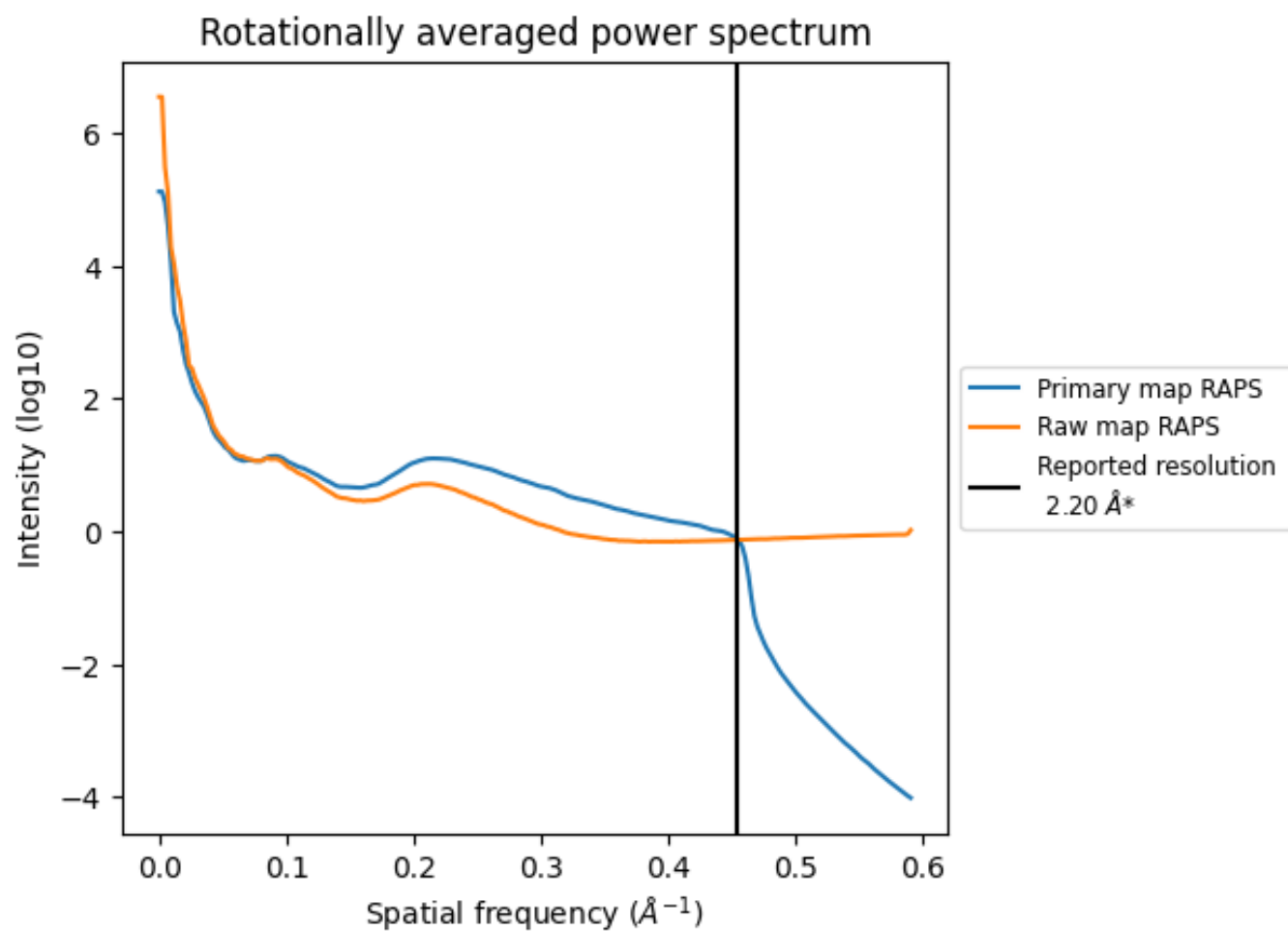
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 169 nm³; this corresponds to an approximate mass of 153 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 ⓘ

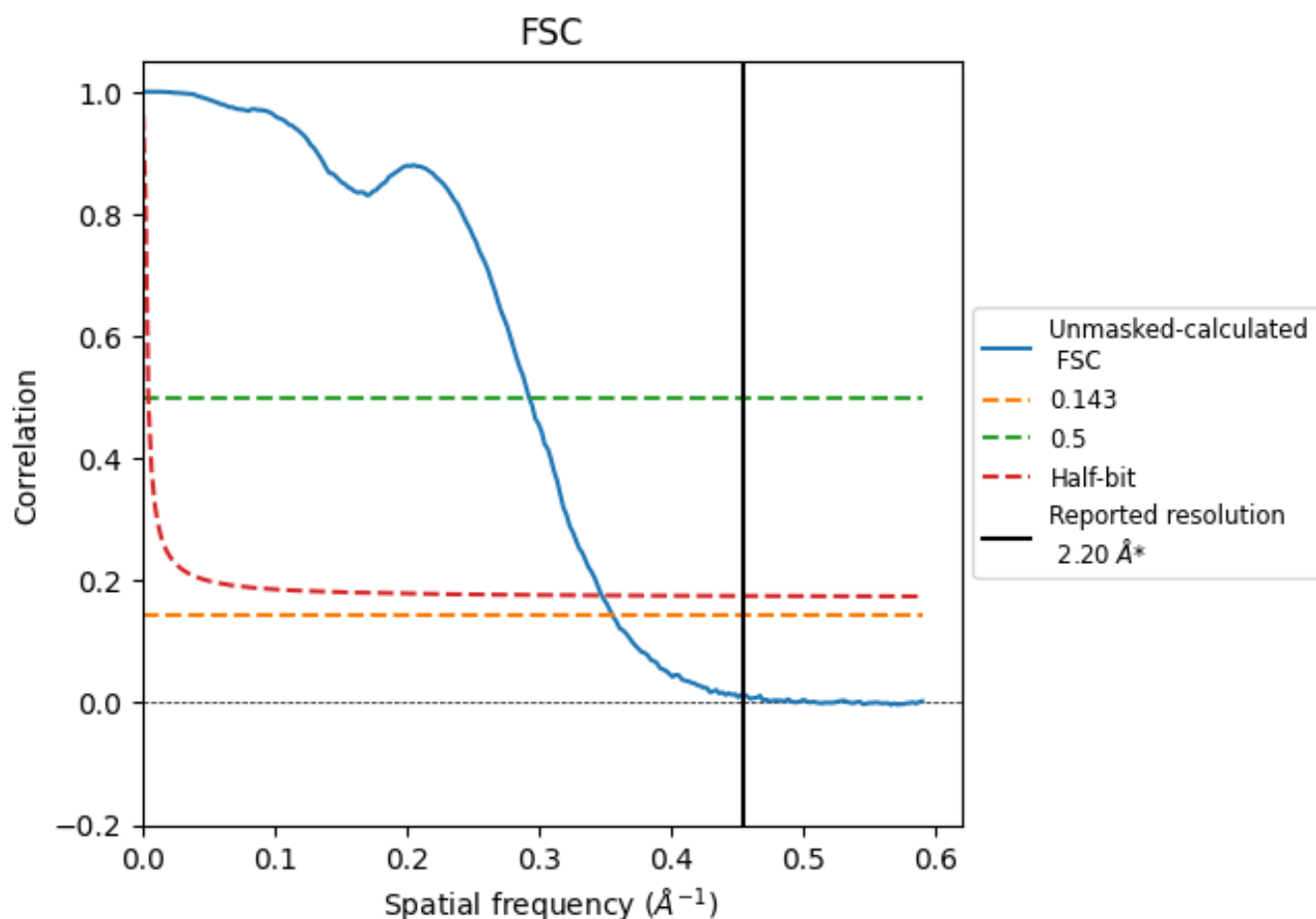


*Reported resolution corresponds to spatial frequency of 0.455 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

8.2 Resolution estimates [i](#)

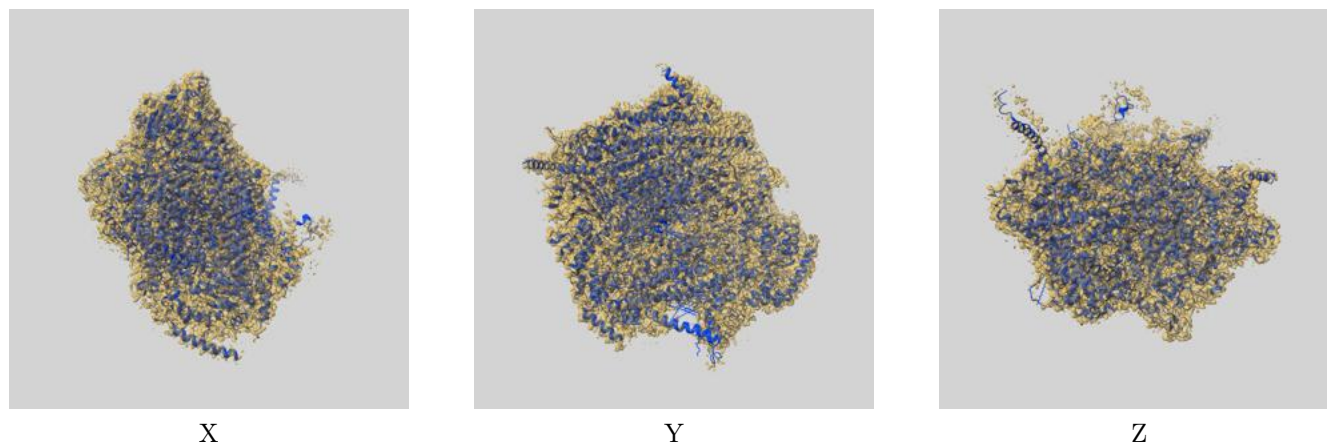
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.81	3.41	2.87

*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 2.81 differs from the reported value 2.2 by more than 10 %

9 Map-model fit [i](#)

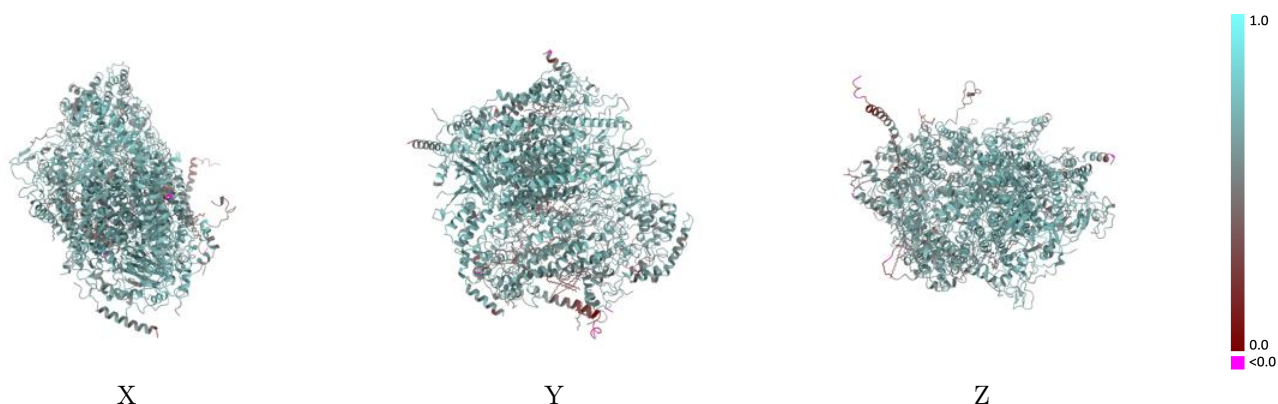
This section contains information regarding the fit between EMDB map EMD-50363 and PDB model 9FQ8. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



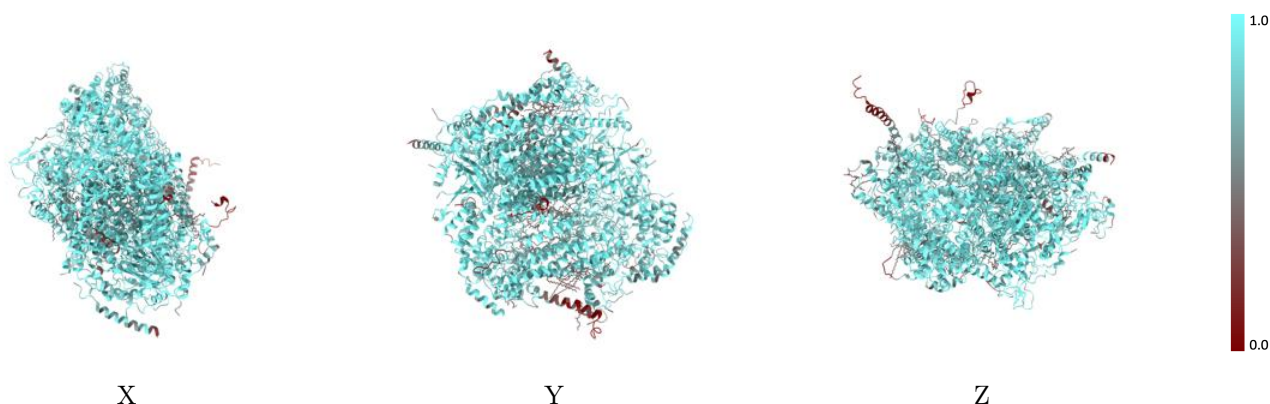
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



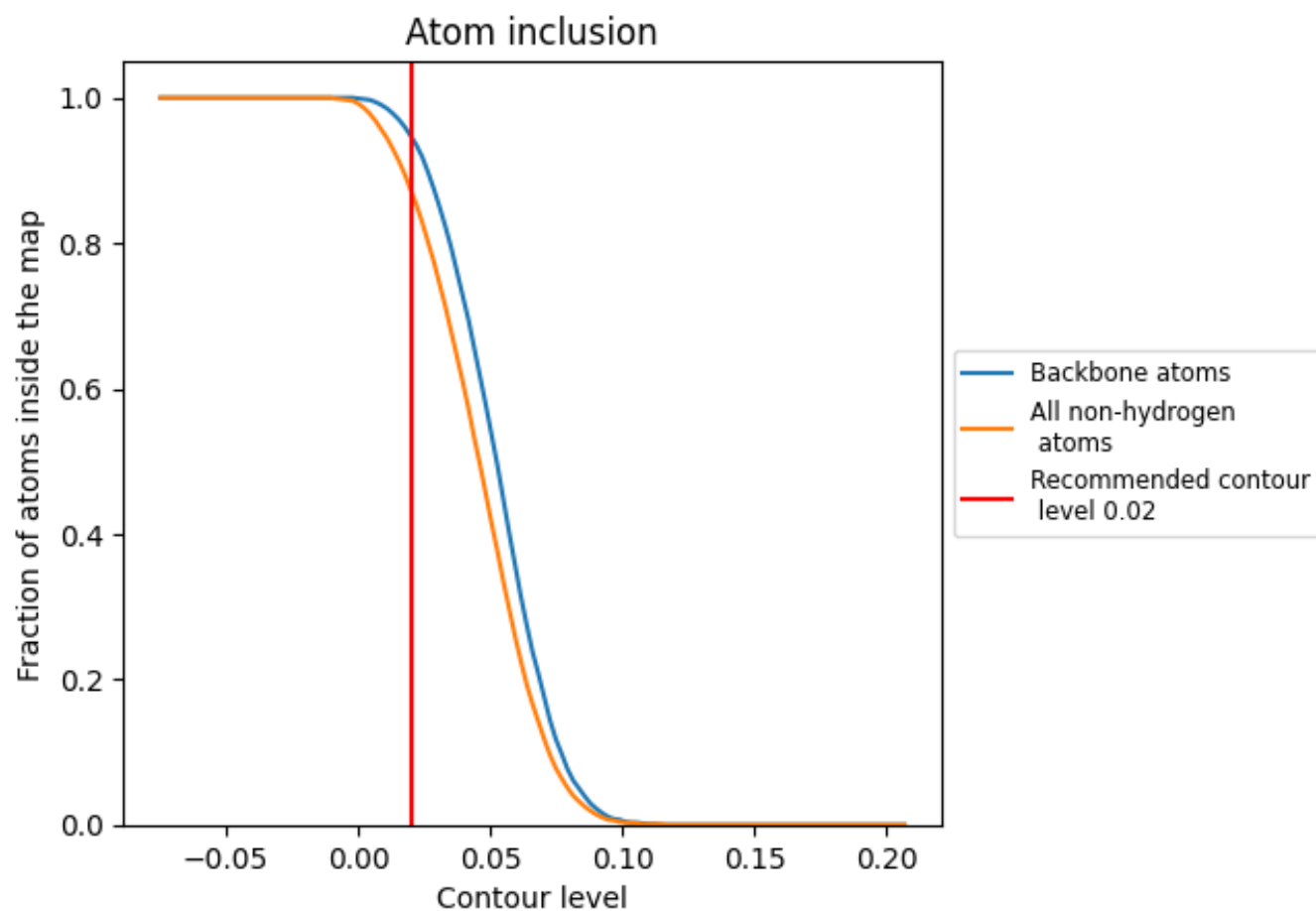
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 87% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8720	 0.6290
4A	 0.8860	 0.6590
4B	 0.6230	 0.4820
4C	 0.6570	 0.5460
4D	 0.8980	 0.6600
4E	 0.8600	 0.5860
4F	 0.7210	 0.5310
4G	 0.9030	 0.6350
4H	 0.8460	 0.5930
4I	 0.9300	 0.6600
4J	 0.8850	 0.5970
4K	 0.7330	 0.5250
4L	 0.8870	 0.6060
4M	 0.8150	 0.6050
4N	 0.9490	 0.6860
4O	 0.8610	 0.6640
4P	 0.9210	 0.6620
4Q	 0.9380	 0.6940
4R	 0.8180	 0.5810
4S	 0.8590	 0.6300
4T	 0.9180	 0.6370
4U	 0.6540	 0.5350
4V	 0.8960	 0.6400
4W	 0.8850	 0.6230
4X	 0.9250	 0.6420
4Y	 0.9310	 0.6740
4Z	 0.9160	 0.6830

