



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:38 PM UTC

PDB ID : 7ZME / pdb_00007zme
EMDB ID : EMD-14796
Title : CryoEM structure of mitochondrial complex I from Chaetomium thermophilum (state 2) - membrane arm
Authors : Laube, E.; Kuehlbrandt, W.
Deposited on : 2022-04-19
Resolution : 2.83 Å (reported)
Based on initial models : 6RFR, 6RFQ

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:

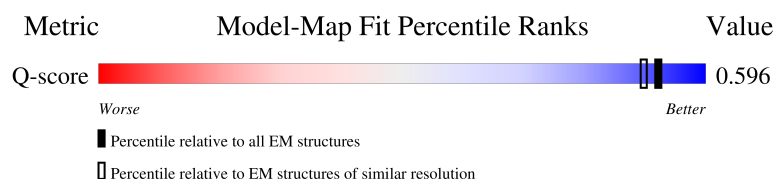
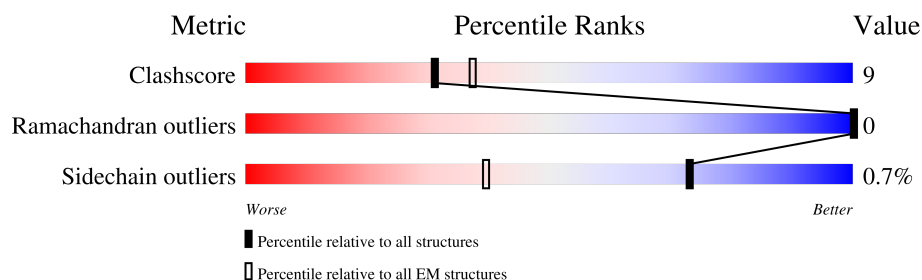
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.83 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.



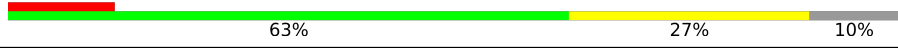
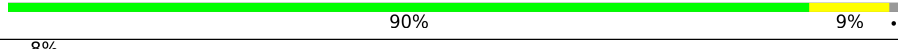
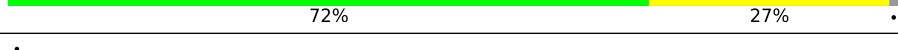
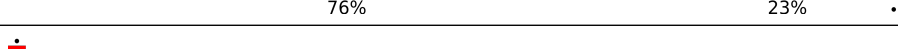
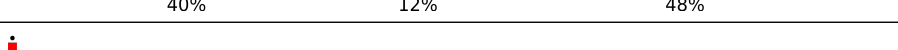
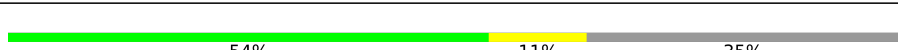
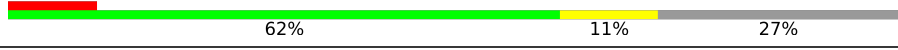
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11847 (2.33 - 3.33)

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	 69% 18% 12%
2	2	571	 77% 19% 4%
3	3	146	 62% 15% 22%
4	4	542	 69% 22% 9%

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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

There are 32 unique types of molecules in this entry. The entry contains 36964 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
			2573	1728	388	446	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
			4456	2993	672	780	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	114	Total	C	N	O	S	0	0
			907	619	132	153	3		

- 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
			5272	3551	792	904	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
			1454	981	219	248	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	77	Total	C	N	O	S	0	0
			658	408	126	118	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
			1375	872	259	242	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	88	Total	C	N	O	S	0	0
			671	450	103	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
			663	418	109	135	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
			610	401	98	111		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	169	Total	C	N	O	S	0	0
			1365	860	254	242	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
			812	519	154	137	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
			1480	941	268	263	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	a	143	Total	C	N	O	S	0	0
			1167	750	195	217	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	60	Total	C	N	O	S	0	0
			490	320	86	82	2		

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

(Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	98	Total	C	N	O	S	0	0
			817	520	144	149	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	e	37	Total	C	N	O	S	0	0
			309	211	54	43	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	80	Total	C	N	O	S	0	0
			677	447	117	111	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	j	73	Total	C	N	O	S	0	0
			603	391	108	101	3		

- 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:

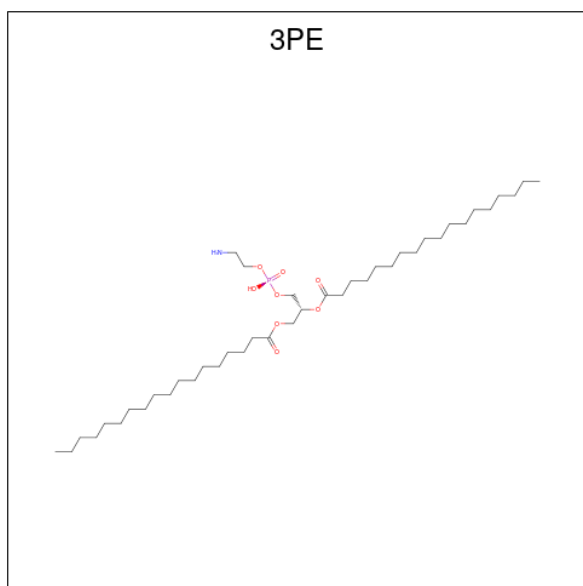
Chain	Residue	Modelled	Actual	Comment	Reference
n	1	MET	-	initiating methionine	UNP G0S086
n	2	LEU	-	insertion	UNP G0S086
n	3	ALA	-	insertion	UNP G0S086
n	4	LEU	-	insertion	UNP G0S086
n	5	ARG	-	insertion	UNP G0S086
n	6	GLN	-	insertion	UNP G0S086
n	7	ARG	-	insertion	UNP G0S086
n	8	ALA	-	insertion	UNP 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	-	amidation	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: $C_{41}H_{82}NO_8P$).



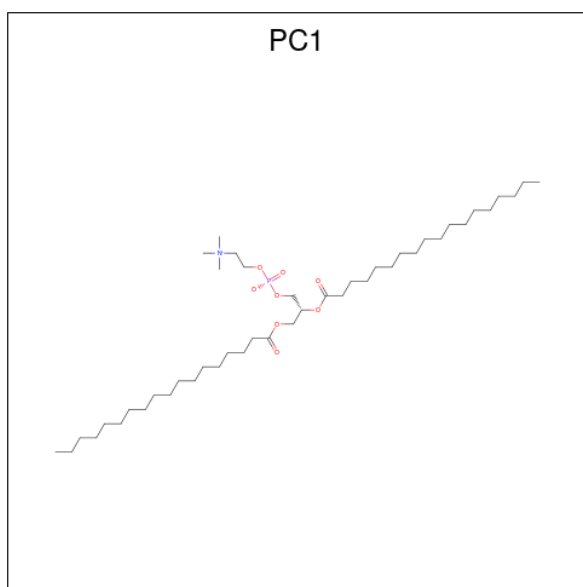
Mol	Chain	Residues	Atoms					AltConf
27	1	1	Total	C	N	O	P	0
			41	31	1	8	1	
27	1	1	Total	C	N	O	P	0
			27	18	1	7	1	
27	4	1	Total	C	N	O	P	0
			34	24	1	8	1	
27	4	1	Total	C	N	O	P	0
			33	23	1	8	1	
27	4	1	Total	C	N	O	P	0
			28	18	1	8	1	
27	5	1	Total	C	N	O	P	0
			40	30	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
27	5	1	Total	C	N	O	P	0
			32	22	1	8	1	
27	5	1	Total	C	N	O	P	0
			42	32	1	8	1	
27	5	1	Total	C	N	O	P	0
			28	18	1	8	1	
27	8	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
			34	24	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
			39	29	1	8	1	
27	n	1	Total	C	N	O	P	0
			39	29	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: $C_{44}H_{88}NO_8P$).



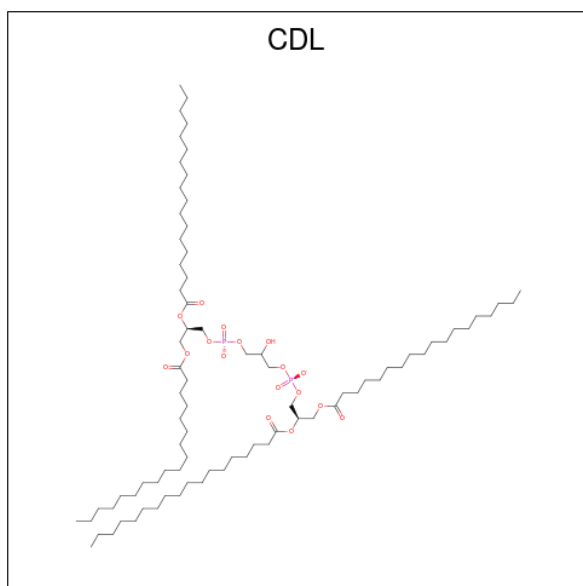
Mol	Chain	Residues	Atoms					AltConf
28	1	1	Total	C	N	O	P	0
			30	20	1	8	1	

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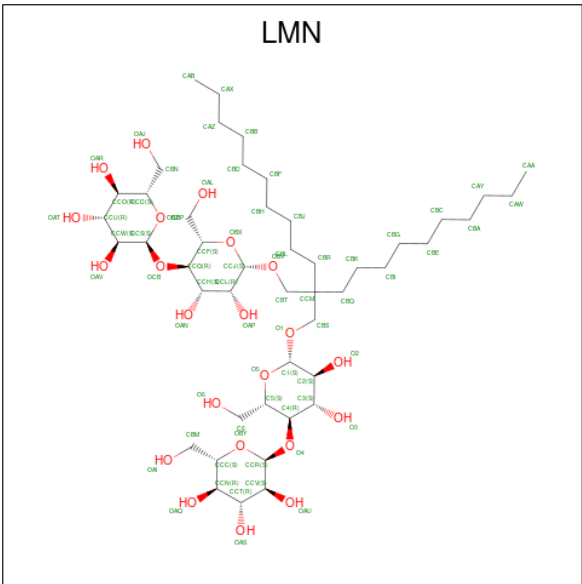
Mol	Chain	Residues	Atoms					AltConf
28	2	1	Total	C	N	O	P	0
			31	21	1	8	1	
28	3	1	Total	C	N	O	P	0
			36	26	1	8	1	
28	4	1	Total	C	N	O	P	0
			45	35	1	8	1	
28	5	1	Total	C	N	O	P	0
			45	35	1	8	1	
28	5	1	Total	C	N	O	P	0
			41	31	1	8	1	
28	n	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



Mol	Chain	Residues	Atoms				AltConf
29	2	1	Total	C	O	P	0
			84	65	17	2	
29	4	1	Total	C	O	P	0
			86	67	17	2	
29	D	1	Total	C	O	P	0
			59	40	17	2	
29	X	1	Total	C	O	P	0
			79	60	17	2	
29	g	1	Total	C	O	P	0
			56	37	17	2	

- 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
			58	41	17	
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	

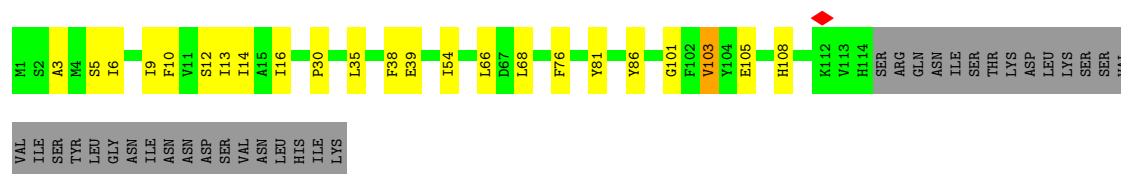
- Molecule 32 is water.

Mol	Chain	Residues	Atoms		AltConf
32	1	62	Total	O	0
			62	62	
32	2	141	Total	O	0
			141	141	
32	3	24	Total	O	0
			24	24	
32	4	84	Total	O	0
			84	84	
32	5	49	Total	O	0
			49	49	
32	6	35	Total	O	0
			35	35	
32	9	19	Total	O	0
			19	19	
32	D	27	Total	O	0
			27	27	
32	J	1	Total	O	0
			1	1	
32	L	11	Total	O	0
			11	11	
32	R	4	Total	O	0
			4	4	
32	S	1	Total	O	0
			1	1	
32	U	36	Total	O	0
			36	36	
32	W	29	Total	O	0
			29	29	
32	X	45	Total	O	0
			45	45	
32	a	11	Total	O	0
			11	11	
32	b	4	Total	O	0
			4	4	
32	d	9	Total	O	0
			9	9	
32	g	10	Total	O	0
			10	10	

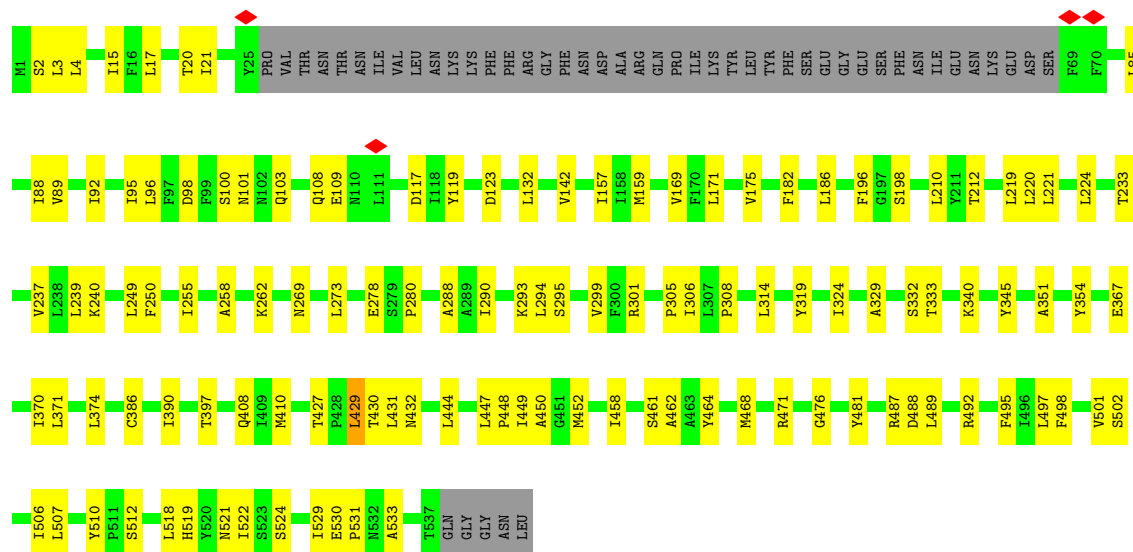
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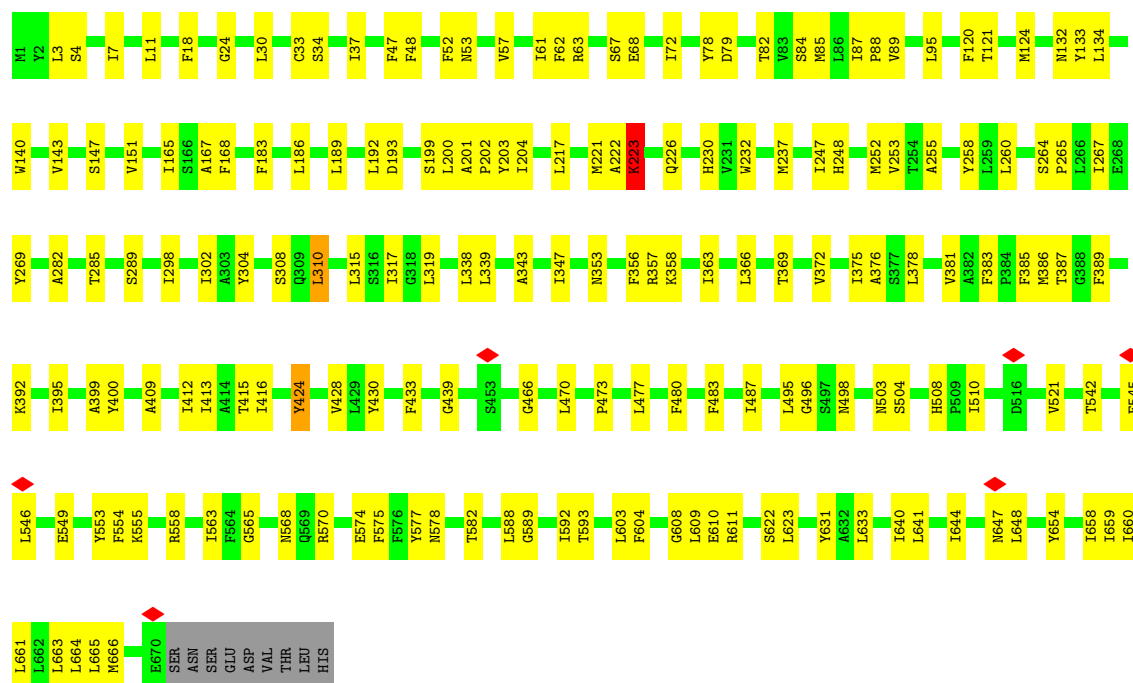
Mol	Chain	Residues	Atoms		AltConf
32	i	4	Total 4	O 4	0
32	j	4	Total 4	O 4	0
32	n	23	Total 23	O 23	0



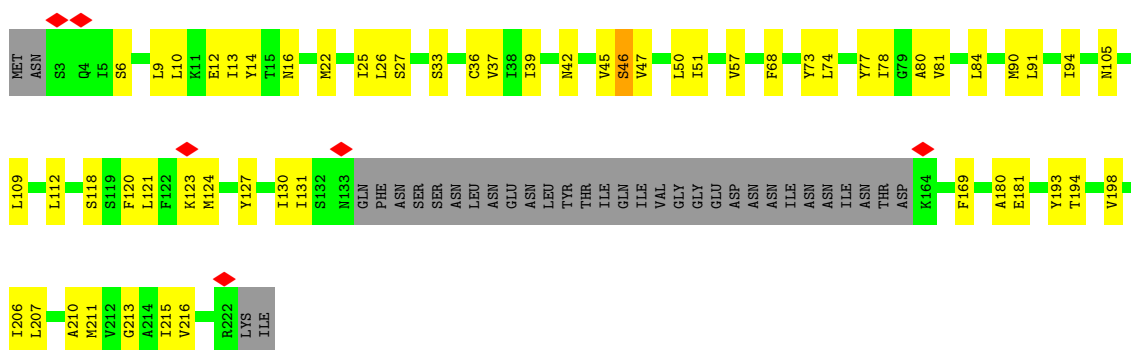
• Molecule 4: NADH-ubiquinone oxidoreductase chain 4



• Molecule 5: NADH-ubiquinone oxidoreductase chain 5



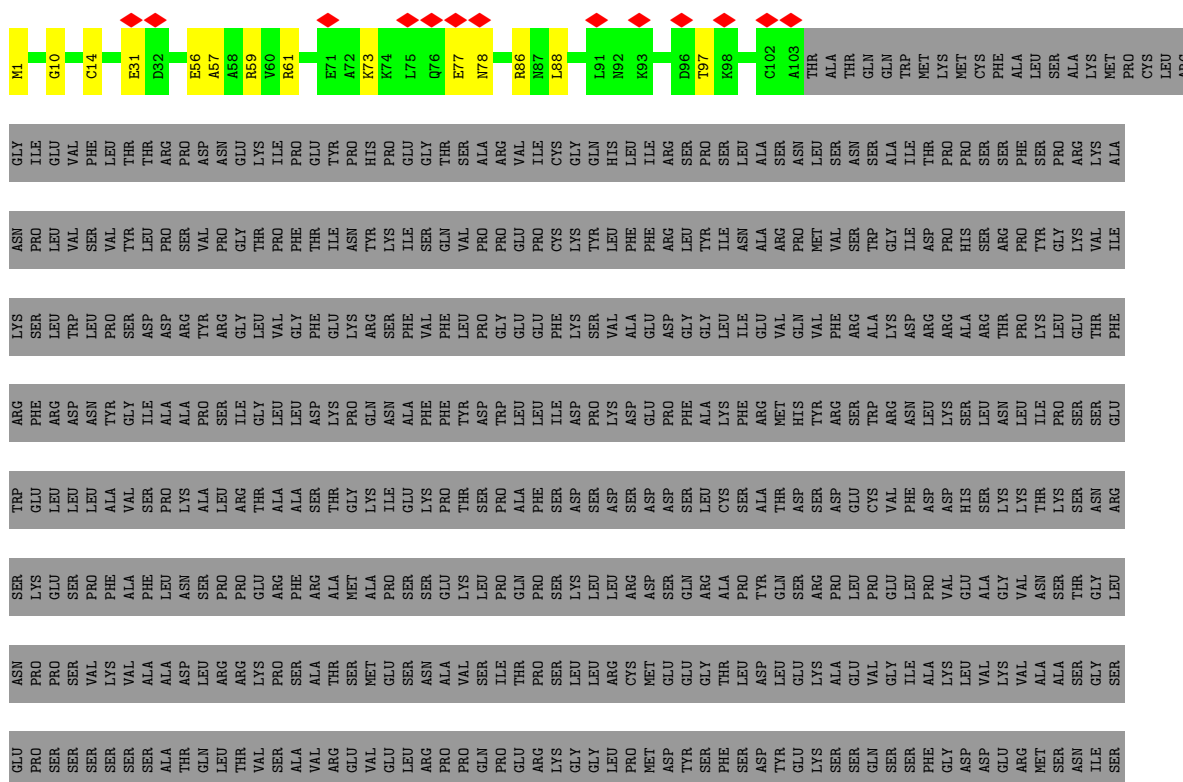
Chain 6: 59% 25% 15%

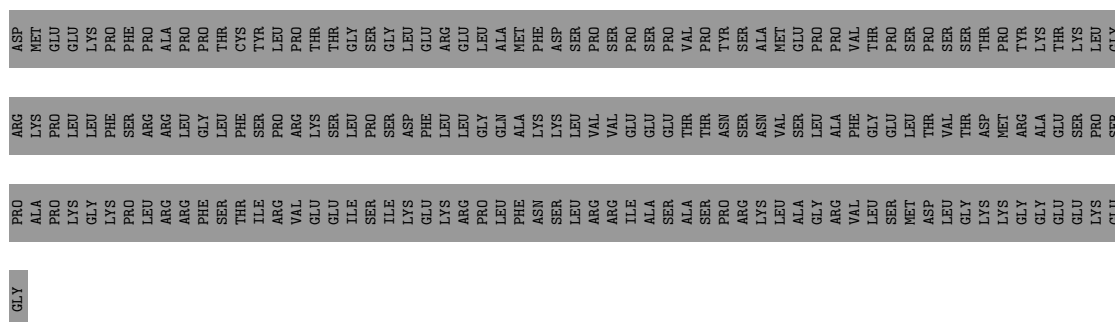


Chain 8:

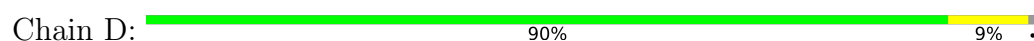


Chain 9: 11% 87%

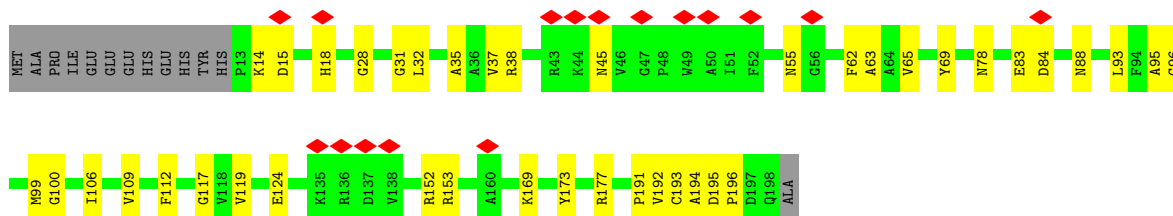




- Molecule 9: Subunit NDUFA1 of NADH-ubiquinone oxidoreductase (Complex I)



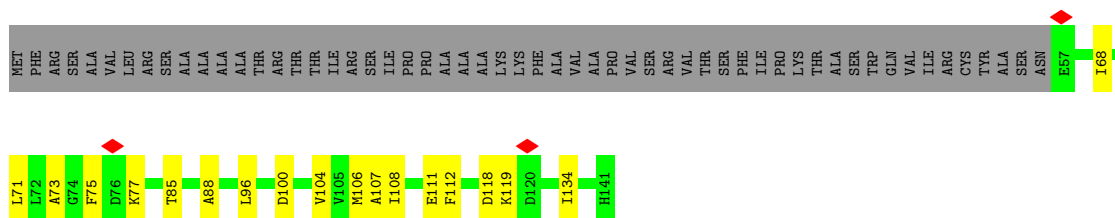
- Molecule 10: NADH-ubiquinone oxidoreductase-like protein



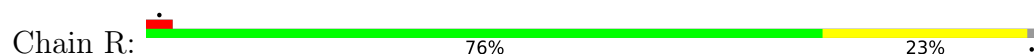
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

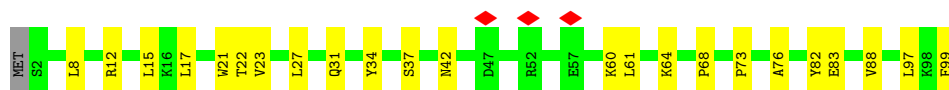


- Molecule 12: Acyl carrier protein



- Molecule 13: Complex I-B22

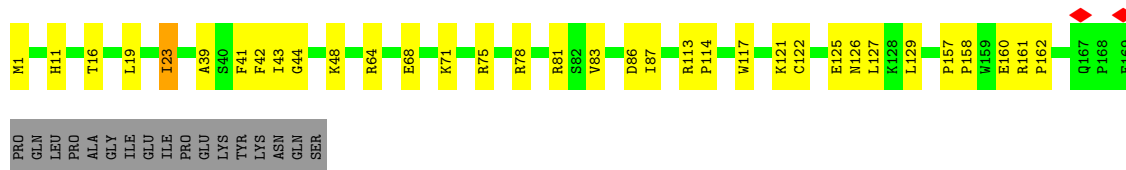




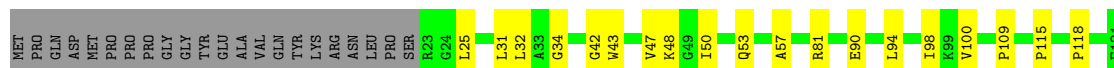
- Molecule 14: Complex I-ESSS



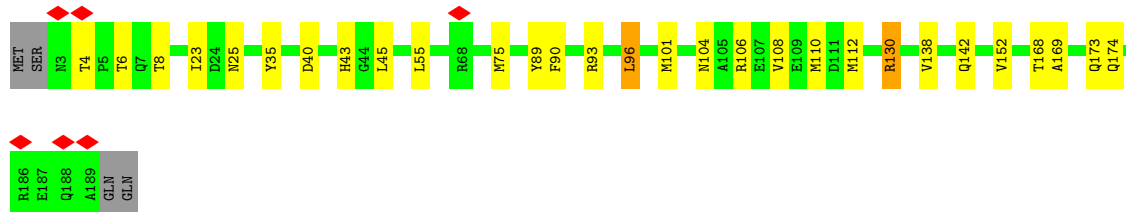
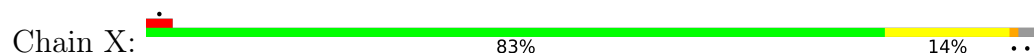
- Molecule 15: NADH-ubiquinone oxidoreductase



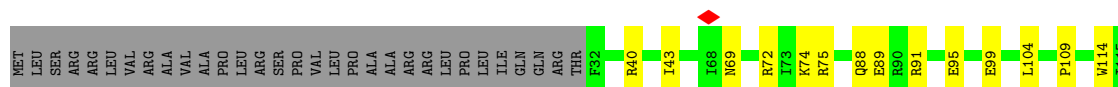
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

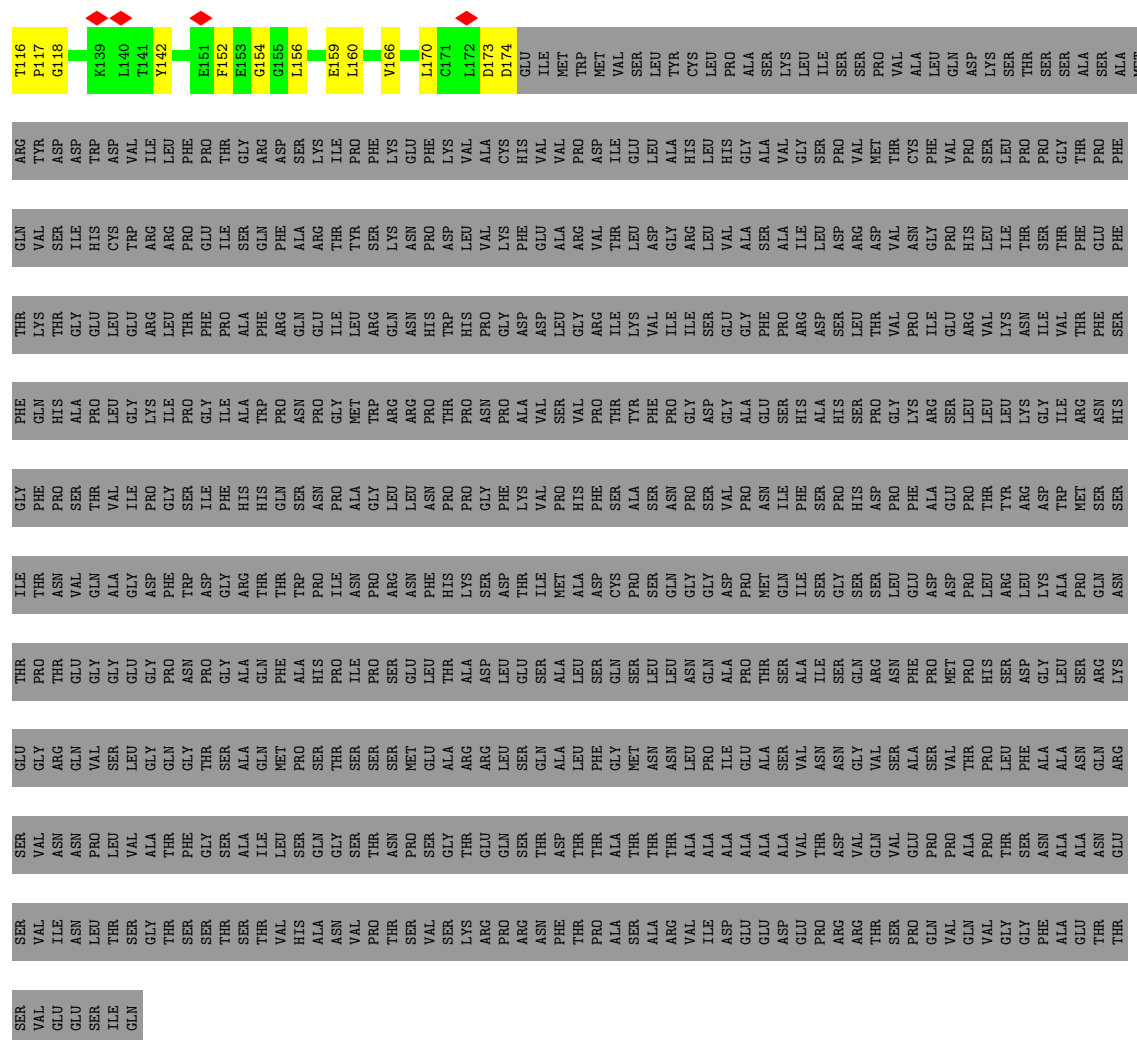


- Molecule 17: NADH-ubiquinone oxidoreductase-like protein

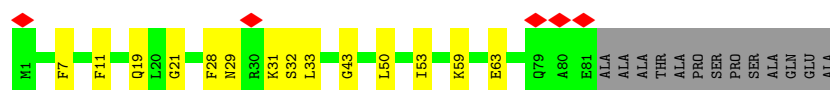


- Molecule 18: NADH dehydrogenase (Ubiquinone)-like protein





- Molecule 19: Subunit NDUFC2 of NADH-ubiquinone oxidoreductase (Complex I)

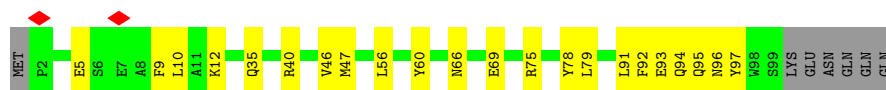


- Molecule 20: Subunit NDUFB3 of NADH-ubiquinone oxidoreductase (Complex I)



- Molecule 21: Subunit NDUFB10 of NADH-ubiquinone oxidoreductase (Complex I)

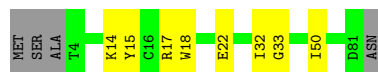
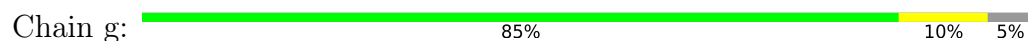




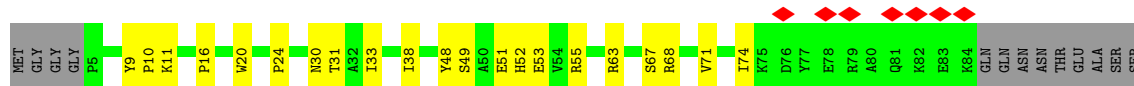
- Molecule 22: Subunit NDUFB2 of NADH-ubiquinone oxidoreductase (Complex I)



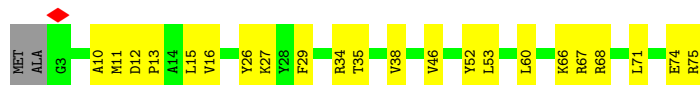
- Molecule 23: Subunit NDUFA3 of NADH-ubiquinone oxidoreductase (Complex I)



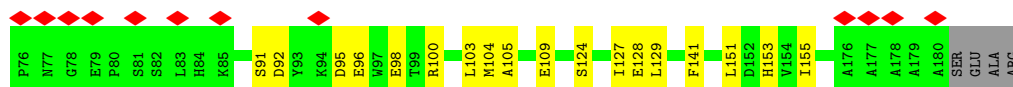
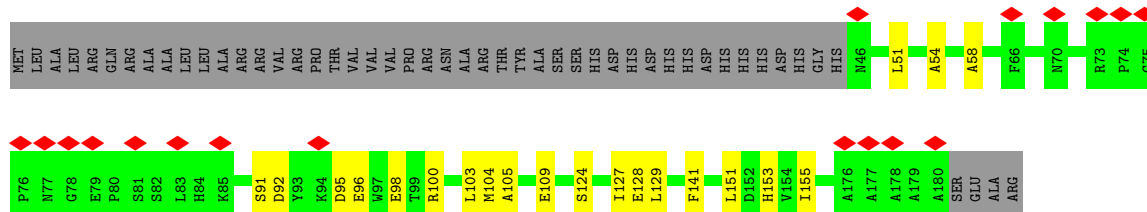
- Molecule 24: Subunit NDUFB6 of NADH-ubiquinone oxidoreductase (Complex I)



- Molecule 25: Subunit NDUFB4 of NADH-ubiquinone oxidoreductase (Complex I)



- Molecule 26: Subunit NDUFB5 of NADH-ubiquinone oxidoreductase (Complex I)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21989	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	2.226	Depositor
Minimum map value	-1.186	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.133	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: ZMP, LMN, 3PE, CDL, PC1

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	0.62	1/2633 (0.0%)	0.91	3/3593 (0.1%)
2	2	0.64	1/4562 (0.0%)	0.94	9/6205 (0.1%)
3	3	0.53	0/934	0.88	2/1269 (0.2%)
4	4	0.49	0/4002	0.76	4/5454 (0.1%)
5	5	0.43	2/5414 (0.0%)	0.68	4/7371 (0.1%)
6	6	0.79	4/1481 (0.3%)	0.99	2/2020 (0.1%)
7	8	0.19	0/671	0.43	0/896
8	9	0.54	0/824	0.82	0/1112
9	D	0.79	1/674 (0.1%)	1.12	0/911
10	J	0.33	0/1400	0.56	0/1892
11	L	0.60	0/677	0.86	0/917
12	Q	0.25	0/673	0.56	1/913 (0.1%)
13	R	0.40	0/832	0.62	0/1133
14	S	0.32	0/635	0.57	0/869
15	U	0.73	1/1403 (0.1%)	1.10	2/1904 (0.1%)
16	W	0.69	0/830	1.17	2/1120 (0.2%)
17	X	0.73	0/1519	1.06	3/2053 (0.1%)
18	a	0.35	0/1204	0.55	0/1632
19	b	0.25	0/701	0.45	0/939
20	c	0.21	0/509	0.42	0/691
21	d	0.31	0/835	0.56	0/1123
22	e	0.48	2/324 (0.6%)	0.50	0/440
23	g	0.58	0/631	0.86	0/868
24	i	0.32	0/706	0.61	2/960 (0.2%)
25	j	0.21	0/617	0.37	0/830
26	n	0.66	2/1092 (0.2%)	0.93	0/1481
All	All	0.54	14/35783 (0.0%)	0.81	34/48596 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	6	181	GLU	C-N	9.50	1.46	1.33
2	2	122	ILE	C-N	8.67	1.45	1.33
6	6	45	VAL	C-N	-8.59	1.21	1.33
5	5	222	ALA	C-N	-8.35	1.22	1.34
6	6	46	SER	C-N	8.22	1.43	1.34
9	D	73	PHE	C-N	-7.23	1.23	1.33
6	6	180	ALA	C-N	7.07	1.43	1.33
26	n	127	ILE	C-N	6.55	1.43	1.33
22	e	14	PHE	C-N	-6.23	1.25	1.33
26	n	128	GLU	C-N	6.11	1.41	1.33
5	5	223	LYS	C-N	5.90	1.42	1.33
15	U	129	LEU	C-N	5.34	1.40	1.33
1	1	202	THR	C-N	-5.27	1.26	1.33
22	e	15	LEU	C-N	5.20	1.40	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	X	130	ARG	N-CA-C	-7.72	103.66	113.23
16	W	25	LEU	N-CA-C	-7.47	103.62	112.89
4	4	182	PHE	CA-CB-CG	6.86	120.66	113.80
2	2	122	ILE	O-C-N	6.63	130.26	122.83
4	4	427	THR	CB-CA-C	6.55	118.90	109.26
12	Q	107	ALA	N-CA-C	-6.54	105.93	114.04
1	1	104	VAL	N-CA-C	-6.08	104.04	112.50
2	2	494	GLU	N-CA-C	-5.93	105.69	113.17
2	2	335	ARG	CB-CA-C	5.92	119.51	109.80
2	2	17	LEU	N-CA-C	-5.82	104.85	112.41
6	6	45	VAL	O-C-N	-5.64	116.40	121.87
4	4	429	LEU	N-CA-C	-5.59	105.19	113.40
2	2	338	ARG	N-CA-C	-5.55	105.77	112.54
17	X	25	ASN	N-CA-C	-5.54	106.36	113.23
1	1	374	ASN	CB-CA-C	5.46	119.95	110.94
1	1	133	ASN	CB-CA-C	5.45	120.36	111.26
3	3	39	GLU	N-CA-C	-5.42	104.01	110.41
15	U	42	PHE	CB-CA-C	5.38	120.00	110.85
2	2	555	LYS	N-CA-C	5.35	116.79	111.07
5	5	304	TYR	CB-CA-C	5.33	119.90	110.85
15	U	41	PHE	CB-CA-C	5.29	119.58	110.79
2	2	67	PHE	CB-CA-C	5.29	120.83	110.67
24	i	31	THR	CB-CA-C	5.28	119.83	110.85
24	i	31	THR	N-CA-C	-5.25	105.64	111.36
2	2	417	GLN	N-CA-C	-5.24	106.40	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	310	LEU	N-CA-C	-5.21	105.28	111.69
17	X	23	ILE	N-CA-C	-5.20	106.73	111.67
5	5	222	ALA	O-C-N	-5.20	116.47	122.09
16	W	31	LEU	N-CA-C	-5.19	105.31	111.69
5	5	424	TYR	CB-CA-C	5.17	119.63	110.85
4	4	495	PHE	CB-CA-C	5.12	119.56	110.85
3	3	103	VAL	N-CA-C	-5.09	105.58	110.72
2	2	363	THR	N-CA-C	-5.06	105.42	112.45
6	6	206	ILE	N-CA-C	-5.02	105.81	110.53

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	2573	0	2696	45	0
2	2	4456	0	4650	81	0
3	3	907	0	922	22	0
4	4	3904	0	4056	92	0
5	5	5272	0	5396	142	0
6	6	1454	0	1538	49	0
7	8	658	0	648	17	0
8	9	807	0	778	10	0
9	D	678	0	642	5	0
10	J	1375	0	1386	37	0
11	L	671	0	737	24	0
12	Q	663	0	638	13	0
13	R	807	0	823	25	0
14	S	610	0	557	18	0
15	U	1365	0	1333	20	0
16	W	812	0	833	16	0
17	X	1480	0	1432	21	0
18	a	1167	0	1104	23	0
19	b	683	0	690	13	0
20	c	490	0	451	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	d	817	0	810	24	0
22	e	309	0	300	5	0
23	g	610	0	620	6	0
24	i	677	0	653	19	0
25	j	603	0	623	17	0
26	n	1061	0	1022	17	0
27	1	68	0	93	2	0
27	4	95	0	112	8	0
27	5	142	0	183	7	0
27	8	36	0	46	1	0
27	J	30	0	34	3	0
27	W	34	0	47	1	0
27	g	75	0	101	6	0
27	n	78	0	110	2	0
28	1	30	0	34	2	0
28	2	31	0	36	0	0
28	3	36	0	46	0	0
28	4	45	0	64	4	0
28	5	86	0	123	8	0
28	n	51	0	76	5	0
29	2	84	0	115	8	0
29	4	86	0	119	8	0
29	D	59	0	62	1	0
29	X	79	0	105	4	0
29	g	56	0	56	3	0
30	2	58	0	77	2	0
30	4	58	0	77	5	0
30	J	69	0	88	0	0
31	Q	36	0	47	5	0
32	1	62	0	0	1	0
32	2	141	0	0	2	0
32	3	24	0	0	1	0
32	4	84	0	0	4	0
32	5	49	0	0	2	0
32	6	35	0	0	0	0
32	9	19	0	0	0	0
32	D	27	0	0	0	0
32	J	1	0	0	0	0
32	L	11	0	0	1	0
32	R	4	0	0	0	0
32	S	1	0	0	0	0
32	U	36	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	W	29	0	0	0	0
32	X	45	0	0	0	0
32	a	11	0	0	0	0
32	b	4	0	0	0	0
32	d	9	0	0	0	0
32	g	10	0	0	0	0
32	i	4	0	0	0	0
32	j	4	0	0	0	0
32	n	23	0	0	0	0
All	All	36964	0	37189	649	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 9.

All (649) 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)
9:D:42:VAL:HG13	9:D:46:ASP:HB2	1.48	0.94
4:4:408:GLN:HA	28:5:701:PC1:H131	1.55	0.87
6:6:127:TYR:O	6:6:131:ILE:HG12	1.76	0.85
5:5:72:ILE:HG23	5:5:132:ASN:HD21	1.43	0.84
28:4:605:PC1:H241	5:5:610:GLU:HG2	1.62	0.81
30:4:604:LMN:HBC	30:4:604:LMN:HBK	1.60	0.81
5:5:221:MET:HG3	5:5:226:GLN:HB2	1.61	0.81
18:a:159:GLU:HA	21:d:69:GLU:HB3	1.63	0.80
10:J:177:ARG:HE	25:j:74:GLU:HG2	1.48	0.78
28:5:701:PC1:H11	28:5:701:PC1:H142	1.65	0.78
2:2:99:ASP:HA	2:2:103:ASN:HD22	1.48	0.77
2:2:181:LEU:HD11	11:L:22:ILE:HG23	1.67	0.76
2:2:17:LEU:HD21	3:3:108:HIS:HA	1.67	0.76
6:6:210:ALA:HA	11:L:69:ILE:HD11	1.68	0.75
2:2:273:THR:HA	2:2:276:THR:HG22	1.66	0.74
5:5:132:ASN:HB2	5:5:192:LEU:HD12	1.69	0.73
15:U:43:ILE:HD13	15:U:83:VAL:HG21	1.72	0.72
2:2:238:TYR:HB3	2:2:242:PHE:HE2	1.54	0.71
13:R:27:LEU:HD12	20:c:28:THR:HG22	1.73	0.71
1:1:82:PRO:HG3	1:1:228:ILE:HG23	1.71	0.71
5:5:124:MET:HE3	5:5:252:MET:HA	1.73	0.70
5:5:124:MET:HE1	5:5:255:ALA:HB2	1.73	0.69
6:6:9:LEU:HB3	16:W:118:PRO:HA	1.74	0.69
15:U:19:LEU:HD22	15:U:23:ILE:HD12	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:578:ASN:HA	5:5:582:THR:HG22	1.74	0.69
6:6:74:LEU:HG	6:6:78:ILE:HD11	1.73	0.69
5:5:439:GLY:O	20:c:43:ARG:NH1	2.26	0.69
15:U:78:ARG:HG2	15:U:81:ARG:HH11	1.58	0.69
7:8:73:MET:HB3	7:8:77:ARG:HG3	1.75	0.68
15:U:122:CYS:O	15:U:126:ASN:ND2	2.26	0.68
6:6:57:VAL:HG11	11:L:34:LEU:HD11	1.76	0.68
4:4:397:THR:HB	25:j:11:MET:HE1	1.76	0.68
8:9:88:LEU:HD12	8:9:97:THR:HG23	1.76	0.68
4:4:249:LEU:HD13	4:4:314:LEU:HD11	1.76	0.67
29:2:601:CDL:CA3	29:2:601:CDL:CA2	2.72	0.67
15:U:121:LYS:NZ	15:U:125:GLU:OE1	2.27	0.67
24:i:9:TYR:O	24:i:11:LYS:NZ	2.27	0.67
6:6:121:LEU:HA	6:6:124:MET:HG3	1.77	0.66
10:J:196:PRO:HG2	21:d:69:GLU:HA	1.77	0.66
29:2:601:CDL:CA3	29:2:601:CDL:HA22	2.25	0.66
4:4:444:LEU:HD12	4:4:448:PRO:HA	1.77	0.66
29:D:101:CDL:H511	29:D:101:CDL:H722	1.78	0.66
2:2:483:ASN:ND2	32:2:703:HOH:O	2.28	0.65
2:2:42:MET:HE2	17:X:93:ARG:HG2	1.79	0.65
5:5:392:LYS:HA	5:5:395:ILE:HD12	1.78	0.65
2:2:216:SER:HB2	2:2:237:PRO:HG3	1.79	0.65
17:X:35:TYR:CE2	17:X:110:MET:HG3	2.32	0.65
20:c:19:PHE:HE1	20:c:24:PHE:HB2	1.62	0.65
17:X:130:ARG:HH11	29:X:201:CDL:CA5	2.10	0.64
1:1:217:VAL:HG21	3:3:38:PHE:HE2	1.63	0.64
4:4:175:VAL:HB	4:4:233:THR:HB	1.80	0.64
5:5:545:GLU:O	20:c:50:ARG:NH2	2.22	0.64
4:4:123:ASP:OD1	4:4:301:ARG:NH2	2.31	0.64
4:4:212:THR:HG23	4:4:262:LYS:HD2	1.78	0.64
2:2:177:LEU:HD21	11:L:22:ILE:HD13	1.79	0.64
6:6:207:LEU:O	6:6:211:MET:HG3	1.97	0.63
15:U:86:ASP:HB3	15:U:127:LEU:HD21	1.78	0.63
1:1:153:LEU:HD21	3:3:66:LEU:HB3	1.80	0.63
5:5:189:LEU:HD21	5:5:204:ILE:HD13	1.79	0.63
5:5:554:PHE:HZ	5:5:563:ILE:HD11	1.62	0.63
1:1:38:MET:HE1	1:1:329:TRP:HA	1.80	0.62
4:4:371:LEU:HD22	4:4:431:LEU:HD11	1.80	0.62
5:5:466:GLY:HA3	5:5:470:LEU:HD23	1.81	0.62
11:L:18:ASN:HD22	11:L:25:MET:HG3	1.64	0.62
4:4:273:LEU:HD21	4:4:345:TYR:HD1	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:506:ILE:HG23	27:4:603:3PE:H261	1.82	0.62
4:4:17:LEU:O	4:4:21:ILE:HG12	1.99	0.62
6:6:112:LEU:HD11	10:J:32:LEU:HG	1.81	0.62
5:5:167:ALA:HA	5:5:232:TRP:HB2	1.81	0.62
2:2:479:VAL:HG11	28:4:605:PC1:H252	1.81	0.61
19:b:59:LYS:O	19:b:63:GLU:HG3	2.00	0.61
2:2:383:ILE:HG21	2:2:432:LEU:HB2	1.81	0.61
5:5:366:LEU:HB3	5:5:369:THR:HB	1.82	0.61
4:4:512:SER:OG	5:5:63:ARG:NH1	2.34	0.61
19:b:29:ASN:HB3	19:b:32:SER:HB2	1.83	0.60
24:i:33:ILE:HD13	26:n:51:LEU:HD11	1.83	0.60
6:6:10:LEU:HD21	8:9:86:ARG:HD2	1.82	0.60
2:2:535:PRO:HA	29:2:601:CDL:H121	1.82	0.60
5:5:641:LEU:HD22	27:5:702:3PE:H3E2	1.84	0.60
7:8:73:MET:HA	7:8:76:LEU:HB3	1.83	0.60
18:a:116:THR:HG22	18:a:118:GLY:H	1.67	0.60
24:i:71:VAL:HG13	24:i:74:ILE:HG12	1.83	0.60
4:4:219:LEU:HD12	4:4:255:ILE:HG12	1.82	0.60
5:5:633:LEU:HD11	6:6:109:LEU:HD11	1.84	0.60
6:6:105:ASN:HD21	10:J:45:ASN:HA	1.67	0.60
13:R:73:PRO:HG2	13:R:76:ALA:HB2	1.83	0.60
5:5:201:ALA:HA	5:5:204:ILE:HD12	1.84	0.59
10:J:152:ARG:HH21	21:d:97:TYR:HB3	1.66	0.59
29:2:601:CDL:CA2	29:2:601:CDL:HA31	2.32	0.59
2:2:155:GLN:NE2	32:2:706:HOH:O	2.35	0.59
5:5:343:ALA:O	5:5:347:ILE:HD12	2.02	0.59
1:1:31:GLU:HG3	1:1:328:ILE:HG12	1.84	0.59
10:J:177:ARG:NE	25:j:74:GLU:HG2	2.17	0.59
4:4:186:LEU:HD11	4:4:212:THR:HG21	1.83	0.58
13:R:88:VAL:HG21	24:i:10:PRO:HG3	1.85	0.58
25:j:29:PHE:CE1	25:j:35:THR:HG21	2.38	0.58
3:3:10:PHE:O	3:3:14:ILE:HG12	2.02	0.58
17:X:112:MET:HG3	17:X:174:GLN:OE1	2.03	0.58
1:1:221:MET:HE1	1:1:232:PHE:HB3	1.86	0.58
3:3:68:LEU:HB3	11:L:61:VAL:HG23	1.85	0.58
4:4:471:ARG:NH2	32:4:707:HOH:O	2.37	0.58
14:S:98:TRP:O	14:S:102:ILE:HG13	2.02	0.58
1:1:370:ILE:HG21	16:W:47:VAL:HA	1.84	0.58
2:2:11:LEU:HD12	29:g:101:CDL:H151	1.84	0.58
4:4:430:THR:HG22	4:4:432:ASN:H	1.69	0.58
17:X:96:LEU:HG	17:X:101:MET:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:37:VAL:O	6:6:46:SER:HB2	2.03	0.58
4:4:157:ILE:HG21	27:4:602:3PE:H341	1.86	0.57
5:5:363:ILE:HB	5:5:433:PHE:HB3	1.86	0.57
11:L:12:ILE:HG23	11:L:13:LEU:HD12	1.85	0.57
29:2:601:CDL:HA22	29:2:601:CDL:HA31	1.85	0.57
5:5:85:MET:HE3	5:5:258:TYR:HB2	1.86	0.57
5:5:68:GLU:HG2	21:d:46:VAL:HG11	1.87	0.57
5:5:661:LEU:HD21	10:J:62:PHE:CE1	2.40	0.57
1:1:9:SER:HB3	3:3:3:ALA:HA	1.86	0.57
16:W:43:TRP:HB3	27:g:102:3PE:H341	1.87	0.57
1:1:360:LEU:HD22	23:g:32:ILE:HG23	1.86	0.57
8:9:1:MET:HA	8:9:14:CYS:HB2	1.87	0.57
15:U:78:ARG:HG2	15:U:81:ARG:NH1	2.20	0.57
6:6:84:LEU:HD21	11:L:27:ILE:HG12	1.87	0.57
3:3:54:ILE:HD13	6:6:90:MET:HB2	1.87	0.56
4:4:519:HIS:CD2	14:S:117:GLN:HE22	2.22	0.56
5:5:203:TYR:CD1	10:J:194:ALA:HA	2.41	0.56
28:5:701:PC1:H142	28:5:701:PC1:C1	2.33	0.56
21:d:12:LYS:HD2	21:d:40:ARG:HH22	1.71	0.56
4:4:332:SER:HB2	4:4:345:TYR:CE2	2.40	0.56
29:4:601:CDL:H132	14:S:94:PHE:HB3	1.87	0.56
13:R:22:THR:HG21	13:R:31:GLN:HE22	1.71	0.56
10:J:35:ALA:HB1	10:J:55:ASN:HB3	1.86	0.56
2:2:161:LEU:HD21	11:L:69:ILE:HD12	1.87	0.56
2:2:292:LEU:HA	2:2:355:LEU:HD11	1.88	0.56
5:5:412:ILE:O	5:5:416:ILE:HD12	2.06	0.56
27:4:602:3PE:H351	27:4:602:3PE:H261	1.88	0.56
23:g:14:LYS:O	23:g:17:ARG:HG3	2.06	0.56
25:j:12:ASP:HB3	25:j:15:LEU:HB2	1.88	0.56
4:4:333:THR:HB	4:4:345:TYR:HD2	1.72	0.55
2:2:148:ILE:HD11	2:2:206:LEU:HD11	1.87	0.55
2:2:61:THR:H	2:2:64:THR:HB	1.71	0.55
4:4:169:VAL:HG11	4:4:294:LEU:HD22	1.88	0.55
18:a:69:ASN:ND2	18:a:99:GLU:OE1	2.39	0.55
10:J:152:ARG:NH1	21:d:93:GLU:O	2.40	0.55
15:U:19:LEU:HG	16:W:81:ARG:HB2	1.89	0.55
2:2:2:ILE:HG22	17:X:152:VAL:HA	1.89	0.55
2:2:91:ILE:HG22	2:2:93:GLU:H	1.71	0.55
2:2:95:SER:H	19:b:31:LYS:NZ	2.05	0.55
1:1:374:ASN:ND2	3:3:81:TYR:H	2.05	0.55
5:5:495:LEU:HD13	7:8:59:GLU:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:42:VAL:HG13	9:D:46:ASP:CB	2.31	0.55
4:4:498:PHE:HE2	29:4:601:CDL:H332	1.71	0.55
29:4:601:CDL:H761	5:5:18:PHE:CE1	2.42	0.55
5:5:498:ASN:ND2	7:8:38:ASN:HB3	2.22	0.55
5:5:622:SER:HB2	18:a:40:ARG:HD2	1.89	0.55
4:4:476:GLY:HA2	18:a:88:GLN:HE22	1.71	0.54
5:5:375:ILE:HG23	5:5:386:MET:HE1	1.89	0.54
6:6:47:VAL:HG22	6:6:81:VAL:HG13	1.89	0.54
5:5:72:ILE:HG23	5:5:132:ASN:ND2	2.20	0.54
5:5:260:LEU:HB2	5:5:317:ILE:HD13	1.89	0.54
7:8:84:ARG:NH2	18:a:142:TYR:O	2.38	0.54
22:e:23:MET:O	22:e:27:ILE:HD12	2.07	0.54
2:2:63:LEU:HD21	2:2:292:LEU:HD23	1.89	0.54
5:5:554:PHE:CZ	5:5:563:ILE:HD11	2.43	0.54
18:a:72:ARG:HG3	18:a:104:LEU:HD11	1.90	0.54
2:2:459:LEU:HD11	4:4:221:LEU:HD22	1.88	0.54
5:5:570:ARG:NE	5:5:574:GLU:OE1	2.40	0.54
4:4:332:SER:HB2	4:4:345:TYR:HE2	1.72	0.54
15:U:71:LYS:HG2	15:U:75:ARG:HH11	1.72	0.54
1:1:168:SER:O	1:1:169:LEU:HB2	2.07	0.54
28:5:701:PC1:H133	24:i:20:TRP:CZ2	2.42	0.54
2:2:430:LEU:HD11	27:4:602:3PE:H281	1.89	0.54
6:6:127:TYR:CD2	6:6:131:ILE:HD11	2.43	0.54
12:Q:73:ALA:O	20:c:38:ARG:NH1	2.41	0.54
26:n:96:GLU:OE2	26:n:100:ARG:NE	2.40	0.54
5:5:264:SER:HA	5:5:267:ILE:HG12	1.89	0.54
5:5:665:LEU:HD11	10:J:62:PHE:CZ	2.43	0.54
17:X:112:MET:HE3	17:X:174:GLN:OE1	2.08	0.53
5:5:61:ILE:HG22	5:5:62:PHE:HD1	1.73	0.53
5:5:95:LEU:HB3	5:5:473:PRO:HB3	1.89	0.53
10:J:100:GLY:HA3	10:J:109:VAL:HA	1.89	0.53
18:a:91:ARG:NH2	18:a:95:GLU:O	2.42	0.53
1:1:353:ILE:HG21	27:1:401:3PE:H2D2	1.90	0.53
29:2:601:CDL:HA22	29:2:601:CDL:HA32	1.90	0.53
5:5:378:LEU:HA	5:5:381:VAL:HG22	1.91	0.53
2:2:292:LEU:HD11	2:2:363:THR:HG23	1.91	0.53
14:S:125:ARG:HG2	14:S:125:ARG:HH21	1.74	0.53
1:1:365:LEU:HA	1:1:370:ILE:HG13	1.91	0.53
4:4:461:SER:HA	4:4:464:TYR:CE2	2.42	0.53
5:5:30:LEU:O	5:5:34:SER:OG	2.24	0.53
24:i:48:TYR:O	24:i:52:HIS:ND1	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:278:PHE:CE1	2:2:282:ILE:HG13	2.44	0.53
10:J:28:GLY:HA3	10:J:63:ALA:HB2	1.91	0.53
24:i:67:SER:O	24:i:71:VAL:HG12	2.07	0.53
4:4:288:ALA:O	4:4:293:LYS:NZ	2.42	0.52
4:4:4:LEU:HG	4:4:171:LEU:HD22	1.91	0.52
5:5:644:ILE:HD13	6:6:120:PHE:CE2	2.43	0.52
16:W:90:GLU:HG3	16:W:94:LEU:HD12	1.90	0.52
2:2:512:ILE:HG22	2:2:520:ILE:HD12	1.92	0.52
4:4:519:HIS:CE1	5:5:67:SER:HA	2.44	0.52
10:J:69:TYR:HB2	10:J:95:ALA:HB2	1.91	0.52
17:X:106:ARG:O	17:X:110:MET:HG2	2.09	0.52
17:X:104:ASN:O	17:X:108:VAL:HG23	2.09	0.52
4:4:239:LEU:HD22	4:4:305:PRO:HB2	1.91	0.52
5:5:4:SER:HA	5:5:7:ILE:HG22	1.91	0.52
5:5:589:GLY:O	5:5:593:THR:HG23	2.09	0.52
1:1:9:SER:HB2	3:3:6:ILE:HD12	1.92	0.52
4:4:92:ILE:O	4:4:95:ILE:HG22	2.09	0.52
6:6:121:LEU:HB3	11:L:5:LEU:HD11	1.91	0.52
21:d:35:GLN:NE2	21:d:94:GLN:OE1	2.39	0.52
4:4:103:GLN:HG3	26:n:98:GLU:HG2	1.92	0.52
30:4:604:LMN:HBK	30:4:604:LMN:CBC	2.37	0.52
4:4:521:ASN:O	4:4:524:SER:OG	2.26	0.52
5:5:339:LEU:HG	5:5:376:ALA:HB1	1.92	0.52
24:i:55:ARG:HH22	24:i:71:VAL:HG21	1.74	0.52
8:9:10:GLY:HA2	26:n:141:PHE:O	2.09	0.51
15:U:1:MET:N	16:W:109:PRO:HD2	2.24	0.51
5:5:558:ARG:NH1	13:R:64:LYS:HE3	2.26	0.51
4:4:367:GLU:HG2	4:4:522:ILE:HD12	1.92	0.51
27:5:703:3PE:H11	27:J:201:3PE:H32	1.92	0.51
6:6:22:MET:HE3	6:6:25:ILE:HB	1.92	0.51
25:j:66:LYS:NZ	25:j:71:LEU:O	2.41	0.51
4:4:117:ASP:HB2	4:4:119:TYR:CZ	2.46	0.51
5:5:132:ASN:HB3	5:5:193:ASP:HA	1.93	0.51
24:i:30:ASN:HD22	26:n:51:LEU:HD23	1.75	0.51
5:5:189:LEU:O	21:d:78:TYR:OH	2.26	0.51
5:5:611:ARG:HH12	27:J:201:3PE:H112	1.74	0.51
18:a:74:LYS:HD2	18:a:104:LEU:HD23	1.91	0.51
2:2:276:THR:HG21	2:2:337:LYS:HE3	1.92	0.51
4:4:273:LEU:HD21	4:4:345:TYR:CD1	2.45	0.51
5:5:644:ILE:HG23	5:5:648:LEU:HD12	1.92	0.51
5:5:661:LEU:HD21	10:J:62:PHE:CD1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:338:LEU:HD11	5:5:372:VAL:HB	1.93	0.50
5:5:575:PHE:HZ	18:a:117:PRO:HD3	1.76	0.50
3:3:103:VAL:HG13	27:g:103:3PE:H241	1.93	0.50
5:5:147:SER:O	5:5:151:VAL:HG23	2.11	0.50
5:5:165:ILE:HG21	28:5:705:PC1:H322	1.92	0.50
9:D:78:PRO:HB2	9:D:80:LYS:NZ	2.26	0.50
25:j:52:TYR:HD1	25:j:53:LEU:HD22	1.76	0.50
2:2:53:LEU:HD11	2:2:60:ILE:HG12	1.92	0.50
4:4:157:ILE:HD13	27:4:602:3PE:H322	1.92	0.50
4:4:329:ALA:HA	4:4:345:TYR:CZ	2.46	0.50
6:6:22:MET:HE2	6:6:26:LEU:HG	1.92	0.50
6:6:68:PHE:HE2	11:L:57:ILE:HD11	1.77	0.50
10:J:191:PRO:HB3	25:j:67:ARG:HB2	1.94	0.50
5:5:412:ILE:O	5:5:415:THR:HG22	2.10	0.50
2:2:313:TYR:O	2:2:317:ILE:HG12	2.12	0.50
4:4:507:LEU:HD11	28:n:202:PC1:H2D2	1.94	0.50
5:5:133:TYR:HB2	5:5:192:LEU:HD13	1.94	0.50
6:6:51:ILE:HB	6:6:81:VAL:HG11	1.93	0.50
19:b:29:ASN:O	19:b:33:LEU:HG	2.12	0.50
2:2:427:LEU:HD23	19:b:21:GLY:HA3	1.94	0.50
5:5:659:ILE:O	5:5:663:LEU:HG	2.11	0.50
10:J:15:ASP:HB3	10:J:18:HIS:HB3	1.93	0.50
1:1:110:GLY:O	1:1:114:MET:HG3	2.11	0.50
5:5:202:PRO:HB3	5:5:269:TYR:CZ	2.46	0.50
26:n:92:ASP:OD1	26:n:92:ASP:N	2.42	0.50
5:5:319:LEU:HD21	5:5:399:ALA:HA	1.94	0.50
6:6:12:GLU:HB3	6:6:16:ASN:HB3	1.93	0.50
8:9:59:ARG:HG3	16:W:98:ILE:HB	1.94	0.50
21:d:9:PHE:O	21:d:10:LEU:HD22	2.12	0.50
2:2:92:PRO:HB3	19:b:29:ASN:HD21	1.77	0.49
5:5:568:ASN:ND2	13:R:68:PRO:HB2	2.28	0.49
5:5:623:LEU:HD11	5:5:666:MET:HE1	1.94	0.49
2:2:276:THR:HG23	2:2:381:PHE:CE1	2.47	0.49
13:R:97:LEU:HD23	13:R:99:PHE:CZ	2.46	0.49
2:2:138:PHE:O	2:2:142:THR:HG23	2.13	0.49
4:4:530:GLU:HB2	4:4:533:ALA:HB3	1.94	0.49
12:Q:96:LEU:HD22	12:Q:100:ASP:HB3	1.94	0.49
17:X:130:ARG:NH1	29:X:201:CDL:OA7	2.46	0.49
18:a:74:LYS:NZ	18:a:109:PRO:O	2.45	0.49
5:5:353:ASN:ND2	5:5:358:LYS:HB2	2.27	0.49
1:1:354:LEU:O	1:1:358:ILE:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:R:31:GLN:HE21	20:c:28:THR:HG23	1.76	0.49
17:X:112:MET:CE	17:X:174:GLN:OE1	2.60	0.49
29:2:601:CDL:H791	19:b:43:GLY:HA2	1.93	0.49
31:Q:201:ZMP:H22	13:R:17:LEU:HD23	1.95	0.49
2:2:99:ASP:HA	2:2:103:ASN:ND2	2.23	0.49
5:5:79:ASP:OD2	5:5:504:SER:OG	2.25	0.49
6:6:127:TYR:HA	6:6:130:ILE:HG12	1.95	0.49
3:3:105:GLU:OE2	6:6:215:ILE:HG12	2.13	0.49
4:4:340:LYS:HE3	32:4:777:HOH:O	2.13	0.49
4:4:351:ALA:HA	4:4:354:TYR:CE2	2.47	0.49
4:4:132:LEU:HD22	4:4:374:LEU:HD12	1.94	0.48
14:S:75:LEU:O	14:S:78:VAL:HG22	2.13	0.48
5:5:549:GLU:HB3	5:5:553:TYR:CE1	2.49	0.48
2:2:525:LEU:HD22	2:2:529:ASN:ND2	2.29	0.48
5:5:553:TYR:CD2	20:c:25:LEU:HD21	2.48	0.48
17:X:4:THR:HG22	17:X:6:THR:H	1.78	0.48
17:X:43:HIS:HB3	17:X:89:TYR:HE2	1.78	0.48
5:5:285:THR:HA	5:5:308:SER:HA	1.93	0.48
5:5:48:PHE:HA	5:5:52:PHE:HD2	1.77	0.48
7:8:73:MET:HG3	7:8:76:LEU:HD23	1.94	0.48
10:J:93:LEU:HD12	10:J:117:GLY:HA3	1.95	0.48
1:1:71:THR:HG23	3:3:35:LEU:HB3	1.95	0.48
4:4:237:VAL:HA	4:4:240:LYS:NZ	2.29	0.48
30:4:604:LMN:HCL	30:4:604:LMN:HBL	1.96	0.48
7:8:67:LYS:HA	7:8:70:VAL:HG22	1.96	0.48
5:5:203:TYR:OH	21:d:75:ARG:NH2	2.46	0.48
10:J:31:GLY:HA2	10:J:62:PHE:CD2	2.49	0.48
1:1:164:MET:HE1	1:1:358:ILE:HG23	1.96	0.48
5:5:3:LEU:HD21	5:5:61:ILE:HD11	1.95	0.48
20:c:43:ARG:O	20:c:48:PHE:HB2	2.14	0.48
5:5:79:ASP:H	5:5:82:THR:HB	1.79	0.48
5:5:357:ARG:HG2	13:R:23:VAL:HG22	1.95	0.48
15:U:117:TRP:CD2	15:U:162:PRO:HA	2.49	0.48
20:c:60:GLY:HA3	22:e:21:ALA:N	2.29	0.47
2:2:92:PRO:O	2:2:95:SER:OG	2.29	0.47
2:2:509:SER:OG	2:2:511:ARG:NH2	2.48	0.47
5:5:24:GLY:HA3	24:i:24:PRO:HD2	1.94	0.47
5:5:508:HIS:CE1	18:a:160:LEU:HD13	2.48	0.47
6:6:9:LEU:HB2	16:W:115:PRO:HG2	1.95	0.47
10:J:84:ASP:N	10:J:84:ASP:OD1	2.47	0.47
4:4:20:THR:HG23	19:b:28:PHE:HE2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:220:PHE:CZ	1:1:221:MET:HE3	2.49	0.47
4:4:269:ASN:ND2	4:4:345:TYR:HE1	2.13	0.47
5:5:253:VAL:HB	5:5:310:LEU:HD11	1.96	0.47
11:L:9:LEU:HA	11:L:12:ILE:HG22	1.97	0.47
25:j:60:LEU:HB2	25:j:75:ARG:NH1	2.30	0.47
1:1:243:MET:SD	32:1:558:HOH:O	2.61	0.47
5:5:11:LEU:HB3	24:i:38:ILE:HG12	1.96	0.47
7:8:14:ARG:HA	7:8:17:MET:HB3	1.95	0.47
4:4:142:VAL:O	4:4:492:ARG:HD2	2.15	0.47
4:4:370:ILE:HD12	4:4:522:ILE:HD11	1.96	0.47
5:5:654:TYR:O	5:5:658:ILE:HG12	2.13	0.47
7:8:18:ARG:HG2	21:d:66:ASN:HD22	1.78	0.47
11:L:63:ALA:HB1	32:L:111:HOH:O	2.15	0.47
1:1:86:LEU:HD11	1:1:234:LEU:HD23	1.97	0.47
19:b:50:LEU:HD23	19:b:53:ILE:HD11	1.97	0.47
6:6:194:THR:HB	17:X:138:VAL:HG11	1.97	0.47
2:2:157:TYR:OH	11:L:66:GLU:HB2	2.14	0.47
2:2:498:ASN:OD1	2:2:500:VAL:HG22	2.15	0.47
5:5:289:SER:HA	5:5:424:TYR:HE2	1.80	0.47
14:S:123:GLU:HB2	21:d:9:PHE:CZ	2.50	0.47
5:5:577:TYR:CE2	28:5:705:PC1:H281	2.51	0.46
27:4:602:3PE:H361	27:4:602:3PE:H332	1.49	0.46
5:5:660:ILE:O	5:5:664:LEU:HG	2.14	0.46
9:D:81:VAL:HB	15:U:11:HIS:HB2	1.98	0.46
12:Q:75:PHE:CZ	12:Q:104:VAL:HG22	2.50	0.46
14:S:125:ARG:HD3	14:S:134:LEU:HD13	1.98	0.46
14:S:136:ASP:OD1	14:S:136:ASP:N	2.47	0.46
4:4:85:LEU:HA	4:4:88:ILE:HD12	1.97	0.46
17:X:8:THR:HB	17:X:168:THR:H	1.80	0.46
1:1:18:VAL:HB	1:1:19:PRO:HD3	1.97	0.46
4:4:386:CYS:HA	4:4:390:ILE:HD12	1.97	0.46
2:2:92:PRO:O	19:b:31:LYS:HD3	2.15	0.46
5:5:53:ASN:OD1	24:i:63:ARG:HG2	2.16	0.46
5:5:353:ASN:HD21	5:5:358:LYS:HB2	1.80	0.46
13:R:34:TYR:O	13:R:37:SER:OG	2.30	0.46
24:i:51:GLU:HB3	24:i:52:HIS:CE1	2.50	0.46
4:4:250:PHE:CB	30:4:604:LMN:HBTA	2.46	0.46
5:5:588:LEU:O	5:5:592:ILE:HG13	2.16	0.46
17:X:55:LEU:HD23	17:X:75:MET:SD	2.56	0.46
5:5:33:CYS:O	5:5:37:ILE:HG12	2.16	0.46
14:S:84:TYR:OH	14:S:90:GLU:OE1	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:49:LYS:NZ	2:2:571:ALA:HB3	2.31	0.46
3:3:30:PRO:HB2	3:3:35:LEU:HD11	1.97	0.46
3:3:68:LEU:HD22	11:L:61:VAL:HA	1.97	0.46
5:5:664:LEU:HD22	10:J:112:PHE:CE1	2.51	0.46
8:9:56:GLU:HB2	16:W:100:VAL:HG11	1.97	0.46
2:2:197:LEU:O	2:2:201:SER:OG	2.22	0.46
2:2:211:ILE:HD11	26:n:129:LEU:HD21	1.97	0.46
4:4:319:TYR:CD2	4:4:447:LEU:HD12	2.51	0.46
4:4:444:LEU:HD23	5:5:183:PHE:HB3	1.98	0.46
10:J:153:ARG:O	21:d:96:ASN:HA	2.15	0.46
2:2:182:LEU:HD11	5:5:631:TYR:HB3	1.98	0.45
4:4:3:LEU:HD22	4:4:89:VAL:HG13	1.98	0.45
5:5:87:ILE:HB	5:5:88:PRO:HD3	1.98	0.45
5:5:400:TYR:HD2	5:5:521:VAL:HG22	1.82	0.45
5:5:298:ILE:O	5:5:302:ILE:HG13	2.16	0.45
5:5:483:PHE:O	5:5:487:ILE:HG13	2.17	0.45
5:5:640:ILE:O	5:5:644:ILE:HG12	2.16	0.45
21:d:91:LEU:O	21:d:95:GLN:HG3	2.16	0.45
1:1:210:ALA:O	1:1:219:GLY:HA3	2.15	0.45
5:5:226:GLN:O	5:5:230:HIS:HB3	2.16	0.45
5:5:387:THR:OG1	5:5:480:PHE:O	2.24	0.45
6:6:33:SER:O	6:6:37:VAL:HG23	2.15	0.45
26:n:151:LEU:O	26:n:155:ILE:HG12	2.16	0.45
5:5:57:VAL:HG12	5:5:78:TYR:HB2	1.99	0.45
5:5:199:SER:OG	21:d:56:LEU:HD21	2.17	0.45
27:8:101:3PE:H221	27:8:101:3PE:H2	1.78	0.45
10:J:169:LYS:HZ3	10:J:173:TYR:HE2	1.62	0.45
2:2:17:LEU:HD13	2:2:17:LEU:HA	1.82	0.45
2:2:54:HIS:HA	17:X:142:GLN:HA	1.97	0.45
2:2:68:HIS:HE1	2:2:140:ILE:HB	1.82	0.45
4:4:410:MET:HG2	4:4:488:ASP:HA	1.98	0.45
29:4:601:CDL:HB31	26:n:54:ALA:HB2	1.99	0.45
7:8:52:GLU:OE2	7:8:56:HIS:NE2	2.49	0.45
24:i:55:ARG:NH2	24:i:71:VAL:HG21	2.31	0.45
3:3:12:SER:O	3:3:16:ILE:HG12	2.17	0.45
5:5:217:LEU:HD12	5:5:217:LEU:HA	1.75	0.45
12:Q:75:PHE:HA	20:c:35:PRO:O	2.16	0.45
31:Q:201:ZMP:O7	13:R:8:LEU:HD21	2.17	0.45
29:g:101:CDL:HB4	29:g:101:CDL:H512	1.48	0.45
1:1:99:GLY:HA3	1:1:102:LEU:HD12	1.99	0.45
2:2:191:LEU:HG	11:L:36:ILE:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:542:THR:HA	5:5:546:LEU:HB2	1.99	0.45
10:J:14:LYS:NZ	10:J:83:GLU:OE2	2.46	0.45
4:4:529:ILE:HG23	21:d:92:PHE:HB3	1.98	0.45
4:4:531:PRO:HG3	10:J:169:LYS:HB3	1.99	0.45
5:5:186:LEU:HG	5:5:192:LEU:HD23	1.98	0.45
7:8:58:TYR:O	7:8:62:GLN:HG2	2.17	0.45
13:R:31:GLN:HG2	20:c:24:PHE:CE1	2.51	0.45
4:4:488:ASP:CG	4:4:489:LEU:H	2.25	0.45
10:J:192:VAL:HG13	25:j:68:ARG:O	2.17	0.45
13:R:60:LYS:O	13:R:64:LYS:N	2.49	0.45
18:a:159:GLU:CD	18:a:159:GLU:H	2.25	0.45
2:2:161:LEU:HD13	6:6:213:GLY:HA3	1.97	0.44
5:5:134:LEU:HB2	5:5:192:LEU:HD11	1.97	0.44
15:U:44:GLY:O	15:U:48:LYS:HB2	2.17	0.44
1:1:46:ALA:O	28:1:403:PC1:H112	2.17	0.44
4:4:220:LEU:O	4:4:224:LEU:HG	2.18	0.44
5:5:603:LEU:O	5:5:608:GLY:HA3	2.18	0.44
6:6:36:CYS:HA	6:6:39:ILE:HG12	1.99	0.44
11:L:18:ASN:HD21	11:L:24:LEU:HB3	1.83	0.44
11:L:37:THR:HG23	11:L:56:ALA:HB1	1.99	0.44
24:i:30:ASN:HD22	26:n:51:LEU:CD2	2.31	0.44
2:2:284:LYS:HE2	2:2:344:THR:HG21	1.98	0.44
2:2:404:LEU:HB2	2:2:407:LYS:HE3	1.98	0.44
6:6:13:ILE:HG23	6:6:14:TYR:H	1.83	0.44
7:8:47:LEU:HD13	7:8:49:TRP:CZ2	2.52	0.44
8:9:73:LYS:HE3	8:9:73:LYS:HB2	1.81	0.44
14:S:125:ARG:HG2	14:S:125:ARG:NH2	2.33	0.44
2:2:242:PHE:HD1	6:6:124:MET:SD	2.41	0.44
3:3:10:PHE:HA	3:3:13:ILE:HG12	1.98	0.44
5:5:124:MET:HE2	5:5:143:VAL:HG11	1.99	0.44
15:U:64:ARG:HG3	15:U:68:GLU:HG3	1.98	0.44
21:d:12:LYS:HD2	21:d:40:ARG:NH2	2.32	0.44
4:4:92:ILE:HG23	27:n:203:3PE:H321	2.00	0.44
4:4:109:GLU:HA	26:n:104:MET:HE2	1.99	0.44
28:5:701:PC1:H11	28:5:701:PC1:C14	2.41	0.44
6:6:12:GLU:HG2	6:6:14:TYR:O	2.18	0.44
10:J:88:ASN:HB2	10:J:124:GLU:HG3	2.00	0.44
13:R:61:LEU:HD13	20:c:19:PHE:HD2	1.82	0.44
14:S:123:GLU:HB2	21:d:9:PHE:CE2	2.52	0.44
15:U:158:PRO:O	15:U:161:ARG:NH1	2.51	0.44
2:2:515:GLU:HG2	2:2:516:LYS:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:290:ILE:HG13	32:4:775:HOH:O	2.17	0.44
27:5:704:3PE:H322	27:5:704:3PE:H351	1.71	0.44
2:2:566:GLN:O	2:2:570:SER:OG	2.28	0.44
4:4:458:ILE:H	4:4:458:ILE:HD12	1.83	0.44
5:5:503:ASN:ND2	21:d:60:TYR:OH	2.51	0.44
16:W:50:ILE:HA	16:W:53:GLN:HG2	2.00	0.44
2:2:167:ARG:O	11:L:80:LEU:HD11	2.16	0.44
2:2:560:MET:HE1	30:2:602:LMN:HBB	1.98	0.44
4:4:15:ILE:HG23	4:4:157:ILE:HG12	1.99	0.44
15:U:83:VAL:O	15:U:87:ILE:HG13	2.18	0.44
28:n:202:PC1:H271	28:n:202:PC1:H2A1	1.79	0.44
4:4:100:SER:OG	21:d:12:LYS:NZ	2.35	0.44
4:4:481:TYR:HA	25:j:10:ALA:HB3	2.00	0.44
5:5:282:ALA:HB2	5:5:315:LEU:HD12	2.00	0.44
5:5:409:ALA:O	5:5:413:ILE:HG12	2.18	0.44
26:n:105:ALA:O	26:n:109:GLU:HG2	2.18	0.44
1:1:113:TYR:HE1	27:1:402:3PE:H232	1.82	0.43
4:4:449:ILE:HG13	4:4:450:ALA:N	2.33	0.43
5:5:120:PHE:CE1	5:5:247:ILE:HG23	2.52	0.43
7:8:27:ARG:HB2	18:a:156:LEU:HD11	1.99	0.43
23:g:33:GLY:HA3	27:g:103:3PE:H2G2	1.99	0.43
5:5:200:LEU:O	5:5:204:ILE:HG13	2.18	0.43
15:U:113:ARG:N	15:U:114:PRO:HD2	2.33	0.43
21:d:79:LEU:HB3	25:j:67:ARG:NH2	2.32	0.43
26:n:95:ASP:N	26:n:95:ASP:OD1	2.51	0.43
4:4:497:LEU:O	4:4:501:VAL:HG22	2.18	0.43
4:4:510:TYR:CG	27:4:603:3PE:H222	2.53	0.43
6:6:131:ILE:HG21	6:6:169:PHE:HZ	1.81	0.43
12:Q:118:ASP:OD1	12:Q:119:LYS:N	2.51	0.43
23:g:18:TRP:CD1	23:g:22:GLU:HG3	2.54	0.43
1:1:218:SER:HB2	1:1:222:THR:HA	2.00	0.43
1:1:322:ILE:O	1:1:326:VAL:HG23	2.19	0.43
2:2:107:TYR:CE2	2:2:109:ARG:HB3	2.53	0.43
2:2:415:ILE:HG22	2:2:487:GLU:HG3	2.00	0.43
6:6:27:SER:HA	11:L:3:ILE:HD12	2.00	0.43
6:6:213:GLY:HA2	6:6:216:VAL:HG12	2.01	0.43
18:a:173:ASP:OD1	18:a:173:ASP:N	2.48	0.43
19:b:7:PHE:O	19:b:11:PHE:N	2.49	0.43
21:d:12:LYS:HB3	21:d:40:ARG:NH1	2.34	0.43
1:1:20:SER:O	1:1:24:ILE:HG12	2.18	0.43
3:3:9:ILE:O	3:3:13:ILE:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:429:LEU:HD12	28:5:701:PC1:H2H1	1.99	0.43
12:Q:71:LEU:HD22	12:Q:111:GLU:HG2	1.99	0.43
18:a:91:ARG:NH1	25:j:12:ASP:OD2	2.44	0.43
4:4:219:LEU:HB2	4:4:258:ALA:CB	2.49	0.43
5:5:121:THR:HG23	32:5:824:HOH:O	2.18	0.43
7:8:37:LEU:HD13	7:8:55:ARG:HA	2.00	0.43
12:Q:112:PHE:CE2	12:Q:134:ILE:HG21	2.53	0.43
14:S:120:ALA:HB3	21:d:47:MET:HG3	1.99	0.43
26:n:153:HIS:H	26:n:153:HIS:CD2	2.37	0.43
2:2:507:ASN:ND2	2:2:524:LEU:HB3	2.34	0.43
5:5:664:LEU:HD13	10:J:112:PHE:CG	2.54	0.43
6:6:6:SER:HA	15:U:16:THR:OG1	2.18	0.43
11:L:27:ILE:O	11:L:30:GLU:HB2	2.19	0.43
1:1:318:VAL:HG22	9:D:15:ILE:HD13	2.01	0.43
2:2:282:ILE:HA	2:2:285:ILE:HD12	2.01	0.43
4:4:2:SER:HB2	4:4:108:GLN:HB2	2.01	0.43
5:5:237:MET:HE1	5:5:248:HIS:HB2	2.00	0.43
5:5:603:LEU:HD11	5:5:611:ARG:HH11	1.83	0.43
1:1:159:ILE:O	1:1:163:ILE:HG12	2.19	0.43
1:1:233:PHE:HD1	1:1:233:PHE:HA	1.66	0.43
2:2:118:GLU:HA	2:2:118:GLU:OE1	2.17	0.43
30:2:602:LMN:HBK	30:2:602:LMN:HBEA	1.85	0.43
4:4:390:ILE:HD13	4:4:489:LEU:HD21	2.00	0.43
14:S:126:ARG:CZ	21:d:5:GLU:HG2	2.49	0.43
18:a:152:PHE:HB3	18:a:156:LEU:HD23	2.00	0.43
22:e:24:TRP:O	22:e:28:PHE:HD1	2.02	0.43
4:4:518:LEU:HG	4:4:522:ILE:CD1	2.48	0.43
10:J:14:LYS:O	10:J:78:ASN:ND2	2.37	0.43
18:a:75:ARG:HD2	18:a:89:GLU:O	2.19	0.43
2:2:363:THR:HG22	2:2:565:VAL:HG22	2.00	0.42
17:X:130:ARG:HH12	29:X:201:CDL:HB21	1.84	0.42
25:j:26:TYR:OH	25:j:27:LYS:HE3	2.19	0.42
1:1:374:ASN:HD21	3:3:81:TYR:H	1.67	0.42
7:8:34:LEU:HD13	7:8:58:TYR:CZ	2.54	0.42
2:2:10:LEU:HA	2:2:127:LEU:HD11	2.02	0.42
2:2:537:SER:HB2	19:b:19:GLN:HG2	2.00	0.42
29:4:601:CDL:H711	24:i:16:PRO:HB3	2.01	0.42
6:6:42:ASN:ND2	6:6:94:ILE:HG23	2.33	0.42
8:9:57:ALA:O	8:9:61:ARG:HB2	2.19	0.42
12:Q:68:ILE:HG13	12:Q:108:ILE:HD11	2.01	0.42
31:Q:201:ZMP:H24A	13:R:17:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:198:SER:HB2	4:4:278:GLU:OE1	2.19	0.42
5:5:647:ASN:HD21	6:6:123:LYS:HE2	1.84	0.42
6:6:118:SER:HB3	11:L:9:LEU:HD11	2.02	0.42
27:g:103:3PE:H32	27:g:103:3PE:H322	1.79	0.42
24:i:49:SER:OG	24:i:53:GLU:OE2	2.28	0.42
1:1:169:LEU:HD23	1:1:169:LEU:HA	1.95	0.42
4:4:462:ALA:HB1	5:5:168:PHE:HE2	1.84	0.42
4:4:502:SER:HA	29:4:601:CDL:H821	2.01	0.42
28:4:605:PC1:H2C1	5:5:609:LEU:HD13	2.01	0.42
1:1:92:GLY:HA3	1:1:242:LEU:HD21	2.02	0.42
4:4:324:ILE:HD11	25:j:46:VAL:HG12	2.01	0.42
5:5:356:PHE:CZ	5:5:428:VAL:HG22	2.54	0.42
5:5:385:PHE:HE2	22:e:31:ALA:HB2	1.84	0.42
12:Q:106:MET:CE	13:R:15:LEU:HD12	2.49	0.42
15:U:157:PRO:HB2	15:U:160:GLU:HG2	2.01	0.42
1:1:340:ASP:OD1	1:1:341:GLN:N	2.53	0.42
4:4:448:PRO:O	4:4:452:MET:HG2	2.20	0.42
4:4:519:HIS:CD2	14:S:117:GLN:NE2	2.86	0.42
10:J:106:ILE:O	10:J:109:VAL:HG22	2.20	0.42
14:S:129:GLU:HG2	14:S:136:ASP:HB3	2.01	0.42
23:g:50:ILE:HD11	27:g:102:3PE:O22	2.19	0.42
2:2:95:SER:H	19:b:31:LYS:HZ2	1.67	0.42
4:4:210:LEU:HD12	28:4:605:PC1:H341	2.01	0.42
5:5:47:PHE:HE1	5:5:84:SER:HA	1.84	0.42
5:5:555:LYS:HD2	13:R:21:TRP:HE3	1.85	0.42
12:Q:106:MET:SD	13:R:12:ARG:HA	2.59	0.42
13:R:82:TYR:CE1	13:R:83:GLU:HG3	2.55	0.42
16:W:43:TRP:HE1	27:g:102:3PE:H3F1	1.85	0.42
1:1:151:TYR:CE1	1:1:201:GLU:HG2	2.54	0.42
2:2:144:ASP:OD2	2:2:204:THR:HG23	2.20	0.42
4:4:295:SER:O	4:4:299:VAL:HG23	2.20	0.42
4:4:306:ILE:C	4:4:308:PRO:HD3	2.44	0.42
4:4:498:PHE:CE2	29:4:601:CDL:H332	2.53	0.42
29:4:601:CDL:H581	26:n:58:ALA:HB2	2.01	0.42
5:5:338:LEU:HD23	5:5:376:ALA:HB2	2.01	0.42
6:6:90:MET:HE3	6:6:91:LEU:HD21	2.02	0.42
16:W:32:LEU:HD23	16:W:32:LEU:HA	1.89	0.42
16:W:48:LYS:HE3	16:W:48:LYS:HB3	1.88	0.42
25:j:13:PRO:HA	25:j:16:VAL:HG22	2.02	0.42
2:2:278:PHE:CD1	2:2:282:ILE:HG13	2.55	0.42
2:2:387:ILE:HG12	2:2:421:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:98:ASP:OD2	4:4:101:ASN:HB2	2.20	0.41
4:4:159:MET:HE3	32:4:745:HOH:O	2.19	0.41
4:4:487:ARG:HH11	14:S:77:GLY:HA3	1.85	0.41
5:5:665:LEU:HD11	10:J:62:PHE:CE1	2.55	0.41
31:Q:201:ZMP:H15	13:R:42:ASN:O	2.19	0.41
14:S:100:SER:HA	27:n:203:3PE:H3C1	2.02	0.41
16:W:34:GLY:HA3	27:W:201:3PE:H292	2.02	0.41
1:1:145:THR:HA	1:1:148:LEU:HD23	2.02	0.41
2:2:259:PRO:HD2	2:2:260:PHE:CE2	2.55	0.41
5:5:89:VAL:HG12	32:5:824:HOH:O	2.19	0.41
5:5:383:PHE:O	5:5:389:PHE:HB2	2.20	0.41
5:5:430:TYR:OH	5:5:545:GLU:HB2	2.19	0.41
7:8:22:VAL:CG2	7:8:27:ARG:HE	2.34	0.41
25:j:34:ARG:O	25:j:38:VAL:HG23	2.20	0.41
28:n:202:PC1:H382	28:n:202:PC1:H3B2	1.83	0.41
4:4:510:TYR:OH	5:5:63:ARG:NH2	2.53	0.41
5:5:61:ILE:HA	24:i:48:TYR:OH	2.20	0.41
5:5:356:PHE:HZ	5:5:428:VAL:HG22	1.85	0.41
12:Q:75:PHE:HB3	12:Q:77:LYS:H	1.86	0.41
24:i:68:ARG:HA	24:i:74:ILE:HD11	2.03	0.41
1:1:49:ILE:O	1:1:52:LEU:HG	2.20	0.41
3:3:76:PHE:HB2	6:6:193:TYR:CZ	2.56	0.41
5:5:264:SER:OG	5:5:265:PRO:HD3	2.19	0.41
12:Q:106:MET:HE1	13:R:15:LEU:HD12	2.03	0.41
1:1:185:LEU:HB3	16:W:42:GLY:HA3	2.03	0.41
1:1:207:PHE:CD1	1:1:342:LEU:HD13	2.55	0.41
2:2:109:ARG:O	2:2:113:ILE:HG12	2.20	0.41
5:5:611:ARG:NH2	27:5:703:3PE:H121	2.35	0.41
18:a:159:GLU:OE2	18:a:159:GLU:N	2.53	0.41
4:4:468:MET:HE2	4:4:468:MET:HB3	1.89	0.41
27:4:603:3PE:H271	27:4:603:3PE:H241	1.91	0.41
30:4:604:LMN:HBL	30:4:604:LMN:HBT	1.82	0.41
5:5:508:HIS:ND1	5:5:510:ILE:HG12	2.35	0.41
12:Q:85:THR:H	12:Q:88:ALA:HB2	1.85	0.41
1:1:34:THR:O	1:1:38:MET:HG3	2.20	0.41
2:2:171:LEU:HD23	2:2:171:LEU:HA	1.92	0.41
2:2:284:LYS:HE2	2:2:344:THR:CG2	2.51	0.41
5:5:496:GLY:HA2	7:8:26:TYR:CE2	2.55	0.41
6:6:213:GLY:O	6:6:216:VAL:HG12	2.20	0.41
10:J:193:CYS:O	10:J:195:ASP:N	2.53	0.41
29:X:201:CDL:H122	29:X:201:CDL:H151	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:85:TYR:CE1	2:2:115:LYS:HA	2.56	0.41
3:3:86:TYR:HD2	6:6:194:THR:HG22	1.86	0.41
4:4:196:PHE:HB2	4:4:280:PRO:HG3	2.03	0.41
5:5:3:LEU:HD23	5:5:3:LEU:HA	1.92	0.41
5:5:565:GLY:HA3	18:a:114:TRP:CZ2	2.55	0.41
5:5:661:LEU:HD12	10:J:65:VAL:HG11	2.03	0.41
6:6:50:LEU:HD13	11:L:27:ILE:HG23	2.01	0.41
31:Q:201:ZMP:H24A	13:R:17:LEU:HD23	2.02	0.41
14:S:98:TRP:CZ3	28:n:202:PC1:H3G2	2.56	0.41
1:1:184:ILE:HG23	1:1:185:LEU:HD22	2.02	0.41
2:2:237:PRO:HG2	2:2:306:LEU:HD11	2.03	0.41
3:3:101:GLY:O	3:3:105:GLU:HG2	2.21	0.41
32:3:307:HOH:O	6:6:211:MET:HE3	2.21	0.41
4:4:408:GLN:HB3	13:R:88:VAL:HG12	2.02	0.41
5:5:140:TRP:CE2	5:5:223:LYS:HD2	2.56	0.41
13:R:97:LEU:HD23	13:R:99:PHE:HZ	1.83	0.41
18:a:154:GLY:C	18:a:170:LEU:HD22	2.46	0.41
18:a:174:ASP:OD1	18:a:174:ASP:N	2.49	0.41
23:g:15:TYR:CZ	29:g:101:CDL:HB62	2.55	0.41
28:n:202:PC1:H2E1	28:n:202:PC1:H2B1	1.82	0.41
2:2:9:LEU:HG	2:2:127:LEU:HD12	2.02	0.41
2:2:79:LEU:HD13	2:2:129:LEU:HD22	2.03	0.41
2:2:88:LYS:HB3	2:2:88:LYS:HE2	1.88	0.41
2:2:321:LEU:HD11	27:5:702:3PE:H392	2.03	0.41
3:3:5:SER:O	3:3:9:ILE:HG12	2.21	0.41
5:5:477:LEU:HD23	5:5:477:LEU:HA	1.89	0.41
6:6:77:TYR:HA	6:6:80:ALA:HB3	2.03	0.41
1:1:53:LEU:HD11	28:1:403:PC1:H331	2.03	0.40
5:5:660:ILE:HD11	10:J:119:VAL:HG11	2.03	0.40
27:5:702:3PE:H371	27:5:702:3PE:H271	2.03	0.40
10:J:38:ARG:HH11	10:J:55:ASN:ND2	2.19	0.40
10:J:96:GLY:HA2	10:J:99:MET:HE3	2.04	0.40
15:U:39:ALA:O	15:U:43:ILE:HG12	2.22	0.40
22:e:41:TRP:N	22:e:41:TRP:CD1	2.89	0.40
2:2:342:TYR:HA	2:2:345:ILE:HD12	2.04	0.40
5:5:604:PHE:HA	27:5:703:3PE:H321	2.03	0.40
11:L:44:SER:OG	11:L:52:GLY:HA3	2.22	0.40
6:6:109:LEU:HD12	10:J:37:VAL:HA	2.03	0.40
1:1:373:VAL:HG21	16:W:57:ALA:HB2	2.03	0.40
5:5:61:ILE:HG22	5:5:62:PHE:CD1	2.55	0.40
5:5:508:HIS:CE1	18:a:166:VAL:HG13	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:22:MET:HE3	6:6:22:MET:O	2.22	0.40
8:9:31:GLU:OE1	26:n:124:SER:OG	2.33	0.40
8:9:77:GLU:HG2	8:9:78:ASN:N	2.36	0.40
17:X:40:ASP:O	17:X:90:PHE:HD1	2.05	0.40
17:X:45:LEU:HD23	17:X:45:LEU:HA	1.93	0.40
2:2:538:ILE:HD12	29:2:601:CDL:H122	2.02	0.40
4:4:96:LEU:HD22	26:n:91:SER:HB3	2.03	0.40
5:5:189:LEU:HD11	5:5:204:ILE:HD11	2.04	0.40
5:5:604:PHE:CE1	27:J:201:3PE:H241	2.57	0.40
17:X:169:ALA:O	17:X:173:GLN:HG3	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	1	330/378 (87%)	317 (96%)	13 (4%)	0	100	100
2	2	554/571 (97%)	545 (98%)	9 (2%)	0	100	100
3	3	112/146 (77%)	108 (96%)	4 (4%)	0	100	100
4	4	490/542 (90%)	479 (98%)	11 (2%)	0	100	100
5	5	668/679 (98%)	638 (96%)	30 (4%)	0	100	100
6	6	186/224 (83%)	178 (96%)	8 (4%)	0	100	100
7	8	75/86 (87%)	71 (95%)	4 (5%)	0	100	100
8	9	101/785 (13%)	100 (99%)	1 (1%)	0	100	100
9	D	79/86 (92%)	78 (99%)	1 (1%)	0	100	100
10	J	184/199 (92%)	179 (97%)	5 (3%)	0	100	100
11	L	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
12	Q	83/141 (59%)	83 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	R	96/99 (97%)	93 (97%)	3 (3%)	0	100	100
14	S	72/143 (50%)	68 (94%)	4 (6%)	0	100	100
15	U	167/186 (90%)	162 (97%)	5 (3%)	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	141/815 (17%)	136 (96%)	5 (4%)	0	100	100
19	b	79/94 (84%)	78 (99%)	1 (1%)	0	100	100
20	c	58/93 (62%)	50 (86%)	8 (14%)	0	100	100
21	d	96/105 (91%)	92 (96%)	4 (4%)	0	100	100
22	e	35/46 (76%)	35 (100%)	0	0	100	100
23	g	76/82 (93%)	74 (97%)	2 (3%)	0	100	100
24	i	78/93 (84%)	75 (96%)	3 (4%)	0	100	100
25	j	71/75 (95%)	68 (96%)	3 (4%)	0	100	100
26	n	133/184 (72%)	129 (97%)	4 (3%)	0	100	100
All	All	4332/6253 (69%)	4198 (97%)	134 (3%)	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	1	284/326 (87%)	275 (97%)	9 (3%)	34	59
2	2	509/518 (98%)	502 (99%)	7 (1%)	59	78
3	3	97/128 (76%)	97 (100%)	0	100	100
4	4	431/477 (90%)	431 (100%)	0	100	100
5	5	579/596 (97%)	578 (100%)	1 (0%)	87	95
6	6	162/203 (80%)	160 (99%)	2 (1%)	63	80
7	8	69/75 (92%)	69 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	9	84/687 (12%)	84 (100%)	0	100	100
9	D	68/69 (99%)	67 (98%)	1 (2%)	57	77
10	J	126/146 (86%)	126 (100%)	0	100	100
11	L	73/76 (96%)	72 (99%)	1 (1%)	59	78
12	Q	72/119 (60%)	72 (100%)	0	100	100
13	R	87/89 (98%)	87 (100%)	0	100	100
14	S	59/111 (53%)	59 (100%)	0	100	100
15	U	149/167 (89%)	148 (99%)	1 (1%)	76	88
16	W	82/102 (80%)	82 (100%)	0	100	100
17	X	145/152 (95%)	144 (99%)	1 (1%)	76	88
18	a	123/697 (18%)	122 (99%)	1 (1%)	73	86
19	b	67/74 (90%)	67 (100%)	0	100	100
20	c	47/80 (59%)	47 (100%)	0	100	100
21	d	87/94 (93%)	87 (100%)	0	100	100
22	e	29/35 (83%)	29 (100%)	0	100	100
23	g	65/69 (94%)	65 (100%)	0	100	100
24	i	68/78 (87%)	68 (100%)	0	100	100
25	j	63/64 (98%)	63 (100%)	0	100	100
26	n	106/150 (71%)	105 (99%)	1 (1%)	70	84
All	All	3731/5382 (69%)	3706 (99%)	25 (1%)	73	88

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	104	VAL
1	1	109	THR
1	1	111	ILE
1	1	134	SER
1	1	148	LEU
1	1	223	GLU
1	1	230	VAL
1	1	233	PHE
1	1	330	THR
2	2	17	LEU
2	2	23	ILE

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Mol	Chain	Res	Type
2	2	60	ILE
2	2	79	LEU
2	2	129	LEU
2	2	164	THR
2	2	564	LEU
5	5	223	LYS
6	6	73	TYR
6	6	198	VAL
9	D	74	GLU
11	L	86	ILE
15	U	23	ILE
17	X	96	LEU
18	a	43	ILE
26	n	103	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	74	ASN
1	1	147	GLN
1	1	203	ASN
1	1	374	ASN
2	2	62	ASN
2	2	119	HIS
2	2	502	ASN
4	4	248	GLN
4	4	309	GLN
5	5	109	HIS
5	5	171	ASN
5	5	353	ASN
5	5	503	ASN
5	5	511	HIS
5	5	562	ASN
6	6	67	ASN
6	6	93	ASN
6	6	105	ASN
6	6	182	ASN
6	6	190	ASN
8	9	8	ASN
8	9	64	GLN
11	L	18	ASN
13	R	24	HIS

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Mol	Chain	Res	Type
13	R	85	ASN
14	S	117	GLN
15	U	56	GLN
15	U	61	ASN
16	W	54	ASN
17	X	65	GLN
17	X	142	GLN
18	a	92	ASN
20	c	39	HIS
21	d	45	GLN
22	e	12	HIS
24	i	29	GLN
26	n	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

32 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	$\# Z > 2$
27	3PE	n	201	-	38,38,50	1.00	4 (10%)	41,43,55	1.15	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CDL	X	201	-	78,78,99	0.32	0	84,90,111	0.41	0
27	3PE	5	702	-	39,39,50	0.31	0	42,44,55	0.37	0
28	PC1	2	603	-	30,30,53	0.34	0	36,38,61	0.37	0
28	PC1	4	605	-	44,44,53	1.04	4 (9%)	50,52,61	1.07	2 (4%)
29	CDL	4	601	-	85,85,99	0.29	0	91,97,111	0.35	0
27	3PE	4	602	-	33,33,50	1.06	4 (12%)	36,38,55	1.14	2 (5%)
28	PC1	5	701	-	44,44,53	0.46	0	50,52,61	0.47	0
28	PC1	n	202	-	50,50,53	0.98	4 (8%)	56,58,61	1.09	2 (3%)
29	CDL	D	101	-	58,58,99	0.34	0	64,70,111	0.45	0
29	CDL	2	601	-	83,83,99	0.32	0	89,95,111	0.37	0
27	3PE	1	401	-	40,40,50	0.41	0	43,45,55	0.44	0
28	PC1	1	403	-	29,29,53	1.28	4 (13%)	35,37,61	1.28	3 (8%)
27	3PE	5	703	-	31,31,50	1.10	4 (12%)	34,36,55	1.17	2 (5%)
27	3PE	4	606	-	27,27,50	1.17	4 (14%)	30,32,55	1.19	2 (6%)
27	3PE	J	201	-	29,29,50	1.13	4 (13%)	32,34,55	1.19	2 (6%)
27	3PE	5	706	-	27,27,50	1.10	3 (11%)	30,32,55	1.17	1 (3%)
27	3PE	W	201	-	33,33,50	0.32	0	34,37,55	0.41	0
27	3PE	n	203	-	38,38,50	0.99	4 (10%)	41,43,55	1.13	2 (4%)
30	LMN	2	602	-	60,60,72	0.21	0	74,80,98	0.41	0
31	ZMP	Q	201	12	30,35,36	0.21	0	34,42,45	0.45	0
27	3PE	1	402	-	26,26,50	0.35	0	28,30,55	0.55	0
28	PC1	3	201	-	35,35,53	0.34	0	41,43,61	0.39	0
27	3PE	5	704	-	41,41,50	0.96	4 (9%)	44,46,55	1.10	2 (4%)
29	CDL	g	101	-	55,55,99	0.35	0	61,67,111	0.56	0
30	LMN	J	202	-	72,72,72	0.17	0	92,98,98	0.29	0
28	PC1	5	705	-	40,40,53	1.10	3 (7%)	46,48,61	1.16	3 (6%)
30	LMN	4	604	-	60,60,72	0.20	0	74,80,98	0.29	0
27	3PE	g	103	-	38,38,50	0.36	0	41,43,55	0.38	0
27	3PE	4	603	-	32,32,50	1.07	4 (12%)	35,37,55	1.18	2 (5%)
27	3PE	8	101	-	35,35,50	1.03	4 (11%)	38,40,55	1.15	2 (5%)
27	3PE	g	102	-	35,35,50	0.34	0	38,40,55	0.48	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
27	3PE	n	201	-	-	14/42/42/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CDL	X	201	-	-	23/89/89/110	-
27	3PE	5	702	-	-	13/43/43/54	-
28	PC1	2	603	-	-	7/34/34/57	-
28	PC1	4	605	-	-	29/48/48/57	-
29	CDL	4	601	-	-	21/96/96/110	-
27	3PE	4	602	-	-	12/37/37/54	-
28	PC1	5	701	-	-	19/48/48/57	-
28	PC1	n	202	-	-	19/54/54/57	-
29	CDL	D	101	-	-	25/69/69/110	-
29	CDL	2	601	-	-	21/94/94/110	-
27	3PE	1	401	-	-	6/44/44/54	-
28	PC1	1	403	-	-	16/32/32/57	-
27	3PE	5	703	-	-	8/35/35/54	-
27	3PE	4	606	-	-	7/31/31/54	-
27	3PE	J	201	-	-	14/33/33/54	-
27	3PE	5	706	-	-	8/30/30/54	-
27	3PE	W	201	-	-	12/36/36/54	-
27	3PE	n	203	-	-	19/42/42/54	-
30	LMN	2	602	-	-	18/44/104/130	0/3/3/4
31	ZMP	Q	201	12	-	8/40/42/43	-
27	3PE	1	402	-	-	8/29/29/54	-
28	PC1	3	201	-	-	10/39/39/57	-
27	3PE	5	704	-	-	14/45/45/54	-
29	CDL	g	101	-	-	15/66/66/110	-
30	LMN	J	202	-	-	11/50/130/130	0/4/4/4
28	PC1	5	705	-	-	22/44/44/57	-
30	LMN	4	604	-	-	15/44/104/130	0/3/3/4
27	3PE	g	103	-	-	15/42/42/54	-
27	3PE	4	603	-	-	20/36/36/54	-
27	3PE	8	101	-	-	16/39/39/54	-
27	3PE	g	102	-	-	15/39/39/54	-

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	5	705	PC1	O21-C2	-2.86	1.39	1.46
27	n	201	3PE	O21-C2	-2.71	1.40	1.46
27	4	606	3PE	O21-C2	-2.67	1.40	1.46
27	5	704	3PE	O21-C2	-2.67	1.40	1.46
27	4	602	3PE	O21-C2	-2.67	1.40	1.46
27	5	706	3PE	O21-C2	-2.66	1.40	1.46
28	1	403	PC1	O21-C2	-2.66	1.40	1.46
27	n	203	3PE	O21-C2	-2.65	1.40	1.46
27	J	201	3PE	O21-C2	-2.64	1.40	1.46
28	n	202	PC1	O21-C2	-2.63	1.40	1.46
27	8	101	3PE	O21-C2	-2.62	1.40	1.46
28	4	605	PC1	O21-C2	-2.61	1.40	1.46
27	5	703	3PE	O21-C2	-2.58	1.40	1.46
27	4	603	3PE	O21-C2	-2.57	1.40	1.46
27	5	703	3PE	O31-C31	2.44	1.40	1.33
27	n	201	3PE	O31-C31	2.44	1.40	1.33
27	J	201	3PE	O31-C31	2.43	1.40	1.33
28	5	705	PC1	O31-C31	2.42	1.40	1.33
27	n	203	3PE	O31-C31	2.41	1.40	1.33
27	4	603	3PE	O31-C31	2.41	1.40	1.33
27	4	606	3PE	O31-C31	2.41	1.40	1.33
28	1	403	PC1	O21-C21	2.40	1.40	1.35
27	8	101	3PE	O31-C31	2.39	1.40	1.33
28	1	403	PC1	O31-C31	2.35	1.40	1.33
27	5	704	3PE	O31-C31	2.34	1.40	1.33
28	n	202	PC1	O31-C31	2.33	1.40	1.33
27	4	602	3PE	O31-C31	2.33	1.40	1.33
28	4	605	PC1	O31-C3	-2.30	1.40	1.45
28	4	605	PC1	O21-C21	2.28	1.40	1.34
27	4	602	3PE	O31-C3	-2.28	1.40	1.45
28	4	605	PC1	O31-C31	2.26	1.39	1.33
27	5	703	3PE	O21-C21	2.23	1.40	1.34
27	J	201	3PE	O31-C3	-2.21	1.40	1.45
27	J	201	3PE	O21-C21	2.20	1.40	1.34
27	5	704	3PE	O31-C3	-2.20	1.40	1.45
28	n	202	PC1	O31-C3	-2.19	1.40	1.45
27	4	603	3PE	O31-C3	-2.18	1.40	1.45
27	8	101	3PE	O31-C3	-2.18	1.40	1.45
27	5	706	3PE	O31-C3	-2.17	1.40	1.45
27	8	101	3PE	O21-C21	2.17	1.40	1.34
27	n	201	3PE	O21-C21	2.17	1.40	1.34
28	n	202	PC1	O21-C21	2.16	1.40	1.34
28	5	705	PC1	O31-C3	-2.16	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	5	703	3PE	O31-C3	-2.16	1.40	1.45
27	4	606	3PE	O21-C21	2.15	1.40	1.34
27	5	706	3PE	O21-C21	2.14	1.40	1.34
27	5	704	3PE	O21-C21	2.14	1.40	1.34
28	1	403	PC1	O31-C3	-2.14	1.40	1.45
27	n	201	3PE	O31-C3	-2.13	1.40	1.45
27	4	606	3PE	O31-C3	-2.12	1.40	1.45
27	n	203	3PE	O21-C21	2.11	1.40	1.34
27	n	203	3PE	O31-C3	-2.11	1.40	1.45
27	4	603	3PE	O21-C21	2.09	1.40	1.34
27	4	602	3PE	O21-C21	2.05	1.40	1.34

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1	403	PC1	O21-C21-C22	5.03	120.05	111.09
27	n	201	3PE	O21-C21-C22	4.14	120.44	111.48
28	4	605	PC1	O21-C21-C22	4.13	120.41	111.48
28	n	202	PC1	O21-C21-C22	4.12	120.39	111.48
27	5	706	3PE	O21-C21-C22	4.11	120.37	111.48
27	n	203	3PE	O21-C21-C22	4.09	120.34	111.48
27	8	101	3PE	O21-C21-C22	4.08	120.30	111.48
27	4	603	3PE	O21-C21-C22	4.06	120.25	111.48
27	J	201	3PE	O21-C21-C22	4.02	120.19	111.48
27	5	703	3PE	O21-C21-C22	3.99	120.12	111.48
28	5	705	PC1	O21-C21-C22	3.98	120.09	111.48
27	5	704	3PE	O21-C21-C22	3.95	120.04	111.48
27	4	602	3PE	O21-C21-C22	3.94	120.01	111.48
27	4	606	3PE	O21-C21-C22	3.89	119.89	111.48
28	5	705	PC1	O31-C31-C32	2.84	120.48	111.83
28	1	403	PC1	O31-C31-C32	2.82	120.43	111.83
27	4	603	3PE	O31-C31-C32	2.80	120.39	111.83
28	4	605	PC1	O31-C31-C32	2.79	120.33	111.83
27	n	203	3PE	O31-C31-C32	2.77	120.29	111.83
27	n	201	3PE	O31-C31-C32	2.75	120.23	111.83
27	5	703	3PE	O31-C31-C32	2.71	120.10	111.83
27	8	101	3PE	O31-C31-C32	2.70	120.08	111.83
27	J	201	3PE	O31-C31-C32	2.69	120.05	111.83
27	4	606	3PE	O31-C31-C32	2.69	120.04	111.83
27	5	704	3PE	O31-C31-C32	2.66	119.95	111.83
27	4	602	3PE	O31-C31-C32	2.60	119.78	111.83
28	n	202	PC1	O31-C31-C32	2.60	119.75	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	5	705	PC1	C11-C12-N	-2.17	108.86	115.82
28	1	403	PC1	C2-O21-C21	-2.05	114.23	117.85

There are no chirality outliers.

All (480) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	1	402	3PE	C11-O13-P-O14
27	4	602	3PE	C1-O11-P-O13
27	4	603	3PE	C1-O11-P-O12
27	4	603	3PE	C1-O11-P-O13
27	4	603	3PE	C1-O11-P-O14
27	4	603	3PE	C11-O13-P-O11
27	4	603	3PE	C11-O13-P-O12
27	4	603	3PE	C11-O13-P-O14
27	4	606	3PE	C11-O13-P-O14
27	4	606	3PE	O21-C2-C3-O31
27	5	702	3PE	C11-O13-P-O14
27	5	704	3PE	C1-O11-P-O14
27	5	704	3PE	C11-O13-P-O11
27	5	704	3PE	C11-O13-P-O12
27	5	704	3PE	O13-C11-C12-N
27	5	706	3PE	C1-O11-P-O12
27	5	706	3PE	C11-O13-P-O14
27	5	706	3PE	C22-C21-O21-C2
27	8	101	3PE	C11-O13-P-O11
27	8	101	3PE	C11-O13-P-O12
27	8	101	3PE	C11-O13-P-O14
27	8	101	3PE	O22-C21-O21-C2
27	8	101	3PE	C22-C21-O21-C2
27	J	201	3PE	C11-O13-P-O11
27	W	201	3PE	C11-O13-P-O11
27	W	201	3PE	C11-O13-P-O12
27	W	201	3PE	C2-C1-O11-P
27	W	201	3PE	O32-C31-O31-C3
27	g	102	3PE	C1-O11-P-O14
27	g	103	3PE	C11-O13-P-O11
27	g	103	3PE	C2-C1-O11-P
27	g	103	3PE	C12-C11-O13-P
27	g	103	3PE	O13-C11-C12-N
27	n	201	3PE	C1-O11-P-O14
27	n	201	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
27	n	201	3PE	O22-C21-O21-C2
27	n	201	3PE	C22-C21-O21-C2
27	n	203	3PE	C1-O11-P-O12
27	n	203	3PE	C1-O11-P-O13
27	n	203	3PE	C1-O11-P-O14
27	n	203	3PE	C11-O13-P-O11
27	n	203	3PE	C11-O13-P-O12
27	n	203	3PE	C11-O13-P-O14
27	n	203	3PE	O22-C21-O21-C2
28	1	403	PC1	C11-O13-P-O14
28	1	403	PC1	C1-O11-P-O12
28	1	403	PC1	C1-O11-P-O14
28	1	403	PC1	C1-O11-P-O13
28	1	403	PC1	O13-C11-C12-N
28	1	403	PC1	C22-C21-O21-C2
28	2	603	PC1	C11-O13-P-O14
28	2	603	PC1	C1-O11-P-O14
28	2	603	PC1	C12-C11-O13-P
28	4	605	PC1	C22-C21-O21-C2
28	5	701	PC1	C11-O13-P-O14
28	5	705	PC1	C11-O13-P-O12
28	5	705	PC1	C11-O13-P-O14
28	5	705	PC1	C11-O13-P-O11
28	5	705	PC1	C1-O11-P-O12
28	5	705	PC1	C1-O11-P-O13
28	5	705	PC1	O13-C11-C12-N
28	n	202	PC1	C1-O11-P-O12
28	n	202	PC1	C1-O11-P-O14
28	n	202	PC1	C1-O11-P-O13
29	2	601	CDL	O1-C1-CA2-OA2
29	2	601	CDL	CA3-OA5-PA1-OA4
29	2	601	CDL	CB2-OB2-PB2-OB3
29	4	601	CDL	OA6-CA4-CA6-OA8
29	4	601	CDL	CB2-OB2-PB2-OB3
29	D	101	CDL	CA2-OA2-PA1-OA3
29	D	101	CDL	CA2-OA2-PA1-OA4
29	D	101	CDL	CA2-OA2-PA1-OA5
29	D	101	CDL	CB3-OB5-PB2-OB2
29	D	101	CDL	CB3-OB5-PB2-OB3
29	D	101	CDL	CB3-OB5-PB2-OB4
29	D	101	CDL	C51-CB5-OB6-CB4
29	g	101	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
29	g	101	CDL	CA2-OA2-PA1-OA5
29	g	101	CDL	OB7-CB5-OB6-CB4
29	g	101	CDL	C51-CB5-OB6-CB4
30	2	602	LMN	OBX-CCJ-OBV-CBT
30	4	604	LMN	CBK-CBQ-CCM-CBR
30	4	604	LMN	CBK-CBQ-CCM-CBS
30	4	604	LMN	CBK-CBQ-CCM-CBT
30	4	604	LMN	OBV-CBT-CCM-CBQ
30	4	604	LMN	OBV-CBT-CCM-CBR
30	4	604	LMN	OBX-CCJ-OBV-CBT
31	Q	201	ZMP	O4-C17-C18-C21
31	Q	201	ZMP	C13-C14-C15-N2
28	1	403	PC1	O22-C21-O21-C2
27	g	103	3PE	O32-C31-O31-C3
27	g	103	3PE	C32-C31-O31-C3
27	4	603	3PE	O32-C31-O31-C3
27	J	201	3PE	O32-C31-O31-C3
27	5	706	3PE	O22-C21-O21-C2
28	4	605	PC1	O22-C21-O21-C2
29	D	101	CDL	OB7-CB5-OB6-CB4
29	X	201	CDL	OB7-CB5-OB6-CB4
27	4	603	3PE	C32-C31-O31-C3
27	n	203	3PE	C22-C21-O21-C2
30	4	604	LMN	CCH-CCQ-OCB-CCS
27	J	201	3PE	C32-C31-O31-C3
27	n	203	3PE	C32-C31-O31-C3
28	4	605	PC1	C32-C31-O31-C3
27	5	702	3PE	O22-C21-O21-C2
29	X	201	CDL	OA7-CA5-OA6-CA4
30	4	604	LMN	OBV-CBT-CCM-CBS
27	8	101	3PE	C32-C31-O31-C3
28	5	705	PC1	C32-C31-O31-C3
29	4	601	CDL	C31-CA7-OA8-CA6
28	3	201	PC1	C32-C33-C34-C35
27	8	101	3PE	O32-C31-O31-C3
27	1	402	3PE	C22-C21-O21-C2
27	5	702	3PE	C22-C21-O21-C2
29	D	101	CDL	C11-CA5-OA6-CA4
29	X	201	CDL	C11-CA5-OA6-CA4
29	X	201	CDL	C51-CB5-OB6-CB4
28	4	605	PC1	O32-C31-O31-C3
27	n	203	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
27	1	402	3PE	O22-C21-O21-C2
28	5	705	PC1	O32-C31-O31-C3
29	4	601	CDL	OA9-CA7-OA8-CA6
29	2	601	CDL	CB2-C1-CA2-OA2
29	X	201	CDL	CA7-C31-C32-C33
30	2	602	LMN	OBZ-CCS-OCB-CCQ
29	D	101	CDL	OA7-CA5-OA6-CA4
29	X	201	CDL	OA5-CA3-CA4-OA6
28	3	201	PC1	O21-C2-C3-O31
27	4	602	3PE	C21-C22-C23-C24
27	4	603	3PE	C31-C32-C33-C34
27	4	603	3PE	C21-C22-C23-C24
27	g	103	3PE	C21-C22-C23-C24
29	4	601	CDL	C51-CB5-OB6-CB4
27	J	201	3PE	C21-C22-C23-C24
27	g	102	3PE	C31-C32-C33-C34
28	5	705	PC1	C21-C22-C23-C24
27	5	704	3PE	C21-C22-C23-C24
28	4	605	PC1	C31-C32-C33-C34
27	4	602	3PE	C22-C21-O21-C2
29	4	601	CDL	C54-C55-C56-C57
29	4	601	CDL	OB7-CB5-OB6-CB4
29	2	601	CDL	C11-CA5-OA6-CA4
27	4	602	3PE	O22-C21-O21-C2
30	2	602	LMN	C2-C1-O1-CBS
29	g	101	CDL	O1-C1-CA2-OA2
27	g	103	3PE	C22-C23-C24-C25
29	2	601	CDL	CB4-CB3-OB5-PB2
29	4	601	CDL	CA4-CA3-OA5-PA1
29	2	601	CDL	OA7-CA5-OA6-CA4
30	2	602	LMN	O5-C1-O1-CBS
30	4	604	LMN	CBJ-CBL-CBR-CCM
27	4	603	3PE	C35-C36-C37-C38
27	5	702	3PE	C33-C34-C35-C36
29	D	101	CDL	C71-C72-C73-C74
27	4	603	3PE	C33-C34-C35-C36
28	5	701	PC1	C21-C22-C23-C24
27	5	704	3PE	C22-C23-C24-C25
27	5	704	3PE	C33-C34-C35-C36
28	4	605	PC1	C29-C2A-C2B-C2C
28	5	701	PC1	C32-C31-O31-C3
27	5	706	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
27	g	102	3PE	C38-C39-C3A-C3B
27	n	201	3PE	C22-C23-C24-C25
28	4	605	PC1	C23-C24-C25-C26
27	n	203	3PE	C36-C37-C38-C39
28	5	701	PC1	C2B-C2C-C2D-C2E
28	5	705	PC1	C32-C33-C34-C35
28	4	605	PC1	C28-C29-C2A-C2B
29	X	201	CDL	C71-CB7-OB8-CB6
28	5	701	PC1	C22-C23-C24-C25
28	n	202	PC1	C23-C24-C25-C26
27	4	602	3PE	C25-C26-C27-C28
28	5	705	PC1	C23-C24-C25-C26
29	X	201	CDL	C15-C16-C17-C18
28	5	705	PC1	C22-C23-C24-C25
27	4	602	3PE	C33-C34-C35-C36
28	4	605	PC1	C35-C36-C37-C38
28	3	201	PC1	C22-C21-O21-C2
28	5	705	PC1	C22-C21-O21-C2
29	D	101	CDL	CB7-C71-C72-C73
27	g	102	3PE	C39-C3A-C3B-C3C
27	4	602	3PE	C22-C23-C24-C25
30	J	202	LMN	CBC-CBE-CBG-CBI
28	5	705	PC1	C35-C36-C37-C38
27	8	101	3PE	C27-C28-C29-C2A
27	n	201	3PE	C21-C22-C23-C24
27	W	201	3PE	C24-C25-C26-C27
28	5	705	PC1	O11-C1-C2-O21
27	W	201	3PE	C22-C21-O21-C2
28	5	701	PC1	C31-C32-C33-C34
30	2	602	LMN	OAL-CBP-CCF-OBX
27	5	706	3PE	O21-C2-C3-O31
29	D	101	CDL	OA6-CA4-CA6-OA8
27	5	702	3PE	C32-C31-O31-C3
28	n	202	PC1	C32-C33-C34-C35
27	g	103	3PE	C2E-C2F-C2G-C2H
27	n	201	3PE	C23-C24-C25-C26
28	1	403	PC1	C35-C36-C37-C38
27	4	606	3PE	C22-C21-O21-C2
27	1	402	3PE	C23-C24-C25-C26
28	n	202	PC1	C3B-C3C-C3D-C3E
28	5	701	PC1	O32-C31-O31-C3
27	8	101	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
27	g	102	3PE	C35-C36-C37-C38
29	2	601	CDL	OB5-CB3-CB4-CB6
29	X	201	CDL	OA5-CA3-CA4-CA6
29	g	101	CDL	OB5-CB3-CB4-CB6
30	J	202	LMN	OAI-CBM-CCC-OBY
29	4	601	CDL	CA5-C11-C12-C13
29	X	201	CDL	OB9-CB7-OB8-CB6
28	5	705	PC1	C31-C32-C33-C34
27	W	201	3PE	C2D-C2E-C2F-C2G
27	8	101	3PE	C31-C32-C33-C34
27	5	703	3PE	C25-C26-C27-C28
30	2	602	LMN	CCL-CCJ-OBV-CBT
27	4	606	3PE	C1-C2-C3-O31
28	3	201	PC1	C1-C2-C3-O31
29	X	201	CDL	CA3-CA4-CA6-OA8
28	n	202	PC1	C29-C2A-C2B-C2C
28	5	705	PC1	C26-C27-C28-C29
27	n	203	3PE	C37-C38-C39-C3A
27	5	702	3PE	C32-C33-C34-C35
29	X	201	CDL	C13-C14-C15-C16
27	5	702	3PE	O32-C31-O31-C3
30	2	602	LMN	C4-C5-C6-O6
27	n	203	3PE	C35-C36-C37-C38
28	5	705	PC1	O22-C21-O21-C2
28	4	605	PC1	C24-C25-C26-C27
30	2	602	LMN	O5-C5-C6-O6
27	5	703	3PE	C22-C23-C24-C25
28	n	202	PC1	C3D-C3E-C3F-C3G
29	g	101	CDL	CB2-C1-CA2-OA2
27	1	402	3PE	O11-C1-C2-O21
29	D	101	CDL	C71-CB7-OB8-CB6
28	5	701	PC1	C28-C29-C2A-C2B
27	n	203	3PE	C3A-C3B-C3C-C3D
28	4	605	PC1	C36-C37-C38-C39
28	4	605	PC1	C2A-C2B-C2C-C2D
27	g	103	3PE	C2B-C2C-C2D-C2E
30	2	602	LMN	CBK-CBQ-CCM-CBR
27	g	102	3PE	O21-C21-C22-C23
29	2	601	CDL	C32-C31-CA7-OA8
29	4	601	CDL	C12-C11-CA5-OA6
31	Q	201	ZMP	O4-C17-C18-C19
27	4	603	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
28	n	202	PC1	C32-C31-O31-C3
29	4	601	CDL	C71-C72-C73-C74
28	5	701	PC1	C22-C21-O21-C2
30	4	604	LMN	CCF-CCQ-OCB-CCS
28	n	202	PC1	C2A-C2B-C2C-C2D
27	g	102	3PE	C32-C33-C34-C35
28	4	605	PC1	C2-C1-O11-P
30	4	604	LMN	CCL-CCJ-OBV-CBT
29	g	101	CDL	CB5-C51-C52-C53
27	4	602	3PE	O11-C1-C2-C3
27	8	101	3PE	O11-C1-C2-C3
28	4	605	PC1	O11-C1-C2-C3
28	5	705	PC1	O11-C1-C2-C3
29	D	101	CDL	C72-C71-CB7-OB8
27	5	704	3PE	C31-C32-C33-C34
27	5	703	3PE	O31-C31-C32-C33
30	4	604	LMN	CAY-CBA-CBC-CBE
28	3	201	PC1	O22-C21-O21-C2
27	1	401	3PE	C23-C24-C25-C26
27	4	602	3PE	C24-C25-C26-C27
27	4	603	3PE	C1-C2-C3-O31
27	5	703	3PE	C1-C2-C3-O31
27	n	201	3PE	C1-C2-C3-O31
29	D	101	CDL	CA3-CA4-CA6-OA8
29	2	601	CDL	C18-C19-C20-C21
27	4	602	3PE	C31-C32-C33-C34
28	4	605	PC1	C11-C12-N-C15
27	5	703	3PE	C24-C25-C26-C27
30	J	202	LMN	C3-C4-O4-CCR
27	W	201	3PE	O22-C21-O21-C2
27	8	101	3PE	O11-C1-C2-O21
29	g	101	CDL	OB5-CB3-CB4-OB6
29	g	101	CDL	C16-C17-C18-C19
28	2	603	PC1	C2-C1-O11-P
29	4	601	CDL	CA7-C31-C32-C33
27	J	201	3PE	O21-C2-C3-O31
27	4	603	3PE	C22-C23-C24-C25
28	4	605	PC1	C32-C33-C34-C35
30	2	602	LMN	CBE-CBG-CBI-CBK
27	5	703	3PE	C29-C2A-C2B-C2C
27	g	102	3PE	C22-C21-O21-C2
30	J	202	LMN	C5-C4-O4-CCR

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Mol	Chain	Res	Type	Atoms
28	1	403	PC1	O31-C31-C32-C33
27	4	603	3PE	O11-C1-C2-C3
27	5	702	3PE	C36-C37-C38-C39
28	n	202	PC1	O32-C31-O31-C3
27	4	606	3PE	O22-C21-O21-C2
28	5	701	PC1	O22-C21-O21-C2
29	D	101	CDL	OB9-CB7-OB8-CB6
28	4	605	PC1	C11-C12-N-C13
27	g	103	3PE	C27-C28-C29-C2A
28	5	701	PC1	C36-C37-C38-C39
27	4	602	3PE	O11-C1-C2-O21
27	4	603	3PE	O11-C1-C2-O21
27	4	606	3PE	O11-C1-C2-O21
27	g	102	3PE	O11-C1-C2-O21
29	2	601	CDL	OB5-CB3-CB4-OB6
27	n	203	3PE	C32-C33-C34-C35
28	1	403	PC1	C1-C2-C3-O31
29	4	601	CDL	CA3-CA4-CA6-OA8
31	Q	201	ZMP	N1-C13-C14-C15
27	8	101	3PE	C33-C34-C35-C36
27	5	702	3PE	C12-C11-O13-P
27	8	101	3PE	C12-C11-O13-P
27	J	201	3PE	C12-C11-O13-P
28	5	701	PC1	C12-C11-O13-P
27	4	603	3PE	O21-C2-C3-O31
27	5	703	3PE	O21-C2-C3-O31
28	1	403	PC1	O21-C2-C3-O31
28	5	705	PC1	O21-C2-C3-O31
29	X	201	CDL	OA6-CA4-CA6-OA8
28	4	605	PC1	C27-C28-C29-C2A
28	5	701	PC1	C25-C26-C27-C28
28	3	201	PC1	C24-C25-C26-C27
29	2	601	CDL	C1-CB2-OB2-PB2
28	2	603	PC1	O13-C11-C12-N
28	n	202	PC1	O13-C11-C12-N
30	J	202	LMN	CCW-CCS-OCB-CCQ
28	n	202	PC1	C21-C22-C23-C24
28	1	403	PC1	C32-C31-O31-C3
28	5	701	PC1	C2E-C2F-C2G-C2H
30	2	602	LMN	OBV-CBT-CCM-CBR
30	J	202	LMN	OBZ-CCS-OCB-CCQ
31	Q	201	ZMP	O2-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
27	1	402	3PE	O11-C1-C2-C3
27	4	606	3PE	O11-C1-C2-C3
27	W	201	3PE	O11-C1-C2-C3
28	3	201	PC1	O11-C1-C2-C3
27	1	401	3PE	C2A-C2B-C2C-C2D
29	2	601	CDL	CB7-C71-C72-C73
28	4	605	PC1	C22-C23-C24-C25
27	n	201	3PE	C2-C1-O11-P
27	n	203	3PE	C2-C1-O11-P
29	X	201	CDL	C38-C39-C40-C41
28	3	201	PC1	O11-C1-C2-O21
28	4	605	PC1	O11-C1-C2-O21
29	4	601	CDL	OA5-CA3-CA4-OA6
28	4	605	PC1	C11-C12-N-C14
30	J	202	LMN	OBY-CCR-O4-C4
27	1	401	3PE	C24-C25-C26-C27
27	g	102	3PE	C3C-C3D-C3E-C3F
29	4	601	CDL	C74-C75-C76-C77
28	5	701	PC1	O21-C2-C3-O31
27	g	102	3PE	C37-C38-C39-C3A
27	J	201	3PE	C1-C2-C3-O31
28	5	705	PC1	C1-C2-C3-O31
30	J	202	LMN	CCV-CCR-O4-C4
28	1	403	PC1	O32-C31-O31-C3
27	g	102	3PE	O22-C21-O21-C2
27	1	401	3PE	C1-O11-P-O14
27	1	401	3PE	C11-O13-P-O14
27	1	402	3PE	C11-O13-P-O11
27	1	402	3PE	C11-O13-P-O12
27	4	602	3PE	C1-O11-P-O14
27	5	704	3PE	C1-O11-P-O13
27	5	706	3PE	C1-O11-P-O13
27	5	706	3PE	C1-O11-P-O14
27	J	201	3PE	C1-O11-P-O12
27	J	201	3PE	C1-O11-P-O13
27	J	201	3PE	C1-O11-P-O14
27	J	201	3PE	C11-O13-P-O12
27	J	201	3PE	C11-O13-P-O14
27	g	102	3PE	C11-O13-P-O14
27	g	103	3PE	C11-O13-P-O14
27	n	201	3PE	C11-O13-P-O14
28	2	603	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
28	3	201	PC1	C11-O13-P-O14
28	4	605	PC1	C11-O13-P-O12
28	4	605	PC1	C11-O13-P-O11
28	4	605	PC1	C1-O11-P-O14
28	n	202	PC1	C11-O13-P-O14
28	n	202	PC1	C11-O13-P-O11
29	2	601	CDL	CA3-OA5-PA1-OA2
29	2	601	CDL	CA3-OA5-PA1-OA3
29	D	101	CDL	CA3-OA5-PA1-OA3
29	g	101	CDL	CB2-OB2-PB2-OB3
29	D	101	CDL	C1-CA2-OA2-PA1
29	D	101	CDL	C13-C14-C15-C16
28	2	603	PC1	C21-C22-C23-C24
29	X	201	CDL	C74-C75-C76-C77
29	2	601	CDL	C24-C25-C26-C27
29	D	101	CDL	CB6-CB4-OB6-CB5
29	4	601	CDL	C12-C13-C14-C15
29	X	201	CDL	C72-C73-C74-C75
27	8	101	3PE	C32-C33-C34-C35
30	J	202	LMN	CAA-CAW-CAY-CBA
29	4	601	CDL	C12-C11-CA5-OA7
29	g	101	CDL	C32-C31-CA7-OA8
30	2	602	LMN	CBK-CBQ-CCM-CBS
29	X	201	CDL	CB4-CB6-OB8-CB7
27	5	704	3PE	C2B-C2C-C2D-C2E
28	n	202	PC1	O31-C31-C32-C33
27	n	203	3PE	C3B-C3C-C3D-C3E
29	4	601	CDL	C34-C35-C36-C37
29	D	101	CDL	C12-C13-C14-C15
27	g	102	3PE	O22-C21-C22-C23
27	g	103	3PE	C29-C2A-C2B-C2C
29	X	201	CDL	C54-C55-C56-C57
29	D	101	CDL	CB4-CB3-OB5-PB2
28	n	202	PC1	C39-C3A-C3B-C3C
28	5	701	PC1	C23-C24-C25-C26
31	Q	201	ZMP	C11-C12-N1-C13
29	X	201	CDL	CB6-CB4-OB6-CB5
28	5	705	PC1	C27-C28-C29-C2A
29	2	601	CDL	C32-C31-CA7-OA9
27	5	702	3PE	C39-C3A-C3B-C3C
27	W	201	3PE	O21-C2-C3-O31
29	g	101	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
27	n	203	3PE	C34-C35-C36-C37
28	1	403	PC1	C34-C35-C36-C37
27	5	702	3PE	C3A-C3B-C3C-C3D
27	n	203	3PE	C3C-C3D-C3E-C3F
30	J	202	LMN	CBB-CBD-CBF-CBH
29	D	101	CDL	CB4-CB6-OB8-CB7
27	1	401	3PE	C2C-C2D-C2E-C2F
29	g	101	CDL	C32-C31-CA7-OA9
27	n	201	3PE	C32-C31-O31-C3
27	5	704	3PE	C2D-C2E-C2F-C2G
27	5	704	3PE	C26-C27-C28-C29
28	4	605	PC1	C26-C27-C28-C29
29	D	101	CDL	C72-C71-CB7-OB9
28	n	202	PC1	C2D-C2E-C2F-C2G
30	2	602	LMN	CCF-CCQ-OCB-CCS
27	n	201	3PE	C32-C33-C34-C35
27	n	201	3PE	O32-C31-O31-C3
27	W	201	3PE	C26-C27-C28-C29
27	8	101	3PE	C2-C1-O11-P
27	5	703	3PE	O32-C31-C32-C33
28	1	403	PC1	C33-C34-C35-C36
29	g	101	CDL	CA3-CA4-OA6-CA5
30	2	602	LMN	CBK-CBQ-CCM-CBT
28	4	605	PC1	C2B-C2C-C2D-C2E
30	2	602	LMN	CCH-CCQ-OCB-CCS
29	2	601	CDL	C17-C18-C19-C20
29	2	601	CDL	CA7-C31-C32-C33
29	2	601	CDL	C77-C78-C79-C80
27	g	102	3PE	O11-C1-C2-C3
29	4	601	CDL	OA5-CA3-CA4-CA6
27	n	201	3PE	C33-C34-C35-C36
28	1	403	PC1	O32-C31-C32-C33
31	Q	201	ZMP	O4-C17-C18-C20
27	5	702	3PE	C34-C35-C36-C37
27	g	103	3PE	C22-C21-O21-C2
30	2	602	LMN	OBV-CBT-CCM-CBQ
30	4	604	LMN	O1-CBS-CCM-CBQ
30	4	604	LMN	O1-CBS-CCM-CBR
30	J	202	LMN	O1-CBS-CCM-CBR
27	W	201	3PE	C1-C2-C3-O31
28	5	701	PC1	C1-C2-C3-O31
29	X	201	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
28	4	605	PC1	O21-C21-C22-C23
29	X	201	CDL	C73-C74-C75-C76
30	2	602	LMN	CBC-CBE-CBG-CBI
27	5	704	3PE	C32-C33-C34-C35
28	n	202	PC1	O11-C1-C2-C3
27	J	201	3PE	O31-C31-C32-C33
29	2	601	CDL	C14-C15-C16-C17
31	Q	201	ZMP	C16-C17-C18-C21
29	X	201	CDL	C14-C15-C16-C17
28	5	701	PC1	C11-C12-N-C15
29	4	601	CDL	CB4-CB3-OB5-PB2
28	5	701	PC1	C27-C28-C29-C2A
28	3	201	PC1	C34-C35-C36-C37
30	2	602	LMN	CAW-CAY-CBA-CBC
28	4	605	PC1	C38-C39-C3A-C3B
27	J	201	3PE	O32-C31-C32-C33
28	4	605	PC1	O22-C21-C22-C23
27	4	603	3PE	C37-C38-C39-C3A
27	g	103	3PE	C26-C27-C28-C29
30	4	604	LMN	CAA-CAW-CAY-CBA
27	5	704	3PE	O21-C21-C22-C23
29	4	601	CDL	C72-C71-CB7-OB8
29	X	201	CDL	C37-C38-C39-C40
27	5	702	3PE	C3B-C3C-C3D-C3E
27	4	603	3PE	O21-C21-C22-C23

There are no ring outliers.

26 monomers are involved in 84 short contacts:

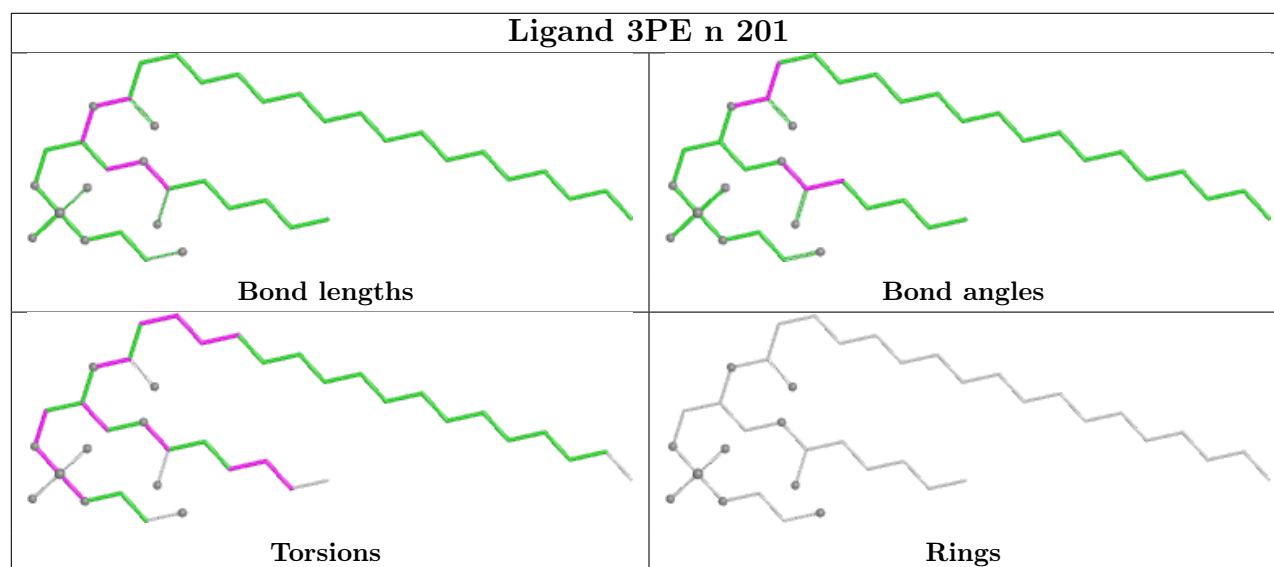
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	X	201	CDL	4	0
27	5	702	3PE	3	0
28	4	605	PC1	4	0
29	4	601	CDL	8	0
27	4	602	3PE	5	0
28	5	701	PC1	6	0
28	n	202	PC1	5	0
29	D	101	CDL	1	0
29	2	601	CDL	8	0
27	1	401	3PE	1	0
28	1	403	PC1	2	0
27	5	703	3PE	3	0

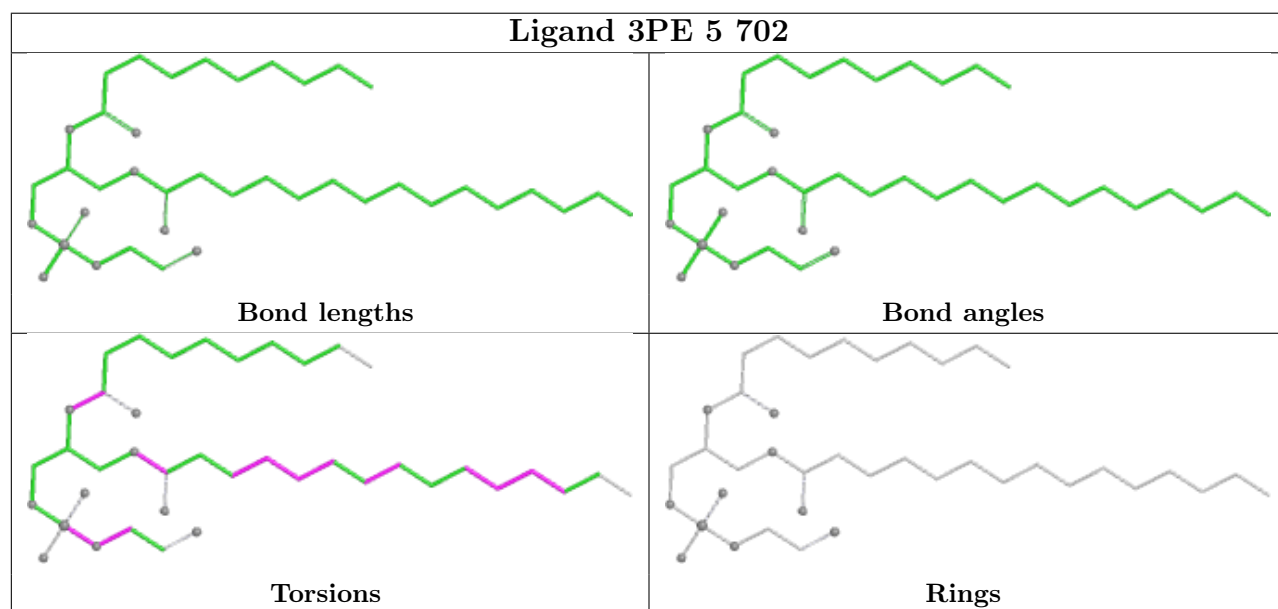
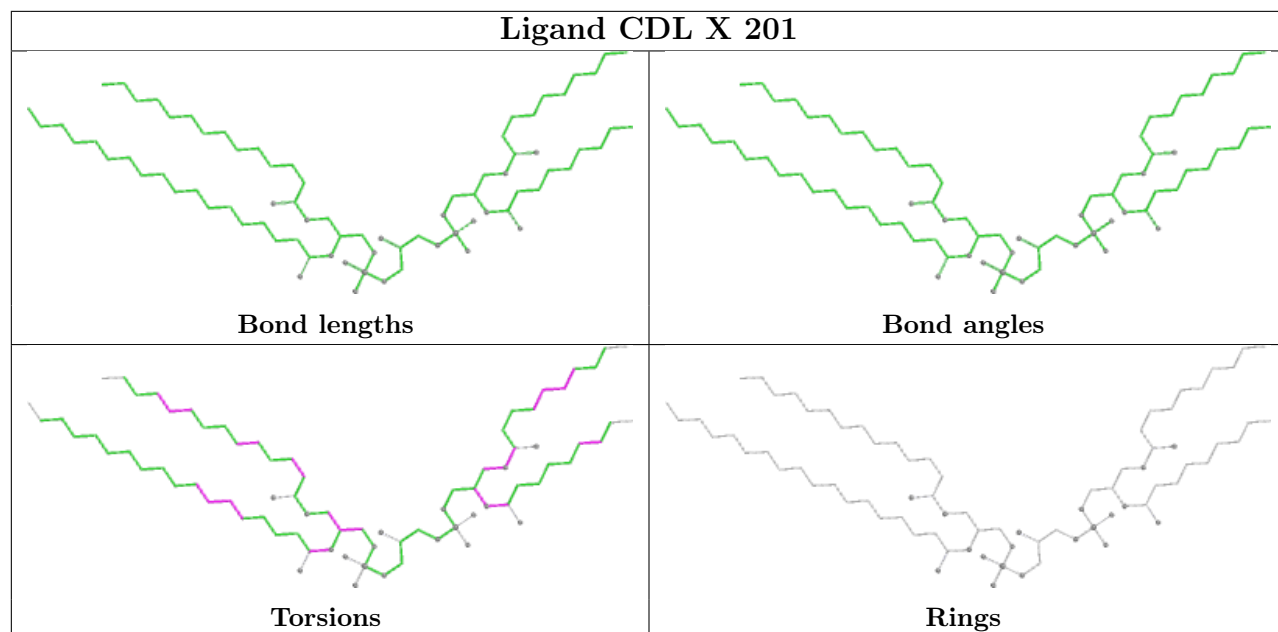
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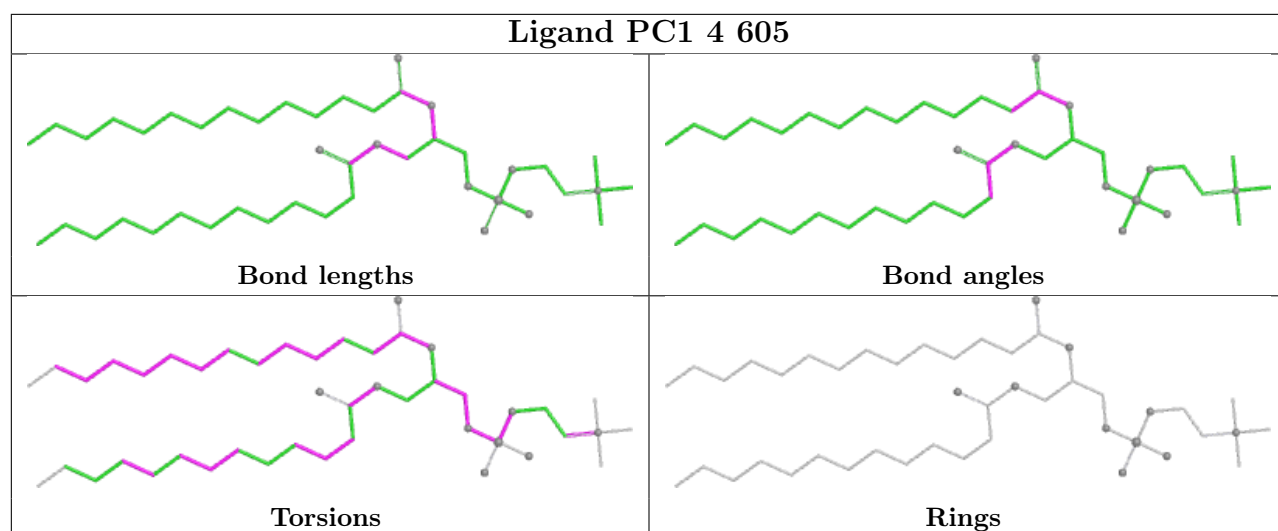
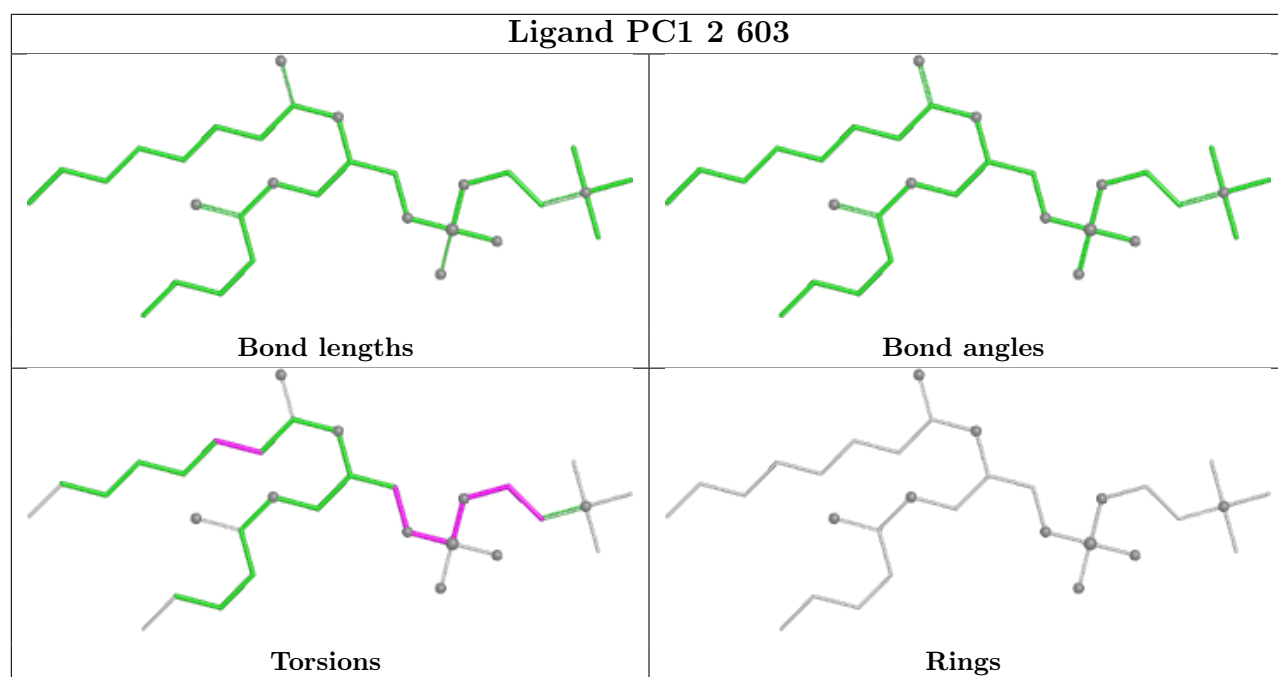
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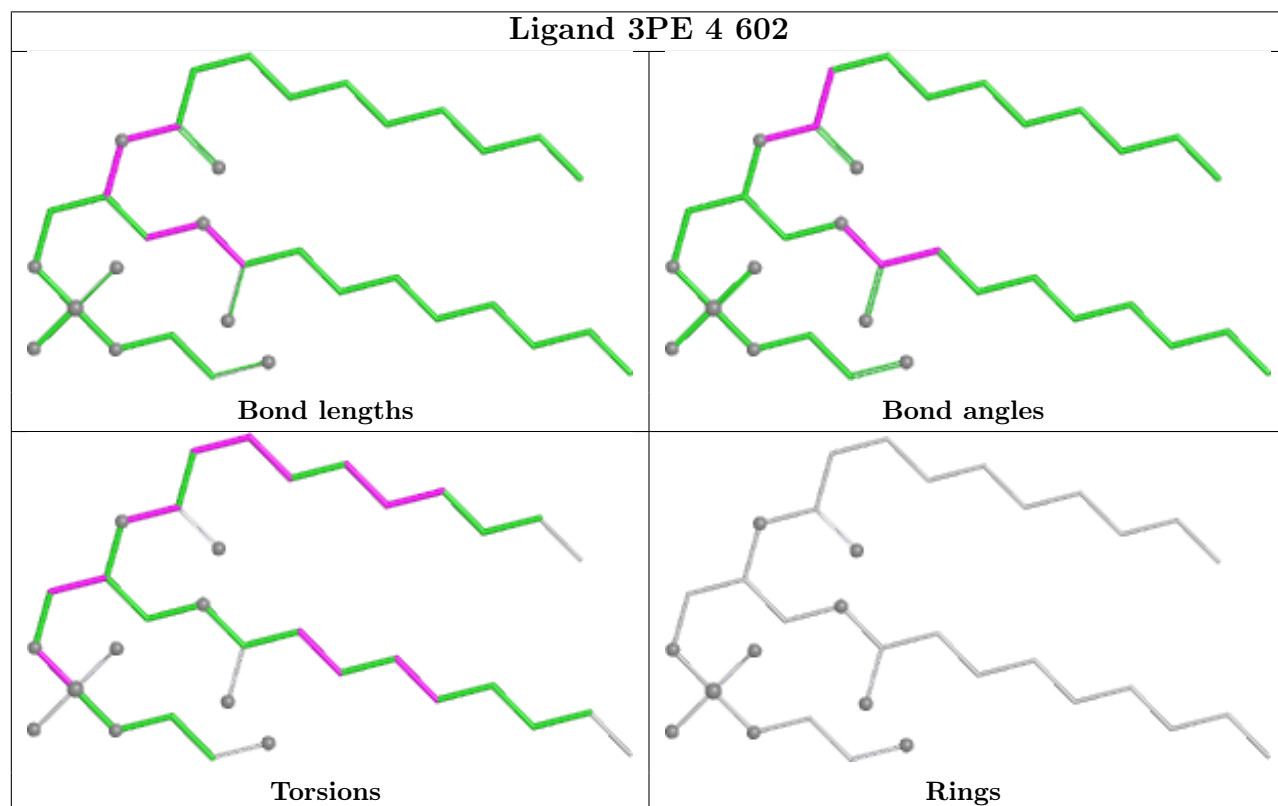
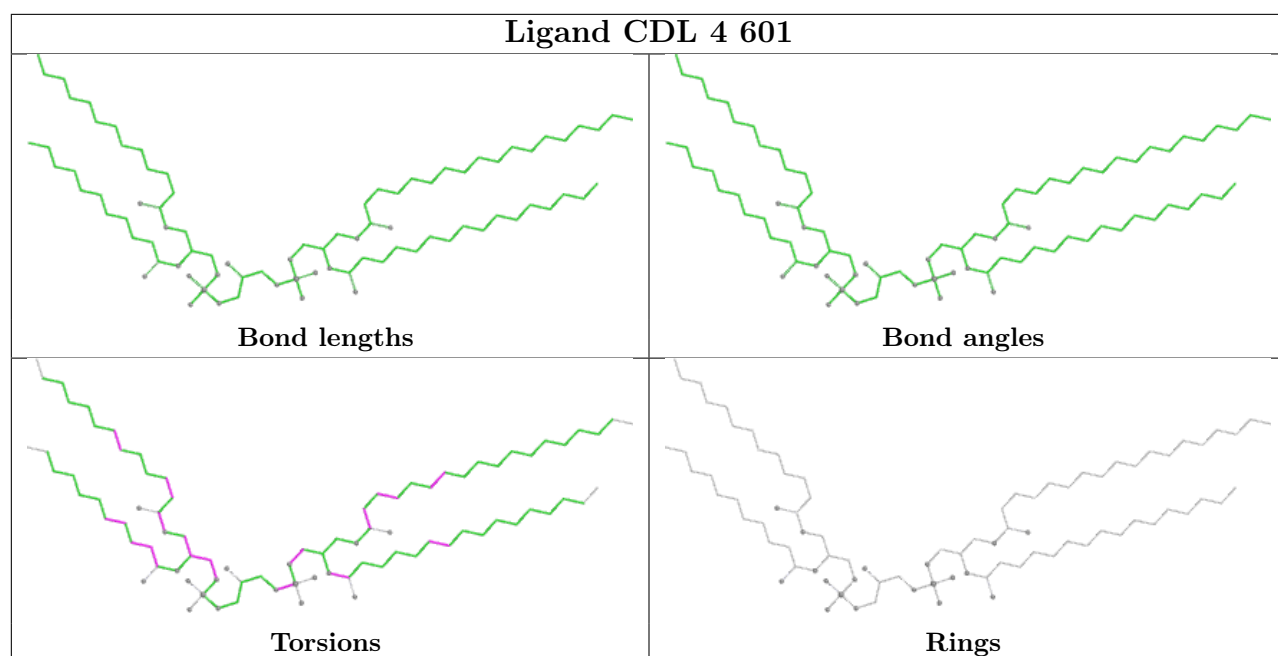
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	J	201	3PE	3	0
27	W	201	3PE	1	0
27	n	203	3PE	2	0
30	2	602	LMN	2	0
31	Q	201	ZMP	5	0
27	1	402	3PE	1	0
27	5	704	3PE	1	0
29	g	101	CDL	3	0
28	5	705	PC1	2	0
30	4	604	LMN	5	0
27	g	103	3PE	3	0
27	4	603	3PE	3	0
27	8	101	3PE	1	0
27	g	102	3PE	3	0

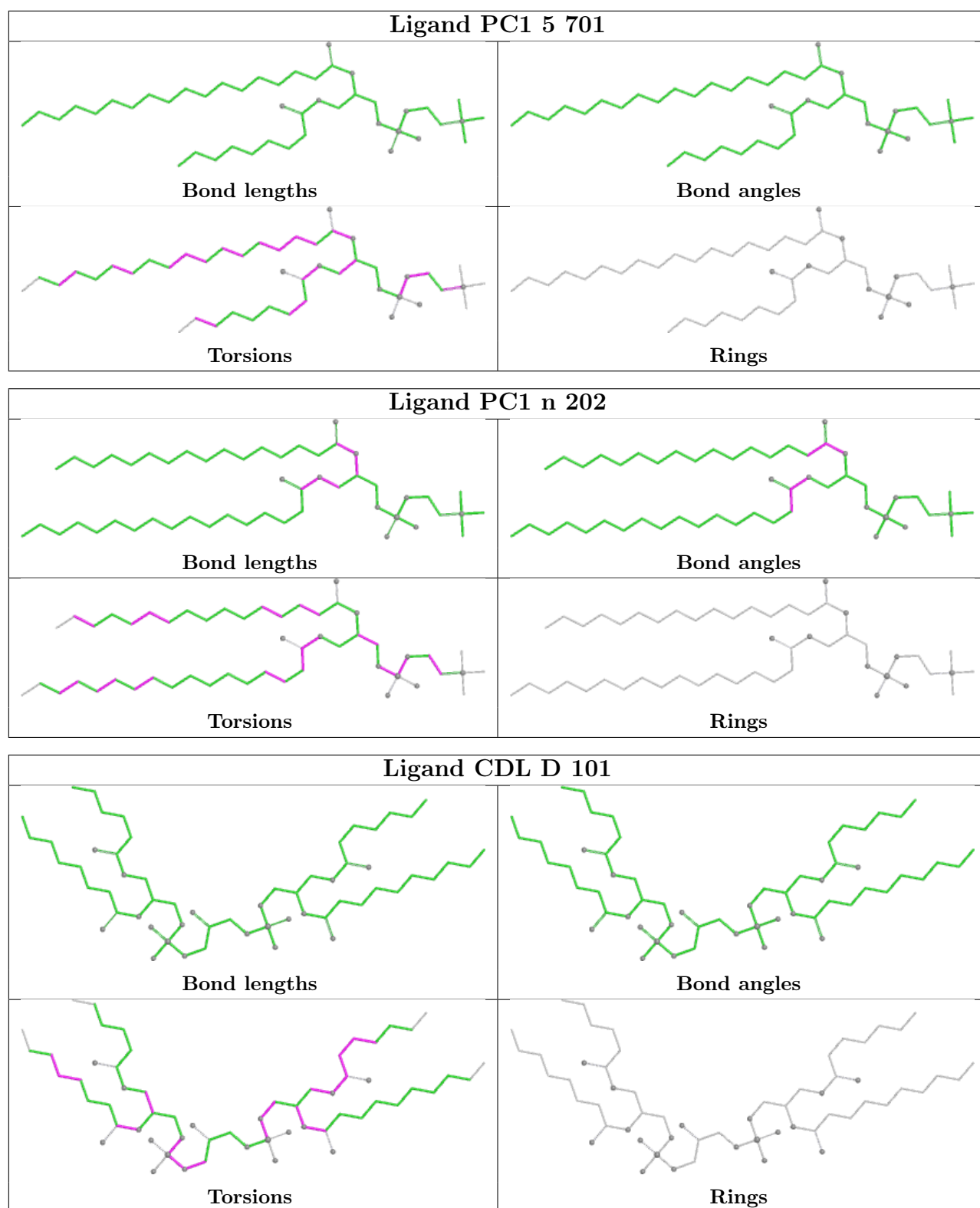
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

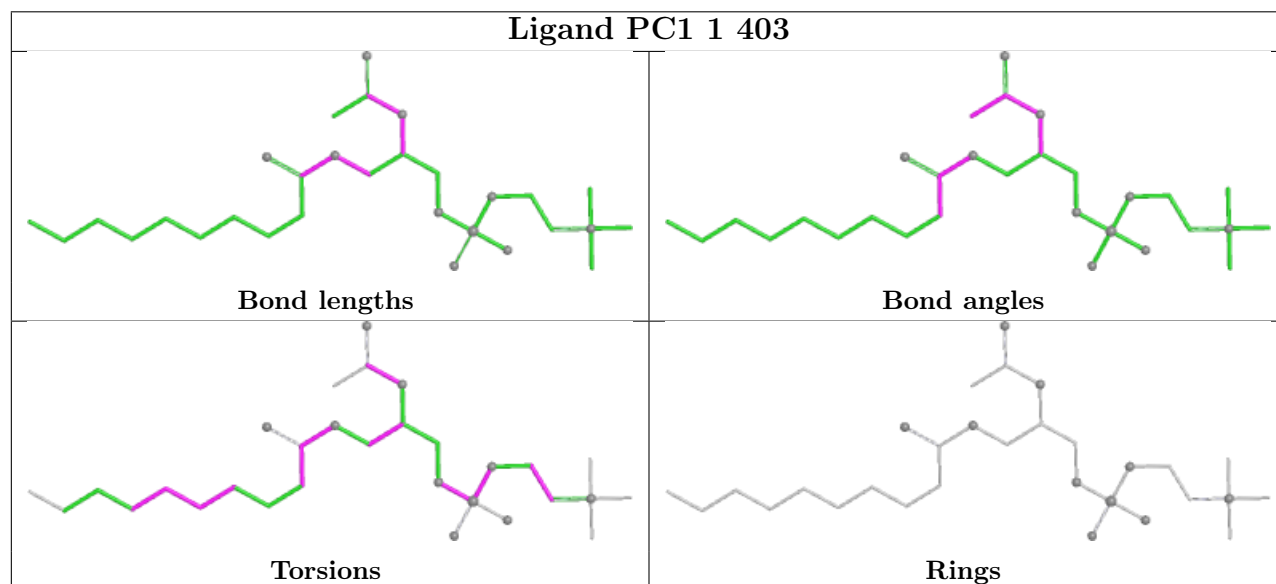
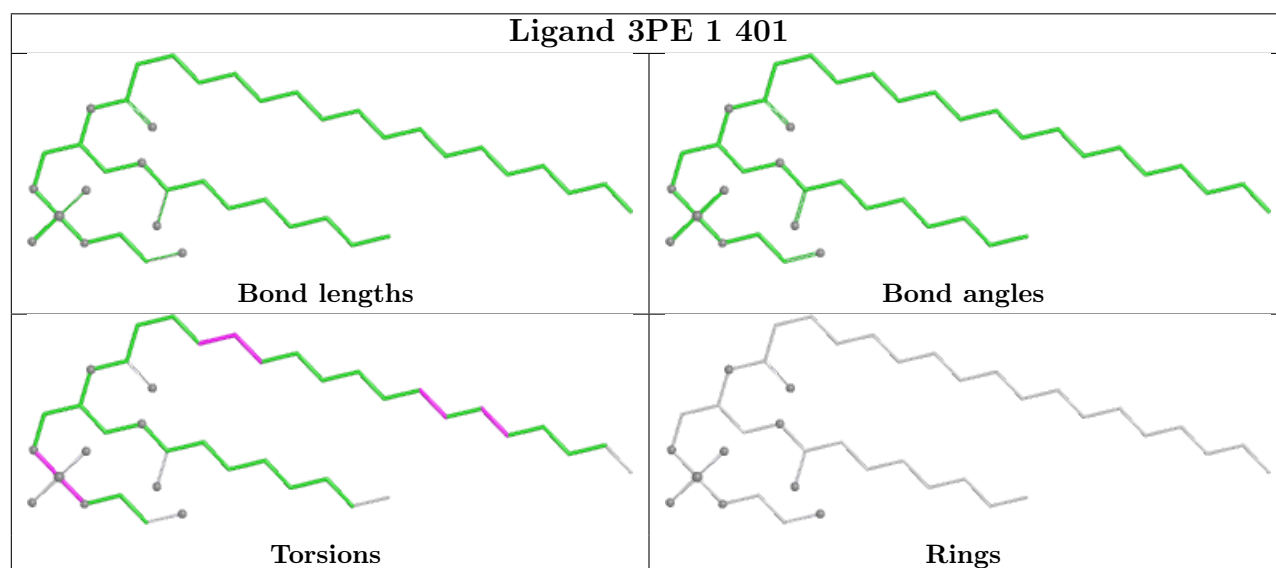
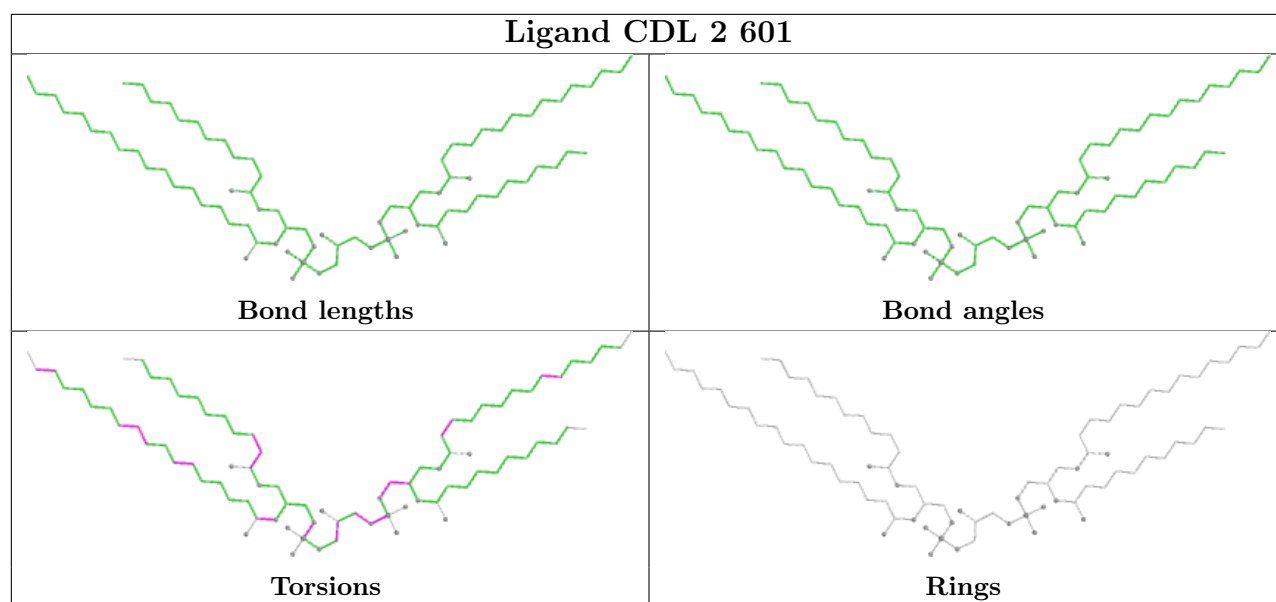


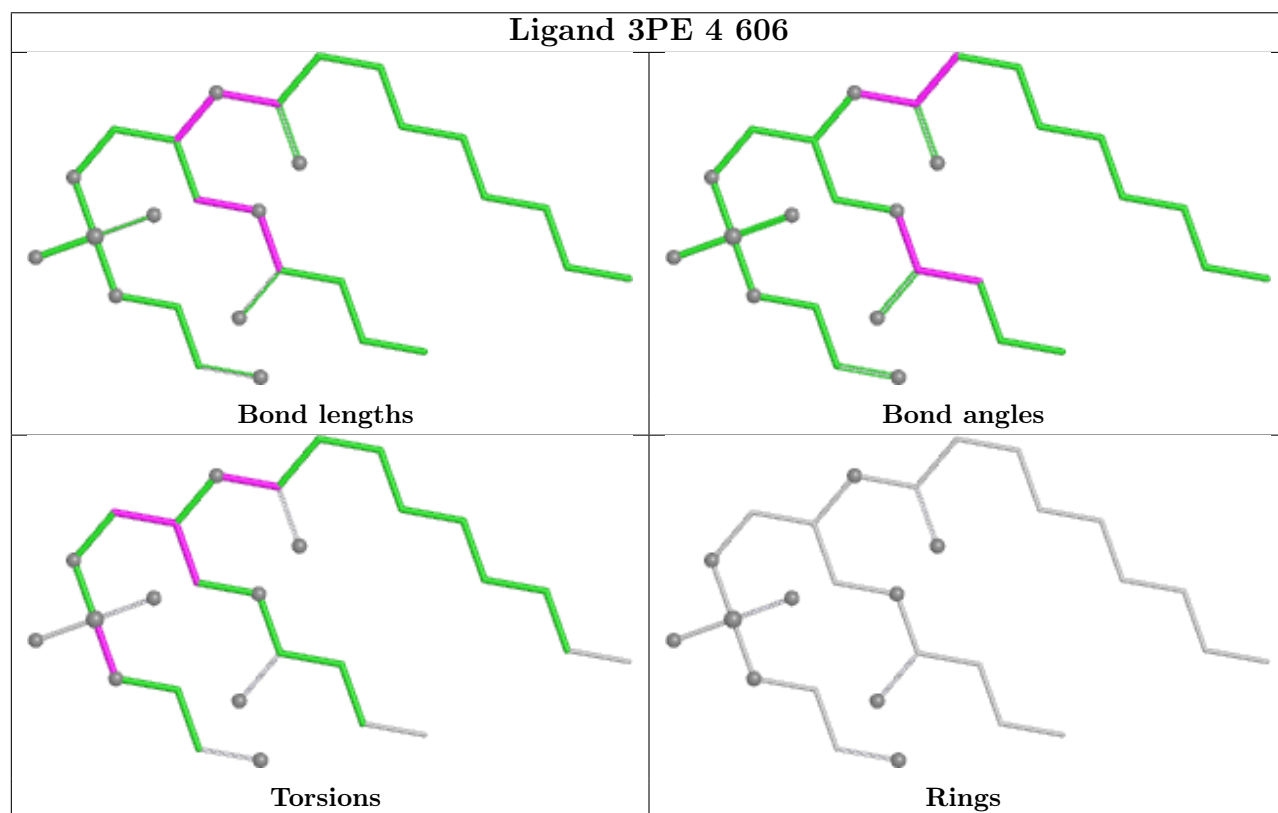
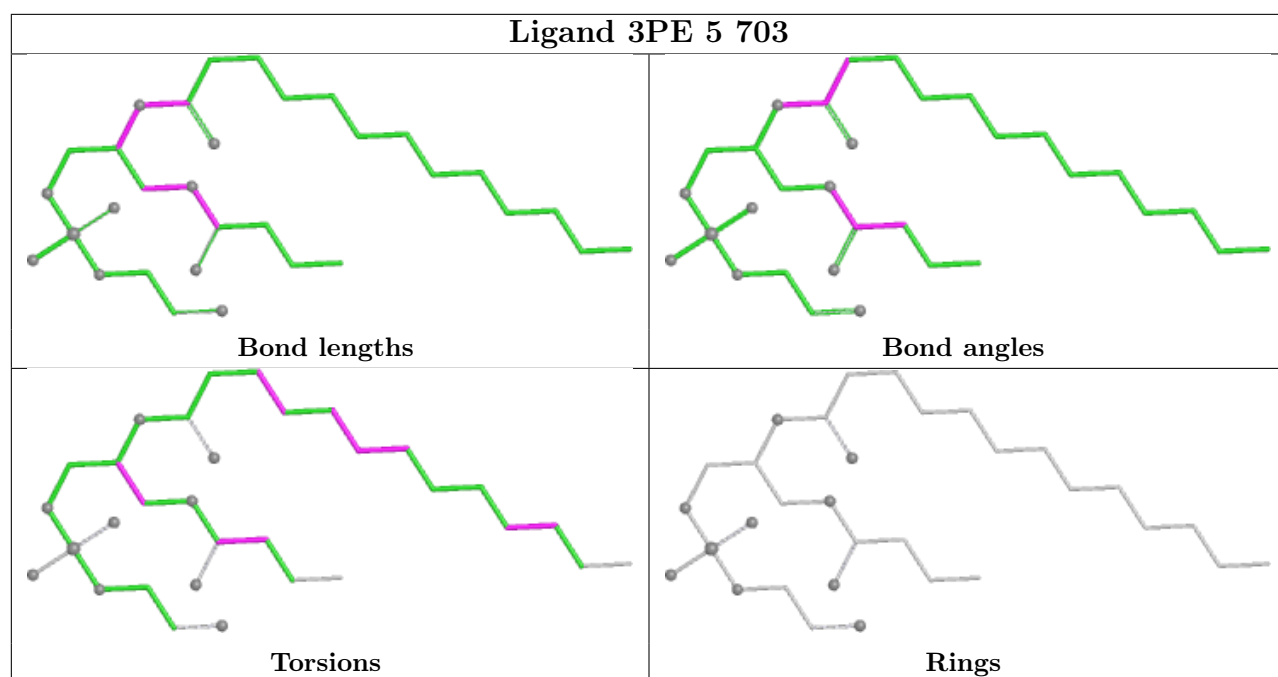




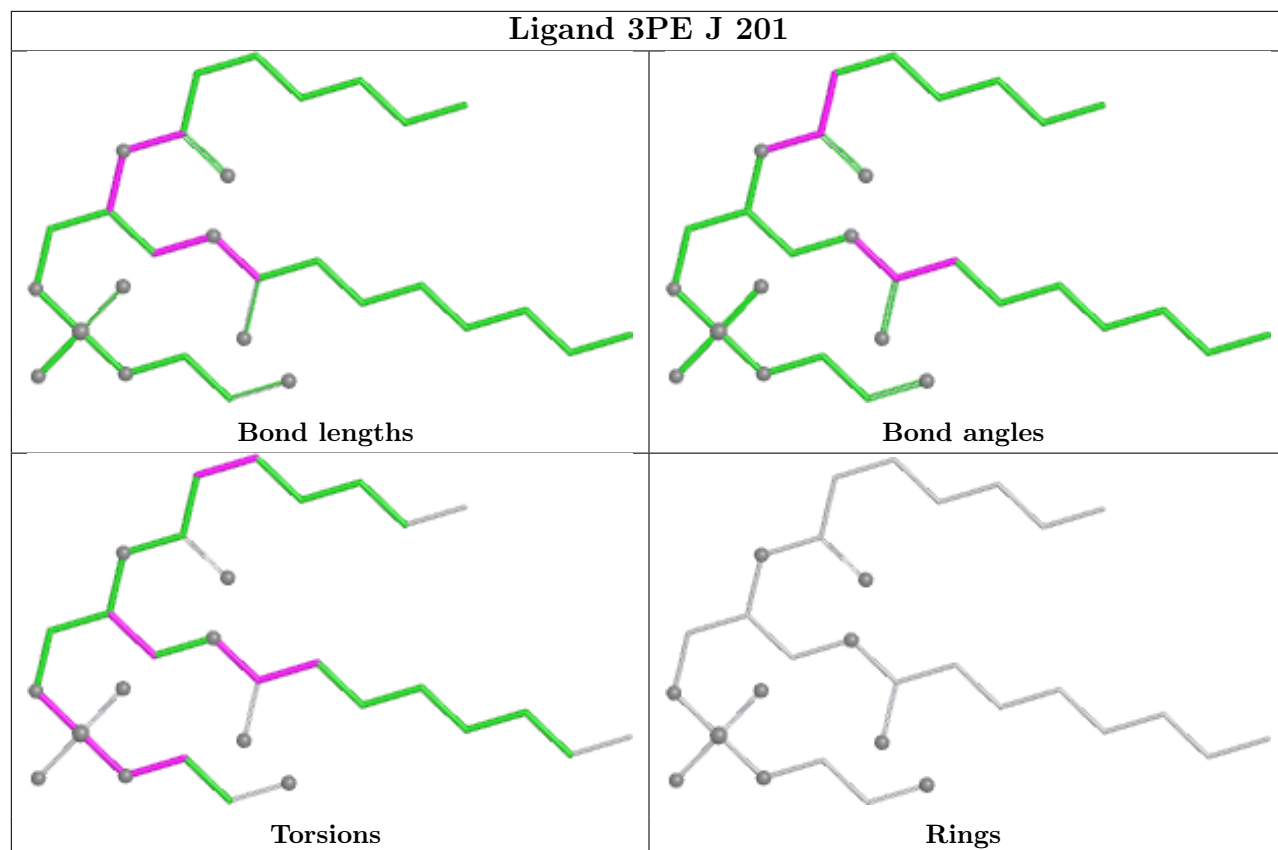




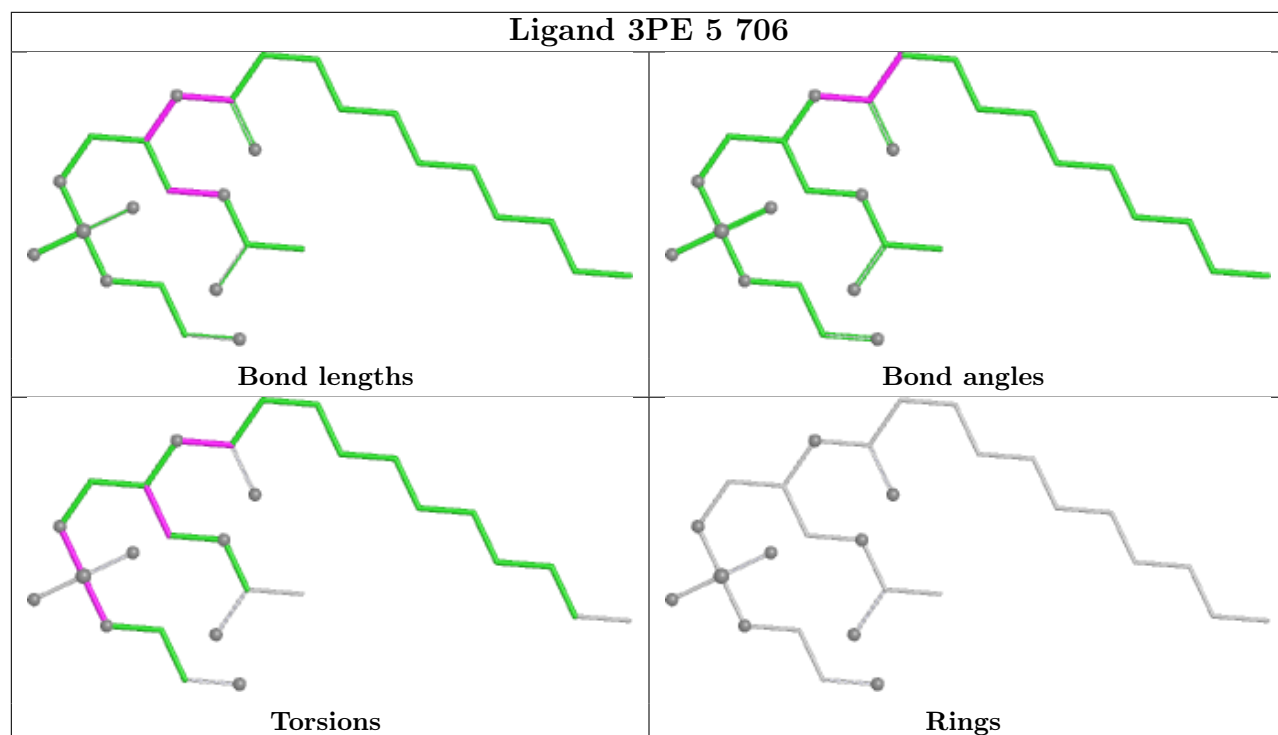


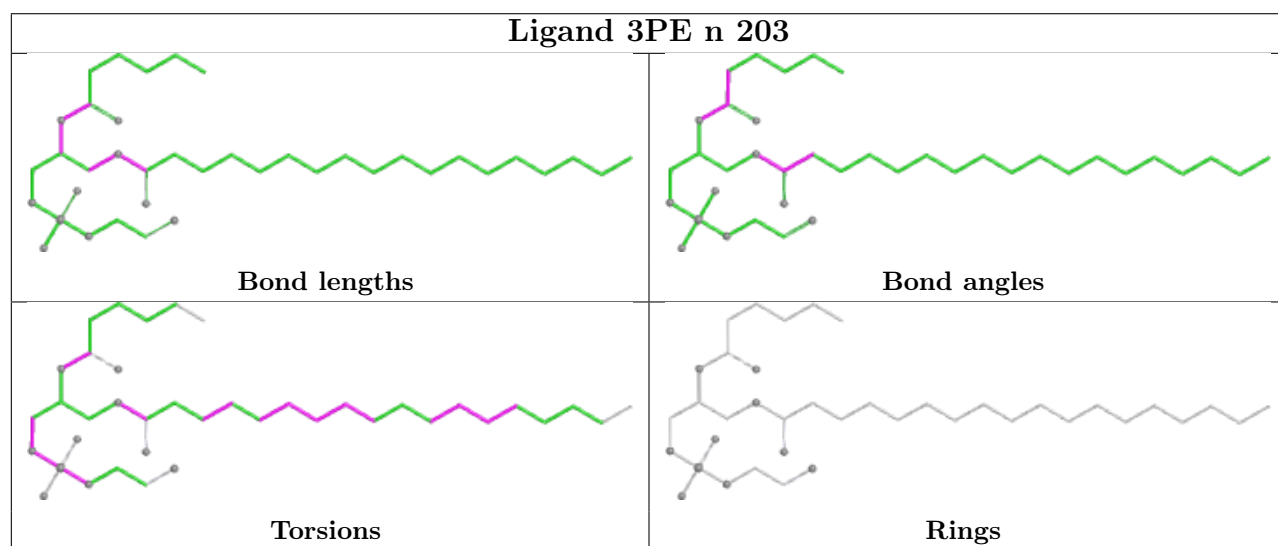
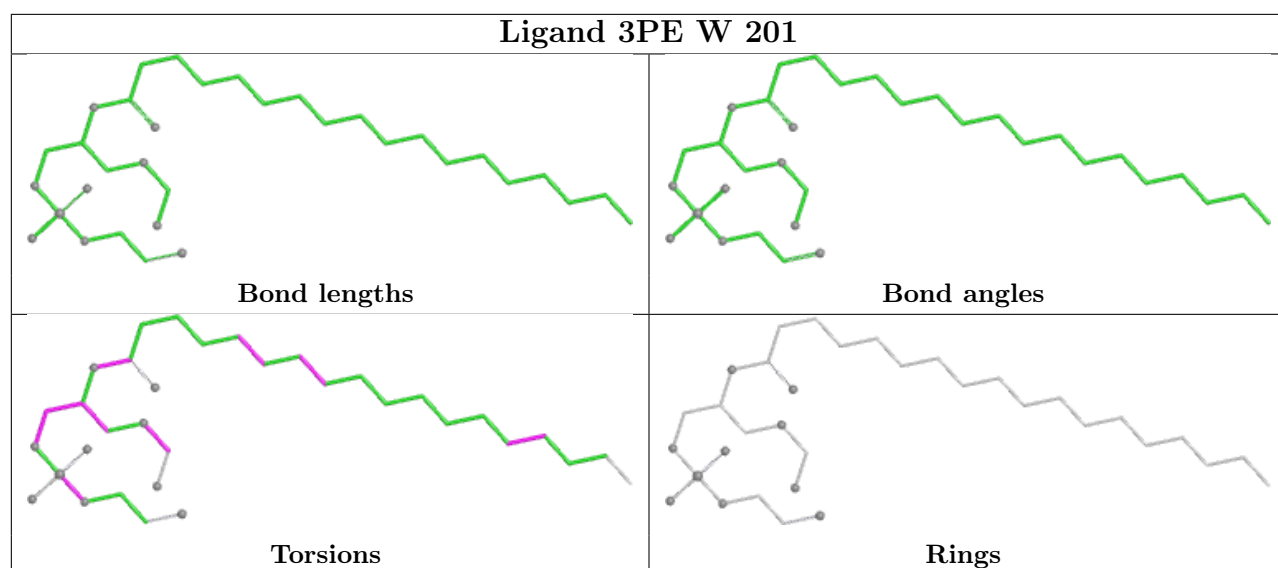


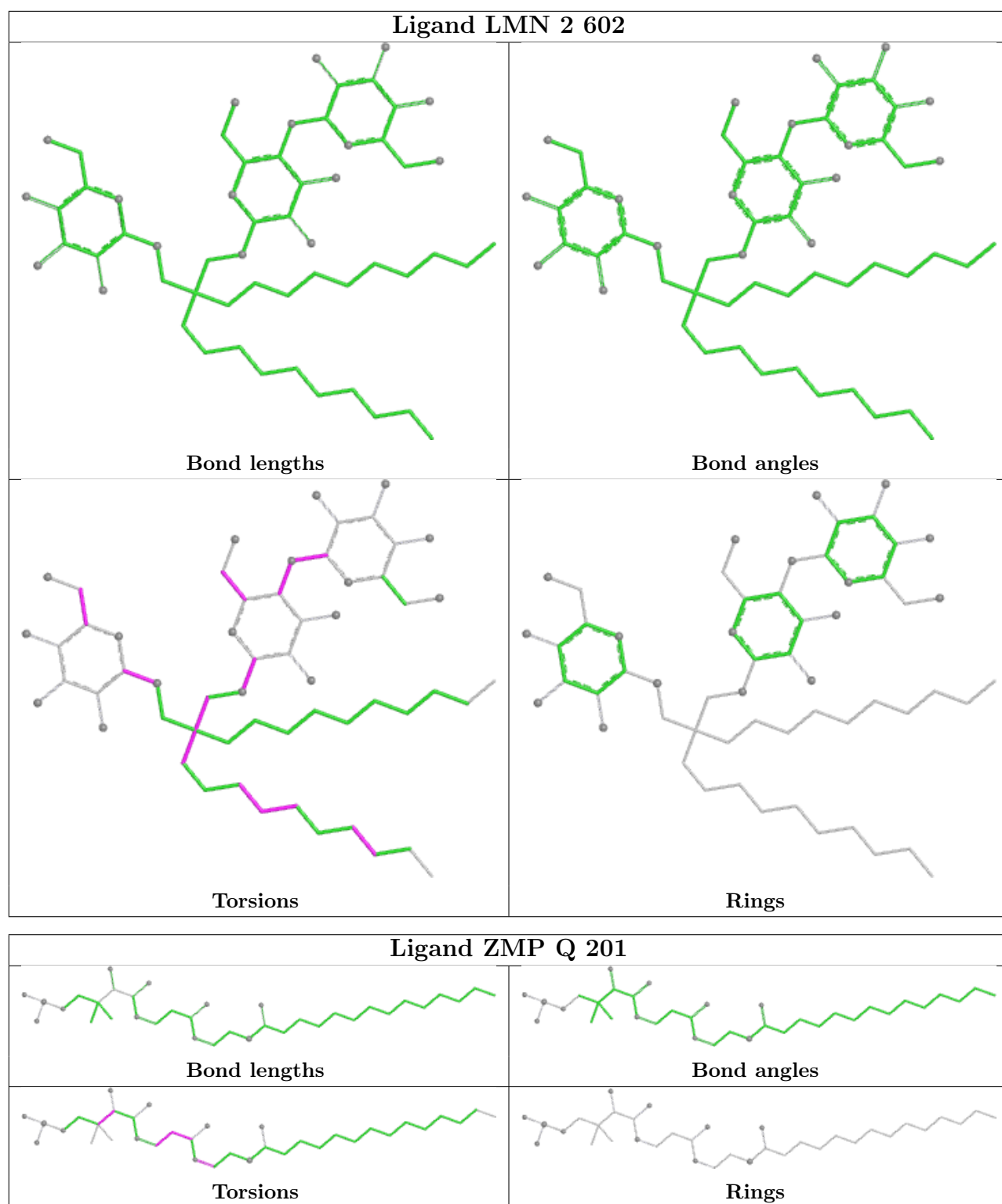
Ligand 3PE J 201

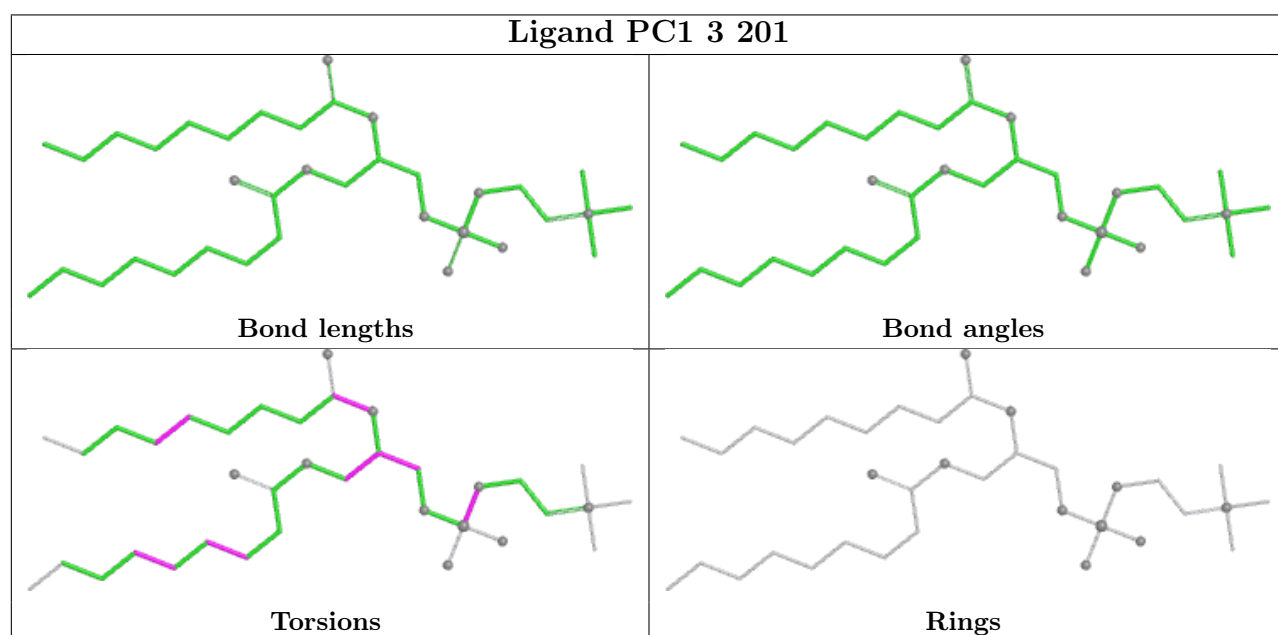
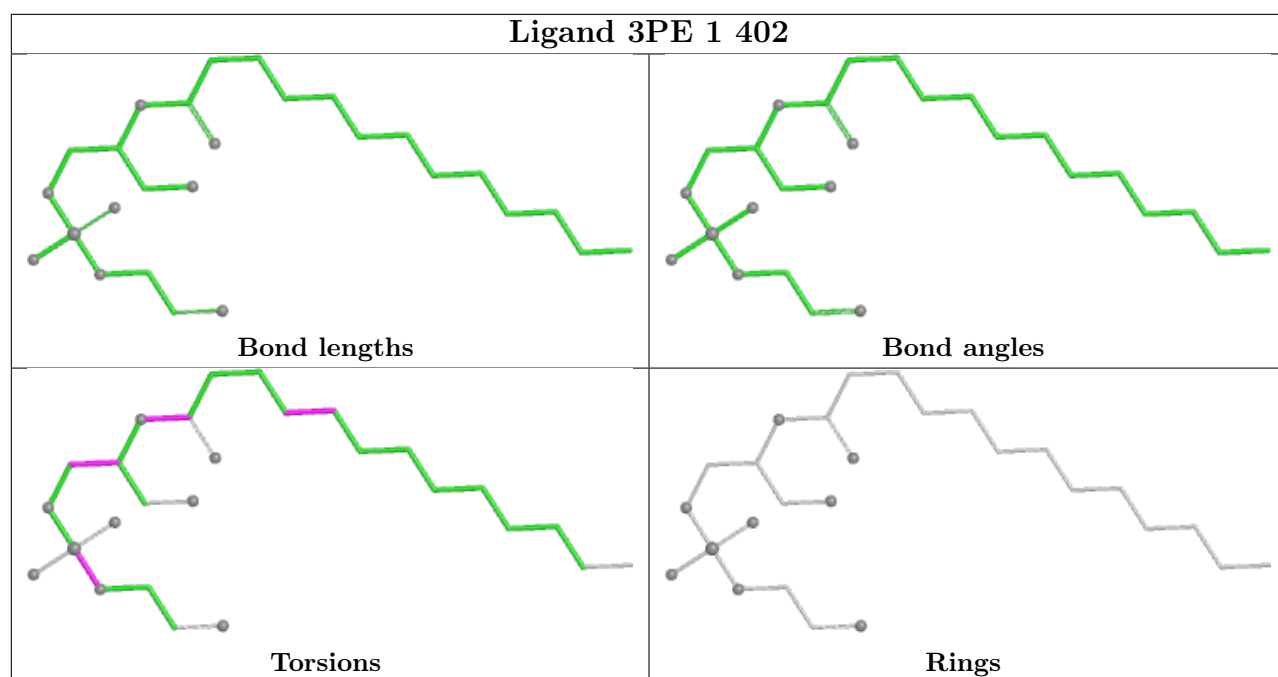


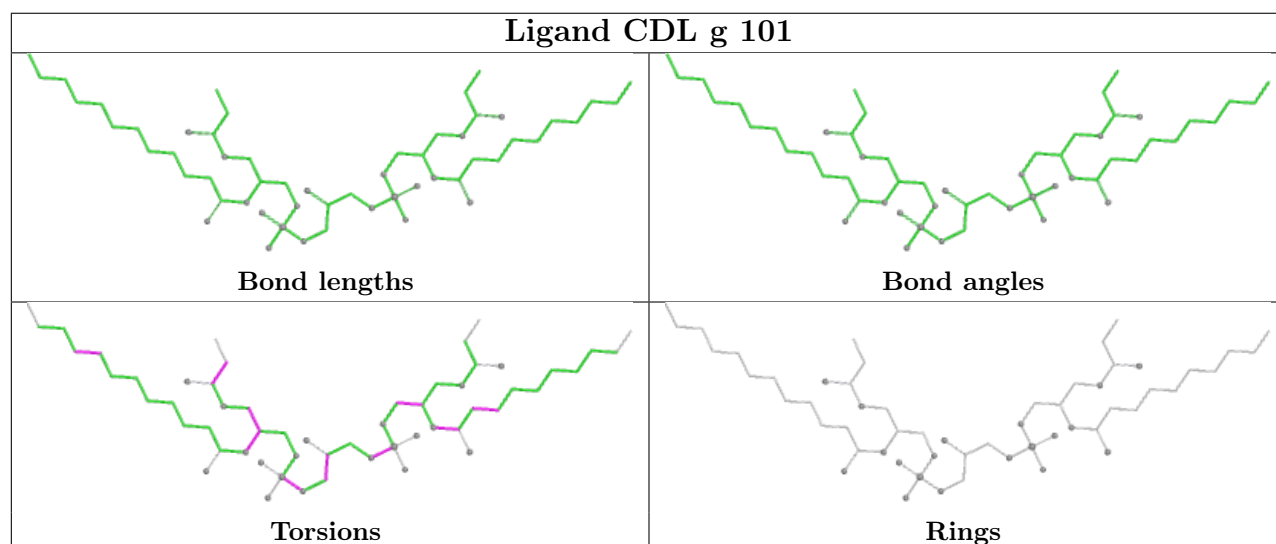
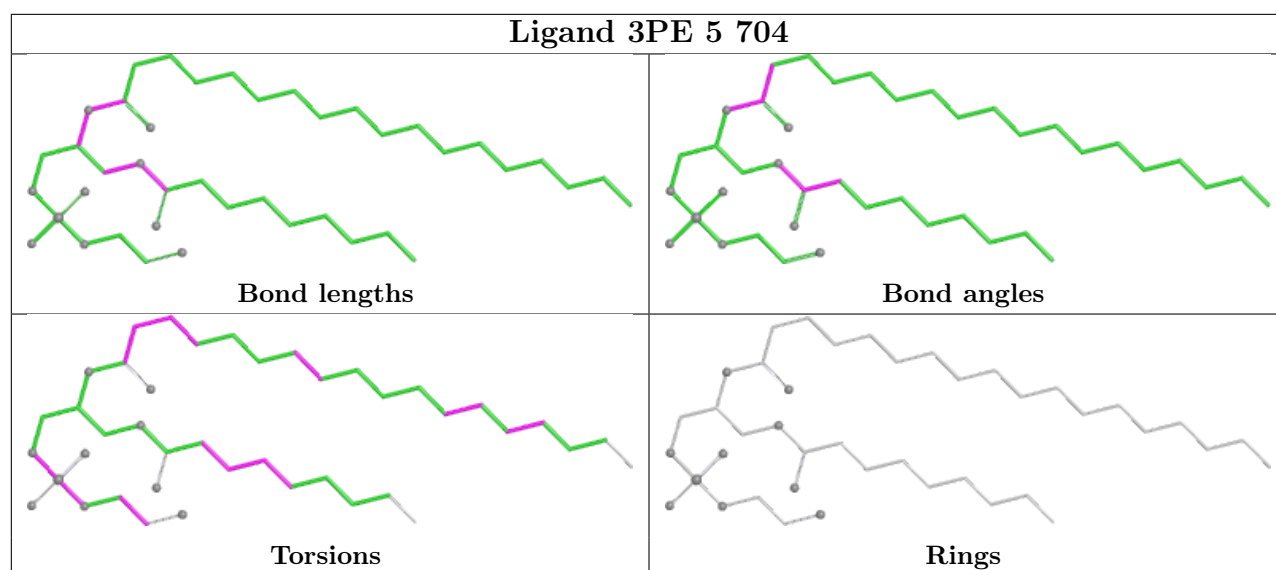
Ligand 3PE 5 706

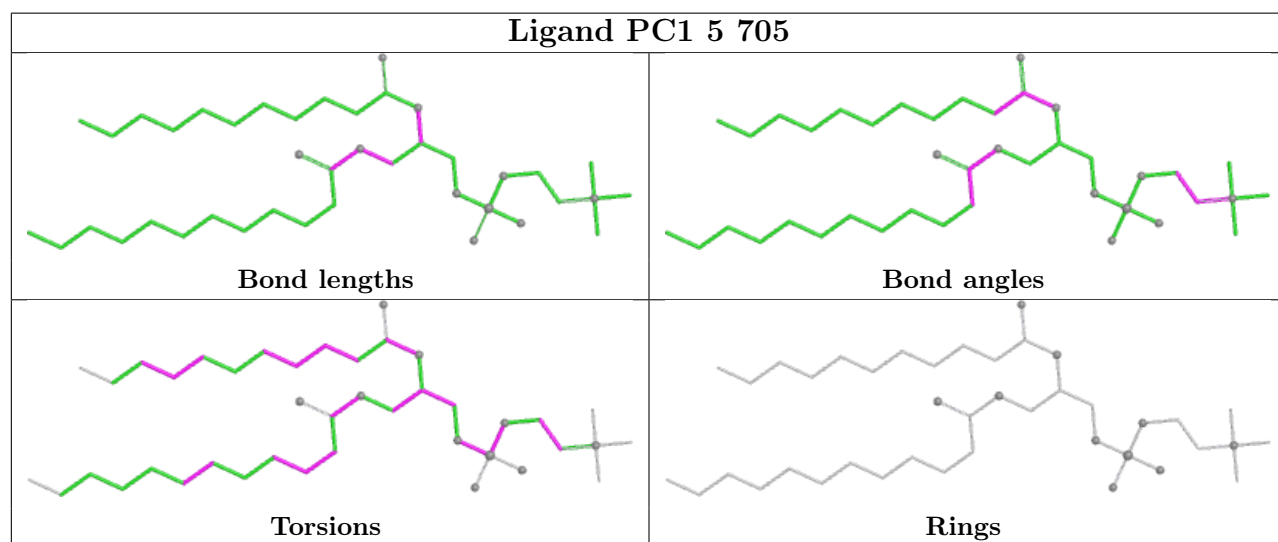
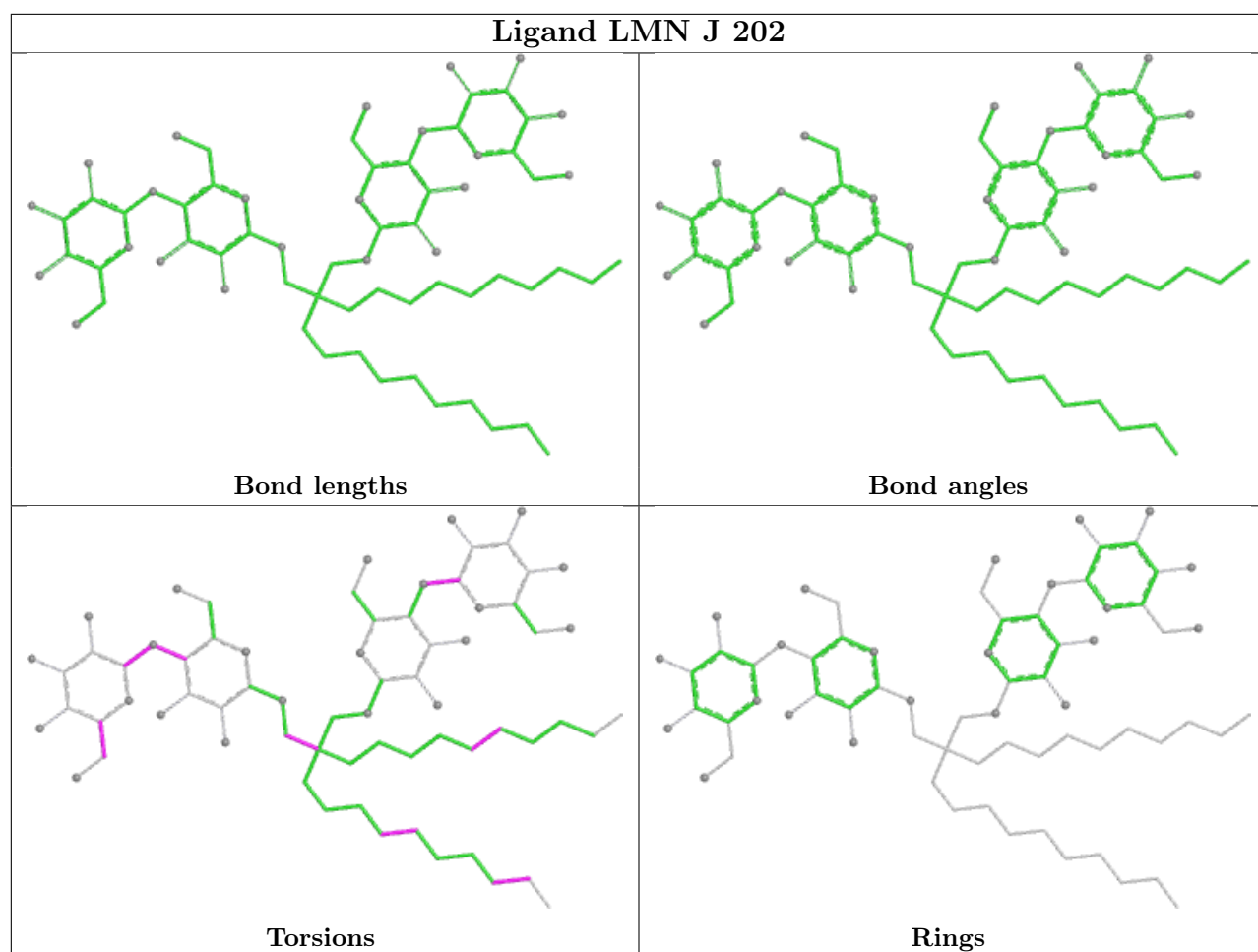


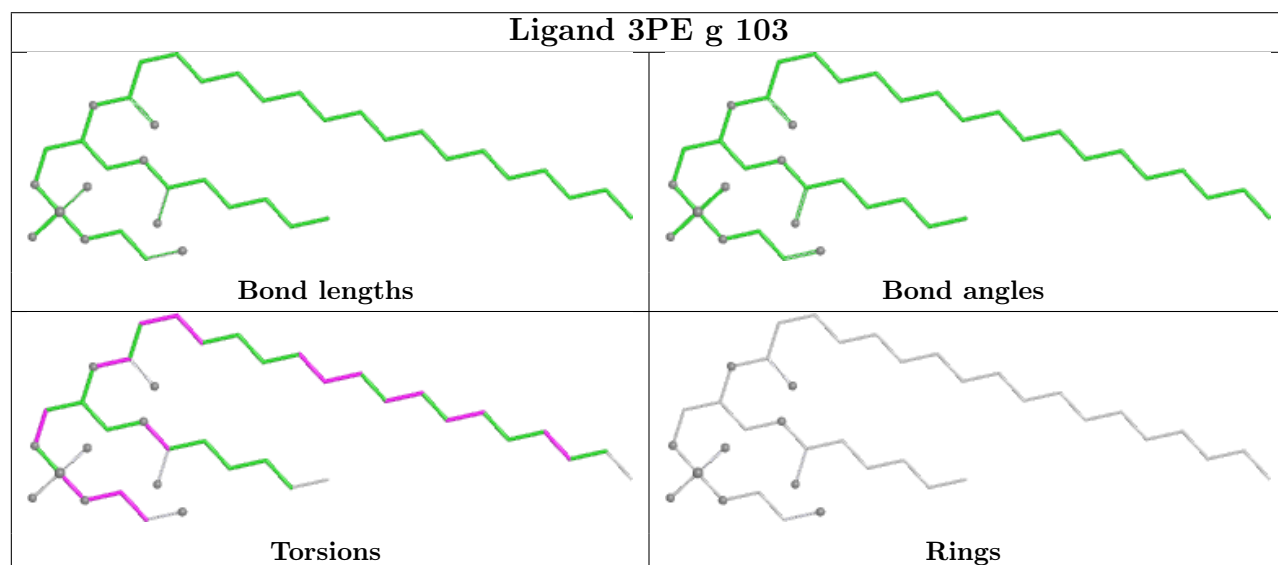
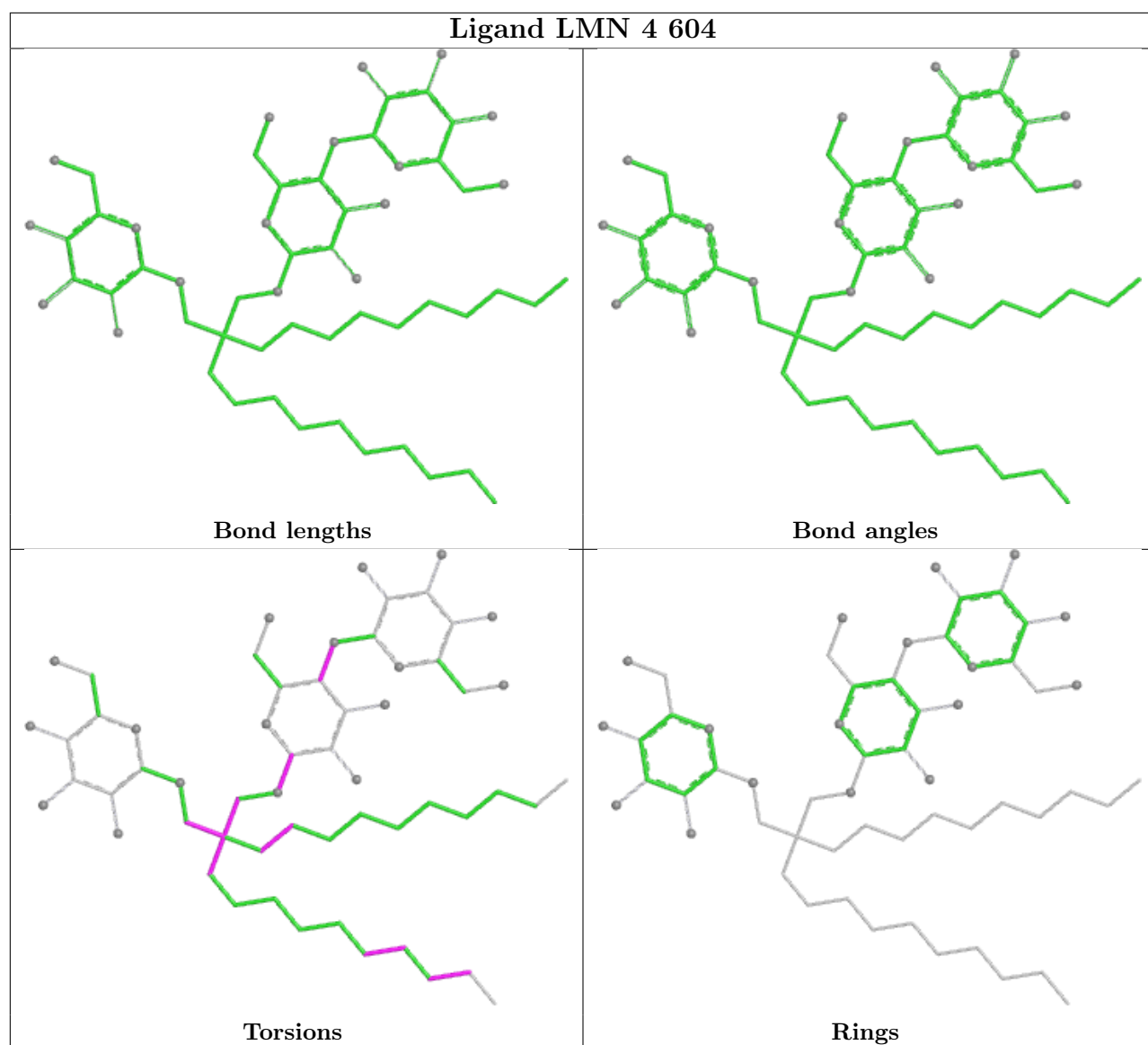


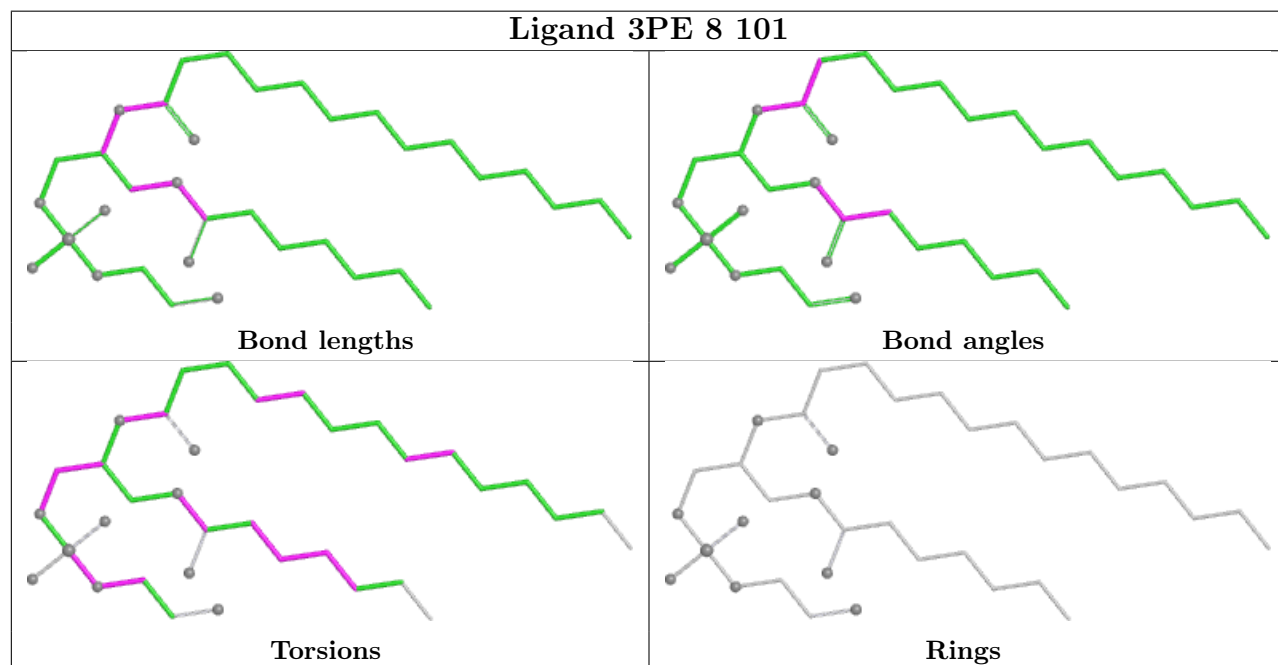
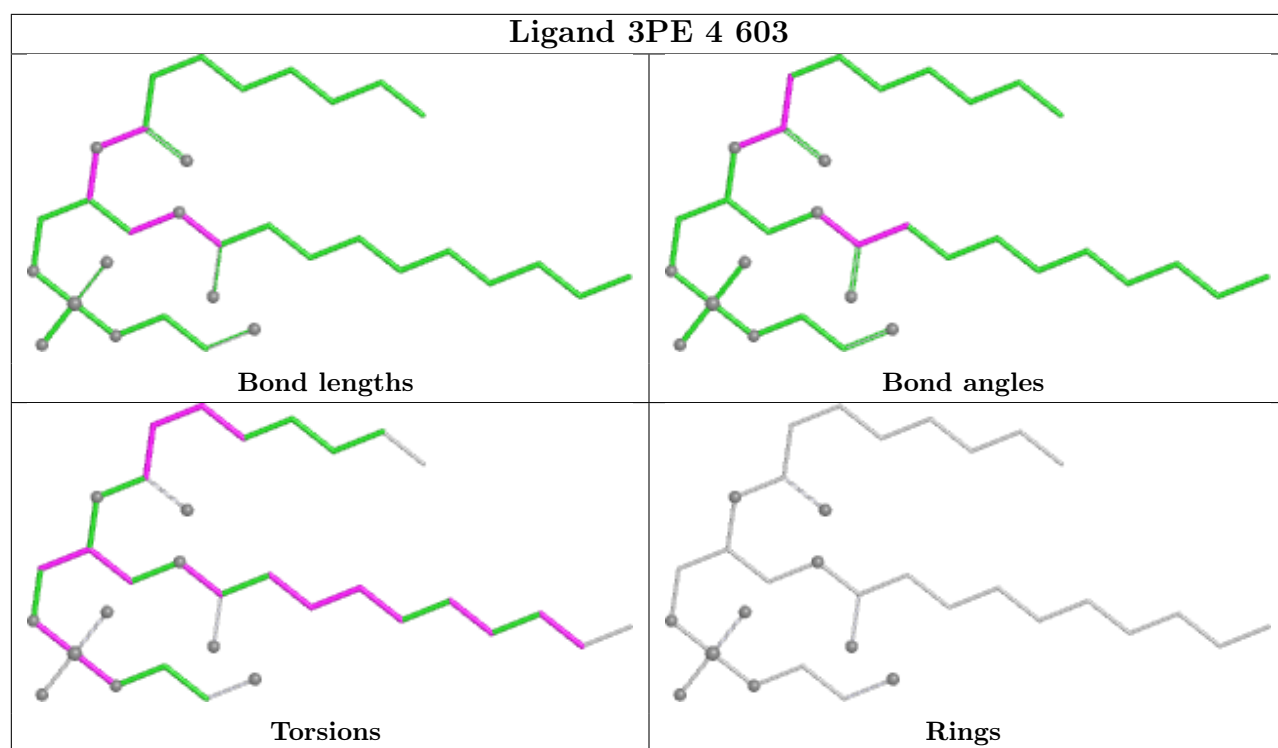


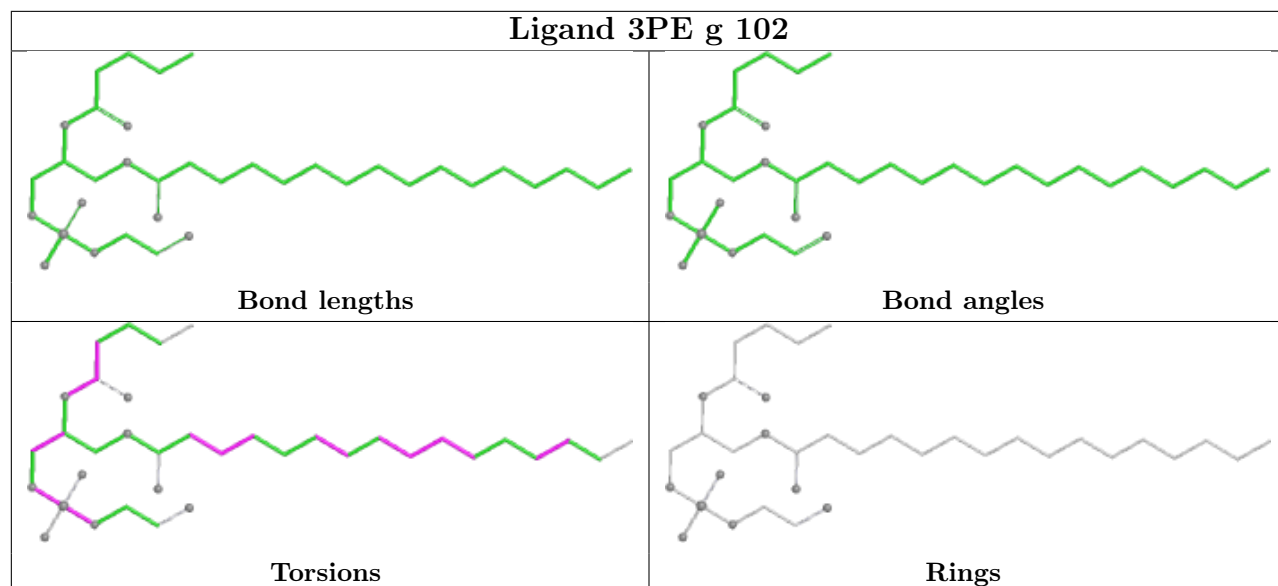












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

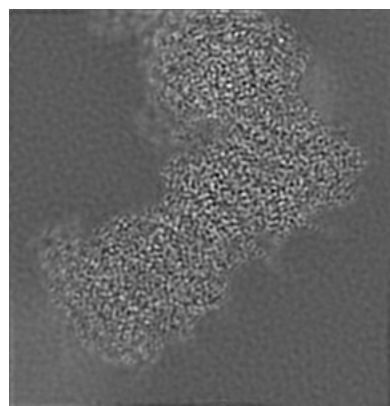
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14796. These allow visual inspection of the internal detail of the map and identification of artifacts.

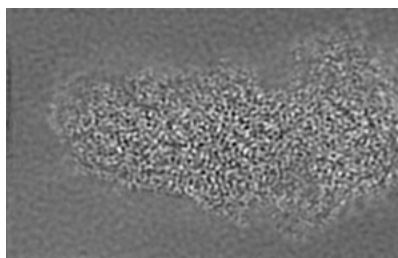
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

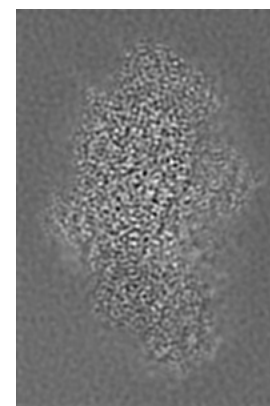
6.1.1 Primary map



X

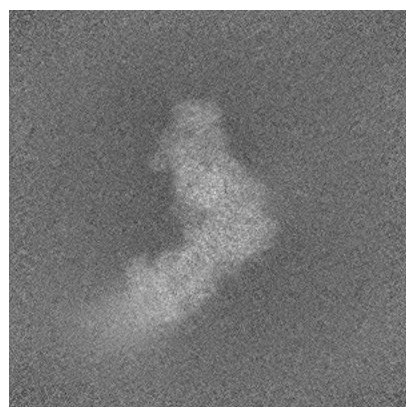


Y

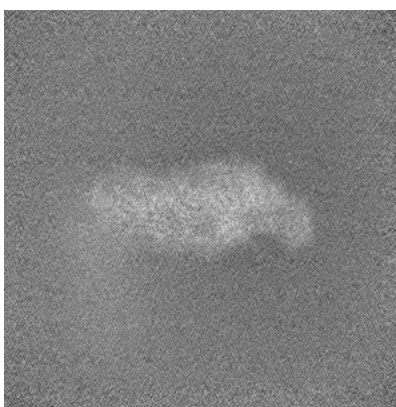


Z

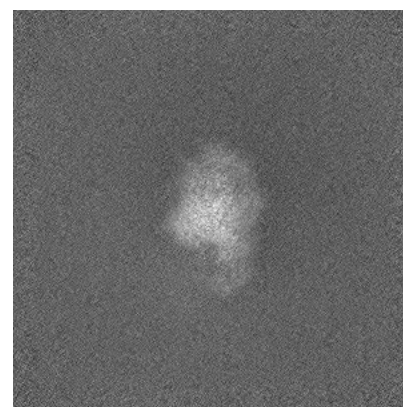
6.1.2 Raw map



X



Y

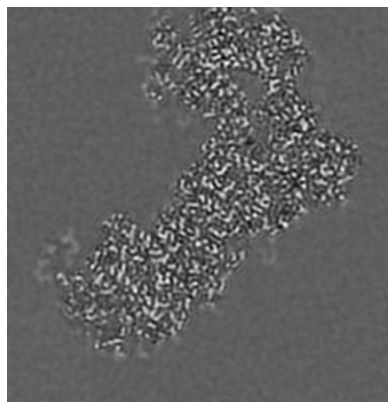


Z

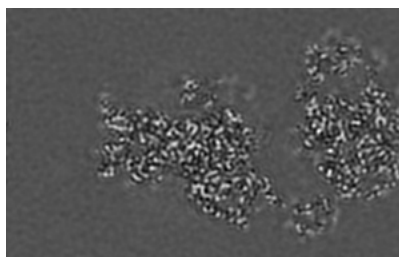
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

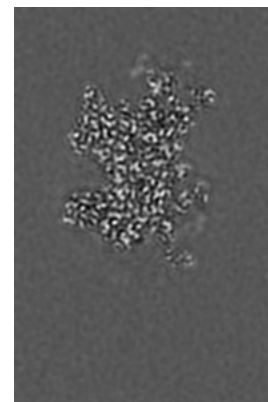
6.2.1 Primary map



X Index: 86

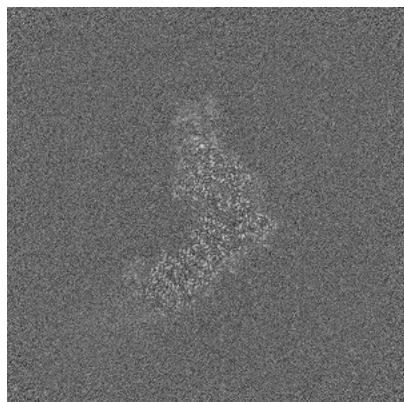


Y Index: 130

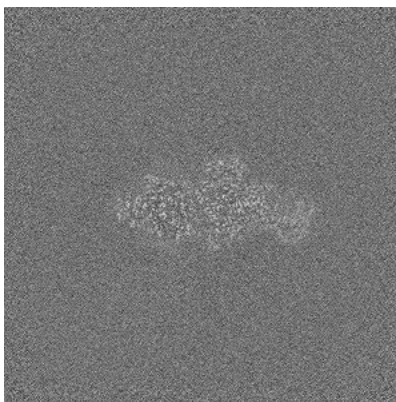


Z Index: 136

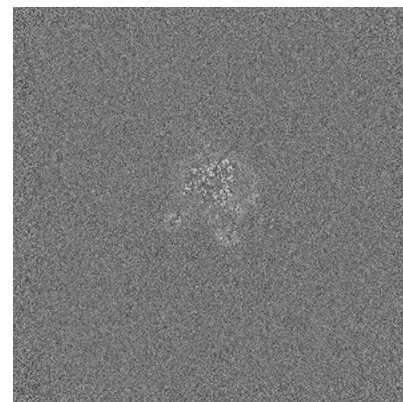
6.2.2 Raw map



X Index: 294



Y Index: 294

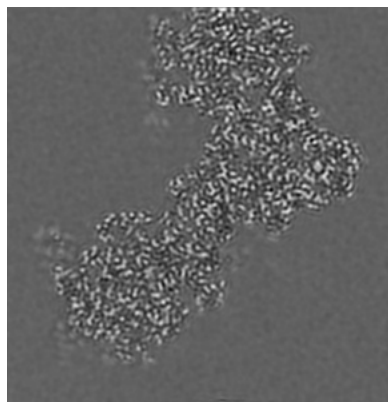


Z Index: 294

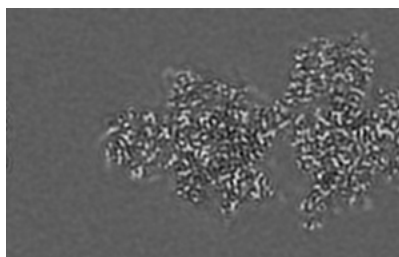
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

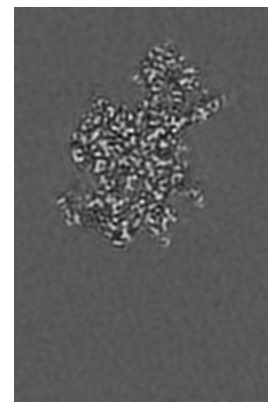
6.3.1 Primary map



X Index: 92

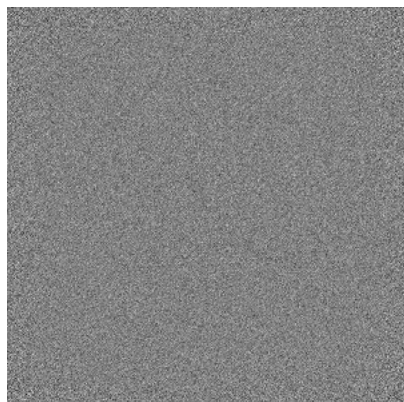


Y Index: 140

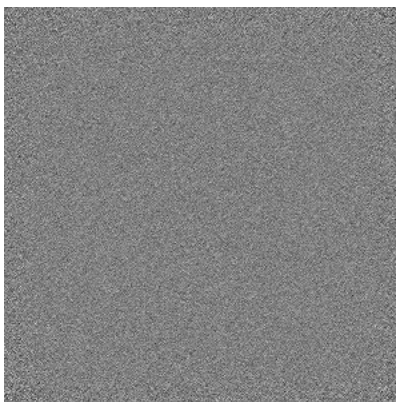


Z Index: 145

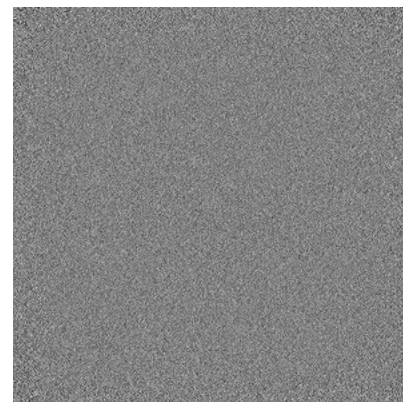
6.3.2 Raw map



X Index: 0



Y Index: 0

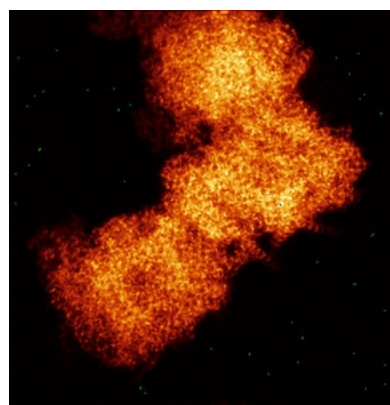


Z Index: 0

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

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

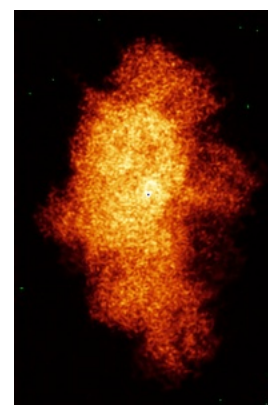
6.4.1 Primary map



X

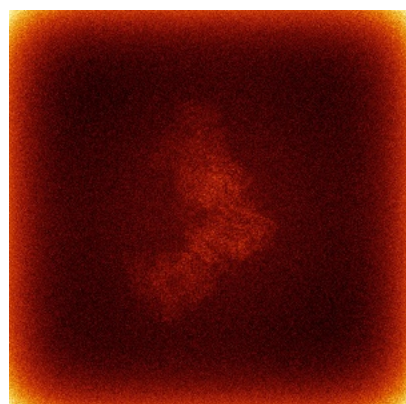


Y

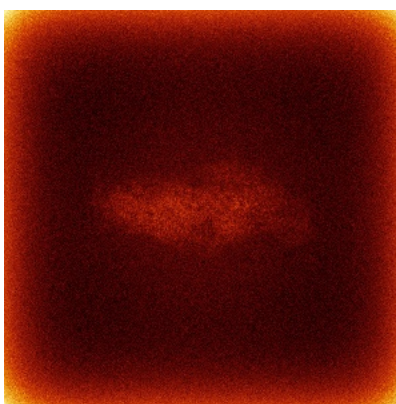


Z

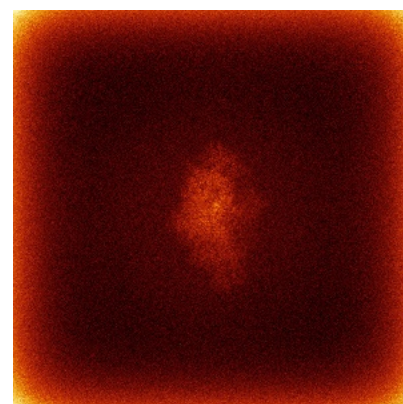
6.4.2 Raw map



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](#)

This section was not generated.

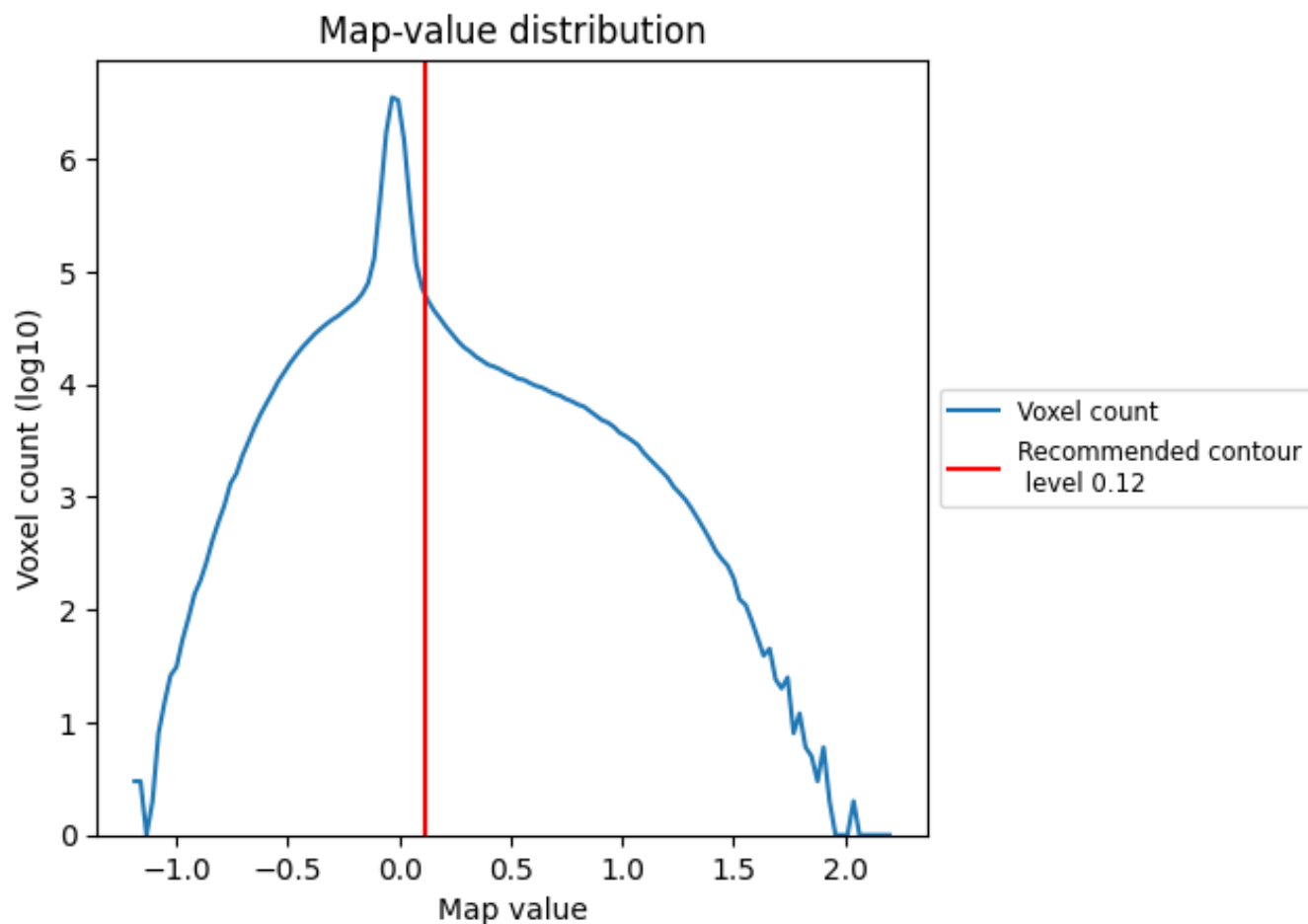
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

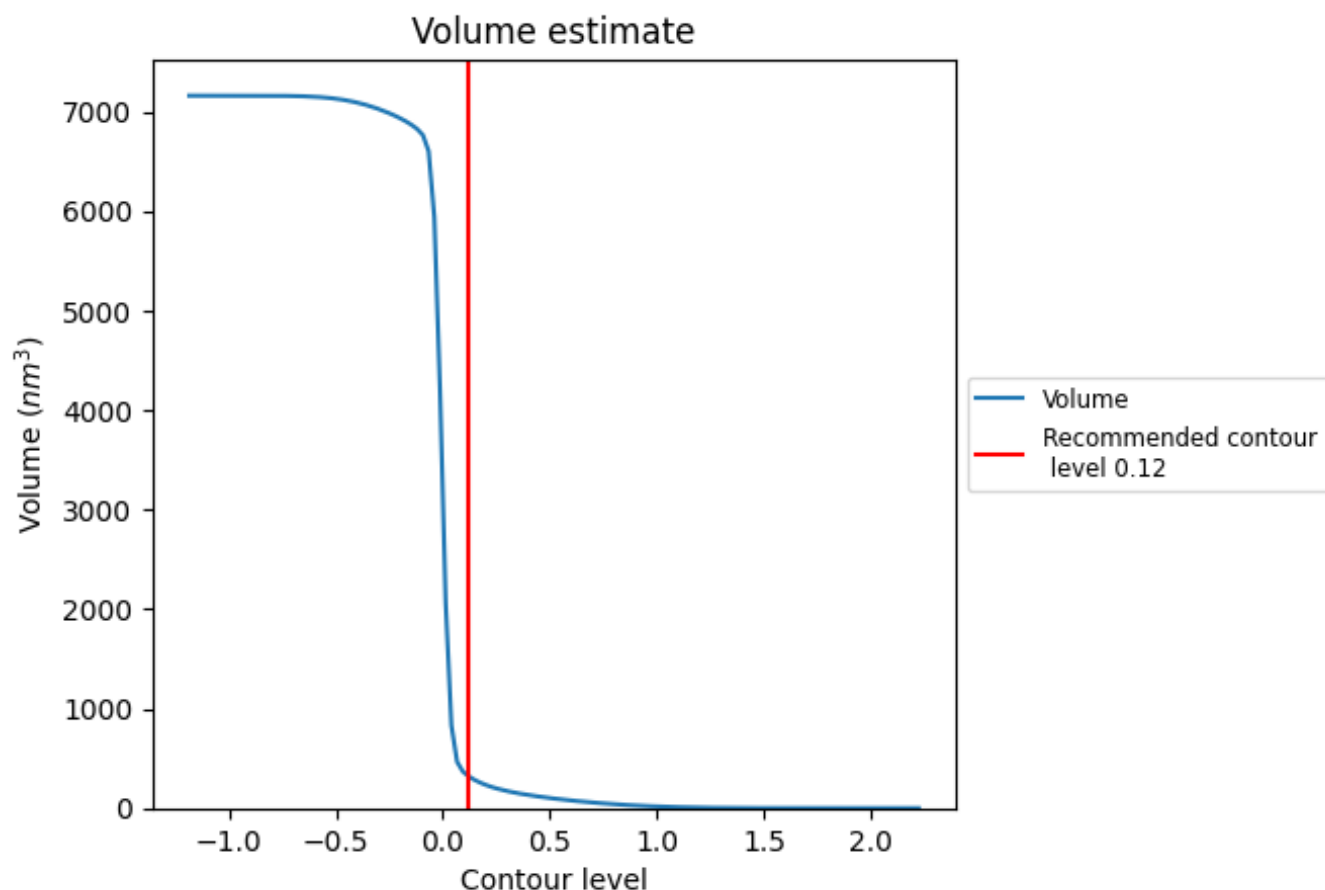
This section contains the results of statistical analysis of the map.

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 320 nm^3 ; this corresponds to an approximate mass of 289 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.

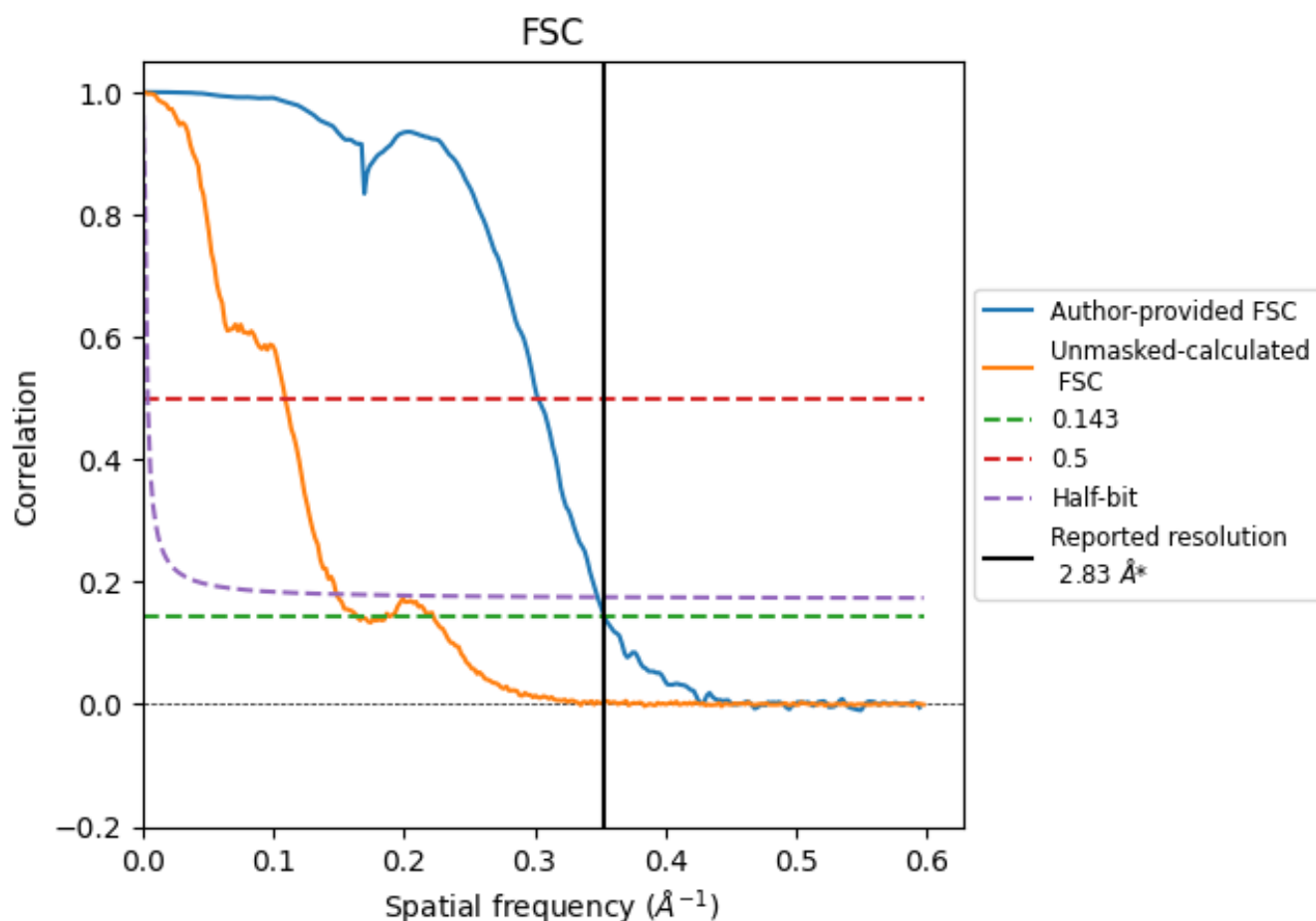
7.3 Rotationally averaged power spectrum [i](#)

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 0.353 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.83	3.31	2.87
Unmasked-calculated*	6.09	9.16	6.74

*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 6.09 differs from the reported value 2.83 by more than 10 %

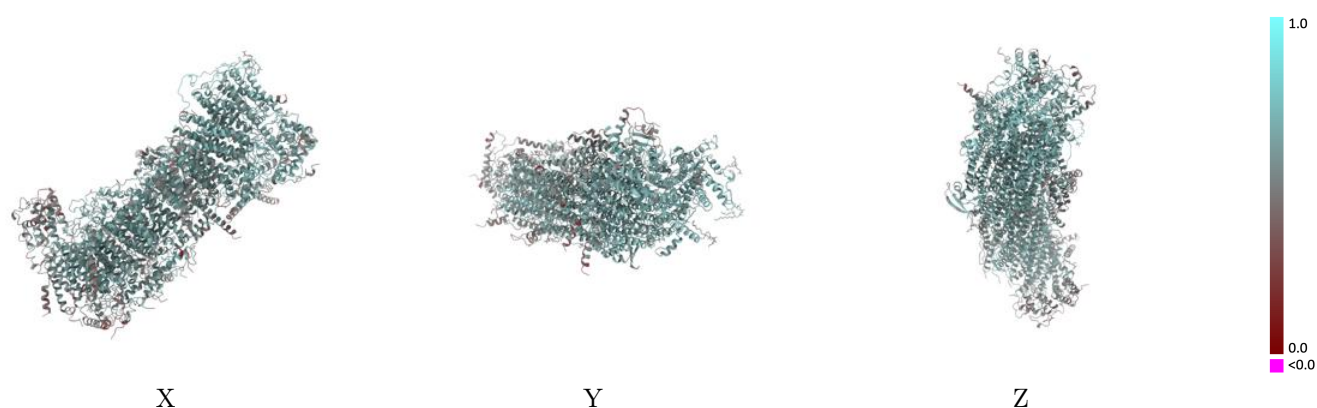
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14796 and PDB model 7ZME. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)

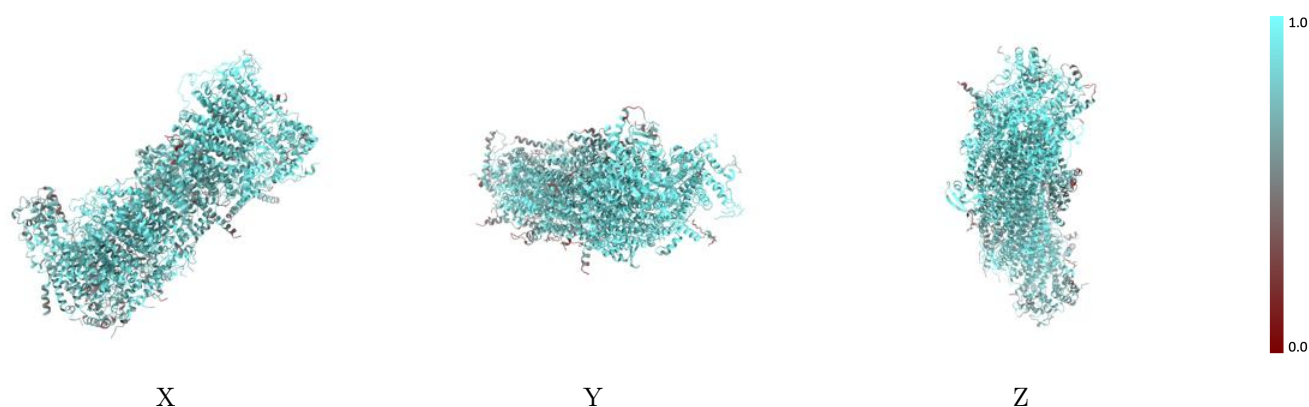
This section was not generated.

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



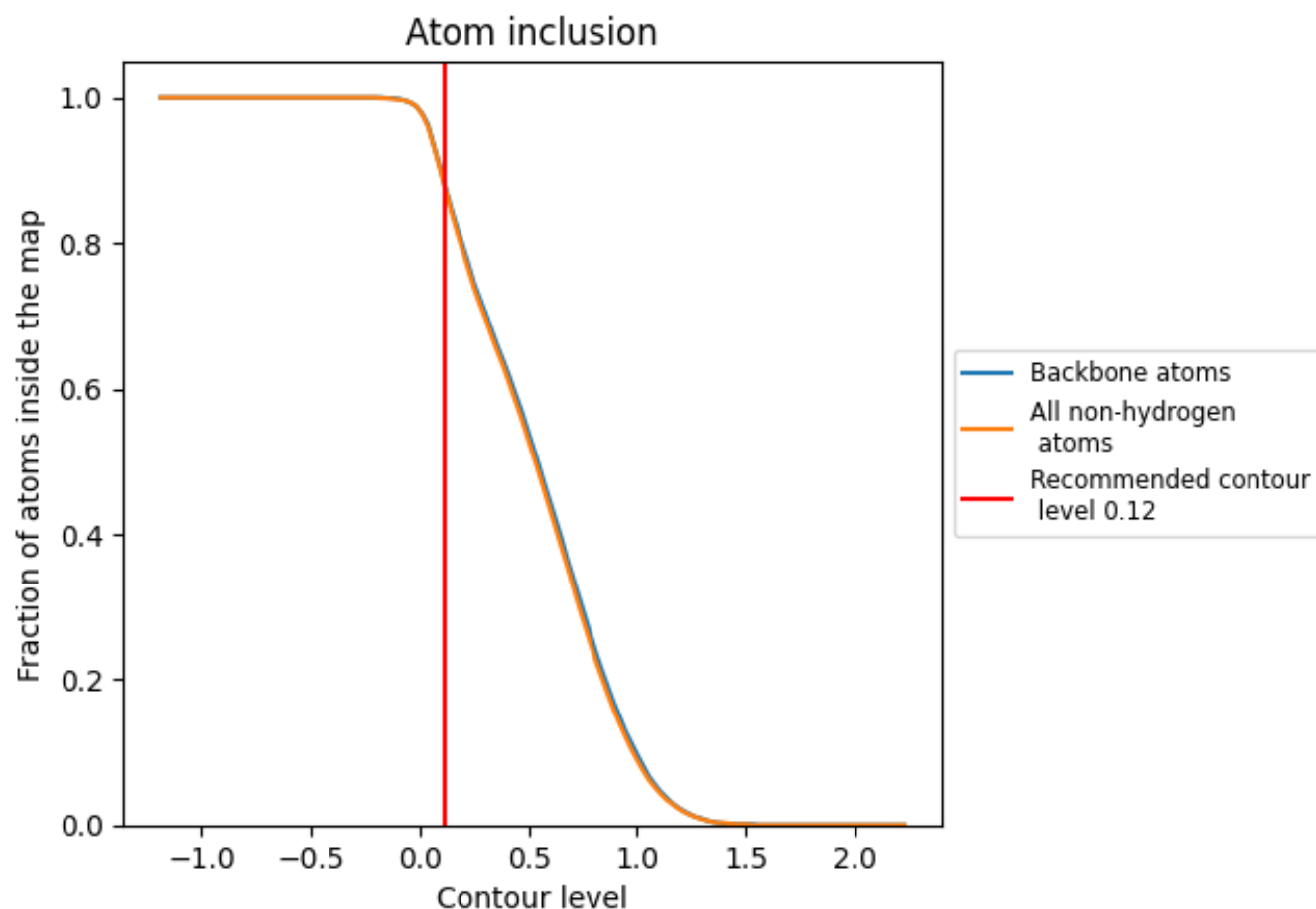
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 88% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8730	 0.5960
1	 0.9560	 0.6450
2	 0.9400	 0.6410
3	 0.9260	 0.6270
4	 0.9260	 0.6290
5	 0.9000	 0.6030
6	 0.8990	 0.6080
8	 0.6260	 0.4540
9	 0.8030	 0.5620
D	 0.9370	 0.6340
J	 0.6970	 0.5030
L	 0.9330	 0.6310
Q	 0.6460	 0.4580
R	 0.7840	 0.5400
S	 0.8510	 0.5740
U	 0.9220	 0.6120
W	 0.9000	 0.6230
X	 0.9160	 0.6160
a	 0.8090	 0.5430
b	 0.8450	 0.5780
c	 0.7230	 0.4780
d	 0.8650	 0.5840
e	 0.7400	 0.5080
g	 0.9010	 0.5920
i	 0.7920	 0.5460
j	 0.9000	 0.5970
n	 0.7100	 0.5340

