



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 08:23 PM UTC

PDB ID : 7ZMH / pdb_00007zmh
EMDB ID : EMD-14798
Title : CryoEM structure of mitochondrial complex I from *Chaetomium thermophilum* (state 1) - membrane arm
Authors : Laube, E.; Kuehlbrandt, W.
Deposited on : 2022-04-19
Resolution : 2.47 Å (reported)
Based on initial models : 6RFQ, 6RFR

This is a wwPDB EM Validation Summary 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

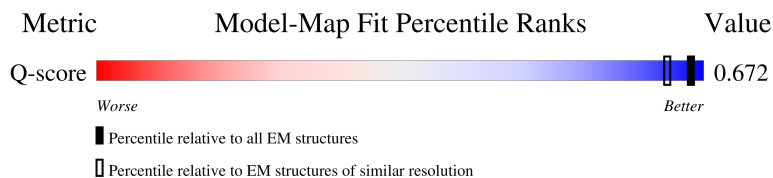
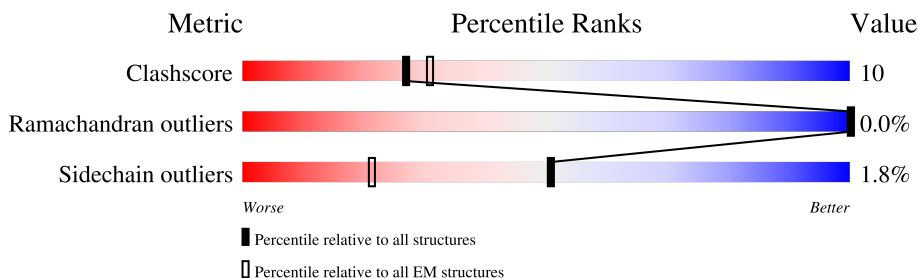
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.47 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.



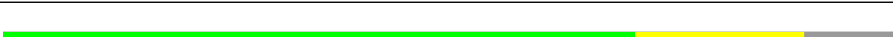
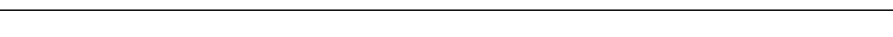
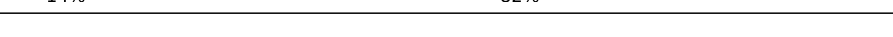
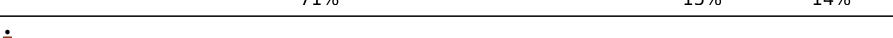
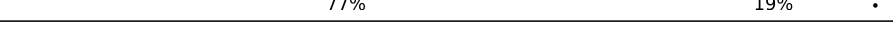
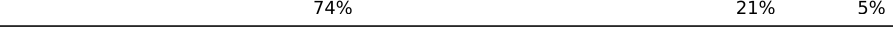
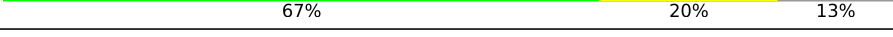
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6086 (1.98 - 2.97)

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	1	378	
2	2	571	
3	3	146	
4	4	542	

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Mol	Chain	Length	Quality of chain
5	5	679	
6	6	224	
7	8	86	
8	9	785	
9	D	86	
10	J	199	
11	L	89	
12	Q	141	
13	R	99	
14	S	143	
15	U	186	
16	W	121	
17	X	191	
18	a	815	
19	b	94	
20	c	93	
21	d	105	
22	e	46	
23	g	82	
24	i	93	
25	j	75	
26	n	184	

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 37605 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 NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	334	Total	C	N	O	S	0	0
			2566	1722	388	445	11		

- Molecule 2 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	558	Total	C	N	O	S	0	0
			4459	2994	672	782	11		

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	101	Total	C	N	O	S	0	0
			788	541	113	132	2		

- Molecule 4 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	494	Total	C	N	O	S	0	0
			3904	2650	572	670	12		

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	670	Total	C	N	O	S	0	0
			5273	3551	792	905	25		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	445	ARG	-	insertion	UNP G1DJA3
5	446	LEU	-	insertion	UNP G1DJA3
5	447	ALA	-	insertion	UNP G1DJA3

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Chain	Residue	Modelled	Actual	Comment	Reference
5	448	ILE	-	insertion	UNP G1DJA3
5	449	ASP	-	insertion	UNP G1DJA3
5	450	ASN	-	insertion	UNP G1DJA3
5	451	PHE	-	insertion	UNP G1DJA3
5	452	PHE	-	insertion	UNP G1DJA3
5	453	SER	-	insertion	UNP G1DJA3
5	454	ALA	-	insertion	UNP G1DJA3
5	455	GLN	-	insertion	UNP G1DJA3
5	456	ALA	-	insertion	UNP G1DJA3
5	457	ILE	-	insertion	UNP G1DJA3
5	458	LYS	-	insertion	UNP G1DJA3

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	190	Total	C	N	O	S	0	0
			1468	988	221	253	6		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	78	Total	C	N	O	S	0	0
			663	411	127	119	6		

- Molecule 8 is a protein called Subunit NDUF5 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	103	Total	C	N	O	S	0	0
			807	500	147	154	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	100	VAL	-	insertion	UNP G0SG48

- Molecule 9 is a protein called Subunit NDUF1 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	85	Total	C	N	O	S	0	0
			678	432	127	115	4		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	186	Total	C	N	O	S	0	0
			1388	877	259	250	2		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	87	Total	C	N	O	S	0	0
			673	453	102	115	3		

- Molecule 12 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	85	Total	C	N	O	S	0	0
			673	422	109	141	1		

- Molecule 13 is a protein called Complex I-B22.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	98	Total	C	N	O	S	0	0
			807	520	149	137	1		

- Molecule 14 is a protein called Complex I-ESSS.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	S	74	Total	C	N	O	0	0
			612	402	98	112		

- Molecule 15 is a protein called NADH-ubiquinone oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	167	Total	C	N	O	S	0	0
			1357	854	253	241	9		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	99	Total	C	N	O	S	0	0
			816	521	154	139	2		

- Molecule 17 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	187	Total	C	N	O	S	0	0
			1484	943	268	265	8		

- Molecule 18 is a protein called NADH dehydrogenase (Ubiquinone)-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	a	144	Total	C	N	O	S	0	0
			1172	753	196	218	5		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	166	VAL	ALA	conflict	UNP G0RXU4
a	168	ALA	MET	conflict	UNP G0RXU4
a	?	-	GLU	deletion	UNP G0RXU4
a	?	-	GLY	deletion	UNP G0RXU4
a	?	-	ASP	deletion	UNP G0RXU4
a	?	-	PRO	deletion	UNP G0RXU4
a	?	-	ASP	deletion	UNP G0RXU4
a	?	-	PRO	deletion	UNP G0RXU4

- Molecule 19 is a protein called Subunit NDUFC2 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	b	81	Total	C	N	O	S	0	0
			683	445	125	110	3		

- Molecule 20 is a protein called Subunit NDUF3 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	c	61	Total	C	N	O	S	0	0
			505	329	91	83	2		

- Molecule 21 is a protein called Subunit NDUF10 of NADH-ubiquinone oxidoreductase

(Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	101	Total	C	N	O	S	0	0
			843	535	149	155	4		

- Molecule 22 is a protein called Subunit NDUF2 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	e	38	Total	C	N	O	S	0	0
			317	215	55	46	1		

- Molecule 23 is a protein called Subunit NDUF3 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	g	78	Total	C	N	O	S	0	0
			610	399	105	105	1		

- Molecule 24 is a protein called Subunit NDUF6 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
24	i	81	Total	C	N	O	S	0	0
			682	450	118	112	2		

- Molecule 25 is a protein called Subunit NDUF4 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	j	75	Total	C	N	O	S	0	0
			616	399	110	103	4		

- Molecule 26 is a protein called Subunit NDUF5 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
26	n	135	Total	C	N	O	S	0	0
			1061	680	186	194	1		

There are 52 discrepancies between the modelled and reference sequences:

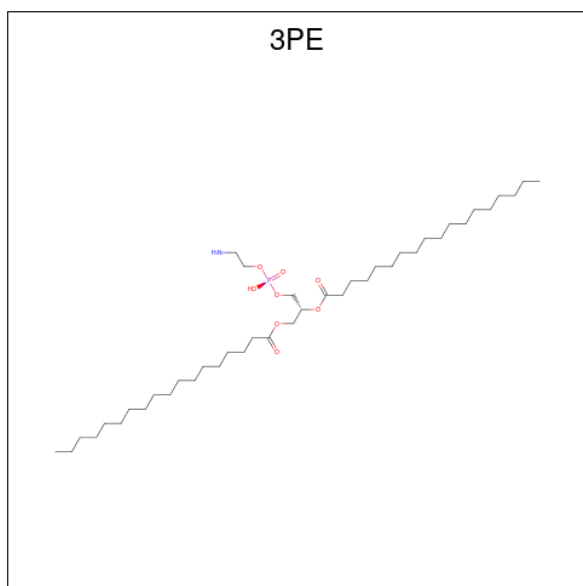
Chain	Residue	Modelled	Actual	Comment	Reference
n	1	MET	-	initiating methionine	UNP G0S086
n	2	LEU	-	insertion	UNP G0S086
n	3	ALA	-	insertion	UNP G0S086
n	4	LEU	-	insertion	UNP G0S086
n	5	ARG	-	insertion	UNP G0S086
n	6	GLN	-	insertion	UNP G0S086
n	7	ARG	-	insertion	UNP G0S086
n	8	ALA	-	insertion	UNP G0S086
n	9	ALA	-	insertion	UNP G0S086
n	10	LEU	-	insertion	UNP G0S086
n	11	LEU	-	insertion	UNP G0S086
n	12	ALA	-	insertion	UNP G0S086
n	13	ARG	-	insertion	UNP G0S086
n	14	ARG	-	insertion	UNP G0S086
n	15	VAL	-	insertion	UNP G0S086
n	16	ARG	-	insertion	UNP G0S086
n	17	PRO	-	insertion	UNP G0S086
n	18	THR	-	insertion	UNP G0S086
n	19	VAL	-	insertion	UNP G0S086
n	20	VAL	-	insertion	UNP G0S086
n	21	VAL	-	insertion	UNP G0S086
n	22	PRO	-	insertion	UNP G0S086
n	23	ARG	-	insertion	UNP G0S086
n	24	ASN	-	insertion	UNP G0S086
n	25	ALA	-	insertion	UNP G0S086
n	26	ARG	-	insertion	UNP G0S086
n	27	THR	-	insertion	UNP G0S086
n	28	TYR	-	insertion	UNP G0S086
n	29	ALA	-	insertion	UNP G0S086
n	30	SER	-	insertion	UNP G0S086
n	31	SER	-	insertion	UNP G0S086
n	32	HIS	-	insertion	UNP G0S086
n	33	ASP	-	insertion	UNP G0S086
n	34	HIS	-	insertion	UNP G0S086
n	35	ASP	-	insertion	UNP G0S086
n	36	HIS	-	insertion	UNP G0S086
n	37	HIS	-	insertion	UNP G0S086
n	38	ASP	-	insertion	UNP G0S086
n	39	HIS	-	insertion	UNP G0S086
n	40	HIS	-	insertion	UNP G0S086
n	41	HIS	-	insertion	UNP G0S086
n	42	ASP	-	insertion	UNP G0S086
n	43	HIS	-	insertion	UNP G0S086

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Chain	Residue	Modelled	Actual	Comment	Reference
n	44	GLY	-	insertion	UNP G0S086
n	45	HIS	-	insertion	UNP G0S086
n	46	ASN	-	insertion	UNP G0S086
n	47	VAL	-	insertion	UNP G0S086
n	48	GLU	-	insertion	UNP G0S086
n	49	GLU	-	insertion	UNP G0S086
n	50	PRO	-	insertion	UNP G0S086
n	51	LEU	-	insertion	UNP G0S086
n	52	GLY	-	insertion	UNP G0S086

- Molecule 27 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



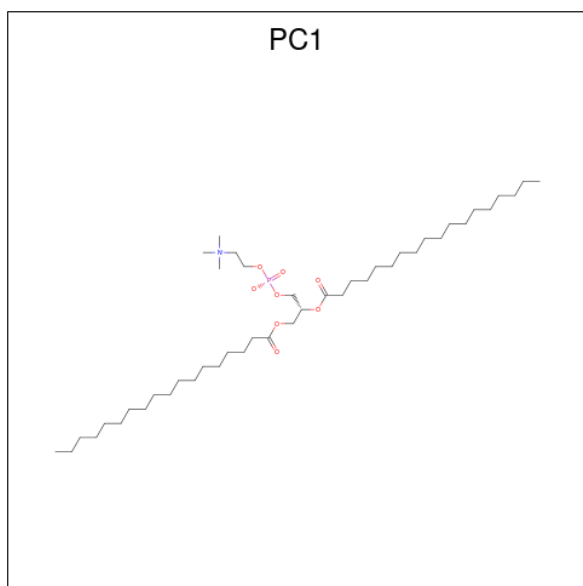
Mol	Chain	Residues	Atoms					AltConf
27	1	1	Total	C	N	O	P	0
			45	35	1	8	1	
27	4	1	Total	C	N	O	P	0
			45	35	1	8	1	
27	4	1	Total	C	N	O	P	0
			34	24	1	8	1	
27	5	1	Total	C	N	O	P	0
			35	25	1	8	1	
27	5	1	Total	C	N	O	P	0
			33	23	1	8	1	
27	5	1	Total	C	N	O	P	0
			35	25	1	8	1	

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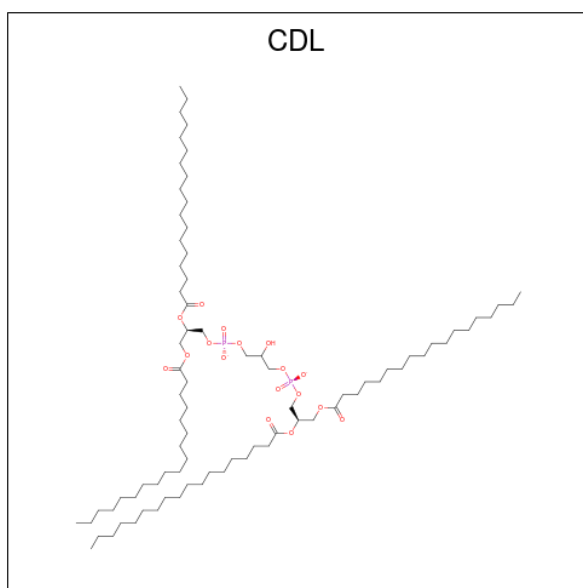
Mol	Chain	Residues	Atoms					AltConf
27	5	1	Total	C	N	O	P	0
			43	33	1	8	1	
27	5	1	Total	C	N	O	P	0
			33	23	1	8	1	
27	6	1	Total	C	N	O	P	0
			36	26	1	8	1	
27	J	1	Total	C	N	O	P	0
			30	20	1	8	1	
27	W	1	Total	C	N	O	P	0
			38	28	1	8	1	
27	W	1	Total	C	N	O	P	0
			39	29	1	8	1	
27	g	1	Total	C	N	O	P	0
			36	26	1	8	1	
27	g	1	Total	C	N	O	P	0
			44	34	1	8	1	
27	i	1	Total	C	N	O	P	0
			41	31	1	8	1	
27	n	1	Total	C	N	O	P	0
			51	41	1	8	1	
27	n	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 28 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
28	1	1	Total	C	N	O	P	0
			42	32	1	8	1	
28	3	1	Total	C	N	O	P	0
			43	33	1	8	1	
28	4	1	Total	C	N	O	P	0
			50	40	1	8	1	
28	5	1	Total	C	N	O	P	0
			54	44	1	8	1	
28	5	1	Total	C	N	O	P	0
			43	33	1	8	1	
28	S	1	Total	C	N	O	P	0
			52	42	1	8	1	
28	X	1	Total	C	N	O	P	0
			39	29	1	8	1	
28	X	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 29 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



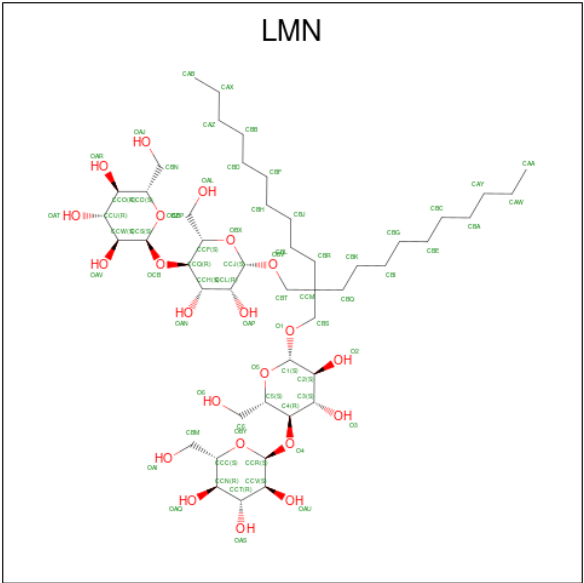
Mol	Chain	Residues	Atoms				AltConf
29	2	1	Total	C	O	P	0
			74	55	17	2	
29	D	1	Total	C	O	P	0
			65	46	17	2	
29	S	1	Total	C	O	P	0
			79	60	17	2	
29	X	1	Total	C	O	P	0
			70	51	17	2	

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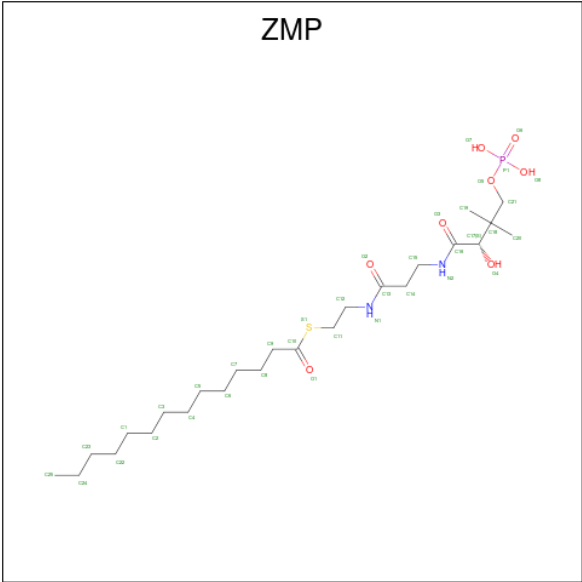
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
29	X	1	79	60	17	2	0

- Molecule 30 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: $C_{47}H_{88}O_{22}$).



Mol	Chain	Residues	Atoms			AltConf
30	2	1	Total	C	O	0
			58	41	17	
30	4	1	Total	C	O	0
			47	35	12	
30	j	1	Total	C	O	0
			69	47	22	

- Molecule 31 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



Mol	Chain	Residues	Atoms						AltConf
31	Q	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	

- Molecule 32 is water.

Mol	Chain	Residues	Atoms		AltConf
32	1	110	Total	O	0
			110	110	
32	2	224	Total	O	0
			224	224	
32	3	25	Total	O	0
			25	25	
32	4	181	Total	O	0
			181	181	
32	5	100	Total	O	0
			100	100	
32	6	52	Total	O	0
			52	52	
32	9	23	Total	O	0
			23	23	
32	D	36	Total	O	0
			36	36	
32	J	1	Total	O	0
			1	1	
32	L	23	Total	O	0
			23	23	
32	Q	1	Total	O	0
			1	1	

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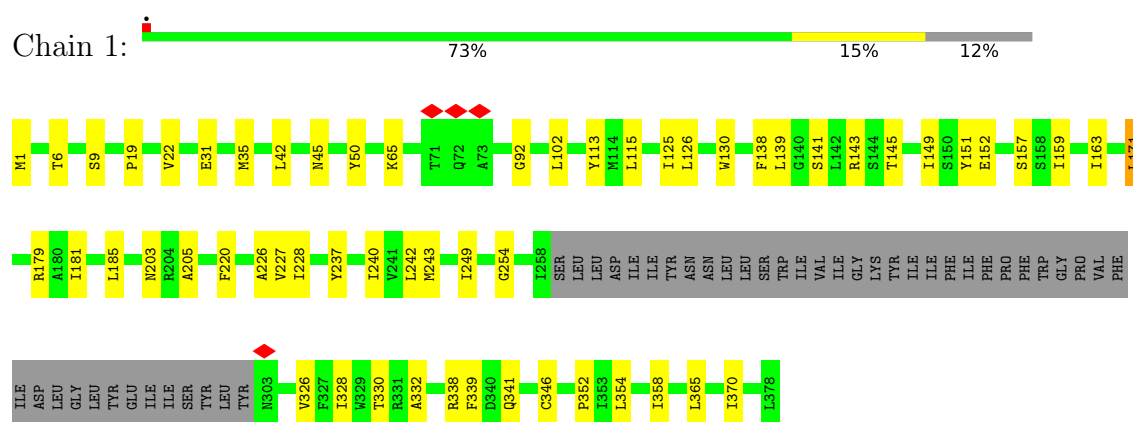
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Mol	Chain	Residues	Atoms		AltConf
32	R	15	Total 15	O 15	0
32	S	6	Total 6	O 6	0
32	U	60	Total 60	O 60	0
32	W	43	Total 43	O 43	0
32	X	71	Total 71	O 71	0
32	a	23	Total 23	O 23	0
32	b	13	Total 13	O 13	0
32	d	18	Total 18	O 18	0
32	g	15	Total 15	O 15	0
32	i	11	Total 11	O 11	0
32	j	18	Total 18	O 18	0
32	n	42	Total 42	O 42	0

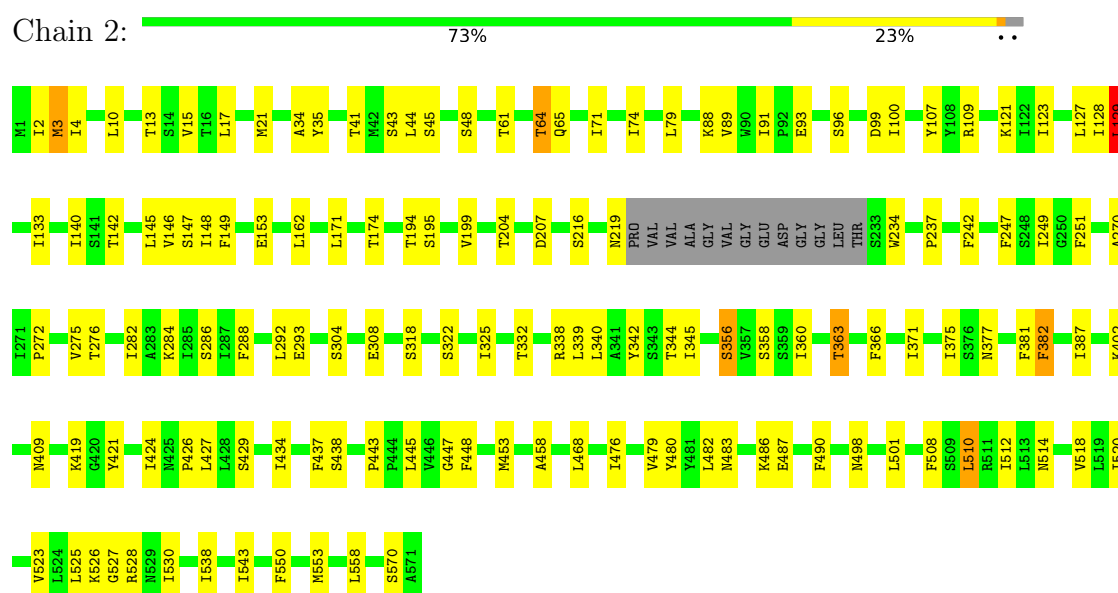
3 Residue-property plots

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: NADH-ubiquinone oxidoreductase chain 1

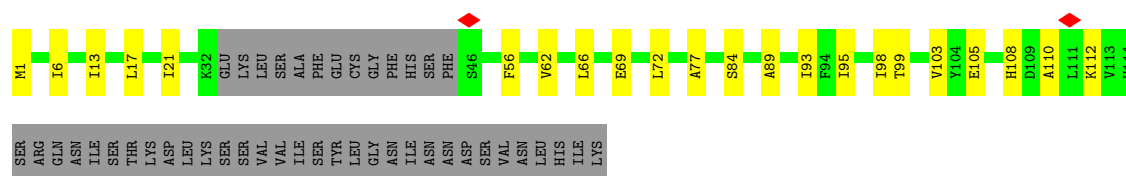


• Molecule 2: NADH dehydrogenase subunit 2



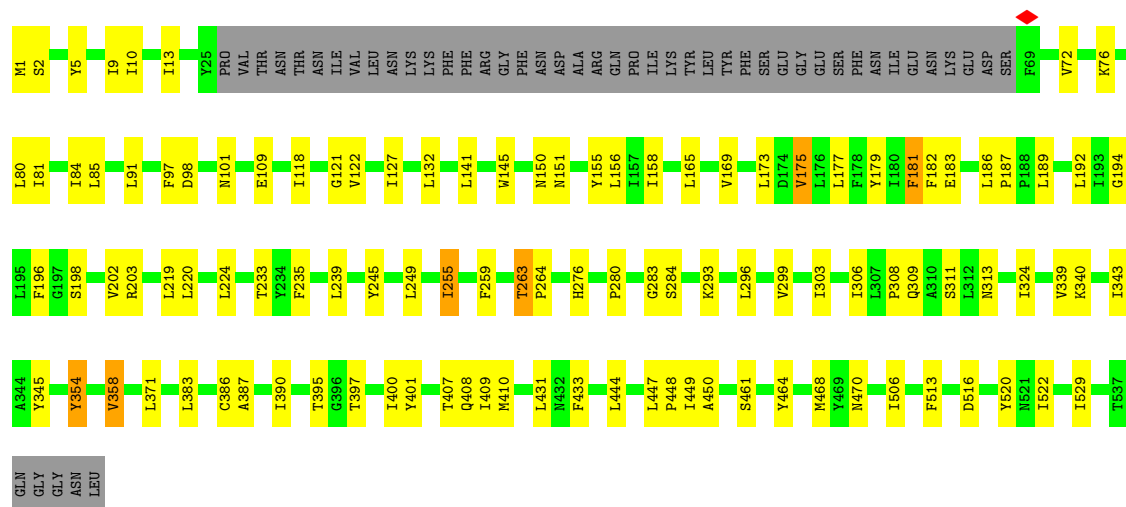
• Molecule 3: NADH-ubiquinone oxidoreductase chain 3





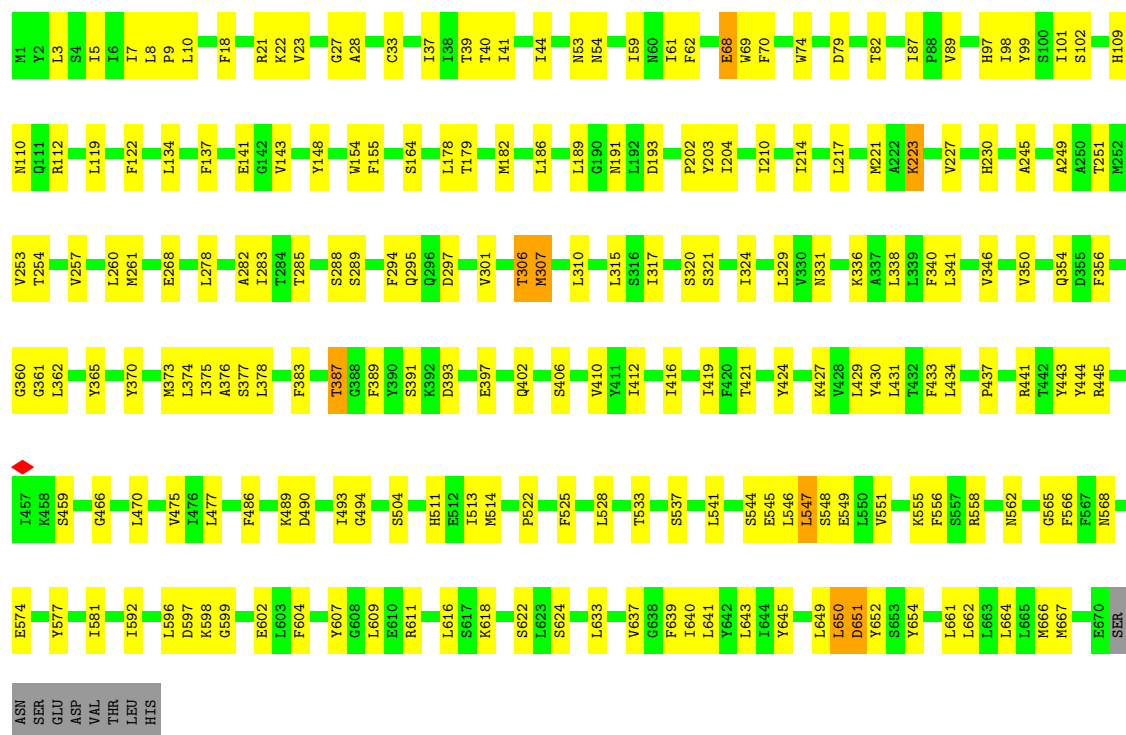
• Molecule 4: NADH-ubiquinone oxidoreductase chain 4

Chain 4: 71% 19% 9%

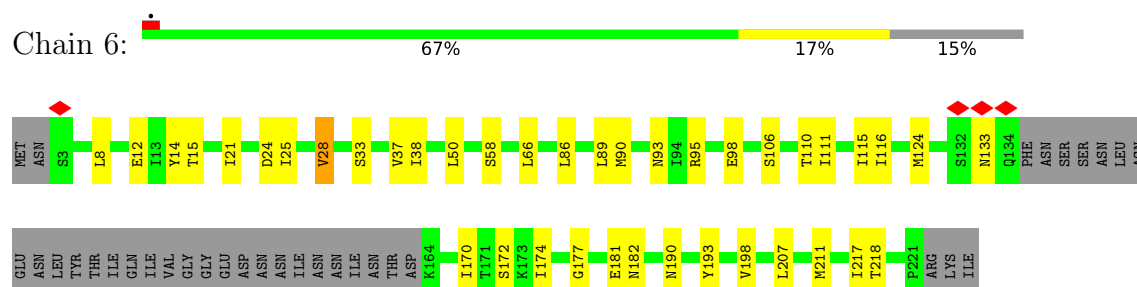


• Molecule 5: NADH-ubiquinone oxidoreductase chain 5

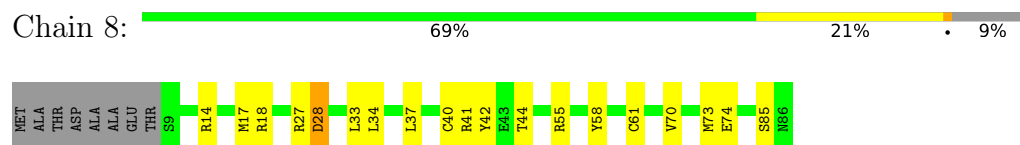
Chain 5: 68% 29% 3%



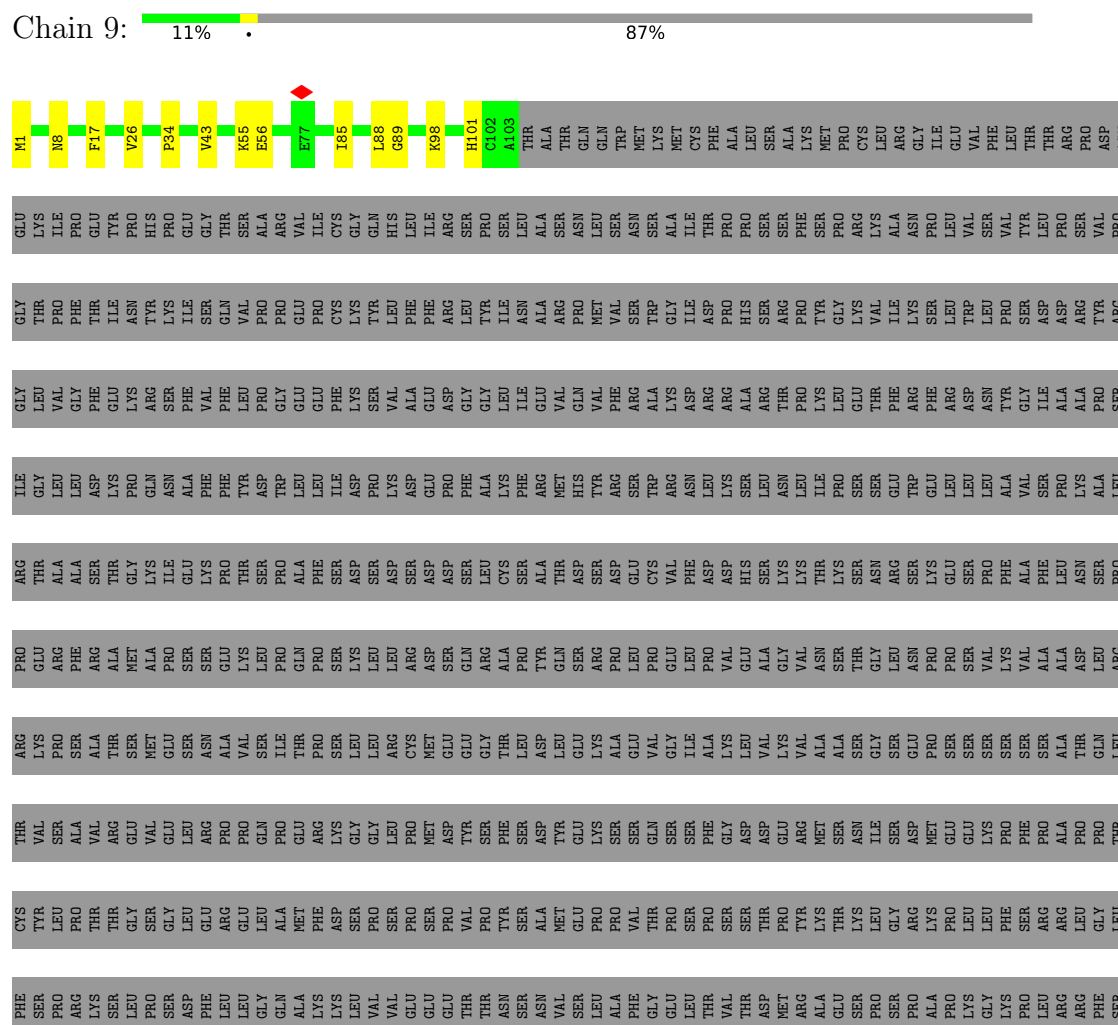
- Molecule 6: NADH-ubiquinone oxidoreductase chain 6



- Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 8: Subunit NDUFS5 of NADH-ubiquinone oxidoreductase (Complex I)



THR
ILE
VAL
GLU
ILE
SER
ILE
LYS
GLU
LYS
ARG
PRO
LEU
PHE
ASN
SER
LEU
ARG
ARG
ILE
ALA
SER
ALA
SER
PRO
ARG
LYS
LYS
ALA
GLY
ARG
VAL
LEU
SER
MET
ASP
LEU
GLY
LYS
LYS
GLY
GLY
GLU
LYS
GLU
GLY

- Molecule 9: Subunit NDUFA1 of NADH-ubiquinone oxidoreductase (Complex I)

Chain D:  73% 26%

MET
P2
E6
I9
M17
K27
V42
W45
D46
K47
E51
R52
R55
R61
D65
R66
P67
P71
G72
F73
E74
N77
P78
W79
K80
V81
X86

- Molecule 10: NADH-ubiquinone oxidoreductase-like protein

Chain J:  66% 28% 7%

MET
ALA
PRO
ILE
GLU
GLU
HIS
GLU
HIS
TYR
HIS
P13
K14
D15
H18
L19
G20
G23
V27
L33
R38
T39
S40
L41
V46
A50
I51
F52
N55
F62
V65
G66
Y69
D70
R80
D84
W85
V86
I90
L93
F94
A95
G96
A97

T98
M99
L101
R108
F112
A113
L120
A121
T122
A123
E124
L130
R131
G132
V133
R136
Y141
E145
R148
K149
I155
E166
I162
R166
K169
P170
Y173
R177
L181
K182
D188
V192
G193
A194
Q198
ALA

- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain L:  73% 24%

MET
N2
I12
L13
G14
N18
N21
I22
I23
L24
I27
S28
I29
S35
M47
I51
G52
G53
T54
Y55
A56
I57
E66
L71
I84
Y88
LYS

- Molecule 12: Acyl carrier protein

Chain Q:  48% 12% 40%

MET
PHE
ARG
SER
ALA
VAL
LEU
ARG
SER
ALA
ALA
ALA
ALA
THR
ARG
THR
THR
ILE
ARG
SER
ILE
PRO
PRO
ALA
ALA
ALA
LYS
LYS
PHE
ALA
VAL
ALA
PRO
VAL
SER
SER
ARG
VAL
THR
SER
PHE
ILE
PRO
LYS
THR
ALA
SER
TRP
GLN
VAL
ILE
ARG
CYS
TYR
ALA
SER
ASN
E57
V62
E63

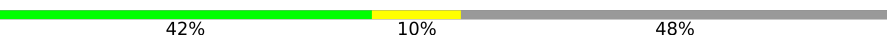
F75
V78
N79
D80
H89
N92
D93
L27
S93
L99
D100
T101
V104
E111
L135
R136
Q137
H141

- Molecule 13: Complex I-B22

Chain R:  81% 17%

MET
S2
L10
Y11
L15
K16
R25
N26
L27
N28
R29
L33
K56
E57
T58
L61
E63
K64
W65
R66
R84
L91
F99

- Molecule 14: Complex I-ESSS

Chain S:  42% 10% 48%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	153568	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.221	Depositor
Minimum map value	-2.124	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.168	Depositor
Recommended contour level	0.12	Depositor
Map size ($\text{\AA}$)	143.964, 218.457, 227.664	wwPDB
Map dimensions	272, 261, 172	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.837, 0.837, 0.837	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: CDL, ZMP, PC1, 3PE, LMN

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	1	0.45	0/2625	0.64	1/3582 (0.0%)
2	2	0.50	4/4565 (0.1%)	0.70	5/6209 (0.1%)
3	3	0.48	0/809	0.76	0/1102
4	4	0.54	2/4002 (0.0%)	0.78	5/5454 (0.1%)
5	5	0.43	4/5415 (0.1%)	0.60	2/7372 (0.0%)
6	6	0.42	0/1495	0.62	1/2038 (0.0%)
7	8	0.57	3/676 (0.4%)	0.54	1/903 (0.1%)
8	9	0.40	0/824	0.63	0/1112
9	D	0.40	0/674	0.67	0/911
10	J	0.39	2/1413 (0.1%)	0.52	1/1908 (0.1%)
11	L	0.42	0/680	0.64	0/921
12	Q	0.67	0/683	1.02	0/926
13	R	0.36	0/832	0.57	0/1133
14	S	0.44	1/637 (0.2%)	0.56	0/872
15	U	0.39	0/1394	0.61	0/1890
16	W	0.42	0/834	0.60	0/1125
17	X	0.45	1/1523 (0.1%)	0.70	2/2058 (0.1%)
18	a	0.37	0/1209	0.59	0/1639
19	b	0.28	0/701	0.38	0/939
20	c	0.24	0/524	0.49	0/710
21	d	0.62	1/861 (0.1%)	0.56	1/1157 (0.1%)
22	e	0.21	0/332	0.32	0/451
23	g	0.29	0/631	0.49	0/868
24	i	0.26	0/711	0.41	0/967
25	j	0.42	0/630	0.62	0/847
26	n	0.26	0/1092	0.37	0/1481
All	All	0.45	18/35772 (0.1%)	0.64	19/48575 (0.0%)

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	d	65	VAL	C-N	15.67	1.58	1.33
7	8	28	ASP	C-N	8.57	1.45	1.33
2	2	510	LEU	C-N	8.34	1.45	1.33
10	J	155	ILE	C-N	6.87	1.43	1.33
2	2	381	PHE	C-N	-6.73	1.24	1.33

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	d	65	VAL	O-C-N	11.94	133.93	121.87
17	X	144	ARG	CG-CD-NE	6.88	127.13	112.00
2	2	129	LEU	N-CA-CB	-6.59	100.44	110.12
17	X	61	ILE	N-CA-C	-6.39	106.56	112.96
1	1	179	ARG	N-CA-C	-6.16	105.03	112.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2566	0	2689	50	0
2	2	4459	0	4652	118	0
3	3	788	0	803	21	0
4	4	3904	0	4056	84	0
5	5	5273	0	5399	162	0
6	6	1468	0	1568	42	0
7	8	663	0	650	12	0
8	9	807	0	778	13	0
9	D	678	0	643	23	0
10	J	1388	0	1393	44	0
11	L	673	0	742	17	0
12	Q	673	0	646	8	0
13	R	807	0	823	13	0
14	S	612	0	562	10	0
15	U	1357	0	1330	31	0
16	W	816	0	837	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	X	1484	0	1436	35	0
18	a	1172	0	1106	21	0
19	b	683	0	690	15	0
20	c	505	0	474	14	0
21	d	843	0	835	14	0
22	e	317	0	304	3	0
23	g	610	0	620	13	0
24	i	682	0	655	18	0
25	j	616	0	640	14	0
26	n	1061	0	1022	21	0
27	1	45	0	64	0	0
27	4	79	0	109	4	0
27	5	179	0	231	10	0
27	6	36	0	46	2	0
27	J	30	0	34	1	0
27	W	77	0	102	5	0
27	g	80	0	108	1	0
27	i	41	0	56	1	0
27	n	90	0	134	2	0
28	1	42	0	58	3	0
28	3	43	0	60	4	0
28	4	50	0	74	11	0
28	5	97	0	148	14	0
28	S	52	0	81	3	0
28	X	71	0	90	4	0
29	2	74	0	92	8	0
29	D	65	0	74	0	0
29	S	79	0	105	3	0
29	X	149	0	189	6	0
30	2	58	0	77	2	0
30	4	47	0	66	2	0
30	j	69	0	88	4	0
31	Q	36	0	47	1	0
32	1	110	0	0	5	0
32	2	224	0	0	25	0
32	3	25	0	0	4	0
32	4	181	0	0	13	0
32	5	100	0	0	11	0
32	6	52	0	0	3	0
32	9	23	0	0	0	0
32	D	36	0	0	3	0
32	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	L	23	0	0	4	0
32	Q	1	0	0	0	0
32	R	15	0	0	1	0
32	S	6	0	0	0	0
32	U	60	0	0	3	0
32	W	43	0	0	4	0
32	X	71	0	0	4	0
32	a	23	0	0	1	0
32	b	13	0	0	1	0
32	d	18	0	0	0	0
32	g	15	0	0	0	0
32	i	11	0	0	1	0
32	j	18	0	0	0	0
32	n	42	0	0	3	0
All	All	37605	0	37486	729	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 10.

The worst 5 of 729 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)
1:1:352:PRO:HB2	32:1:554:HOH:O	1.68	0.93
1:1:130:TRP:HB2	6:6:90:MET:HE3	1.48	0.92
5:5:3:LEU:HD21	5:5:59:ILE:HG12	1.53	0.90
5:5:288:SER:HB3	5:5:307:MET:HE2	1.60	0.81
10:J:27:VAL:HG21	10:J:66:GLY:HA3	1.60	0.81

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	330/378 (87%)	317 (96%)	13 (4%)	0	100	100
2	2	554/571 (97%)	545 (98%)	8 (1%)	1 (0%)	43	61
3	3	97/146 (66%)	93 (96%)	4 (4%)	0	100	100
4	4	490/542 (90%)	479 (98%)	11 (2%)	0	100	100
5	5	668/679 (98%)	636 (95%)	31 (5%)	1 (0%)	48	66
6	6	186/224 (83%)	183 (98%)	3 (2%)	0	100	100
7	8	76/86 (88%)	71 (93%)	5 (7%)	0	100	100
8	9	101/785 (13%)	101 (100%)	0	0	100	100
9	D	79/86 (92%)	78 (99%)	1 (1%)	0	100	100
10	J	184/199 (92%)	178 (97%)	6 (3%)	0	100	100
11	L	85/89 (96%)	85 (100%)	0	0	100	100
12	Q	83/141 (59%)	82 (99%)	1 (1%)	0	100	100
13	R	96/99 (97%)	94 (98%)	2 (2%)	0	100	100
14	S	72/143 (50%)	72 (100%)	0	0	100	100
15	U	165/186 (89%)	163 (99%)	2 (1%)	0	100	100
16	W	97/121 (80%)	97 (100%)	0	0	100	100
17	X	185/191 (97%)	182 (98%)	3 (2%)	0	100	100
18	a	142/815 (17%)	136 (96%)	6 (4%)	0	100	100
19	b	79/94 (84%)	77 (98%)	2 (2%)	0	100	100
20	c	59/93 (63%)	55 (93%)	4 (7%)	0	100	100
21	d	99/105 (94%)	97 (98%)	2 (2%)	0	100	100
22	e	36/46 (78%)	35 (97%)	1 (3%)	0	100	100
23	g	76/82 (93%)	73 (96%)	3 (4%)	0	100	100
24	i	79/93 (85%)	76 (96%)	3 (4%)	0	100	100
25	j	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
26	n	133/184 (72%)	129 (97%)	4 (3%)	0	100	100
All	All	4324/6253 (69%)	4206 (97%)	116 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	5	68	GLU
2	2	570	SER

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	1	283/326 (87%)	281 (99%)	2 (1%)	76	88
2	2	510/518 (98%)	501 (98%)	9 (2%)	51	74
3	3	82/128 (64%)	82 (100%)	0	100	100
4	4	431/477 (90%)	423 (98%)	8 (2%)	50	73
5	5	580/596 (97%)	568 (98%)	12 (2%)	47	71
6	6	168/203 (83%)	165 (98%)	3 (2%)	51	74
7	8	69/75 (92%)	68 (99%)	1 (1%)	59	79
8	9	84/687 (12%)	82 (98%)	2 (2%)	43	67
9	D	68/69 (99%)	67 (98%)	1 (2%)	57	78
10	J	129/146 (88%)	129 (100%)	0	100	100
11	L	74/76 (97%)	67 (90%)	7 (10%)	8	15
12	Q	75/119 (63%)	69 (92%)	6 (8%)	11	21
13	R	87/89 (98%)	84 (97%)	3 (3%)	32	57
14	S	60/111 (54%)	58 (97%)	2 (3%)	33	58
15	U	149/167 (89%)	149 (100%)	0	100	100
16	W	83/102 (81%)	79 (95%)	4 (5%)	23	43
17	X	146/152 (96%)	144 (99%)	2 (1%)	59	79
18	a	123/697 (18%)	121 (98%)	2 (2%)	55	77
19	b	67/74 (90%)	67 (100%)	0	100	100
20	c	49/80 (61%)	49 (100%)	0	100	100
21	d	90/94 (96%)	90 (100%)	0	100	100
22	e	30/35 (86%)	30 (100%)	0	100	100
23	g	65/69 (94%)	62 (95%)	3 (5%)	24	45
24	i	68/78 (87%)	67 (98%)	1 (2%)	57	78
25	j	64/64 (100%)	64 (100%)	0	100	100
26	n	106/150 (71%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3740/5382 (70%)	3672 (98%)	68 (2%)	51 74

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	W	38	LEU
16	W	68	ILE
23	g	10	SER
5	5	387	THR
5	5	289	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
17	X	162	ASN
17	X	173	GLN
19	b	29	ASN
9	D	77	ASN
8	9	84	GLN

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 ⓘ

34 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
28	PC1	X	204	-	31,31,53	1.24	4 (12%)	37,39,61	1.12	2 (5%)
27	3PE	n	202	-	38,38,50	1.01	4 (10%)	41,43,55	1.14	2 (4%)
27	3PE	4	601	-	44,44,50	0.92	4 (9%)	47,49,55	1.11	2 (4%)
29	CDL	S	201	-	78,78,99	0.99	8 (10%)	84,90,111	1.15	4 (4%)
27	3PE	g	102	-	43,43,50	0.93	4 (9%)	46,48,55	1.10	2 (4%)
28	PC1	1	402	-	41,41,53	1.09	4 (9%)	47,49,61	1.09	2 (4%)
27	3PE	5	707	-	32,32,50	1.07	4 (12%)	35,37,55	1.18	2 (5%)
27	3PE	5	704	-	34,34,50	1.05	4 (11%)	37,39,55	1.21	2 (5%)
28	PC1	X	203	-	38,38,53	1.12	4 (10%)	44,46,61	1.09	2 (4%)
27	3PE	W	202	-	38,38,50	0.99	4 (10%)	41,43,55	1.11	3 (7%)
27	3PE	g	101	-	35,35,50	1.02	4 (11%)	38,40,55	1.18	2 (5%)
28	PC1	5	706	-	42,42,53	1.09	5 (11%)	48,50,61	1.16	2 (4%)
28	PC1	4	603	-	49,49,53	1.00	4 (8%)	55,57,61	1.16	3 (5%)
29	CDL	X	202	-	78,78,99	0.98	7 (8%)	84,90,111	1.19	5 (5%)
27	3PE	J	201	-	29,29,50	1.13	4 (13%)	32,34,55	1.17	2 (6%)
29	CDL	2	601	-	73,73,99	0.34	0	79,85,111	0.51	0
27	3PE	5	703	-	32,32,50	1.07	4 (12%)	35,37,55	1.13	2 (5%)
27	3PE	n	201	-	50,50,50	0.88	4 (8%)	53,55,55	1.12	2 (3%)
27	3PE	6	301	-	35,35,50	1.05	4 (11%)	38,40,55	1.22	2 (5%)
28	PC1	3	201	-	42,42,53	1.07	4 (9%)	48,50,61	1.11	2 (4%)
28	PC1	5	701	-	53,53,53	1.00	5 (9%)	59,61,61	1.27	4 (6%)
27	3PE	4	604	-	33,33,50	1.06	4 (12%)	36,38,55	1.16	2 (5%)
30	LMN	2	602	-	60,60,72	1.74	11 (18%)	74,80,98	1.10	4 (5%)
27	3PE	5	705	-	42,42,50	0.95	4 (9%)	45,47,55	1.15	2 (4%)
27	3PE	5	702	-	34,34,50	1.04	4 (11%)	37,39,55	1.14	2 (5%)
27	3PE	W	201	-	37,37,50	1.00	4 (10%)	40,42,55	1.13	2 (5%)
30	LMN	4	602	-	48,48,72	1.87	13 (27%)	56,62,98	1.06	2 (3%)
31	ZMP	Q	201	12	30,35,36	0.24	0	34,42,45	0.44	0
29	CDL	D	101	-	64,64,99	1.09	8 (12%)	70,76,111	1.16	4 (5%)
29	CDL	X	201	-	69,69,99	1.04	7 (10%)	75,81,111	1.18	5 (6%)
28	PC1	S	202	-	51,51,53	0.97	4 (7%)	57,59,61	1.09	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	3PE	1	401	-	44,44,50	0.93	4 (9%)	47,49,55	1.21	4 (8%)
30	LMN	j	101	-	72,72,72	1.65	14 (19%)	92,98,98	1.08	6 (6%)
27	3PE	i	101	-	40,40,50	0.97	4 (10%)	43,45,55	1.16	2 (4%)

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
28	PC1	X	204	-	-	14/35/35/57	-
27	3PE	n	202	-	-	22/42/42/54	-
27	3PE	4	601	-	-	14/48/48/54	-
29	CDL	S	201	-	-	34/89/89/110	-
27	3PE	g	102	-	-	18/47/47/54	-
28	PC1	1	402	-	-	22/45/45/57	-
27	3PE	5	707	-	-	10/36/36/54	-
27	3PE	5	704	-	-	11/38/38/54	-
28	PC1	X	203	-	-	18/42/42/57	-
27	3PE	W	202	-	-	14/42/42/54	-
27	3PE	g	101	-	-	14/39/39/54	-
28	PC1	5	706	-	-	22/46/46/57	-
28	PC1	4	603	-	-	26/53/53/57	-
29	CDL	X	202	-	-	43/89/89/110	-
27	3PE	J	201	-	-	15/33/33/54	-
29	CDL	2	601	-	-	24/84/84/110	-
27	3PE	5	703	-	-	17/36/36/54	-
27	3PE	n	201	-	-	19/54/54/54	-
27	3PE	6	301	-	-	20/39/39/54	-
28	PC1	3	201	-	-	13/46/46/57	-
28	PC1	5	701	-	-	27/57/57/57	-
27	3PE	4	604	-	-	12/37/37/54	-
30	LMN	2	602	-	-	25/44/104/130	0/3/3/4
27	3PE	5	705	-	-	15/46/46/54	-
27	3PE	5	702	-	-	15/38/38/54	-
27	3PE	W	201	-	-	14/41/41/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMN	4	602	-	-	24/38/78/130	0/2/2/4
31	ZMP	Q	201	12	-	10/40/42/43	-
29	CDL	D	101	-	-	27/75/75/110	-
29	CDL	X	201	-	-	25/80/80/110	-
28	PC1	S	202	-	-	17/55/55/57	-
27	3PE	1	401	-	-	18/48/48/54	-
30	LMN	j	101	-	-	23/50/130/130	0/4/4/4
27	3PE	i	101	-	-	18/44/44/54	-

The worst 5 of 170 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	j	101	LMN	O5-C1	4.66	1.53	1.41
30	4	602	LMN	O5-C1	4.65	1.53	1.41
30	2	602	LMN	O5-C1	4.62	1.53	1.41
30	j	101	LMN	CBS-CCM	4.36	1.63	1.53
30	4	602	LMN	CBS-CCM	4.31	1.63	1.53

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	4	603	PC1	O21-C21-C22	4.94	122.17	111.48
28	5	701	PC1	O21-C21-C22	4.92	122.12	111.48
28	5	706	PC1	O21-C21-C22	4.63	121.50	111.48
27	1	401	3PE	O21-C21-C22	4.54	121.30	111.48
27	5	704	3PE	O21-C21-C22	4.38	120.96	111.48

There are no chirality outliers.

5 of 660 torsion outliers are listed below:

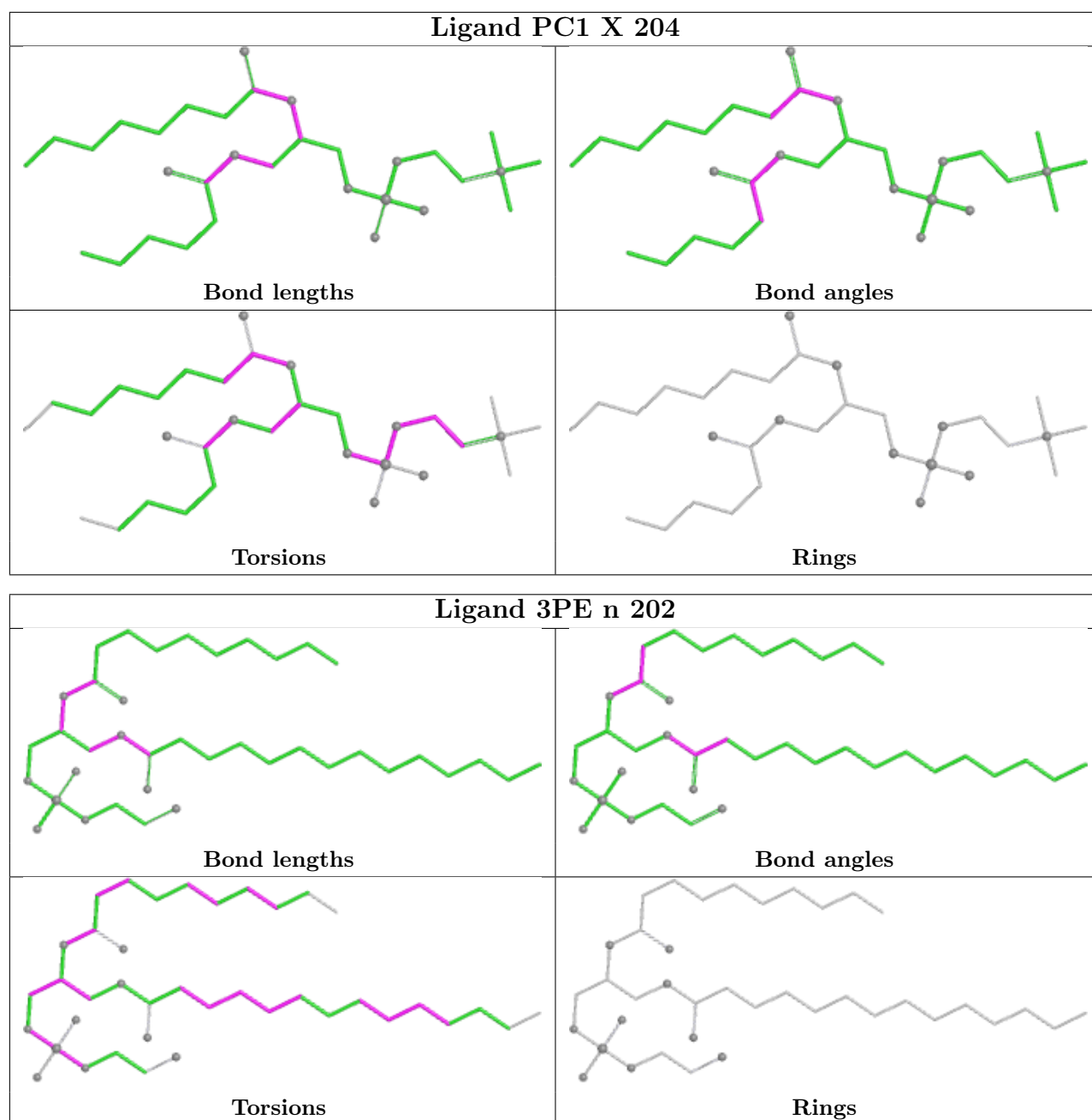
Mol	Chain	Res	Type	Atoms
27	1	401	3PE	C1-O11-P-O12
27	1	401	3PE	C1-O11-P-O13
27	1	401	3PE	C1-O11-P-O14
27	4	604	3PE	C11-O13-P-O11
27	4	604	3PE	O22-C21-O21-C2

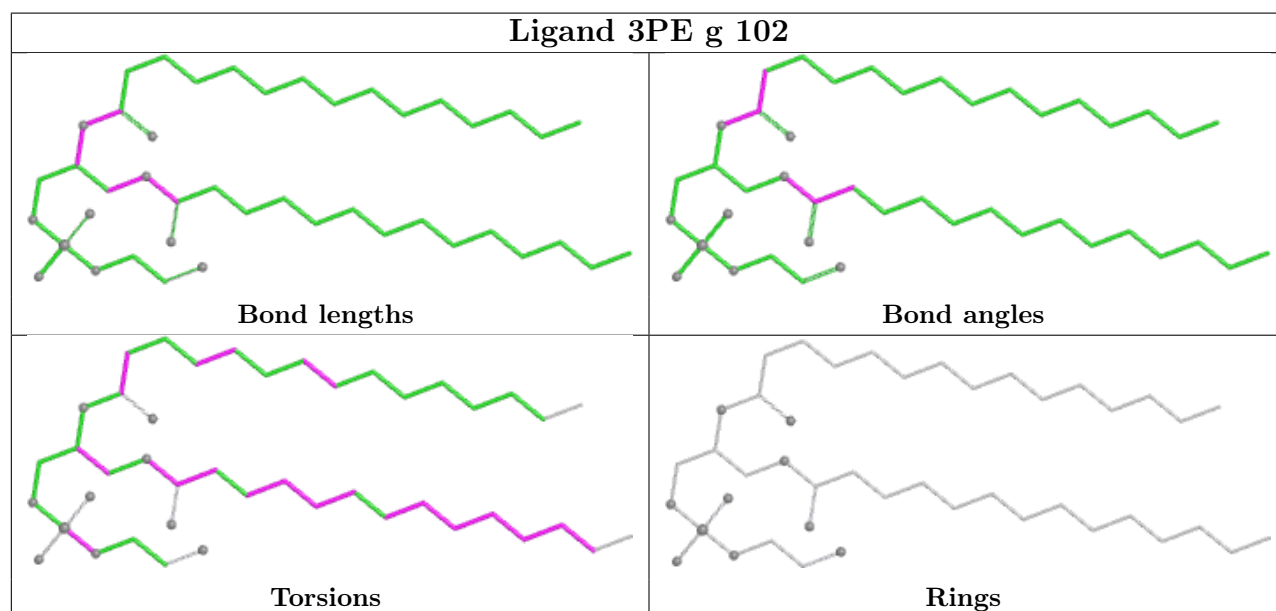
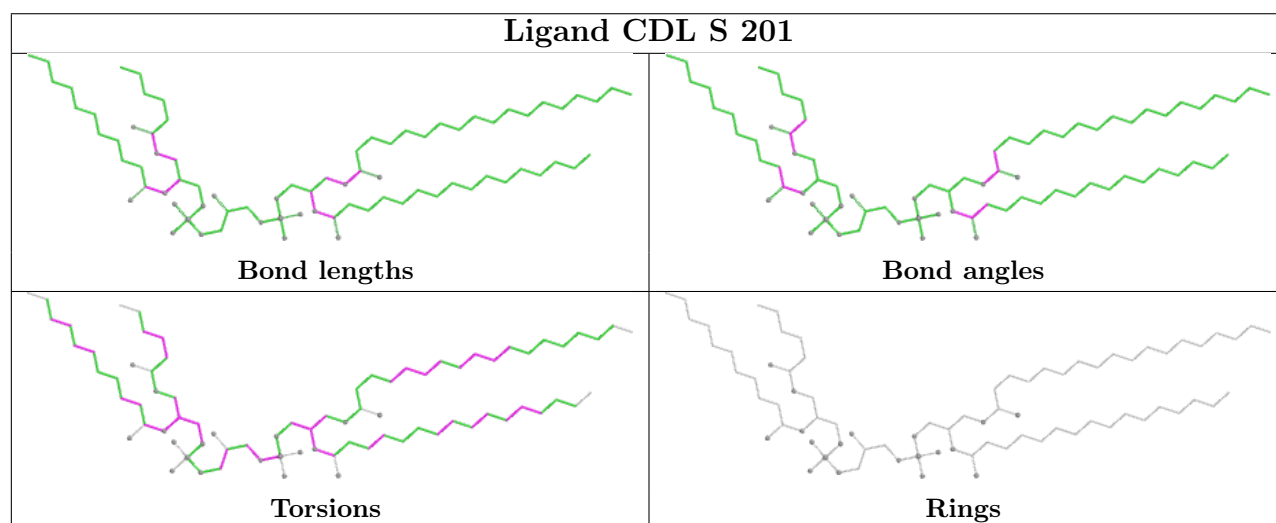
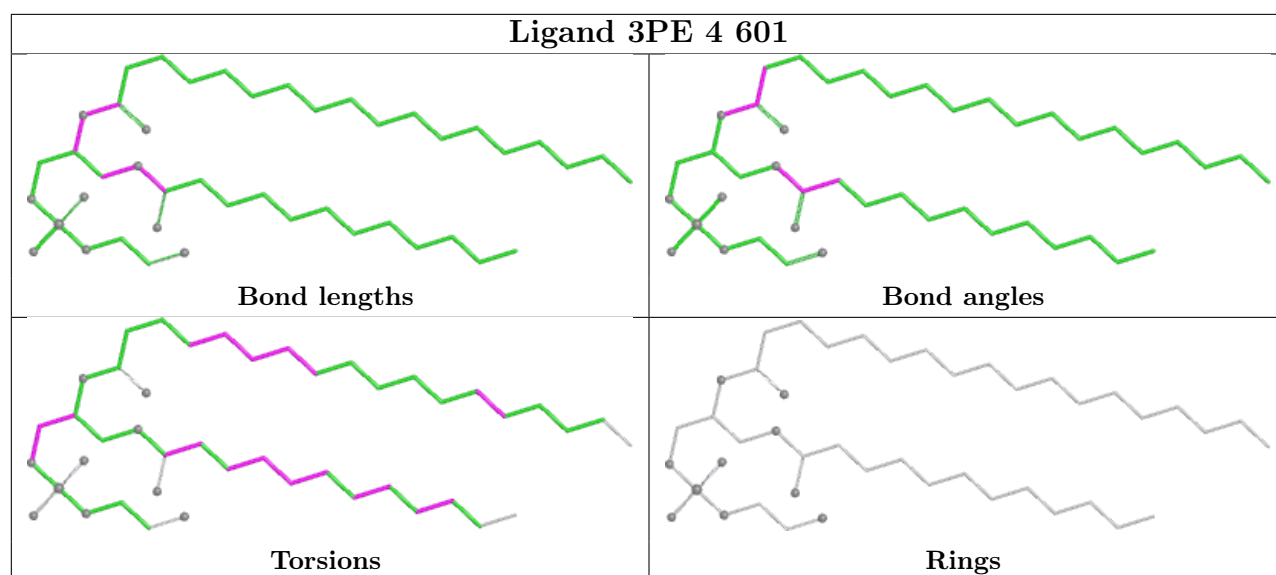
There are no ring outliers.

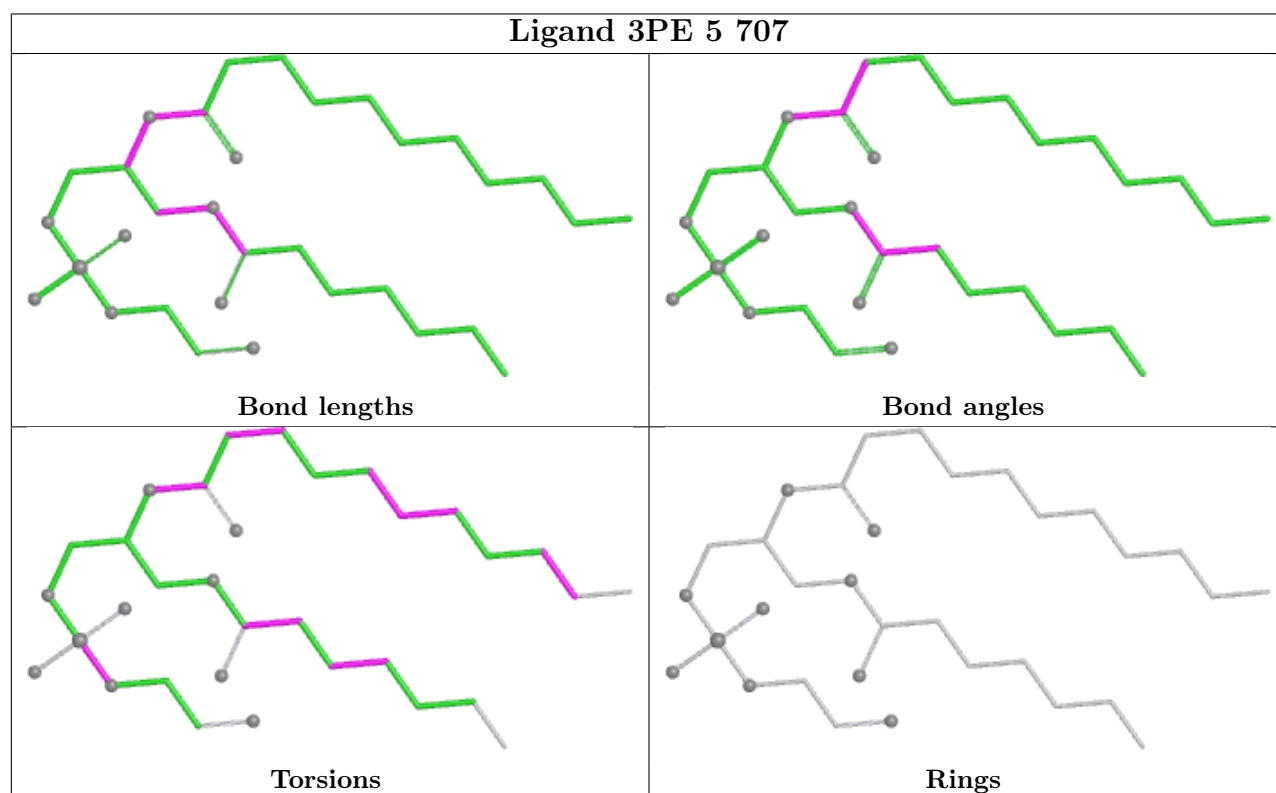
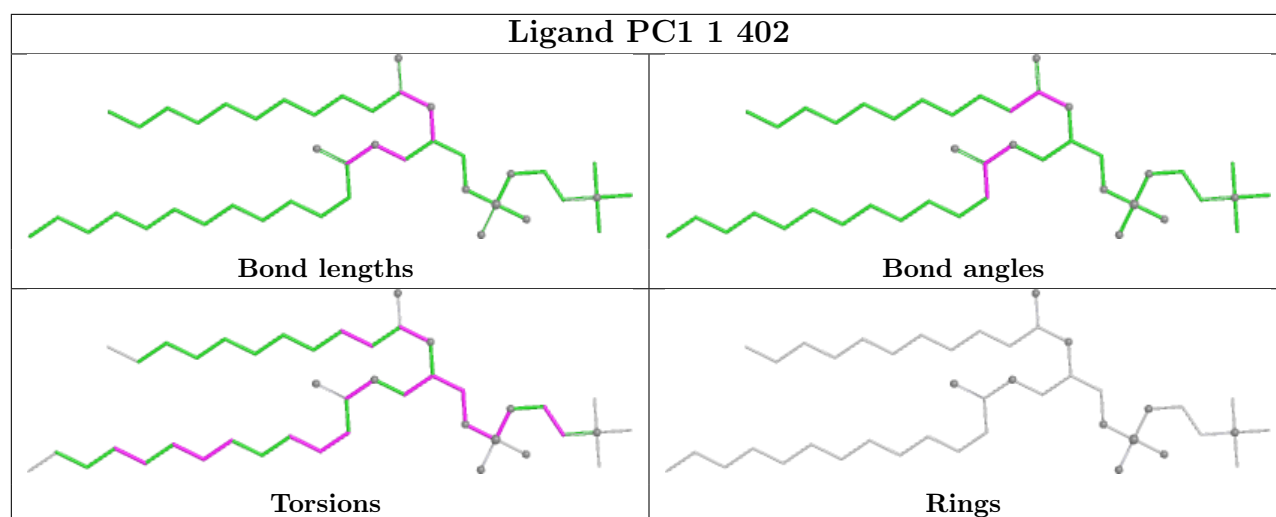
29 monomers are involved in 89 short contacts:

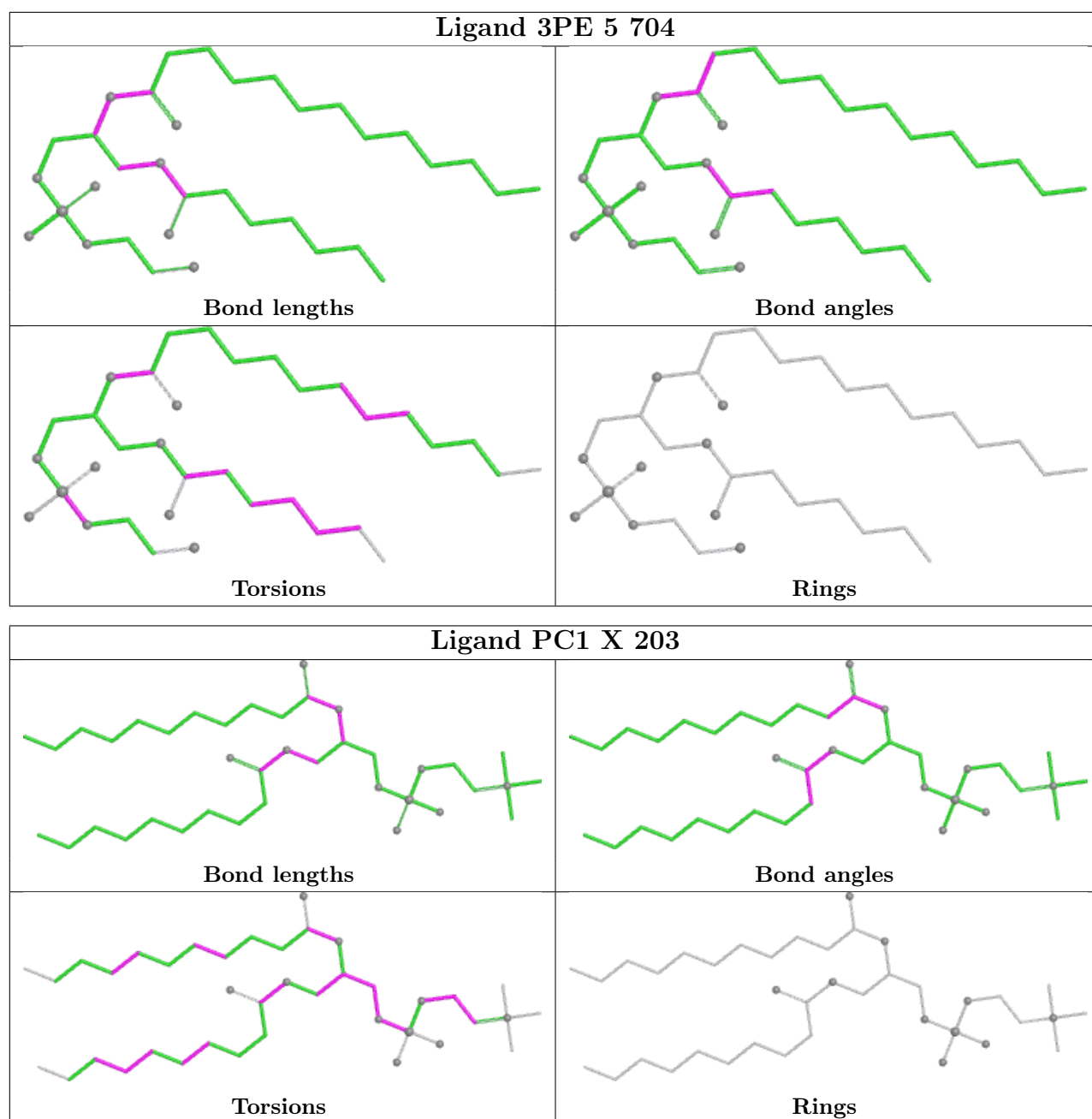
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	X	204	PC1	2	0
27	4	601	3PE	4	0
29	S	201	CDL	3	0
28	1	402	PC1	3	0
27	5	707	3PE	2	0
27	5	704	3PE	3	0
28	X	203	PC1	2	0
27	W	202	3PE	3	0
27	g	101	3PE	1	0
28	5	706	PC1	2	0
28	4	603	PC1	11	0
29	X	202	CDL	5	0
27	J	201	3PE	1	0
29	2	601	CDL	8	0
27	5	703	3PE	3	0
27	n	201	3PE	2	0
27	6	301	3PE	2	0
28	3	201	PC1	4	0
28	5	701	PC1	12	0
30	2	602	LMN	2	0
27	5	705	3PE	1	0
27	5	702	3PE	1	0
27	W	201	3PE	2	0
30	4	602	LMN	2	0
31	Q	201	ZMP	1	0
29	X	201	CDL	1	0
28	S	202	PC1	3	0
30	j	101	LMN	4	0
27	i	101	3PE	1	0

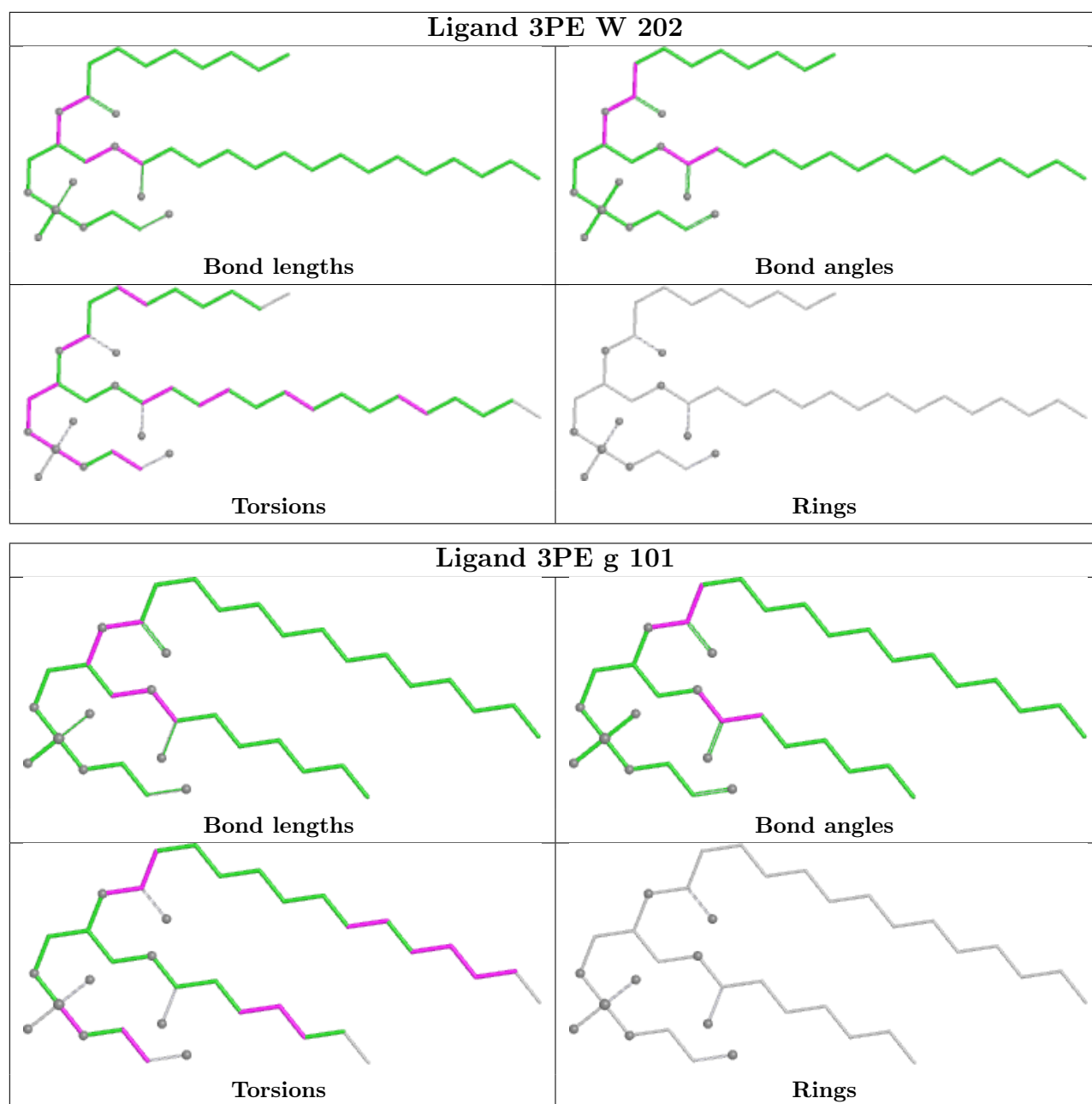
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

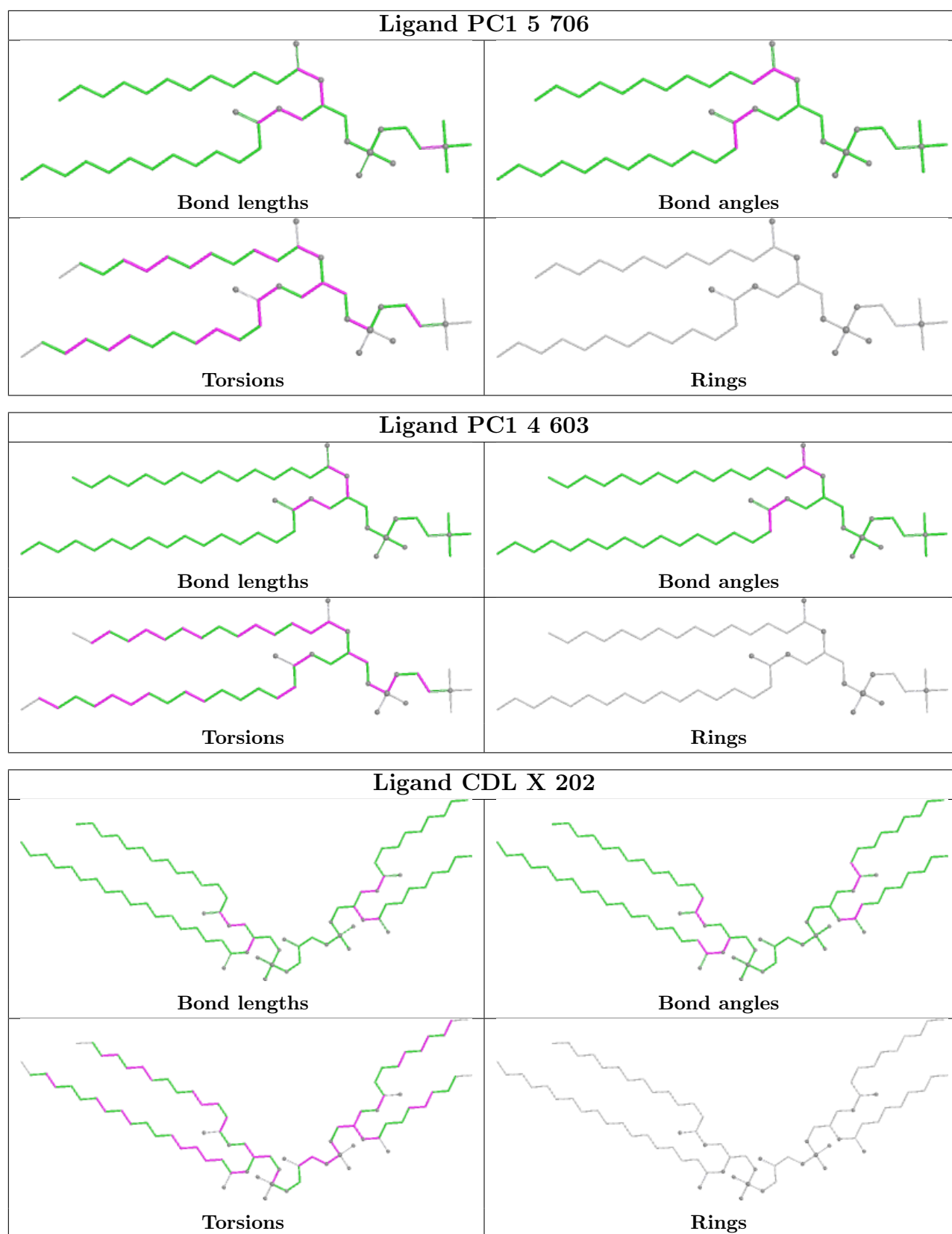


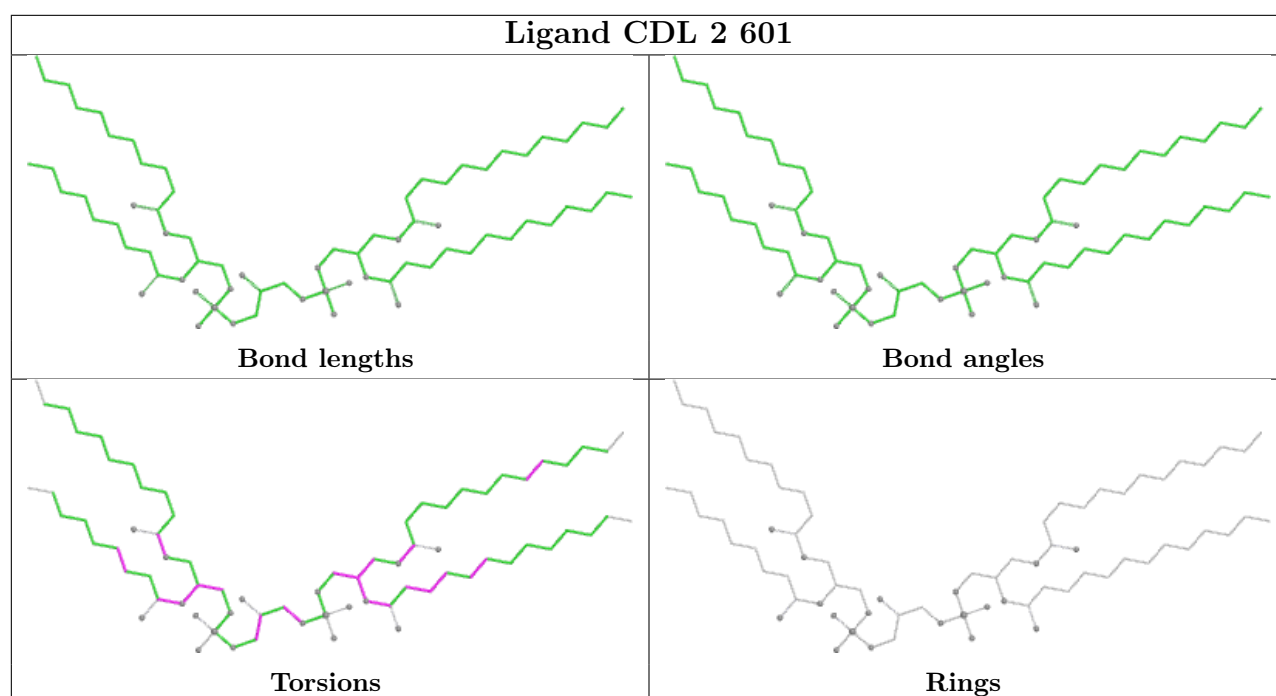
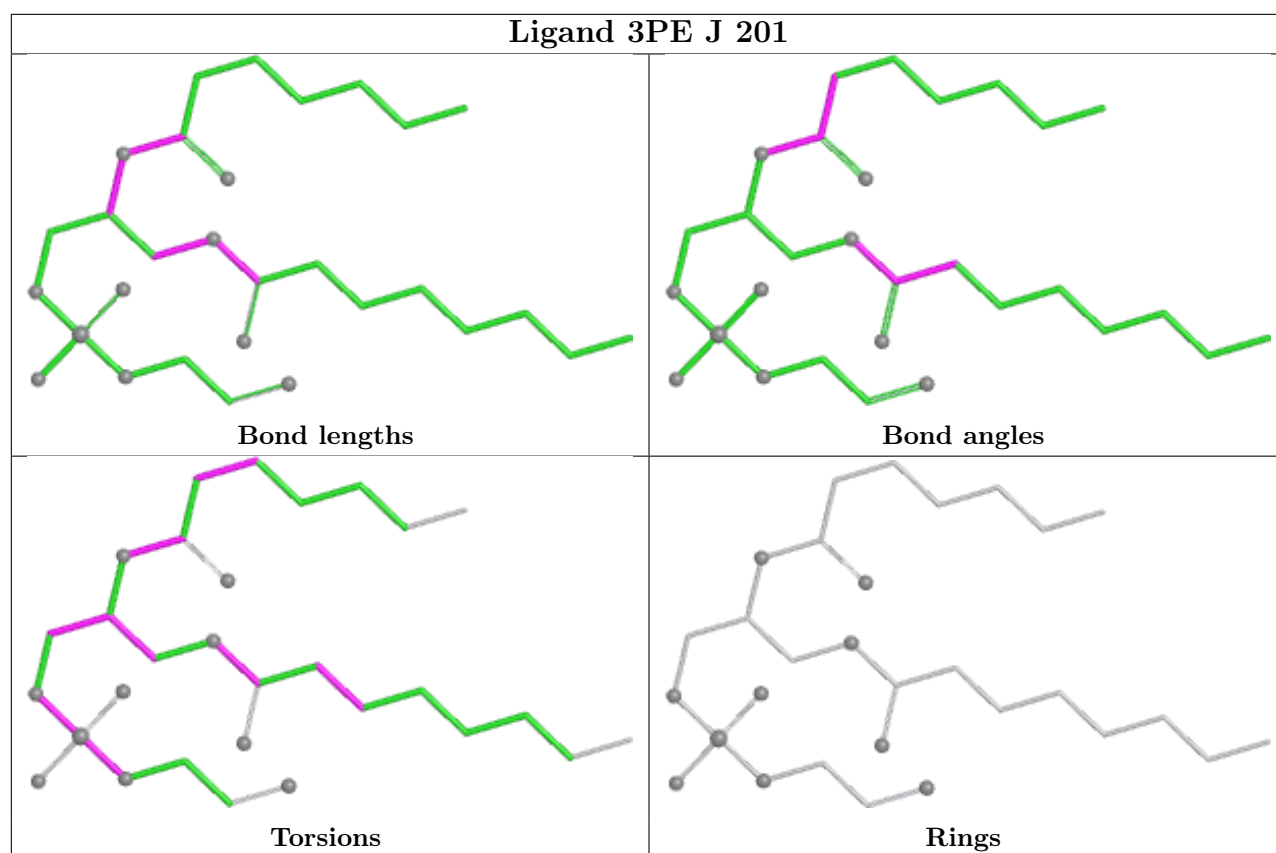


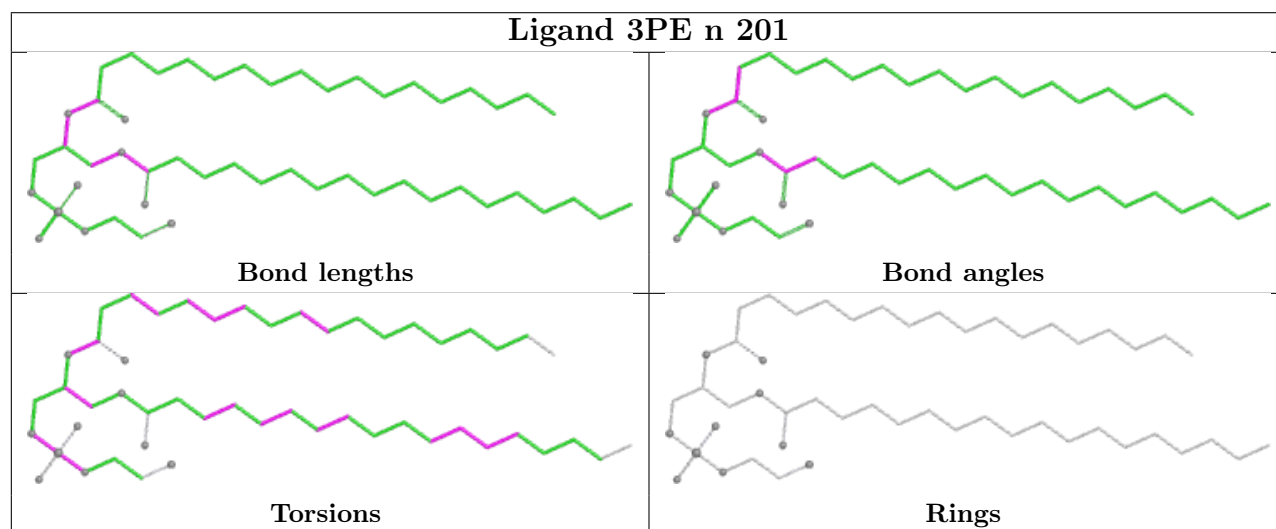
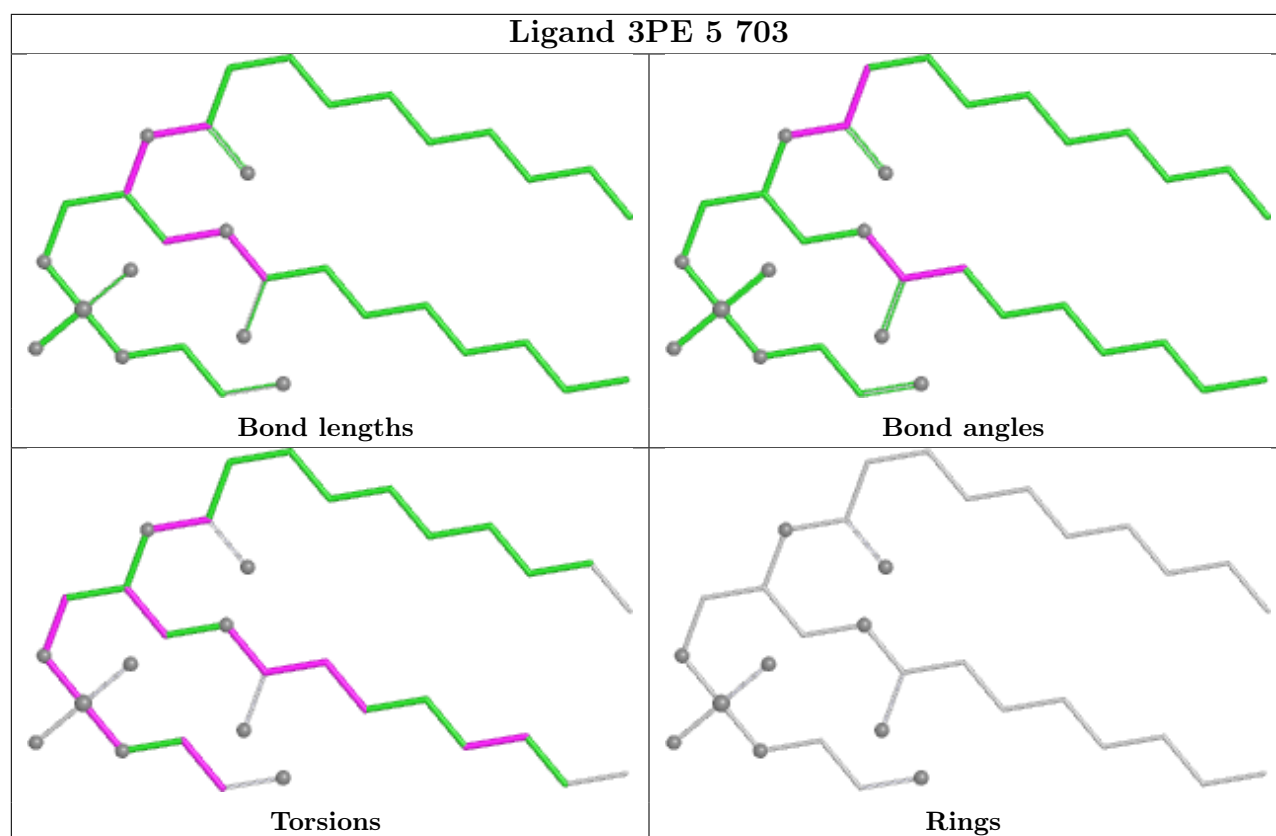


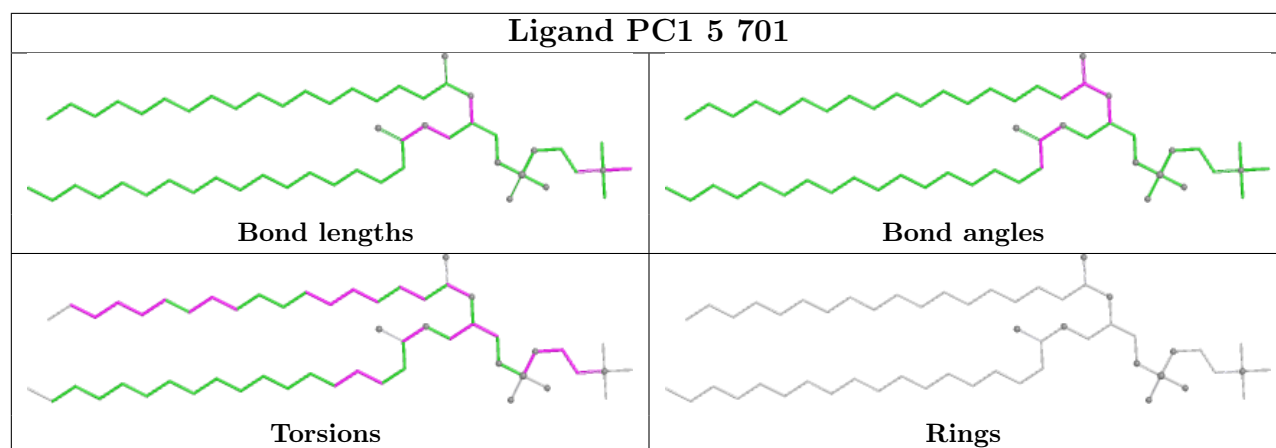
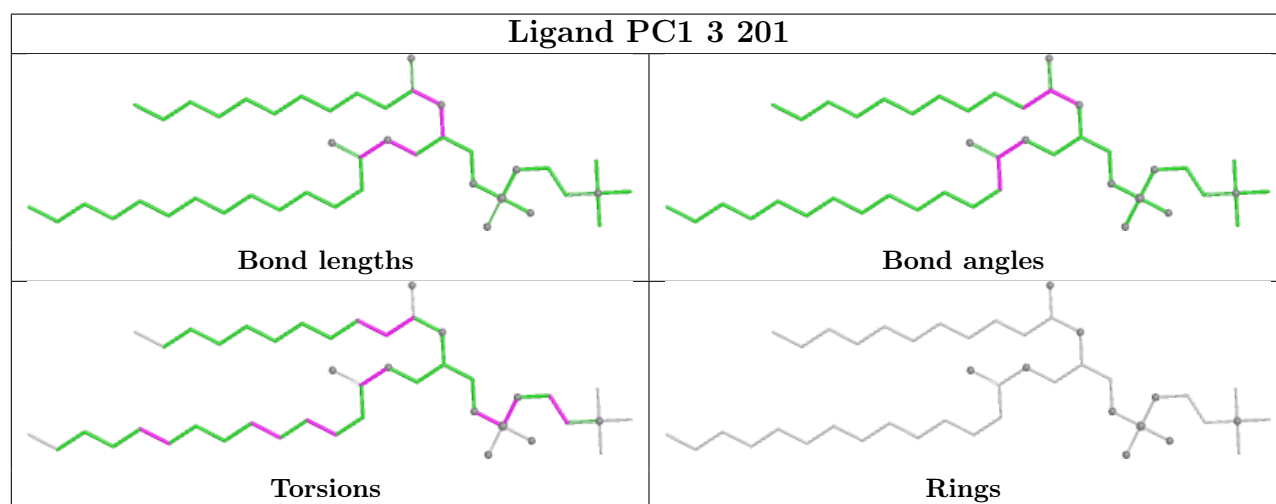
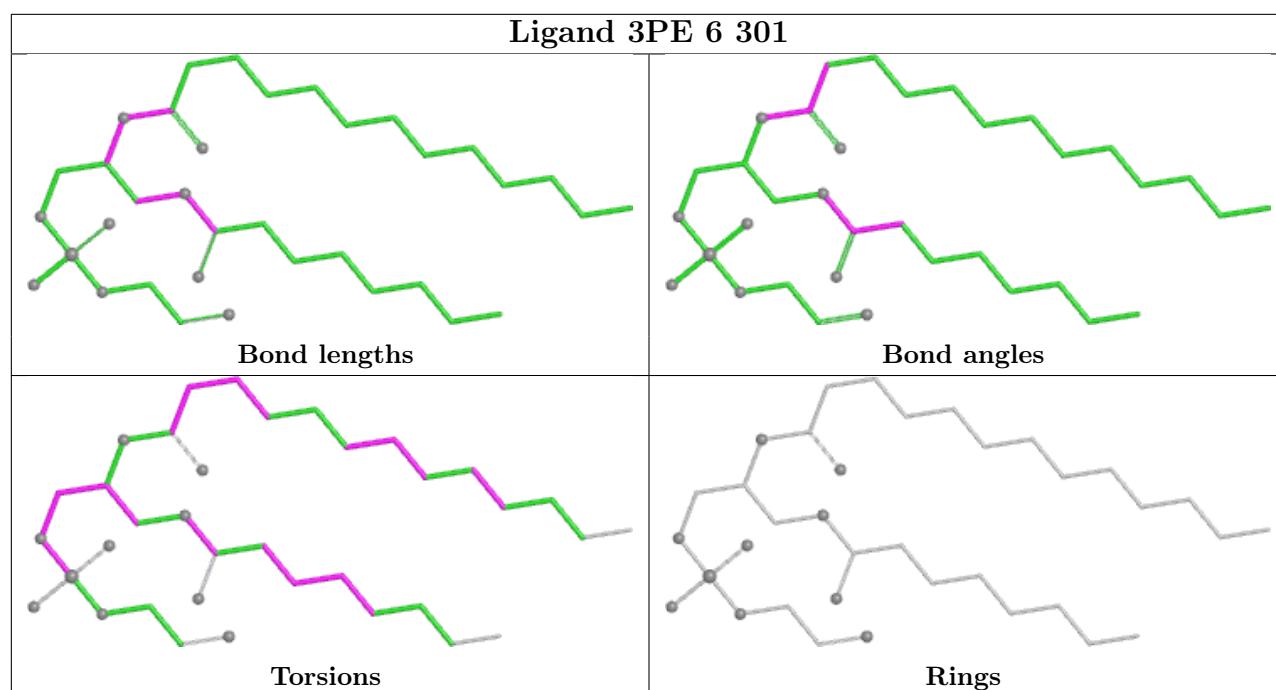


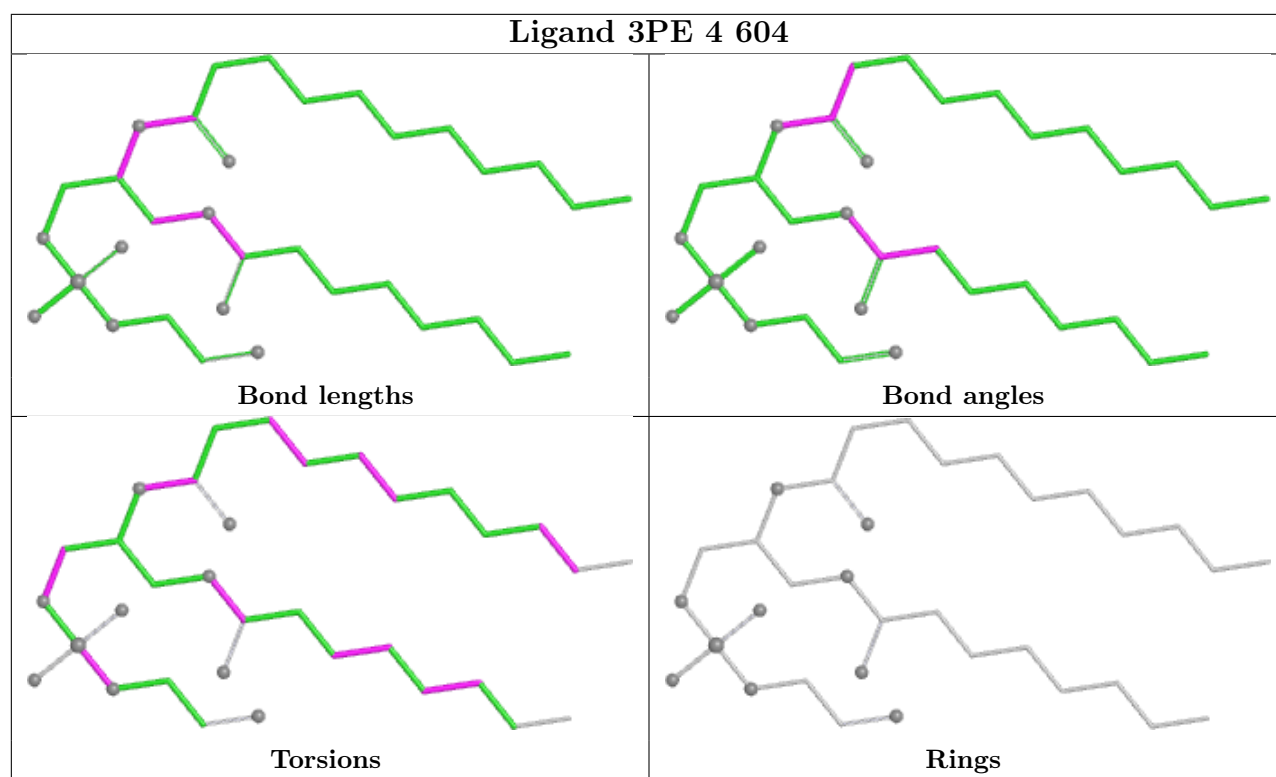


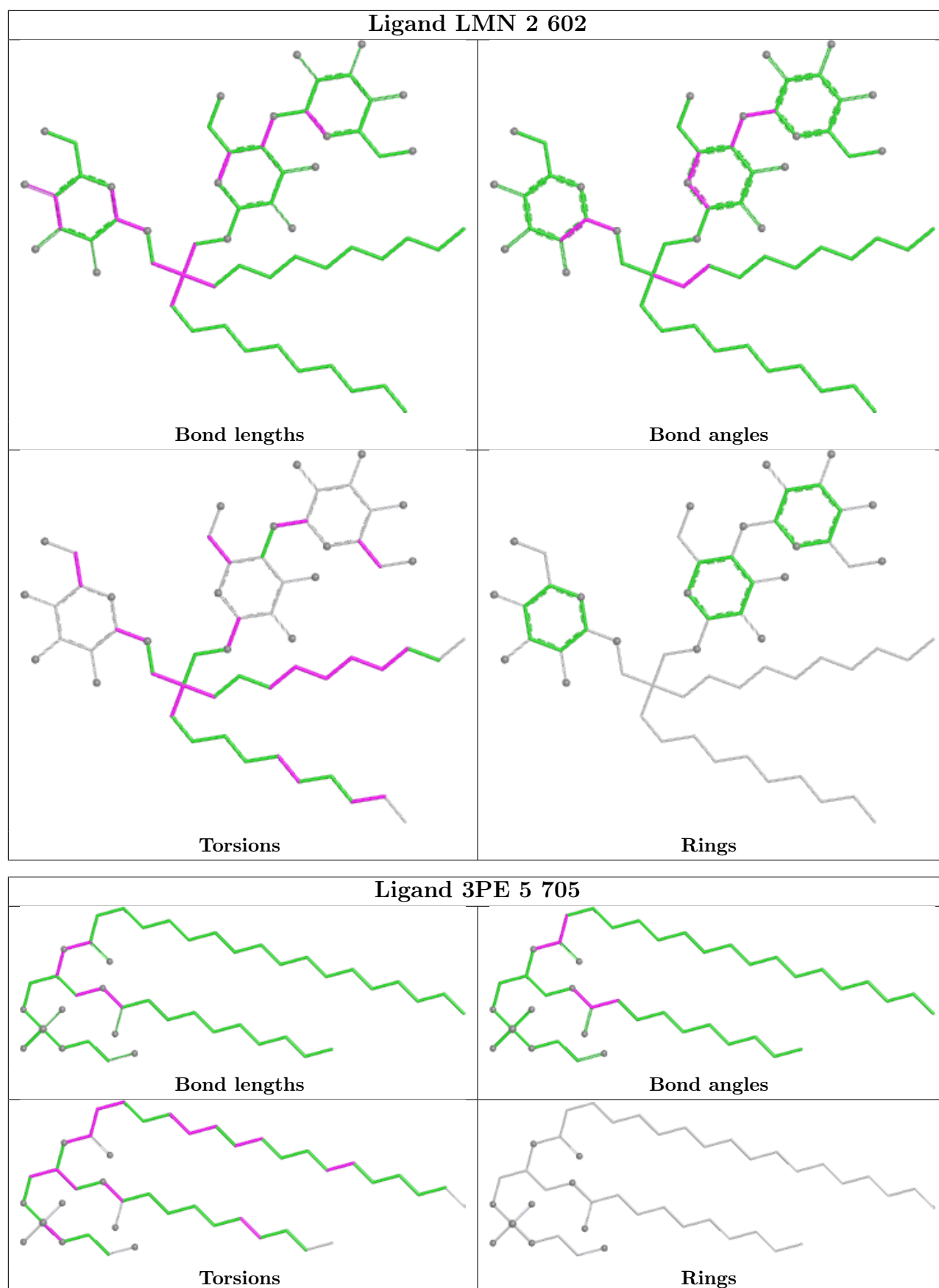


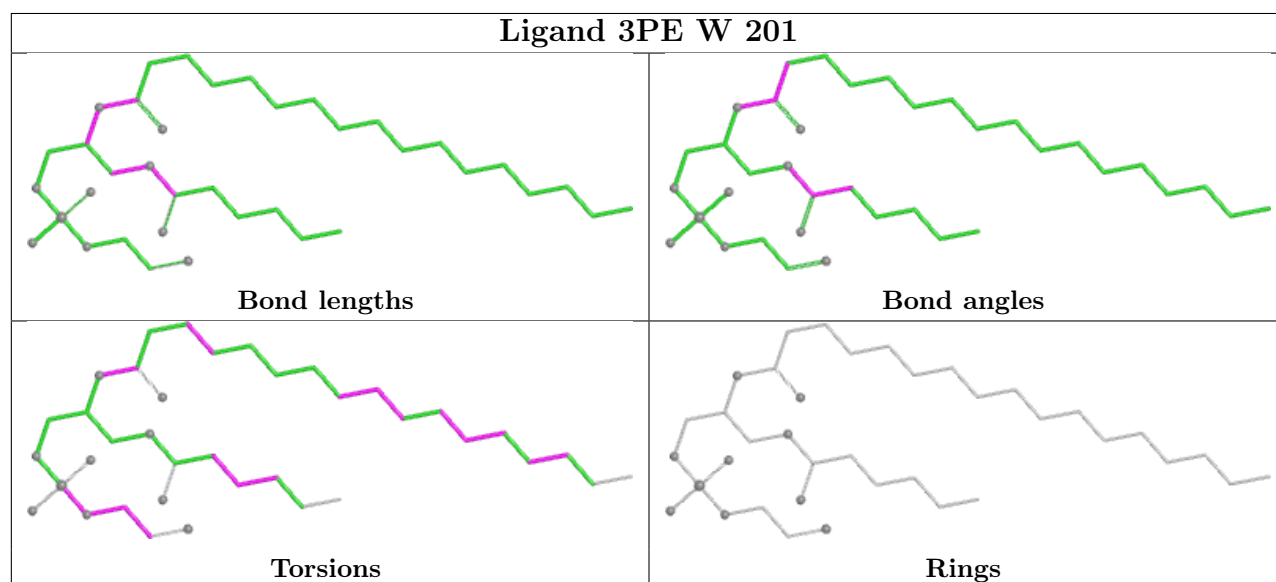
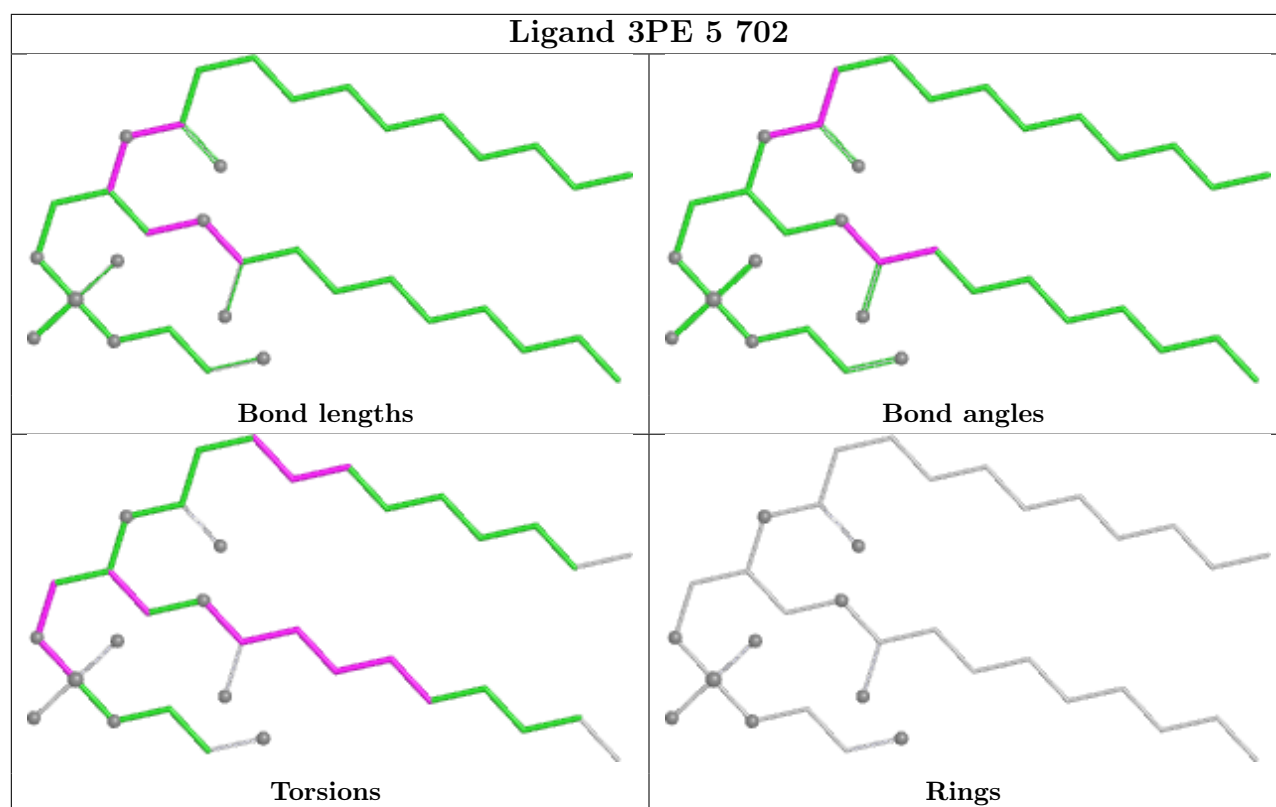


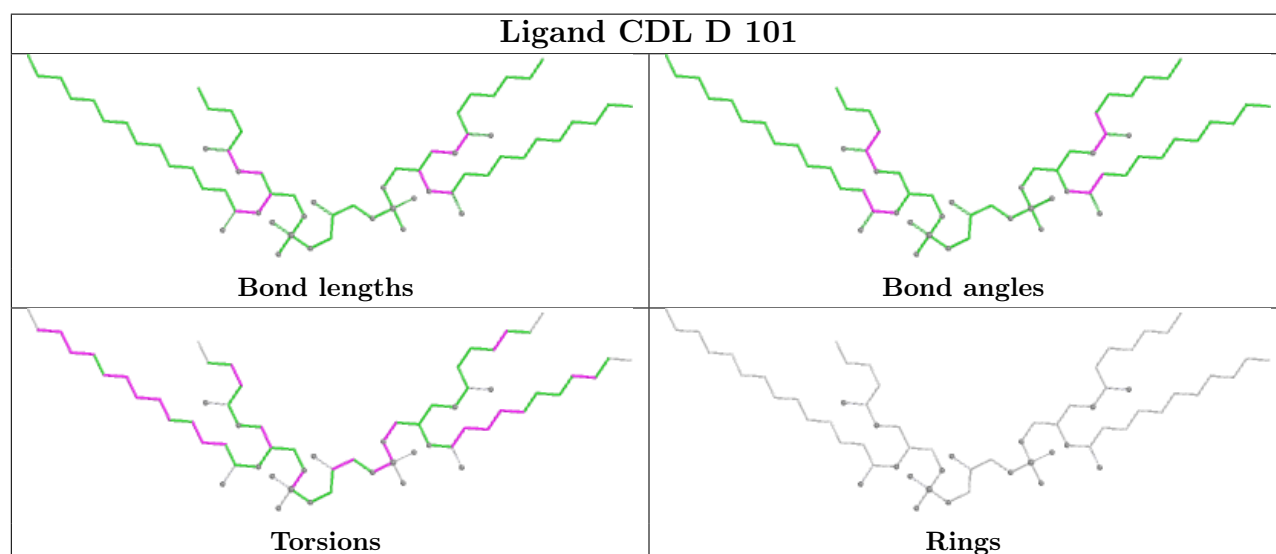
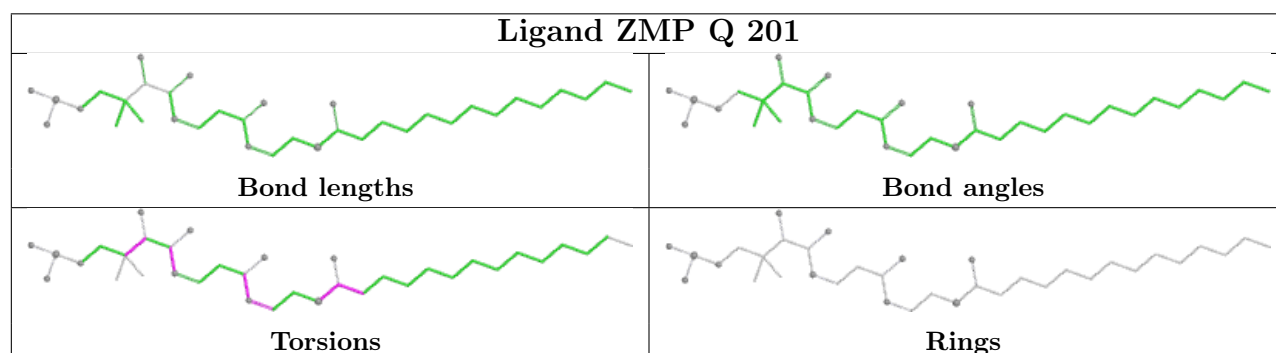
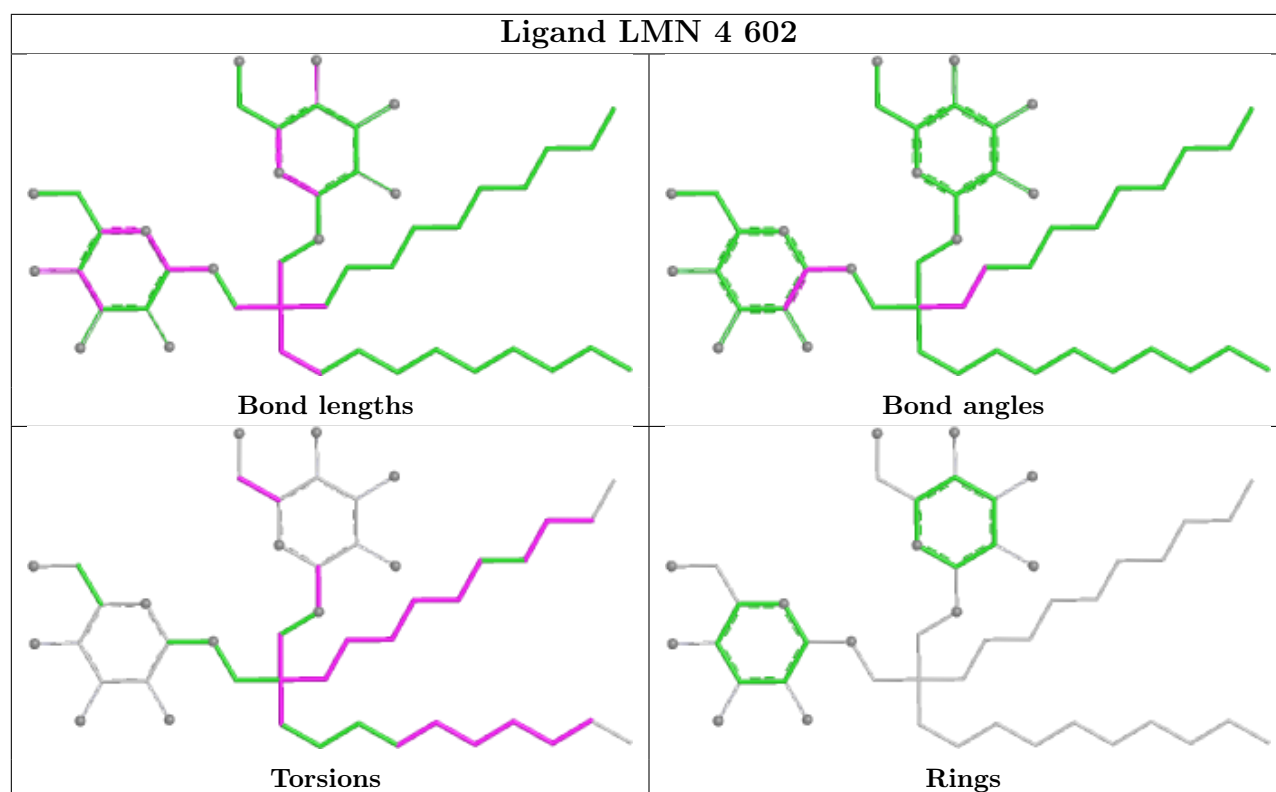


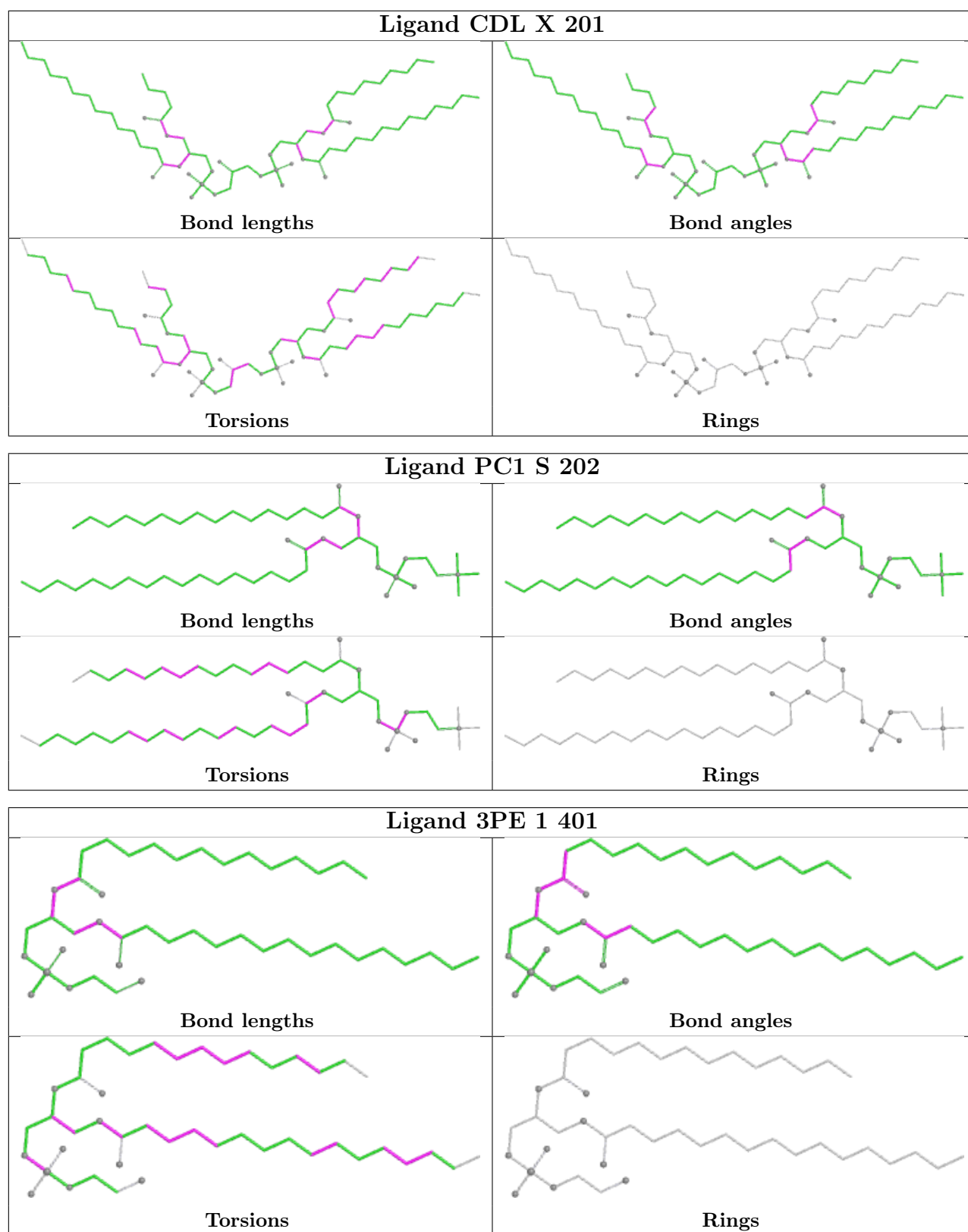


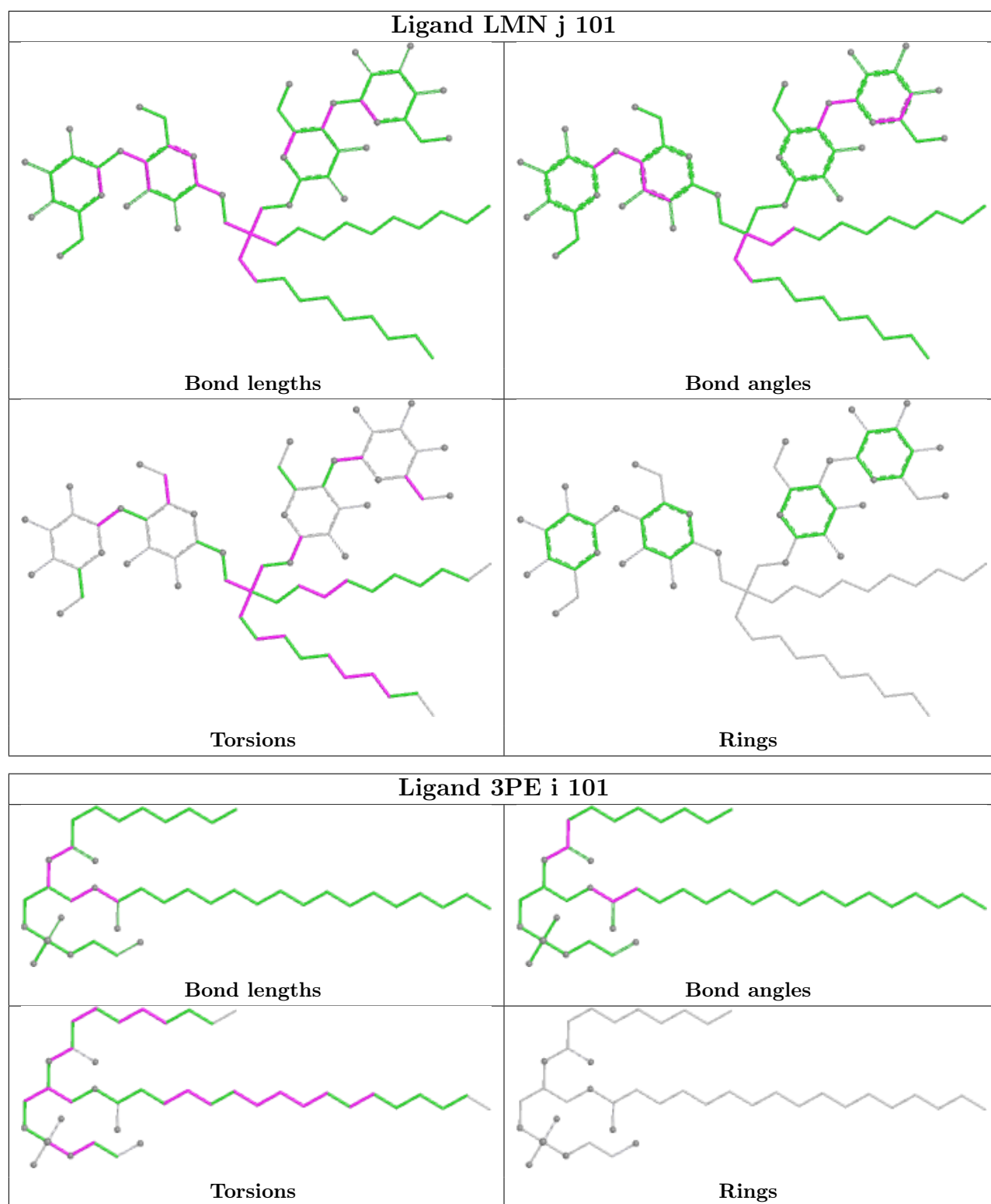












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

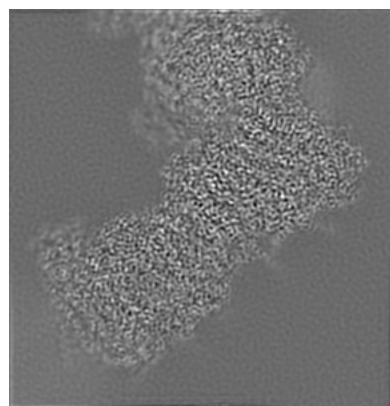
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14798. These allow visual inspection of the internal detail of the map and identification of artifacts.

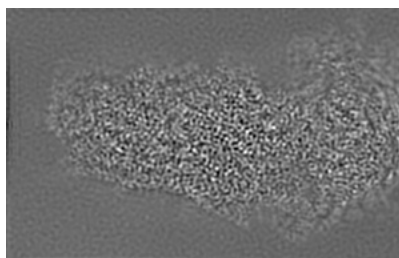
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

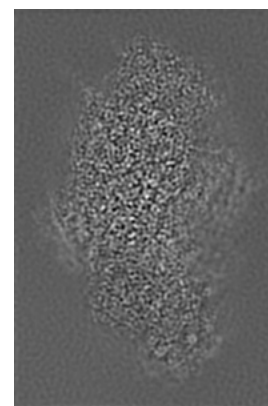
6.1.1 Primary map



X

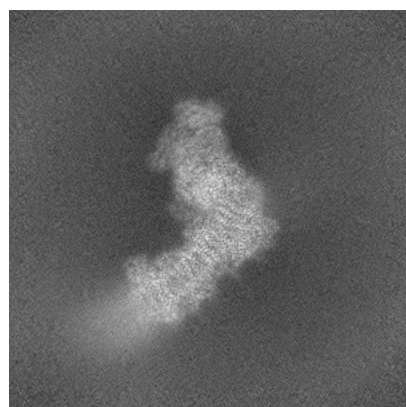


Y

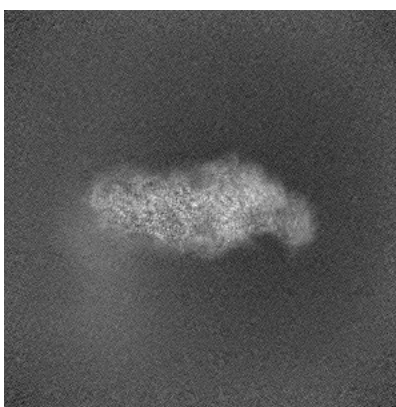


Z

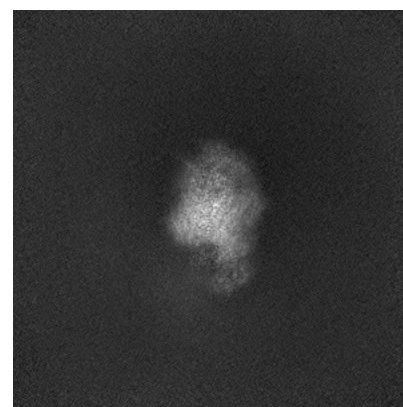
6.1.2 Raw map



X



Y

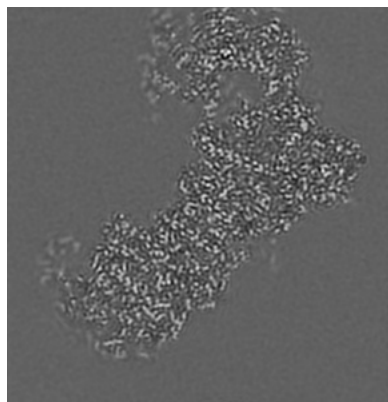


Z

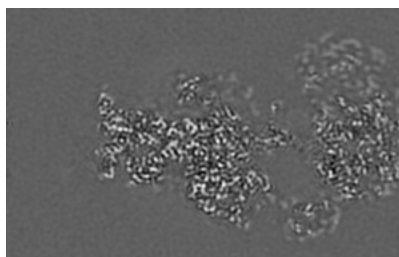
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

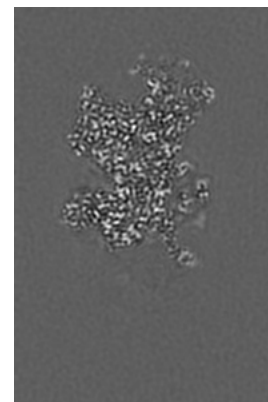
6.2.1 Primary map



X Index: 86

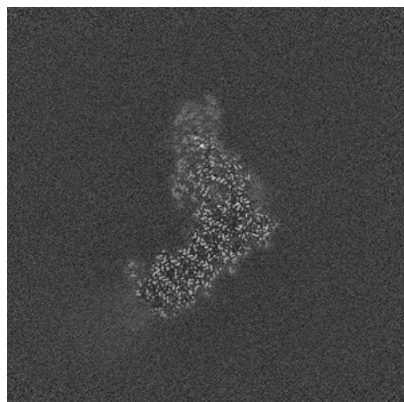


Y Index: 130

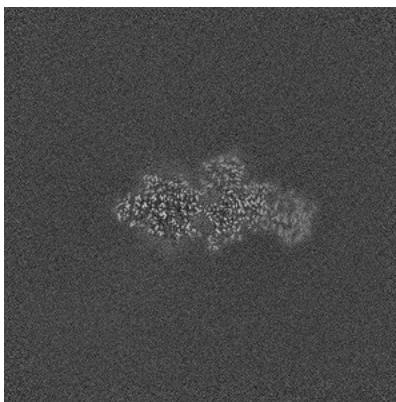


Z Index: 136

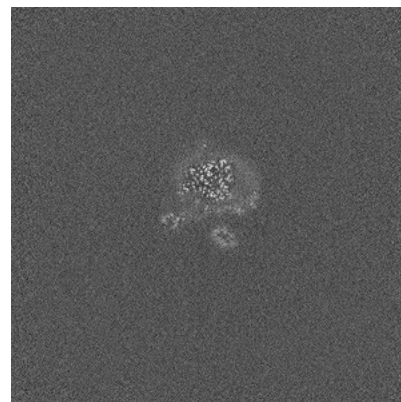
6.2.2 Raw map



X Index: 294



Y Index: 294

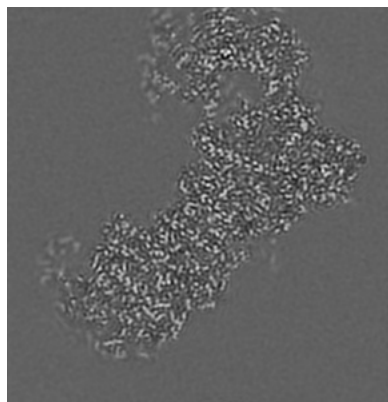


Z Index: 294

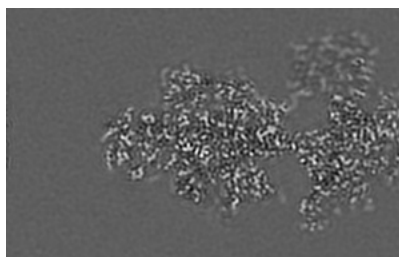
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

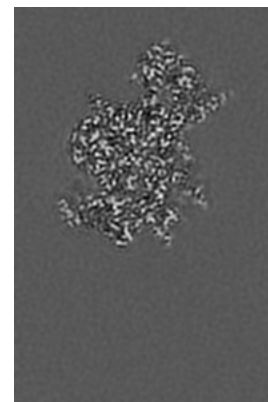
6.3.1 Primary map



X Index: 86

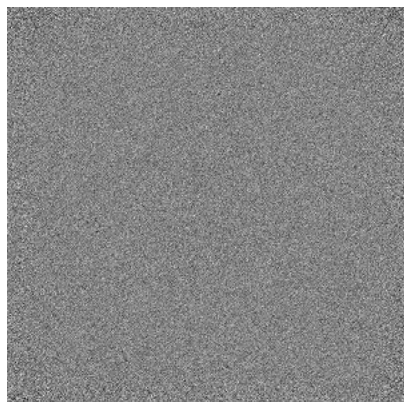


Y Index: 140

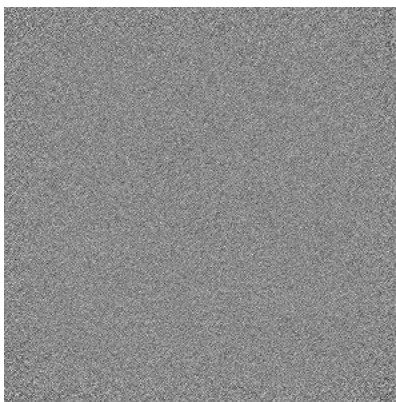


Z Index: 145

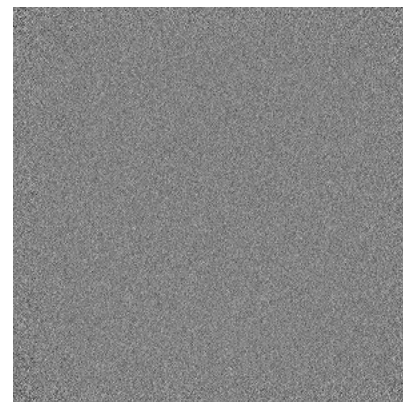
6.3.2 Raw map



X Index: 0



Y Index: 0

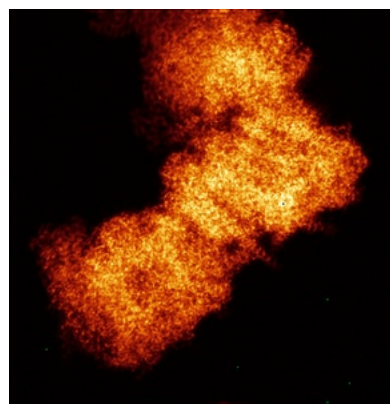


Z Index: 0

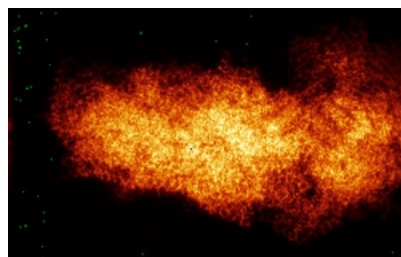
The images above show the largest variance slices of the map in three orthogonal directions.

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

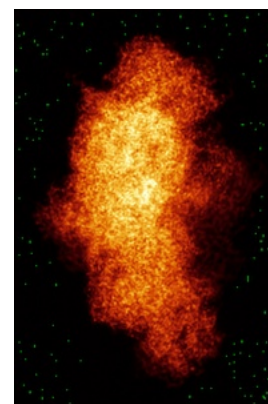
6.4.1 Primary map



X

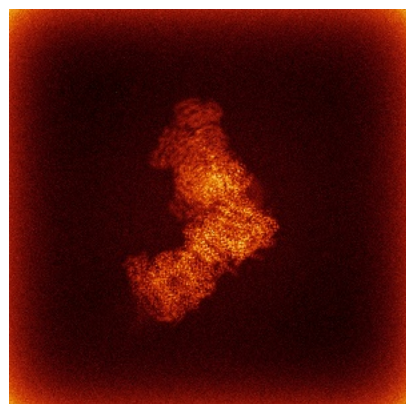


Y

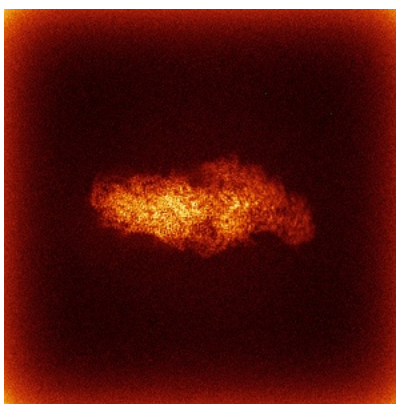


Z

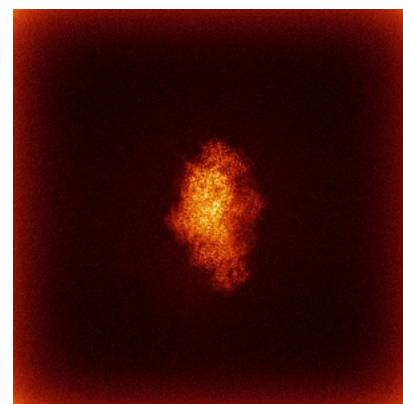
6.4.2 Raw map



X



Y

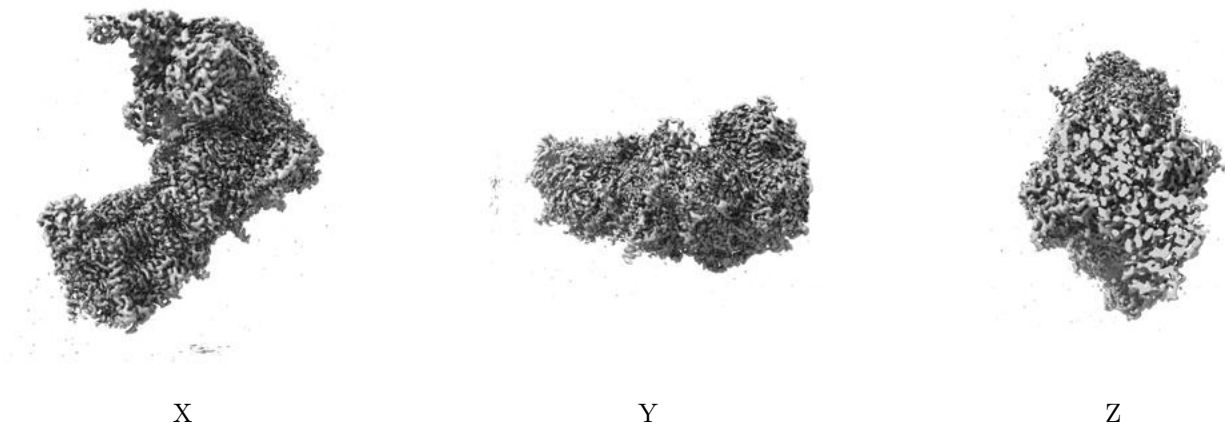


Z

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.

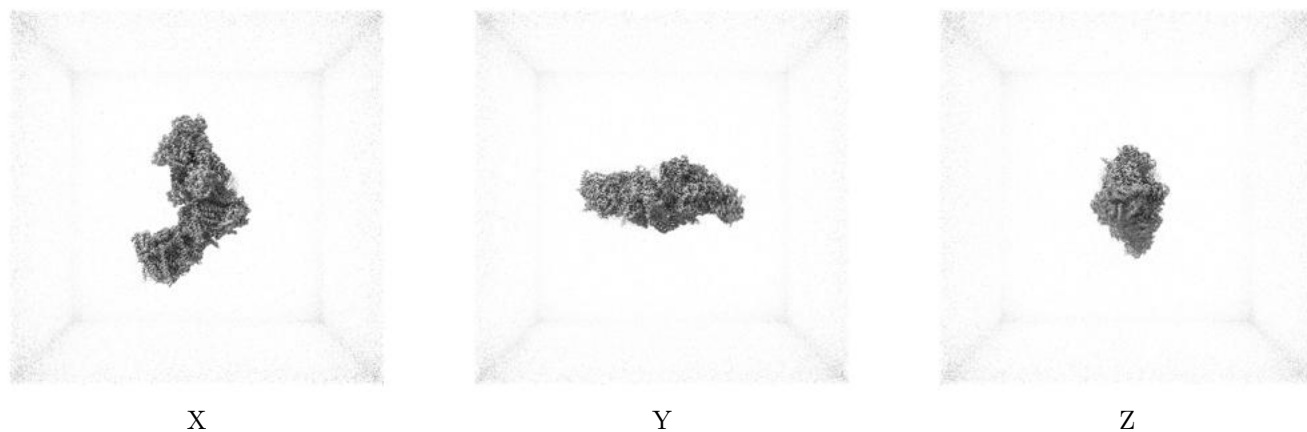
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

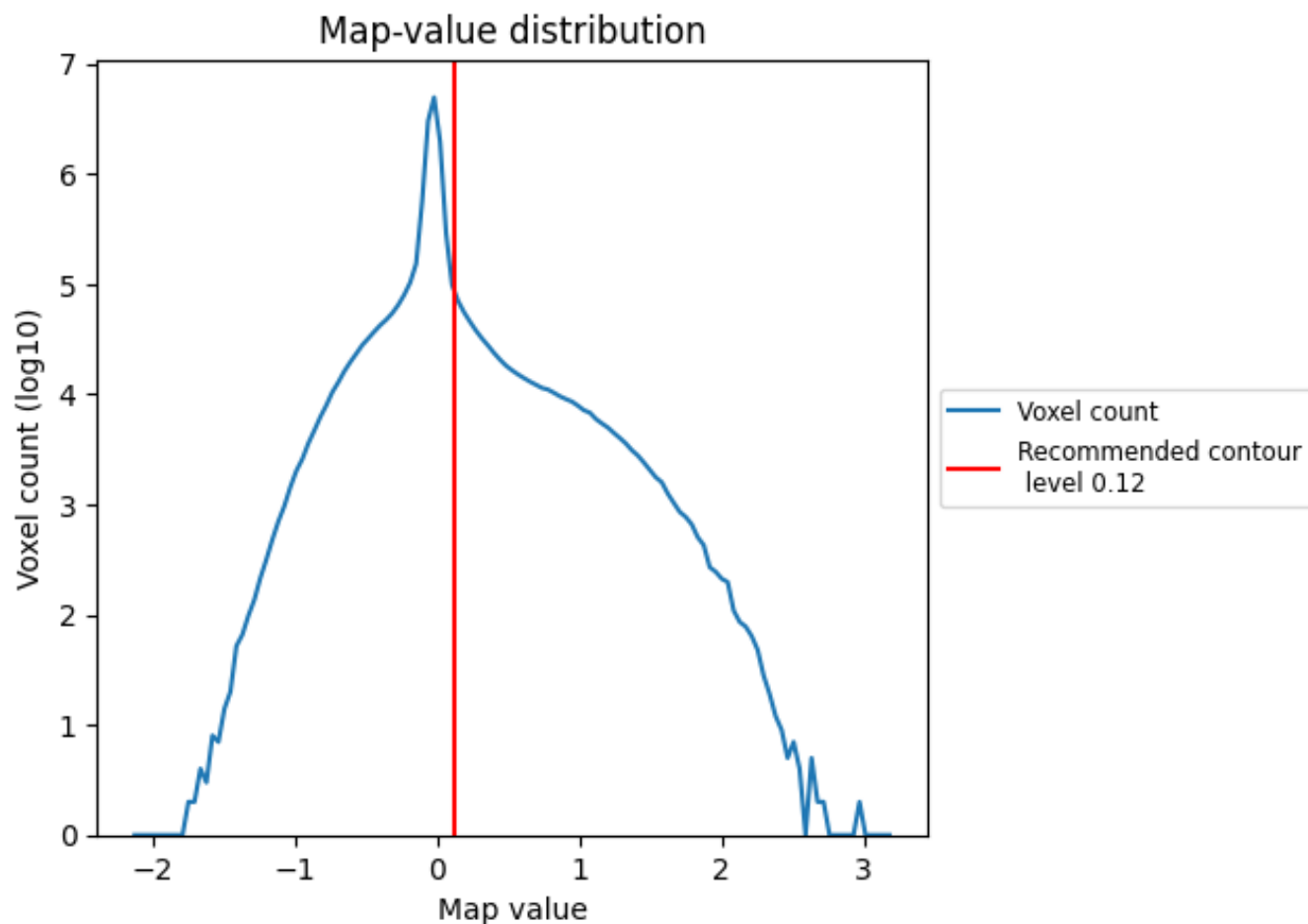
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

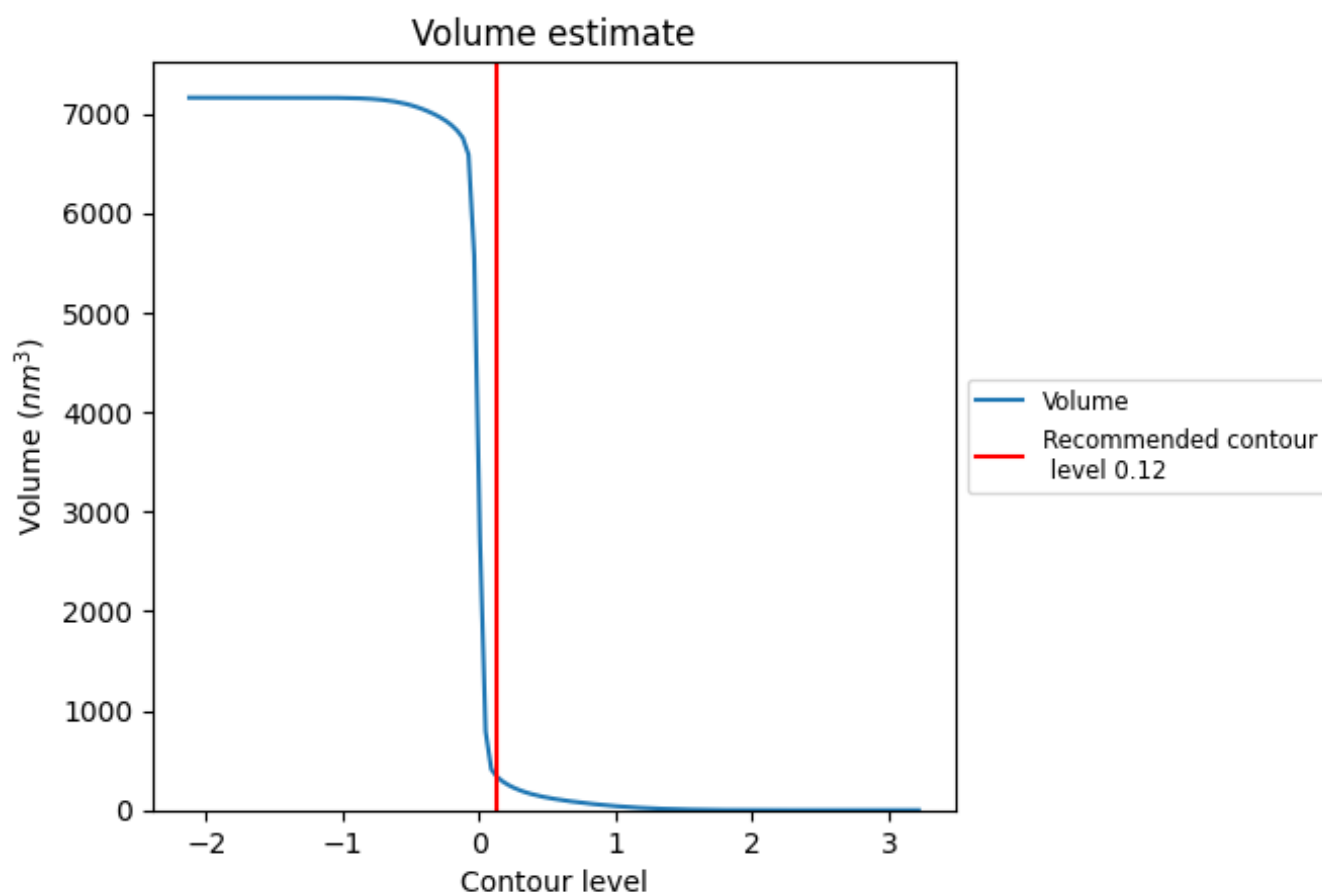
This section contains the results of statistical analysis of the map.

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 354 nm³; this corresponds to an approximate mass of 319 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.

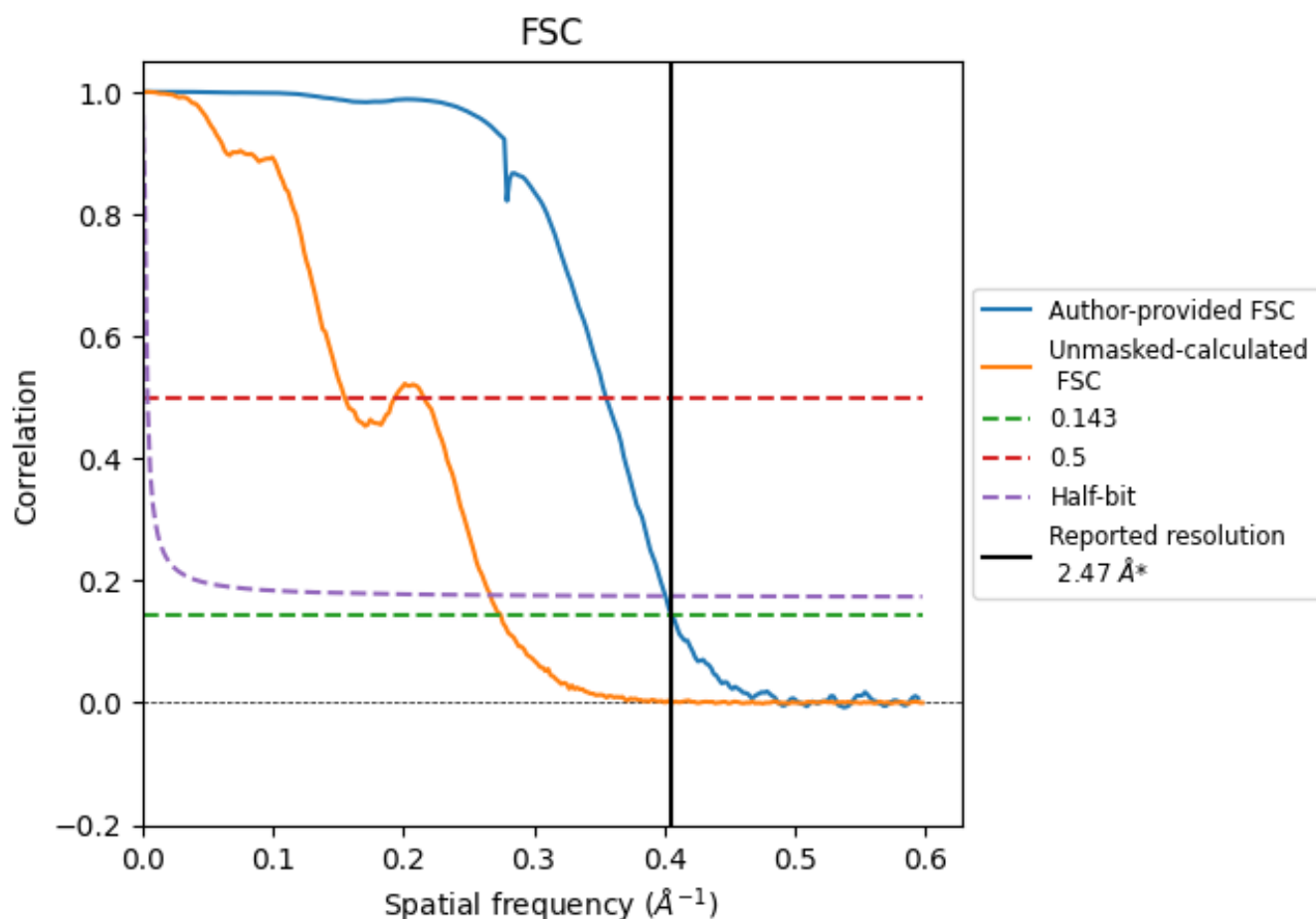
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.405 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

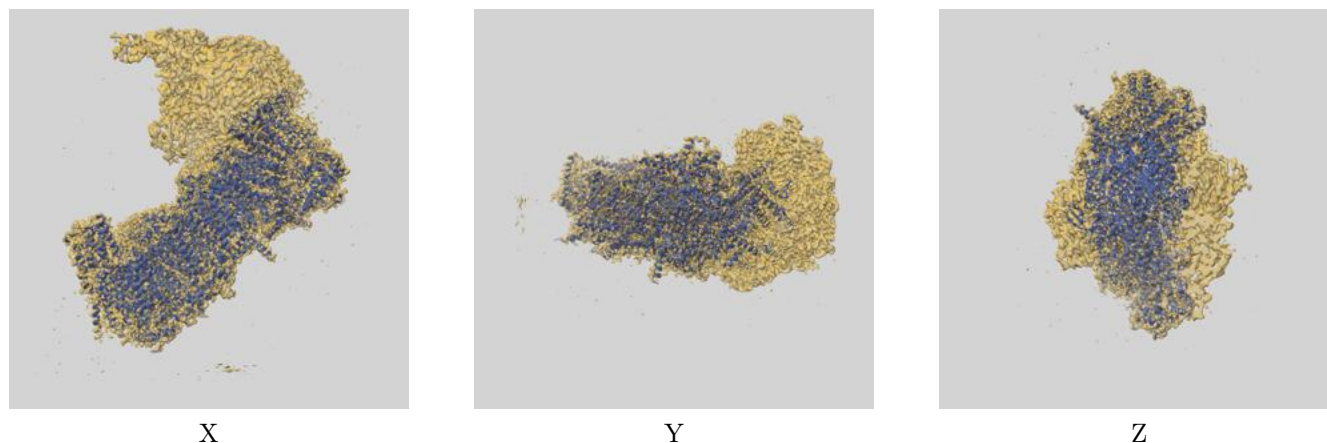
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.47	-	-
Author-provided FSC curve	2.47	2.82	2.50
Unmasked-calculated*	3.64	6.45	3.75

*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 3.64 differs from the reported value 2.47 by more than 10 %

9 Map-model fit [i](#)

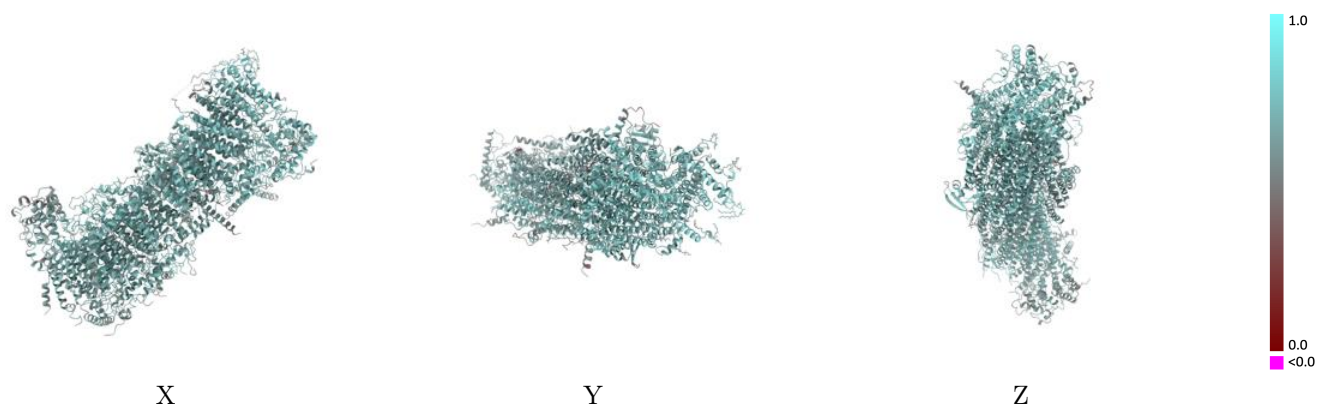
This section contains information regarding the fit between EMDB map EMD-14798 and PDB model 7ZMH. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



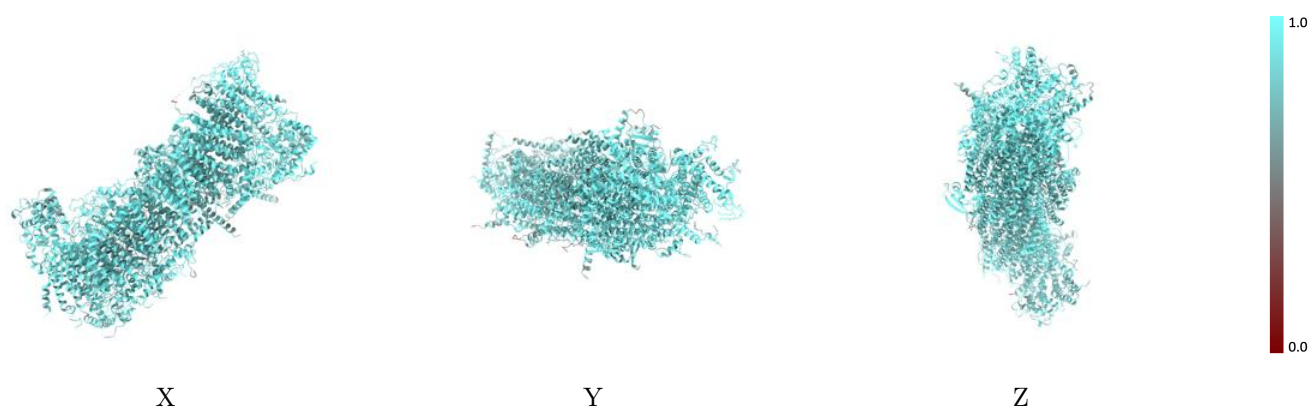
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



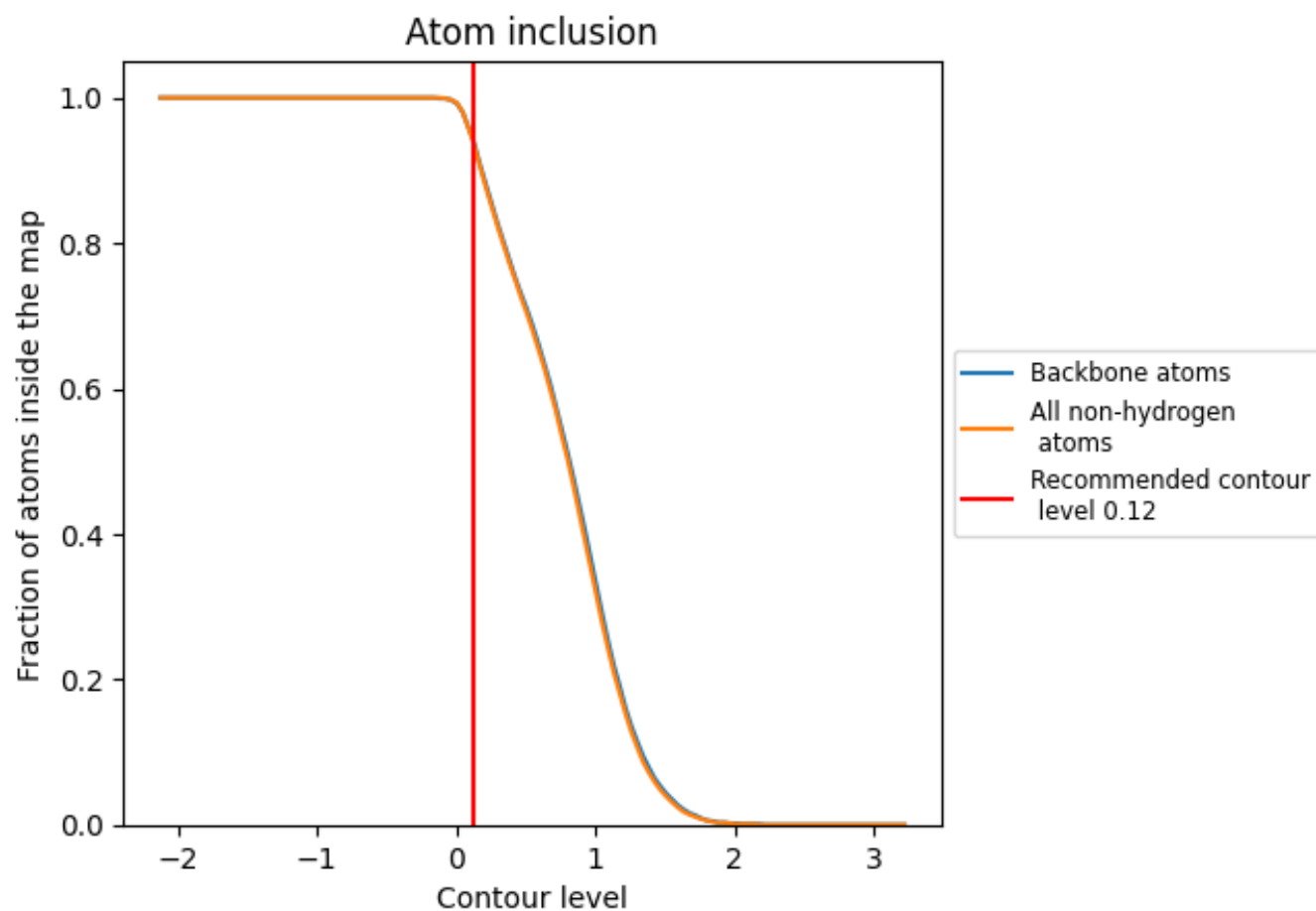
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9410	 0.6720
1	 0.9560	 0.6940
2	 0.9720	 0.7080
3	 0.9260	 0.6630
4	 0.9740	 0.7030
5	 0.9660	 0.6790
6	 0.9380	 0.6790
8	 0.8910	 0.5970
9	 0.8910	 0.6450
D	 0.9920	 0.7050
J	 0.8880	 0.6120
L	 0.9760	 0.7070
Q	 0.8060	 0.5640
R	 0.9000	 0.6270
S	 0.9300	 0.6450
U	 0.9660	 0.6880
W	 0.9440	 0.6790
X	 0.9490	 0.6820
a	 0.9150	 0.6300
b	 0.9210	 0.6620
c	 0.8910	 0.5780
d	 0.9420	 0.6730
e	 0.9060	 0.6070
g	 0.9510	 0.6660
i	 0.8990	 0.6460
j	 0.9380	 0.6700
n	 0.8610	 0.6280

