



Full wwPDB EM Validation Report ⓘ

Dec 19, 2022 – 02:38 PM JST

PDB ID : 7VZ8
EMDB ID : EMD-32222
Title : Membrane arm of deactive state CI from Q1-NADH dataset
Authors : Gu, J.; Yang, M.
Deposited on : 2021-11-15
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

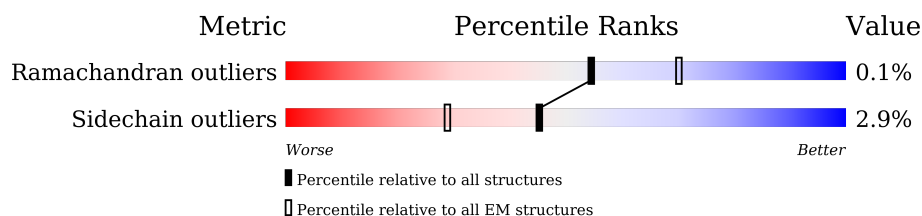
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	Q	40	<div> <div>25%</div> <div>100%</div> </div>
2	S	70	<div> <div>99%</div> </div>
3	U	83	<div> <div>8%</div> <div>96%</div> </div>
4	V	140	<div> <div>31%</div> <div>98%</div> </div>
5	W	113	<div> <div>98%</div> </div>
6	X	88	<div> <div>6%</div> <div>99%</div> </div>
7	Y	70	<div> <div>24%</div> <div>99%</div> </div>
8	Z	84	<div> <div>21%</div> <div>100%</div> </div>
9	a	140	<div> <div>99%</div> </div>

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Mol	Chain	Length	Quality of chain
10	b	126	
11	c	156	
12	d	175	
13	e	107	
14	f	42	
15	g	121	
16	h	105	
17	i	347	
18	j	113	
19	k	98	
20	l	603	
21	m	175	
22	n	56	
23	o	128	
24	p	178	
25	r	459	
26	s	318	
27	u	171	
28	v	124	
29	w	320	

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 39019 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 dehydrogenase [ubiquinone] iron-sulfur protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	40	Total	C	N	O	S	0	0
			333	217	56	59	1		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	70	Total	C	N	O	S	0	0
			567	364	104	94	5		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	U	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	113	Total	C	N	O	S	0	0
			949	614	160	167	8		

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	88	Total	C	N	O	S	0	0
			696	449	103	139	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	70	Total	C	N	O	S	0	0
			597	392	98	106	1		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	84	Total	C	N	O	S	0	0
			674	437	116	120	1		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	140	Total	C	N	O	S	0	0
			1165	762	199	201	3		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	103	Total	C	N	O	S	0	0
			879	573	158	147	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	156	Total	C	N	O	S	0	0
			1315	853	213	241	8		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	175	Total	C	N	O	S	0	0
			1461	916	265	272	8		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	107	Total	C	N	O	S	0	0
			890	568	145	173	4		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	f	42	Total	C	N	O	0	0
			342	225	58	59		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

- Molecule 17 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	i	347	Total	C	N	O	S	0	0
			2710	1782	420	462	46		

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	99	Total	C	N	O	S	0	0
			800	545	118	132	5		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	k	97	Total	C	N	O	S	0	0
			740	488	112	127	13		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	603	Total	C	N	O	S	0	0
			4782	3172	740	819	51		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	126	Total	C	N	O	S	0	0
			925	622	135	162	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	n	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	o	128	Total	C	N	O	S	0	0
			1062	691	182	189			

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	p	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

- Molecule 25 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	r	459	Total	C	N	O	S	0	0
			3631	2412	572	609	38		

- Molecule 26 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	s	303	Total	C	N	O	S	0	0
			2394	1607	369	397	21		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	u	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

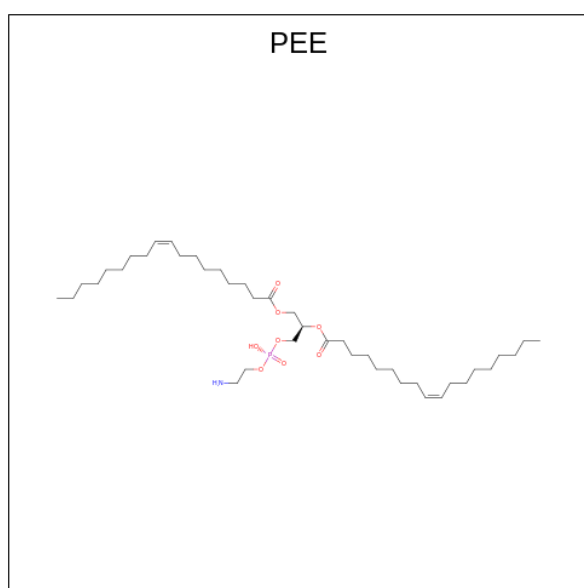
- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	v	124	Total	C	N	O	S	0	0
			1028	642	195	182	9		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10.

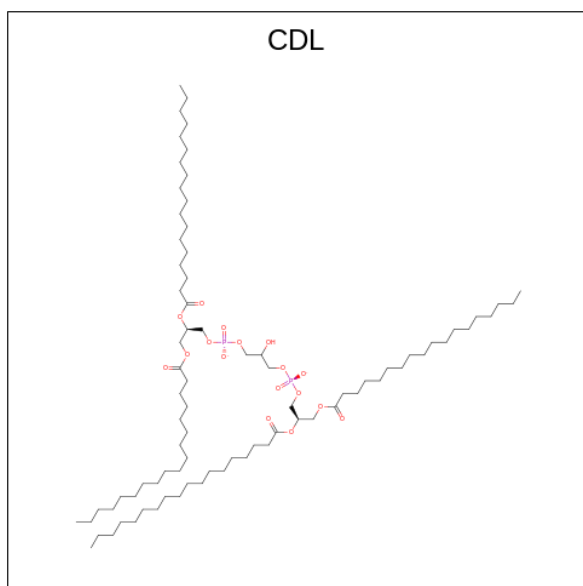
Mol	Chain	Residues	Atoms					AltConf	Trace
29	w	320	Total	C	N	O	S	0	0
			2582	1643	438	491	10		

- Molecule 30 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
30	Q	1	Total	C	N	O	P	0
			47	37	1	8	1	
30	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	b	1	Total	C	N	O	P	0
			46	36	1	8	1	
30	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
30	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
30	r	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	s	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 31 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



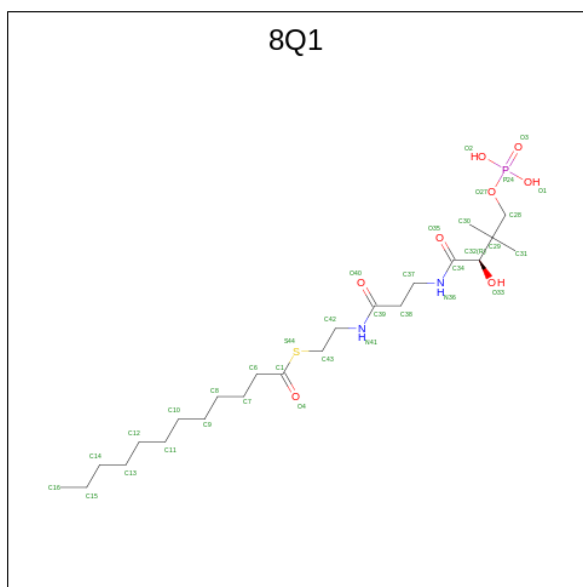
Mol	Chain	Residues	Atoms				AltConf
31	V	1	Total	C	O	P	0
			71	52	17	2	
31	a	1	Total	C	O	P	0
			91	72	17	2	
31	i	1	Total	C	O	P	0
			66	47	17	2	
31	l	1	Total	C	O	P	0
			100	81	17	2	

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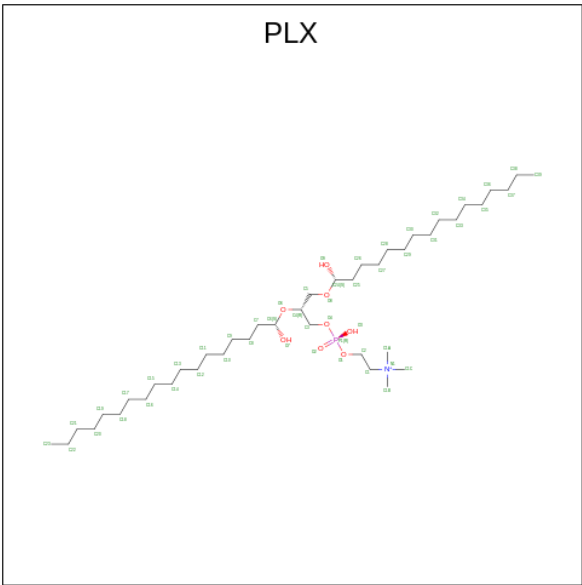
Mol	Chain	Residues	Atoms				AltConf
31	r	1	Total	C	O	P	0
			199	161	34	4	
31	r	1	Total	C	O	P	0
			199	161	34	4	

- Molecule 32 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



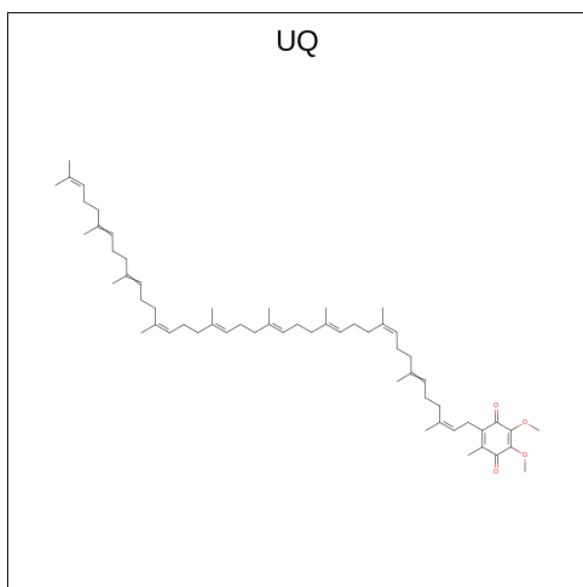
Mol	Chain	Residues	Atoms						AltConf
32	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 33 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOXOL (three-letter code: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



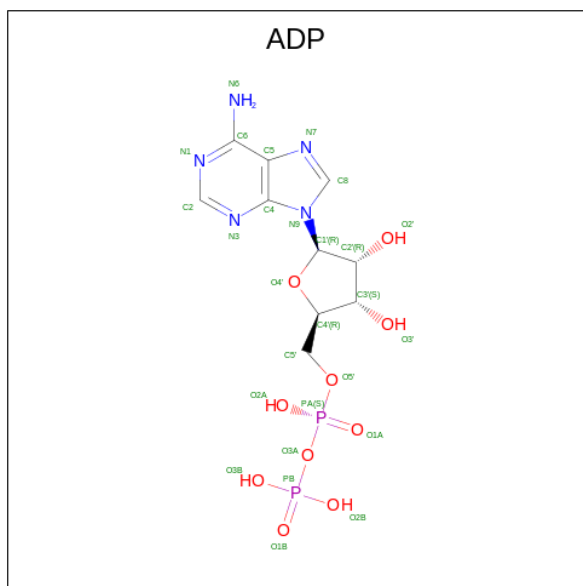
Mol	Chain	Residues	Atoms					AltConf
33	e	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	m	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	r	1	Total	C	N	O	P	0
			104	84	2	16	2	
33	r	1	Total	C	N	O	P	0
			104	84	2	16	2	

- Molecule 34 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
34	s	1	Total	C	O	0
			28	24	4	

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
35	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

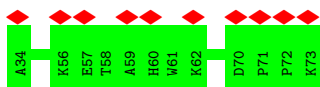
- Molecule 36 is water.

Mol	Chain	Residues	Atoms	AltConf
36	Q	5	Total O 5 5	0
36	S	7	Total O 7 7	0
36	U	3	Total O 3 3	0
36	W	3	Total O 3 3	0
36	Z	1	Total O 1 1	0
36	c	4	Total O 4 4	0
36	d	1	Total O 1 1	0
36	e	2	Total O 2 2	0
36	g	2	Total O 2 2	0
36	h	4	Total O 4 4	0
36	i	64	Total O 64 64	0
36	j	13	Total O 13 13	0
36	k	17	Total O 17 17	0
36	l	55	Total O 55 55	0
36	m	11	Total O 11 11	0
36	n	2	Total O 2 2	0
36	p	2	Total O 2 2	0
36	r	83	Total O 83 83	0
36	s	61	Total O 61 61	0
36	u	2	Total O 2 2	0
36	w	3	Total O 3 3	0

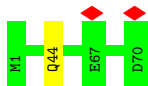
3 Residue-property plots

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

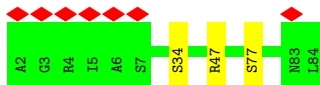
- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2



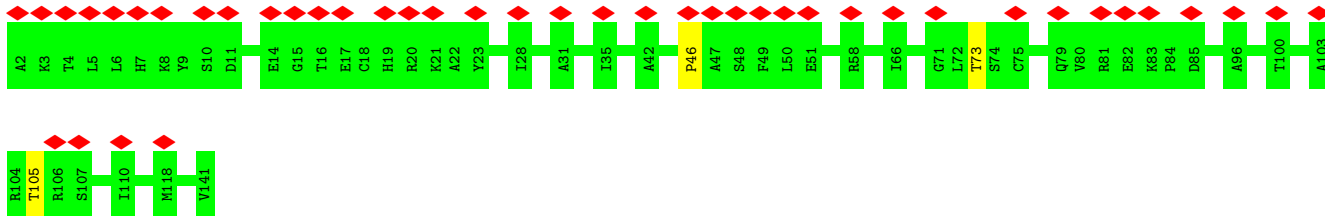
- Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



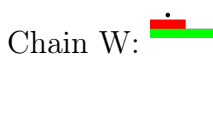
- Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

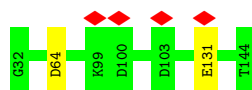


- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

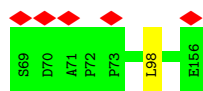


- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

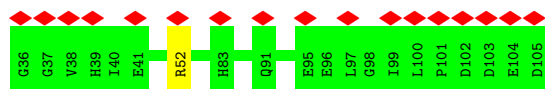




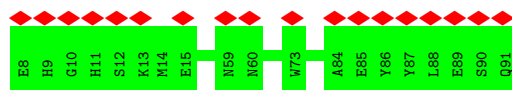
- Molecule 6: Acyl carrier protein



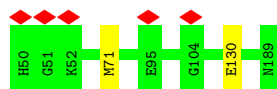
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2



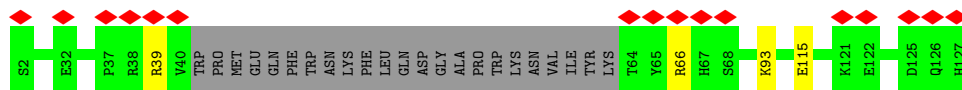
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



- Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5



- Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



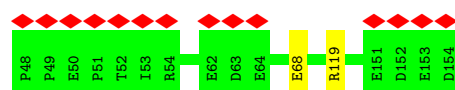
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8



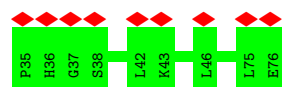
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



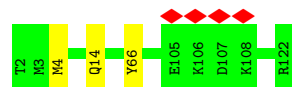
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11



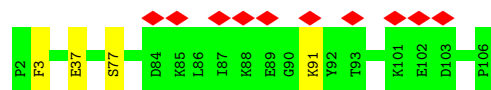
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 subunit C1



- Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2



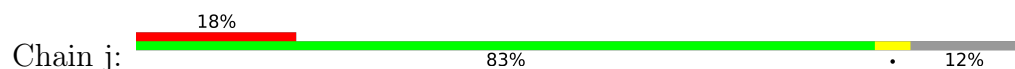
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

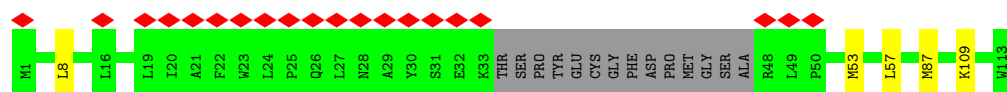


- Molecule 17: NADH-ubiquinone oxidoreductase chain 2

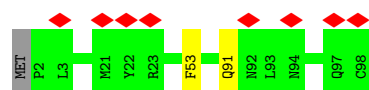


- Molecule 18: NADH-ubiquinone oxidoreductase chain 3





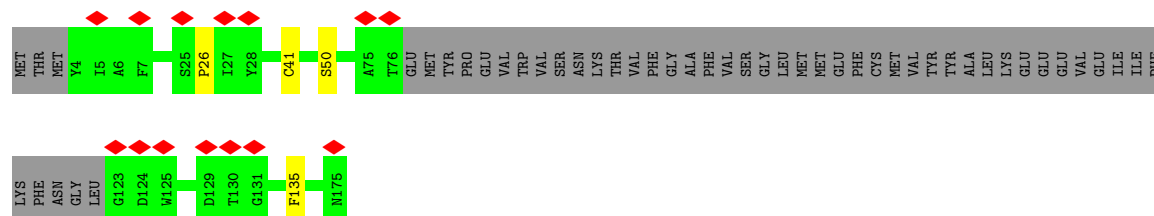
- Molecule 19: NADH-ubiquinone oxidoreductase chain 4L



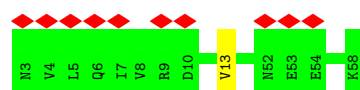
- Molecule 20: NADH-ubiquinone oxidoreductase chain 5



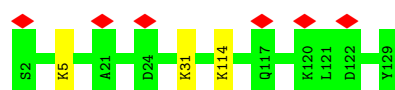
- Molecule 21: NADH-ubiquinone oxidoreductase chain 6



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9





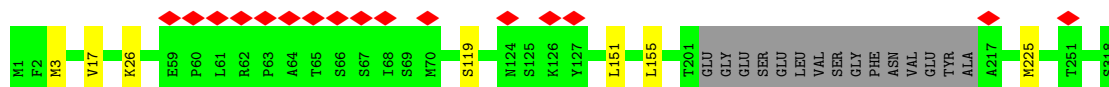
- Molecule 25: NADH-ubiquinone oxidoreductase chain 4

Chain r: 98%



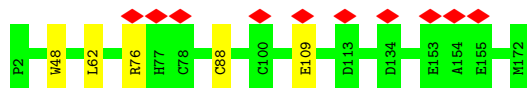
- Molecule 26: NADH-ubiquinone oxidoreductase chain 1

Chain s: 5% 93% 5%



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u: 6% 97%



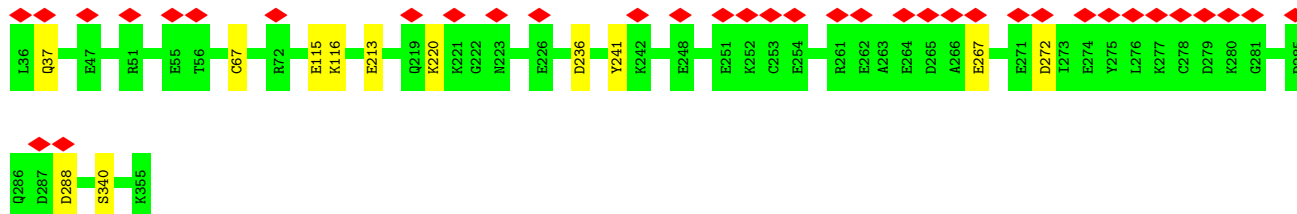
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v: 21% 91% 9%



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10

Chain w: 11% 96%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	209056	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.074	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	263.496, 263.496, 263.496	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.54895, 0.54895, 0.54895	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, 8Q1, UQ, PLX, CDL, PEE

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	Q	0.26	0/350	0.42	0/483
2	S	0.26	0/582	0.49	0/783
3	U	0.25	0/664	0.43	0/912
4	V	0.25	0/1042	0.45	0/1411
5	W	0.27	0/973	0.48	0/1312
6	X	0.26	0/708	0.44	0/959
7	Y	0.26	0/623	0.46	0/853
8	Z	0.25	0/695	0.44	0/939
9	a	0.28	0/1199	0.48	0/1623
10	b	0.27	0/906	0.53	0/1232
11	c	0.27	0/1371	0.47	0/1875
12	d	0.27	0/1494	0.51	0/2015
13	e	0.27	0/916	0.48	0/1246
14	f	0.25	0/350	0.40	0/473
15	g	0.29	0/1031	0.48	0/1394
16	h	0.26	0/889	0.50	0/1190
17	i	0.26	0/2773	0.45	0/3768
18	j	0.27	0/819	0.48	0/1117
19	k	0.26	0/751	0.44	0/1018
20	l	0.27	0/4911	0.46	0/6679
21	m	0.28	0/947	0.48	0/1286
22	n	0.24	0/491	0.48	0/663
23	o	0.27	0/1092	0.49	0/1481
24	p	0.29	0/1590	0.53	0/2155
25	r	0.27	0/3723	0.47	0/5078
26	s	0.27	0/2464	0.47	0/3369
27	u	0.27	0/1436	0.49	0/1938
28	v	0.26	0/1052	0.56	0/1411
29	w	0.27	0/2642	0.49	0/3580
All	All	0.27	0/38484	0.48	0/52243

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	38/40 (95%)	38 (100%)	0	0	100	100
2	S	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
3	U	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
4	V	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	22	46
5	W	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	Y	68/70 (97%)	63 (93%)	5 (7%)	0	100	100
8	Z	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
9	a	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
10	b	99/126 (79%)	93 (94%)	6 (6%)	0	100	100
11	c	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
12	d	173/175 (99%)	171 (99%)	2 (1%)	0	100	100
13	e	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
14	f	40/42 (95%)	40 (100%)	0	0	100	100
15	g	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
16	h	103/105 (98%)	100 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	i	345/347 (99%)	332 (96%)	13 (4%)	0	100	100
18	j	95/113 (84%)	89 (94%)	6 (6%)	0	100	100
19	k	95/98 (97%)	89 (94%)	6 (6%)	0	100	100
20	l	601/603 (100%)	583 (97%)	18 (3%)	0	100	100
21	m	122/175 (70%)	108 (88%)	13 (11%)	1 (1%)	19	43
22	n	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
23	o	126/128 (98%)	118 (94%)	8 (6%)	0	100	100
24	p	176/178 (99%)	164 (93%)	11 (6%)	1 (1%)	25	50
25	r	457/459 (100%)	447 (98%)	10 (2%)	0	100	100
26	s	299/318 (94%)	286 (96%)	13 (4%)	0	100	100
27	u	169/171 (99%)	162 (96%)	7 (4%)	0	100	100
28	v	122/124 (98%)	115 (94%)	7 (6%)	0	100	100
29	w	318/320 (99%)	307 (96%)	10 (3%)	1 (0%)	41	66
All	All	4582/4750 (96%)	4404 (96%)	174 (4%)	4 (0%)	54	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	V	46	PRO
24	p	174	PRO
21	m	26	PRO
29	w	340	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	34/34 (100%)	34 (100%)	0	100	100
2	S	58/58 (100%)	57 (98%)	1 (2%)	60	84
3	U	69/69 (100%)	66 (96%)	3 (4%)	29	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	V	101/101 (100%)	99 (98%)	2 (2%)	55	81
5	W	99/99 (100%)	97 (98%)	2 (2%)	55	81
6	X	77/81 (95%)	76 (99%)	1 (1%)	69	87
7	Y	62/63 (98%)	61 (98%)	1 (2%)	62	85
8	Z	65/65 (100%)	65 (100%)	0	100	100
9	a	122/122 (100%)	120 (98%)	2 (2%)	62	85
10	b	98/119 (82%)	94 (96%)	4 (4%)	30	59
11	c	141/141 (100%)	138 (98%)	3 (2%)	53	80
12	d	155/155 (100%)	150 (97%)	5 (3%)	39	68
13	e	99/99 (100%)	97 (98%)	2 (2%)	55	81
14	f	35/38 (92%)	35 (100%)	0	100	100
15	g	108/108 (100%)	105 (97%)	3 (3%)	43	73
16	h	93/93 (100%)	89 (96%)	4 (4%)	29	57
17	i	311/311 (100%)	301 (97%)	10 (3%)	39	68
18	j	88/99 (89%)	83 (94%)	5 (6%)	20	44
19	k	84/85 (99%)	82 (98%)	2 (2%)	49	77
20	l	536/537 (100%)	518 (97%)	18 (3%)	37	66
21	m	95/141 (67%)	92 (97%)	3 (3%)	39	68
22	n	53/53 (100%)	52 (98%)	1 (2%)	57	82
23	o	113/113 (100%)	110 (97%)	3 (3%)	44	74
24	p	159/159 (100%)	157 (99%)	2 (1%)	69	87
25	r	410/410 (100%)	403 (98%)	7 (2%)	60	84
26	s	263/275 (96%)	256 (97%)	7 (3%)	44	74
27	u	153/153 (100%)	148 (97%)	5 (3%)	38	67
28	v	104/111 (94%)	93 (89%)	11 (11%)	6	15
29	w	281/283 (99%)	270 (96%)	11 (4%)	32	61
All	All	4066/4175 (97%)	3948 (97%)	118 (3%)	45	71

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S	44	GLN
3	U	34	SER

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Mol	Chain	Res	Type
3	U	47	ARG
3	U	77	SER
4	V	73	THR
4	V	105	THR
5	W	64	ASP
5	W	131	GLU
6	X	98	LEU
7	Y	52	ARG
9	a	71	MET
9	a	130	GLU
10	b	39	ARG
10	b	66	ARG
10	b	93	LYS
10	b	115	GLU
11	c	53	LYS
11	c	91	ASP
11	c	185	GLU
12	d	15	ARG
12	d	16	ARG
12	d	60	ARG
12	d	79	GLU
12	d	127	LYS
13	e	68	GLU
13	e	119	ARG
15	g	4	MET
15	g	14	GLN
15	g	66	TYR
16	h	3	PHE
16	h	37	GLU
16	h	77	SER
16	h	91	LYS
17	i	1	MET
17	i	67	SER
17	i	68	MET
17	i	88	LYS
17	i	104	MET
17	i	146	SER
17	i	148	SER
17	i	244	MET
17	i	257	LEU
17	i	278	MET
18	j	8	LEU

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Mol	Chain	Res	Type
18	j	53	MET
18	j	57	LEU
18	j	87	MET
18	j	109	LYS
19	k	53	PHE
19	k	91	GLN
20	l	1	MET
20	l	52	LEU
20	l	59	GLN
20	l	60	GLU
20	l	71	LEU
20	l	197	ASP
20	l	293	ILE
20	l	336	LYS
20	l	340	PHE
20	l	349	SER
20	l	357	ARG
20	l	359	MET
20	l	383	MET
20	l	391	SER
20	l	393	ASP
20	l	500	LEU
20	l	525	MET
20	l	554	ASP
21	m	41	CYS
21	m	50	SER
21	m	135	PHE
22	n	13	VAL
23	o	5	LYS
23	o	31	LYS
23	o	114	LYS
24	p	48	PHE
24	p	142	GLU
25	r	59	ASP
25	r	140	THR
25	r	168	GLN
25	r	304	GLN
25	r	332	THR
25	r	375	LEU
25	r	378	GLU
26	s	3	MET
26	s	17	VAL

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Mol	Chain	Res	Type
26	s	26	LYS
26	s	119	SER
26	s	151	LEU
26	s	155	LEU
26	s	225	MET
27	u	48	TRP
27	u	62	LEU
27	u	76	ARG
27	u	88	CYS
27	u	109	GLU
28	v	14	SER
28	v	21	ARG
28	v	34	ARG
28	v	36	GLU
28	v	57	ASP
28	v	65	GLN
28	v	69	CYS
28	v	78	LEU
28	v	94	ASP
28	v	107	ARG
28	v	115	ARG
29	w	37	GLN
29	w	67	CYS
29	w	115	GLU
29	w	116	LYS
29	w	213	GLU
29	w	220	LYS
29	w	236	ASP
29	w	241	TYR
29	w	267	GLU
29	w	272	ASP
29	w	288	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
15	g	119	HIS
17	i	221	HIS
19	k	91	GLN
20	l	2	ASN
29	w	107	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

21 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$
31	CDL	r	503	-	98,98,99	0.93	4 (4%)	104,110,111	1.10	7 (6%)
30	PEE	U	101	-	50,50,50	1.15	6 (12%)	53,55,55	0.94	2 (3%)
30	PEE	s	401	-	50,50,50	1.15	6 (12%)	53,55,55	1.00	2 (3%)
31	CDL	V	201	-	70,70,99	1.22	8 (11%)	76,82,111	0.99	4 (5%)
33	PLX	r	502	-	51,51,51	1.13	4 (7%)	55,59,59	0.63	1 (1%)
31	CDL	r	505	-	99,99,99	1.08	8 (8%)	105,111,111	0.85	4 (3%)
30	PEE	l	702	-	45,45,50	1.22	6 (13%)	48,50,55	0.99	2 (4%)
31	CDL	i	401	-	65,65,99	1.28	8 (12%)	71,77,111	1.03	4 (5%)
33	PLX	r	504	-	51,51,51	1.14	4 (7%)	55,59,59	0.65	1 (1%)
34	UQ	s	402	-	28,28,63	0.52	0	34,37,79	1.17	4 (11%)
30	PEE	m	202	-	40,40,50	1.14	5 (12%)	43,45,55	1.01	2 (4%)
30	PEE	Q	101	-	46,46,50	1.20	6 (13%)	49,51,55	1.01	2 (4%)
32	8Q1	X	201	6	31,34,34	1.69	6 (19%)	40,43,43	1.59	7 (17%)
30	PEE	b	201	-	45,45,50	1.21	6 (13%)	48,50,55	0.96	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	ADP	w	401	-	24,29,29	3.12	6 (25%)	29,45,45	1.43	4 (13%)
30	PEE	r	501	-	50,50,50	1.15	6 (12%)	53,55,55	1.00	2 (3%)
33	PLX	m	201	-	51,51,51	1.15	4 (7%)	55,59,59	0.60	1 (1%)
31	CDL	a	201	-	90,90,99	1.12	9 (10%)	96,102,111	0.96	4 (4%)
33	PLX	e	201	-	51,51,51	1.13	4 (7%)	55,59,59	0.59	1 (1%)
33	PLX	g	201	-	51,51,51	1.12	3 (5%)	55,59,59	0.63	1 (1%)
31	CDL	l	701	-	99,99,99	1.08	8 (8%)	105,111,111	0.86	4 (3%)

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
31	CDL	r	503	-	-	37/109/109/110	-
30	PEE	U	101	-	-	22/54/54/54	-
30	PEE	s	401	-	-	23/54/54/54	-
31	CDL	V	201	-	-	48/81/81/110	-
33	PLX	r	502	-	-	27/55/55/55	-
31	CDL	r	505	-	-	68/110/110/110	-
30	PEE	l	702	-	-	22/49/49/54	-
31	CDL	i	401	-	-	42/76/76/110	-
33	PLX	r	504	-	-	24/55/55/55	-
34	UQ	s	402	-	-	6/21/45/87	0/1/1/1
30	PEE	m	202	-	-	17/44/44/54	-
30	PEE	Q	101	-	-	25/50/50/54	-
32	8Q1	X	201	6	-	20/41/41/41	-
30	PEE	b	201	-	-	21/49/49/54	-
35	ADP	w	401	-	-	3/12/32/32	0/3/3/3
30	PEE	r	501	-	-	27/54/54/54	-
33	PLX	m	201	-	-	30/55/55/55	-
31	CDL	a	201	-	-	42/101/101/110	-
33	PLX	e	201	-	-	32/55/55/55	-
33	PLX	g	201	-	-	24/55/55/55	-
31	CDL	l	701	-	-	51/110/110/110	-

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	w	401	ADP	C3'-C4'	-8.80	1.30	1.53
35	w	401	ADP	O4'-C4'	7.72	1.62	1.45
35	w	401	ADP	O4'-C1'	-6.86	1.31	1.41
32	X	201	8Q1	C34-N36	5.42	1.45	1.33
32	X	201	8Q1	C39-N41	5.30	1.45	1.33
31	r	503	CDL	OA8-CA7	4.29	1.45	1.33
31	r	503	CDL	OB8-CB7	4.20	1.45	1.33
31	r	503	CDL	OB6-CB5	4.06	1.45	1.34
31	r	503	CDL	OA6-CA5	4.05	1.45	1.34
35	w	401	ADP	C6-N6	3.87	1.48	1.34
30	l	702	PEE	C18-C19	3.72	1.53	1.31
30	r	501	PEE	C18-C19	3.70	1.53	1.31
30	b	201	PEE	C18-C19	3.70	1.53	1.31
30	U	101	PEE	C18-C19	3.70	1.53	1.31
30	m	202	PEE	C18-C19	3.69	1.53	1.31
30	Q	101	PEE	C18-C19	3.68	1.53	1.31
30	s	401	PEE	C18-C19	3.68	1.53	1.31
30	r	501	PEE	C39-C38	3.65	1.53	1.31
30	b	201	PEE	C39-C38	3.65	1.52	1.31
30	U	101	PEE	C39-C38	3.63	1.52	1.31
30	Q	101	PEE	C39-C38	3.63	1.52	1.31
30	l	702	PEE	C39-C38	3.63	1.52	1.31
30	s	401	PEE	C39-C38	3.62	1.52	1.31
31	V	201	CDL	OA8-CA7	3.53	1.43	1.33
31	i	401	CDL	OA8-CA7	3.52	1.43	1.33
31	l	701	CDL	OA8-CA7	3.42	1.43	1.33
35	w	401	ADP	O2'-C2'	-3.40	1.35	1.43
31	r	505	CDL	OA8-CA7	3.39	1.43	1.33
31	a	201	CDL	OA8-CA7	3.38	1.43	1.33
31	i	401	CDL	OB6-CB5	3.15	1.43	1.34
35	w	401	ADP	O3'-C3'	3.08	1.50	1.43
31	r	505	CDL	OB8-CB7	3.00	1.42	1.33
31	l	701	CDL	OA6-CA5	2.99	1.42	1.34
31	V	201	CDL	OB6-CB5	2.99	1.42	1.34
31	r	505	CDL	OB6-CB5	2.99	1.42	1.34
31	i	401	CDL	OA6-CA5	2.98	1.42	1.34
31	i	401	CDL	OB8-CB7	2.98	1.42	1.33
31	V	201	CDL	OA6-CA5	2.96	1.42	1.34
31	a	201	CDL	OB6-CB5	2.96	1.42	1.34
31	l	701	CDL	OB8-CB7	2.96	1.42	1.33
31	a	201	CDL	OA6-CA5	2.95	1.42	1.34
31	a	201	CDL	OB8-CB7	2.94	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	V	201	CDL	OB8-CB7	2.94	1.41	1.33
31	r	505	CDL	OA6-CA5	2.92	1.42	1.34
31	l	701	CDL	OB6-CB5	2.91	1.42	1.34
33	r	504	PLX	O6-C4	-2.90	1.40	1.44
33	g	201	PLX	O6-C4	-2.76	1.40	1.44
33	e	201	PLX	O6-C4	-2.68	1.41	1.44
33	m	201	PLX	O6-C4	-2.59	1.41	1.44
31	r	505	CDL	OA6-CA4	-2.54	1.40	1.46
30	Q	101	PEE	O3-C30	2.49	1.40	1.33
30	b	201	PEE	O3-C30	2.47	1.40	1.33
30	U	101	PEE	O2-C2	-2.46	1.40	1.46
30	s	401	PEE	O2-C2	-2.45	1.40	1.46
30	l	702	PEE	O2-C2	-2.44	1.40	1.46
31	a	201	CDL	OA6-CA4	-2.44	1.40	1.46
30	r	501	PEE	O2-C2	-2.43	1.40	1.46
30	b	201	PEE	O2-C2	-2.42	1.40	1.46
30	s	401	PEE	O3-C30	2.42	1.40	1.33
30	U	101	PEE	O3-C30	2.41	1.40	1.33
33	r	502	PLX	C7-C6	2.40	1.55	1.50
30	Q	101	PEE	O2-C2	-2.40	1.40	1.46
33	m	201	PLX	C7-C6	2.38	1.55	1.50
31	V	201	CDL	OA6-CA4	-2.38	1.40	1.46
30	l	702	PEE	O3-C30	2.36	1.40	1.33
30	r	501	PEE	O3-C30	2.35	1.40	1.33
31	i	401	CDL	OA6-CA4	-2.35	1.40	1.46
31	l	701	CDL	OB6-CB4	-2.33	1.40	1.46
32	X	201	8Q1	C1-S44	2.32	1.81	1.76
31	l	701	CDL	OA6-CA4	-2.31	1.40	1.46
30	m	202	PEE	O2-C2	-2.31	1.40	1.46
30	m	202	PEE	O3-C30	2.31	1.40	1.33
33	e	201	PLX	C7-C6	2.30	1.55	1.50
30	Q	101	PEE	O2-C10	2.29	1.40	1.34
30	m	202	PEE	O2-C10	2.28	1.40	1.34
32	X	201	8Q1	O40-C39	-2.26	1.18	1.23
33	r	502	PLX	O6-C4	-2.26	1.41	1.44
31	i	401	CDL	PB2-OB2	2.25	1.68	1.59
30	l	702	PEE	O3-C3	-2.24	1.40	1.45
32	X	201	8Q1	O35-C34	-2.24	1.18	1.23
30	U	101	PEE	O2-C10	2.24	1.40	1.34
33	g	201	PLX	C7-C6	2.24	1.55	1.50
30	l	702	PEE	O2-C10	2.23	1.40	1.34
30	b	201	PEE	O2-C10	2.22	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	s	401	PEE	O2-C10	2.21	1.40	1.34
32	X	201	8Q1	C6-C1	2.21	1.53	1.50
31	V	201	CDL	PB2-OB2	2.20	1.68	1.59
31	i	401	CDL	PB2-OB5	2.18	1.68	1.59
31	a	201	CDL	OB6-CB4	-2.18	1.41	1.46
31	r	505	CDL	PB2-OB5	2.17	1.68	1.59
31	r	505	CDL	PB2-OB2	2.16	1.68	1.59
31	V	201	CDL	PB2-OB5	2.16	1.68	1.59
30	r	501	PEE	O3-C3	-2.16	1.40	1.45
31	a	201	CDL	PB2-OB2	2.15	1.68	1.59
31	r	505	CDL	OB6-CB4	-2.15	1.41	1.46
33	r	504	PLX	C7-C6	2.14	1.55	1.50
33	m	201	PLX	P1-O4	2.13	1.67	1.59
30	r	501	PEE	O2-C10	2.13	1.40	1.34
33	r	502	PLX	P1-O4	2.13	1.67	1.59
30	m	202	PEE	O3-C3	-2.13	1.40	1.45
33	r	504	PLX	P1-O4	2.13	1.67	1.59
30	U	101	PEE	O3-C3	-2.12	1.40	1.45
31	l	701	CDL	PB2-OB2	2.11	1.67	1.59
31	V	201	CDL	OB6-CB4	-2.11	1.41	1.46
30	s	401	PEE	O3-C3	-2.11	1.40	1.45
31	i	401	CDL	OB6-CB4	-2.11	1.41	1.46
31	l	701	CDL	PB2-OB5	2.09	1.67	1.59
33	m	201	PLX	P1-O1	2.08	1.67	1.59
33	g	201	PLX	P1-O4	2.07	1.67	1.59
31	a	201	CDL	PB2-OB5	2.05	1.67	1.59
33	e	201	PLX	P1-O4	2.04	1.67	1.59
30	Q	101	PEE	O3-C3	-2.03	1.40	1.45
33	e	201	PLX	P1-O1	2.03	1.67	1.59
30	b	201	PEE	O3-C3	-2.02	1.40	1.45
33	r	502	PLX	P1-O1	2.02	1.67	1.59
33	r	504	PLX	P1-O1	2.01	1.67	1.59
31	a	201	CDL	C11-CA5	2.00	1.56	1.50

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	201	8Q1	C6-C1-S44	6.24	120.72	113.46
31	r	503	CDL	OA6-CA5-C11	4.78	121.81	111.50
35	w	401	ADP	N3-C2-N1	-4.47	121.69	128.68
31	i	401	CDL	OA6-CA5-C11	4.37	120.92	111.50
31	a	201	CDL	OA6-CA5-C11	4.36	120.90	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	V	201	CDL	OB6-CB5-C51	4.29	120.74	111.50
31	a	201	CDL	OB6-CB5-C51	4.22	120.59	111.50
30	m	202	PEE	O2-C10-C11	4.15	120.45	111.50
30	s	401	PEE	O2-C10-C11	4.11	120.35	111.50
31	l	701	CDL	OA6-CA5-C11	4.09	120.32	111.50
30	Q	101	PEE	O2-C10-C11	4.07	120.28	111.50
30	r	501	PEE	O2-C10-C11	4.06	120.25	111.50
31	i	401	CDL	OB6-CB5-C51	3.91	119.93	111.50
31	r	505	CDL	OB6-CB5-C51	3.89	119.89	111.50
30	l	702	PEE	O2-C10-C11	3.86	119.83	111.50
31	l	701	CDL	OB6-CB5-C51	3.75	119.58	111.50
31	r	503	CDL	OB6-CB5-C51	3.74	119.57	111.50
30	U	101	PEE	O2-C10-C11	3.69	119.46	111.50
31	r	505	CDL	OA6-CA5-C11	3.68	119.42	111.50
30	b	201	PEE	O2-C10-C11	3.67	119.40	111.50
32	X	201	8Q1	O4-C1-C6	-3.57	119.78	123.99
31	r	503	CDL	CA4-OA6-CA5	-3.35	109.53	117.79
31	V	201	CDL	OA6-CA5-C11	3.35	120.14	110.80
34	s	402	UQ	C7-C6-C1	3.33	122.49	118.48
31	r	503	CDL	OB8-CB7-C71	2.95	121.17	111.91
30	l	702	PEE	O3-C30-C31	2.81	120.74	111.91
30	s	401	PEE	O3-C30-C31	2.79	120.66	111.91
35	w	401	ADP	O4'-C1'-C2'	-2.79	102.85	106.93
31	V	201	CDL	OA8-CA7-C31	2.77	120.59	111.91
30	r	501	PEE	O3-C30-C31	2.74	120.52	111.91
31	a	201	CDL	OB8-CB7-C71	2.73	120.46	111.91
31	i	401	CDL	OA8-CA7-C31	2.71	120.41	111.91
31	r	503	CDL	OA8-CA7-C31	2.68	120.32	111.91
32	X	201	8Q1	C38-C39-N41	2.66	120.89	116.42
35	w	401	ADP	PA-O3A-PB	-2.65	123.74	132.83
30	b	201	PEE	O3-C30-C31	2.62	120.12	111.91
31	V	201	CDL	OB8-CB7-C71	2.61	120.09	111.91
34	s	402	UQ	C6-C5-C4	2.60	121.24	119.18
31	l	701	CDL	OB8-CB7-C71	2.60	120.06	111.91
31	r	505	CDL	OA8-CA7-C31	2.60	120.05	111.91
31	r	505	CDL	OB8-CB7-C71	2.60	120.05	111.91
30	U	101	PEE	O3-C30-C31	2.58	120.01	111.91
33	g	201	PLX	C1A-N1-C1	2.57	120.42	109.92
34	s	402	UQ	C8-C7-C6	2.56	118.96	112.05
30	Q	101	PEE	O3-C30-C31	2.56	119.94	111.91
31	i	401	CDL	OB8-CB7-C71	2.54	119.89	111.91
33	r	504	PLX	C1A-N1-C1	2.49	120.10	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	l	701	CDL	OA8-CA7-C31	2.48	119.68	111.91
33	e	201	PLX	C1A-N1-C1	2.46	119.97	109.92
30	m	202	PEE	O3-C30-C31	2.45	119.58	111.91
33	r	502	PLX	C1A-N1-C1	2.41	119.79	109.92
32	X	201	8Q1	O4-C1-S44	-2.40	119.50	122.61
31	a	201	CDL	OA8-CA7-C31	2.33	119.20	111.91
33	m	201	PLX	C1A-N1-C1	2.32	119.40	109.92
31	r	503	CDL	OA6-CA5-OA7	-2.32	118.11	123.70
32	X	201	8Q1	C43-S44-C1	2.16	108.60	101.87
34	s	402	UQ	CM5-C5-C6	-2.12	120.94	124.40
35	w	401	ADP	C4-C5-N7	-2.09	107.22	109.40
32	X	201	8Q1	C37-C38-C39	2.09	115.83	112.36
32	X	201	8Q1	C38-C37-N36	-2.08	107.69	111.90
31	r	503	CDL	OB8-CB7-OB9	-2.02	118.50	123.59

There are no chirality outliers.

All (611) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	U	101	PEE	C17-C18-C19-C20
30	U	101	PEE	C1-O3P-P-O1P
30	b	201	PEE	C1-O3P-P-O1P
30	l	702	PEE	C11-C10-O2-C2
30	l	702	PEE	C4-O4P-P-O2P
30	l	702	PEE	C4-O4P-P-O1P
30	m	202	PEE	C11-C10-O2-C2
30	m	202	PEE	O4-C10-O2-C2
30	s	401	PEE	O4P-C4-C5-N
31	V	201	CDL	CB2-C1-CA2-OA2
31	V	201	CDL	CA2-C1-CB2-OB2
31	V	201	CDL	OA9-CA7-OA8-CA6
31	V	201	CDL	C31-CA7-OA8-CA6
31	V	201	CDL	CB2-OB2-PB2-OB3
31	a	201	CDL	CA2-OA2-PA1-OA3
31	a	201	CDL	CA2-OA2-PA1-OA4
31	a	201	CDL	CA3-OA5-PA1-OA4
31	a	201	CDL	CB3-OB5-PB2-OB4
31	i	401	CDL	CA2-OA2-PA1-OA4
31	i	401	CDL	CA3-OA5-PA1-OA2
31	i	401	CDL	CA3-OA5-PA1-OA3
31	i	401	CDL	CA3-OA5-PA1-OA4
31	l	701	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
31	l	701	CDL	CA2-OA2-PA1-OA3
31	l	701	CDL	CB2-OB2-PB2-OB3
31	l	701	CDL	CB2-OB2-PB2-OB4
31	l	701	CDL	CB2-OB2-PB2-OB5
31	l	701	CDL	CB3-OB5-PB2-OB3
31	l	701	CDL	OB6-CB4-CB6-OB8
31	r	503	CDL	CA3-OA5-PA1-OA3
31	r	503	CDL	CB3-OB5-PB2-OB4
31	r	505	CDL	CB2-C1-CA2-OA2
31	r	505	CDL	CA2-OA2-PA1-OA3
31	r	505	CDL	CA2-OA2-PA1-OA4
31	r	505	CDL	CA3-OA5-PA1-OA3
31	r	505	CDL	CA3-OA5-PA1-OA4
31	r	505	CDL	C51-CB5-OB6-CB4
32	X	201	8Q1	C1-C6-C7-C8
32	X	201	8Q1	O4-C1-S44-C43
32	X	201	8Q1	C6-C1-S44-C43
32	X	201	8Q1	C28-C29-C32-C34
32	X	201	8Q1	C28-C29-C32-O33
32	X	201	8Q1	C30-C29-C32-C34
32	X	201	8Q1	C30-C29-C32-O33
32	X	201	8Q1	C31-C29-C32-C34
32	X	201	8Q1	C31-C29-C32-O33
32	X	201	8Q1	N36-C37-C38-C39
32	X	201	8Q1	C28-O27-P24-O2
32	X	201	8Q1	C28-O27-P24-O1
33	e	201	PLX	O7-C6-O6-C4
33	e	201	PLX	C3-O4-P1-O2
33	e	201	PLX	C2-O1-P1-O4
33	e	201	PLX	C2-O1-P1-O2
33	e	201	PLX	C2-O1-P1-O3
33	e	201	PLX	O9-C24-O8-C5
33	e	201	PLX	O9-C24-C25-C26
33	g	201	PLX	O7-C6-O6-C4
33	g	201	PLX	C3-O4-P1-O2
33	g	201	PLX	C25-C24-O8-C5
33	m	201	PLX	O7-C6-C7-C8
33	m	201	PLX	C7-C6-O6-C4
33	m	201	PLX	O7-C6-O6-C4
33	m	201	PLX	C3-O4-P1-O3
33	r	502	PLX	O7-C6-O6-C4
33	r	502	PLX	C5-C4-O6-C6

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Mol	Chain	Res	Type	Atoms
33	r	502	PLX	O9-C24-O8-C5
33	r	502	PLX	O9-C24-C25-C26
34	s	402	UQ	C1-C6-C7-C8
34	s	402	UQ	C5-C6-C7-C8
34	s	402	UQ	C9-C11-C12-C13
34	s	402	UQ	C14-C16-C17-C18
35	w	401	ADP	C5'-O5'-PA-O3A
30	Q	101	PEE	O4-C10-O2-C2
30	l	702	PEE	O4-C10-O2-C2
31	r	505	CDL	OB7-CB5-OB6-CB4
30	Q	101	PEE	C11-C10-O2-C2
30	b	201	PEE	C31-C30-O3-C3
31	i	401	CDL	C31-CA7-OA8-CA6
31	r	505	CDL	C71-CB7-OB8-CB6
30	b	201	PEE	C37-C38-C39-C40
30	s	401	PEE	C37-C38-C39-C40
30	b	201	PEE	O5-C30-O3-C3
31	i	401	CDL	OA9-CA7-OA8-CA6
31	r	505	CDL	OB9-CB7-OB8-CB6
31	r	503	CDL	O1-C1-CA2-OA2
30	l	702	PEE	C31-C30-O3-C3
31	l	701	CDL	C71-CB7-OB8-CB6
31	i	401	CDL	C31-C32-C33-C34
31	l	701	CDL	C11-C12-C13-C14
33	m	201	PLX	C28-C29-C30-C31
33	r	502	PLX	C9-C10-C11-C12
33	r	502	PLX	C30-C31-C32-C33
33	e	201	PLX	C12-C13-C14-C15
33	g	201	PLX	C7-C8-C9-C10
30	m	202	PEE	C31-C30-O3-C3
30	l	702	PEE	O5-C30-O3-C3
31	l	701	CDL	OB9-CB7-OB8-CB6
31	i	401	CDL	C71-CB7-OB8-CB6
31	l	701	CDL	C35-C36-C37-C38
30	m	202	PEE	O5-C30-O3-C3
31	i	401	CDL	C37-C38-C39-C40
31	l	701	CDL	CA2-C1-CB2-OB2
30	U	101	PEE	C31-C30-O3-C3
31	a	201	CDL	C71-CB7-OB8-CB6
31	r	503	CDL	C31-CA7-OA8-CA6
31	l	701	CDL	C59-C60-C61-C62
30	l	702	PEE	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
31	V	201	CDL	O1-C1-CA2-OA2
31	l	701	CDL	O1-C1-CA2-OA2
31	r	505	CDL	OB6-CB4-CB6-OB8
30	r	501	PEE	C10-C11-C12-C13
30	U	101	PEE	O5-C30-O3-C3
31	r	505	CDL	C74-C75-C76-C77
30	r	501	PEE	C17-C18-C19-C20
31	V	201	CDL	C74-C75-C76-C77
30	Q	101	PEE	C10-C11-C12-C13
31	i	401	CDL	CB7-C71-C72-C73
31	l	701	CDL	CB5-C51-C52-C53
31	r	505	CDL	CA7-C31-C32-C33
31	r	505	CDL	CB7-C71-C72-C73
30	s	401	PEE	C30-C31-C32-C33
31	a	201	CDL	CA7-C31-C32-C33
31	i	401	CDL	OB9-CB7-OB8-CB6
31	V	201	CDL	O1-C1-CB2-OB2
31	i	401	CDL	O1-C1-CA2-OA2
31	r	505	CDL	O1-C1-CA2-OA2
31	a	201	CDL	OB9-CB7-OB8-CB6
31	r	503	CDL	OA9-CA7-OA8-CA6
30	U	101	PEE	C1-O3P-P-O4P
30	l	702	PEE	C4-O4P-P-O3P
30	r	501	PEE	C1-O3P-P-O4P
31	V	201	CDL	CA2-OA2-PA1-OA5
31	V	201	CDL	CB2-OB2-PB2-OB5
31	a	201	CDL	CA2-OA2-PA1-OA5
31	a	201	CDL	CA3-OA5-PA1-OA2
31	a	201	CDL	CB3-OB5-PB2-OB2
31	i	401	CDL	CA2-OA2-PA1-OA5
31	i	401	CDL	CB3-OB5-PB2-OB2
31	l	701	CDL	CB3-OB5-PB2-OB2
31	r	503	CDL	CA2-OA2-PA1-OA5
31	r	503	CDL	CA3-OA5-PA1-OA2
31	r	503	CDL	CB3-OB5-PB2-OB2
31	r	505	CDL	CA2-OA2-PA1-OA5
31	r	505	CDL	CA3-OA5-PA1-OA2
31	r	505	CDL	CB3-OB5-PB2-OB2
33	e	201	PLX	C3-O4-P1-O1
33	m	201	PLX	C3-O4-P1-O1
33	r	502	PLX	C3-O4-P1-O1
31	V	201	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
31	r	505	CDL	C51-C52-C53-C54
31	i	401	CDL	CB2-C1-CA2-OA2
31	i	401	CDL	C14-C15-C16-C17
31	V	201	CDL	C56-C57-C58-C59
31	r	505	CDL	C20-C21-C22-C23
33	m	201	PLX	C34-C35-C36-C37
31	i	401	CDL	CA7-C31-C32-C33
31	l	701	CDL	C37-C38-C39-C40
31	r	505	CDL	C41-C42-C43-C44
33	e	201	PLX	C13-C14-C15-C16
33	m	201	PLX	C7-C8-C9-C10
30	U	101	PEE	C11-C10-O2-C2
30	r	501	PEE	C12-C13-C14-C15
31	r	505	CDL	C43-C44-C45-C46
31	r	505	CDL	C55-C56-C57-C58
31	r	505	CDL	C60-C61-C62-C63
31	r	505	CDL	C71-C72-C73-C74
33	e	201	PLX	C25-C26-C27-C28
33	e	201	PLX	C33-C34-C35-C36
33	g	201	PLX	C28-C29-C30-C31
33	r	502	PLX	C16-C17-C18-C19
33	r	504	PLX	C28-C29-C30-C31
30	Q	101	PEE	C12-C13-C14-C15
31	a	201	CDL	C11-C12-C13-C14
33	e	201	PLX	C29-C30-C31-C32
33	m	201	PLX	C25-C26-C27-C28
33	r	502	PLX	C27-C28-C29-C30
33	r	504	PLX	C14-C15-C16-C17
33	r	504	PLX	C29-C30-C31-C32
30	b	201	PEE	C12-C13-C14-C15
31	i	401	CDL	C52-C53-C54-C55
30	l	702	PEE	C23-C24-C25-C26
30	r	501	PEE	C31-C32-C33-C34
31	a	201	CDL	C32-C33-C34-C35
31	i	401	CDL	C35-C36-C37-C38
30	l	702	PEE	C31-C32-C33-C34
31	a	201	CDL	C75-C76-C77-C78
31	r	503	CDL	C58-C59-C60-C61
33	r	504	PLX	C31-C32-C33-C34
33	g	201	PLX	C11-C10-C9-C8
33	g	201	PLX	C30-C31-C32-C33
33	g	201	PLX	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
31	V	201	CDL	C55-C56-C57-C58
31	a	201	CDL	C37-C38-C39-C40
31	r	505	CDL	C58-C59-C60-C61
31	r	505	CDL	C75-C76-C77-C78
30	b	201	PEE	C33-C34-C35-C36
31	i	401	CDL	C71-C72-C73-C74
31	l	701	CDL	C39-C40-C41-C42
31	l	701	CDL	C40-C41-C42-C43
31	r	505	CDL	C17-C18-C19-C20
33	e	201	PLX	C28-C29-C30-C31
30	m	202	PEE	C11-C12-C13-C14
30	s	401	PEE	C12-C13-C14-C15
33	e	201	PLX	C14-C15-C16-C17
33	g	201	PLX	C27-C28-C29-C30
33	r	502	PLX	C13-C14-C15-C16
30	U	101	PEE	O4-C10-O2-C2
30	U	101	PEE	C34-C35-C36-C37
31	V	201	CDL	C54-C55-C56-C57
31	r	505	CDL	C35-C36-C37-C38
33	r	502	PLX	C15-C16-C17-C18
31	i	401	CDL	C36-C37-C38-C39
33	g	201	PLX	C14-C15-C16-C17
33	g	201	PLX	C9-C10-C11-C12
33	g	201	PLX	C33-C34-C35-C36
33	r	502	PLX	C12-C13-C14-C15
33	e	201	PLX	C2-C1-N1-C1A
31	l	701	CDL	C54-C55-C56-C57
31	r	505	CDL	C73-C74-C75-C76
33	e	201	PLX	C10-C11-C12-C13
33	g	201	PLX	C10-C11-C12-C13
33	m	201	PLX	C13-C14-C15-C16
33	r	502	PLX	C7-C8-C9-C10
31	l	701	CDL	C14-C15-C16-C17
33	m	201	PLX	C35-C36-C37-C38
31	r	505	CDL	CA5-C11-C12-C13
31	V	201	CDL	OB9-CB7-OB8-CB6
30	U	101	PEE	C41-C42-C43-C44
33	m	201	PLX	C12-C13-C14-C15
31	V	201	CDL	C60-C61-C62-C63
31	a	201	CDL	C21-C22-C23-C24
31	a	201	CDL	C73-C74-C75-C76
31	r	505	CDL	C61-C62-C63-C64

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Mol	Chain	Res	Type	Atoms
33	m	201	PLX	C15-C16-C17-C18
31	l	701	CDL	CB7-C71-C72-C73
31	l	701	CDL	CA3-CA4-CA6-OA8
30	b	201	PEE	C17-C18-C19-C20
31	l	701	CDL	C57-C58-C59-C60
31	l	701	CDL	C75-C76-C77-C78
33	m	201	PLX	C27-C28-C29-C30
30	s	401	PEE	C10-C11-C12-C13
31	r	505	CDL	C31-CA7-OA8-CA6
30	r	501	PEE	C11-C10-O2-C2
31	a	201	CDL	C17-C18-C19-C20
31	a	201	CDL	C56-C57-C58-C59
31	V	201	CDL	CA7-C31-C32-C33
30	Q	101	PEE	C35-C36-C37-C38
33	r	504	PLX	C11-C10-C9-C8
31	r	505	CDL	CB5-C51-C52-C53
31	r	503	CDL	CB2-C1-CA2-OA2
31	V	201	CDL	C59-C60-C61-C62
31	r	505	CDL	C23-C24-C25-C26
33	m	201	PLX	C33-C34-C35-C36
31	V	201	CDL	C52-C53-C54-C55
31	r	505	CDL	C33-C34-C35-C36
30	s	401	PEE	C33-C34-C35-C36
31	V	201	CDL	C11-CA5-OA6-CA4
30	r	501	PEE	C41-C42-C43-C44
31	r	505	CDL	C82-C83-C84-C85
33	g	201	PLX	C25-C26-C27-C28
30	s	401	PEE	C17-C18-C19-C20
31	r	505	CDL	OA9-CA7-OA8-CA6
31	r	505	CDL	C37-C38-C39-C40
30	Q	101	PEE	C19-C20-C21-C22
30	r	501	PEE	O4-C10-O2-C2
31	r	503	CDL	OA7-CA5-OA6-CA4
30	s	401	PEE	C31-C30-O3-C3
31	r	503	CDL	C51-C52-C53-C54
31	r	505	CDL	C14-C15-C16-C17
31	r	505	CDL	C52-C53-C54-C55
33	e	201	PLX	C27-C28-C29-C30
33	r	504	PLX	C10-C11-C12-C13
31	r	503	CDL	C20-C21-C22-C23
31	r	505	CDL	C62-C63-C64-C65
33	r	504	PLX	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
31	a	201	CDL	C54-C55-C56-C57
31	r	503	CDL	C11-CA5-OA6-CA4
31	a	201	CDL	OA5-CA3-CA4-OA6
31	r	505	CDL	C76-C77-C78-C79
30	b	201	PEE	C31-C32-C33-C34
31	V	201	CDL	OA7-CA5-OA6-CA4
31	l	701	CDL	OA6-CA4-CA6-OA8
31	r	505	CDL	OA6-CA4-CA6-OA8
32	X	201	8Q1	C9-C10-C11-C12
33	e	201	PLX	C2-C1-N1-C1C
33	r	504	PLX	C13-C14-C15-C16
33	g	201	PLX	C13-C14-C15-C16
30	r	501	PEE	C13-C14-C15-C16
30	U	101	PEE	C36-C37-C38-C39
30	m	202	PEE	C4-O4P-P-O3P
31	r	505	CDL	CB2-OB2-PB2-OB5
33	g	201	PLX	C3-O4-P1-O1
30	s	401	PEE	O5-C30-O3-C3
30	l	702	PEE	O3P-C1-C2-C3
31	V	201	CDL	OB5-CB3-CB4-CB6
31	a	201	CDL	OA5-CA3-CA4-CA6
33	m	201	PLX	O4-C3-C4-C5
31	l	701	CDL	C62-C63-C64-C65
31	r	505	CDL	C78-C79-C80-C81
31	a	201	CDL	C35-C36-C37-C38
31	V	201	CDL	C75-C76-C77-C78
31	i	401	CDL	C11-C12-C13-C14
31	l	701	CDL	C12-C13-C14-C15
31	l	701	CDL	C32-C33-C34-C35
30	l	702	PEE	C32-C33-C34-C35
31	i	401	CDL	C32-C33-C34-C35
30	r	501	PEE	C36-C37-C38-C39
31	r	505	CDL	CB3-CB4-CB6-OB8
33	m	201	PLX	C3-C4-C5-O8
33	m	201	PLX	C26-C27-C28-C29
33	r	502	PLX	C3-C4-C5-O8
33	r	502	PLX	C28-C29-C30-C31
33	r	504	PLX	C3-C4-C5-O8
31	V	201	CDL	C62-C63-C64-C65
31	l	701	CDL	C73-C74-C75-C76
31	a	201	CDL	C31-C32-C33-C34
30	s	401	PEE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
30	s	401	PEE	C22-C23-C24-C25
31	a	201	CDL	C52-C53-C54-C55
31	r	505	CDL	C56-C57-C58-C59
30	r	501	PEE	C11-C12-C13-C14
31	a	201	CDL	C15-C16-C17-C18
33	e	201	PLX	C11-C12-C13-C14
32	X	201	8Q1	C28-O27-P24-O3
30	r	501	PEE	C20-C21-C22-C23
33	e	201	PLX	C2-C1-N1-C1B
31	l	701	CDL	C52-C53-C54-C55
30	l	702	PEE	O2-C2-C3-O3
31	i	401	CDL	OB6-CB4-CB6-OB8
31	r	503	CDL	C52-C53-C54-C55
31	l	701	CDL	C55-C56-C57-C58
31	a	201	CDL	C71-C72-C73-C74
31	V	201	CDL	C58-C59-C60-C61
31	l	701	CDL	C64-C65-C66-C67
30	U	101	PEE	C30-C31-C32-C33
31	V	201	CDL	C84-C85-C86-C87
30	r	501	PEE	C40-C41-C42-C43
31	i	401	CDL	OB5-CB3-CB4-CB6
33	g	201	PLX	C35-C36-C37-C38
31	a	201	CDL	CB5-C51-C52-C53
31	r	505	CDL	C57-C58-C59-C60
34	s	402	UQ	C15-C14-C16-C17
30	Q	101	PEE	C21-C22-C23-C24
31	r	505	CDL	C54-C55-C56-C57
33	r	502	PLX	C33-C34-C35-C36
31	r	503	CDL	C51-CB5-OB6-CB4
30	U	101	PEE	C21-C22-C23-C24
33	r	504	PLX	C11-C12-C13-C14
31	l	701	CDL	C33-C34-C35-C36
33	r	504	PLX	C30-C31-C32-C33
31	V	201	CDL	C53-C54-C55-C56
31	r	505	CDL	CA3-CA4-CA6-OA8
30	U	101	PEE	C40-C41-C42-C43
33	e	201	PLX	C7-C8-C9-C10
33	e	201	PLX	C5-C4-O6-C6
33	g	201	PLX	O9-C24-C25-C26
33	r	504	PLX	O7-C6-C7-C8
31	V	201	CDL	OB5-CB3-CB4-OB6
33	m	201	PLX	O4-C3-C4-O6

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Mol	Chain	Res	Type	Atoms
30	s	401	PEE	C19-C20-C21-C22
30	l	702	PEE	C24-C25-C26-C27
30	m	202	PEE	C13-C14-C15-C16
31	r	505	CDL	C64-C65-C66-C67
33	e	201	PLX	C31-C32-C33-C34
33	e	201	PLX	C16-C17-C18-C19
30	U	101	PEE	C22-C23-C24-C25
31	r	505	CDL	C42-C43-C44-C45
31	V	201	CDL	C71-C72-C73-C74
31	V	201	CDL	C79-C80-C81-C82
31	i	401	CDL	C33-C34-C35-C36
31	l	701	CDL	C63-C64-C65-C66
33	e	201	PLX	C9-C10-C11-C12
30	Q	101	PEE	C2-C1-O3P-P
31	a	201	CDL	C60-C61-C62-C63
33	m	201	PLX	C30-C31-C32-C33
30	Q	101	PEE	C22-C23-C24-C25
31	i	401	CDL	C73-C74-C75-C76
33	m	201	PLX	C14-C15-C16-C17
33	e	201	PLX	O8-C24-C25-C26
31	a	201	CDL	OB5-CB3-CB4-CB6
33	g	201	PLX	O4-C3-C4-C5
31	a	201	CDL	C23-C24-C25-C26
30	Q	101	PEE	C16-C17-C18-C19
30	r	501	PEE	C38-C39-C40-C41
30	Q	101	PEE	C23-C24-C25-C26
32	X	201	8Q1	O33-C32-C34-N36
33	r	504	PLX	C25-C26-C27-C28
30	m	202	PEE	C3-C2-O2-C10
31	r	503	CDL	OB7-CB5-OB6-CB4
30	Q	101	PEE	C24-C25-C26-C27
30	Q	101	PEE	C1-C2-C3-O3
30	b	201	PEE	C1-C2-C3-O3
30	r	501	PEE	C1-C2-C3-O3
31	r	505	CDL	CB4-CB3-OB5-PB2
33	e	201	PLX	C3-C4-C5-O8
31	i	401	CDL	OB5-CB3-CB4-OB6
33	e	201	PLX	C15-C16-C17-C18
30	Q	101	PEE	O2-C2-C3-O3
30	r	501	PEE	O2-C2-C3-O3
33	e	201	PLX	O6-C4-C5-O8
33	r	504	PLX	O6-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
31	l	701	CDL	C34-C35-C36-C37
30	m	202	PEE	C33-C34-C35-C36
31	V	201	CDL	C51-CB5-OB6-CB4
30	s	401	PEE	C15-C16-C17-C18
33	r	502	PLX	C31-C32-C33-C34
30	U	101	PEE	C37-C38-C39-C40
30	m	202	PEE	C31-C32-C33-C34
31	r	505	CDL	C79-C80-C81-C82
31	V	201	CDL	CB3-OB5-PB2-OB2
31	l	701	CDL	CA2-OA2-PA1-OA5
31	l	701	CDL	C74-C75-C76-C77
31	r	503	CDL	CA4-CA3-OA5-PA1
30	Q	101	PEE	C1-O3P-P-O1P
30	U	101	PEE	C1-O3P-P-O2P
30	m	202	PEE	C4-O4P-P-O2P
30	m	202	PEE	C4-O4P-P-O1P
30	r	501	PEE	C1-O3P-P-O2P
30	r	501	PEE	C1-O3P-P-O1P
30	r	501	PEE	C4-O4P-P-O1P
31	V	201	CDL	CA2-OA2-PA1-OA4
31	V	201	CDL	CB3-OB5-PB2-OB3
31	a	201	CDL	CA3-OA5-PA1-OA3
31	a	201	CDL	CB3-OB5-PB2-OB3
31	i	401	CDL	CB2-OB2-PB2-OB3
31	i	401	CDL	CB3-OB5-PB2-OB4
31	r	503	CDL	CA2-OA2-PA1-OA3
31	r	503	CDL	CA3-OA5-PA1-OA4
31	r	505	CDL	CB2-OB2-PB2-OB3
31	r	505	CDL	CB2-OB2-PB2-OB4
31	r	505	CDL	CB3-OB5-PB2-OB3
33	m	201	PLX	C3-O4-P1-O2
33	r	502	PLX	C3-O4-P1-O2
33	r	502	PLX	C2-O1-P1-O3
35	w	401	ADP	C5'-O5'-PA-O2A
30	s	401	PEE	O3P-C1-C2-C3
30	b	201	PEE	C21-C22-C23-C24
31	r	505	CDL	C44-C45-C46-C47
33	m	201	PLX	C25-C24-O8-C5
33	r	504	PLX	C25-C24-O8-C5
31	V	201	CDL	C80-C81-C82-C83
31	l	701	CDL	C77-C78-C79-C80
31	V	201	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
31	r	505	CDL	C39-C40-C41-C42
31	i	401	CDL	OA5-CA3-CA4-OA6
33	g	201	PLX	O4-C3-C4-O6
30	l	702	PEE	C38-C39-C40-C41
31	r	503	CDL	CB5-C51-C52-C53
30	l	702	PEE	C1-C2-C3-O3
31	i	401	CDL	CB3-CB4-CB6-OB8
31	l	701	CDL	CB3-CB4-CB6-OB8
31	i	401	CDL	OA6-CA4-CA6-OA8
33	m	201	PLX	O6-C4-C5-O8
33	r	502	PLX	O6-C4-C5-O8
31	a	201	CDL	C57-C58-C59-C60
30	U	101	PEE	C38-C39-C40-C41
31	V	201	CDL	C64-C65-C66-C67
32	X	201	8Q1	C7-C8-C9-C10
33	r	504	PLX	C6-C7-C8-C9
31	l	701	CDL	C15-C16-C17-C18
33	r	504	PLX	O6-C6-C7-C8
30	m	202	PEE	O3-C30-C31-C32
31	i	401	CDL	C39-C40-C41-C42
33	r	502	PLX	C10-C11-C12-C13
30	s	401	PEE	C18-C19-C20-C21
31	r	503	CDL	C35-C36-C37-C38
33	r	502	PLX	C14-C15-C16-C17
33	r	504	PLX	C27-C28-C29-C30
31	i	401	CDL	OA5-CA3-CA4-CA6
31	r	505	CDL	C31-C32-C33-C34
30	Q	101	PEE	C30-C31-C32-C33
30	r	501	PEE	C31-C30-O3-C3
30	s	401	PEE	O3P-C1-C2-O2
31	a	201	CDL	OB5-CB3-CB4-OB6
34	s	402	UQ	C13-C14-C16-C17
30	U	101	PEE	C23-C24-C25-C26
31	i	401	CDL	C75-C76-C77-C78
31	r	505	CDL	C34-C35-C36-C37
33	r	504	PLX	C35-C36-C37-C38
30	r	501	PEE	O5-C30-O3-C3
30	b	201	PEE	O2-C2-C3-O3
30	U	101	PEE	C12-C13-C14-C15
31	V	201	CDL	CA3-OA5-PA1-OA2
31	l	701	CDL	CA3-OA5-PA1-OA2
31	r	503	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
33	r	504	PLX	C2-O1-P1-O4
31	r	505	CDL	C11-C12-C13-C14
30	m	202	PEE	C16-C17-C18-C19
31	V	201	CDL	C12-C11-CA5-OA6
30	Q	101	PEE	C38-C39-C40-C41
31	r	503	CDL	C39-C40-C41-C42
30	l	702	PEE	C30-C31-C32-C33
33	r	502	PLX	C29-C30-C31-C32
31	r	505	CDL	C13-C14-C15-C16
30	b	201	PEE	C18-C19-C20-C21
31	r	503	CDL	C53-C54-C55-C56
30	l	702	PEE	C14-C15-C16-C17
31	V	201	CDL	C82-C83-C84-C85
30	b	201	PEE	C39-C40-C41-C42
33	e	201	PLX	C24-C25-C26-C27
31	V	201	CDL	OA6-CA4-CA6-OA8
31	V	201	CDL	C12-C11-CA5-OA7
31	V	201	CDL	OB6-CB4-CB6-OB8
33	g	201	PLX	O8-C24-C25-C26
33	m	201	PLX	O6-C6-C7-C8
30	s	401	PEE	C34-C35-C36-C37
31	a	201	CDL	C36-C37-C38-C39
30	r	501	PEE	C32-C33-C34-C35
31	l	701	CDL	C44-C45-C46-C47
31	r	503	CDL	C56-C57-C58-C59
32	X	201	8Q1	O27-C28-C29-C30
30	l	702	PEE	C19-C20-C21-C22
33	m	201	PLX	C11-C12-C13-C14
33	r	502	PLX	C2-O1-P1-O4
31	i	401	CDL	C72-C73-C74-C75
30	l	702	PEE	C15-C16-C17-C18
30	Q	101	PEE	O3P-C1-C2-C3
33	r	504	PLX	C34-C35-C36-C37
32	X	201	8Q1	C42-C43-S44-C1
31	a	201	CDL	OB6-CB4-CB6-OB8
33	m	201	PLX	C19-C20-C21-C22
31	r	503	CDL	C24-C25-C26-C27
30	Q	101	PEE	C17-C18-C19-C20
32	X	201	8Q1	C10-C11-C12-C13
33	e	201	PLX	C19-C20-C21-C22
35	w	401	ADP	C4'-C5'-O5'-PA
33	m	201	PLX	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
30	Q	101	PEE	C32-C33-C34-C35
30	r	501	PEE	C18-C19-C20-C21
31	V	201	CDL	CA3-CA4-CA6-OA8
30	s	401	PEE	C14-C15-C16-C17
33	m	201	PLX	C4-C5-O8-C24
30	U	101	PEE	C43-C44-C45-C46
30	b	201	PEE	C15-C16-C17-C18
30	Q	101	PEE	C36-C37-C38-C39
31	i	401	CDL	CB5-C51-C52-C53
31	r	503	CDL	C82-C83-C84-C85
31	i	401	CDL	C15-C16-C17-C18
31	a	201	CDL	C32-C31-CA7-OA8
30	b	201	PEE	O4-C10-O2-C2
30	Q	101	PEE	C31-C32-C33-C34
30	b	201	PEE	C34-C35-C36-C37
33	g	201	PLX	C16-C17-C18-C19
31	r	505	CDL	C36-C37-C38-C39
31	a	201	CDL	C76-C77-C78-C79
31	l	701	CDL	OA7-CA5-OA6-CA4
30	Q	101	PEE	C1-O3P-P-O4P
31	a	201	CDL	C41-C42-C43-C44
30	l	702	PEE	C36-C37-C38-C39
30	m	202	PEE	C18-C19-C20-C21
30	s	401	PEE	C16-C17-C18-C19
30	s	401	PEE	O4-C10-O2-C2
31	l	701	CDL	C32-C31-CA7-OA8
31	r	505	CDL	C63-C64-C65-C66
30	Q	101	PEE	C18-C19-C20-C21
30	m	202	PEE	C23-C24-C25-C26
31	i	401	CDL	CA3-CA4-CA6-OA8
31	r	503	CDL	OA5-CA3-CA4-OA6
31	V	201	CDL	C32-C31-CA7-OA8
33	r	504	PLX	C2-C1-N1-C1A
30	s	401	PEE	C21-C22-C23-C24
31	r	503	CDL	C74-C75-C76-C77
33	m	201	PLX	C18-C19-C20-C21
30	Q	101	PEE	C14-C15-C16-C17
30	r	501	PEE	C34-C35-C36-C37
31	l	701	CDL	C43-C44-C45-C46
31	r	505	CDL	C32-C33-C34-C35
30	l	702	PEE	C16-C17-C18-C19
31	r	503	CDL	C12-C11-CA5-OA6

Continued on next page...

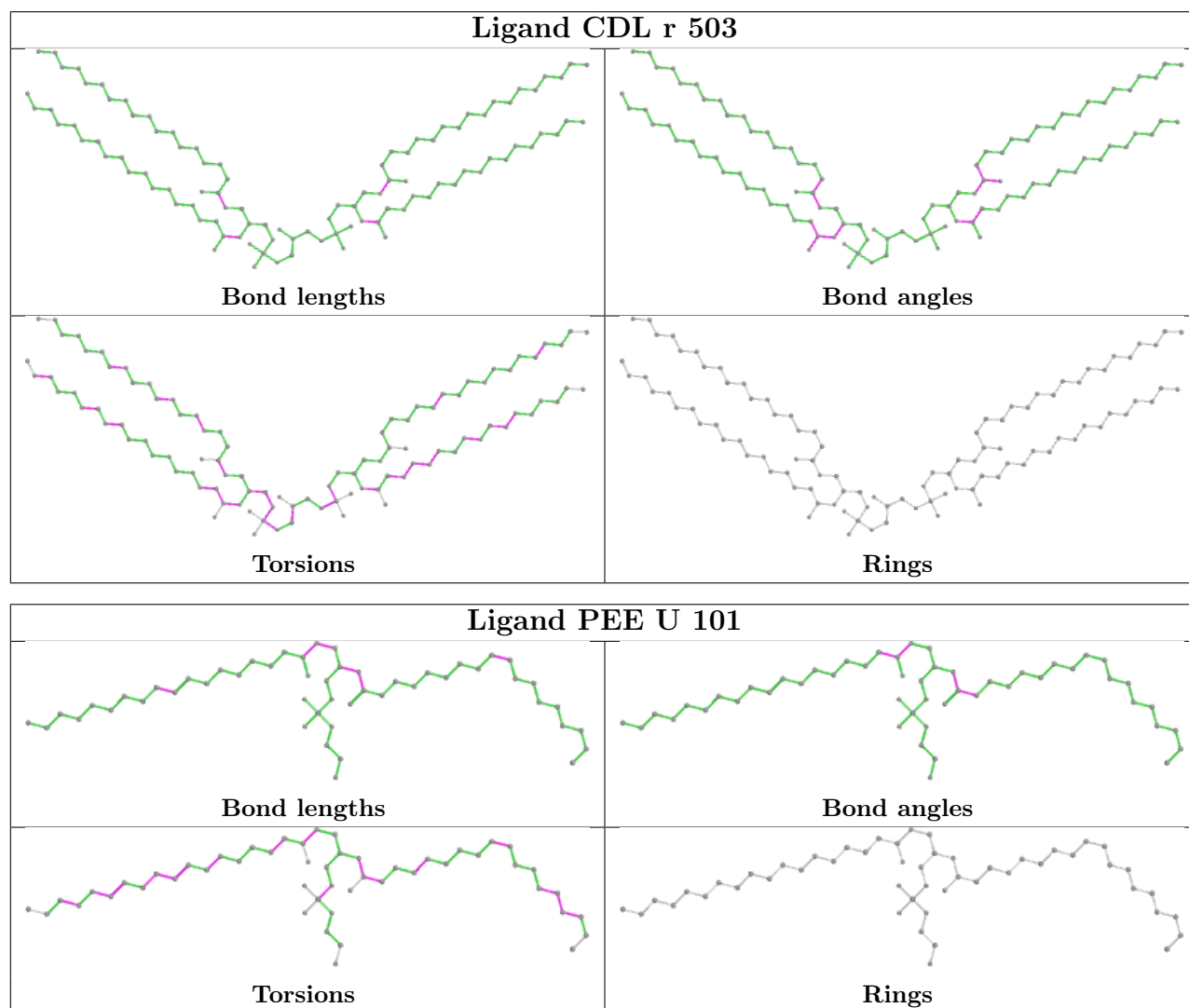
Continued from previous page...

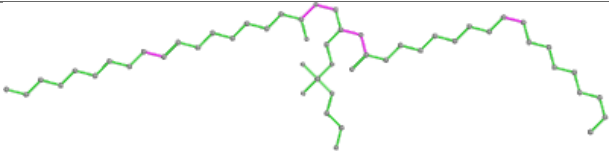
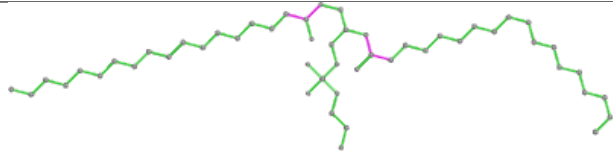
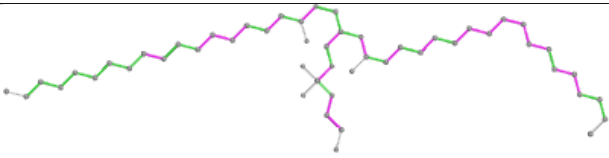
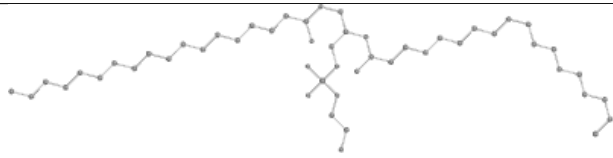
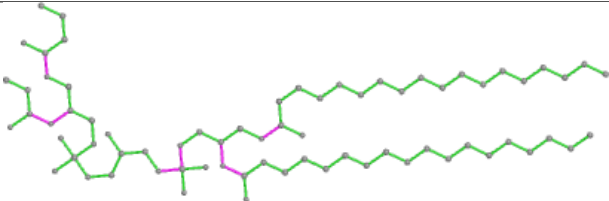
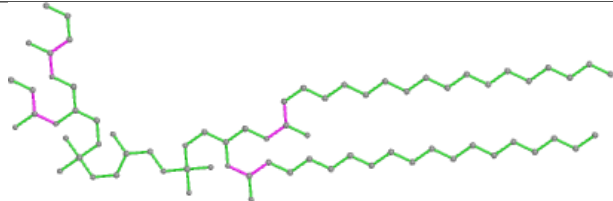
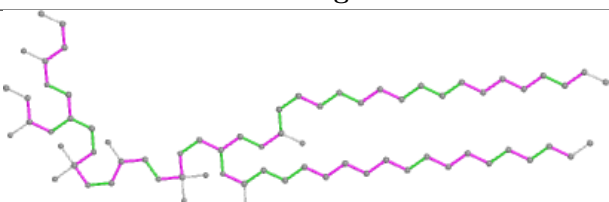
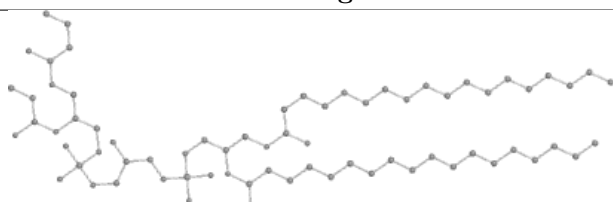
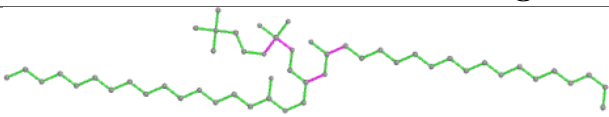
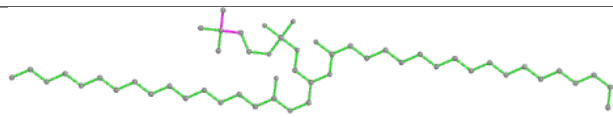
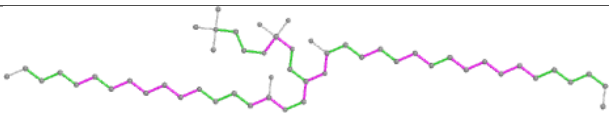
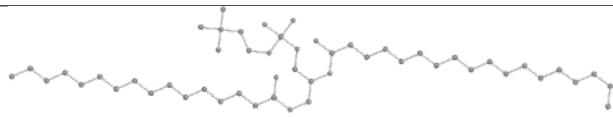
Mol	Chain	Res	Type	Atoms
31	r	503	CDL	C59-C60-C61-C62
31	l	701	CDL	C12-C11-CA5-OA6
30	m	202	PEE	C24-C25-C26-C27
30	b	201	PEE	C11-C10-O2-C2
31	l	701	CDL	C11-CA5-OA6-CA4
30	b	201	PEE	C14-C15-C16-C17
33	r	502	PLX	O8-C24-C25-C26
31	r	503	CDL	C18-C19-C20-C21
30	b	201	PEE	C38-C39-C40-C41
30	r	501	PEE	C43-C44-C45-C46
33	r	504	PLX	C7-C8-C9-C10
31	a	201	CDL	CB3-CB4-CB6-OB8
33	g	201	PLX	C3-C4-C5-O8
31	i	401	CDL	CB2-OB2-PB2-OB5
30	s	401	PEE	C1-O3P-P-O1P
31	V	201	CDL	CA3-OA5-PA1-OA3
31	r	503	CDL	CB2-OB2-PB2-OB3
33	r	502	PLX	C3-O4-P1-O3
31	r	503	CDL	C32-C33-C34-C35
31	l	701	CDL	C32-C31-CA7-OA9
32	X	201	8Q1	O27-C28-C29-C31
30	r	501	PEE	C5-C4-O4P-P
30	s	401	PEE	C5-C4-O4P-P
33	g	201	PLX	C1-C2-O1-P1
33	r	502	PLX	C25-C24-O8-C5
31	V	201	CDL	C32-C31-CA7-OA9
31	r	503	CDL	CA5-C11-C12-C13
33	r	504	PLX	C2-C1-N1-C1C
30	U	101	PEE	O2-C10-C11-C12
31	a	201	CDL	C72-C71-CB7-OB8
31	l	701	CDL	CB2-C1-CA2-OA2
31	r	505	CDL	C83-C84-C85-C86
31	l	701	CDL	C12-C11-CA5-OA7
31	r	503	CDL	C12-C11-CA5-OA7
30	b	201	PEE	C16-C17-C18-C19
30	b	201	PEE	C36-C37-C38-C39
31	i	401	CDL	C13-C14-C15-C16
30	r	501	PEE	C24-C25-C26-C27
31	r	505	CDL	C81-C82-C83-C84
30	U	101	PEE	O4-C10-C11-C12
31	a	201	CDL	CA5-C11-C12-C13
31	V	201	CDL	C81-C82-C83-C84

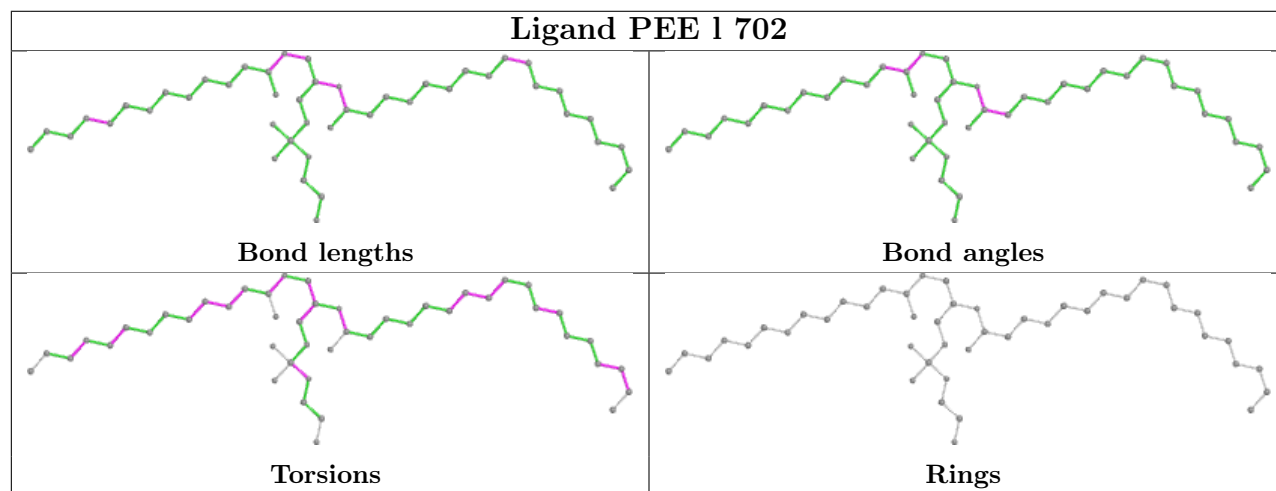
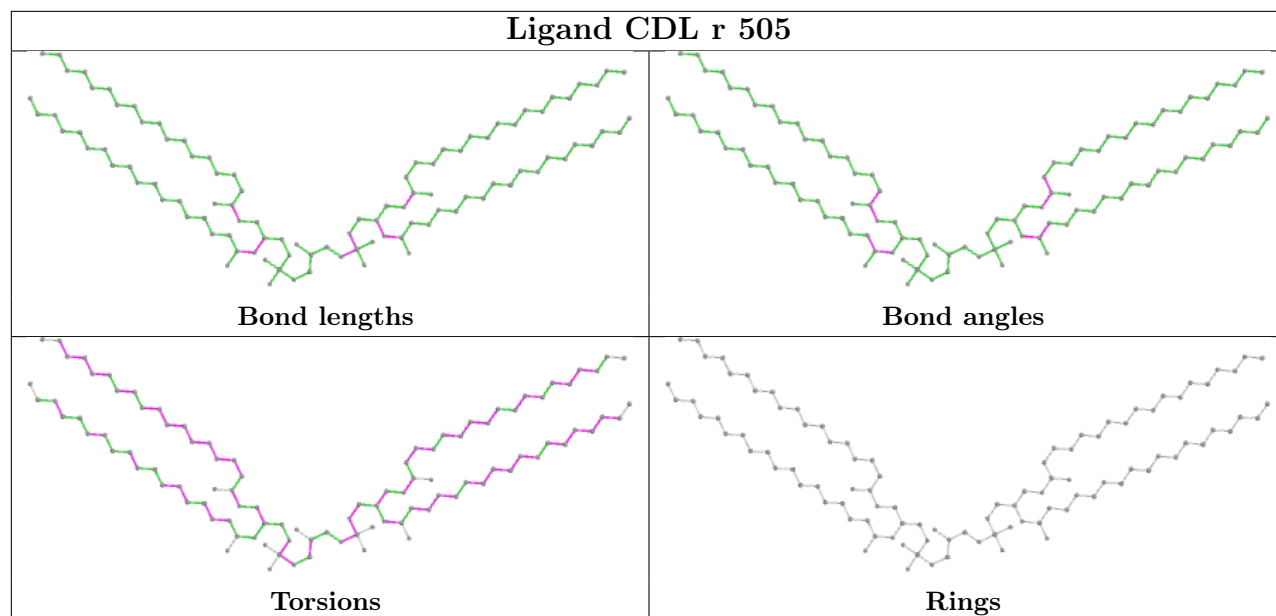
There are no ring outliers.

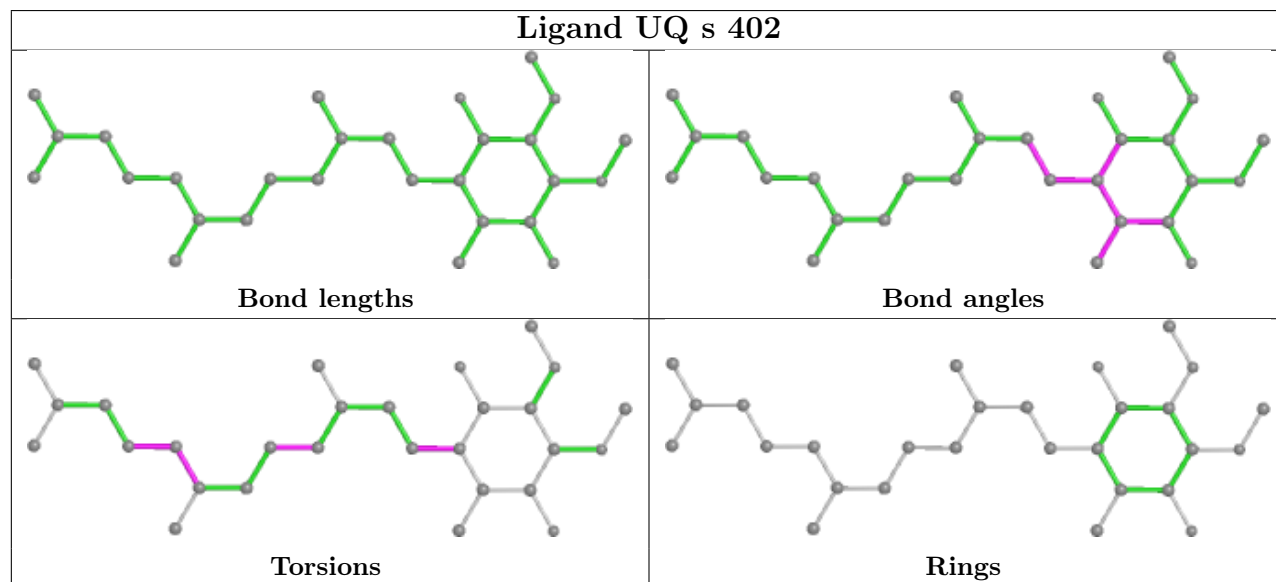
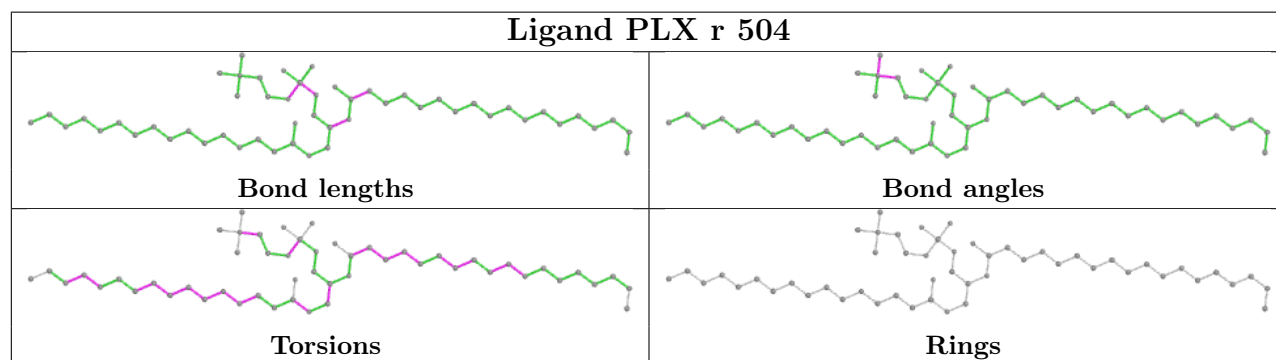
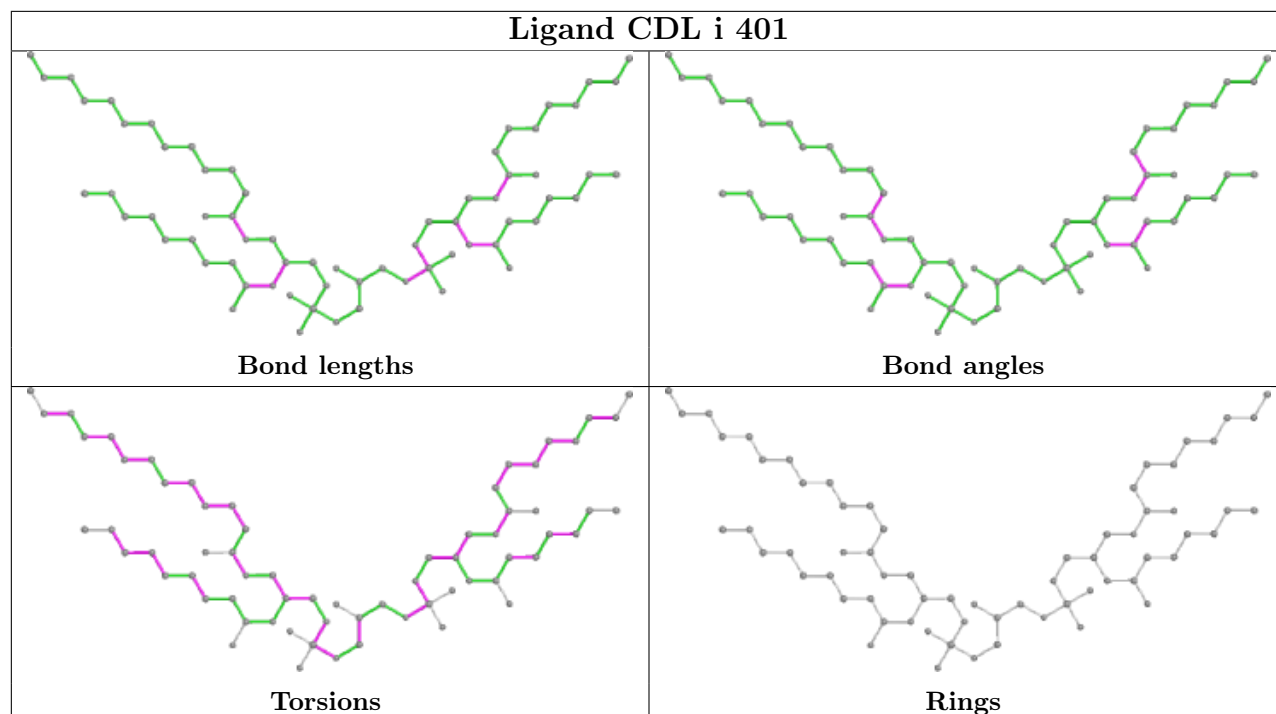
No monomer is involved in short contacts.

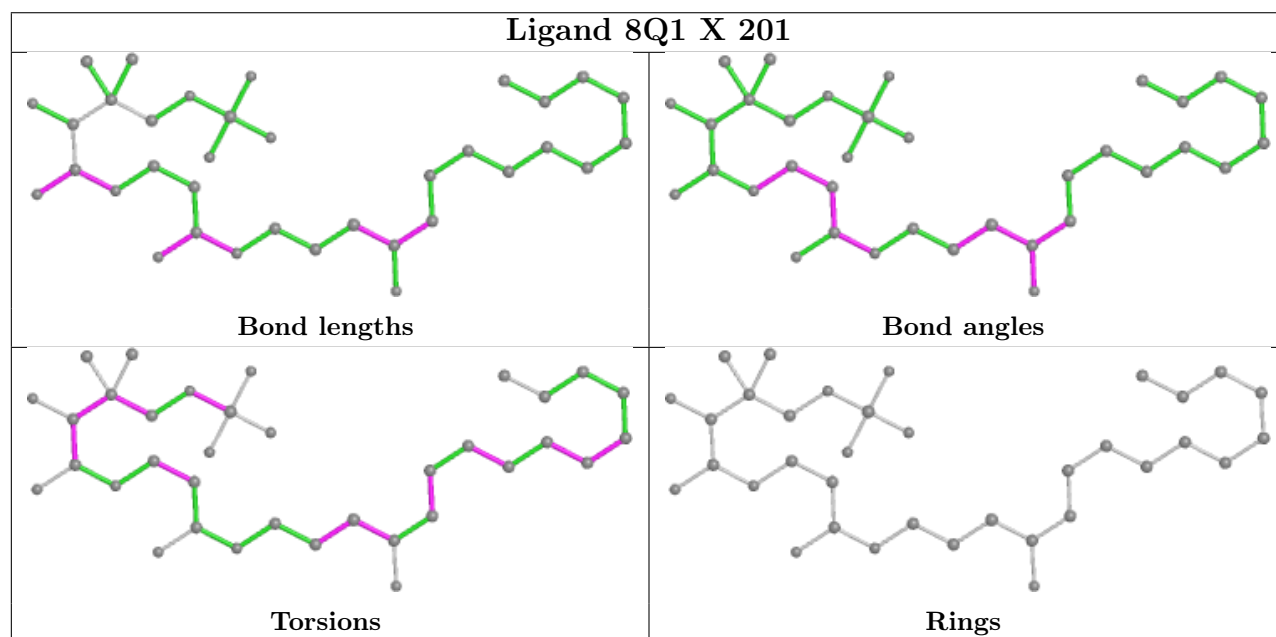
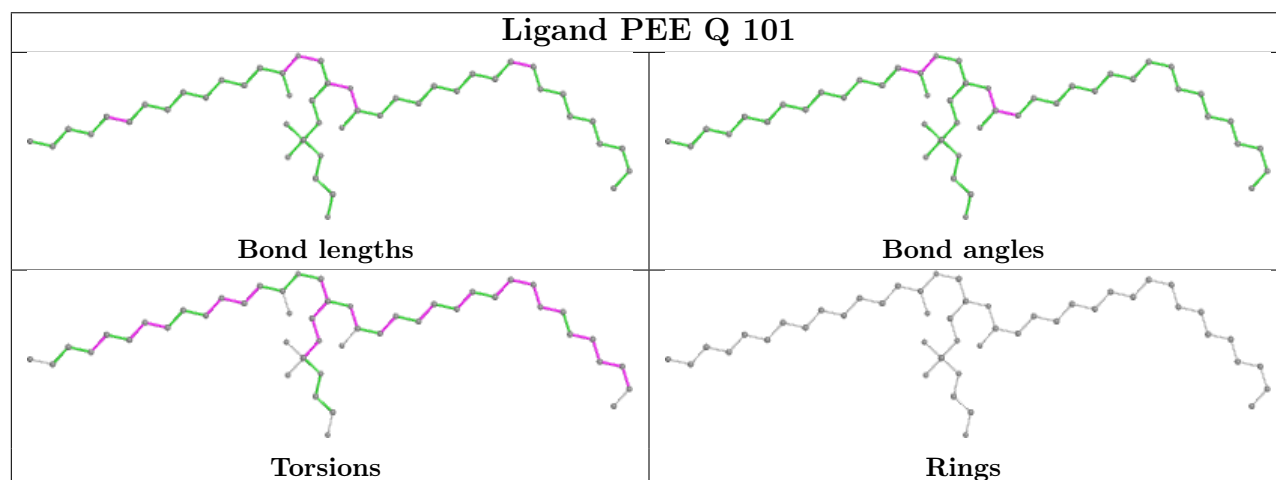
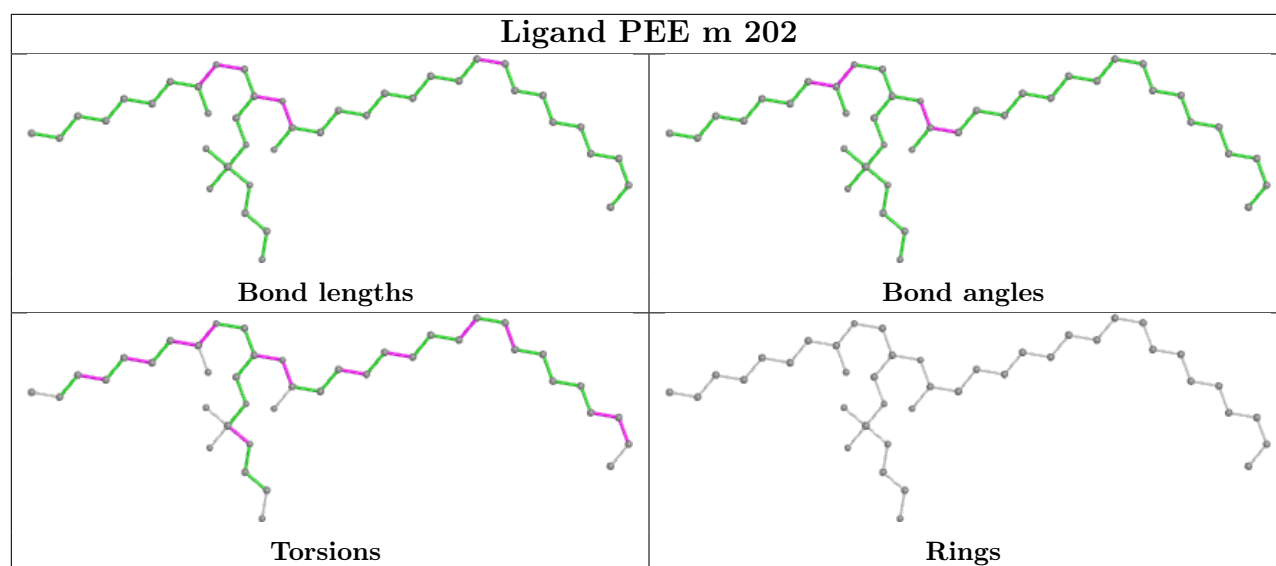
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

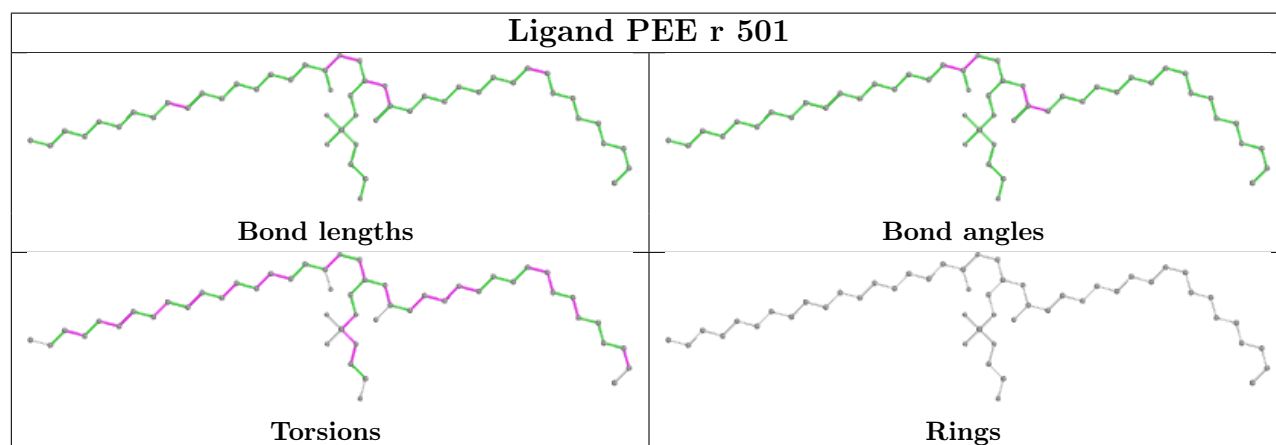
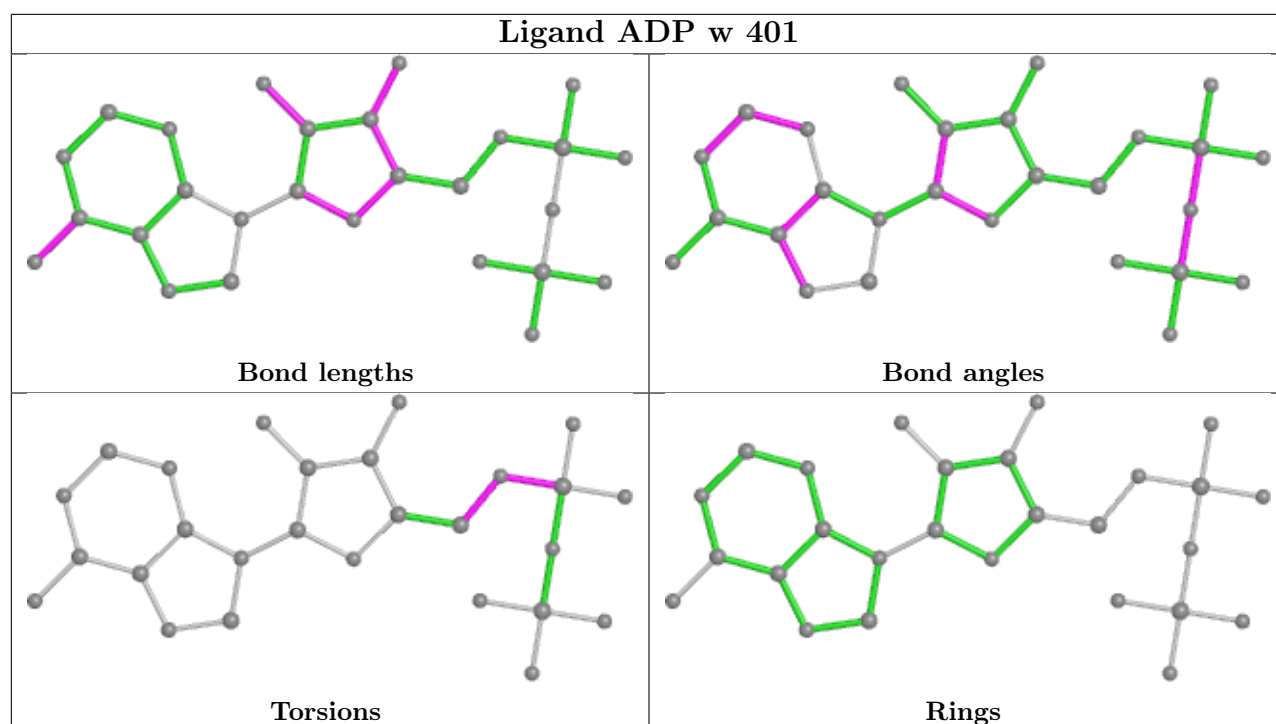
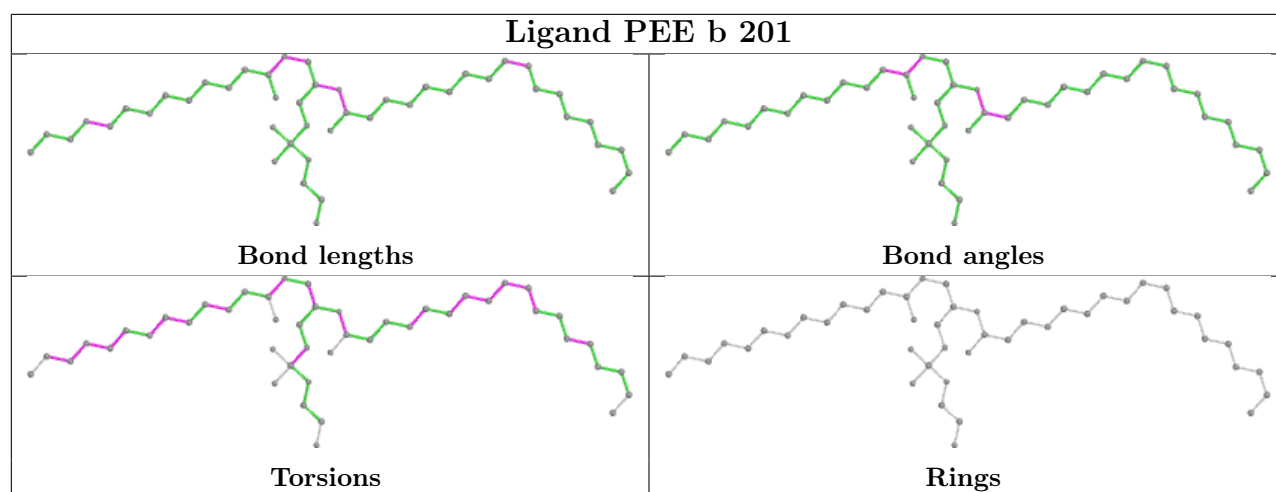


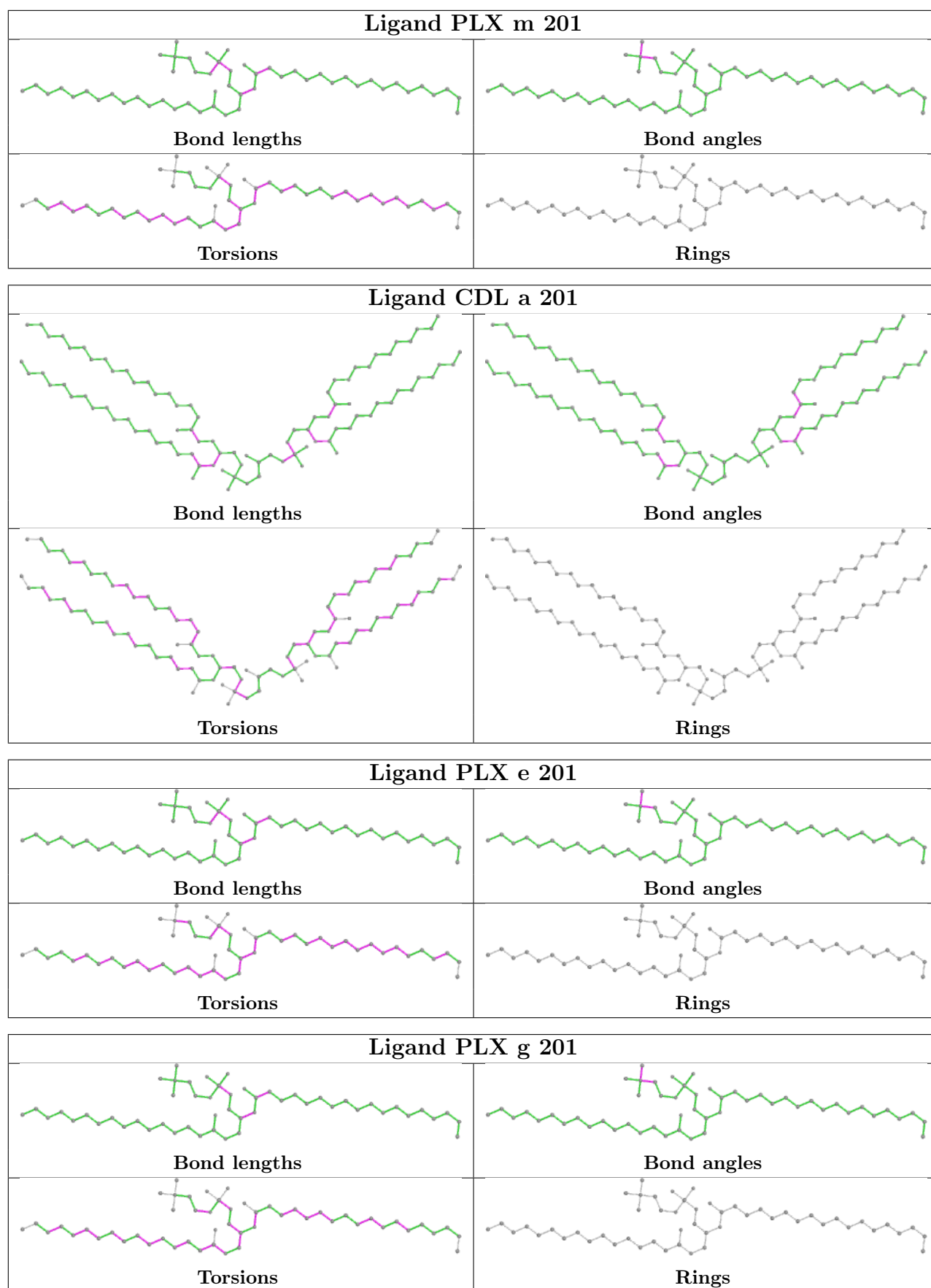
Ligand PEE s 401	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CDL V 201	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PLX r 502	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

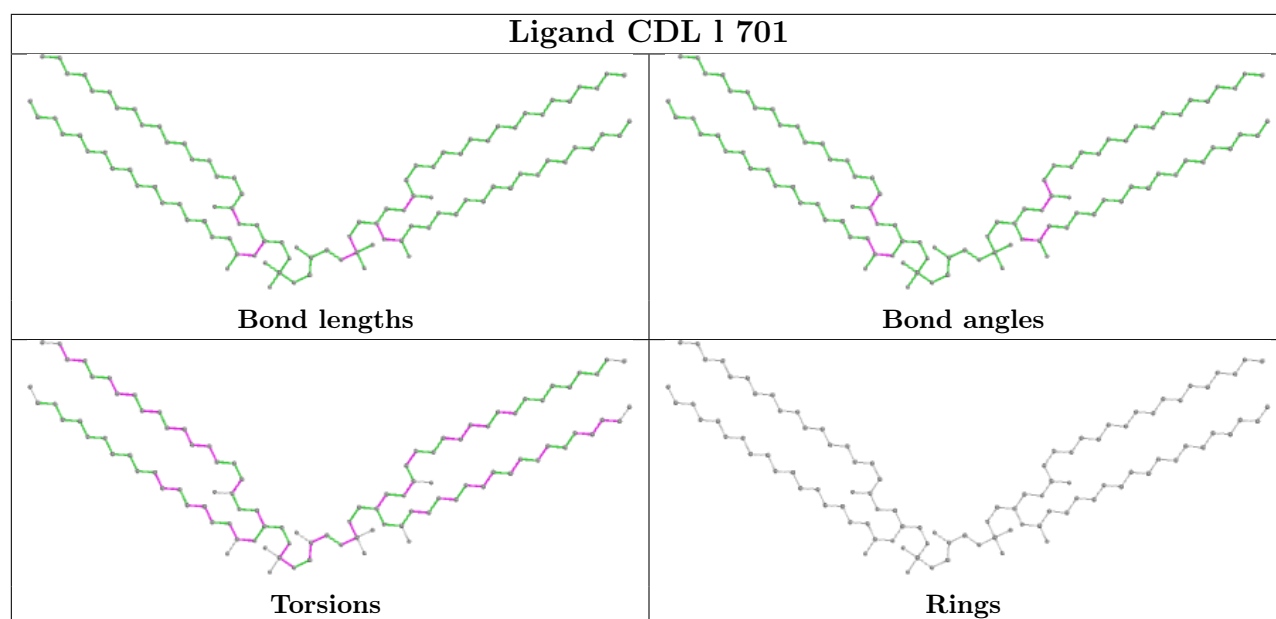












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

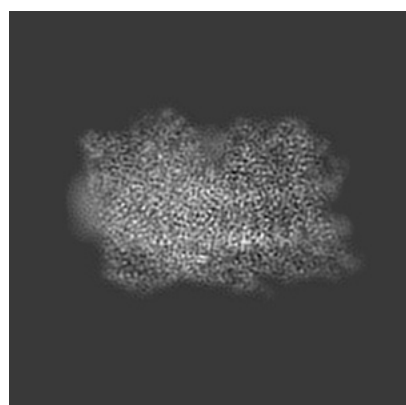
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32222. These allow visual inspection of the internal detail of the map and identification of artifacts.

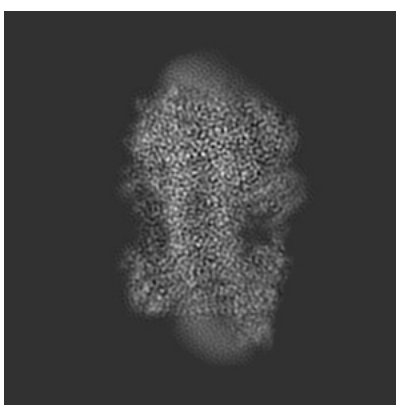
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

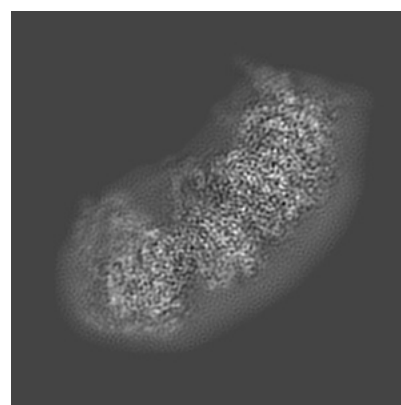
6.1.1 Primary map



X



Y

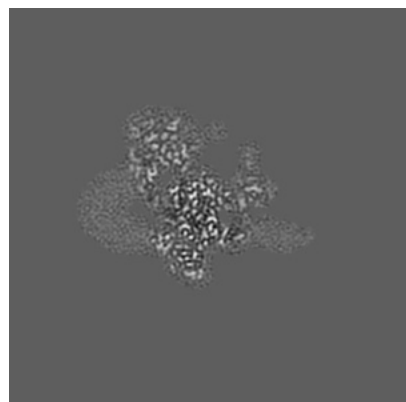


Z

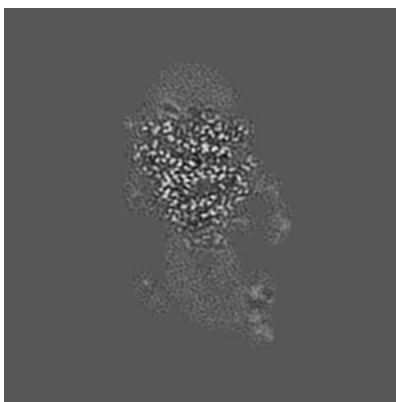
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

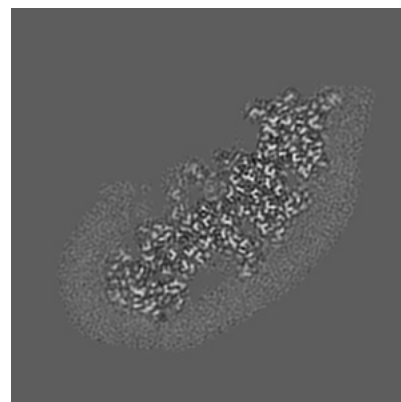
6.2.1 Primary map



X Index: 240



Y Index: 240

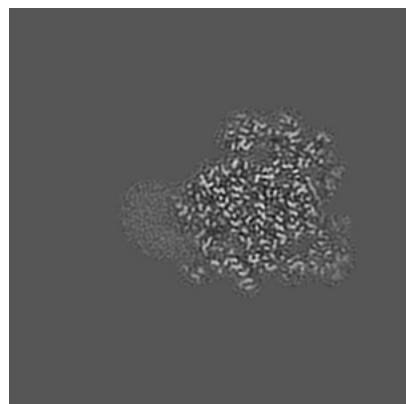


Z Index: 240

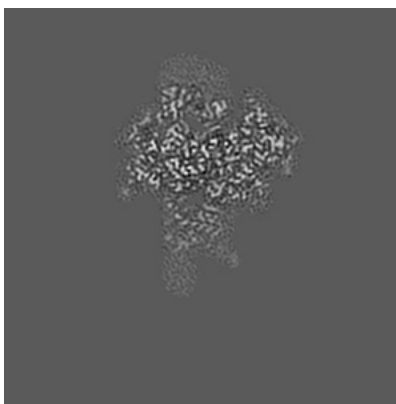
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

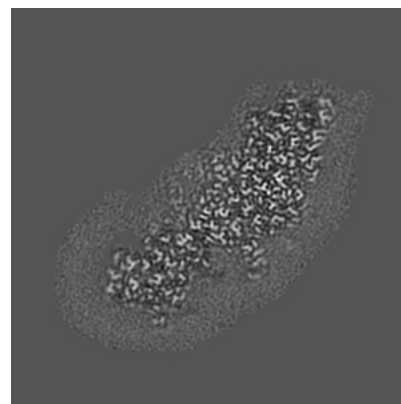
6.3.1 Primary map



X Index: 323



Y Index: 281

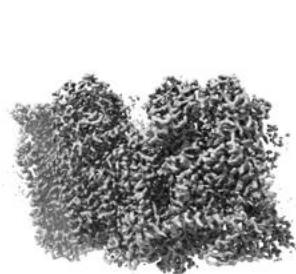


Z Index: 254

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

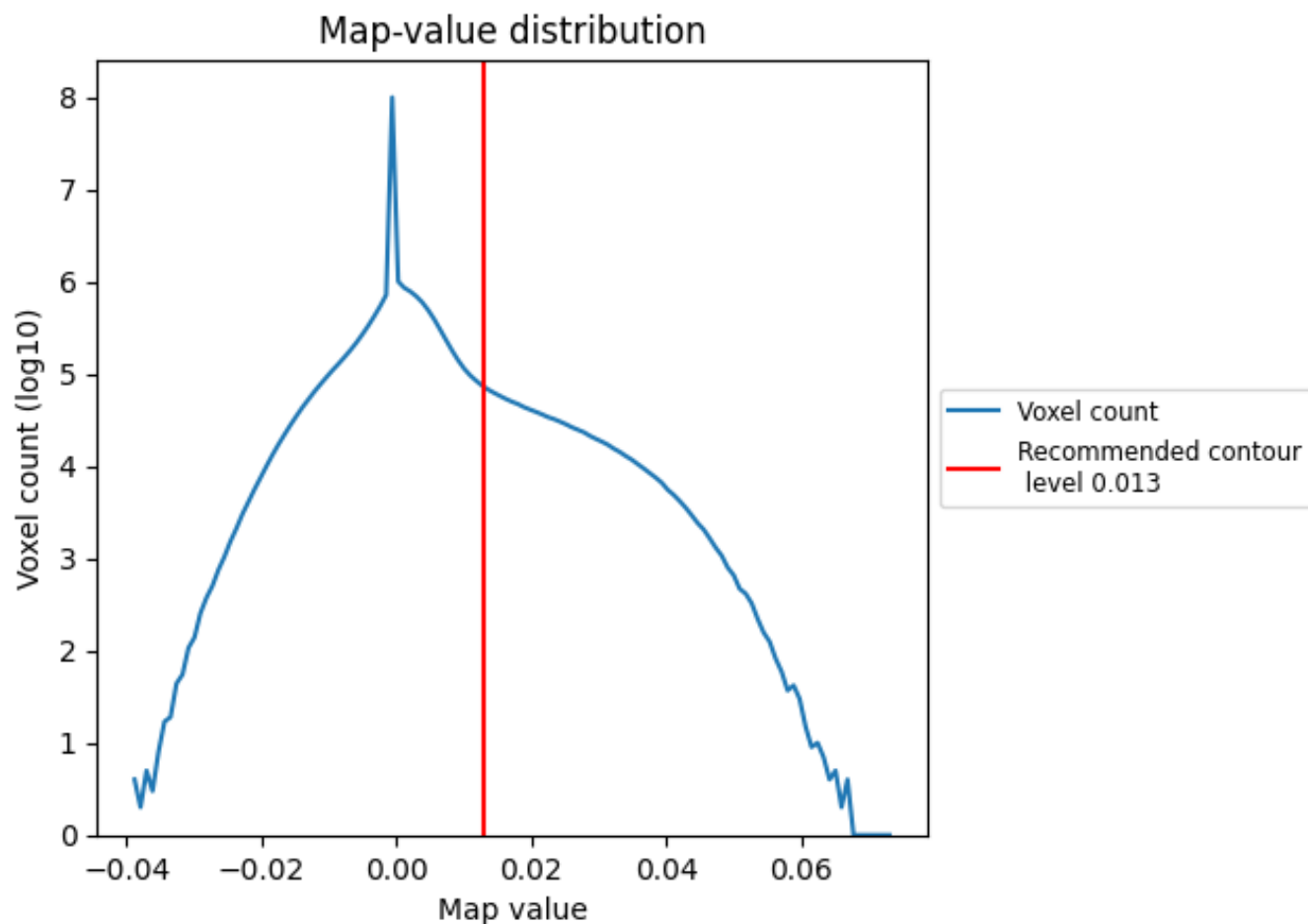
6.5 Mask visualisation

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

7 Map analysis [i](#)

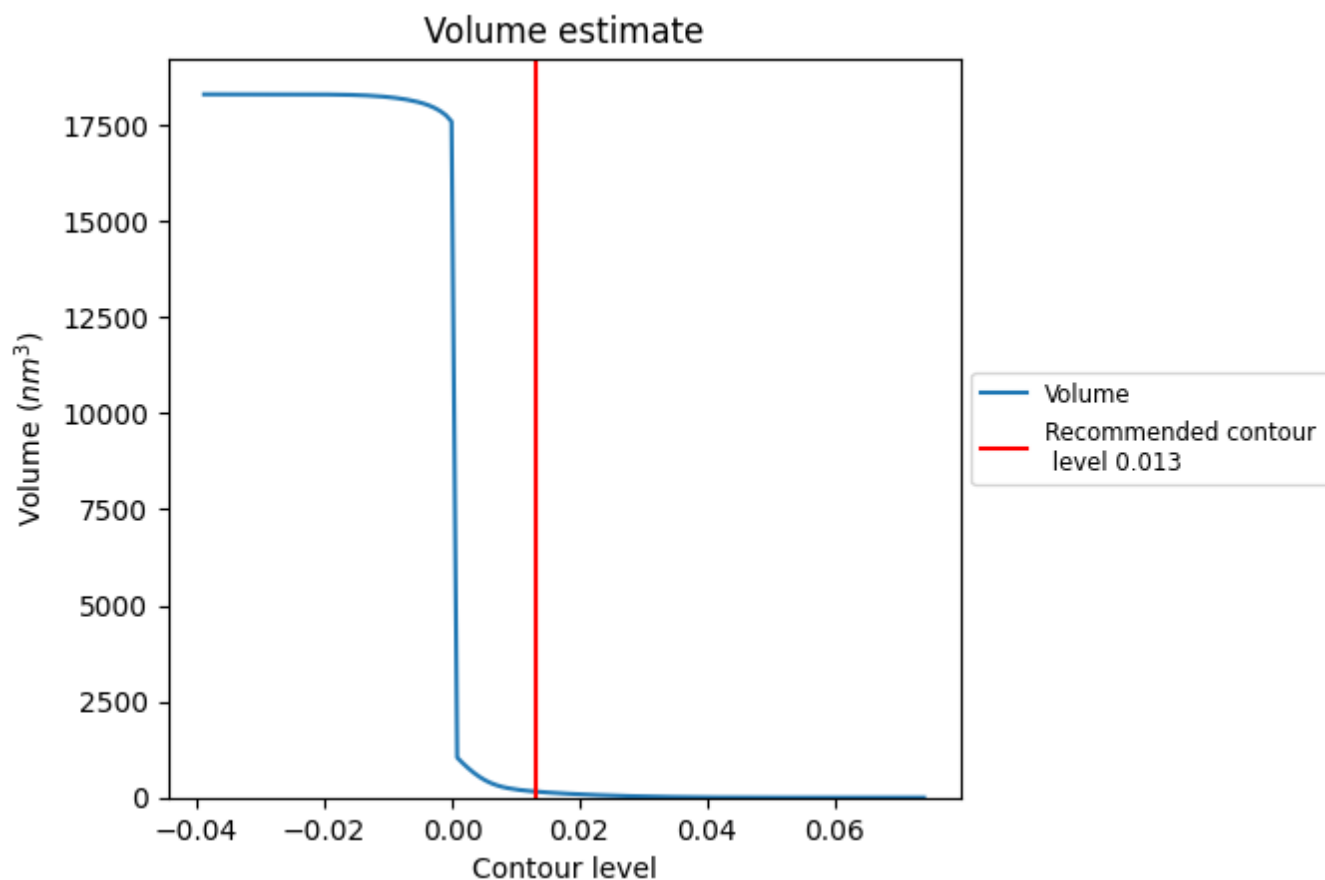
This section contains the results of statistical analysis of the map.

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.

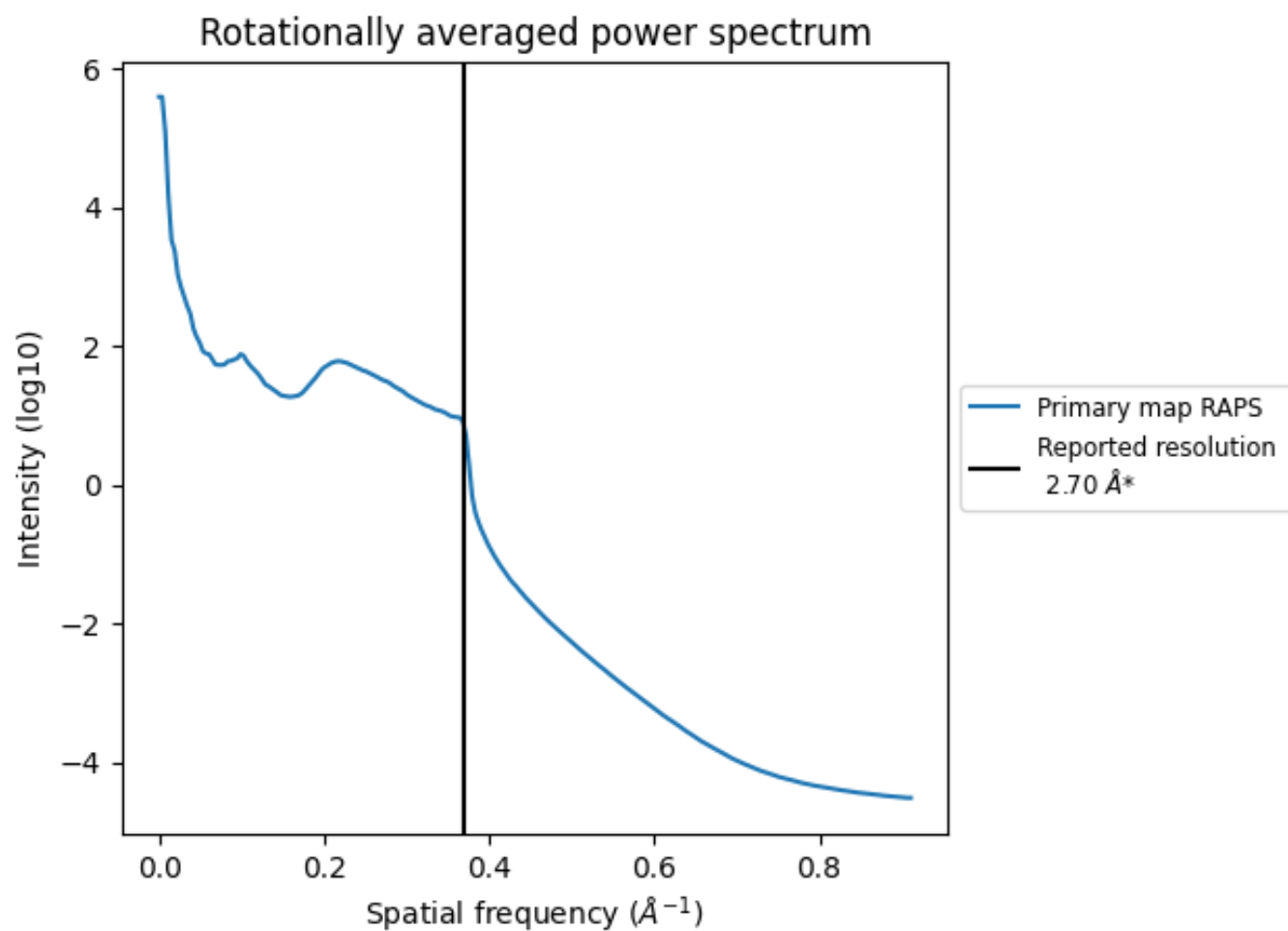
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 158 nm³; this corresponds to an approximate mass of 143 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

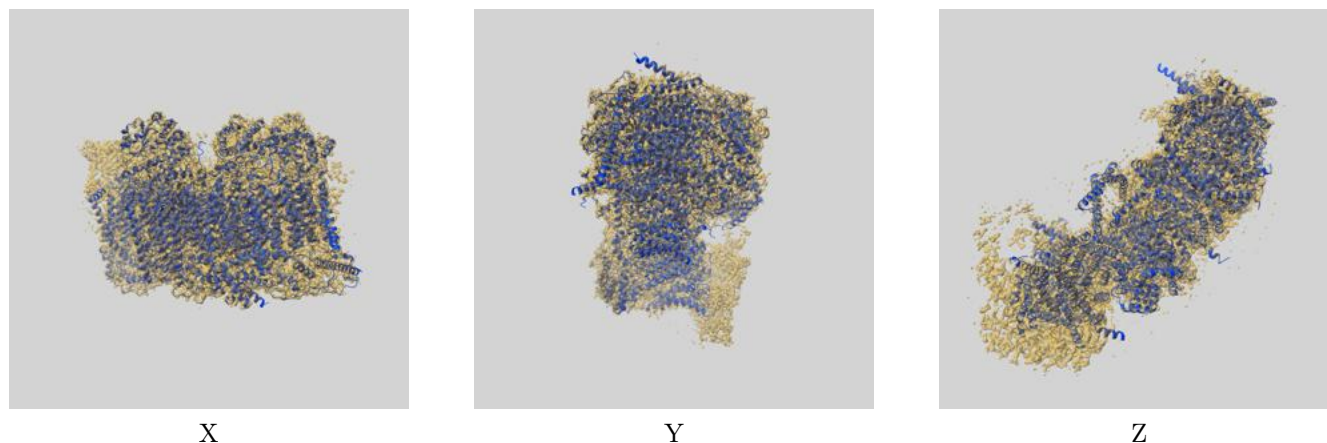
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

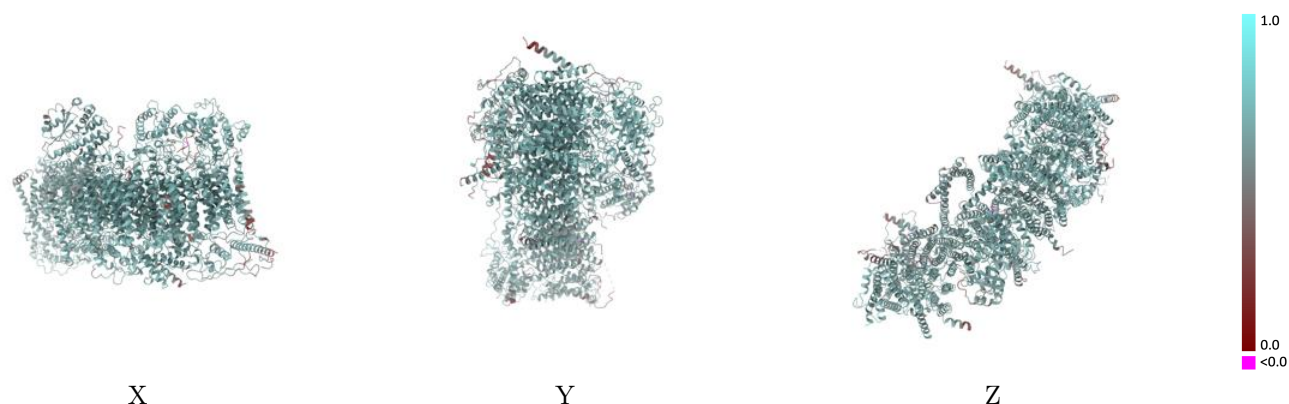
This section contains information regarding the fit between EMDB map EMD-32222 and PDB model 7VZ8. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



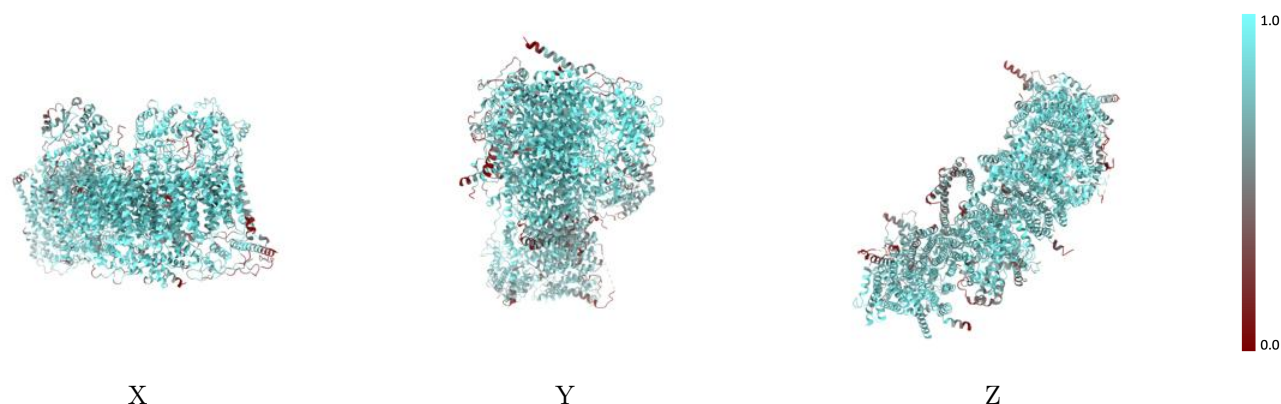
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



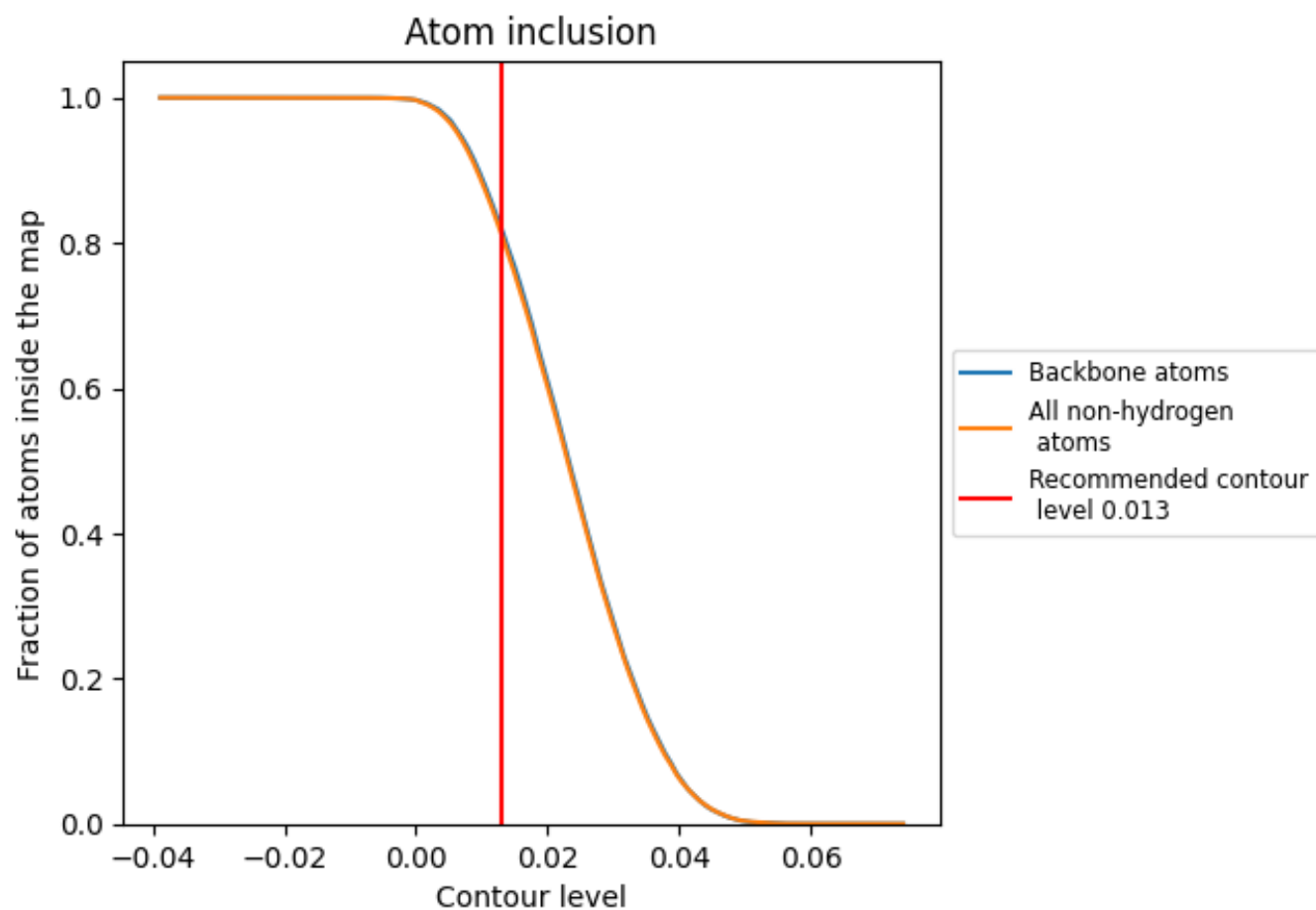
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.013).





























































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 81% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8120	 0.6280
Q	 0.6622	 0.5990
S	 0.8318	 0.6210
U	 0.7441	 0.5990
V	 0.5354	 0.5630
W	 0.8400	 0.6390
X	 0.8262	 0.6180
Y	 0.6718	 0.5850
Z	 0.6261	 0.5420
a	 0.8692	 0.6490
b	 0.7140	 0.5850
c	 0.8389	 0.6360
d	 0.8120	 0.6300
e	 0.7709	 0.6100
f	 0.6677	 0.5770
g	 0.8854	 0.6520
h	 0.7955	 0.6260
i	 0.9328	 0.6640
j	 0.6982	 0.5790
k	 0.7970	 0.6290
l	 0.8884	 0.6560
m	 0.7617	 0.6040
n	 0.7091	 0.5960
o	 0.8222	 0.6400
p	 0.8639	 0.6380
r	 0.9139	 0.6580
s	 0.8322	 0.6300
u	 0.7914	 0.6210
v	 0.6586	 0.5770
w	 0.7375	 0.6070

