



## Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 09:40 PM JST

PDB ID : 5XTD / pdb\_00005xt  
EMDB ID : EMD-6773  
Title : Cryo-EM structure of human respiratory complex I  
Authors : Gu, J.; Wu, M.; Yang, M.  
Deposited on : 2017-06-19  
Resolution : 3.70 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](mailto: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>.

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

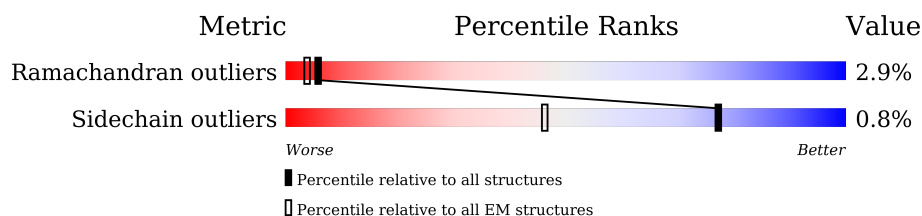
EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

# 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 3.70 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	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	431	<div> <div>60%</div> <div>98%</div> <div>.</div> </div>
2	B	176	<div> <div>6%</div> <div>99%</div> <div>.</div> </div>
3	C	156	<div> <div>.</div> <div>97%</div> <div>.</div> </div>
4	E	113	<div> <div>50%</div> <div>97%</div> <div>.</div> </div>
5	F	83	<div> <div>54%</div> <div>100%</div> <div>.</div> </div>
6	G	85	<div> <div>91%</div> <div>98%</div> <div>.</div> </div>
6	X	85	<div> <div>95%</div> <div>5%</div> <div>.</div> </div>
7	H	112	<div> <div>51%</div> <div>96%</div> <div>.</div> </div>
8	I	110	<div> <div>45%</div> <div>81%</div> <div>5%</div> <div>14%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
9	J	337	
10	K	33	
11	L	118	
12	M	687	
13	N	143	
14	O	212	
15	P	208	
16	Q	430	
17	S	70	
18	T	95	
19	U	83	
20	V	140	
21	W	138	
22	Y	59	
23	Z	80	
24	a	138	
25	b	128	
26	c	153	
27	d	171	
28	e	97	
29	f	47	
30	g	119	
31	h	104	
32	i	347	
33	j	115	

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Mol	Chain	Length	Quality of chain
34	k	97	<p>10% 93% 6% .</p>
35	l	603	<p>94% 5% .</p>
36	m	174	<p>10% 94% 6% .</p>
37	n	56	<p>11% 96% .</p>
38	o	128	<p>97% .</p>
39	p	172	<p>98% .</p>
40	r	459	<p>98% .</p>
41	s	318	<p>97% .</p>
42	u	169	<p>97% .</p>
43	v	137	<p>10% 77% . 19%</p>
44	w	320	<p>18% 97% .</p>

## 2 Entry composition [i](#)

There are 52 unique types of molecules in this entry. The entry contains 66789 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] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3322	2096	594	612	20		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	176	Total	C	N	O	S	0	0
			1420	893	243	271	13		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	156	Total	C	N	O	S	0	0
			1249	794	227	214	14		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	113	Total	C	N	O	S	0	0
			968	623	178	162	5		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	83	Total	C	N	O	S	0	0
			670	422	124	122	2		

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	85	Total	C	N	O	S	0	0
			672	434	99	134	5		
6	X	85	Total	C	N	O	S	0	0
			686	442	101	138	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			922	593	157	169	3		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	95	Total	C	N	O	S	0	0
			769	483	146	138	2		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	337	Total	C	N	O	S	0	0
			2712	1759	482	463	8		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	33	Total	C	N	O	S	0	0
			274	173	47	53	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	118	Total	C	N	O	S	0	0
			964	608	173	179	4		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	687	Total	C	N	O	S	0	0
			5274	3310	917	1009	38		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	143	Total	C	N	O	S	0	0
			1195	770	210	212	3		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	212	Total	C	N	O	S	0	0
			1643	1047	276	310	10		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1730	1117	297	313	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	430	Total	C	N	O	S	0	0
			3460	2214	599	624	23		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			568	367	101	96	4		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	95	Total	C	N	O	S	0	0
			742	459	138	142	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	83	Total	C	N	O	S	0	0
			647	427	105	113	2		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	140	Total	C	N	O	S	0	0
			1038	668	178	187	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	138	Total	C	N	O	S	0	0
			1135	727	202	200	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	59	Total	C	N	O	S	0	0
			533	354	87	91	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	80	Total	C	N	O	S	0	0
			648	426	110	110	2		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	138	Total	C	N	O	S	0	0
			1174	771	199	202	2		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	124	Total	C	N	O	S	0	0
			1059	697	181	176	5		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	153	Total	C	N	O	S	0	0
			1236	795	208	222	11		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	171	Total	C	N	O	S	0	0
			1418	885	262	259	12		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	97	Total	C	N	O	S	0	0
			810	522	132	152	4		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	47	Total	C	N	O	0	0
			405	269	69	67		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	119	Total	C	N	O	S	0	0
			1004	658	173	169	4		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	104	Total	C	N	O	S	0	0
			863	546	161	150	6		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	347	Total	C	N	O	S	0	0
			2735	1819	421	470	25		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	115	Total	C	N	O	S	0	0
			919	626	132	152	9		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	97	Total	C	N	O	S	0	0
			740	487	113	127	13		

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	603	Total	C	N	O	S	0	0
			4717	3119	742	823	33		

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	174	Total	C	N	O	S	0	0
			1313	879	194	229	11		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	56	Total	C	N	O	S	0	0
			473	305	85	80	3		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit

4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	128	Total	C	N	O	S	0	0
			1066	685	192	187	2		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	172	Total	C	N	O	S	0	0
			1495	961	265	261	8		

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	459	Total	C	N	O	S	0	0
			3629	2411	569	619	30		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	318	Total	C	N	O	S	0	0
			2509	1678	380	435	16		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	169	Total	C	N	O	S	0	0
			1394	886	247	252	9		

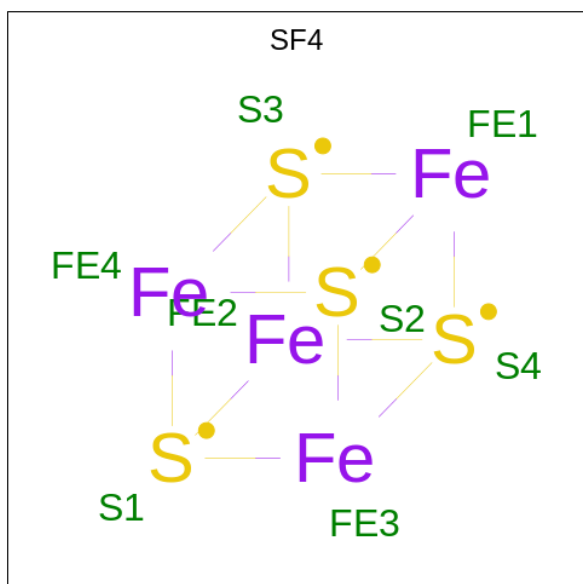
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	111	Total	C	N	O	S	0	0
			921	569	187	156	9		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

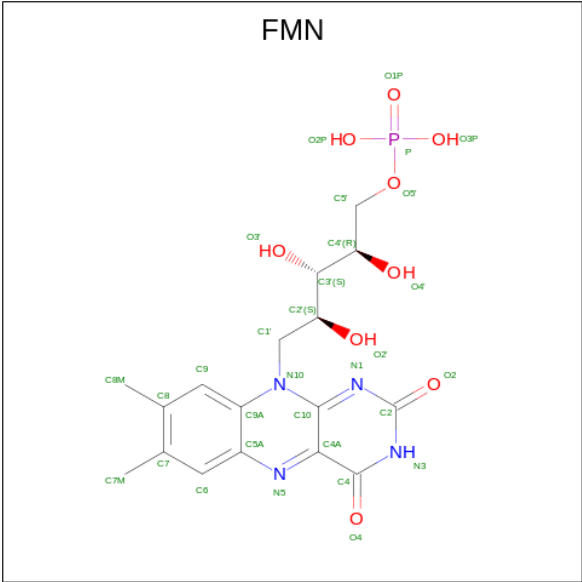
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2474	1573	429	464	8		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



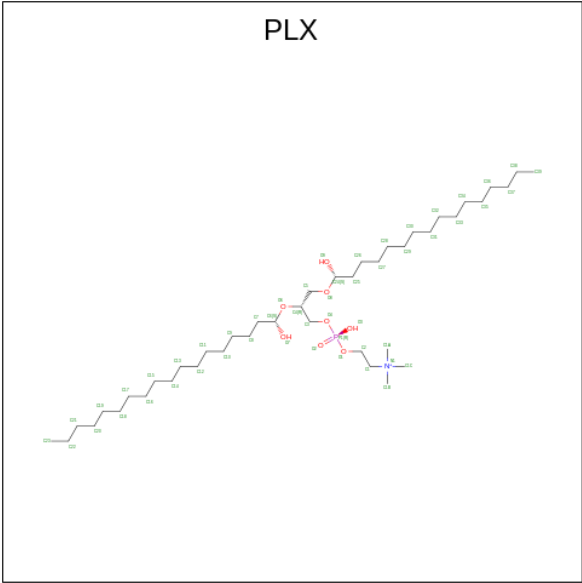
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$ ).



Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 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-TRIOL (CCD ID: PLX) (formula: C<sub>42</sub>H<sub>89</sub>NO<sub>8</sub>P).



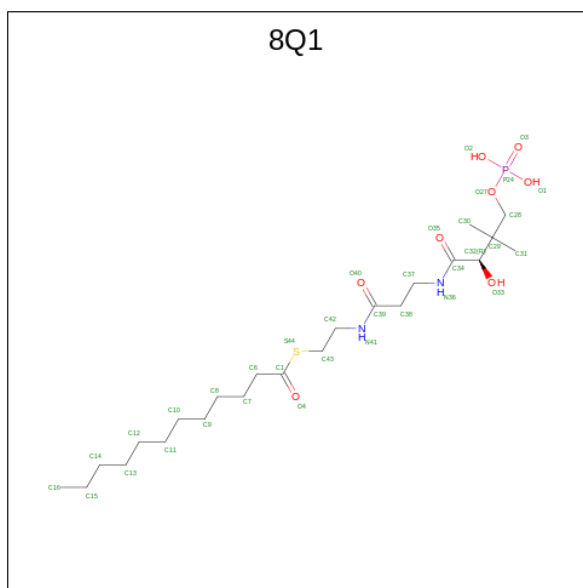
Mol	Chain	Residues	Atoms					AltConf
47	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	U	1	Total	C	N	O	P	0
			52	42	1	8	1	

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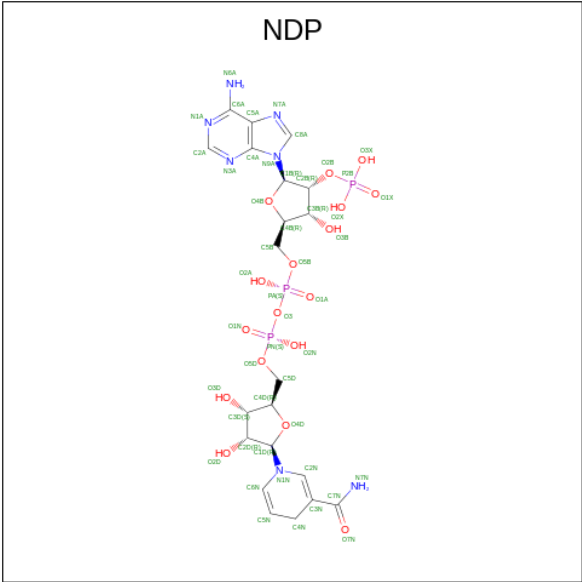
Mol	Chain	Residues	Atoms					AltConf
47	V	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	b	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 48 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula:  $C_{23}H_{45}N_2O_8PS$ ).



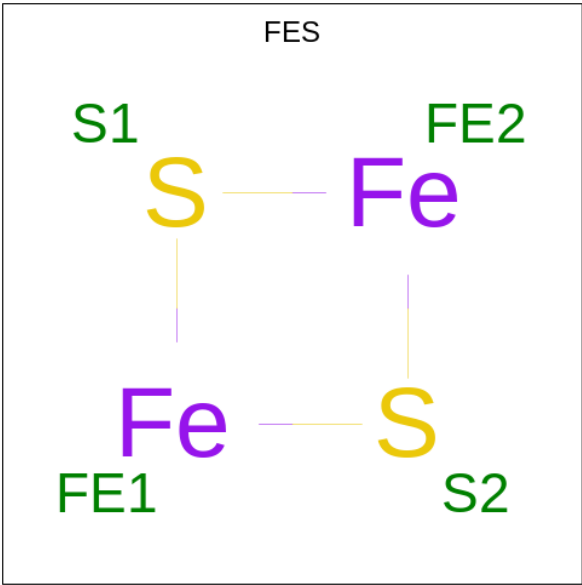
Mol	Chain	Residues	Atoms						AltConf
48	E	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
48	p	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 49 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



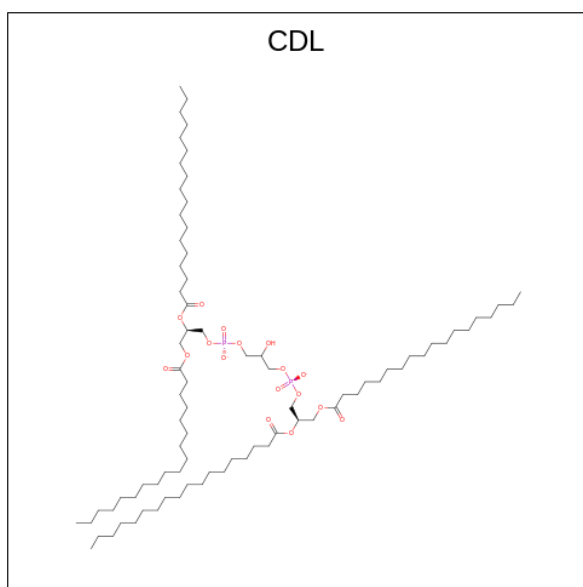
Mol	Chain	Residues	Atoms					AltConf
49	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 50 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



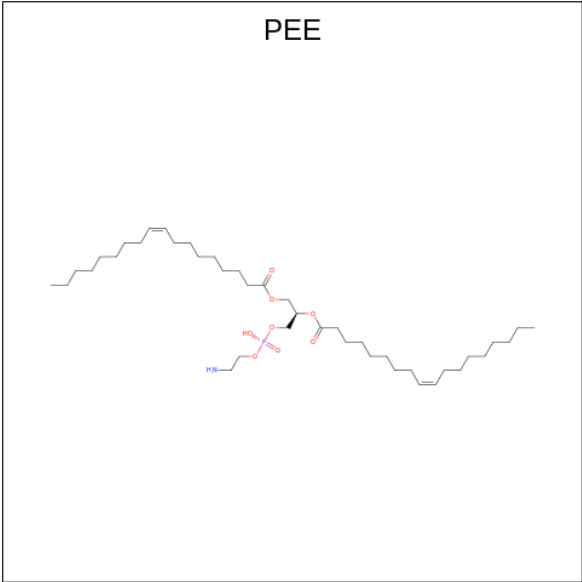
Mol	Chain	Residues	Atoms			AltConf
50	M	1	Total	Fe	S	0
			4	2	2	
50	O	1	Total	Fe	S	0
			4	2	2	

- Molecule 51 is CARDIOLIPIN (CCD ID: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				AltConf
51	V	1	Total	C	O	P	0
			63	44	17	2	
51	i	1	Total	C	O	P	0
			64	45	17	2	
51	l	1	Total	C	O	P	0
			64	45	17	2	
51	l	1	Total	C	O	P	0
			64	45	17	2	
51	n	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 52 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula:  $C_{41}H_{78}NO_8P$ ).

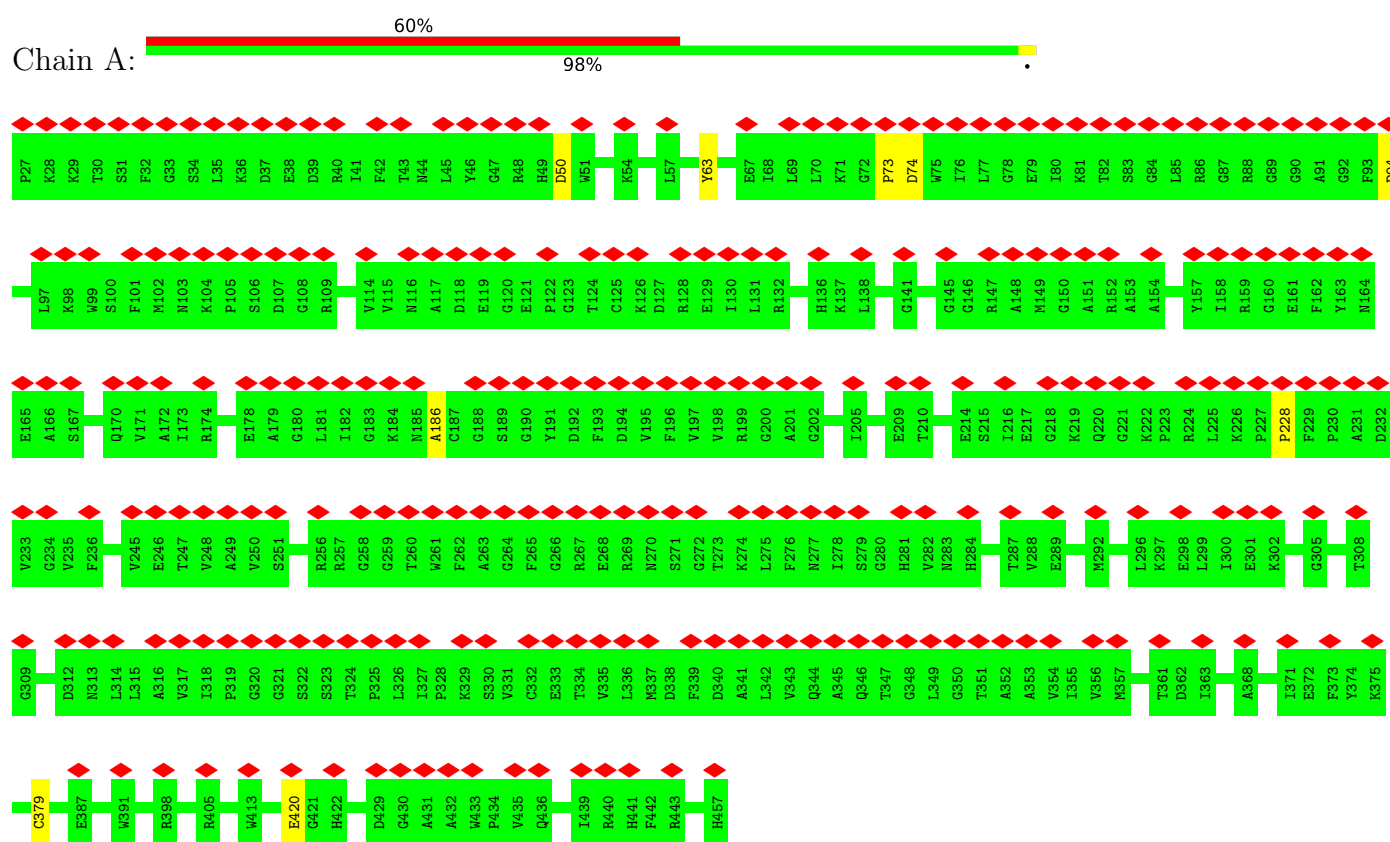


Mol	Chain	Residues	Atoms					AltConf
52	V	1	Total	C	N	O	P	0
			51	41	1	8	1	
52	W	1	Total	C	N	O	P	0
			51	41	1	8	1	
52	1	1	Total	C	N	O	P	0
			49	39	1	8	1	
52	1	1	Total	C	N	O	P	0
			51	41	1	8	1	

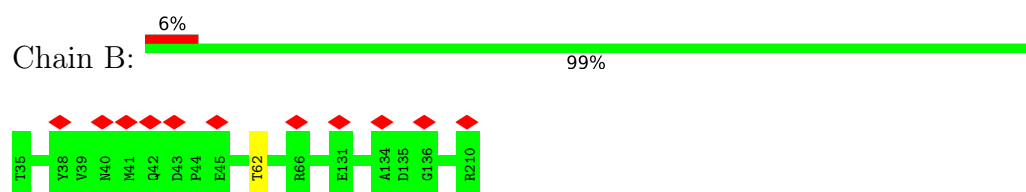
### 3 Residue-property plots

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] flavoprotein 1, mitochondrial



- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

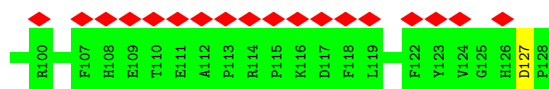
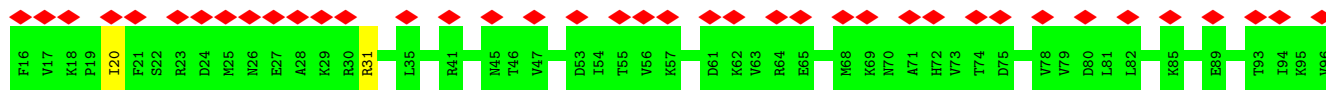


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

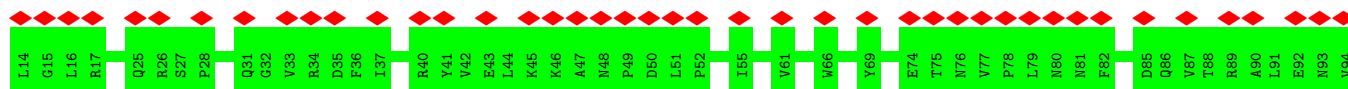




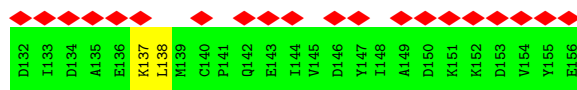
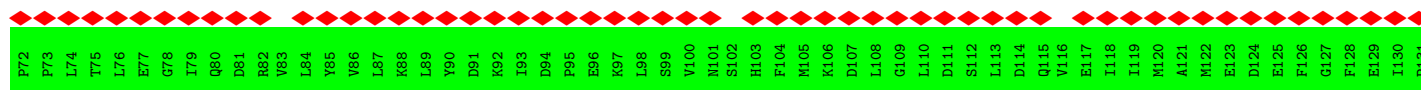
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 6: Acyl carrier protein, mitochondrial

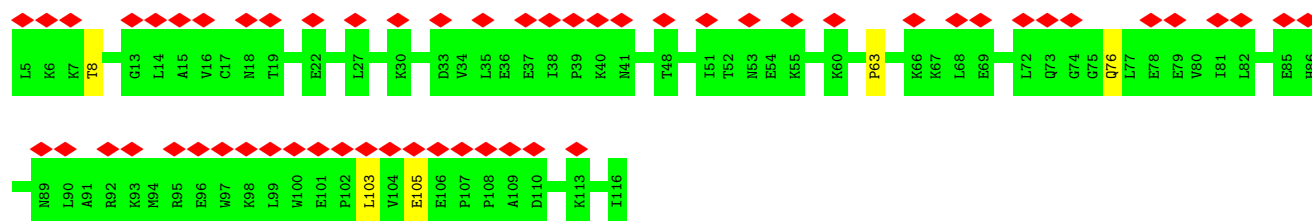


- Molecule 6: Acyl carrier protein, mitochondrial

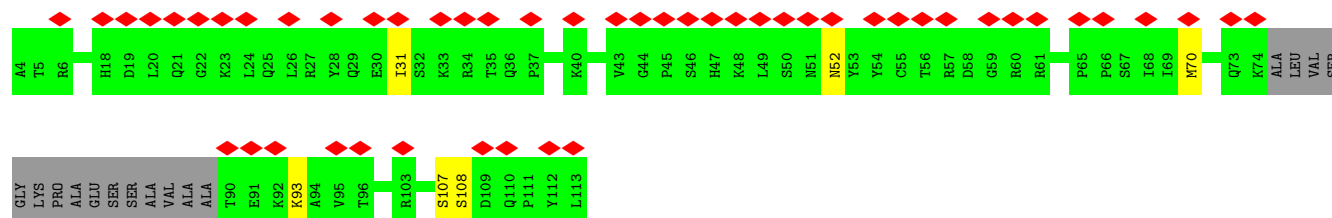
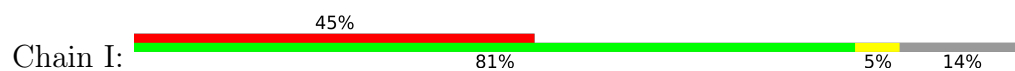


- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

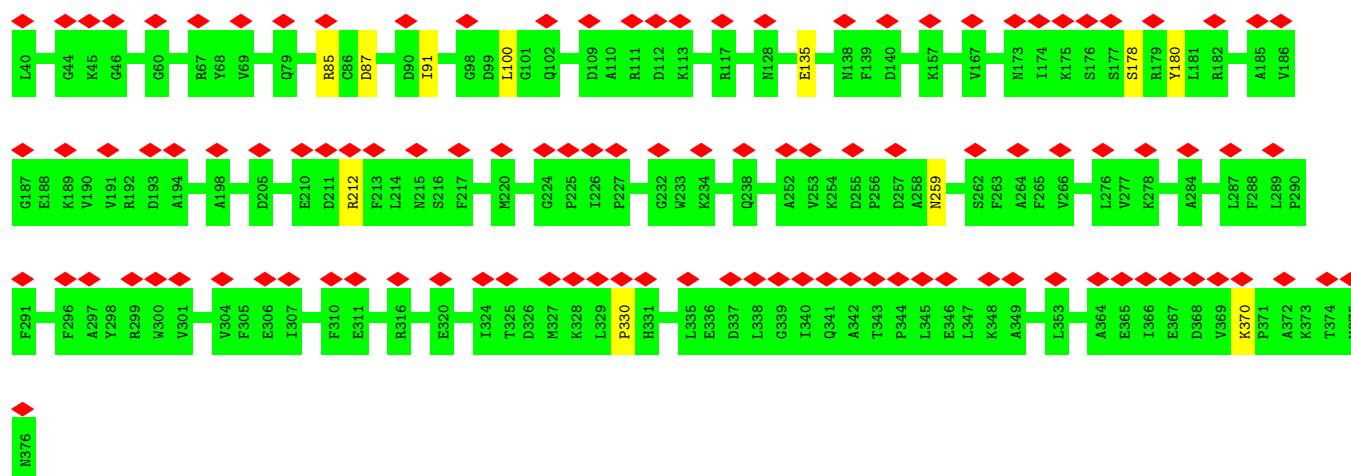




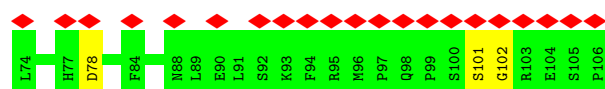
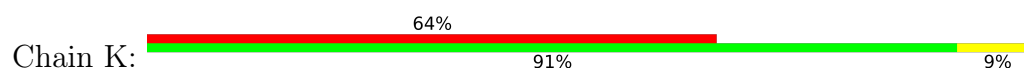
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

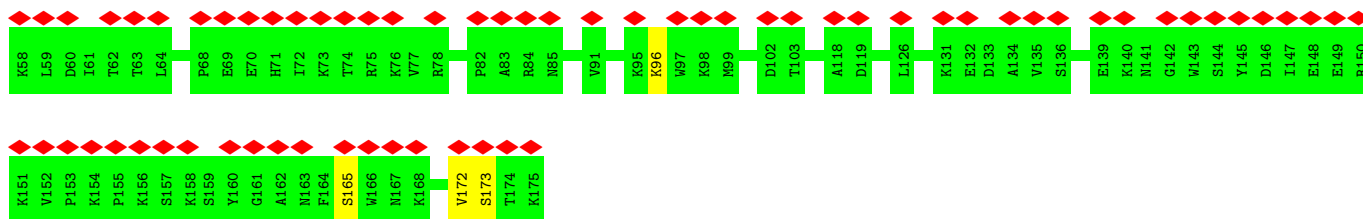


- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

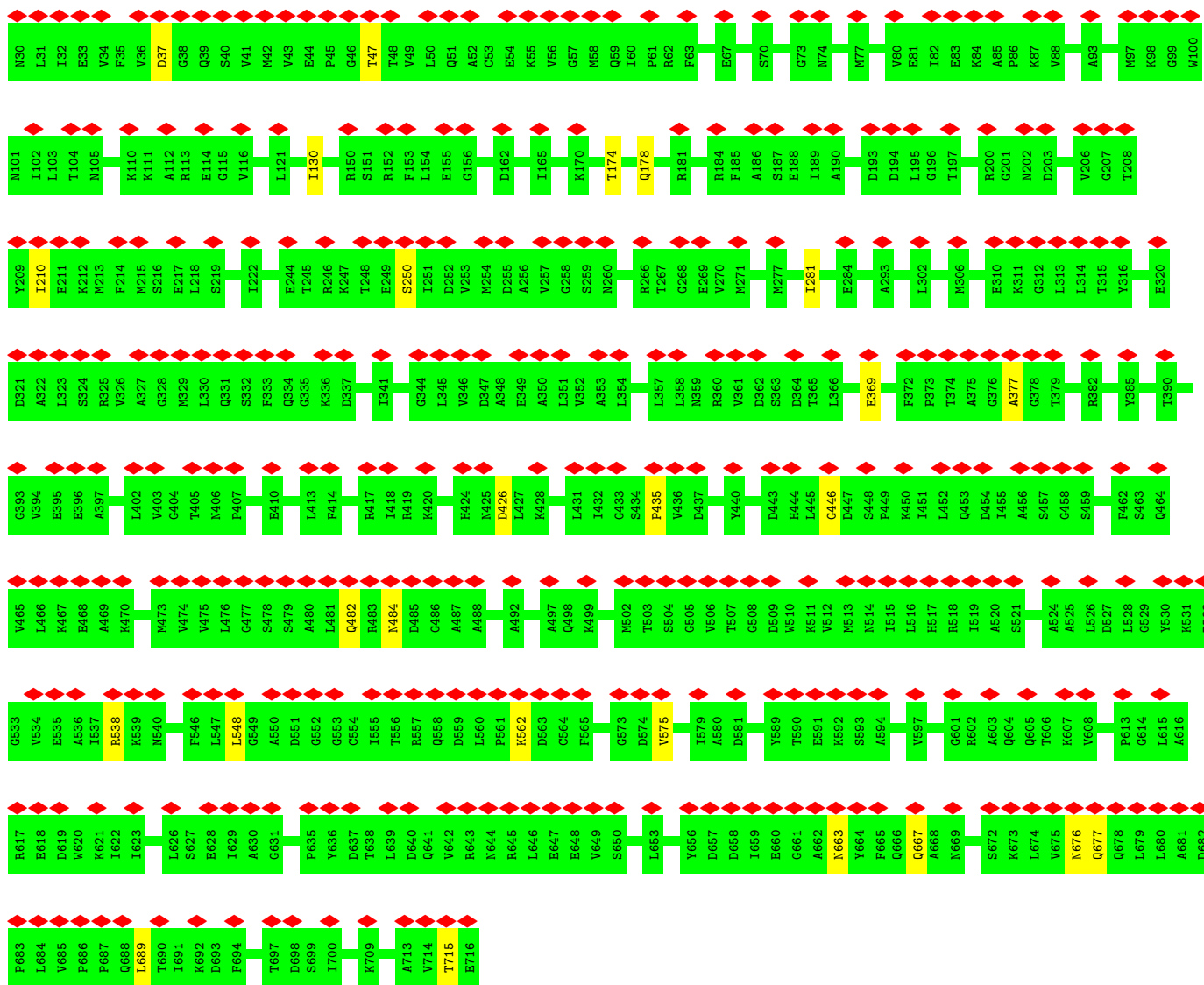


- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



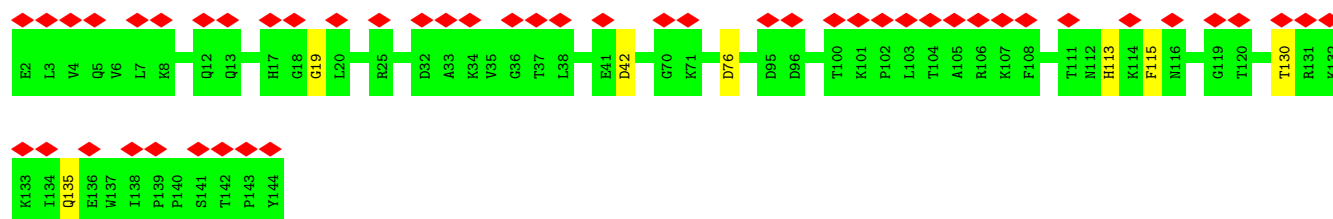


- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

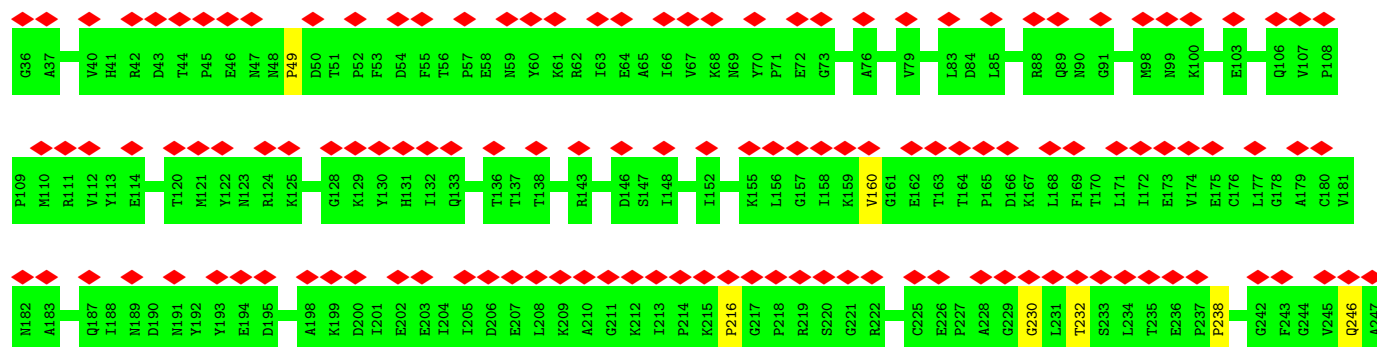


- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

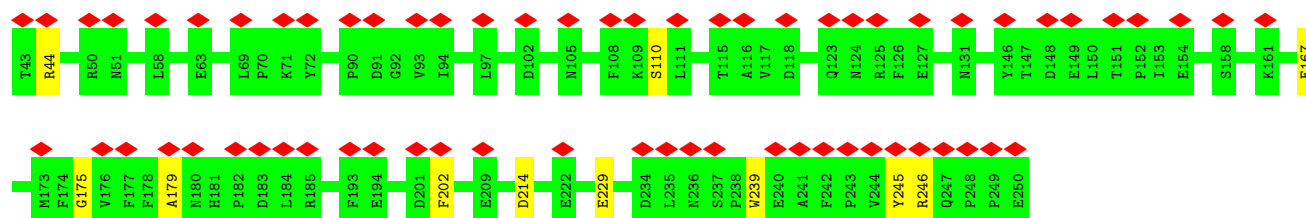




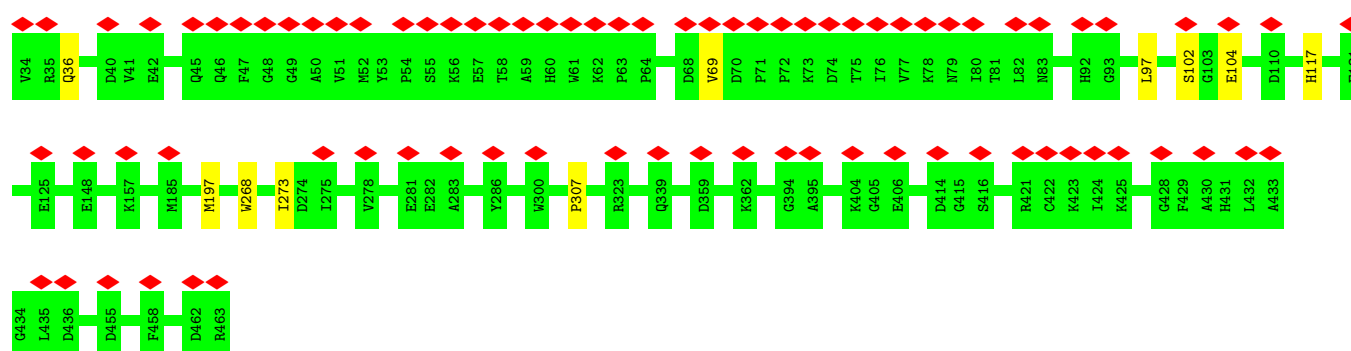
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



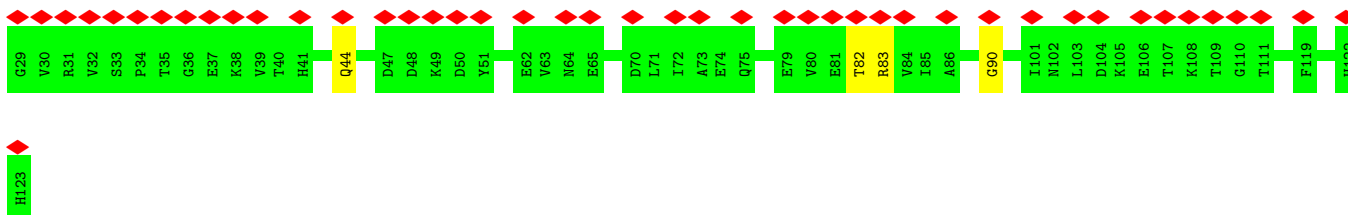
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S:  97%



- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T:  47% 96%



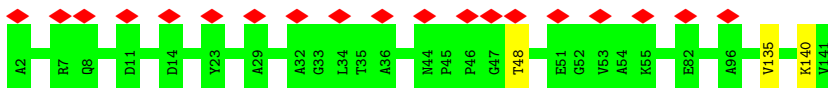
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:  99%



- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:  14% 98%




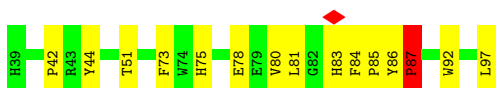
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:  97%




- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y:  75% 24%



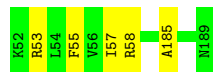
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z:  100%


There are no outlier residues recorded for this chain.

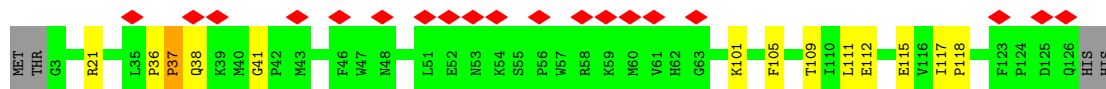
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:  96%



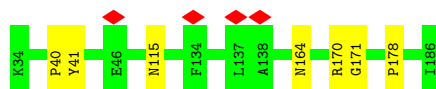
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain b:  87%



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c:  95%



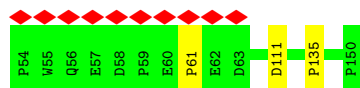
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d:  95%



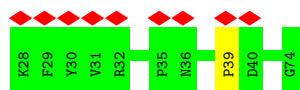
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e:  97%



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f:  98%



- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g: 95% 5%



- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h: 94% 6%



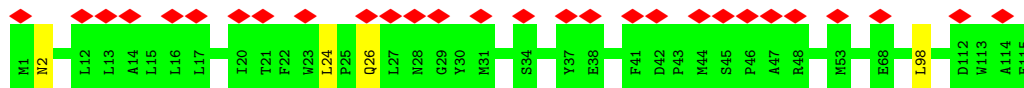
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain i: 98% 2%



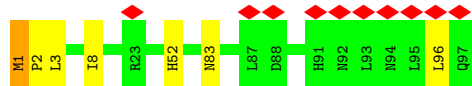
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j: 24% 97% 1%



- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

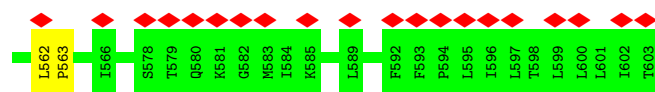
Chain k: 10% 93% 6%



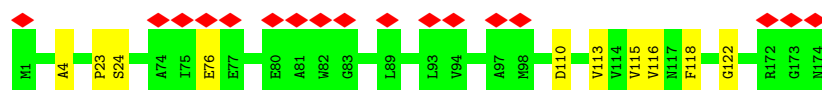
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l: 94% 5%

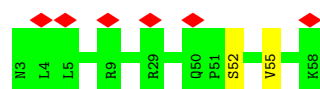




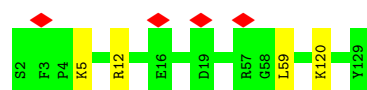
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6



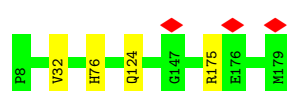
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

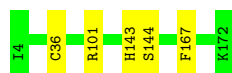


- Molecule 41: NADH-ubiquinone oxidoreductase chain 1




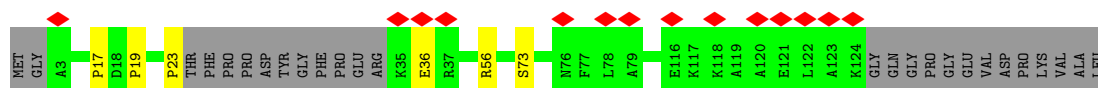
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:  97%



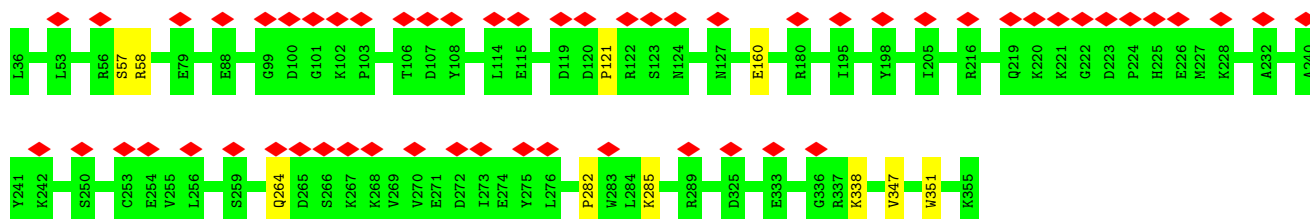
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v:  10% 77% 19%



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain w:  18% 97%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	167761	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 ( $e^-/\text{\AA}^2$ )	1.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.325	Depositor
Minimum map value	-0.134	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0525	Depositor
Map size ( $\text{\AA}$ )	519.83997, 519.83997, 519.83997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.083, 1.083, 1.083	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, FMN, 8Q1, SF4, PLX, CDL, FES, 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	A	0.30	0/3398	0.49	0/4590
2	B	0.50	0/1452	0.57	0/1964
3	C	0.58	0/1280	0.57	0/1732
4	E	0.34	0/993	0.54	0/1335
5	F	0.28	0/682	0.52	0/922
6	G	0.33	0/684	0.53	0/926
6	X	0.57	0/698	0.61	0/942
7	H	0.33	0/941	0.59	0/1275
8	I	0.29	0/788	0.54	0/1066
9	J	0.34	0/2785	0.52	0/3771
10	K	0.27	0/282	0.47	0/381
11	L	0.33	0/987	0.53	0/1331
12	M	0.32	0/5362	0.53	0/7266
13	N	0.37	0/1236	0.55	0/1681
14	O	0.29	0/1682	0.51	0/2289
15	P	0.38	0/1780	0.59	0/2424
16	Q	0.43	0/3552	0.59	1/4815 (0.0%)
17	S	0.60	0/583	0.64	0/785
18	T	0.31	0/755	0.47	0/1017
19	U	0.52	0/670	0.63	0/920
20	V	0.51	0/1065	0.61	0/1450
21	W	0.57	0/1166	0.66	0/1579
22	Y	0.52	0/559	0.73	3/763 (0.4%)
23	Z	0.45	0/669	0.53	0/899
24	a	0.68	0/1209	0.65	0/1639
25	b	0.59	1/1095 (0.1%)	0.69	4/1480 (0.3%)
26	c	0.58	0/1287	0.58	0/1761
27	d	0.63	0/1445	0.65	1/1945 (0.1%)
28	e	0.61	0/835	0.62	0/1134
29	f	0.48	0/418	0.58	0/566
30	g	0.64	0/1035	0.63	0/1398
31	h	0.62	0/884	0.65	0/1182

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	i	0.67	0/2808	0.77	2/3843 (0.1%)
33	j	0.55	0/945	0.69	1/1292 (0.1%)
34	k	0.68	1/751 (0.1%)	0.79	1/1019 (0.1%)
35	l	0.61	1/4840 (0.0%)	0.69	3/6611 (0.0%)
36	m	0.68	0/1346	0.67	0/1832
37	n	0.49	0/484	0.62	0/652
38	o	0.54	0/1093	0.61	0/1479
39	p	0.59	0/1549	0.59	0/2098
40	r	0.70	0/3723	0.76	2/5089 (0.0%)
41	s	0.62	0/2580	0.73	0/3539
42	u	0.57	0/1433	0.61	0/1937
43	v	0.48	0/934	0.67	3/1241 (0.2%)
44	w	0.44	0/2533	0.56	0/3440
All	All	0.51	3/67276 (0.0%)	0.62	21/91300 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
44	w	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	118	PRO	N-CD	5.18	1.55	1.47
34	k	2	PRO	N-CD	5.14	1.55	1.47
35	l	231	PRO	N-CD	5.05	1.54	1.47

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	i	323	THR	C-N-CD	-7.37	104.38	120.60
22	Y	92	TRP	N-CA-C	-7.00	92.10	111.00
27	d	2	PRO	N-CA-CB	6.79	111.44	103.30
22	Y	87	PRO	CA-N-CD	-6.57	102.30	111.50
25	b	36	PRO	C-N-CD	6.22	141.46	128.40
32	i	323	THR	C-N-CA	6.05	147.42	122.00
43	v	17	PRO	N-CA-CB	5.93	110.42	103.30
43	v	23	PRO	N-CA-CB	5.90	110.38	103.30
35	l	197	ASP	C-N-CD	5.88	140.74	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	105	PHE	C-N-CD	5.81	140.60	128.40
34	k	1	MET	C-N-CD	5.75	140.47	128.40
35	l	90	ILE	C-N-CD	5.72	140.41	128.40
43	v	19	PRO	N-CA-CB	5.69	110.13	103.30
35	l	230	HIS	C-N-CD	5.68	140.33	128.40
25	b	117	ILE	C-N-CD	5.67	140.31	128.40
16	Q	97	LEU	CA-CB-CG	5.65	128.29	115.30
25	b	37	PRO	CA-N-CD	-5.41	103.93	111.50
33	j	98	LEU	CB-CG-CD2	-5.40	101.82	111.00
22	Y	86	TYR	C-N-CD	5.12	139.15	128.40
40	r	408	LEU	CA-CB-CG	-5.10	103.58	115.30
40	r	238	LEU	CB-CG-CD2	-5.08	102.36	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	w	338	LYS	Peptide

## 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	A	429/431 (100%)	396 (92%)	24 (6%)	9 (2%)	5	33
2	B	174/176 (99%)	163 (94%)	10 (6%)	1 (1%)	22	54
3	C	154/156 (99%)	136 (88%)	13 (8%)	5 (3%)	3	27
4	E	111/113 (98%)	101 (91%)	8 (7%)	2 (2%)	7	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
6	G	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	5	30
6	X	83/85 (98%)	73 (88%)	6 (7%)	4 (5%)	2	19
7	H	110/112 (98%)	100 (91%)	5 (4%)	5 (4%)	2	19
8	I	91/110 (83%)	79 (87%)	6 (7%)	6 (7%)	1	14
9	J	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	5	33
10	K	31/33 (94%)	27 (87%)	1 (3%)	3 (10%)	0	7
11	L	116/118 (98%)	104 (90%)	8 (7%)	4 (3%)	3	26
12	M	685/687 (100%)	608 (89%)	54 (8%)	23 (3%)	3	26
13	N	141/143 (99%)	119 (84%)	15 (11%)	7 (5%)	1	18
14	O	210/212 (99%)	188 (90%)	15 (7%)	7 (3%)	3	26
15	P	206/208 (99%)	173 (84%)	22 (11%)	11 (5%)	1	18
16	Q	428/430 (100%)	397 (93%)	24 (6%)	7 (2%)	8	37
17	S	68/70 (97%)	61 (90%)	5 (7%)	2 (3%)	3	28
18	T	93/95 (98%)	87 (94%)	2 (2%)	4 (4%)	2	20
19	U	81/83 (98%)	76 (94%)	4 (5%)	1 (1%)	11	41
20	V	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	5	32
21	W	136/138 (99%)	127 (93%)	5 (4%)	4 (3%)	3	28
22	Y	57/59 (97%)	50 (88%)	1 (2%)	6 (10%)	0	6
23	Z	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
24	a	136/138 (99%)	121 (89%)	12 (9%)	3 (2%)	5	32
25	b	122/128 (95%)	107 (88%)	10 (8%)	5 (4%)	2	22
26	c	151/153 (99%)	129 (85%)	15 (10%)	7 (5%)	2	19
27	d	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	22	54
28	e	95/97 (98%)	83 (87%)	9 (10%)	3 (3%)	3	27
29	f	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	5	32
30	g	117/119 (98%)	105 (90%)	6 (5%)	6 (5%)	1	18
31	h	102/104 (98%)	86 (84%)	10 (10%)	6 (6%)	1	16
32	i	345/347 (99%)	324 (94%)	15 (4%)	6 (2%)	7	36
33	j	113/115 (98%)	103 (91%)	7 (6%)	3 (3%)	4	29
34	k	95/97 (98%)	88 (93%)	4 (4%)	3 (3%)	3	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	l	601/603 (100%)	551 (92%)	38 (6%)	12 (2%)	6	34
36	m	172/174 (99%)	150 (87%)	12 (7%)	10 (6%)	1	16
37	n	54/56 (96%)	50 (93%)	2 (4%)	2 (4%)	2	24
38	o	126/128 (98%)	113 (90%)	9 (7%)	4 (3%)	3	27
39	p	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	7	35
40	r	457/459 (100%)	420 (92%)	28 (6%)	9 (2%)	6	34
41	s	316/318 (99%)	286 (90%)	21 (7%)	9 (3%)	4	28
42	u	167/169 (99%)	152 (91%)	10 (6%)	5 (3%)	3	27
43	v	107/137 (78%)	90 (84%)	14 (13%)	3 (3%)	4	28
44	w	318/320 (99%)	281 (88%)	28 (9%)	9 (3%)	4	28
All	All	8097/8236 (98%)	7338 (91%)	526 (6%)	233 (3%)	6	28

All (233) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	TYR
1	A	73	PRO
1	A	379	CYS
2	B	62	THR
12	M	37	ASP
12	M	47	THR
12	M	178	GLN
12	M	210	ILE
12	M	369	GLU
13	N	115	PHE
14	O	232	THR
14	O	246	GLN
15	P	167	GLU
17	S	60	TYR
18	T	82	THR
19	U	71	GLN
21	W	34	SER
6	X	155	TYR
22	Y	84	PHE
24	a	58	ARG
26	c	115	ASN
26	c	178	PRO
27	d	2	PRO

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Mol	Chain	Res	Type
31	h	20	ILE
32	i	91	ASN
32	i	323	THR
33	j	24	LEU
33	j	26	GLN
34	k	52	HIS
35	l	450	LEU
36	m	115	VAL
36	m	116	VAL
36	m	118	PHE
37	n	55	VAL
40	r	52	CYS
40	r	346	GLN
44	w	57	SER
44	w	282	PRO
44	w	347	VAL
3	C	84	PHE
3	C	165	SER
4	E	20	ILE
4	E	127	ASP
6	G	138	LEU
7	H	105	GLU
8	I	31	ILE
8	I	93	LYS
8	I	107	SER
9	J	87	ASP
11	L	173	SER
12	M	250	SER
12	M	482	GLN
12	M	484	ASN
12	M	562	LYS
12	M	663	ASN
12	M	676	ASN
13	N	19	GLY
13	N	76	ASP
14	O	49	PRO
14	O	160	VAL
16	Q	104	GLU
16	Q	117	HIS
18	T	44	GLN
20	V	135	VAL
20	V	140	LYS

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Mol	Chain	Res	Type
21	W	11	PRO
22	Y	44	TYR
22	Y	51	THR
24	a	57	ILE
24	a	185	ALA
25	b	101	LYS
26	c	170	ARG
30	g	9	PRO
31	h	3	PHE
31	h	24	GLU
31	h	43	CYS
33	j	2	ASN
35	l	73	THR
35	l	512	LYS
36	m	122	GLY
37	n	52	SER
40	r	45	ILE
40	r	188	ASN
40	r	250	LEU
40	r	421	HIS
41	s	203	GLY
41	s	213	ILE
41	s	217	ALA
41	s	316	PRO
43	v	56	ARG
44	w	264	GLN
44	w	285	LYS
1	A	74	ASP
7	H	8	THR
7	H	63	PRO
8	I	52	ASN
9	J	135	GLU
9	J	178	SER
10	K	101	SER
11	L	165	SER
12	M	538	ARG
12	M	677	GLN
12	M	689	LEU
12	M	715	THR
13	N	113	HIS
14	O	238	PRO
15	P	44	ARG

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Mol	Chain	Res	Type
15	P	179	ALA
15	P	214	ASP
15	P	229	GLU
16	Q	36	GLN
16	Q	197	MET
18	T	83	ARG
6	X	140	CYS
22	Y	85	PRO
25	b	37	PRO
25	b	109	THR
26	c	164	ASN
28	e	61	PRO
28	e	111	ASP
30	g	10	LEU
30	g	12	PHE
30	g	50	ARG
32	i	87	THR
34	k	83	ASN
34	k	96	LEU
35	l	65	ASN
35	l	451	LEU
35	l	511	LEU
35	l	549	PRO
35	l	554	ASP
35	l	563	PRO
36	m	4	ALA
36	m	76	GLU
36	m	110	ASP
38	o	5	LYS
38	o	12	ARG
40	r	139	GLN
41	s	38	ASN
42	u	36	CYS
42	u	101	ARG
42	u	143	HIS
43	v	73	SER
44	w	351	TRP
1	A	50	ASP
1	A	186	ALA
3	C	156	GLY
7	H	76	GLN
8	I	108	SER

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Mol	Chain	Res	Type
9	J	100	LEU
9	J	330	PRO
9	J	370	LYS
10	K	78	ASP
11	L	172	VAL
12	M	377	ALA
12	M	426	ASP
13	N	42	ASP
13	N	130	THR
14	O	216	PRO
14	O	230	GLY
15	P	175	GLY
15	P	246	ARG
17	S	36	LYS
21	W	16	TYR
6	X	74	LEU
22	Y	42	PRO
22	Y	87	PRO
25	b	115	GLU
26	c	40	PRO
26	c	41	TYR
30	g	49	ARG
30	g	56	GLY
31	h	32	ARG
31	h	45	HIS
32	i	150	ASN
35	l	249	SER
35	l	387	THR
35	l	562	LEU
38	o	59	LEU
38	o	120	LYS
39	p	76	HIS
40	r	251	ASN
41	s	208	VAL
41	s	288	LEU
41	s	289	LEU
42	u	167	PHE
43	v	36	GLU
1	A	228	PRO
1	A	420	GLU
7	H	103	LEU
9	J	259	ASN

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Mol	Chain	Res	Type
12	M	281	ILE
12	M	548	LEU
12	M	667	GLN
15	P	110	SER
15	P	202	PHE
15	P	239	TRP
15	P	245	TYR
16	Q	102	SER
20	V	48	THR
6	X	153	ASP
26	c	171	GLY
32	i	92	GLN
36	m	113	VAL
39	p	175	ARG
42	u	144	SER
44	w	58	ARG
44	w	121	PRO
44	w	160	GLU
3	C	102	ASP
6	G	137	LYS
8	I	70	MET
11	L	96	LYS
12	M	446	GLY
13	N	135	GLN
18	T	90	GLY
25	b	41	GLY
29	f	39	PRO
36	m	24	SER
39	p	32	VAL
40	r	205	VAL
12	M	435	PRO
21	W	10	MET
41	s	241	ILE
1	A	94	PRO
12	M	575	VAL
36	m	23	PRO
3	C	144	PRO
16	Q	307	PRO
16	Q	69	VAL
10	K	102	GLY
32	i	338	PRO
28	e	135	PRO

### 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	A	346/346 (100%)	346 (100%)	0	100	100
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	106/106 (100%)	105 (99%)	1 (1%)	75	84
5	F	74/74 (100%)	74 (100%)	0	100	100
6	G	74/79 (94%)	74 (100%)	0	100	100
6	X	78/79 (99%)	78 (100%)	0	100	100
7	H	100/100 (100%)	100 (100%)	0	100	100
8	I	87/96 (91%)	87 (100%)	0	100	100
9	J	292/292 (100%)	288 (99%)	4 (1%)	62	76
10	K	32/32 (100%)	32 (100%)	0	100	100
11	L	107/107 (100%)	107 (100%)	0	100	100
12	M	576/577 (100%)	574 (100%)	2 (0%)	91	94
13	N	129/129 (100%)	129 (100%)	0	100	100
14	O	181/181 (100%)	181 (100%)	0	100	100
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	371/371 (100%)	369 (100%)	2 (0%)	86	92
17	S	59/59 (100%)	59 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	72/72 (100%)	72 (100%)	0	100	100
20	V	102/102 (100%)	102 (100%)	0	100	100
21	W	119/119 (100%)	119 (100%)	0	100	100
22	Y	57/57 (100%)	49 (86%)	8 (14%)	3	17
23	Z	62/63 (98%)	62 (100%)	0	100	100
24	a	124/124 (100%)	122 (98%)	2 (2%)	58	74
25	b	118/122 (97%)	114 (97%)	4 (3%)	32	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	c	124/137 (90%)	124 (100%)	0	100	100
27	d	145/154 (94%)	137 (94%)	8 (6%)	18	45
28	e	90/90 (100%)	90 (100%)	0	100	100
29	f	43/43 (100%)	43 (100%)	0	100	100
30	g	105/105 (100%)	105 (100%)	0	100	100
31	h	90/90 (100%)	90 (100%)	0	100	100
32	i	314/314 (100%)	314 (100%)	0	100	100
33	j	102/103 (99%)	102 (100%)	0	100	100
34	k	85/85 (100%)	82 (96%)	3 (4%)	31	56
35	l	531/532 (100%)	511 (96%)	20 (4%)	28	53
36	m	137/137 (100%)	137 (100%)	0	100	100
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	114/114 (100%)	114 (100%)	0	100	100
39	p	157/157 (100%)	156 (99%)	1 (1%)	84	90
40	r	416/416 (100%)	416 (100%)	0	100	100
41	s	278/278 (100%)	278 (100%)	0	100	100
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	89/121 (74%)	89 (100%)	0	100	100
44	w	249/288 (86%)	249 (100%)	0	100	100
All	All	7093/7209 (98%)	7038 (99%)	55 (1%)	77	85

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	31	ARG
9	J	85	ARG
9	J	91	ILE
9	J	180	TYR
9	J	212	ARG
12	M	130	ILE
12	M	174	THR
16	Q	268	TRP
16	Q	273	ILE
22	Y	73	PHE
22	Y	75	HIS

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Mol	Chain	Res	Type
22	Y	78	GLU
22	Y	80	VAL
22	Y	81	LEU
22	Y	83	HIS
22	Y	87	PRO
22	Y	97	LEU
24	a	53	ARG
24	a	55	PHE
25	b	21	ARG
25	b	38	GLN
25	b	111	LEU
25	b	112	GLU
27	d	54	ARG
27	d	55	TYR
27	d	57	TYR
27	d	60	ARG
27	d	61	GLN
27	d	113	GLN
27	d	115	TYR
27	d	117	GLN
34	k	1	MET
34	k	3	LEU
34	k	8	ILE
35	l	25	ASN
35	l	59	GLN
35	l	87	MET
35	l	88	MET
35	l	94	LEU
35	l	95	PHE
35	l	97	THR
35	l	99	SER
35	l	191	LEU
35	l	193	SER
35	l	195	SER
35	l	196	TRP
35	l	197	ASP
35	l	217	LEU
35	l	218	LEU
35	l	223	LYS
35	l	226	GLN
35	l	447	ASN
35	l	450	LEU

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Mol	Chain	Res	Type
35	l	452	ASN
39	p	124	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (142) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	116	ASN
1	A	164	ASN
1	A	170	GLN
1	A	284	HIS
1	A	313	ASN
1	A	441	HIS
2	B	184	ASN
3	C	95	HIS
4	E	48	HIS
4	E	49	GLN
4	E	51	GLN
4	E	70	ASN
5	F	62	GLN
5	F	81	ASN
6	G	80	GLN
7	H	50	GLN
7	H	73	GLN
7	H	76	GLN
7	H	83	GLN
7	H	111	GLN
8	I	73	GLN
9	J	71	ASN
9	J	102	GLN
9	J	183	ASN
10	K	77	HIS
11	L	71	HIS
11	L	86	ASN
12	M	384	ASN
12	M	425	ASN
12	M	444	HIS
12	M	460	HIS
12	M	464	GLN
12	M	498	GLN
12	M	514	ASN
12	M	688	GLN

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Mol	Chain	Res	Type
13	N	91	HIS
13	N	113	HIS
13	N	135	GLN
14	O	59	ASN
14	O	69	ASN
14	O	189	ASN
14	O	191	ASN
15	P	74	GLN
15	P	82	ASN
15	P	105	ASN
15	P	124	ASN
15	P	247	GLN
16	Q	38	GLN
16	Q	147	ASN
16	Q	182	ASN
16	Q	183	HIS
16	Q	190	HIS
16	Q	233	HIS
16	Q	234	GLN
16	Q	339	GLN
16	Q	431	HIS
16	Q	442	HIS
16	Q	454	GLN
17	S	44	HIS
17	S	68	ASN
18	T	64	ASN
21	W	8	GLN
21	W	61	GLN
21	W	112	HIS
21	W	135	HIS
22	Y	75	HIS
24	a	90	ASN
24	a	189	ASN
25	b	14	GLN
25	b	83	HIS
25	b	89	HIS
25	b	126	GLN
26	c	56	ASN
26	c	84	HIS
26	c	154	GLN
27	d	59	HIS
27	d	61	GLN

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Mol	Chain	Res	Type
27	d	85	GLN
27	d	113	GLN
27	d	117	GLN
27	d	138	GLN
30	g	60	GLN
30	g	96	HIS
32	i	83	GLN
32	i	112	HIS
32	i	150	ASN
32	i	186	HIS
32	i	222	ASN
33	j	10	ASN
34	k	7	ASN
34	k	94	ASN
35	l	4	HIS
35	l	59	GLN
35	l	139	GLN
35	l	192	HIS
35	l	199	GLN
35	l	205	ASN
35	l	226	GLN
35	l	248	HIS
35	l	274	GLN
35	l	296	ASN
35	l	320	ASN
35	l	332	HIS
35	l	348	HIS
35	l	394	HIS
35	l	400	ASN
35	l	442	ASN
35	l	446	ASN
35	l	534	HIS
35	l	569	HIS
35	l	580	GLN
36	m	45	ASN
36	m	117	ASN
37	n	40	ASN
38	o	62	ASN
38	o	126	HIS
39	p	75	GLN
40	r	48	ASN
40	r	168	HIS

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Mol	Chain	Res	Type
40	r	390	ASN
40	r	415	GLN
40	r	425	ASN
41	s	93	ASN
41	s	169	GLN
41	s	235	ASN
42	u	30	HIS
42	u	31	HIS
42	u	64	ASN
42	u	77	HIS
42	u	99	HIS
42	u	104	GLN
42	u	143	HIS
43	v	43	GLN
43	v	61	HIS
43	v	85	HIS
43	v	92	HIS
44	w	85	HIS
44	w	111	ASN
44	w	132	GLN
44	w	149	HIS
44	w	257	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](#)

30 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
47	PLX	r	502	-	51,51,51	0.64	0	55,59,59	0.67	1 (1%)
51	CDL	n	101	-	63,63,99	1.24	5 (7%)	69,75,111	1.07	4 (5%)
49	NDP	J	401	-	45,52,52	0.95	2 (4%)	53,80,80	1.32	4 (7%)
45	SF4	A	501	1	0,12,12	-	-	-		
45	SF4	B	301	2	0,12,12	-	-	-		
47	PLX	g	203	-	51,51,51	0.78	1 (1%)	55,59,59	0.58	1 (1%)
51	CDL	l	704	-	63,63,99	1.26	5 (7%)	69,75,111	1.01	4 (5%)
52	PEE	l	702	-	50,50,50	1.16	6 (12%)	53,55,55	0.99	2 (3%)
48	8Q1	p	201	-	31,34,34	1.67	5 (16%)	40,43,43	1.57	5 (12%)
51	CDL	i	401	-	63,63,99	1.21	5 (7%)	69,75,111	1.04	5 (7%)
47	PLX	g	201	-	51,51,51	0.82	1 (1%)	55,59,59	0.69	1 (1%)
45	SF4	M	801	12	0,12,12	-	-	-		
47	PLX	B	303	-	51,51,51	0.77	1 (1%)	55,59,59	0.68	1 (1%)
48	8Q1	E	201	-	31,34,34	1.64	6 (19%)	40,43,43	1.39	7 (17%)
45	SF4	M	802	12	0,12,12	-	-	-		
45	SF4	B	302	2	0,12,12	-	-	-		
47	PLX	U	101	-	51,51,51	0.74	1 (1%)	55,59,59	0.72	2 (3%)
45	SF4	C	301	3	0,12,12	-	-	-		
50	FES	O	301	14	0,4,4	-	-	-		
47	PLX	g	202	-	51,51,51	0.75	1 (1%)	55,59,59	0.61	1 (1%)
47	PLX	V	203	-	51,51,51	0.78	1 (1%)	55,59,59	0.59	1 (1%)
47	PLX	r	501	-	51,51,51	0.74	1 (1%)	55,59,59	0.65	1 (1%)
52	PEE	V	202	-	50,50,50	1.16	6 (12%)	53,55,55	0.91	2 (3%)
47	PLX	b	201	-	51,51,51	0.57	0	55,59,59	0.64	0
52	PEE	l	701	-	48,48,50	1.34	4 (8%)	51,53,55	0.96	2 (3%)
51	CDL	V	201	-	61,61,99	1.21	5 (8%)	64,71,111	0.94	3 (4%)
51	CDL	l	703	-	63,63,99	1.21	5 (7%)	69,75,111	1.07	4 (5%)
46	FMN	A	502	-	33,33,33	1.40	6 (18%)	48,50,50	1.34	8 (16%)
52	PEE	W	201	-	50,50,50	1.14	6 (12%)	53,55,55	0.97	2 (3%)
50	FES	M	803	-	0,4,4	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	PLX	r	502	-	-	36/55/55/55	-
51	CDL	n	101	-	-	33/74/74/110	-
49	NDP	J	401	-	-	15/30/77/77	0/5/5/5
45	SF4	A	501	1	-	-	0/6/5/5
45	SF4	B	301	2	-	-	0/6/5/5
47	PLX	g	203	-	-	24/55/55/55	-
51	CDL	l	704	-	-	44/74/74/110	-
52	PEE	l	702	-	-	27/54/54/54	-
48	8Q1	p	201	-	-	19/41/41/41	-
51	CDL	i	401	-	-	39/74/74/110	-
47	PLX	g	201	-	-	25/55/55/55	-
45	SF4	M	801	12	-	-	0/6/5/5
47	PLX	B	303	-	-	21/55/55/55	-
48	8Q1	E	201	-	-	18/41/41/41	-
45	SF4	M	802	12	-	-	0/6/5/5
45	SF4	B	302	2	-	-	0/6/5/5
47	PLX	U	101	-	-	22/55/55/55	-
45	SF4	C	301	3	-	-	0/6/5/5
50	FES	O	301	14	-	-	0/1/1/1
47	PLX	g	202	-	-	25/55/55/55	-
47	PLX	V	203	-	-	26/55/55/55	-
47	PLX	r	501	-	-	28/55/55/55	-
52	PEE	V	202	-	-	27/54/54/54	-
47	PLX	b	201	-	-	27/55/55/55	-
52	PEE	l	701	-	-	32/52/52/54	-
51	CDL	V	201	-	-	42/69/69/110	-
51	CDL	l	703	-	-	38/74/74/110	-
46	FMN	A	502	-	-	7/18/18/18	0/3/3/3
52	PEE	W	201	-	-	32/54/54/54	-
50	FES	M	803	-	-	-	0/1/1/1

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	p	201	8Q1	C34-N36	5.30	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	E	201	8Q1	C34-N36	5.24	1.45	1.33
48	p	201	8Q1	C39-N41	5.24	1.45	1.33
48	E	201	8Q1	C39-N41	4.93	1.44	1.33
46	A	502	FMN	C9A-C5A	4.42	1.48	1.41
51	l	704	CDL	OB8-CB7	4.36	1.46	1.33
51	n	101	CDL	OA6-CA5	4.31	1.46	1.34
51	l	703	CDL	OA6-CA5	4.28	1.46	1.34
51	V	201	CDL	OA6-CA5	4.26	1.46	1.34
51	l	703	CDL	OB8-CB7	4.24	1.45	1.33
51	V	201	CDL	OB8-CB7	4.18	1.45	1.33
52	l	701	PEE	C39-C38	4.17	1.55	1.31
51	l	704	CDL	OA8-CA7	4.15	1.45	1.33
51	l	704	CDL	OA6-CA5	4.14	1.46	1.34
52	l	701	PEE	O3-C30	4.12	1.45	1.33
52	l	701	PEE	C18-C19	4.11	1.55	1.31
51	n	101	CDL	OB8-CB7	4.10	1.45	1.33
51	i	401	CDL	OB8-CB7	4.05	1.45	1.33
51	i	401	CDL	OA6-CA5	4.01	1.45	1.34
51	n	101	CDL	OA8-CA7	3.92	1.44	1.33
51	l	703	CDL	OA8-CA7	3.82	1.44	1.33
52	l	702	PEE	C18-C19	3.78	1.53	1.31
52	V	202	PEE	C18-C19	3.75	1.53	1.31
51	i	401	CDL	OA8-CA7	3.74	1.44	1.33
52	W	201	PEE	C18-C19	3.74	1.53	1.31
52	V	202	PEE	C39-C38	3.71	1.53	1.31
52	l	702	PEE	C39-C38	3.70	1.53	1.31
52	W	201	PEE	C39-C38	3.67	1.53	1.31
51	l	704	CDL	OB6-CB5	3.31	1.43	1.34
52	l	701	PEE	O2-C10	3.31	1.43	1.34
51	n	101	CDL	OB6-CB5	3.29	1.43	1.34
51	l	703	CDL	OB6-CB5	3.23	1.43	1.34
51	V	201	CDL	OB6-CB5	3.13	1.43	1.34
49	J	401	NDP	C6N-C5N	3.11	1.38	1.33
51	i	401	CDL	OB6-CB5	3.10	1.43	1.34
46	A	502	FMN	C8-C7	3.07	1.48	1.40
46	A	502	FMN	C4-N3	-3.04	1.33	1.38
51	V	201	CDL	OA8-CA7	3.00	1.44	1.33
47	B	303	PLX	O6-C4	-2.97	1.40	1.44
47	g	203	PLX	O6-C4	-2.92	1.40	1.44
47	V	203	PLX	O6-C4	-2.82	1.40	1.44
47	g	201	PLX	O6-C4	-2.79	1.40	1.44
51	n	101	CDL	OB6-CB4	-2.75	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	V	201	CDL	OB6-CB4	-2.62	1.40	1.46
47	U	101	PLX	O6-C4	-2.54	1.41	1.44
51	i	401	CDL	OB6-CB4	-2.51	1.40	1.46
47	g	202	PLX	O6-C4	-2.48	1.41	1.44
48	E	201	8Q1	O35-C34	-2.48	1.18	1.23
48	p	201	8Q1	O35-C34	-2.46	1.18	1.23
52	V	202	PEE	O2-C10	2.41	1.41	1.34
52	l	702	PEE	O2-C10	2.39	1.41	1.34
47	r	501	PLX	O6-C4	-2.37	1.41	1.44
51	l	704	CDL	OB6-CB4	-2.36	1.40	1.46
51	l	703	CDL	OB6-CB4	-2.34	1.40	1.46
48	E	201	8Q1	C1-S44	2.34	1.81	1.76
48	E	201	8Q1	O40-C39	-2.34	1.18	1.23
48	p	201	8Q1	O40-C39	-2.34	1.18	1.23
52	l	702	PEE	O3-C30	2.33	1.40	1.33
46	A	502	FMN	C5A-N5	-2.26	1.35	1.39
52	l	702	PEE	O2-C2	-2.25	1.41	1.46
48	p	201	8Q1	C1-S44	2.25	1.81	1.76
52	V	202	PEE	O2-C2	-2.25	1.41	1.46
52	W	201	PEE	O3-C30	2.24	1.39	1.33
52	V	202	PEE	O3-C30	2.24	1.39	1.33
52	W	201	PEE	O2-C10	2.22	1.40	1.34
52	V	202	PEE	O3-C3	-2.22	1.40	1.45
48	E	201	8Q1	C6-C1	2.22	1.53	1.50
52	W	201	PEE	O2-C2	-2.19	1.41	1.46
52	l	702	PEE	O3-C3	-2.18	1.40	1.45
52	W	201	PEE	O3-C3	-2.15	1.40	1.45
46	A	502	FMN	C4A-N5	2.14	1.34	1.30
46	A	502	FMN	C2-N3	-2.03	1.34	1.39
49	J	401	NDP	C5A-C4A	2.03	1.46	1.40

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	p	201	8Q1	C6-C1-S44	6.03	120.47	113.46
49	J	401	NDP	PN-O3-PA	-5.21	114.94	132.83
48	E	201	8Q1	C6-C1-S44	4.56	118.77	113.46
52	l	702	PEE	O2-C10-C11	4.38	120.95	111.50
51	l	703	CDL	OA6-CA5-C11	4.16	120.48	111.50
51	i	401	CDL	OA6-CA5-C11	4.13	120.39	111.50
51	l	704	CDL	OA6-CA5-C11	4.11	120.36	111.50
51	V	201	CDL	OB6-CB5-C51	4.09	120.32	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	n	101	CDL	OB6-CB5-C51	4.08	120.29	111.50
52	l	701	PEE	O2-C10-C11	4.01	120.14	111.50
51	l	703	CDL	OB6-CB5-C51	3.94	120.00	111.50
51	l	704	CDL	OB6-CB5-C51	3.92	119.96	111.50
51	n	101	CDL	OA6-CA5-C11	3.92	119.94	111.50
49	J	401	NDP	N3A-C2A-N1A	-3.76	122.81	128.68
52	W	201	PEE	O2-C10-C11	3.69	119.45	111.50
48	p	201	8Q1	O4-C1-C6	-3.63	119.70	123.99
52	V	202	PEE	O2-C10-C11	3.59	119.25	111.50
51	i	401	CDL	OB6-CB5-C51	3.51	119.06	111.50
51	V	201	CDL	OA6-CA5-C11	3.44	118.92	111.50
51	l	703	CDL	OA8-CA7-C31	2.99	121.28	111.91
52	V	202	PEE	O3-C30-C31	2.85	120.86	111.91
52	l	702	PEE	O3-C30-C31	2.85	120.84	111.91
46	A	502	FMN	C4-C4A-N5	2.82	122.25	118.23
48	E	201	8Q1	C43-S44-C1	2.79	110.56	101.87
46	A	502	FMN	C4A-C10-N1	-2.76	118.33	124.73
51	i	401	CDL	OB8-CB7-C71	2.75	120.55	111.91
51	n	101	CDL	OA8-CA7-C31	2.74	120.49	111.91
48	E	201	8Q1	C32-C34-N36	2.73	122.01	116.58
51	l	704	CDL	OA8-CA7-C31	2.72	120.45	111.91
48	p	201	8Q1	C43-S44-C1	2.71	110.31	101.87
52	W	201	PEE	O3-C30-C31	2.70	120.38	111.91
51	n	101	CDL	OB8-CB7-C71	2.69	120.36	111.91
51	l	703	CDL	OB8-CB7-C71	2.68	120.32	111.91
51	l	704	CDL	OB8-CB7-C71	2.67	120.28	111.91
48	p	201	8Q1	C38-C39-N41	2.55	120.71	116.42
48	E	201	8Q1	O4-C1-C6	-2.53	121.00	123.99
51	V	201	CDL	OB8-CB7-C71	2.53	119.86	111.91
48	E	201	8Q1	C42-N41-C39	-2.43	118.33	122.84
49	J	401	NDP	C4A-C5A-N7A	-2.42	106.87	109.40
46	A	502	FMN	C4A-C10-N10	2.42	120.02	116.48
51	i	401	CDL	OA8-CA7-C31	2.41	119.47	111.91
48	E	201	8Q1	C37-N36-C34	-2.39	118.33	122.59
47	B	303	PLX	C1C-N1-C1	2.36	119.59	109.92
47	V	203	PLX	C1C-N1-C1	2.32	119.40	109.92
46	A	502	FMN	O2-C2-N1	-2.31	118.00	121.83
47	U	101	PLX	C1C-N1-C1	2.29	119.30	109.92
52	l	701	PEE	O3-C30-C31	2.29	119.10	111.91
47	g	203	PLX	C1C-N1-C1	2.27	119.21	109.92
46	A	502	FMN	C4-N3-C2	-2.22	121.54	125.64
49	J	401	NDP	C3D-C2D-C1D	2.21	105.62	101.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	g	201	PLX	C1C-N1-C1	2.20	118.93	109.92
47	g	202	PLX	C1C-N1-C1	2.19	118.90	109.92
46	A	502	FMN	C4A-C4-N3	2.15	118.66	113.19
48	p	201	8Q1	O4-C1-S44	-2.15	119.83	122.61
46	A	502	FMN	C10-N1-C2	2.14	121.18	116.90
48	E	201	8Q1	O35-C34-N36	-2.12	118.45	122.99
46	A	502	FMN	N3-C2-N1	2.10	123.51	119.38
47	r	502	PLX	C2-C1-N1	-2.09	108.79	115.78
47	U	101	PLX	C5-C4-C3	-2.08	106.87	111.79
47	r	501	PLX	C1C-N1-C1	2.06	118.35	109.92
51	i	401	CDL	OA6-CA5-OA7	-2.01	118.86	123.70

There are no chirality outliers.

All (607) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	C1'-C2'-C3'-O3'
46	A	502	FMN	C1'-C2'-C3'-C4'
46	A	502	FMN	C3'-C4'-C5'-O5'
46	A	502	FMN	O4'-C4'-C5'-O5'
47	B	303	PLX	C2-O1-P1-O2
47	B	303	PLX	N1-C1-C2-O1
47	U	101	PLX	O7-C6-C7-C8
47	U	101	PLX	O7-C6-O6-C4
47	U	101	PLX	C3-O4-P1-O2
47	U	101	PLX	N1-C1-C2-O1
47	U	101	PLX	O9-C24-C25-C26
47	V	203	PLX	O7-C6-C7-C8
47	V	203	PLX	N1-C1-C2-O1
47	V	203	PLX	O9-C24-C25-C26
47	b	201	PLX	O7-C6-O6-C4
47	b	201	PLX	N1-C1-C2-O1
47	b	201	PLX	O9-C24-O8-C5
47	g	201	PLX	O7-C6-C7-C8
47	g	201	PLX	O7-C6-O6-C4
47	g	201	PLX	C3-C4-O6-C6
47	g	202	PLX	C2-O1-P1-O4
47	g	202	PLX	C2-O1-P1-O2
47	g	202	PLX	C2-O1-P1-O3
47	g	202	PLX	O9-C24-O8-C5
47	g	203	PLX	O7-C6-O6-C4
47	g	203	PLX	C2-O1-P1-O2

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Mol	Chain	Res	Type	Atoms
47	g	203	PLX	C25-C24-O8-C5
47	r	501	PLX	C3-O4-P1-O1
47	r	501	PLX	C3-O4-P1-O2
47	r	501	PLX	C3-O4-P1-O3
47	r	501	PLX	O8-C24-C25-C26
47	r	502	PLX	C7-C6-O6-C4
47	r	502	PLX	C3-O4-P1-O1
47	r	502	PLX	C3-O4-P1-O2
47	r	502	PLX	C3-O4-P1-O3
47	r	502	PLX	C2-O1-P1-O2
47	r	502	PLX	N1-C1-C2-O1
47	r	502	PLX	O9-C24-C25-C26
48	E	201	8Q1	C1-C6-C7-C8
48	E	201	8Q1	O4-C1-S44-C43
48	E	201	8Q1	C6-C1-S44-C43
48	E	201	8Q1	C29-C32-C34-N36
48	E	201	8Q1	C29-C32-C34-O35
48	E	201	8Q1	C42-C43-S44-C1
48	E	201	8Q1	C28-O27-P24-O3
48	E	201	8Q1	C28-O27-P24-O2
48	E	201	8Q1	C28-O27-P24-O1
48	p	201	8Q1	C1-C6-C7-C8
48	p	201	8Q1	O4-C1-S44-C43
48	p	201	8Q1	C6-C1-S44-C43
48	p	201	8Q1	C28-C29-C32-C34
48	p	201	8Q1	C28-C29-C32-O33
48	p	201	8Q1	C30-C29-C32-C34
48	p	201	8Q1	C31-C29-C32-C34
48	p	201	8Q1	C31-C29-C32-O33
48	p	201	8Q1	C28-O27-P24-O2
48	p	201	8Q1	C28-O27-P24-O1
49	J	401	NDP	C5B-O5B-PA-O1A
49	J	401	NDP	C5D-O5D-PN-O1N
51	V	201	CDL	CB2-C1-CA2-OA2
51	V	201	CDL	CA2-OA2-PA1-OA3
51	V	201	CDL	CA2-OA2-PA1-OA4
51	V	201	CDL	CA2-OA2-PA1-OA5
51	V	201	CDL	CA3-OA5-PA1-OA3
51	V	201	CDL	CA3-OA5-PA1-OA4
51	V	201	CDL	OA9-CA7-OA8-CA6
51	V	201	CDL	C51-CB5-OB6-CB4
51	i	401	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
51	i	401	CDL	CB2-C1-CA2-OA2
51	i	401	CDL	CA2-OA2-PA1-OA3
51	i	401	CDL	CA2-OA2-PA1-OA4
51	i	401	CDL	CA2-OA2-PA1-OA5
51	i	401	CDL	CA3-OA5-PA1-OA3
51	i	401	CDL	CA3-OA5-PA1-OA4
51	i	401	CDL	OA6-CA4-CA6-OA8
51	i	401	CDL	CB2-OB2-PB2-OB4
51	i	401	CDL	CB3-OB5-PB2-OB3
51	i	401	CDL	CB3-OB5-PB2-OB4
51	l	703	CDL	CA2-OA2-PA1-OA3
51	l	703	CDL	OB7-CB5-OB6-CB4
51	l	704	CDL	CA2-OA2-PA1-OA3
51	l	704	CDL	CA2-OA2-PA1-OA4
51	l	704	CDL	CA3-OA5-PA1-OA2
51	l	704	CDL	CA3-OA5-PA1-OA4
51	l	704	CDL	C11-CA5-OA6-CA4
51	l	704	CDL	CB2-OB2-PB2-OB3
51	n	101	CDL	CA2-OA2-PA1-OA3
51	n	101	CDL	CA2-OA2-PA1-OA4
51	n	101	CDL	CA2-OA2-PA1-OA5
51	n	101	CDL	OA7-CA5-OA6-CA4
51	n	101	CDL	C11-CA5-OA6-CA4
51	n	101	CDL	CB2-OB2-PB2-OB3
51	n	101	CDL	CB2-OB2-PB2-OB4
51	n	101	CDL	C51-CB5-OB6-CB4
52	V	202	PEE	C2-C1-O3P-P
52	V	202	PEE	O4P-C4-C5-N
52	W	201	PEE	C4-O4P-P-O3P
52	W	201	PEE	C4-O4P-P-O1P
52	l	701	PEE	C11-C10-O2-C2
52	l	701	PEE	C4-O4P-P-O2P
52	l	701	PEE	C4-O4P-P-O1P
51	l	704	CDL	OA9-CA7-OA8-CA6
51	l	704	CDL	OB9-CB7-OB8-CB6
51	n	101	CDL	OA9-CA7-OA8-CA6
51	V	201	CDL	OB7-CB5-OB6-CB4
51	l	704	CDL	OA7-CA5-OA6-CA4
51	n	101	CDL	OB7-CB5-OB6-CB4
52	l	701	PEE	O4-C10-O2-C2
51	l	704	CDL	C31-CA7-OA8-CA6
51	l	704	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
51	n	101	CDL	C31-CA7-OA8-CA6
51	n	101	CDL	C71-CB7-OB8-CB6
51	l	703	CDL	C51-CB5-OB6-CB4
48	E	201	8Q1	C38-C39-N41-C42
52	W	201	PEE	C17-C18-C19-C20
52	l	701	PEE	C37-C38-C39-C40
52	l	702	PEE	C37-C38-C39-C40
51	n	101	CDL	OB9-CB7-OB8-CB6
52	l	702	PEE	O5-C30-O3-C3
51	l	703	CDL	O1-C1-CA2-OA2
51	l	704	CDL	O1-C1-CA2-OA2
51	i	401	CDL	C11-CA5-OA6-CA4
52	W	201	PEE	C21-C22-C23-C24
52	V	202	PEE	C20-C21-C22-C23
47	r	502	PLX	C16-C17-C18-C19
52	l	701	PEE	C32-C33-C34-C35
49	J	401	NDP	O4B-C4B-C5B-O5B
49	J	401	NDP	C3B-C4B-C5B-O5B
52	l	702	PEE	C31-C30-O3-C3
47	g	203	PLX	C26-C27-C28-C29
47	r	501	PLX	C10-C11-C12-C13
47	b	201	PLX	C4-C3-O4-P1
47	b	201	PLX	C14-C15-C16-C17
47	g	203	PLX	C30-C31-C32-C33
47	r	502	PLX	C30-C31-C32-C33
52	W	201	PEE	C32-C33-C34-C35
49	J	401	NDP	C1B-C2B-O2B-P2B
47	g	202	PLX	C10-C11-C12-C13
48	E	201	8Q1	O40-C39-N41-C42
51	l	703	CDL	CB2-C1-CA2-OA2
47	r	502	PLX	C12-C13-C14-C15
51	i	401	CDL	C31-C32-C33-C34
52	W	201	PEE	C31-C30-O3-C3
51	l	703	CDL	C73-C74-C75-C76
51	l	703	CDL	OB5-CB3-CB4-OB6
52	W	201	PEE	C12-C13-C14-C15
52	l	701	PEE	C34-C35-C36-C37
51	V	201	CDL	O1-C1-CA2-OA2
51	l	703	CDL	O1-C1-CB2-OB2
47	r	501	PLX	C12-C13-C14-C15
52	W	201	PEE	O5-C30-O3-C3
51	V	201	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
51	i	401	CDL	OA7-CA5-OA6-CA4
47	V	203	PLX	C13-C14-C15-C16
51	l	704	CDL	CB5-C51-C52-C53
51	n	101	CDL	CA7-C31-C32-C33
52	l	702	PEE	C10-C11-C12-C13
52	l	702	PEE	C17-C18-C19-C20
52	W	201	PEE	C15-C16-C17-C18
51	i	401	CDL	CA5-C11-C12-C13
52	V	202	PEE	C10-C11-C12-C13
52	l	701	PEE	C30-C31-C32-C33
47	r	501	PLX	C27-C28-C29-C30
51	n	101	CDL	C31-C32-C33-C34
51	i	401	CDL	C31-CA7-OA8-CA6
49	J	401	NDP	C3B-C2B-O2B-P2B
52	l	701	PEE	C39-C40-C41-C42
52	V	202	PEE	C17-C18-C19-C20
52	l	701	PEE	C17-C18-C19-C20
47	B	303	PLX	C2-O1-P1-O4
47	U	101	PLX	C3-O4-P1-O1
47	b	201	PLX	C3-O4-P1-O1
47	g	201	PLX	C3-O4-P1-O1
47	g	202	PLX	C3-O4-P1-O1
47	g	203	PLX	C2-O1-P1-O4
47	r	502	PLX	C2-O1-P1-O4
51	V	201	CDL	CA3-OA5-PA1-OA2
51	V	201	CDL	CB3-OB5-PB2-OB2
51	i	401	CDL	CA3-OA5-PA1-OA2
51	i	401	CDL	CB2-OB2-PB2-OB5
51	i	401	CDL	CB3-OB5-PB2-OB2
51	l	703	CDL	CB3-OB5-PB2-OB2
51	l	704	CDL	CA2-OA2-PA1-OA5
51	n	101	CDL	CB2-OB2-PB2-OB5
52	V	202	PEE	C1-O3P-P-O4P
52	W	201	PEE	C1-O3P-P-O4P
52	l	701	PEE	C4-O4P-P-O3P
52	V	202	PEE	C31-C30-O3-C3
51	l	703	CDL	CA2-C1-CB2-OB2
51	l	703	CDL	C71-CB7-OB8-CB6
47	B	303	PLX	O6-C6-C7-C8
47	U	101	PLX	O6-C6-C7-C8
47	g	203	PLX	O8-C24-C25-C26
47	g	201	PLX	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
51	l	704	CDL	C51-CB5-OB6-CB4
47	B	303	PLX	C27-C28-C29-C30
47	g	201	PLX	C7-C8-C9-C10
47	g	202	PLX	C7-C8-C9-C10
47	g	203	PLX	C29-C30-C31-C32
51	l	704	CDL	C31-C32-C33-C34
51	n	101	CDL	C12-C13-C14-C15
51	n	101	CDL	C13-C14-C15-C16
52	W	201	PEE	C14-C15-C16-C17
52	l	701	PEE	C22-C23-C24-C25
47	g	203	PLX	C34-C35-C36-C37
52	l	702	PEE	C20-C21-C22-C23
51	l	704	CDL	OB7-CB5-OB6-CB4
51	n	101	CDL	CB5-C51-C52-C53
48	p	201	8Q1	C11-C12-C13-C14
51	V	201	CDL	C71-C72-C73-C74
52	l	701	PEE	C21-C22-C23-C24
47	r	501	PLX	C13-C14-C15-C16
47	r	502	PLX	C14-C15-C16-C17
52	V	202	PEE	C12-C13-C14-C15
52	l	702	PEE	C33-C34-C35-C36
51	l	703	CDL	CB7-C71-C72-C73
51	l	704	CDL	CB7-C71-C72-C73
47	U	101	PLX	C33-C34-C35-C36
51	l	704	CDL	C51-C52-C53-C54
52	V	202	PEE	C40-C41-C42-C43
47	U	101	PLX	C10-C11-C12-C13
47	U	101	PLX	C35-C36-C37-C38
47	b	201	PLX	C16-C17-C18-C19
47	b	201	PLX	C29-C30-C31-C32
47	g	203	PLX	C15-C16-C17-C18
47	r	502	PLX	C11-C12-C13-C14
47	r	502	PLX	C10-C11-C12-C13
48	p	201	8Q1	C6-C7-C8-C9
47	U	101	PLX	C19-C20-C21-C22
47	U	101	PLX	C12-C13-C14-C15
47	U	101	PLX	C9-C10-C11-C12
47	V	203	PLX	C10-C11-C12-C13
47	b	201	PLX	C27-C28-C29-C30
47	g	202	PLX	C14-C15-C16-C17
48	E	201	8Q1	C12-C13-C14-C15
51	i	401	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
52	l	702	PEE	C40-C41-C42-C43
47	B	303	PLX	C9-C10-C11-C12
47	B	303	PLX	C28-C29-C30-C31
47	r	502	PLX	C9-C10-C11-C12
51	l	704	CDL	C32-C33-C34-C35
47	b	201	PLX	C18-C19-C20-C21
47	g	201	PLX	C16-C17-C18-C19
52	V	202	PEE	C14-C15-C16-C17
52	l	702	PEE	C34-C35-C36-C37
51	l	704	CDL	CA7-C31-C32-C33
47	U	101	PLX	C7-C8-C9-C10
47	V	203	PLX	C25-C26-C27-C28
47	g	201	PLX	C10-C11-C12-C13
51	l	703	CDL	C51-C52-C53-C54
52	l	702	PEE	C21-C22-C23-C24
47	b	201	PLX	C25-C26-C27-C28
51	l	703	CDL	C11-C12-C13-C14
47	V	203	PLX	C32-C33-C34-C35
47	g	202	PLX	C9-C10-C11-C12
51	n	101	CDL	C51-C52-C53-C54
51	n	101	CDL	CB7-C71-C72-C73
52	l	701	PEE	C20-C21-C22-C23
47	r	502	PLX	C32-C33-C34-C35
48	E	201	8Q1	N41-C42-C43-S44
47	g	203	PLX	C10-C11-C12-C13
52	V	202	PEE	C34-C35-C36-C37
52	V	202	PEE	O5-C30-O3-C3
47	B	303	PLX	C12-C13-C14-C15
47	g	203	PLX	C17-C18-C19-C20
47	r	502	PLX	C26-C27-C28-C29
52	W	201	PEE	C37-C38-C39-C40
47	g	203	PLX	C7-C8-C9-C10
47	r	502	PLX	C25-C26-C27-C28
51	i	401	CDL	C34-C35-C36-C37
51	i	401	CDL	OA9-CA7-OA8-CA6
47	g	202	PLX	C11-C12-C13-C14
48	p	201	8Q1	C7-C8-C9-C10
47	B	303	PLX	O7-C6-C7-C8
47	g	203	PLX	O9-C24-C25-C26
47	r	501	PLX	O9-C24-C25-C26
47	r	502	PLX	O7-C6-C7-C8
47	g	203	PLX	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
47	r	501	PLX	C7-C8-C9-C10
51	i	401	CDL	C11-C12-C13-C14
51	l	703	CDL	C33-C34-C35-C36
46	A	502	FMN	O2'-C2'-C3'-O3'
47	r	501	PLX	C35-C36-C37-C38
51	i	401	CDL	C32-C33-C34-C35
52	V	202	PEE	C43-C44-C45-C46
51	l	703	CDL	OB9-CB7-OB8-CB6
52	l	701	PEE	C13-C14-C15-C16
52	l	701	PEE	C41-C42-C43-C44
51	V	201	CDL	OA7-CA5-OA6-CA4
46	A	502	FMN	O2'-C2'-C3'-C4'
47	V	203	PLX	C11-C12-C13-C14
48	p	201	8Q1	C12-C13-C14-C15
52	W	201	PEE	C23-C24-C25-C26
51	l	703	CDL	C31-CA7-OA8-CA6
51	V	201	CDL	C11-CA5-OA6-CA4
47	g	201	PLX	C32-C33-C34-C35
47	r	501	PLX	C26-C27-C28-C29
51	V	201	CDL	CB5-C51-C52-C53
51	i	401	CDL	CB5-C51-C52-C53
51	n	101	CDL	C55-C56-C57-C58
52	W	201	PEE	C41-C42-C43-C44
52	l	701	PEE	C15-C16-C17-C18
52	l	702	PEE	C19-C20-C21-C22
47	r	502	PLX	C7-C8-C9-C10
47	r	502	PLX	C36-C37-C38-C39
51	i	401	CDL	C73-C74-C75-C76
52	V	202	PEE	C31-C32-C33-C34
47	r	502	PLX	C20-C21-C22-C23
51	n	101	CDL	C71-C72-C73-C74
52	l	702	PEE	C31-C32-C33-C34
51	i	401	CDL	C71-CB7-OB8-CB6
47	b	201	PLX	C30-C31-C32-C33
47	g	202	PLX	C26-C27-C28-C29
52	W	201	PEE	C43-C44-C45-C46
51	i	401	CDL	C51-CB5-OB6-CB4
47	r	502	PLX	C35-C36-C37-C38
51	V	201	CDL	C14-C15-C16-C17
47	B	303	PLX	C29-C30-C31-C32
47	b	201	PLX	C32-C33-C34-C35
47	r	501	PLX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
52	V	202	PEE	C19-C20-C21-C22
52	W	201	PEE	C19-C20-C21-C22
47	g	203	PLX	C35-C36-C37-C38
47	b	201	PLX	C11-C12-C13-C14
47	g	202	PLX	C11-C10-C9-C8
51	l	704	CDL	C13-C14-C15-C16
51	l	703	CDL	OA9-CA7-OA8-CA6
47	r	502	PLX	C17-C18-C19-C20
52	l	701	PEE	C23-C24-C25-C26
52	l	701	PEE	C40-C41-C42-C43
52	l	701	PEE	C16-C17-C18-C19
47	g	201	PLX	C2-O1-P1-O4
51	l	703	CDL	CA2-OA2-PA1-OA5
47	B	303	PLX	C15-C16-C17-C18
51	n	101	CDL	C34-C35-C36-C37
51	l	704	CDL	OB5-CB3-CB4-CB6
52	l	701	PEE	O3P-C1-C2-C3
47	r	502	PLX	C15-C16-C17-C18
52	l	702	PEE	C42-C43-C44-C45
47	B	303	PLX	C11-C10-C9-C8
51	l	704	CDL	CB2-C1-CA2-OA2
51	i	401	CDL	OB7-CB5-OB6-CB4
51	V	201	CDL	C12-C13-C14-C15
51	n	101	CDL	C33-C34-C35-C36
52	W	201	PEE	C33-C34-C35-C36
47	r	501	PLX	C3-C4-C5-O8
51	l	703	CDL	CA3-CA4-CA6-OA8
52	V	202	PEE	C41-C42-C43-C44
47	r	501	PLX	C18-C19-C20-C21
52	W	201	PEE	C44-C45-C46-C47
47	g	201	PLX	C26-C27-C28-C29
47	U	101	PLX	O8-C24-C25-C26
52	l	702	PEE	C12-C13-C14-C15
51	i	401	CDL	OB9-CB7-OB8-CB6
48	p	201	8Q1	C13-C14-C15-C16
47	b	201	PLX	C20-C21-C22-C23
47	V	203	PLX	C7-C8-C9-C10
52	l	701	PEE	C42-C43-C44-C45
52	l	702	PEE	C44-C45-C46-C47
52	l	701	PEE	C2-C1-O3P-P
51	V	201	CDL	OA5-CA3-CA4-OA6
47	U	101	PLX	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
52	W	201	PEE	O2-C2-C3-O3
51	l	703	CDL	C75-C76-C77-C78
48	p	201	8Q1	C30-C29-C32-O33
51	i	401	CDL	C52-C51-CB5-OB6
47	V	203	PLX	C16-C17-C18-C19
51	i	401	CDL	C35-C36-C37-C38
51	V	201	CDL	C72-C73-C74-C75
52	W	201	PEE	C34-C35-C36-C37
47	U	101	PLX	C11-C10-C9-C8
47	V	203	PLX	C12-C13-C14-C15
47	g	201	PLX	C17-C18-C19-C20
47	g	201	PLX	C27-C28-C29-C30
51	l	703	CDL	OB5-CB3-CB4-CB6
52	W	201	PEE	O3P-C1-C2-C3
47	V	203	PLX	C31-C32-C33-C34
47	r	501	PLX	C25-C26-C27-C28
51	V	201	CDL	C52-C53-C54-C55
47	B	303	PLX	C30-C31-C32-C33
47	U	101	PLX	C28-C29-C30-C31
47	b	201	PLX	C13-C14-C15-C16
52	l	702	PEE	C11-C10-O2-C2
47	b	201	PLX	C11-C10-C9-C8
47	U	101	PLX	C27-C28-C29-C30
47	b	201	PLX	C36-C37-C38-C39
47	g	201	PLX	C3-C4-C5-O8
51	V	201	CDL	CB3-CB4-CB6-OB8
51	i	401	CDL	CA3-CA4-CA6-OA8
52	W	201	PEE	C1-C2-C3-O3
47	r	502	PLX	C27-C28-C29-C30
48	p	201	8Q1	C10-C11-C12-C13
48	E	201	8Q1	C7-C8-C9-C10
47	r	501	PLX	C28-C29-C30-C31
52	W	201	PEE	C13-C14-C15-C16
51	V	201	CDL	C53-C54-C55-C56
47	b	201	PLX	C5-C4-O6-C6
47	g	202	PLX	C5-C4-O6-C6
47	r	501	PLX	O7-C6-C7-C8
47	b	201	PLX	C35-C36-C37-C38
51	l	704	CDL	OA5-CA3-CA4-OA6
47	V	203	PLX	C26-C27-C28-C29
51	l	703	CDL	OA6-CA4-CA6-OA8
51	V	201	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
47	g	201	PLX	C20-C21-C22-C23
47	g	203	PLX	C4-C3-O4-P1
47	r	501	PLX	C4-C3-O4-P1
51	l	704	CDL	C73-C74-C75-C76
47	r	501	PLX	C19-C20-C21-C22
51	l	703	CDL	C15-C16-C17-C18
51	n	101	CDL	CA5-C11-C12-C13
52	W	201	PEE	O4-C10-O2-C2
52	W	201	PEE	C11-C10-O2-C2
47	B	303	PLX	C11-C12-C13-C14
52	l	702	PEE	O4-C10-O2-C2
47	B	303	PLX	C32-C33-C34-C35
52	l	701	PEE	C31-C32-C33-C34
51	V	201	CDL	C75-C76-C77-C78
47	r	501	PLX	C30-C31-C32-C33
47	g	202	PLX	C30-C31-C32-C33
47	g	202	PLX	O4-C3-C4-O6
51	V	201	CDL	OB5-CB3-CB4-OB6
51	l	703	CDL	OA5-CA3-CA4-OA6
52	V	202	PEE	C33-C34-C35-C36
52	V	202	PEE	C32-C33-C34-C35
47	b	201	PLX	O6-C4-C5-O8
47	r	501	PLX	O6-C4-C5-O8
51	V	201	CDL	OA6-CA4-CA6-OA8
51	V	201	CDL	OB6-CB4-CB6-OB8
48	E	201	8Q1	C6-C7-C8-C9
49	J	401	NDP	C5B-O5B-PA-O3
49	J	401	NDP	C5D-O5D-PN-O3
51	l	704	CDL	C12-C13-C14-C15
47	r	502	PLX	C24-C25-C26-C27
47	r	502	PLX	C34-C35-C36-C37
47	g	201	PLX	C35-C36-C37-C38
52	l	701	PEE	C24-C25-C26-C27
52	l	702	PEE	C11-C12-C13-C14
51	n	101	CDL	C35-C36-C37-C38
51	n	101	CDL	C11-C12-C13-C14
51	l	704	CDL	CB2-OB2-PB2-OB5
47	r	501	PLX	C31-C32-C33-C34
52	W	201	PEE	C31-C32-C33-C34
47	r	502	PLX	C4-C3-O4-P1
51	l	704	CDL	CA4-CA3-OA5-PA1
47	b	201	PLX	C3-O4-P1-O2

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Mol	Chain	Res	Type	Atoms
47	g	201	PLX	C3-O4-P1-O3
47	g	202	PLX	C3-O4-P1-O2
47	g	202	PLX	C3-O4-P1-O3
47	r	502	PLX	C2-O1-P1-O3
49	J	401	NDP	C5B-O5B-PA-O2A
49	J	401	NDP	C5D-O5D-PN-O2N
51	V	201	CDL	CB3-OB5-PB2-OB4
51	i	401	CDL	CB2-OB2-PB2-OB3
51	l	703	CDL	CA2-OA2-PA1-OA4
51	l	703	CDL	CB3-OB5-PB2-OB4
51	l	704	CDL	CA3-OA5-PA1-OA3
51	n	101	CDL	CA3-OA5-PA1-OA3
52	V	202	PEE	C1-O3P-P-O1P
47	g	202	PLX	O4-C3-C4-C5
51	V	201	CDL	OA5-CA3-CA4-CA6
51	V	201	CDL	OB5-CB3-CB4-CB6
51	l	703	CDL	OA5-CA3-CA4-CA6
51	l	704	CDL	OA5-CA3-CA4-CA6
47	r	501	PLX	C15-C16-C17-C18
47	U	101	PLX	C25-C24-O8-C5
47	b	201	PLX	C1-C2-O1-P1
47	g	203	PLX	C1-C2-O1-P1
47	r	501	PLX	C25-C24-O8-C5
52	W	201	PEE	C10-C11-C12-C13
47	V	203	PLX	C19-C20-C21-C22
47	g	203	PLX	C19-C20-C21-C22
51	V	201	CDL	C74-C75-C76-C77
51	l	704	CDL	OB5-CB3-CB4-OB6
52	l	701	PEE	O3P-C1-C2-O2
47	V	203	PLX	C14-C15-C16-C17
47	g	203	PLX	C3-C4-C5-O8
47	r	502	PLX	C3-C4-C5-O8
47	g	203	PLX	O6-C4-C5-O8
47	r	502	PLX	O6-C4-C5-O8
51	l	704	CDL	OA6-CA4-CA6-OA8
47	g	201	PLX	C24-C25-C26-C27
47	r	502	PLX	O8-C24-C25-C26
48	E	201	8Q1	O33-C32-C34-O35
47	g	202	PLX	O7-C6-C7-C8
51	l	704	CDL	C15-C16-C17-C18
47	B	303	PLX	C20-C21-C22-C23
47	U	101	PLX	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
49	J	401	NDP	O4D-C1D-N1N-C6N
47	r	502	PLX	C11-C10-C9-C8
51	n	101	CDL	C73-C74-C75-C76
47	g	201	PLX	C14-C15-C16-C17
51	V	201	CDL	CA3-CA4-OA6-CA5
51	l	703	CDL	CB6-CB4-OB6-CB5
51	l	704	CDL	CA6-CA4-OA6-CA5
52	l	701	PEE	C3-C2-O2-C10
52	l	702	PEE	C3-C2-O2-C10
51	V	201	CDL	CB7-C71-C72-C73
51	i	401	CDL	C32-C31-CA7-OA8
51	V	201	CDL	C55-C56-C57-C58
51	n	101	CDL	C53-C54-C55-C56
51	l	703	CDL	CA7-C31-C32-C33
52	V	202	PEE	C11-C10-O2-C2
51	n	101	CDL	C15-C16-C17-C18
47	U	101	PLX	C2-O1-P1-O4
47	V	203	PLX	C3-O4-P1-O1
47	g	203	PLX	C3-O4-P1-O1
51	V	201	CDL	CB2-OB2-PB2-OB5
51	l	703	CDL	CB2-OB2-PB2-OB5
52	V	202	PEE	C4-O4P-P-O3P
52	l	701	PEE	C1-O3P-P-O4P
52	l	702	PEE	C4-O4P-P-O3P
49	J	401	NDP	C2D-C1D-N1N-C6N
47	V	203	PLX	C29-C30-C31-C32
47	V	203	PLX	C3-C4-C5-O8
47	b	201	PLX	C28-C29-C30-C31
47	r	501	PLX	C11-C10-C9-C8
51	l	703	CDL	C34-C35-C36-C37
51	l	704	CDL	C1-CB2-OB2-PB2
52	V	202	PEE	C23-C24-C25-C26
52	V	202	PEE	O4-C10-O2-C2
52	V	202	PEE	C35-C36-C37-C38
52	l	702	PEE	C23-C24-C25-C26
52	l	701	PEE	O4P-C4-C5-N
47	g	202	PLX	C15-C16-C17-C18
47	g	201	PLX	C19-C20-C21-C22
47	V	203	PLX	O6-C6-C7-C8
47	g	201	PLX	O6-C6-C7-C8
51	i	401	CDL	C1-CB2-OB2-PB2
51	i	401	CDL	CB4-CB3-OB5-PB2

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Mol	Chain	Res	Type	Atoms
51	l	703	CDL	CA4-CA3-OA5-PA1
52	W	201	PEE	C11-C12-C13-C14
47	B	303	PLX	C6-C7-C8-C9
47	V	203	PLX	C6-C7-C8-C9
51	l	703	CDL	CB5-C51-C52-C53
47	g	201	PLX	C25-C26-C27-C28
48	E	201	8Q1	O27-C28-C29-C30
48	p	201	8Q1	O27-C28-C29-C31
51	V	201	CDL	C11-C12-C13-C14
47	g	203	PLX	C3-C4-O6-C6
47	r	501	PLX	C5-C4-O6-C6
52	V	202	PEE	C21-C22-C23-C24
47	V	203	PLX	C33-C34-C35-C36
51	i	401	CDL	C72-C71-CB7-OB8
48	p	201	8Q1	C42-C43-S44-C1
47	g	201	PLX	O6-C4-C5-O8
47	B	303	PLX	C7-C8-C9-C10
51	i	401	CDL	C52-C51-CB5-OB7
51	V	201	CDL	C73-C74-C75-C76
51	l	704	CDL	CA3-CA4-CA6-OA8
47	g	202	PLX	C16-C17-C18-C19
47	r	502	PLX	C28-C29-C30-C31
47	g	201	PLX	O4-C3-C4-O6
47	V	203	PLX	C24-C25-C26-C27
48	E	201	8Q1	O33-C32-C34-N36
51	l	704	CDL	C32-C31-CA7-OA8
52	W	201	PEE	C35-C36-C37-C38
51	l	703	CDL	C32-C31-CA7-OA8
52	W	201	PEE	C1-C2-O2-C10
47	g	202	PLX	C27-C28-C29-C30
47	B	303	PLX	C14-C15-C16-C17
47	V	203	PLX	C35-C36-C37-C38
52	V	202	PEE	C30-C31-C32-C33
47	b	201	PLX	C3-C4-C5-O8
51	V	201	CDL	CA3-CA4-CA6-OA8
49	J	401	NDP	O4D-C4D-C5D-O5D
47	r	502	PLX	C33-C34-C35-C36
49	J	401	NDP	O4D-C1D-N1N-C2N
51	l	704	CDL	C35-C36-C37-C38
47	B	303	PLX	O9-C24-C25-C26
52	l	701	PEE	C38-C39-C40-C41
52	l	702	PEE	C18-C19-C20-C21

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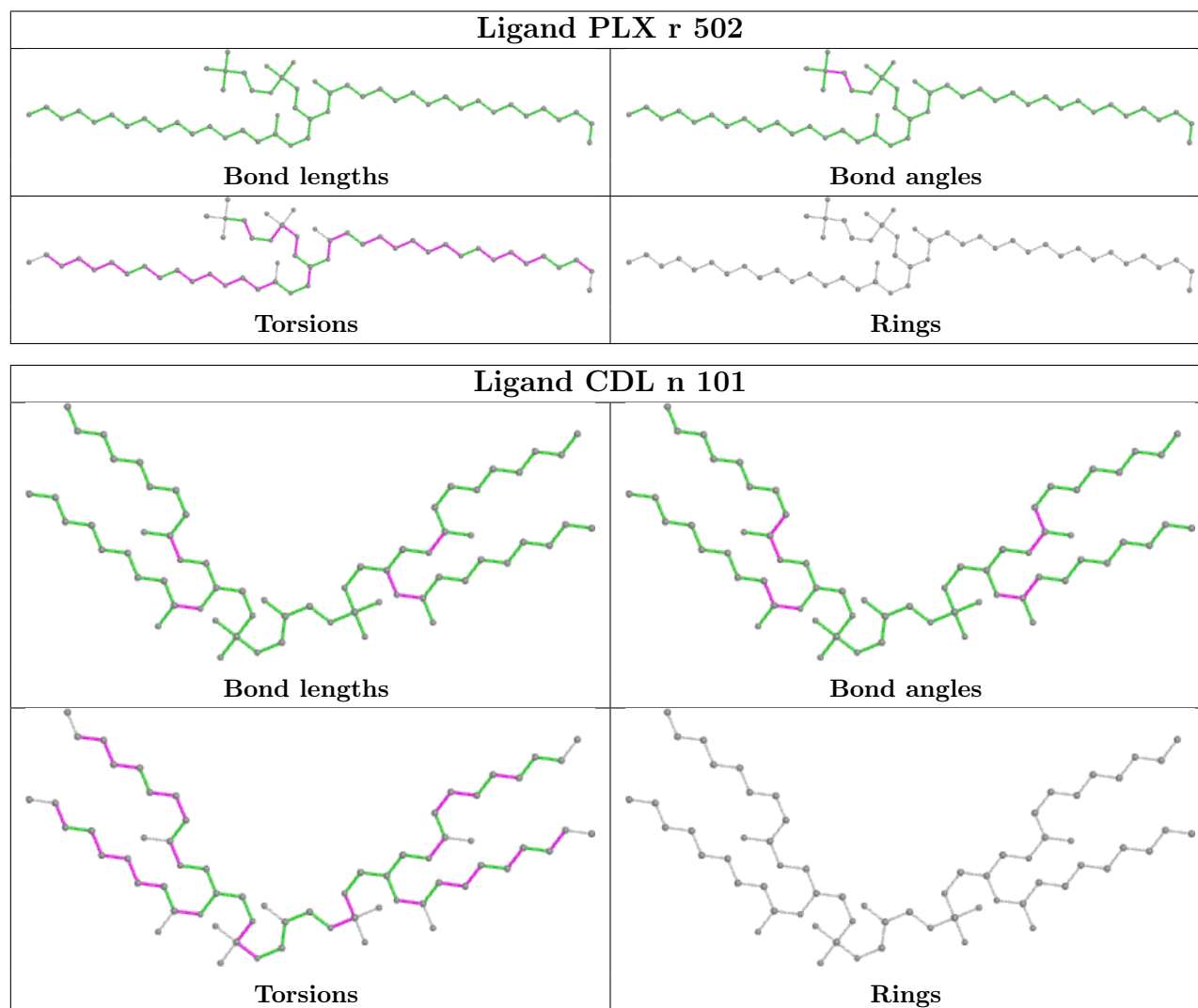
Mol	Chain	Res	Type	Atoms
51	l	703	CDL	C32-C31-CA7-OA9
51	l	703	CDL	C32-C33-C34-C35
52	l	702	PEE	C1-C2-C3-O3
47	b	201	PLX	C24-C25-C26-C27
52	l	702	PEE	C22-C23-C24-C25
47	B	303	PLX	C4-C3-O4-P1
47	V	203	PLX	C17-C18-C19-C20
47	V	203	PLX	C3-O4-P1-O2
47	g	201	PLX	C3-O4-P1-O2
51	l	703	CDL	CA3-OA5-PA1-OA3
51	l	704	CDL	CB3-OB5-PB2-OB3
51	n	101	CDL	CB3-OB5-PB2-OB3
52	l	702	PEE	C4-O4P-P-O1P
51	V	201	CDL	C12-C11-CA5-OA7
51	l	704	CDL	C32-C31-CA7-OA9
52	l	701	PEE	C33-C34-C35-C36
47	r	501	PLX	C14-C15-C16-C17
47	b	201	PLX	C25-C24-O8-C5
47	g	202	PLX	C25-C24-O8-C5
52	W	201	PEE	C5-C4-O4P-P
49	J	401	NDP	C2D-C1D-N1N-C2N
52	V	202	PEE	C39-C40-C41-C42
52	l	702	PEE	C41-C42-C43-C44
52	l	702	PEE	C32-C33-C34-C35
51	l	704	CDL	C52-C51-CB5-OB6
51	l	704	CDL	C74-C75-C76-C77
47	g	202	PLX	C6-C7-C8-C9
47	g	202	PLX	C24-C25-C26-C27
52	l	701	PEE	C11-C12-C13-C14
46	A	502	FMN	N10-C1'-C2'-O2'
47	V	203	PLX	C15-C16-C17-C18
47	g	203	PLX	C36-C37-C38-C39
52	W	201	PEE	C42-C43-C44-C45
51	l	704	CDL	C52-C51-CB5-OB7
51	V	201	CDL	C52-C51-CB5-OB6

There are no ring outliers.

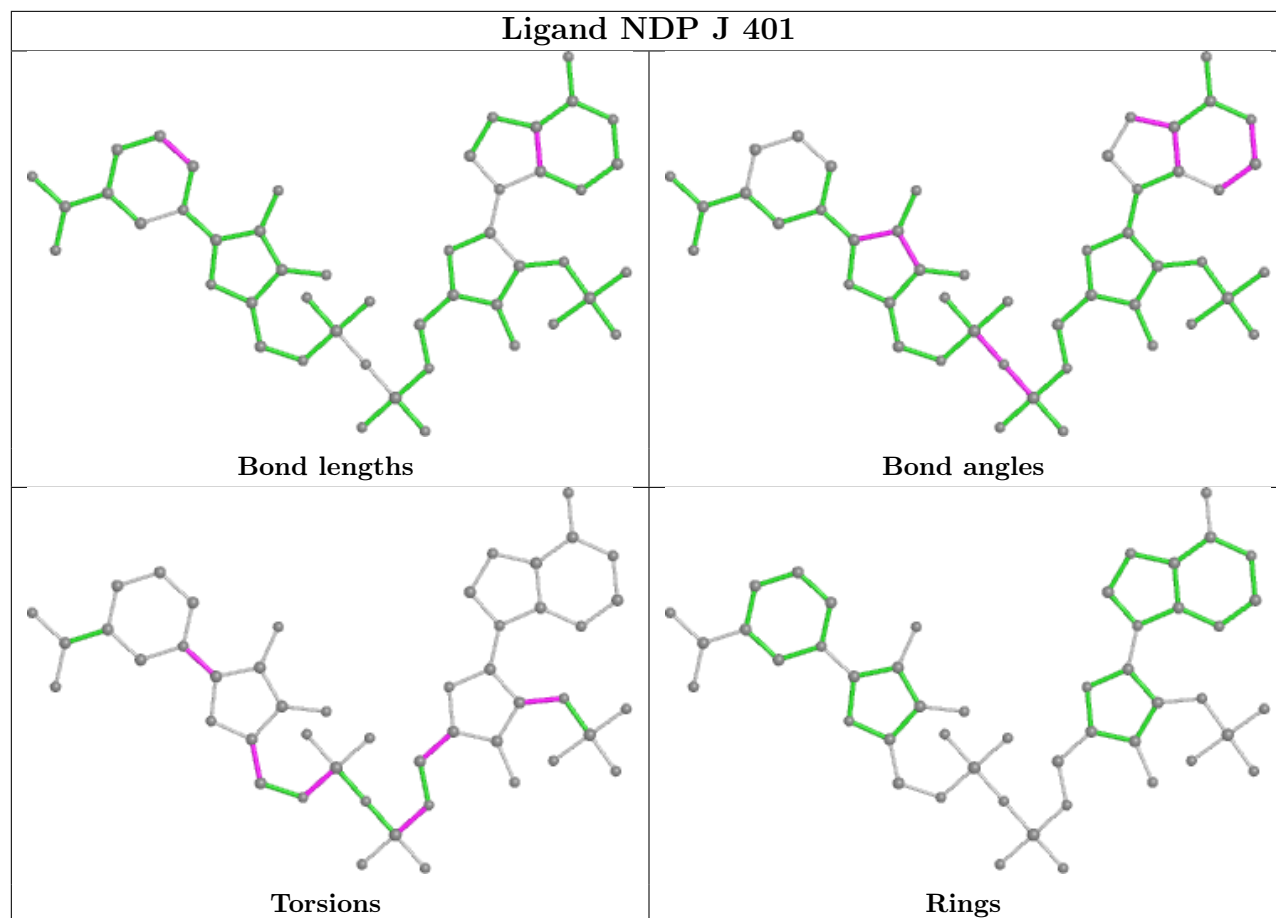
No monomer is involved in short contacts.

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

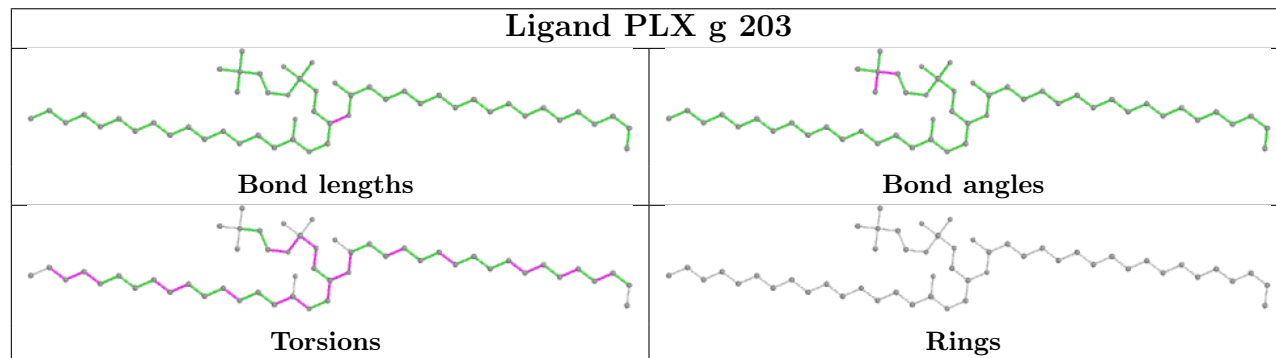
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

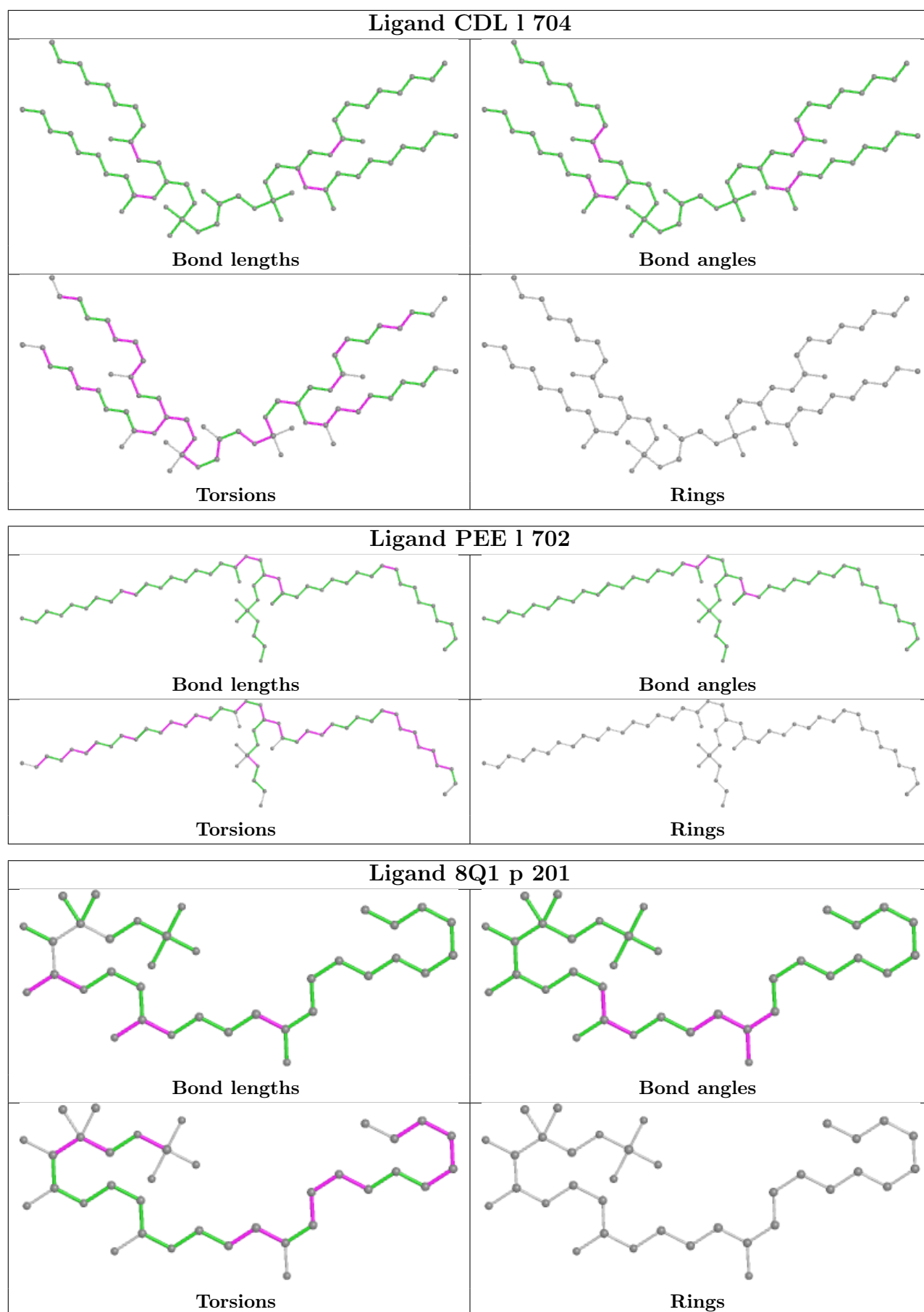


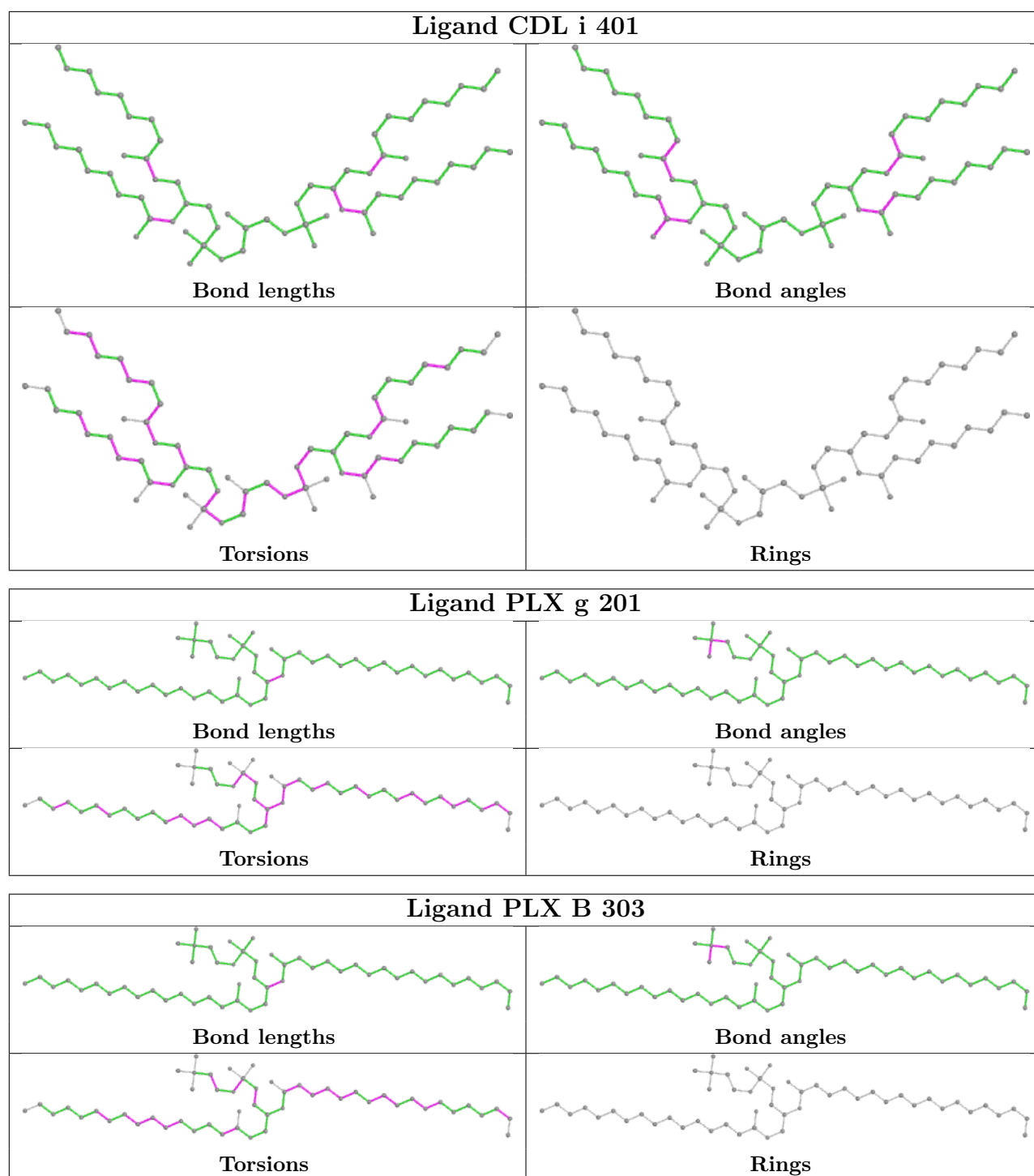
## Ligand NDP J 401

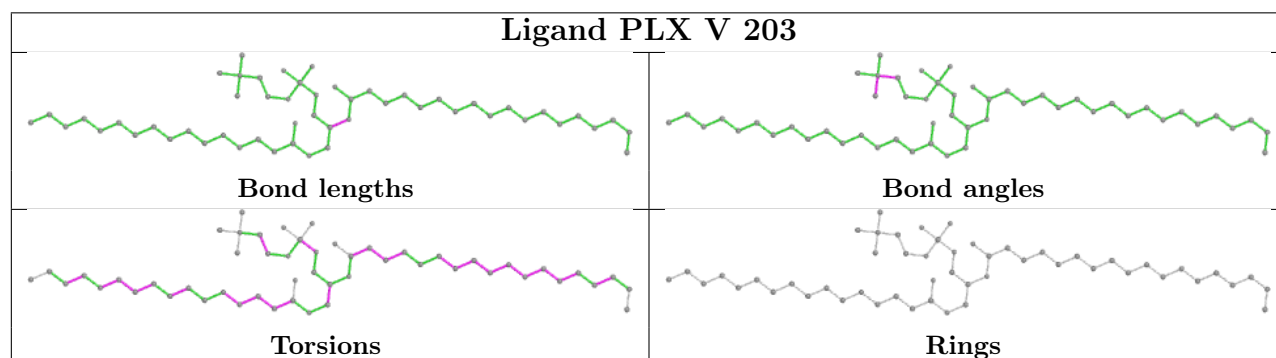
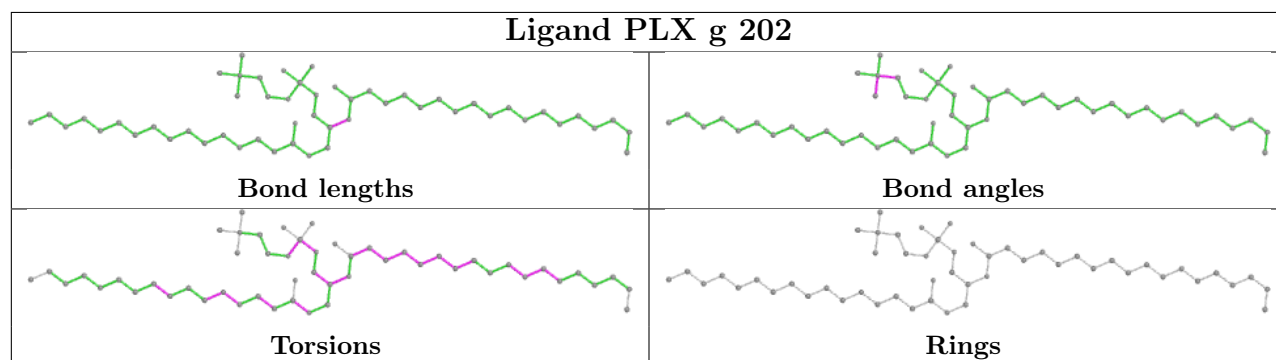
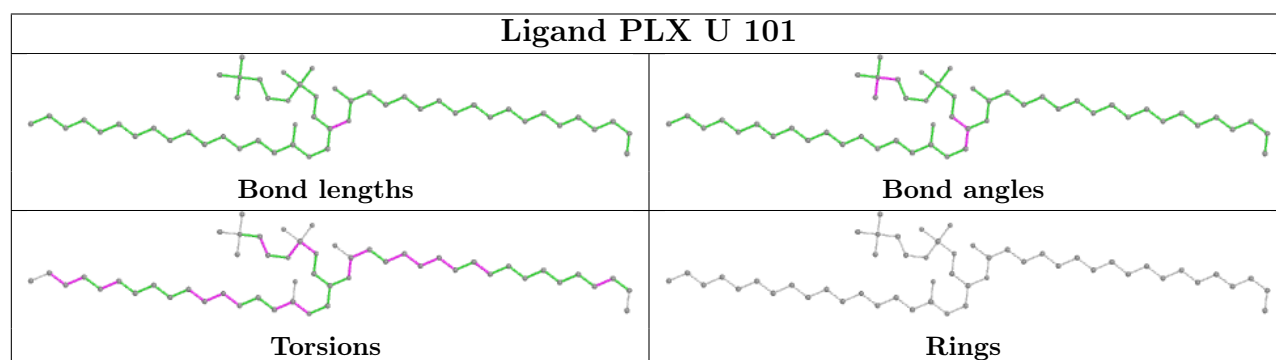
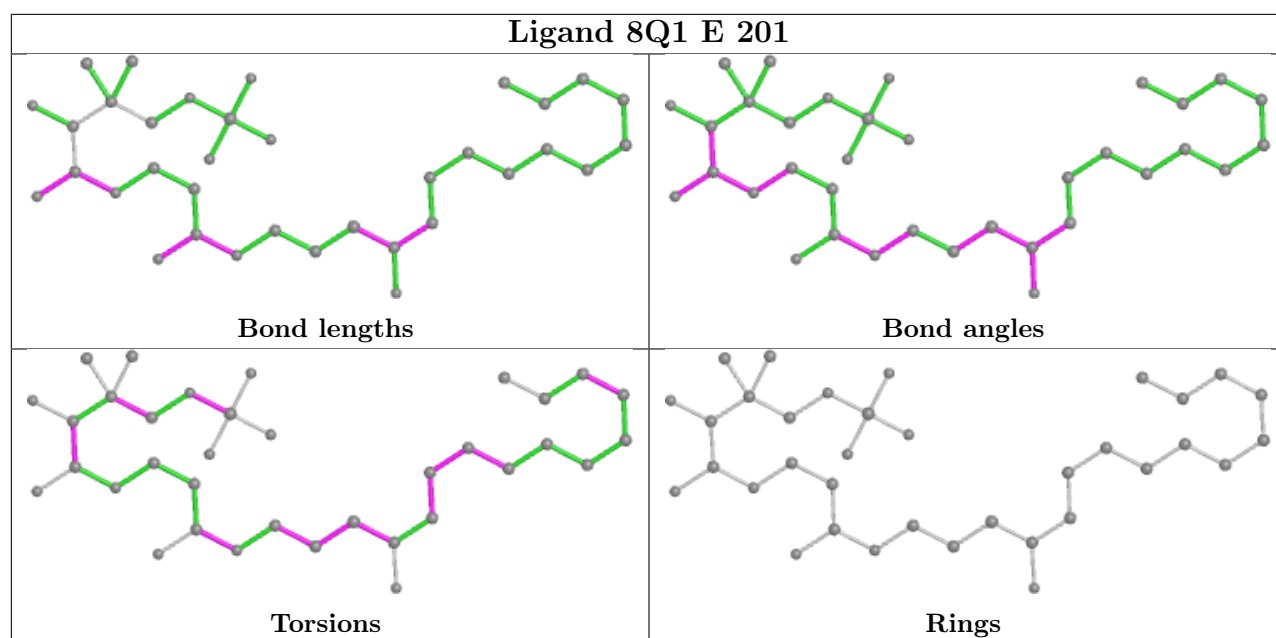


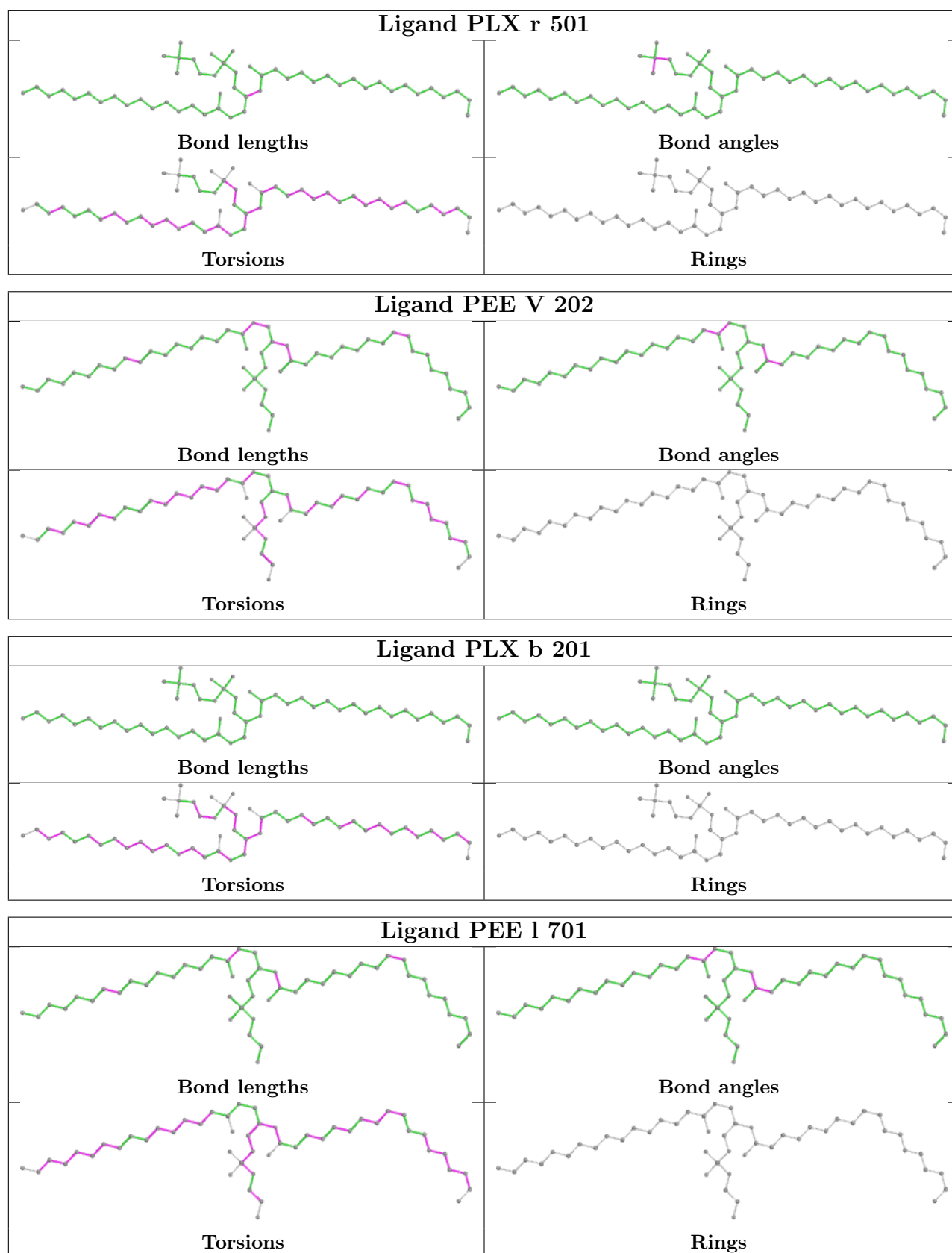
## Ligand PLX g 203

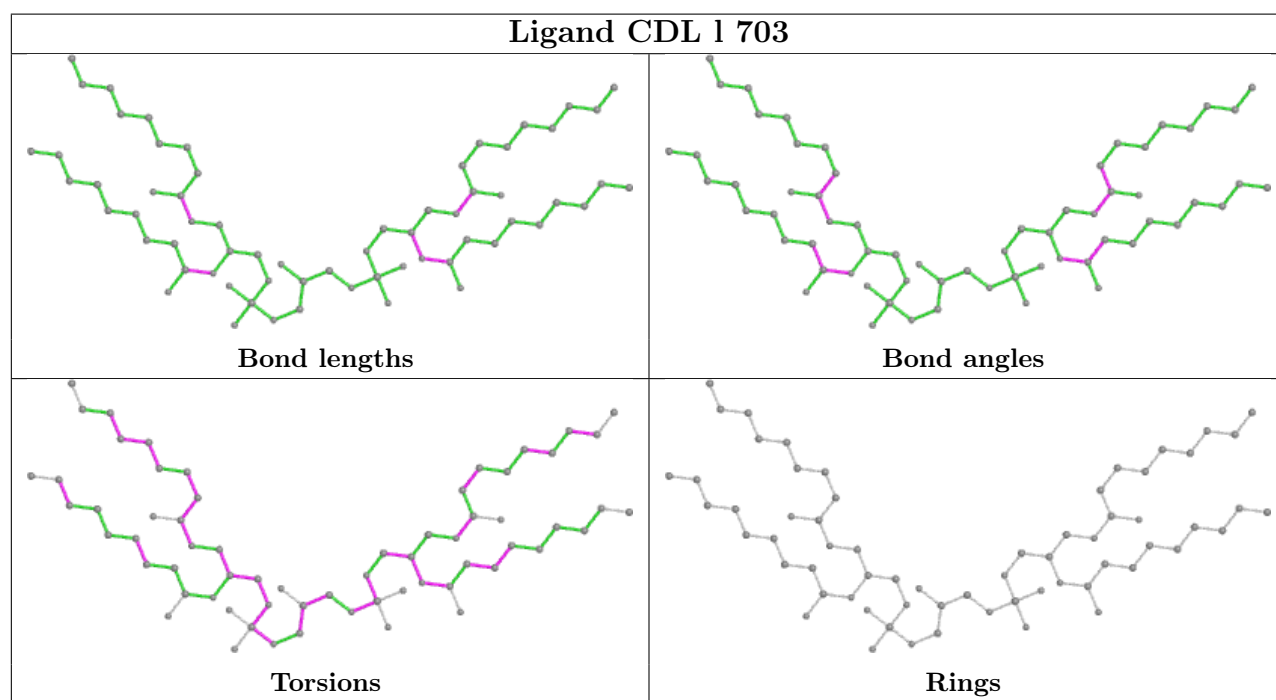
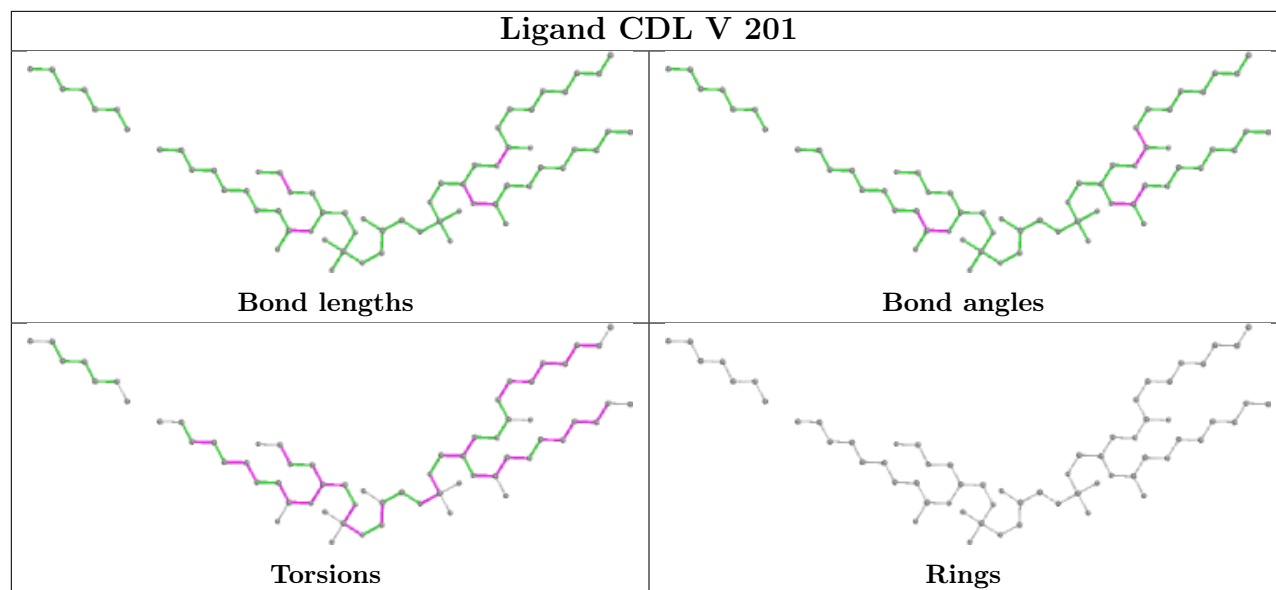


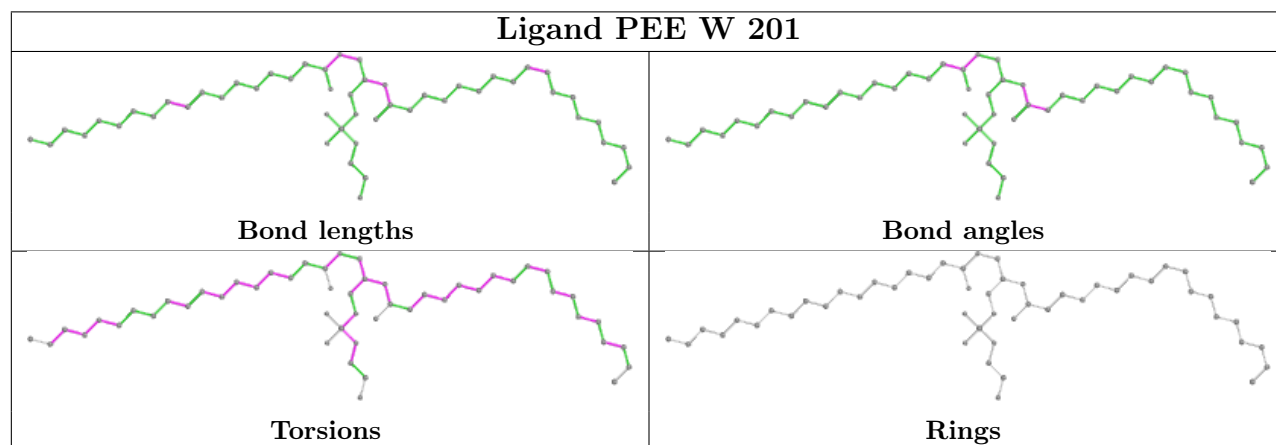
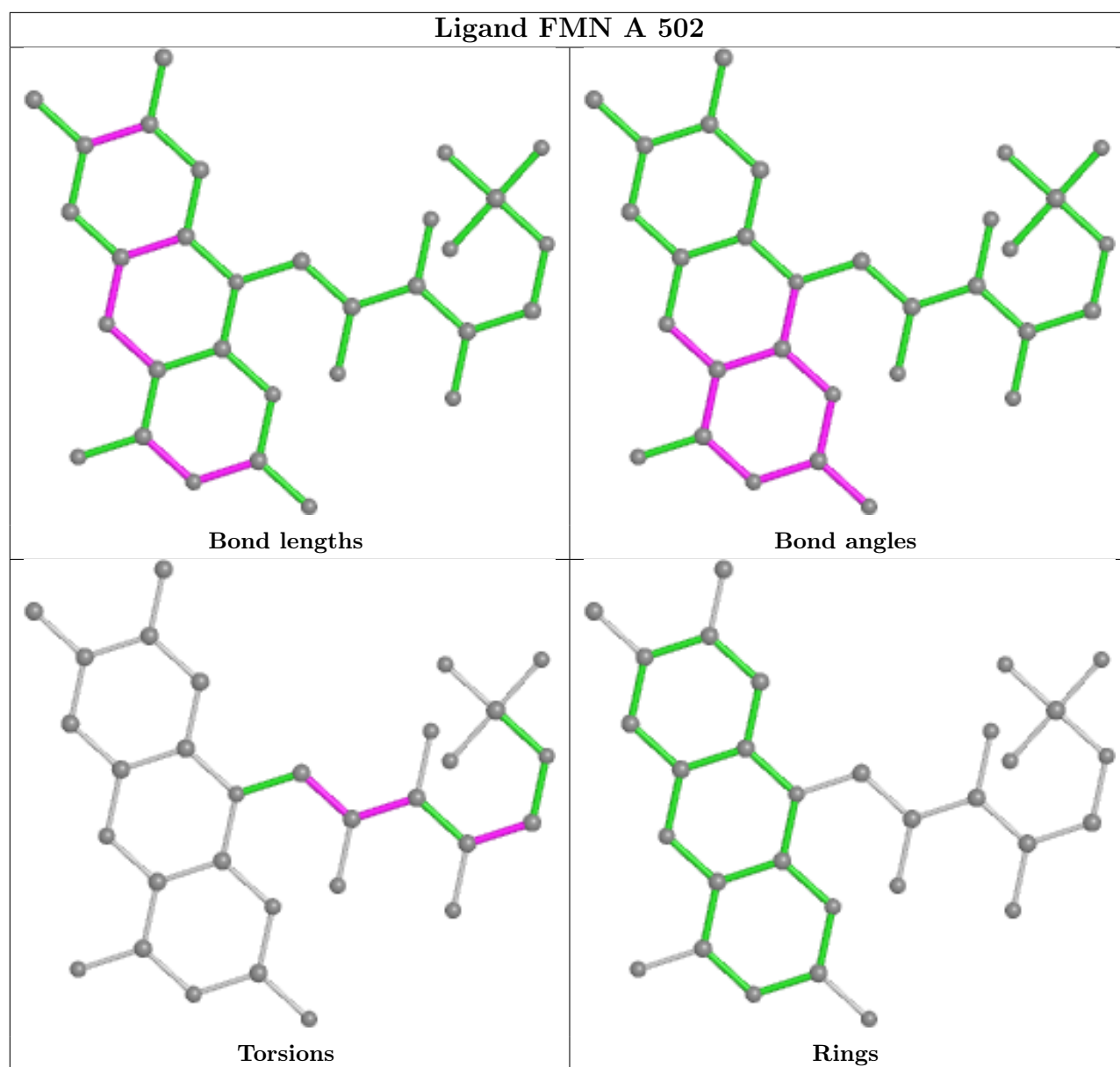












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

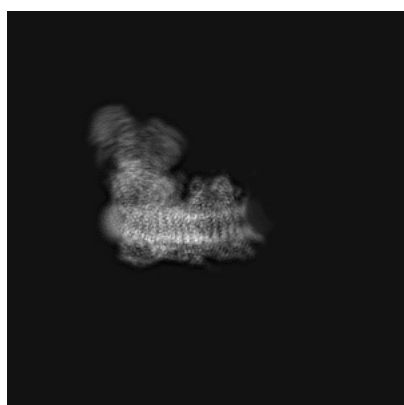
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6773. These allow visual inspection of the internal detail of the map and identification of artifacts.

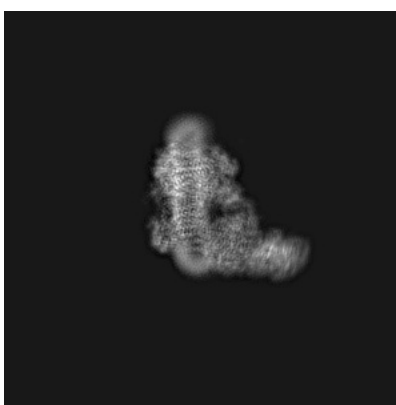
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

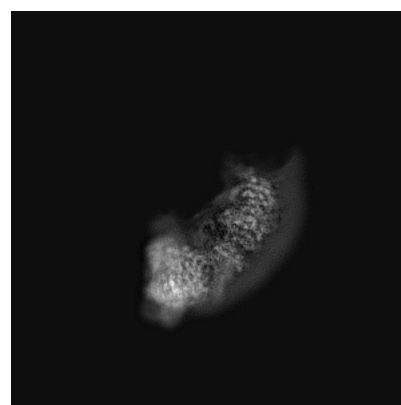
#### 6.1.1 Primary map



X



Y



Z

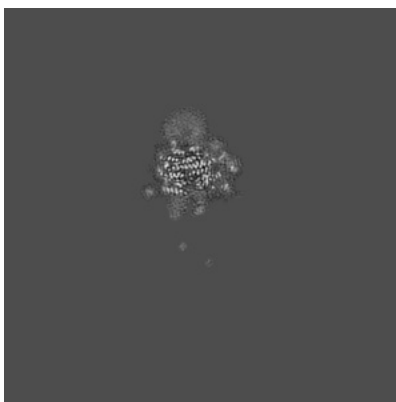
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

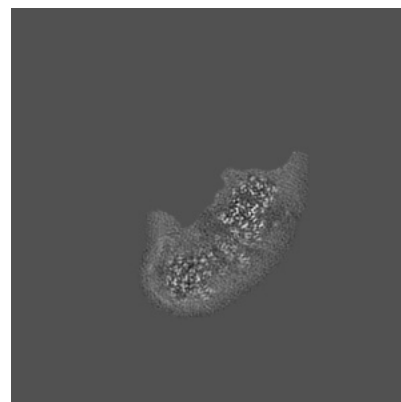
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

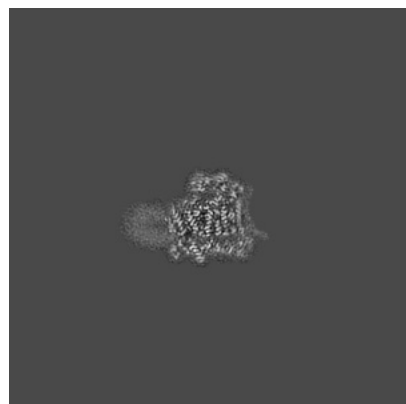


Z Index: 240

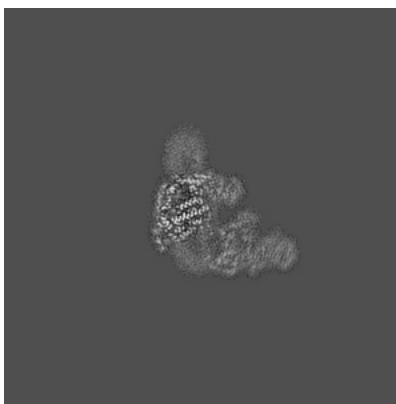
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

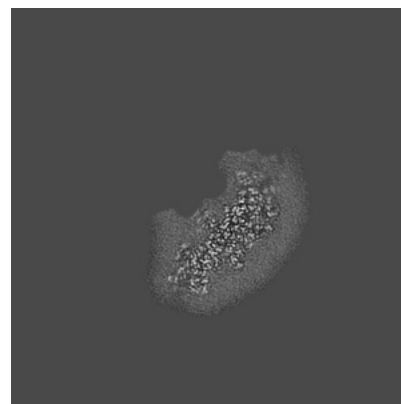
### 6.3.1 Primary map



X Index: 290



Y Index: 183

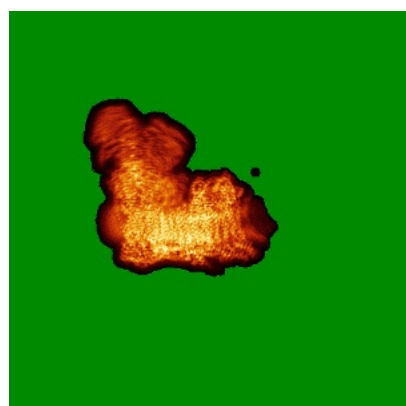


Z Index: 208

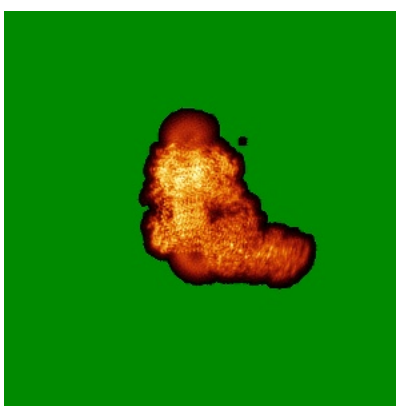
The images above show the largest variance slices of the map in three orthogonal directions.

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

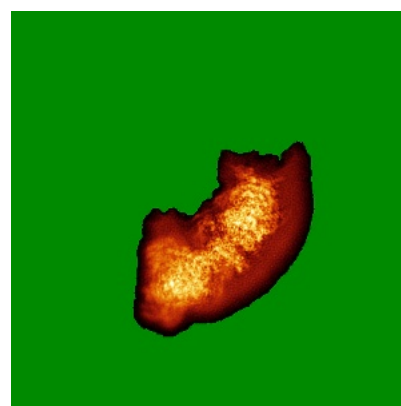
### 6.4.1 Primary map



X



Y



Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0525. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

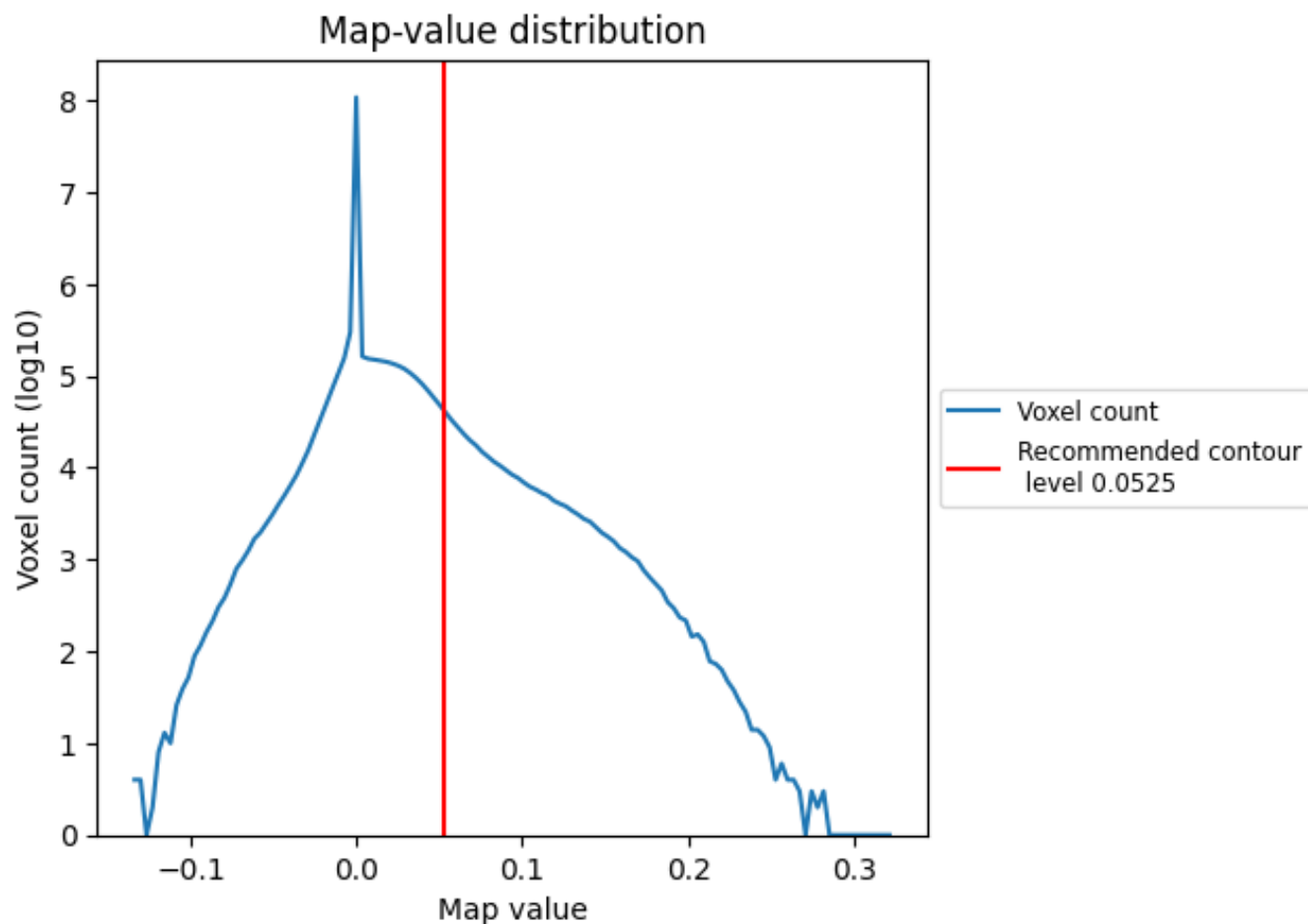
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

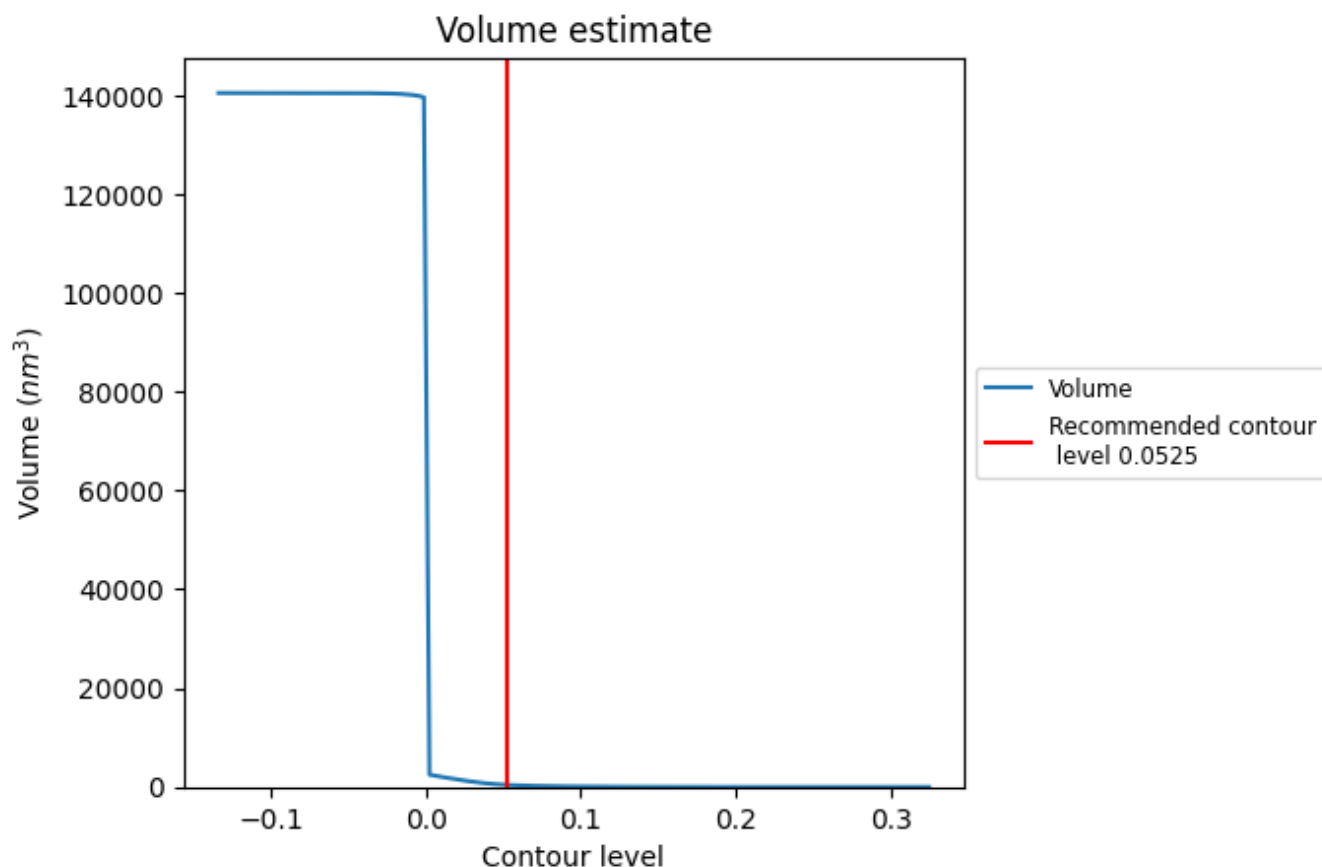
This section contains the results of statistical analysis of the map.

### 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.

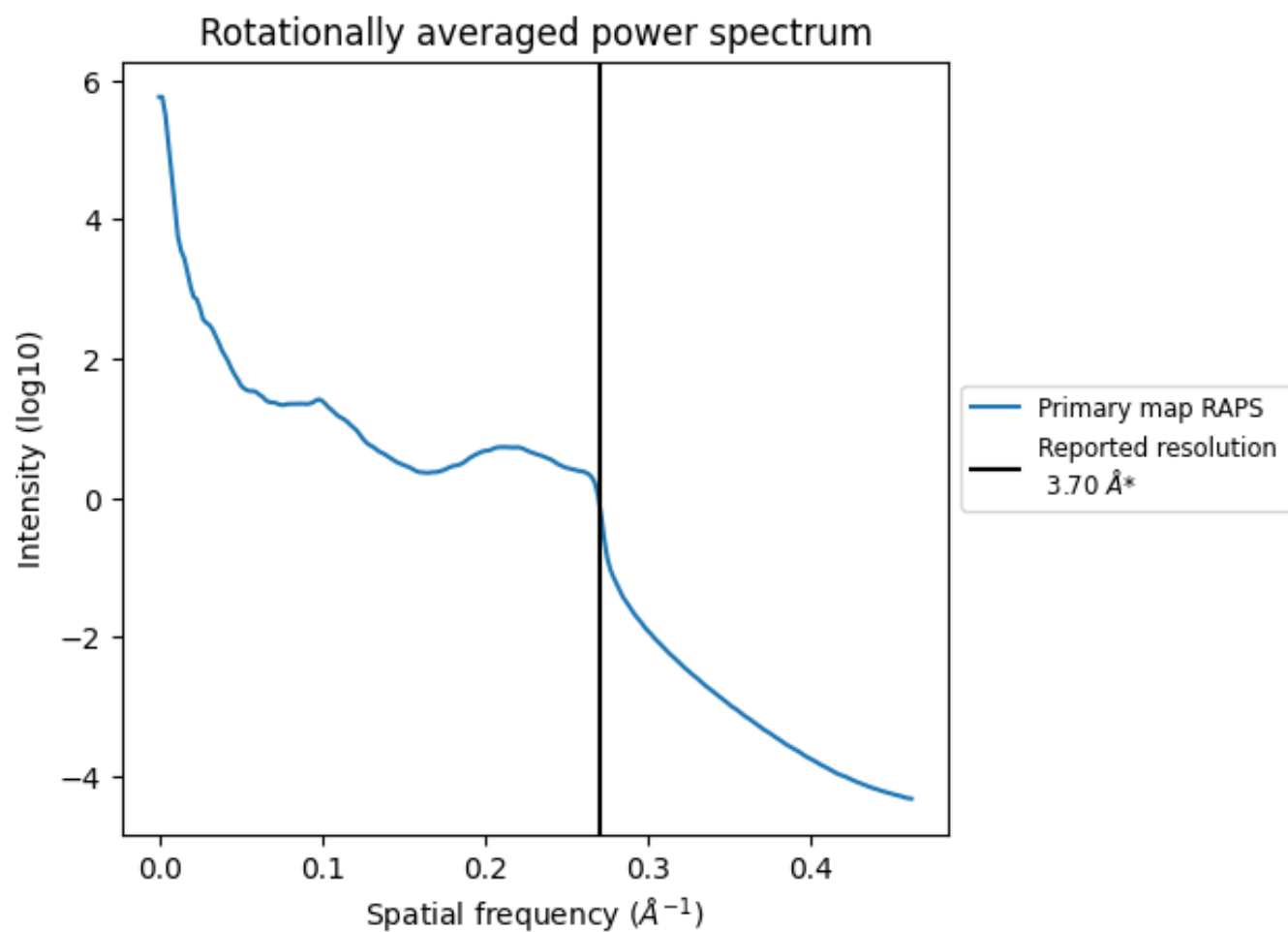
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 412 nm<sup>3</sup>; this corresponds to an approximate mass of 372 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 0.270 Å<sup>-1</sup>

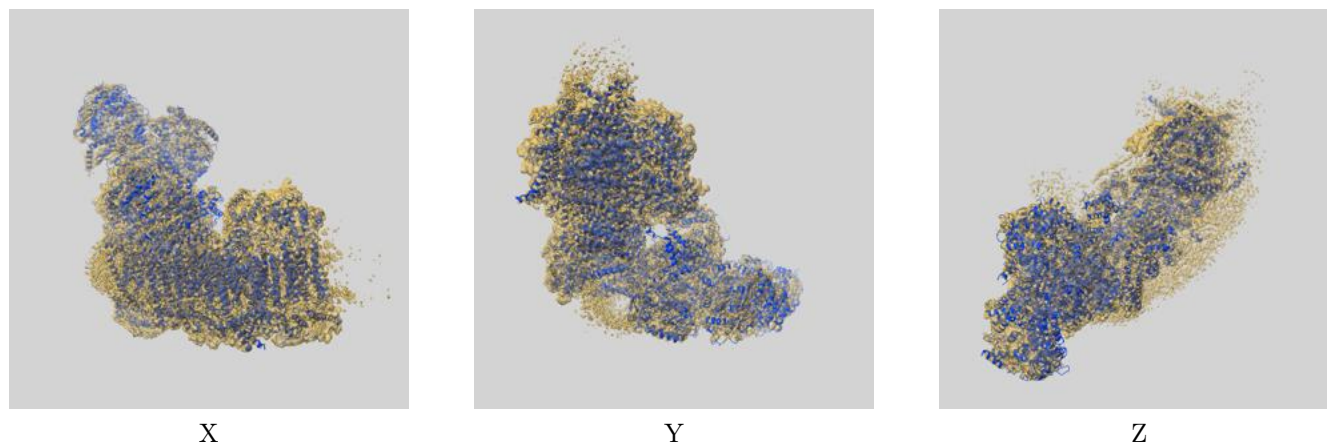
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

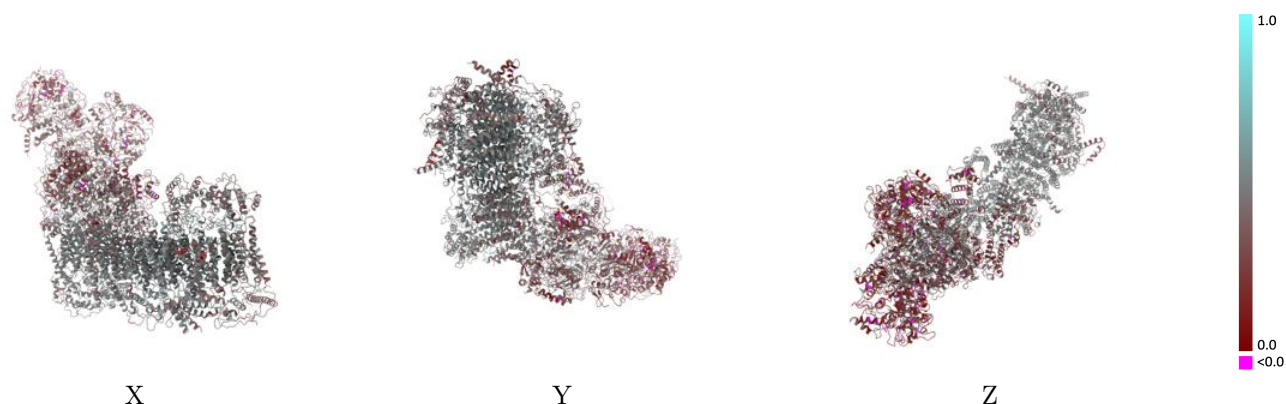
This section contains information regarding the fit between EMDB map EMD-6773 and PDB model 5XTD. Per-residue inclusion information can be found in section [3](#) on page [18](#).

### 9.1 Map-model overlay [i](#)



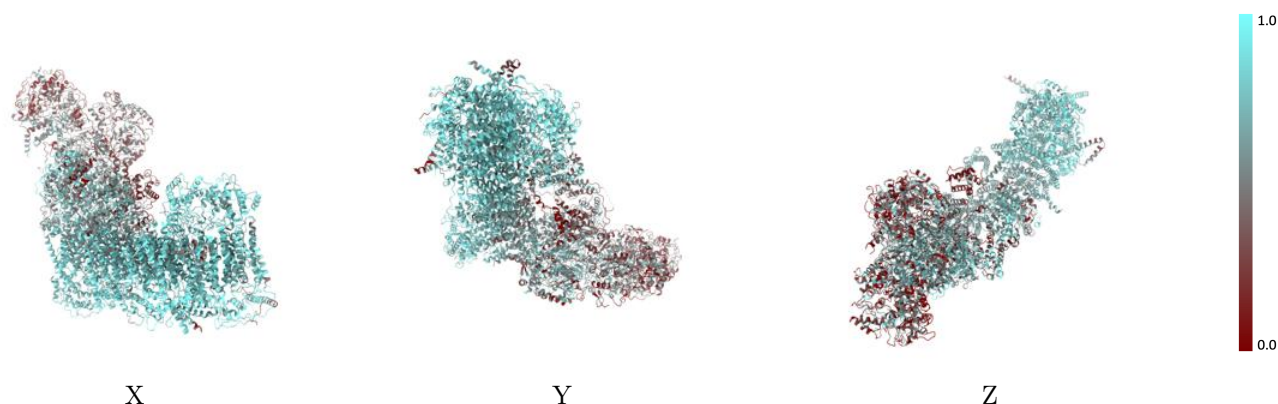
The images above show the 3D surface view of the map at the recommended contour level 0.0525 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



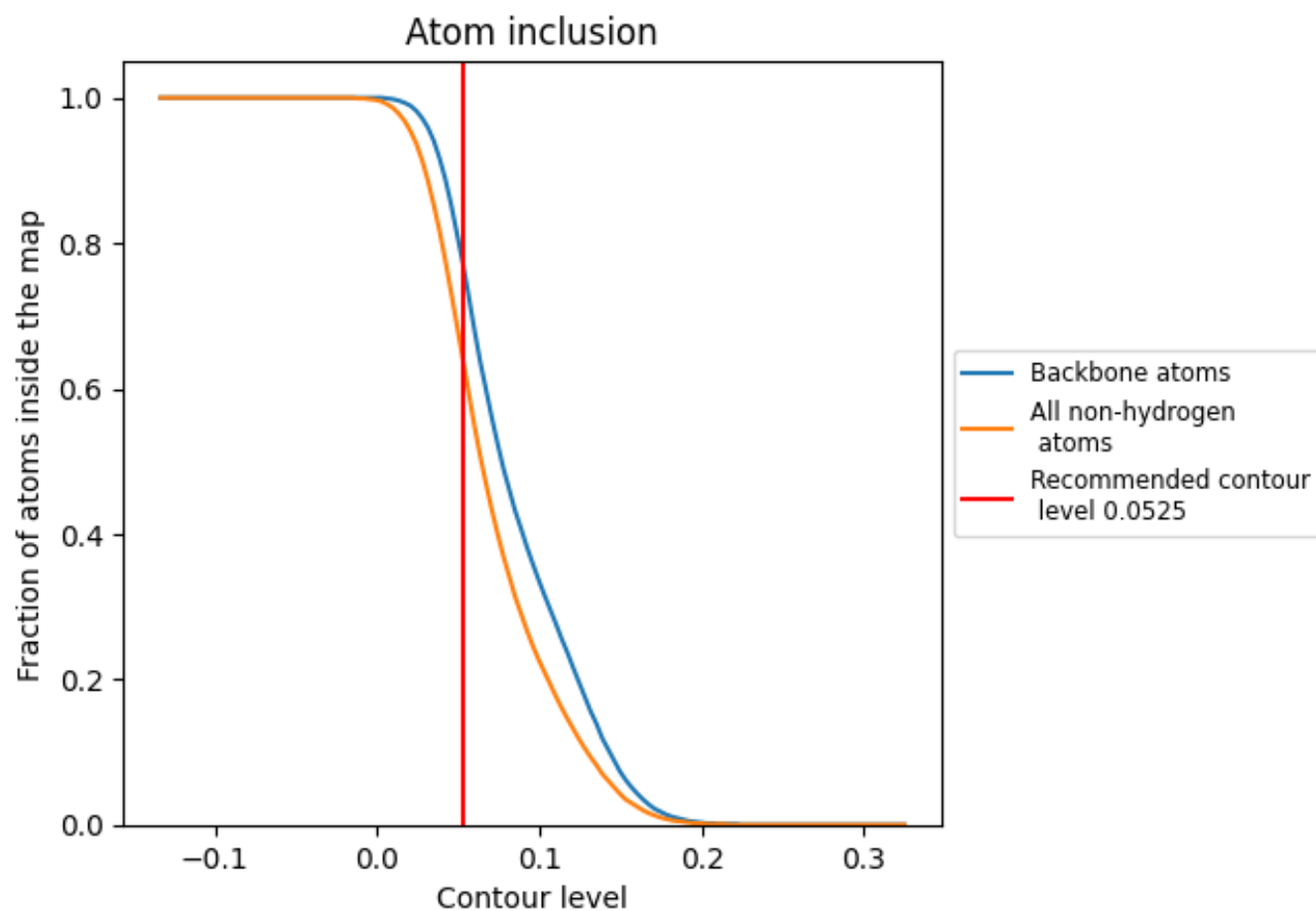
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0525).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 64% 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 (0.0525) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6410	 0.4010
A	 0.3440	 0.2340
B	 0.7530	 0.4320
C	 0.7910	 0.4590
E	 0.3910	 0.3140
F	 0.3690	 0.2200
G	 0.1290	 0.2310
H	 0.4360	 0.2870
I	 0.4070	 0.3250
J	 0.5260	 0.3290
K	 0.3020	 0.2340
L	 0.3510	 0.2970
M	 0.4030	 0.2840
N	 0.5340	 0.3760
O	 0.3390	 0.2460
P	 0.5330	 0.3350
Q	 0.6230	 0.3820
S	 0.8200	 0.4740
T	 0.4140	 0.3560
U	 0.7870	 0.4510
V	 0.6180	 0.4430
W	 0.8030	 0.4550
X	 0.7880	 0.4390
Y	 0.8360	 0.4350
Z	 0.7600	 0.4170
a	 0.8660	 0.5000
b	 0.7050	 0.3980
c	 0.8320	 0.4840
d	 0.8260	 0.4620
e	 0.7660	 0.4730
f	 0.6670	 0.3950
g	 0.7960	 0.4890
h	 0.8170	 0.4660
i	 0.7810	 0.5020
j	 0.6040	 0.4120



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Chain	Atom inclusion	Q-score
k	 0.7110	 0.4750
l	 0.7560	 0.4770
m	 0.7010	 0.4490
n	 0.7370	 0.4510
o	 0.7890	 0.4710
p	 0.8180	 0.4600
r	 0.8290	 0.5080
s	 0.7680	 0.4730
u	 0.8410	 0.4560
v	 0.7170	 0.3930
w	 0.6340	 0.3910