



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 07:43 PM UTC

PDB ID : 7QSK / pdb_00007qsk
EMDB ID : EMD-14132
Title : Bovine complex I in lipid nanodisc, Active-Q10
Authors : Chung, I.; Bridges, H.R.; Hirst, J.
Deposited on : 2022-01-13
Resolution : 2.84 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

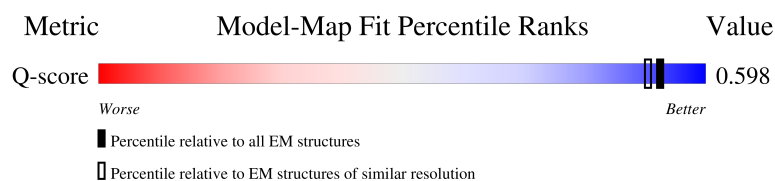
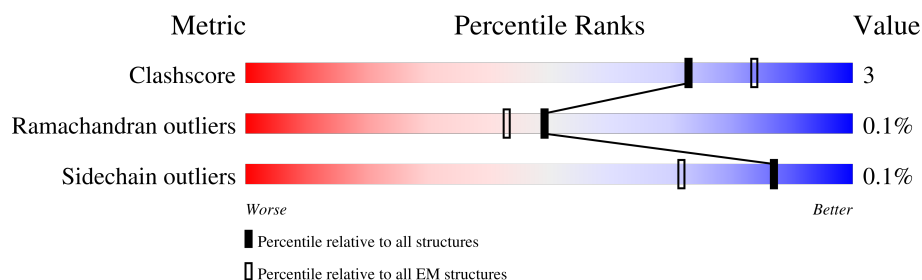
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.84 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



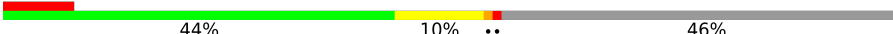
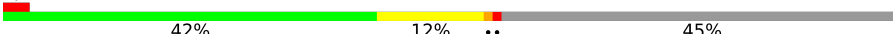
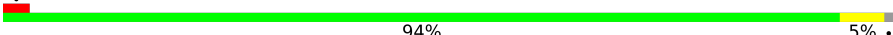
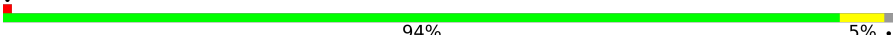
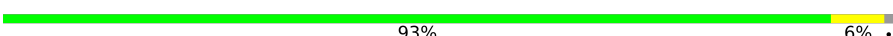
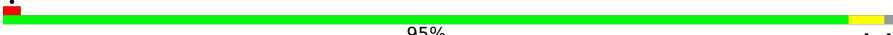
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11884 (2.34 - 3.34)

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	A	115	
2	B	216	
3	C	266	
4	D	463	

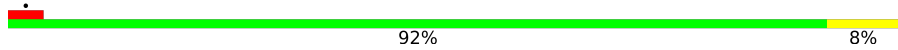
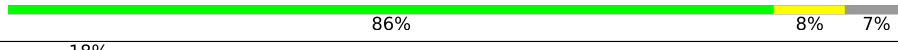
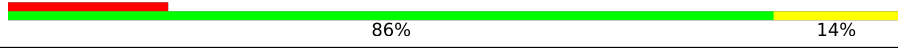
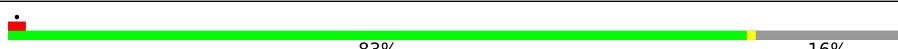
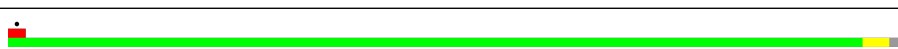
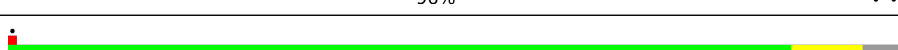
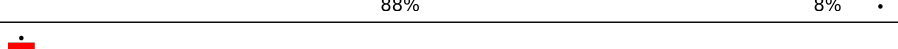
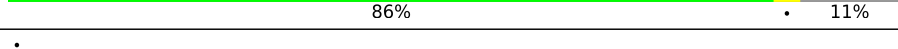
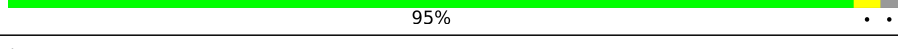
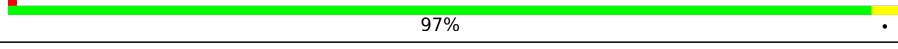
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	d	120	
30	e	106	
31	f	57	
32	g	154	
33	h	189	
34	i	127	
35	j	108	
36	k	98	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	109	

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 69986 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	115	Total	C	N	O	S	0	0
			921	622	133	159	7		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	155	Total	C	N	O	S	0	0
			1241	792	224	211	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	209	Total	C	N	O	S	0	0
			1738	1120	298	317	3		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	430	Total	C	N	O	S	0	0
			3459	2209	596	629	25		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	variant	UNP P17694

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1659	1059	278	312	10		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	432	Total	C	N	O	S	2	0
			3347	2111	598	618	20		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	699	Total	C	N	O	S	1	0
			5366	3362	934	1030	40		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	318	Total	C	N	O	S	1	0
			2517	1687	386	421	23		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	175	Total	C	N	O	S	0	0
			1345	906	191	236	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			745	486	112	131	16		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			4802	3195	737	827	43		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3654	2436	570	609	39		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	347	Total	C	N	O	S	0	0
			2733	1817	416	457	43		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	320	Total	C	N	O	S	0	0
			2589	1662	429	488	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	255	LYS	ASN	variant	UNP P34942

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	342	Total	C	N	O	S	1	0
			2768	1792	489	482	5		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	129	Total	C	N	O	S	0	0
			1049	659	188	199	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	96	Total	C	N	O	S	0	0
			740	454	140	143	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	87	Total	C	N	O	S	0	0
			700	440	131	127	2		

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	85	Total	C	N	O	S	0	0
			688	444	101	138	5		
20	U	86	Total	C	N	O	S	0	0
			693	447	102	139	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	115	Total	C	N	O	S	0	0
			928	600	157	168	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	115	Total	C	N	O	S	0	0
			976	625	181	166	4		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	171	Total	C	N	O	S	0	0
			1402	887	253	252	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	140	Total	C	N	O	S	0	0
			1030	657	176	191	6		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	141	Total	C	N	O	S	0	0
			1152	740	201	202	9		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	70	Total	C	N	O	S	0	0
			569	365	104	95	5		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	83	Total	C	N	O	S	0	0
			651	425	109	115	2		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	49	Total	C	N	O	0	0
			414	273	70	71		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	120	Total	C	N	O	S	0	0
			999	650	172	172	5		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	99	Total	C	N	O	S	0	0
			829	523	158	142	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	57	Total	C	N	O	S	0	0
			492	322	86	82	2		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	100	Total	C	N	O	S	0	0
			839	539	139	157	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	138	Total	C	N	O	S	0	0
			1154	759	196	197	2		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	127	Total	C	N	O	S	0	0
			1097	722	191	183	1		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	71	Total	C	N	O	S	0	0
			597	390	99	107	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	81	Total	C	N	O	S	0	0
			653	427	110	114	2		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	156	Total	C	N	O	S	0	0
			1314	850	216	240	8		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	128	Total	C	N	O	S	0	0
			1067	684	188	195			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	172	Total	C	N	O	S	0	0
			1492	955	273	257	7		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	122	Total	C	N	O	S	0	0
			1048	653	201	185	9		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	173	Total	C	N	O	S	0	0
			1453	910	268	267	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

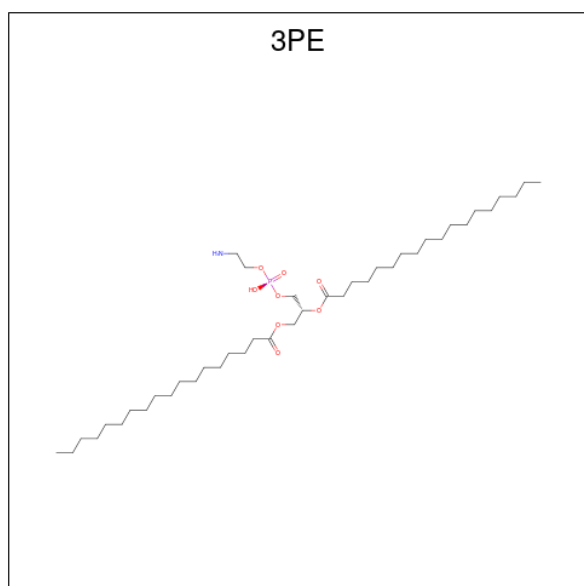
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	95	Total	C	N	O	S	0	0
			776	490	144	139	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	45	Total	C	N	O	S	1	0
			391	244	71	75	1		

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



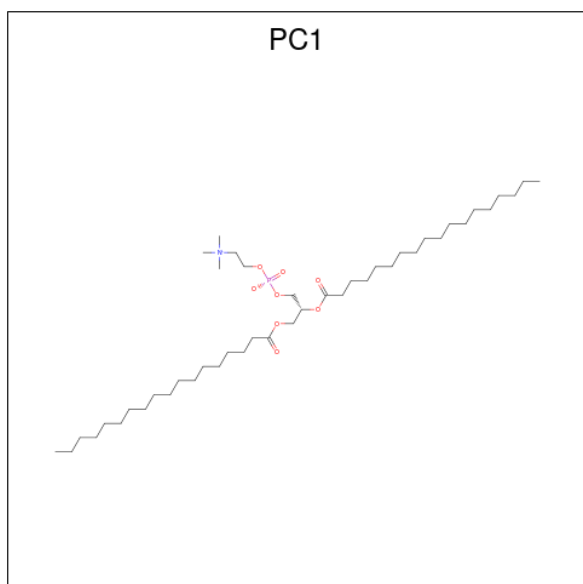
Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
45	H	1	Total	C	N	O	P	0
			36	26	1	8	1	
45	K	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	L	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
45	L	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	M	1	Total	C	N	O	P	0
			49	39	1	8	1	

Continued on next page...

Continued from previous page...

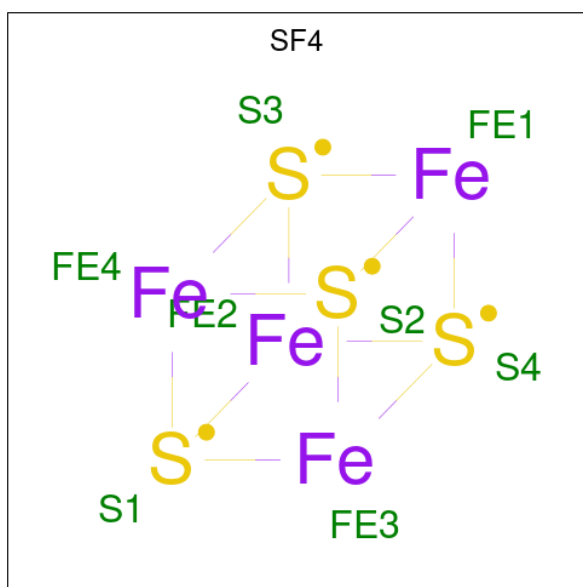
Mol	Chain	Residues	Atoms					AltConf
45	M	1	Total	C	N	O	P	0
			45	35	1	8	1	
45	M	1	Total	C	N	O	P	0
			48	38	1	8	1	
45	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	P	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	Y	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	Y	1	Total	C	N	O	P	0
			40	30	1	8	1	
45	Y	1	Total	C	N	O	P	0
			30	20	1	8	1	
45	Y	1	Total	C	N	O	P	0
			33	23	1	8	1	
45	Y	1	Total	C	N	O	P	0
			27	17	1	8	1	
45	d	1	Total	C	N	O	P	0
			49	39	1	8	1	
45	m	1	Total	C	N	O	P	0
			50	40	1	8	1	
45	m	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



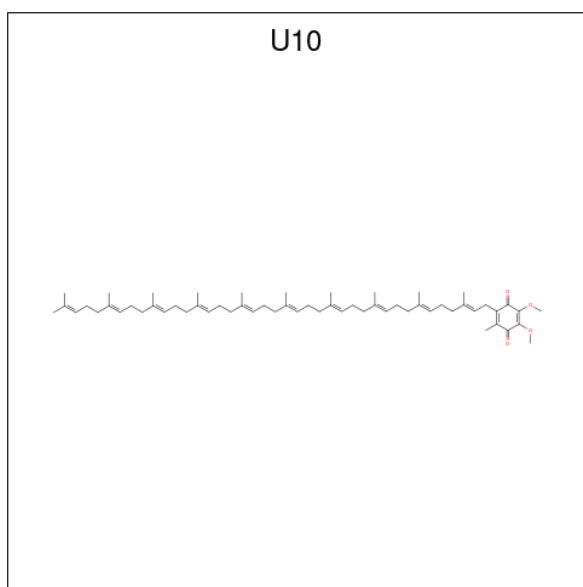
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	A	1	Total	C	N	O	P	0
			33	23	1	8	1	
46	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	I	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	M	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	Y	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	Z	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	d	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	g	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	h	1	Total	C	N	O	P	0
			47	37	1	8	1	
46	q	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	q	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



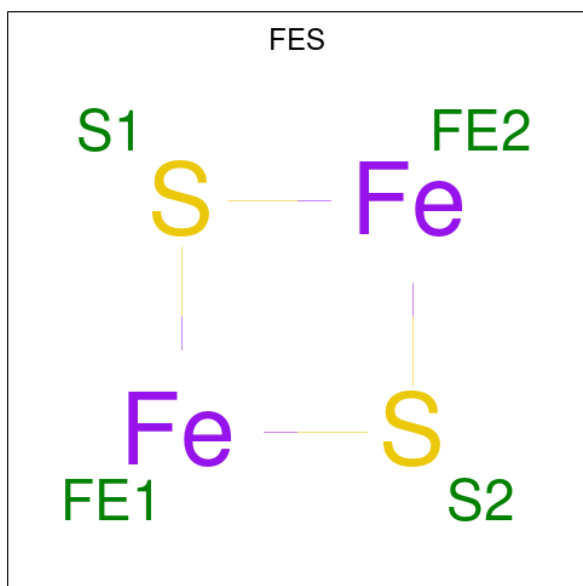
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 48 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



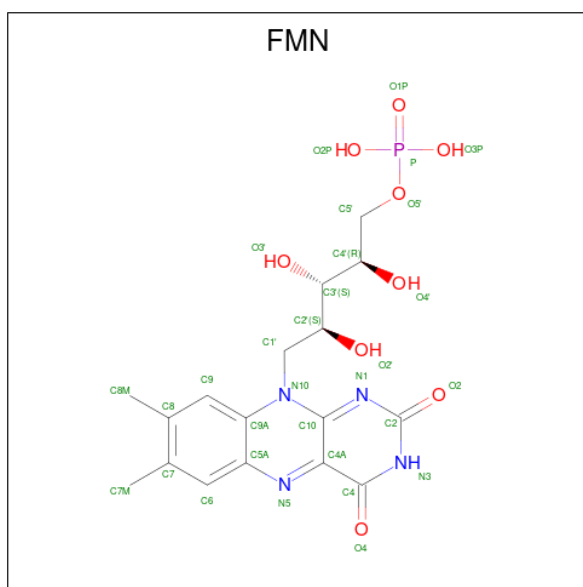
Mol	Chain	Residues	Atoms			AltConf
48	D	1	Total	C	O	0
			63	59	4	

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
49	E	1	Total	Fe	S	0
			4	2	2	
49	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 50 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).

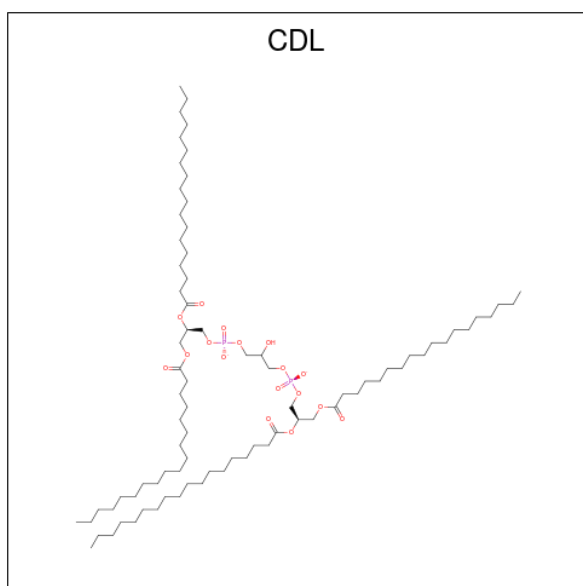


Mol	Chain	Residues	Atoms					AltConf
50	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 51 is POTASSIUM ION (CCD ID: K) (formula: K).

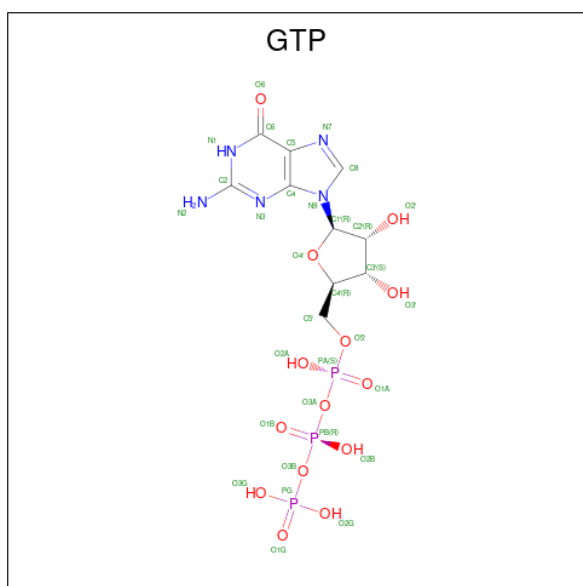
Mol	Chain	Residues	Atoms	AltConf
51	G	1	Total K 1 1	0

- Molecule 52 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$).



Mol	Chain	Residues	Atoms				AltConf
52	H	1	Total	C	O	P	0
			51	32	17	2	
52	L	1	Total	C	O	P	0
			76	57	17	2	
52	N	1	Total	C	O	P	0
			62	43	17	2	
52	X	1	Total	C	O	P	0
			86	67	17	2	
52	d	1	Total	C	O	P	0
			65	46	17	2	
52	h	1	Total	C	O	P	0
			80	61	17	2	
52	r	1	Total	C	O	P	0
			61	42	17	2	

- Molecule 53 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



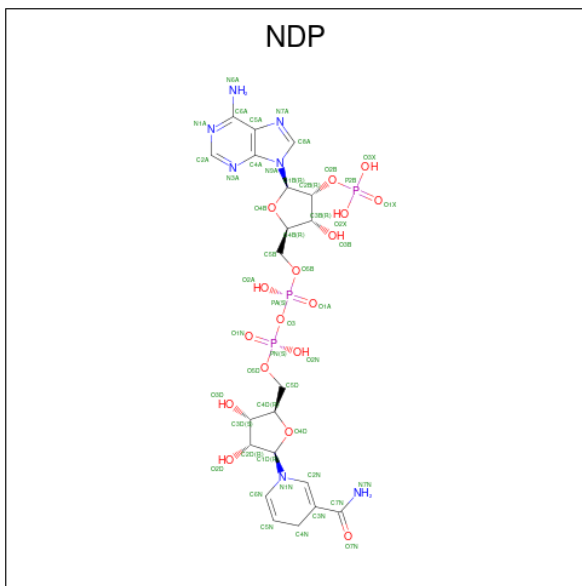
Mol	Chain	Residues	Atoms					AltConf
53	O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	O	1	Total	Mg	0
			1	1	

- Molecule 55 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).

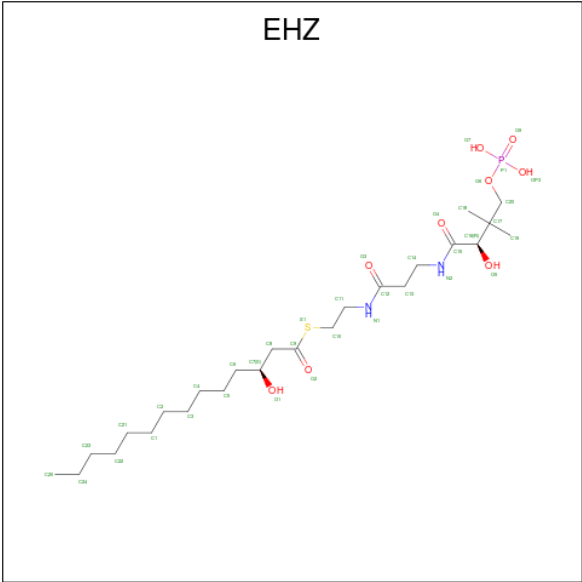


Mol	Chain	Residues	Atoms					AltConf
55	P	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

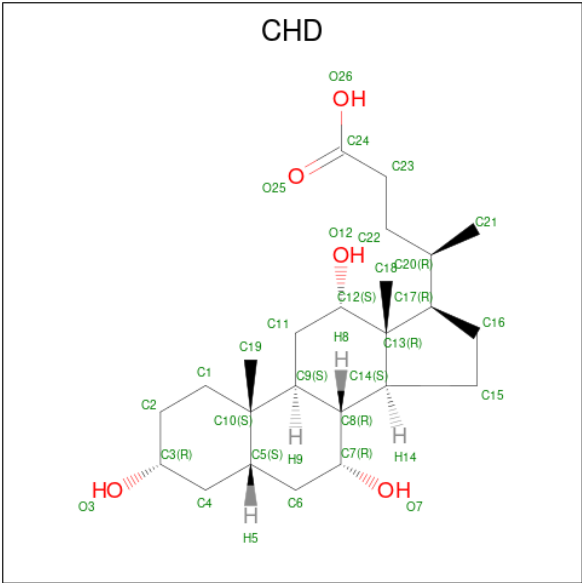
Mol	Chain	Residues	Atoms	AltConf
56	R	1	Total Zn 1 1	0

- Molecule 57 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).



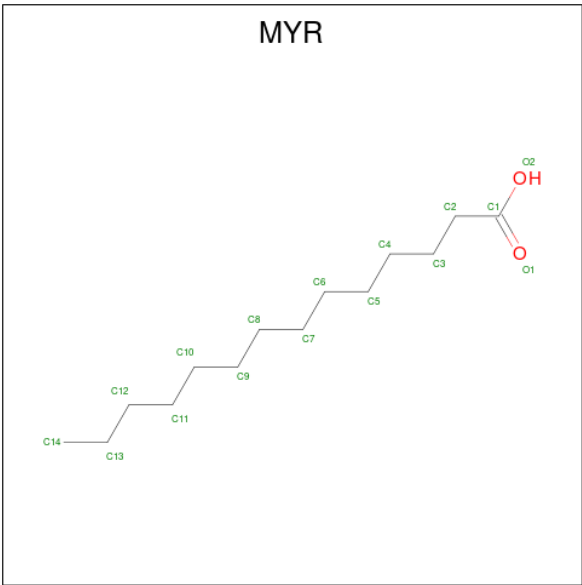
Mol	Chain	Residues	Atoms					AltConf
57	T	1	Total	C	N	O	P	S
			37	25	2	8	1	1
57	U	1	Total	C	N	O	P	S
			37	25	2	8	1	1

- Molecule 58 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



Mol	Chain	Residues	Atoms			AltConf
58	i	1	Total	C	O	0
			29	24	5	

- Molecule 59 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).



Mol	Chain	Residues	Atoms			AltConf
59	o	1	Total	C	O	0
			15	14	1	

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		AltConf
60	A	19	Total	O	0
			19	19	
60	B	46	Total	O	0
			46	46	
60	C	42	Total	O	0
			42	42	
60	D	107	Total	O	0
			107	107	
60	E	10	Total	O	0
			10	10	
60	F	42	Total	O	0
			42	42	
60	G	128	Total	O	0
			128	128	
60	H	60	Total	O	0
			60	60	
60	I	52	Total	O	0
			52	52	
60	J	25	Total	O	0
			25	25	
60	K	8	Total	O	0
			8	8	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
60	L	55	Total 55	O 55	0
60	M	61	Total 61	O 61	0
60	N	38	Total 38	O 38	0
60	O	15	Total 15	O 15	0
60	P	41	Total 41	O 41	0
60	Q	50	Total 50	O 50	0
60	R	11	Total 11	O 11	0
60	T	2	Total 2	O 2	0
60	U	7	Total 7	O 7	0
60	V	5	Total 5	O 5	0
60	W	11	Total 11	O 11	0
60	X	13	Total 13	O 13	0
60	Z	31	Total 31	O 31	0
60	a	14	Total 14	O 14	0
60	b	2	Total 2	O 2	0
60	c	1	Total 1	O 1	0
60	d	13	Total 13	O 13	0
60	e	13	Total 13	O 13	0
60	f	2	Total 2	O 2	0
60	g	8	Total 8	O 8	0
60	h	16	Total 16	O 16	0

Continued on next page...

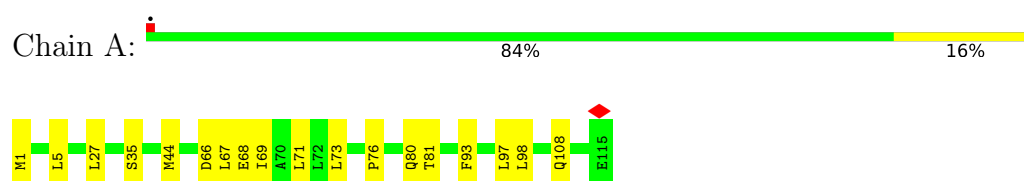
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
60	i	4	Total 4	O 4	0
60	j	2	Total 2	O 2	0
60	k	1	Total 1	O 1	0
60	l	10	Total 10	O 10	0
60	m	11	Total 11	O 11	0
60	n	19	Total 19	O 19	0
60	o	5	Total 5	O 5	0
60	p	20	Total 20	O 20	0
60	q	24	Total 24	O 24	0
60	r	13	Total 13	O 13	0
60	s	3	Total 3	O 3	0

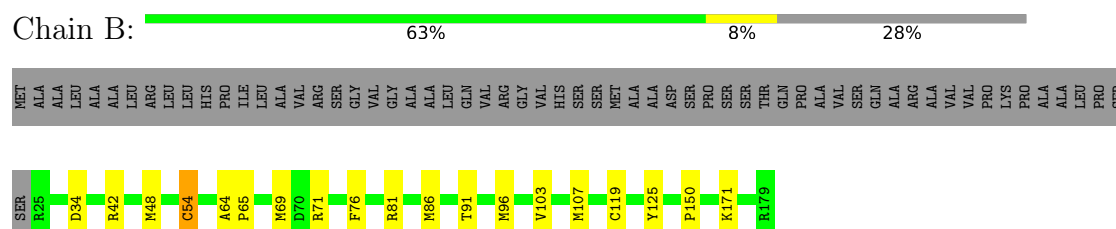
3 Residue-property plots [i](#)

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

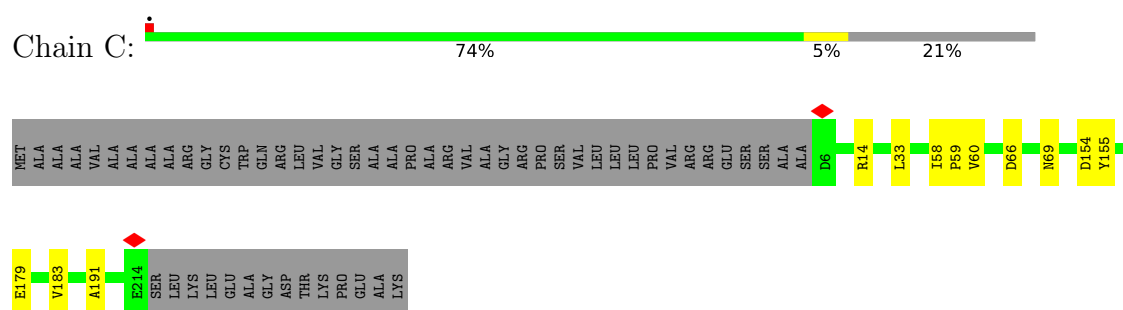
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



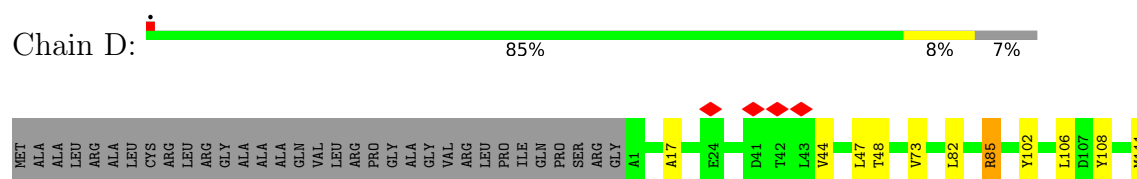
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



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



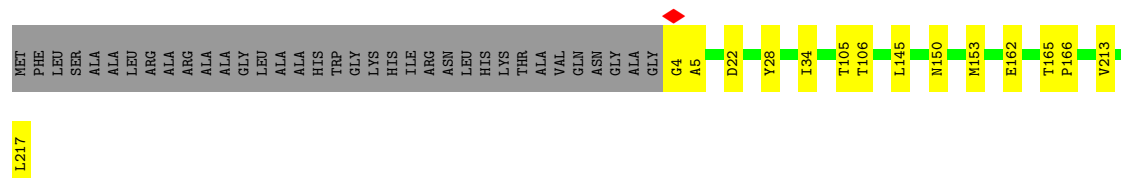
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial





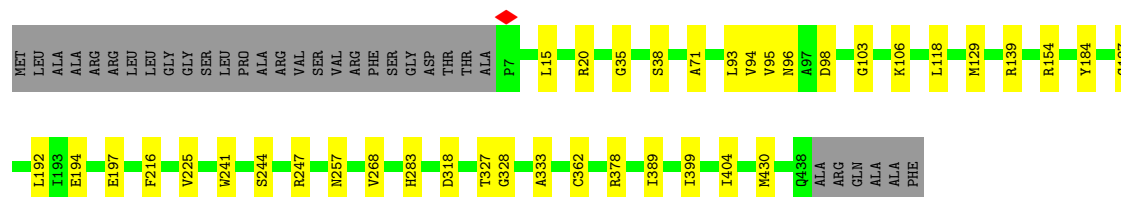
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E: 80% 6% 14%



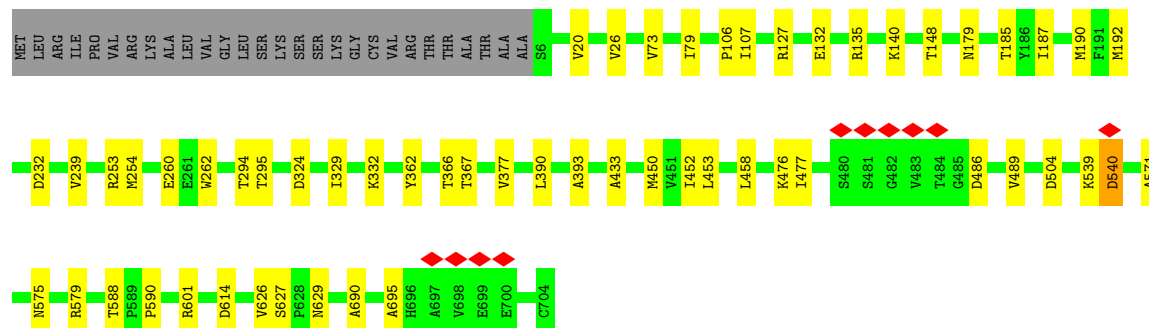
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F: 85% 8% 7%



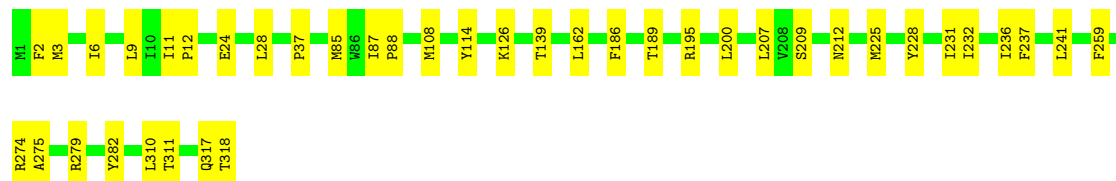
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G: 88% 8% 4%



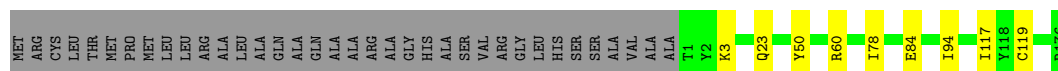
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H: 87% 13% 0%



- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:  79% 17%



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:  91% 9%



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  86% 14%

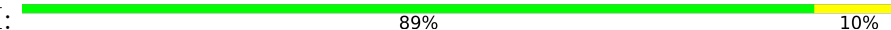


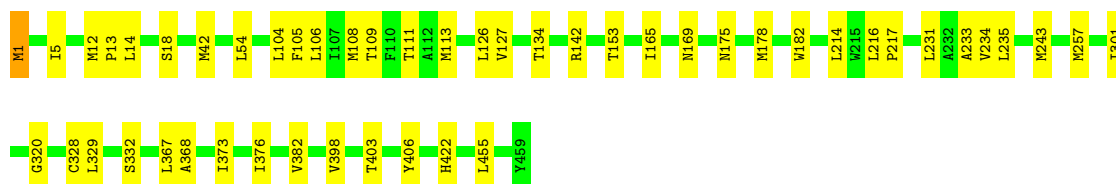
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:  89% 11%

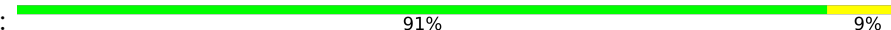


- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:  89% 10%



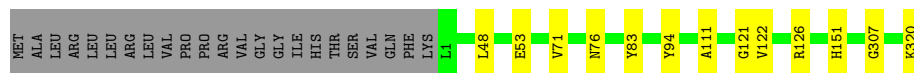
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:  91% 9%



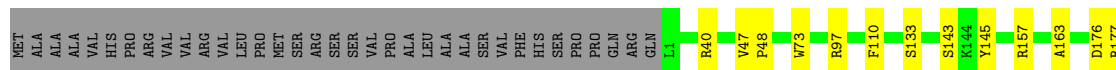
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O: 90% 7%



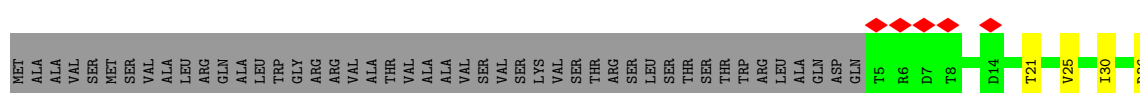
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P: 83% 7% 10%



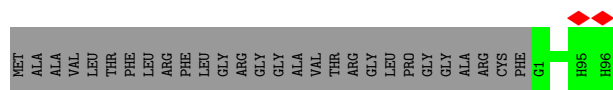
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q: 68% 6% 26%



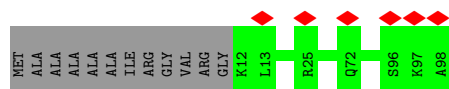
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R: 77% 23%

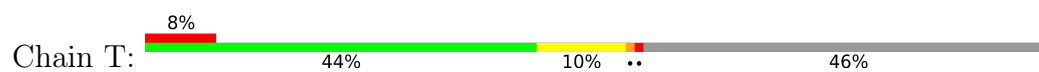


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S: 6% 88% 12%



- Molecule 20: Acyl carrier protein, mitochondrial



MET ALA VAL ARG VAL CYS ALA ARG VAL ASP VAL ARG LEU PRO THR PHE ALA PRO PRO PRO PRO LEU ARG PRO LEU THR LEU ALA ALA ALA ARG PRO LEU THR THR PHE ALA ALA GLU THR THR ARG ARG PRO GLY ALA ALA PRO LEU PRO ALA LEU VAL LEU ALA GLN VAL PRO GLY ARG

VAL THR GLN LEU ARG CYS GLN TYR ASP ALA P4 P5 L6 E9 D13 R14 V15 L19 D23 K24 I25 D26 D27 E28 K29 L30 S31 S32 N33 S34 K37 K38 D39 S44 L45 D46 M52 E61 I65 E68 K64 Y67 E68

- Molecule 20: Acyl carrier protein, mitochondrial



MET ALA VAL ARG VAL CYS ALA ARG VAL ASP VAL ARG LEU PRO THR PHE ALA ALA GLU THR THR ARG ARG PRO GLY ALA ALA PRO LEU PRO ALA LEU VAL LEU ALA GLN VAL PRO GLY ARG

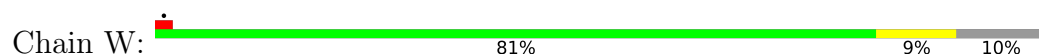
VAL THR GLN LEU ARG CYS GLN TYR ASP A3 P4 P5 V15 L16 Y17 Y18 L19 K20 L21 P27 E28 K29 L30 S31 V32 N33 S34 K37 S44 M52 E57 E61 D64 I65 D66 A67 E68 E68

- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



MET A1 G2 L3 Q49 I50 E53 M57 R70 Q82 I115

- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



MET ALA SER GLY LEU ARG GLN ALA VAL ALA S14 R33 W39 Y40 R41 H48 R64 I73 V79 G86 V96 T101 R114 P115 K116 D127 P128

- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



MET P1 E16 N39 M43 W47 M63 C87 C99 D120 L121 D156 M171

- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



MET A1 E2 T3 V4 L5 R6 D10 I11 F48 V52 T104 V140

- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:  87% 11% .



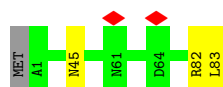
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:  97% .



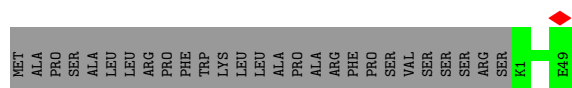
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:  95% . .



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c:  64% 36%



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:  92% 8%



- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:  86% 8% 7%

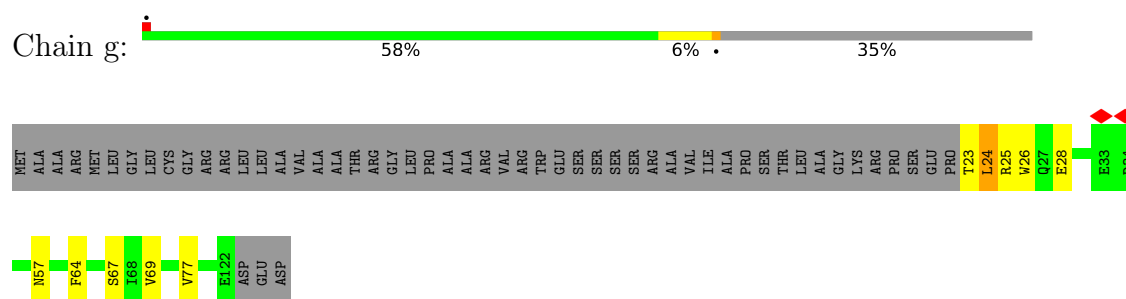


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

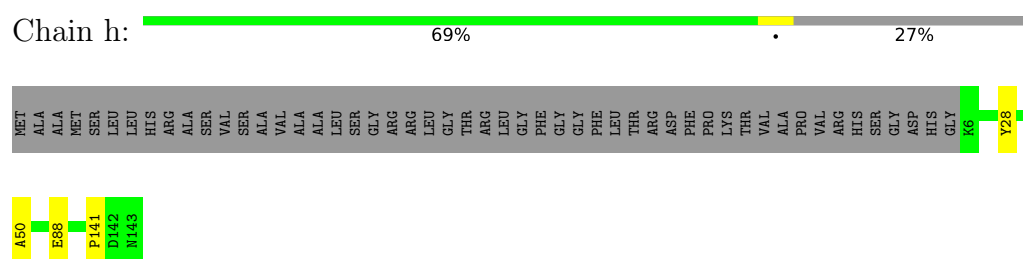
Chain f:  18% 86% 14%



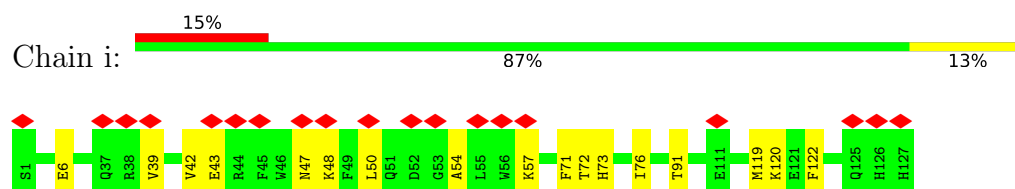
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



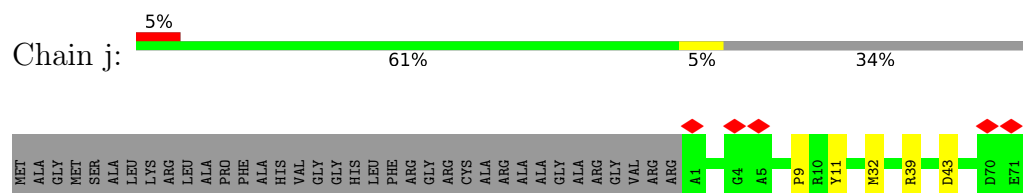
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



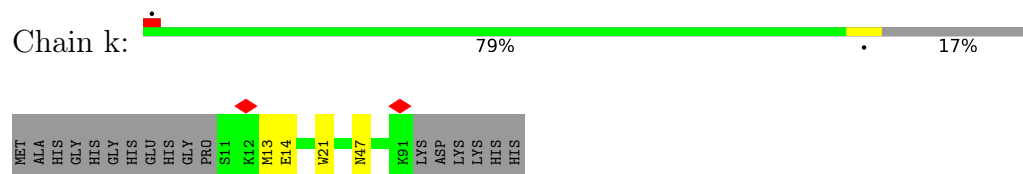
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



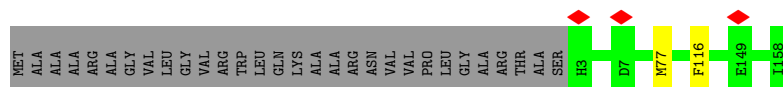
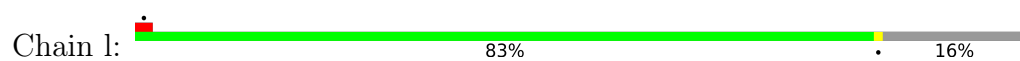
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



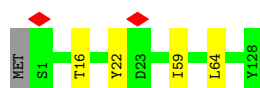
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



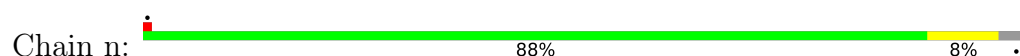
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



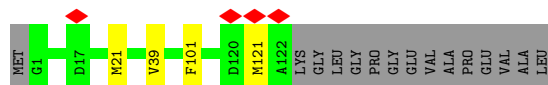
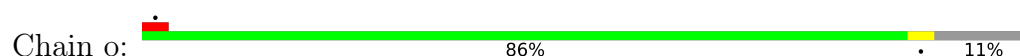
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



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



- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



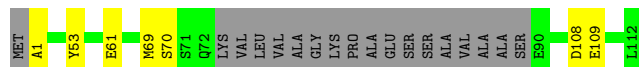
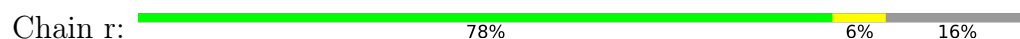
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



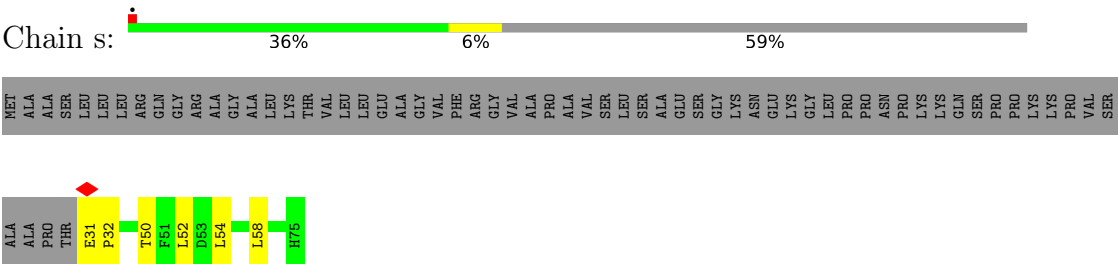
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



● Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23449	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 ($e^-/\text{\AA}^2$)	40.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	31.499	Depositor
Minimum map value	-14.518	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.943	Depositor
Recommended contour level	5	Depositor
Map size (Å)	479.744, 479.744, 479.744	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7496, 0.7496, 0.7496	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAC, AME, GTP, ZN, U10, K, NDP, FES, PC1, FME, 3PE, MG, FMN, CDL, 2MR, CHD, AYA, MYR, SF4, EH2

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	0.28	0/936	0.29	0/1281
2	B	0.31	0/1272	0.40	1/1720 (0.1%)
3	C	0.28	0/1789	0.31	0/2436
4	D	0.29	0/3537	0.30	0/4794
5	E	0.25	0/1699	0.32	0/2312
6	F	0.25	0/3424	0.30	0/4627
7	G	0.27	0/5457	0.33	0/7397
8	H	0.33	0/2579	0.37	0/3524
9	I	0.30	0/1445	0.33	0/1956
10	J	0.25	0/1370	0.29	0/1859
11	K	0.28	0/745	0.33	0/1008
12	L	0.26	0/4920	0.29	0/6694
13	M	0.29	0/3738	0.32	0/5097
14	N	0.28	0/2792	0.31	0/3800
15	O	0.24	0/2651	0.27	0/3587
16	P	0.26	0/2847	0.31	0/3864
17	Q	0.26	0/1072	0.31	0/1449
18	R	0.26	0/753	0.29	0/1014
19	S	0.22	0/711	0.29	0/956
20	T	0.29	0/700	0.63	1/944 (0.1%)
20	U	0.36	0/705	0.68	1/952 (0.1%)
21	V	0.25	0/948	0.26	0/1284
22	W	0.25	0/1000	0.31	0/1344
23	X	0.25	0/1439	0.33	0/1942
24	Y	0.23	0/1042	0.28	0/1414
25	Z	0.26	0/1181	0.30	0/1592
26	a	0.26	0/584	0.31	0/786
27	b	0.23	0/672	0.33	0/923
28	c	0.23	0/427	0.27	0/579
29	d	0.26	0/1018	0.32	0/1375
30	e	0.23	0/850	0.36	0/1136

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.23	0/505	0.39	0/681
32	g	0.31	0/865	0.41	1/1175 (0.1%)
33	h	0.26	0/1188	0.30	0/1607
34	i	0.23	0/1127	0.39	1/1534 (0.1%)
35	j	0.22	0/624	0.27	0/855
36	k	0.20	0/672	0.27	0/906
37	l	0.24	0/1369	0.32	0/1873
38	m	0.25	0/1094	0.29	0/1480
39	n	0.24	0/1545	0.30	0/2092
40	o	0.25	0/1073	0.34	0/1437
41	p	0.24	0/1486	0.30	0/2004
42	q	0.25	0/1250	0.31	0/1698
43	r	0.25	0/789	0.31	0/1068
44	s	0.20	0/403	0.27	0/545
All	All	0.27	0/68293	0.32	5/92601 (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
4	D	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	U	28	GLU	CA-CB-CG	6.21	126.51	114.10
20	T	28	GLU	CA-CB-CG	6.19	126.47	114.10
2	B	54	CYS	CA-CB-SG	5.50	127.05	114.40
32	g	57	ASN	N-CA-C	-5.12	106.54	112.89
34	i	39	VAL	CG1-CB-CG2	5.08	121.97	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	85	2MR	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	921	0	952	19	0
2	B	1241	0	1251	20	0
3	C	1738	0	1685	9	0
4	D	3459	0	3405	32	0
5	E	1659	0	1664	9	0
6	F	3347	0	3297	24	0
7	G	5366	0	5378	41	0
8	H	2517	0	2631	33	0
9	I	1414	0	1370	10	0
10	J	1345	0	1352	14	0
11	K	745	0	785	14	0
12	L	4802	0	4960	44	0
13	M	3654	0	3852	37	0
14	N	2733	0	2912	24	0
15	O	2589	0	2566	7	0
16	P	2768	0	2782	24	0
17	Q	1049	0	1045	10	0
18	R	740	0	714	0	0
19	S	700	0	719	0	0
20	T	688	0	684	13	0
20	U	693	0	688	18	0
21	V	928	0	972	4	0
22	W	976	0	991	13	0
23	X	1402	0	1381	7	0
24	Y	1030	0	1039	5	0
25	Z	1152	0	1151	16	0
26	a	569	0	568	2	0
27	b	651	0	662	2	0
28	c	414	0	415	0	0
29	d	999	0	988	6	0
30	e	829	0	829	7	0
31	f	492	0	501	7	0
32	g	839	0	790	8	0
33	h	1154	0	1168	6	0
34	i	1097	0	1108	12	0
35	j	597	0	536	4	0
36	k	653	0	639	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	l	1314	0	1210	2	0
38	m	1067	0	1067	4	0
39	n	1492	0	1438	12	0
40	o	1048	0	1018	3	0
41	p	1453	0	1425	5	0
42	q	1209	0	1182	2	0
43	r	776	0	782	5	0
44	s	391	0	361	4	0
45	A	47	0	71	0	0
45	H	36	0	46	0	0
45	K	44	0	62	0	0
45	L	135	0	201	2	0
45	M	142	0	212	2	0
45	N	51	0	82	7	0
45	P	35	0	44	0	0
45	Y	161	0	195	1	0
45	d	49	0	75	0	0
45	m	91	0	136	2	0
46	A	103	0	128	1	0
46	B	46	0	66	0	0
46	I	98	0	150	1	0
46	M	35	0	44	0	0
46	Y	46	0	66	0	0
46	Z	48	0	73	7	0
46	d	39	0	52	0	0
46	g	44	0	65	0	0
46	h	47	0	71	1	0
46	q	97	0	145	1	0
47	B	8	0	0	1	0
47	F	8	0	0	0	0
47	G	16	0	0	0	0
47	I	16	0	0	0	0
48	D	63	0	90	2	0
49	E	4	0	0	0	0
49	G	4	0	0	0	0
50	F	31	0	19	0	0
51	G	1	0	0	0	0
52	H	51	0	46	0	0
52	L	76	0	99	0	0
52	N	62	0	68	0	0
52	X	86	0	125	1	0
52	d	65	0	77	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	h	80	0	104	1	0
52	r	61	0	66	0	0
53	O	32	0	12	1	0
54	O	1	0	0	0	0
55	P	48	0	26	3	0
56	R	1	0	0	0	0
57	T	37	0	0	2	0
57	U	37	0	0	2	0
58	i	29	0	37	1	0
59	o	15	0	27	0	0
60	A	19	0	0	2	0
60	B	46	0	0	1	0
60	C	42	0	0	0	0
60	D	107	0	0	1	0
60	E	10	0	0	0	0
60	F	42	0	0	2	0
60	G	128	0	0	3	0
60	H	60	0	0	3	0
60	I	52	0	0	1	0
60	J	25	0	0	0	0
60	K	8	0	0	0	0
60	L	55	0	0	2	0
60	M	61	0	0	2	0
60	N	38	0	0	3	0
60	O	15	0	0	0	0
60	P	41	0	0	3	0
60	Q	50	0	0	3	0
60	R	11	0	0	0	0
60	T	2	0	0	1	0
60	U	7	0	0	0	0
60	V	5	0	0	0	0
60	W	11	0	0	1	0
60	X	13	0	0	0	0
60	Z	31	0	0	1	0
60	a	14	0	0	0	0
60	b	2	0	0	0	0
60	c	1	0	0	0	0
60	d	13	0	0	0	0
60	e	13	0	0	0	0
60	f	2	0	0	0	0
60	g	8	0	0	0	0
60	h	16	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	i	4	0	0	0	0
60	j	2	0	0	0	0
60	k	1	0	0	0	0
60	l	10	0	0	0	0
60	m	11	0	0	0	0
60	n	19	0	0	0	0
60	o	5	0	0	0	0
60	p	20	0	0	1	0
60	q	24	0	0	0	0
60	r	13	0	0	1	0
60	s	3	0	0	0	0
All	All	69986	0	69693	460	0

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

All (460) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:HD11	11:K:68:ALA:HB3	1.44	0.96
20:U:31:SER:HG	20:U:34:SER:HG	1.06	0.95
14:N:263:LYS:HG3	60:N:522:HOH:O	1.68	0.94
7:G:190:MET:HE3	7:G:695:ALA:HB2	1.50	0.93
7:G:433:ALA:O	7:G:476:LYS:NZ	2.02	0.91
12:L:439:THR:OG1	20:U:57:GLU:OE1	1.90	0.90
20:T:31:SER:HG	20:T:34:SER:HG	1.07	0.89
8:H:209:SER:OG	8:H:212:ASN:OD1	1.91	0.89
14:N:182:SER:OG	14:N:293:TYR:OH	1.92	0.88
13:M:14:LEU:O	13:M:18:SER:OG	1.94	0.85
21:V:49:GLN:NE2	21:V:53:GLU:OE2	2.11	0.84
46:Z:201:PC1:H133	46:Z:201:PC1:O12	1.77	0.84
20:T:68:GLU:OE2	22:W:33:ARG:NH2	2.11	0.82
29:d:45:ASP:OD2	29:d:64:TYR:OH	1.98	0.81
8:H:24:GLU:OE2	8:H:274:ARG:NH1	2.15	0.80
20:T:28:GLU:OE1	20:T:28:GLU:N	2.13	0.79
16:P:97:ARG:NH1	55:P:501:NDP:O1A	2.16	0.79
20:U:28:GLU:OE1	20:U:28:GLU:N	2.12	0.79
1:A:80:GLN:OE1	8:H:317:GLN:NE2	2.14	0.79
17:Q:47:SER:OG	60:Q:201:HOH:O	1.99	0.79
16:P:143:SER:OG	16:P:282:ASP:OD1	2.01	0.78
8:H:311:THR:OG1	25:Z:51:MET:SD	2.41	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:318:THR:O	60:H:701:HOH:O	2.00	0.77
7:G:26:VAL:HG13	7:G:79:ILE:HD13	1.65	0.77
25:Z:21:TYR:OH	43:r:108:ASP:OD2	2.02	0.77
60:A:319:HOH:O	10:J:141:MET:SD	2.42	0.76
57:U:101:EHZ:O3	39:n:11:HIS:NE2	2.20	0.75
7:G:232:ASP:OD2	60:G:901:HOH:O	2.03	0.75
2:B:48:MET:O	60:B:301:HOH:O	2.04	0.75
8:H:318:THR:OG1	60:H:702:HOH:O	2.03	0.75
32:g:67:SER:OG	33:h:28:TYR:O	2.05	0.74
3:C:179:GLU:OE1	16:P:40:ARG:NH1	2.23	0.72
10:J:124:ASP:OD1	11:K:2:SER:OG	2.07	0.72
13:M:328:CYS:O	60:M:1001:HOH:O	2.07	0.72
16:P:263:TYR:CE2	16:P:284:VAL:HG22	2.25	0.71
20:U:17:TYR:HH	36:k:21:TRP:CD1	2.08	0.71
17:Q:106:GLU:OE1	60:Q:202:HOH:O	2.07	0.71
16:P:330:GLU:OE2	22:W:48:HIS:ND1	2.19	0.70
17:Q:36:ARG:NE	17:Q:106:GLU:OE1	2.24	0.70
57:T:101:EHZ:O1	60:T:201:HOH:O	2.08	0.69
39:n:34:ASP:OD1	39:n:35:LYS:N	2.26	0.69
4:D:393:ALA:O	60:D:801:HOH:O	2.09	0.69
13:M:127:VAL:HG11	45:N:401:3PE:H3I2	1.73	0.69
20:U:3:ALA:O	20:U:4:PRO:C	2.36	0.69
6:F:184:TYR:OH	60:F:601:HOH:O	2.09	0.68
8:H:236:ILE:HG23	8:H:259:PHE:HZ	1.58	0.68
17:Q:82:LEU:O	60:Q:203:HOH:O	2.11	0.67
1:A:67:LEU:HD11	11:K:68:ALA:CB	2.23	0.67
4:D:371:LYS:HE2	4:D:424:VAL:HG23	1.77	0.67
58:i:201:CHD:H212	58:i:201:CHD:H12	1.77	0.67
25:Z:94:GLU:OE1	60:Z:301:HOH:O	2.12	0.67
15:O:94:TYR:OH	15:O:151:HIS:ND1	2.24	0.67
15:O:83:TYR:OH	53:O:401:GTP:O2'	2.11	0.66
15:O:111:ALA:HB1	15:O:122:VAL:HG21	1.78	0.66
7:G:601:ARG:NH2	7:G:614:ASP:OD1	2.28	0.66
12:L:26:THR:O	12:L:26:THR:HG22	1.95	0.66
13:M:126:LEU:HD21	13:M:153:THR:HG21	1.77	0.66
17:Q:36:ARG:NH1	17:Q:106:GLU:OE2	2.29	0.65
3:C:183:VAL:O	22:W:101:THR:OG1	2.11	0.65
1:A:67:LEU:HD13	11:K:65:VAL:HA	1.79	0.65
20:T:46:ASP:OD1	22:W:64:ARG:NH2	2.30	0.64
8:H:236:ILE:HG23	8:H:259:PHE:CZ	2.31	0.64
22:W:127:ASP:OD1	60:W:201:HOH:O	2.15	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:i:119:MET:HE3	34:i:122:PHE:CE1	2.31	0.64
13:M:42:MET:HE1	32:g:77:VAL:HG22	1.79	0.64
14:N:83:GLN:OE1	14:N:85:THR:N	2.31	0.64
8:H:310:LEU:HD12	8:H:311:THR:HG23	1.80	0.63
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.32	0.63
20:U:17:TYR:OH	36:k:21:TRP:NE1	2.32	0.63
3:C:14:ARG:NH1	43:r:61:GLU:O	2.32	0.63
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.32	0.63
14:N:257:LEU:HD21	45:N:401:3PE:H3I3	1.80	0.62
6:F:378:ARG:NE	7:G:132:GLU:OE2	2.23	0.62
13:M:105:PHE:O	13:M:109:THR:OG1	2.05	0.62
33:h:49:GLU:OE1	52:h:201:CDL:O1	2.14	0.62
2:B:91:THR:OG1	2:B:119:CYS:SG	2.57	0.62
12:L:392:LYS:NZ	12:L:416:THR:HG23	2.14	0.62
41:p:92:ARG:NH1	60:p:201:HOH:O	2.32	0.62
2:B:54:CYS:HB3	4:D:108:TYR:CG	2.35	0.62
4:D:154:VAL:HG13	4:D:297:TYR:HE1	1.64	0.62
33:h:50:ALA:HB2	41:p:60:TYR:CE2	2.35	0.61
5:E:105:THR:HG22	5:E:106:THR:H	1.64	0.61
25:Z:68:ARG:NH2	25:Z:72:MET:SD	2.73	0.61
12:L:35:TYR:OH	34:i:73:HIS:NE2	2.23	0.61
34:i:54:ALA:HB3	34:i:57:LYS:HG2	1.82	0.61
43:r:69:MET:SD	43:r:70:SER:N	2.73	0.61
1:A:5:LEU:HD21	8:H:3:MET:SD	2.41	0.60
4:D:326:ASP:OD1	7:G:127:ARG:NH2	2.33	0.60
38:m:16:THR:O	38:m:22:TYR:OH	2.12	0.60
39:n:15:VAL:HG22	39:n:63:LEU:HD13	1.83	0.60
12:L:373:LEU:HD23	12:L:431:LEU:HD11	1.84	0.60
6:F:15:LEU:O	6:F:20:ARG:NH1	2.34	0.60
7:G:332:LYS:NZ	60:G:909:HOH:O	2.35	0.60
20:U:68:GLU:OE1	20:U:68:GLU:HA	2.02	0.60
13:M:422:HIS:HB2	38:m:59:ILE:HD12	1.83	0.59
1:A:68:GLU:OE1	1:A:98:LEU:HD13	2.02	0.59
13:M:134:THR:O	13:M:142:ARG:NE	2.29	0.59
16:P:263:TYR:CD2	16:P:284:VAL:HG13	2.37	0.59
25:Z:140:PHE:O	46:Z:201:PC1:H142	2.03	0.59
20:T:68:GLU:HA	20:T:68:GLU:OE1	2.02	0.59
13:M:178:MET:SD	41:p:81:VAL:HG11	2.43	0.58
4:D:300:ARG:NH2	4:D:420:THR:O	2.36	0.58
48:D:701:U10:H453	8:H:225:MET:HG2	1.86	0.58
20:U:52:MET:HE1	39:n:23:LEU:HB3	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:44:VAL:O	4:D:44:VAL:HG13	2.02	0.58
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.34	0.58
1:A:27:LEU:HD12	46:A:202:PC1:H133	1.84	0.58
29:d:2:MET:HE3	29:d:82:MET:HE3	1.84	0.58
7:G:107:ILE:HG23	9:I:78:ILE:HD12	1.85	0.57
9:I:3:LYS:NZ	43:r:109:GLU:OE2	2.35	0.57
21:V:57:MET:HE2	21:V:70:ARG:HB3	1.87	0.57
15:O:71:VAL:HG22	15:O:76:ASN:HA	1.87	0.57
2:B:125:TYR:HB2	9:I:117:ILE:CG2	2.35	0.57
7:G:140:LYS:O	7:G:148:THR:OG1	2.18	0.57
4:D:47:LEU:HD21	8:H:126:LYS:HD3	1.87	0.56
4:D:165:THR:OG1	8:H:275:ALA:O	2.15	0.56
16:P:97:ARG:HE	55:P:501:NDP:H8A	1.69	0.56
42:q:65:THR:O	42:q:73:THR:OG1	2.23	0.56
34:i:47:ASN:OD1	34:i:48:LYS:N	2.40	0.55
60:H:717:HOH:O	46:Z:201:PC1:H132	2.07	0.55
6:F:154:ARG:HA	44:s:58:LEU:HD21	1.89	0.55
7:G:329:ILE:HD11	7:G:626:VAL:HG21	1.89	0.55
43:r:53:TYR:OH	60:r:301:HOH:O	2.18	0.55
10:J:45:LEU:HD21	46:Z:201:PC1:H231	1.89	0.55
4:D:73:VAL:HG21	4:D:414:VAL:HG21	1.89	0.55
6:F:247:ARG:NH2	6:F:318:ASP:OD2	2.38	0.54
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.90	0.54
7:G:20:VAL:HG21	7:G:73:VAL:HG21	1.88	0.54
16:P:48:PRO:HB2	16:P:73:TRP:CD1	2.43	0.54
16:P:176:ASP:OD1	16:P:177:ARG:N	2.41	0.54
20:U:17:TYR:HH	36:k:21:TRP:NE1	2.06	0.54
6:F:93:LEU:HD13	6:F:129:MET:HE1	1.90	0.54
7:G:190:MET:HE1	7:G:690:ALA:HB1	1.89	0.54
20:U:57:GLU:OE2	35:j:11:TYR:OH	2.25	0.54
13:M:113:MET:HG2	13:M:175:ASN:OD1	2.08	0.54
33:h:141:PRO:O	60:h:301:HOH:O	2.19	0.53
14:N:236:LYS:HG3	14:N:237:THR:HG23	1.89	0.53
7:G:190:MET:HE3	7:G:695:ALA:CB	2.30	0.53
23:X:120:ASP:OD1	23:X:121:LEU:N	2.37	0.53
1:A:80:GLN:HB3	8:H:317:GLN:HE21	1.73	0.53
1:A:80:GLN:NE2	60:A:303:HOH:O	2.41	0.53
41:p:130:GLN:O	41:p:134:VAL:HG23	2.09	0.53
16:P:263:TYR:CE2	16:P:284:VAL:HG13	2.44	0.52
12:L:474:PRO:O	60:L:801:HOH:O	2.18	0.52
40:o:121:MET:HE2	40:o:121:MET:HA	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:f:7:VAL:HG12	31:f:7:VAL:O	2.09	0.52
4:D:106:LEU:HD11	4:D:391:ILE:HD13	1.91	0.52
12:L:286:LEU:HD22	12:L:411:MET:SD	2.50	0.52
32:g:23:THR:O	32:g:24:LEU:HG	2.10	0.52
12:L:251:THR:O	12:L:254:VAL:HG22	2.09	0.52
8:H:195:ARG:HD3	8:H:231:ILE:HD11	1.92	0.51
12:L:230:HIS:N	12:L:231:PRO:CD	2.73	0.51
16:P:157:ARG:NH2	16:P:163:ALA:O	2.41	0.51
34:i:119:MET:HE3	34:i:122:PHE:HE1	1.74	0.51
15:O:307:GLY:O	15:O:320:LYS:NZ	2.33	0.51
20:T:6:LEU:HD12	20:T:84:LYS:HD2	1.91	0.51
12:L:392:LYS:HZ1	12:L:416:THR:HG23	1.74	0.51
13:M:108:MET:HE1	52:X:201:CDL:H221	1.92	0.51
11:K:43:MET:HE1	14:N:72:MET:HE1	1.92	0.51
25:Z:129:ALA:O	25:Z:133:VAL:HG23	2.11	0.51
1:A:93:PHE:O	1:A:97:LEU:HD13	2.10	0.51
6:F:118:LEU:HD13	6:F:225:VAL:HG13	1.94	0.51
13:M:178:MET:HE1	13:M:182:TRP:CZ2	2.46	0.50
7:G:393:ALA:O	60:G:902:HOH:O	2.19	0.50
20:U:4:PRO:HG3	35:j:9:PRO:HG3	1.92	0.50
13:M:403:THR:HA	13:M:406:TYR:CE1	2.46	0.50
8:H:200:LEU:HD13	8:H:282:TYR:HB3	1.92	0.50
9:I:119:CYS:O	60:I:301:HOH:O	2.18	0.50
20:T:31:SER:OG	20:T:34:SER:OG	2.06	0.50
7:G:366:THR:O	7:G:367:THR:OG1	2.16	0.50
12:L:264:TYR:N	12:L:265:PRO:CD	2.74	0.50
14:N:289:ASN:HA	14:N:292:PHE:CE1	2.47	0.50
40:o:21:MET:HE1	40:o:101:PHE:CD2	2.47	0.50
5:E:22:ASP:OD1	5:E:28:TYR:OH	2.30	0.50
7:G:453:LEU:HD21	7:G:458:LEU:HD21	1.94	0.49
20:T:68:GLU:OE2	22:W:33:ARG:CZ	2.59	0.49
46:h:202:PC1:H2D1	46:h:202:PC1:H2I2	1.92	0.49
7:G:627:SER:OG	7:G:629:ASN:OD1	2.29	0.49
39:n:142:GLU:OE2	39:n:157:ARG:NH2	2.39	0.49
4:D:111:MET:SD	4:D:111:MET:N	2.85	0.49
12:L:69:LEU:HD11	13:M:455:LEU:CD1	2.43	0.49
7:G:539:LYS:O	7:G:540:ASP:HB2	2.13	0.49
30:e:85:LEU:O	30:e:89:GLY:N	2.46	0.49
12:L:419:THR:HA	12:L:422:TYR:CE1	2.48	0.49
42:q:144:TYR:O	42:q:145:LYS:C	2.56	0.49
4:D:154:VAL:HG11	4:D:225:LEU:HD21	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:15:VAL:O	20:U:19:LEU:HD12	2.13	0.49
45:M:902:3PE:H3B1	14:N:284:ILE:HG21	1.95	0.49
16:P:253:PHE:C	16:P:254:LEU:HD12	2.38	0.49
32:g:64:PHE:O	32:g:69:VAL:HG23	2.13	0.49
8:H:200:LEU:HD23	8:H:279:ARG:HD3	1.94	0.48
13:M:329:LEU:O	13:M:332:SER:OG	2.26	0.48
6:F:96:ASN:ND2	6:F:187:GLY:O	2.45	0.48
20:T:15:VAL:O	20:T:19:LEU:HD12	2.12	0.48
32:g:26:TRP:CD1	32:g:28:GLU:HB2	2.47	0.48
3:C:58:ILE:HB	3:C:59:PRO:HD3	1.96	0.48
5:E:4:GLY:O	5:E:5:ALA:HB3	2.13	0.48
12:L:331:THR:HB	12:L:387:THR:HG22	1.95	0.48
12:L:558:LEU:HD21	45:m:402:3PE:H2H2	1.95	0.48
16:P:176:ASP:O	16:P:177:ARG:HB2	2.13	0.48
44:s:31:GLU:N	44:s:32:PRO:CD	2.76	0.48
3:C:154:ASP:OD1	3:C:155:TYR:N	2.47	0.48
7:G:362:TYR:OH	7:G:504:ASP:OD1	2.22	0.48
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.96	0.48
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.48	0.48
20:U:64:ASP:OD2	39:n:17:ARG:HG2	2.14	0.48
6:F:194:GLU:OE2	17:Q:133:LYS:NZ	2.29	0.48
25:Z:140:PHE:CZ	46:Z:201:PC1:H151	2.49	0.48
6:F:94:VAL:HG11	6:F:192:LEU:HD22	1.96	0.48
8:H:87:ILE:N	8:H:88:PRO:CD	2.77	0.48
12:L:537:ALA:HB3	12:L:538:PRO:HD3	1.96	0.48
12:L:556:ILE:HG22	12:L:557:TRP:N	2.29	0.48
13:M:231:LEU:HA	13:M:235:LEU:HD12	1.95	0.48
4:D:108:TYR:CZ	4:D:424:VAL:HG13	2.49	0.48
31:f:39:ASN:N	33:h:88:GLU:OE1	2.45	0.48
13:M:243:MET:HB3	13:M:301:ILE:HG21	1.96	0.47
16:P:145:TYR:CD2	16:P:286:ARG:HD3	2.48	0.47
10:J:123:GLY:O	10:J:126:VAL:HG22	2.14	0.47
2:B:69:MET:HE1	2:B:76:PHE:CE2	2.50	0.47
8:H:139:THR:HB	10:J:65:MET:SD	2.53	0.47
46:Z:201:PC1:H141	26:a:39:ALA:O	2.14	0.47
34:i:50:LEU:HD23	34:i:50:LEU:H	1.79	0.47
13:M:165:ILE:HG21	14:N:268:GLN:HA	1.94	0.47
11:K:56:ALA:O	11:K:59:MET:HG3	2.14	0.47
12:L:529:PHE:HB3	12:L:530:PRO:HD3	1.96	0.47
22:W:96:VAL:HG12	22:W:96:VAL:O	2.15	0.47
7:G:239:VAL:HG23	7:G:253:ARG:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:233:LEU:HB3	12:L:234:PRO:HD3	1.97	0.47
7:G:575:ASN:OD1	7:G:579:ARG:N	2.48	0.47
13:M:422:HIS:CB	38:m:59:ILE:HD12	2.43	0.47
16:P:133:SER:O	55:P:501:NDP:H6N	2.15	0.47
1:A:44:MET:HG2	22:W:96:VAL:HB	1.97	0.47
14:N:324:THR:HG22	14:N:325:PHE:CD1	2.50	0.47
34:i:120:LYS:CG	40:o:39:VAL:HG13	2.45	0.47
2:B:125:TYR:CE2	4:D:102:TYR:CD1	3.02	0.47
7:G:377:VAL:HG13	7:G:452:ILE:HD12	1.97	0.47
7:G:588:THR:HG21	17:Q:63:GLU:HA	1.97	0.47
13:M:106:LEU:HD13	13:M:234:VAL:HG11	1.96	0.47
7:G:329:ILE:CD1	7:G:626:VAL:HG21	2.45	0.46
12:L:375:VAL:HG22	35:j:32:MET:SD	2.55	0.46
4:D:259:MET:HE1	4:D:405:MET:HE1	1.97	0.46
12:L:24:PHE:O	12:L:24:PHE:CG	2.69	0.46
13:M:12:MET:HB2	13:M:13:PRO:HD3	1.96	0.46
6:F:362:CYS:HB3	6:F:404:ILE:HD12	1.98	0.46
11:K:42:VAL:O	11:K:46:LEU:HD13	2.15	0.46
15:O:48:LEU:HD22	15:O:121:GLY:HA3	1.96	0.46
1:A:69:ILE:O	1:A:73:LEU:N	2.43	0.46
6:F:95:VAL:HG11	6:F:118:LEU:HD11	1.97	0.46
13:M:178:MET:HE1	13:M:182:TRP:CE2	2.50	0.46
14:N:335:MET:HE2	45:N:401:3PE:C2B	2.45	0.46
57:U:101:EHZ:O3	39:n:11:HIS:CD2	2.68	0.46
23:X:39:ASN:OD1	25:Z:73:PRO:HG2	2.16	0.46
30:e:17:MET:O	30:e:17:MET:HG2	2.16	0.46
5:E:165:THR:HG22	5:E:166:PRO:HD2	1.98	0.46
7:G:324:ASP:HB3	7:G:571:ALA:HB1	1.98	0.46
7:G:486:ASP:OD1	7:G:486:ASP:O	2.33	0.46
12:L:245:ALA:O	12:L:249:SER:OG	2.33	0.46
7:G:294:THR:HG23	7:G:295:THR:N	2.30	0.46
14:N:335:MET:HE2	45:N:401:3PE:H2B1	1.96	0.46
20:U:21:LEU:HD13	36:k:47:ASN:HA	1.97	0.46
5:E:34:ILE:HD11	44:s:52:LEU:HD22	1.97	0.46
8:H:28:LEU:HD13	8:H:275:ALA:HB2	1.97	0.46
8:H:114:TYR:OH	10:J:61:LEU:O	2.31	0.46
8:H:207:LEU:O	8:H:209:SER:N	2.47	0.46
4:D:158:ALA:HB1	4:D:163:ALA:HB3	1.98	0.46
12:L:76:LEU:HD21	12:L:196:TRP:HE3	1.81	0.46
12:L:357:ARG:O	12:L:436:ARG:NE	2.41	0.46
1:A:71:LEU:O	10:J:147:TYR:OH	2.27	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:539:LYS:O	7:G:540:ASP:CB	2.63	0.45
11:K:56:ALA:C	11:K:58:MET:N	2.74	0.45
48:D:701:U10:H321	48:D:701:U10:H301	1.82	0.45
12:L:562:LEU:CB	12:L:563:PRO:CD	2.94	0.45
8:H:87:ILE:HG12	8:H:88:PRO:HD3	1.97	0.45
13:M:5:ILE:HD11	13:M:108:MET:HG2	1.98	0.45
16:P:258:LEU:HD23	16:P:263:TYR:HB2	1.99	0.45
8:H:85:MET:SD	8:H:108:MET:HB2	2.56	0.45
34:i:6:GLU:OE1	39:n:157:ARG:NH1	2.49	0.45
36:k:14:GLU:O	36:k:14:GLU:HG2	2.17	0.45
10:J:141:MET:HE3	30:e:26:HIS:CD2	2.51	0.45
20:U:28:GLU:H	20:U:28:GLU:CD	2.13	0.45
39:n:23:LEU:CD2	39:n:43:LEU:HD23	2.47	0.45
12:L:397:GLU:CG	12:L:482:MET:HE1	2.47	0.45
20:T:52:MET:CE	22:W:41:ARG:HD3	2.46	0.45
33:h:32:THR:O	33:h:36:VAL:HG23	2.17	0.45
39:n:132:TRP:O	39:n:136:VAL:HG23	2.17	0.45
6:F:98:ASP:O	6:F:139:ARG:HD2	2.17	0.45
16:P:233:PRO:HD3	16:P:307:ALA:HB1	1.98	0.45
6:F:389:ILE:HG13	6:F:430:MET:HE1	1.99	0.45
20:U:4:PRO:O	20:U:5:PRO:C	2.57	0.45
35:j:39:ARG:O	35:j:43:ASP:N	2.49	0.45
2:B:64:ALA:HB1	2:B:65:PRO:CD	2.47	0.45
8:H:186:PHE:O	8:H:189:THR:OG1	2.34	0.45
6:F:399:ILE:HG22	6:F:399:ILE:O	2.16	0.44
7:G:135:ARG:NH1	7:G:179:ASN:OD1	2.50	0.44
8:H:237:PHE:CE2	8:H:241:LEU:HD11	2.52	0.44
31:f:49:LYS:O	31:f:50:PRO:C	2.60	0.44
4:D:184:VAL:O	9:I:60:ARG:NH1	2.42	0.44
45:M:903:3PE:H3A1	14:N:335:MET:HE1	1.99	0.44
16:P:189:GLY:O	60:P:601:HOH:O	2.21	0.44
20:T:37:MET:HE1	20:T:44:SER:HA	2.00	0.44
4:D:149:ASN:OD1	4:D:371:LYS:NZ	2.51	0.44
12:L:405:ASN:ND2	37:l:116:PHE:O	2.48	0.44
14:N:242:VAL:HG11	45:N:401:3PE:C25	2.47	0.44
16:P:286:ARG:NH1	60:P:606:HOH:O	2.49	0.44
7:G:254:MET:HA	7:G:260:GLU:O	2.17	0.44
8:H:162:LEU:HD21	8:H:237:PHE:HE1	1.81	0.44
13:M:104:LEU:HG	13:M:108:MET:HE2	2.00	0.44
24:Y:48:PHE:O	24:Y:52:VAL:HG23	2.18	0.44
2:B:86:MET:CE	2:B:103:VAL:HG23	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:17:ALA:HB1	11:K:98:CYS:SG	2.58	0.44
12:L:183:ILE:HG21	13:M:382:VAL:HG11	1.99	0.44
13:M:127:VAL:HG11	45:N:401:3PE:C3I	2.44	0.44
23:X:43:MET:HE2	25:Z:73:PRO:HG3	2.00	0.44
1:A:108:GLN:HB2	10:J:169:MET:HE1	2.00	0.44
11:K:56:ALA:O	11:K:59:MET:N	2.43	0.44
24:Y:104:THR:HG22	24:Y:104:THR:O	2.17	0.44
36:k:13:MET:O	36:k:14:GLU:C	2.60	0.44
2:B:54:CYS:HB3	4:D:108:TYR:CB	2.47	0.44
2:B:71:ARG:NH1	9:I:50:TYR:O	2.51	0.44
3:C:191:ALA:O	17:Q:74:SER:OG	2.19	0.44
13:M:54:LEU:O	13:M:113:MET:HE2	2.18	0.44
17:Q:25:VAL:HB	17:Q:30:ILE:HD11	1.99	0.44
32:g:23:THR:HG22	32:g:24:LEU:N	2.33	0.44
3:C:66:ASP:O	21:V:82:GLN:NE2	2.51	0.44
16:P:196:LEU:HG	16:P:196:LEU:O	2.18	0.44
20:U:37:MET:HE1	20:U:44:SER:HA	1.99	0.44
14:N:337:LEU:N	14:N:338:PRO:CD	2.81	0.43
16:P:283:LYS:NZ	60:P:605:HOH:O	2.50	0.43
57:T:101:EHZ:O3	22:W:79:VAL:HG22	2.16	0.43
4:D:161:ILE:HG22	4:D:161:ILE:O	2.16	0.43
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.53	0.43
34:i:72:THR:HA	34:i:76:ILE:HD12	2.00	0.43
10:J:167:VAL:HG22	14:N:42:PRO:HG3	2.00	0.43
12:L:426:ILE:O	12:L:430:ALA:HB3	2.19	0.43
13:M:233:ALA:HA	13:M:320:GLY:HA2	2.00	0.43
29:d:18:ALA:HB2	29:d:81:TYR:CD1	2.53	0.43
2:B:150:PRO:HB3	47:B:201:SF4:S1	2.59	0.43
7:G:185:THR:O	7:G:187:ILE:N	2.47	0.43
13:M:1:FME:HE3	13:M:111:THR:HG21	2.01	0.43
22:W:39:TRP:HZ2	22:W:86:GLY:O	2.01	0.43
5:E:150:ASN:HB3	5:E:162:GLU:HB3	2.01	0.43
12:L:63:ILE:O	12:L:79:SER:HA	2.19	0.43
6:F:94:VAL:HG11	6:F:192:LEU:CD2	2.49	0.43
14:N:63:GLN:OE1	60:N:501:HOH:O	2.21	0.43
12:L:559:GLU:CD	13:M:214:LEU:HD13	2.43	0.43
23:X:43:MET:O	23:X:47:TRP:HE3	2.01	0.43
14:N:115:VAL:HB	14:N:116:PRO:HD3	2.01	0.43
15:O:53:GLU:OE1	15:O:126:ARG:NH1	2.48	0.43
25:Z:101:VAL:HG13	25:Z:102:PRO:HD2	2.01	0.43
29:d:45:ASP:OD2	52:d:203:CDL:O1	2.28	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:g:24:LEU:O	32:g:25:ARG:HB2	2.17	0.43
2:B:64:ALA:HB1	2:B:65:PRO:HD2	2.00	0.43
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.51	0.43
6:F:71:ALA:N	60:F:610:HOH:O	2.47	0.43
3:C:33:LEU:HD13	3:C:60:VAL:HG22	2.00	0.43
13:M:169:ASN:OD1	60:M:1002:HOH:O	2.21	0.43
12:L:342:CYS:SG	12:L:372:ALA:HB3	2.59	0.42
4:D:212:TYR:CD1	25:Z:19:ILE:HD11	2.54	0.42
7:G:190:MET:HB3	7:G:192:MET:HG2	2.01	0.42
17:Q:21:THR:HG21	22:W:73:ILE:HD11	2.00	0.42
34:i:91:THR:HA	41:p:4:TRP:HZ3	1.84	0.42
36:k:14:GLU:OE1	36:k:14:GLU:N	2.52	0.42
3:C:69:ASN:OD1	21:V:50:ILE:HG21	2.19	0.42
2:B:71:ARG:HA	8:H:37:PRO:HA	2.00	0.42
6:F:35:GLY:O	6:F:38:SER:OG	2.22	0.42
25:Z:13:VAL:HG13	25:Z:14:GLY:N	2.34	0.42
29:d:63:LEU:HD23	52:d:203:CDL:OA9	2.19	0.42
4:D:212:TYR:HD1	25:Z:19:ILE:HD11	1.85	0.42
10:J:126:VAL:HG23	10:J:127:ILE:HG23	2.01	0.42
23:X:16:GLU:OE1	23:X:16:GLU:N	2.52	0.42
23:X:63:ASN:OD1	25:Z:81:ARG:NH2	2.51	0.42
5:E:213:VAL:HG13	5:E:217:LEU:HD22	1.99	0.42
7:G:477:ILE:HD11	7:G:489:VAL:HG11	2.01	0.42
12:L:479:GLN:NE2	60:L:807:HOH:O	2.52	0.42
12:L:530:PRO:O	12:L:534:HIS:HB2	2.20	0.42
16:P:209:ASP:OD2	16:P:308:THR:N	2.51	0.42
1:A:66:ASP:O	1:A:69:ILE:HG12	2.20	0.42
6:F:241:TRP:O	6:F:244:SER:OG	2.37	0.42
10:J:157:THR:HG22	11:K:66:PHE:HE1	1.84	0.42
12:L:140:LEU:HD22	12:L:182:PHE:CZ	2.55	0.42
12:L:302:ILE:HG22	12:L:340:PHE:CZ	2.55	0.42
12:L:358:LYS:HG3	39:n:79:TYR:CE1	2.54	0.42
13:M:216:LEU:HB3	13:M:217:PRO:HD3	2.01	0.42
16:P:47:VAL:O	16:P:47:VAL:HG12	2.20	0.42
24:Y:11:ILE:O	24:Y:11:ILE:HG13	2.20	0.42
2:B:42:ARG:NH2	46:q:201:PC1:O14	2.47	0.42
7:G:366:THR:HB	7:G:450:MET:HE3	2.01	0.42
10:J:44:VAL:HG12	10:J:49:GLY:HA3	2.01	0.42
45:L:701:3PE:H2H1	13:M:398:VAL:HG22	2.01	0.42
2:B:34:ASP:OD2	2:B:171:LYS:HA	2.20	0.42
31:f:11:TRP:O	31:f:14:VAL:HG22	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:165:THR:CG2	5:E:166:PRO:HD2	2.50	0.41
6:F:106:LYS:HB3	6:F:257:ASN:HD21	1.85	0.41
11:K:56:ALA:O	11:K:58:MET:N	2.53	0.41
6:F:268:VAL:HG21	6:F:283:HIS:ND1	2.36	0.41
8:H:11:ILE:HB	8:H:12:PRO:HD3	2.02	0.41
12:L:578:THR:O	12:L:580:GLN:N	2.53	0.41
23:X:87:CYS:HB3	23:X:99:CYS:SG	2.60	0.41
24:Y:3:THR:HG23	24:Y:4:VAL:N	2.34	0.41
29:d:4:GLY:O	29:d:5:ARG:C	2.63	0.41
30:e:16:TRP:CE3	30:e:17:MET:HB2	2.56	0.41
31:f:20:PHE:CE2	31:f:24:TYR:CE2	3.08	0.41
31:f:20:PHE:CE2	31:f:24:TYR:HE2	2.38	0.41
1:A:73:LEU:O	1:A:76:PRO:HD2	2.19	0.41
2:B:86:MET:HE1	2:B:103:VAL:HG23	2.02	0.41
2:B:103:VAL:O	2:B:107:MET:HG3	2.21	0.41
11:K:59:MET:HG3	11:K:60:PRO:HD3	2.01	0.41
14:N:146:PHE:N	14:N:147:PRO:CD	2.83	0.41
37:l:77:MET:HE1	38:m:64:LEU:CD1	2.50	0.41
1:A:35:SER:O	2:B:81:ARG:NH2	2.53	0.41
14:N:46:LYS:NZ	14:N:126:SER:OG	2.53	0.41
14:N:174:GLN:NE2	60:N:503:HOH:O	2.54	0.41
24:Y:6:ARG:HG2	24:Y:10:ASP:OD2	2.19	0.41
6:F:197:GLU:OE2	6:F:216:PHE:N	2.53	0.41
12:L:48:MET:HE2	45:L:704:3PE:H3A1	2.02	0.41
20:T:52:MET:HE2	22:W:41:ARG:HD3	2.02	0.41
44:s:50:THR:O	44:s:54:LEU:HD13	2.20	0.41
34:i:71:PHE:CE2	34:i:76:ILE:HD11	2.56	0.41
9:I:84:GLU:HB2	9:I:94:ILE:HD12	2.02	0.41
12:L:392:LYS:HZ3	12:L:416:THR:HG23	1.85	0.41
13:M:373:ILE:HA	13:M:376:ILE:HD12	2.02	0.41
1:A:44:MET:CE	4:D:48:THR:HG22	2.51	0.41
6:F:327:THR:OG1	6:F:328:GLY:N	2.54	0.41
12:L:356:ILE:O	12:L:436:ARG:NH2	2.54	0.41
16:P:110:PHE:CZ	16:P:145:TYR:CE1	3.09	0.41
4:D:424:VAL:O	4:D:427:GLU:HG2	2.20	0.41
7:G:366:THR:O	7:G:366:THR:HG22	2.20	0.41
11:K:13:THR:O	11:K:17:VAL:HG23	2.20	0.41
12:L:131:LEU:HD23	12:L:131:LEU:C	2.46	0.41
13:M:42:MET:HE1	32:g:77:VAL:CG2	2.49	0.41
14:N:257:LEU:CD2	45:N:401:3PE:H3I3	2.49	0.41
25:Z:127:LEU:HD23	30:e:82:ARG:CD	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:e:86:ILE:HD11	30:e:91:TYR:HD2	1.86	0.41
1:A:81:THR:O	27:b:45:ASN:ND2	2.54	0.41
4:D:145:THR:OG1	4:D:181:TYR:OH	2.34	0.41
5:E:145:LEU:HD12	5:E:153:MET:SD	2.61	0.41
10:J:38:GLY:HA3	46:Z:201:PC1:H382	2.03	0.41
20:U:27:PRO:O	20:U:30:LEU:HB3	2.21	0.41
31:f:49:LYS:HG2	31:f:50:PRO:HD2	2.03	0.41
6:F:103:GLY:O	6:F:333:ALA:HB1	2.20	0.40
7:G:262:TRP:HB2	7:G:390:LEU:HD11	2.02	0.40
14:N:277:ILE:HD13	45:Y:803:3PE:H241	2.04	0.40
2:B:96:MET:SD	4:D:82:LEU:HD23	2.62	0.40
7:G:106:PRO:HB2	9:I:78:ILE:HD11	2.04	0.40
20:T:27:PRO:O	20:T:30:LEU:HB3	2.21	0.40
34:i:42:VAL:HG23	34:i:43:GLU:N	2.36	0.40
8:H:9:LEU:HD12	26:a:19:PRO:HB3	2.03	0.40
8:H:232:ILE:O	8:H:236:ILE:HG13	2.22	0.40
25:Z:68:ARG:O	25:Z:72:MET:HG3	2.22	0.40
4:D:233:ARG:NH1	9:I:23:GLN:O	2.53	0.40
4:D:343:GLU:OE2	4:D:343:GLU:N	2.50	0.40
4:D:371:LYS:CE	4:D:424:VAL:HG23	2.49	0.40
7:G:107:ILE:CG2	9:I:78:ILE:HD12	2.50	0.40
2:B:91:THR:HA	2:B:119:CYS:HB3	2.04	0.40
46:I:201:PC1:H143	46:I:201:PC1:H111	1.89	0.40
13:M:257:MET:HE1	45:m:401:3PE:H371	2.03	0.40
13:M:367:LEU:O	13:M:368:ALA:HB3	2.21	0.40
27:b:82:ARG:O	27:b:83:LEU:C	2.65	0.40
30:e:86:ILE:HD13	30:e:91:TYR:O	2.22	0.40
39:n:27:GLU:OE1	39:n:33:ARG:NH1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
2	B	153/216 (71%)	146 (95%)	7 (5%)	0	100	100
3	C	207/266 (78%)	203 (98%)	4 (2%)	0	100	100
4	D	427/463 (92%)	411 (96%)	16 (4%)	0	100	100
5	E	212/249 (85%)	204 (96%)	8 (4%)	0	100	100
6	F	432/464 (93%)	420 (97%)	12 (3%)	0	100	100
7	G	698/727 (96%)	669 (96%)	27 (4%)	2 (0%)	36	55
8	H	317/318 (100%)	305 (96%)	12 (4%)	0	100	100
9	I	174/212 (82%)	170 (98%)	4 (2%)	0	100	100
10	J	173/175 (99%)	164 (95%)	8 (5%)	1 (1%)	21	39
11	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
12	L	604/606 (100%)	581 (96%)	22 (4%)	1 (0%)	43	62
13	M	457/459 (100%)	452 (99%)	5 (1%)	0	100	100
14	N	345/347 (99%)	333 (96%)	12 (4%)	0	100	100
15	O	318/343 (93%)	315 (99%)	3 (1%)	0	100	100
16	P	341/380 (90%)	332 (97%)	9 (3%)	0	100	100
17	Q	127/175 (73%)	124 (98%)	3 (2%)	0	100	100
18	R	94/124 (76%)	91 (97%)	3 (3%)	0	100	100
19	S	85/99 (86%)	81 (95%)	4 (5%)	0	100	100
20	T	83/156 (53%)	80 (96%)	3 (4%)	0	100	100
20	U	84/156 (54%)	80 (95%)	4 (5%)	0	100	100
21	V	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
22	W	113/128 (88%)	106 (94%)	7 (6%)	0	100	100
23	X	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
24	Y	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
25	Z	139/144 (96%)	134 (96%)	5 (4%)	0	100	100
26	a	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
27	b	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
28	c	47/76 (62%)	47 (100%)	0	0	100	100
29	d	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
30	e	97/106 (92%)	95 (98%)	2 (2%)	0	100	100
31	f	55/57 (96%)	52 (94%)	3 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	g	98/154 (64%)	94 (96%)	3 (3%)	1 (1%)	12	24
33	h	136/189 (72%)	133 (98%)	3 (2%)	0	100	100
34	i	125/127 (98%)	122 (98%)	3 (2%)	0	100	100
35	j	69/108 (64%)	67 (97%)	2 (3%)	0	100	100
36	k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100
37	l	154/186 (83%)	148 (96%)	6 (4%)	0	100	100
38	m	126/129 (98%)	119 (94%)	7 (6%)	0	100	100
39	n	170/179 (95%)	168 (99%)	2 (1%)	0	100	100
40	o	120/137 (88%)	115 (96%)	5 (4%)	0	100	100
41	p	171/176 (97%)	169 (99%)	2 (1%)	0	100	100
42	q	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
43	r	91/113 (80%)	87 (96%)	4 (4%)	0	100	100
44	s	44/109 (40%)	42 (96%)	2 (4%)	0	100	100
All	All	8204/9212 (89%)	7947 (97%)	252 (3%)	5 (0%)	49	69

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	590	PRO
10	J	24	PRO
12	L	562	LEU
7	G	540	ASP
32	g	24	LEU

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	100/100 (100%)	100 (100%)	0	100	100
2	B	131/175 (75%)	131 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	190/228 (83%)	190 (100%)	0	100	100
4	D	370/392 (94%)	370 (100%)	0	100	100
5	E	183/205 (89%)	183 (100%)	0	100	100
6	F	348/368 (95%)	348 (100%)	0	100	100
7	G	587/608 (96%)	587 (100%)	0	100	100
8	H	275/274 (100%)	275 (100%)	0	100	100
9	I	151/175 (86%)	151 (100%)	0	100	100
10	J	141/141 (100%)	141 (100%)	0	100	100
11	K	85/85 (100%)	85 (100%)	0	100	100
12	L	533/533 (100%)	533 (100%)	0	100	100
13	M	412/412 (100%)	412 (100%)	0	100	100
14	N	315/315 (100%)	315 (100%)	0	100	100
15	O	283/303 (93%)	283 (100%)	0	100	100
16	P	297/327 (91%)	297 (100%)	0	100	100
17	Q	116/153 (76%)	116 (100%)	0	100	100
18	R	79/97 (81%)	79 (100%)	0	100	100
19	S	77/82 (94%)	77 (100%)	0	100	100
20	T	79/135 (58%)	74 (94%)	5 (6%)	16	34
20	U	79/135 (58%)	74 (94%)	5 (6%)	16	34
21	V	101/102 (99%)	101 (100%)	0	100	100
22	W	107/114 (94%)	107 (100%)	0	100	100
23	X	154/155 (99%)	154 (100%)	0	100	100
24	Y	101/102 (99%)	101 (100%)	0	100	100
25	Z	120/121 (99%)	120 (100%)	0	100	100
26	a	59/59 (100%)	59 (100%)	0	100	100
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	45/68 (66%)	45 (100%)	0	100	100
29	d	105/105 (100%)	105 (100%)	0	100	100
30	e	89/96 (93%)	89 (100%)	0	100	100
31	f	54/54 (100%)	54 (100%)	0	100	100
32	g	91/131 (70%)	91 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	h	121/158 (77%)	121 (100%)	0	100	100
34	i	120/120 (100%)	120 (100%)	0	100	100
35	j	61/84 (73%)	61 (100%)	0	100	100
36	k	63/76 (83%)	63 (100%)	0	100	100
37	l	140/159 (88%)	140 (100%)	0	100	100
38	m	114/115 (99%)	114 (100%)	0	100	100
39	n	156/161 (97%)	156 (100%)	0	100	100
40	o	110/120 (92%)	110 (100%)	0	100	100
41	p	155/157 (99%)	155 (100%)	0	100	100
42	q	131/131 (100%)	131 (100%)	0	100	100
43	r	85/97 (88%)	85 (100%)	0	100	100
44	s	45/92 (49%)	45 (100%)	0	100	100
All	All	7229/7892 (92%)	7219 (100%)	10 (0%)	87	96

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	T	28	GLU
20	T	32	VAL
20	T	61	GLU
20	T	65	ILE
20	T	68	GLU
20	U	28	GLU
20	U	32	VAL
20	U	61	GLU
20	U	65	ILE
20	U	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	19	HIS
3	C	46	ASN
4	D	84	HIS
6	F	200	GLN
6	F	402	HIS
6	F	421	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	182	GLN
7	G	517	ASN
9	I	123	GLN
9	I	168	ASN
11	K	52	HIS
12	L	56	HIS
12	L	269	ASN
12	L	328	HIS
13	M	168	GLN
13	M	169	ASN
13	M	366	ASN
15	O	114	HIS
15	O	287	HIS
16	P	36	ASN
16	P	44	GLN
16	P	102	GLN
17	Q	67	ASN
19	S	80	ASN
21	V	82	GLN
22	W	126	HIS
23	X	105	GLN
25	Z	61	GLN
29	d	6	GLN
30	e	26	HIS
30	e	96	HIS
33	h	124	HIS
35	j	58	GLN
37	l	87	ASN
37	l	104	HIS
41	p	143	HIS
42	q	52	ASN
42	q	72	ASN
43	r	46	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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
12	FME	L	1	12	8,9,10	0.98	0	8,9,11	0.72	0
43	AYA	r	1	43	6,7,8	1.26	1 (16%)	6,8,10	0.95	0
13	FME	M	1	13	8,9,10	1.01	0	8,9,11	0.95	1 (12%)
10	FME	J	1	10	8,9,10	1.01	0	8,9,11	0.84	0
1	FME	A	1	1	8,9,10	0.98	0	8,9,11	1.11	1 (12%)
34	SAC	i	1	34	7,8,9	0.97	0	7,9,11	1.09	0
14	FME	N	1	14	8,9,10	0.96	0	8,9,11	1.13	0
8	FME	H	1	8	8,9,10	0.98	0	8,9,11	1.03	0
11	FME	K	1	11	8,9,10	0.97	0	8,9,11	0.86	0
24	AYA	Y	1	24	6,7,8	1.30	1 (16%)	6,8,10	1.19	1 (16%)
29	AME	d	1	29	9,10,11	1.51	2 (22%)	9,11,13	1.39	1 (11%)
4	2MR	D	85	4	10,12,13	2.76	4 (40%)	5,13,15	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	L	1	12	-	2/7/9/11	-
43	AYA	r	1	43	-	0/5/6/8	-
13	FME	M	1	13	-	1/7/9/11	-
10	FME	J	1	10	-	4/7/9/11	-
1	FME	A	1	1	-	5/7/9/11	-
34	SAC	i	1	34	-	1/7/8/10	-
14	FME	N	1	14	-	3/7/9/11	-
8	FME	H	1	8	-	3/7/9/11	-
11	FME	K	1	11	-	4/7/9/11	-
24	AYA	Y	1	24	-	1/5/6/8	-
29	AME	d	1	29	-	5/9/10/12	-
4	2MR	D	85	4	-	0/10/13/15	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.14	1.44	1.33
4	D	85	2MR	CZ-NE	4.84	1.44	1.34
4	D	85	2MR	O-C	4.27	1.36	1.20
29	d	1	AME	CT1-N	3.40	1.45	1.34
24	Y	1	AYA	CA-N	-2.59	1.43	1.46
43	r	1	AYA	CA-N	-2.45	1.43	1.46
4	D	85	2MR	CQ1-NH1	-2.16	1.42	1.46
29	d	1	AME	OT-CT1	-2.01	1.18	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	1	AYA	CB-CA-N	2.61	112.63	109.68
1	A	1	FME	C-CA-N	2.23	113.80	109.50
13	M	1	FME	C-CA-N	2.03	113.42	109.50
29	d	1	AME	CT2-CT1-N	2.00	119.44	116.12

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	C-CA-CB-CG
8	H	1	FME	C-CA-CB-CG
10	J	1	FME	O1-CN-N-CA
10	J	1	FME	N-CA-CB-CG
10	J	1	FME	C-CA-CB-CG
11	K	1	FME	O1-CN-N-CA
12	L	1	FME	O1-CN-N-CA
14	N	1	FME	O1-CN-N-CA
14	N	1	FME	CB-CA-N-CN
24	Y	1	AYA	O-C-CA-CB
29	d	1	AME	C-CA-CB-CG
29	d	1	AME	O-C-CA-CB
34	i	1	SAC	CB-CA-N-C1A
8	H	1	FME	CA-CB-CG-SD
12	L	1	FME	CA-CB-CG-SD
11	K	1	FME	N-CA-CB-CG
11	K	1	FME	C-CA-CB-CG
13	M	1	FME	C-CA-CB-CG
14	N	1	FME	N-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A	1	FME	CB-CG-SD-CE
29	d	1	AME	CB-CG-SD-CE
10	J	1	FME	CB-CG-SD-CE
29	d	1	AME	C-CA-N-CT1
1	A	1	FME	CB-CA-N-CN
1	A	1	FME	N-CA-CB-CG
8	H	1	FME	N-CA-CB-CG
29	d	1	AME	CB-CA-N-CT1
11	K	1	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 59 ligands modelled in this entry, 3 are monoatomic - leaving 56 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
45	3PE	H	601	-	35,35,50	1.04	4 (11%)	38,40,55	1.08	2 (5%)
46	PC1	q	202	-	48,48,53	0.99	4 (8%)	54,56,61	1.04	2 (3%)
52	CDL	H	602	-	50,50,99	1.21	8 (16%)	56,62,111	1.21	4 (7%)
52	CDL	X	201	-	85,85,99	0.94	8 (9%)	91,97,111	1.05	4 (4%)
45	3PE	M	901	-	48,48,50	0.88	4 (8%)	51,53,55	1.04	2 (3%)
46	PC1	d	202	-	38,38,53	1.15	4 (10%)	44,46,61	1.10	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	FMN	F	501	-	33,33,33	1.08	2 (6%)	48,50,50	1.20	6 (12%)
46	PC1	A	202	-	34,34,53	1.19	4 (11%)	40,42,61	1.09	2 (5%)
47	SF4	B	201	2	0,12,12	-	-	-	-	-
45	3PE	d	201	-	48,48,50	0.89	4 (8%)	51,53,55	1.05	2 (3%)
49	FES	E	301	5	0,4,4	-	-	-	-	-
53	GTP	O	401	54	33,34,34	3.29	14 (42%)	50,54,54	1.87	15 (30%)
45	3PE	m	401	-	49,49,50	0.88	4 (8%)	52,54,55	1.11	2 (3%)
46	PC1	I	204	-	43,43,53	1.06	4 (9%)	49,51,61	1.07	2 (4%)
45	3PE	A	201	-	46,46,50	0.90	4 (8%)	49,51,55	1.07	2 (4%)
46	PC1	q	201	-	47,47,53	1.03	4 (8%)	53,55,61	1.05	2 (3%)
45	3PE	Y	804	-	32,32,50	1.06	4 (12%)	35,37,55	1.07	2 (5%)
46	PC1	Y	806	-	45,45,53	1.03	4 (8%)	51,53,61	1.01	2 (3%)
47	SF4	F	502	6	0,12,12	-	-	-	-	-
57	EHZ	U	101	20	31,36,37	1.52	5 (16%)	36,44,47	2.72	8 (22%)
58	CHD	i	201	-	32,32,32	3.29	10 (31%)	51,51,51	3.34	25 (49%)
45	3PE	P	502	-	34,34,50	1.04	4 (11%)	37,39,55	1.24	2 (5%)
45	3PE	Y	802	-	39,39,50	0.97	4 (10%)	42,44,55	1.10	2 (4%)
57	EHZ	T	101	20	31,36,37	1.51	5 (16%)	36,44,47	2.72	8 (22%)
45	3PE	L	701	-	45,45,50	0.92	4 (8%)	48,50,55	1.10	2 (4%)
45	3PE	m	402	-	40,40,50	0.97	4 (10%)	43,45,55	1.16	2 (4%)
45	3PE	M	903	-	47,47,50	0.90	4 (8%)	50,52,55	1.07	2 (4%)
47	SF4	G	801	7	0,12,12	-	-	-	-	-
45	3PE	L	704	-	43,43,50	0.94	4 (9%)	46,48,55	1.10	2 (4%)
52	CDL	N	402	-	61,61,99	1.11	8 (13%)	67,73,111	1.24	4 (5%)
55	NDP	P	501	-	51,52,52	2.25	7 (13%)	71,80,80	1.58	15 (21%)
45	3PE	L	703	-	44,44,50	0.91	4 (9%)	47,49,55	1.06	2 (4%)
47	SF4	I	202	9	0,12,12	-	-	-	-	-
46	PC1	M	904	-	34,34,53	1.19	4 (11%)	40,42,61	1.08	2 (5%)
46	PC1	A	203	-	34,34,53	1.19	4 (11%)	40,42,61	1.08	2 (5%)
52	CDL	L	702	-	75,75,99	1.02	8 (10%)	81,87,111	1.06	4 (4%)
45	3PE	Y	803	-	29,29,50	1.12	4 (13%)	32,34,55	1.20	2 (6%)
47	SF4	I	203	9	0,12,12	-	-	-	-	-
59	MYR	o	201	40	13,14,15	0.99	0	12,13,15	0.56	0
47	SF4	G	802	7	0,12,12	-	-	-	-	-
52	CDL	d	203	-	64,64,99	1.08	7 (10%)	70,76,111	1.07	4 (5%)
46	PC1	Z	201	-	47,47,53	0.47	0	53,55,61	0.61	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PC1	h	202	-	46,46,53	1.03	4 (8%)	52,54,61	1.06	2 (3%)
45	3PE	M	902	-	44,44,50	0.92	4 (9%)	47,49,55	1.09	2 (4%)
46	PC1	I	201	-	53,53,53	0.96	4 (7%)	59,61,61	1.00	2 (3%)
48	U10	D	701	-	63,63,63	2.74	17 (26%)	78,79,79	1.93	21 (26%)
45	3PE	Y	805	-	26,26,50	1.19	4 (15%)	29,31,55	1.16	2 (6%)
46	PC1	B	202	-	45,45,53	1.04	4 (8%)	51,53,61	1.00	2 (3%)
46	PC1	g	201	-	43,43,53	1.06	4 (9%)	49,51,61	1.09	2 (4%)
49	FES	G	803	7	0,4,4	-	-	-	-	-
52	CDL	h	201	-	79,79,99	0.98	8 (10%)	85,91,111	1.11	4 (4%)
52	CDL	r	201	-	60,60,99	1.12	8 (13%)	66,72,111	1.17	4 (6%)
45	3PE	Y	801	-	30,30,50	1.10	4 (13%)	33,35,55	1.07	2 (6%)
45	3PE	K	101	-	43,43,50	0.93	4 (9%)	46,48,55	1.16	3 (6%)
46	PC1	A	204	-	32,32,53	1.26	5 (15%)	38,40,61	1.17	2 (5%)
45	3PE	N	401	-	50,50,50	0.84	4 (8%)	53,55,55	1.08	2 (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
45	3PE	H	601	-	-	19/39/39/54	-
46	PC1	q	202	-	-	19/52/52/57	-
52	CDL	H	602	-	-	28/61/61/110	-
52	CDL	X	201	-	-	44/96/96/110	-
45	3PE	M	901	-	-	23/52/52/54	-
46	PC1	d	202	-	-	18/42/42/57	-
50	FMN	F	501	-	-	2/18/18/18	0/3/3/3
46	PC1	A	202	-	-	22/38/38/57	-
47	SF4	B	201	2	-	-	0/6/5/5
45	3PE	d	201	-	-	21/52/52/54	-
53	GTP	O	401	54	-	5/22/38/38	0/3/3/3
49	FES	E	301	5	-	-	0/1/1/1
45	3PE	m	401	-	-	23/53/53/54	-
46	PC1	I	204	-	-	18/47/47/57	-
45	3PE	A	201	-	-	24/50/50/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PC1	q	201	-	-	14/51/51/57	-
45	3PE	Y	804	-	-	16/36/36/54	-
46	PC1	Y	806	-	-	16/49/49/57	-
57	EHZ	U	101	20	-	13/42/44/45	-
58	CHD	i	201	-	-	2/9/74/74	0/4/4/4
47	SF4	F	502	6	-	-	0/6/5/5
45	3PE	P	502	-	-	16/38/38/54	-
45	3PE	Y	802	-	-	21/43/43/54	-
57	EHZ	T	101	20	-	13/42/44/45	-
45	3PE	L	701	-	-	21/49/49/54	-
45	3PE	m	402	-	-	26/44/44/54	-
45	3PE	M	903	-	-	20/51/51/54	-
52	CDL	N	402	-	-	37/71/71/110	-
45	3PE	L	704	-	-	15/47/47/54	-
47	SF4	G	801	7	-	-	0/6/5/5
55	NDP	P	501	-	-	7/34/77/77	0/5/5/5
45	3PE	L	703	-	-	21/48/48/54	-
47	SF4	I	202	9	-	-	0/6/5/5
46	PC1	M	904	-	-	18/38/38/57	-
46	PC1	A	203	-	-	15/38/38/57	-
52	CDL	L	702	-	-	31/86/86/110	-
45	3PE	Y	803	-	-	9/33/33/54	-
59	MYR	o	201	40	-	6/12/12/13	-
47	SF4	I	203	9	-	-	0/6/5/5
52	CDL	d	203	-	-	21/75/75/110	-
47	SF4	G	802	7	-	-	0/6/5/5
46	PC1	Z	201	-	-	17/51/51/57	-
46	PC1	h	202	-	-	24/50/50/57	-
45	3PE	M	902	-	-	18/48/48/54	-
46	PC1	I	201	-	-	20/57/57/57	-
48	U10	D	701	-	-	30/63/87/87	0/1/1/1
45	3PE	Y	805	-	-	10/30/30/54	-
46	PC1	B	202	-	-	11/49/49/57	-
46	PC1	g	201	-	-	16/47/47/57	-
52	CDL	h	201	-	-	31/90/90/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	FES	G	803	7	-	-	0/1/1/1
52	CDL	r	201	-	-	20/71/71/110	-
45	3PE	Y	801	-	-	25/34/34/54	-
45	3PE	K	101	-	-	22/47/47/54	-
46	PC1	A	204	-	-	12/36/36/57	-
45	3PE	N	401	-	-	30/54/54/54	-

All (244) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	P	501	NDP	P2B-O2B	12.65	1.81	1.59
58	i	201	CHD	C11-C12	8.74	1.67	1.53
53	O	401	GTP	O6-C6	8.73	1.40	1.23
58	i	201	CHD	C16-C15	7.04	1.73	1.54
53	O	401	GTP	C5-N7	6.69	1.52	1.39
58	i	201	CHD	C8-C9	6.45	1.66	1.53
48	D	701	U10	C38-C39	6.35	1.47	1.33
48	D	701	U10	C48-C49	6.34	1.47	1.33
48	D	701	U10	C13-C14	6.18	1.47	1.33
48	D	701	U10	C33-C34	6.05	1.47	1.33
48	D	701	U10	C28-C29	6.04	1.47	1.33
48	D	701	U10	C23-C24	6.02	1.46	1.33
48	D	701	U10	C8-C9	6.00	1.46	1.33
48	D	701	U10	C43-C44	5.98	1.46	1.33
48	D	701	U10	C18-C19	5.93	1.46	1.33
58	i	201	CHD	C13-C17	5.83	1.65	1.55
58	i	201	CHD	C20-C17	-5.72	1.44	1.54
48	D	701	U10	O4-C4	-5.66	1.23	1.36
48	D	701	U10	O3-C3	-5.41	1.23	1.36
58	i	201	CHD	O12-C12	-5.35	1.34	1.43
58	i	201	CHD	C6-C5	5.31	1.62	1.53
53	O	401	GTP	PA-O3A	5.13	1.65	1.59
53	O	401	GTP	PB-O3A	5.07	1.65	1.59
53	O	401	GTP	PB-O3B	5.03	1.64	1.59
48	D	701	U10	C53-C54	4.94	1.47	1.32
57	T	101	EHZ	C12-N1	4.94	1.45	1.33
57	U	101	EHZ	C12-N1	4.92	1.45	1.33
53	O	401	GTP	C2-N1	4.91	1.49	1.37
53	O	401	GTP	C2-N2	4.65	1.45	1.34
53	O	401	GTP	C2-N3	4.63	1.44	1.33
57	U	101	EHZ	C15-N2	4.62	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	T	101	EHZ	C15-N2	4.57	1.44	1.33
53	O	401	GTP	C8-N9	-4.31	1.27	1.37
55	P	501	NDP	PN-O5D	3.97	1.74	1.59
58	i	201	CHD	C15-C14	3.79	1.62	1.54
53	O	401	GTP	C4-N9	-3.76	1.28	1.38
55	P	501	NDP	PA-O3	3.74	1.63	1.59
58	i	201	CHD	C6-C7	3.52	1.59	1.52
48	D	701	U10	C4-C5	-3.50	1.38	1.48
55	P	501	NDP	O2B-C2B	-3.40	1.32	1.44
50	F	501	FMN	C4A-N5	3.27	1.37	1.30
48	D	701	U10	C3-C2	-3.27	1.39	1.48
52	L	702	CDL	OA6-CA4	-2.99	1.39	1.46
52	X	201	CDL	OA6-CA4	-2.91	1.39	1.46
53	O	401	GTP	O4'-C1'	2.90	1.48	1.42
52	r	201	CDL	OB6-CB4	-2.90	1.39	1.46
52	h	201	CDL	OA6-CA4	-2.86	1.39	1.46
46	I	204	PC1	O21-C2	-2.86	1.39	1.46
48	D	701	U10	C6-C5	-2.83	1.38	1.46
52	L	702	CDL	OB6-CB4	-2.83	1.40	1.46
46	B	202	PC1	O21-C2	-2.82	1.40	1.46
45	K	101	3PE	O21-C2	-2.82	1.40	1.46
46	d	202	PC1	O21-C2	-2.82	1.40	1.46
52	h	201	CDL	OB6-CB4	-2.82	1.40	1.46
45	A	201	3PE	O21-C2	-2.81	1.40	1.46
46	I	201	PC1	O21-C2	-2.79	1.40	1.46
46	q	201	PC1	O21-C2	-2.79	1.40	1.46
52	r	201	CDL	OA6-CA4	-2.77	1.40	1.46
46	h	202	PC1	O21-C2	-2.77	1.40	1.46
46	g	201	PC1	O21-C2	-2.77	1.40	1.46
52	N	402	CDL	OA6-CA4	-2.77	1.40	1.46
52	H	602	CDL	OB6-CB4	-2.76	1.40	1.46
45	M	902	3PE	O21-C2	-2.76	1.40	1.46
52	d	203	CDL	OA6-CA4	-2.76	1.40	1.46
46	A	202	PC1	O21-C2	-2.75	1.40	1.46
45	L	704	3PE	O21-C2	-2.75	1.40	1.46
45	Y	802	3PE	O21-C2	-2.74	1.40	1.46
46	A	203	PC1	O21-C2	-2.73	1.40	1.46
45	Y	805	3PE	O21-C2	-2.72	1.40	1.46
45	m	402	3PE	O21-C2	-2.71	1.40	1.46
45	M	901	3PE	O21-C2	-2.71	1.40	1.46
45	L	701	3PE	O21-C2	-2.71	1.40	1.46
45	L	703	3PE	O21-C2	-2.69	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	Y	803	3PE	O21-C2	-2.68	1.40	1.46
48	D	701	U10	C6-C1	2.67	1.40	1.35
46	M	904	PC1	O21-C2	-2.66	1.40	1.46
45	M	903	3PE	O21-C2	-2.66	1.40	1.46
52	d	203	CDL	OB6-CB4	-2.66	1.40	1.46
52	N	402	CDL	OB6-CB4	-2.65	1.40	1.46
45	m	401	3PE	O21-C2	-2.64	1.40	1.46
46	Y	806	PC1	O21-C2	-2.64	1.40	1.46
45	H	601	3PE	O21-C2	-2.64	1.40	1.46
45	d	201	3PE	O21-C2	-2.59	1.40	1.46
57	U	101	EHZ	O4-C15	-2.58	1.18	1.23
57	T	101	EHZ	O4-C15	-2.56	1.18	1.23
52	X	201	CDL	OA8-CA7	2.56	1.40	1.33
46	A	204	PC1	O21-C2	-2.55	1.40	1.46
52	d	203	CDL	OA8-CA7	2.55	1.40	1.33
52	H	602	CDL	OA6-CA4	-2.54	1.40	1.46
52	X	201	CDL	OB8-CB7	2.52	1.40	1.33
52	H	602	CDL	OB8-CB7	2.50	1.40	1.33
57	U	101	EHZ	O3-C12	-2.50	1.18	1.23
45	K	101	3PE	O31-C3	-2.50	1.39	1.45
52	L	702	CDL	OA8-CA7	2.49	1.40	1.33
46	q	202	PC1	O31-C31	2.49	1.40	1.33
45	Y	804	3PE	O21-C2	-2.48	1.40	1.46
46	h	202	PC1	O31-C31	2.48	1.40	1.33
52	L	702	CDL	OB8-CB7	2.48	1.40	1.33
52	r	201	CDL	OB8-CB7	2.48	1.40	1.33
57	T	101	EHZ	O3-C12	-2.46	1.18	1.23
50	F	501	FMN	C10-N1	2.46	1.38	1.33
46	I	201	PC1	O31-C31	2.45	1.40	1.33
46	d	202	PC1	O31-C31	2.45	1.40	1.33
46	I	204	PC1	O31-C31	2.45	1.40	1.33
52	h	201	CDL	OA8-CA7	2.45	1.40	1.33
45	H	601	3PE	O31-C31	2.43	1.40	1.33
45	N	401	3PE	O21-C2	-2.42	1.40	1.46
45	Y	801	3PE	O31-C31	2.42	1.40	1.33
46	M	904	PC1	O31-C31	2.41	1.40	1.33
52	H	602	CDL	OA8-CA7	2.41	1.40	1.33
45	P	502	3PE	O31-C31	2.41	1.40	1.33
52	r	201	CDL	OA8-CA7	2.41	1.40	1.33
46	B	202	PC1	O31-C31	2.40	1.40	1.33
52	h	201	CDL	OB8-CB6	-2.40	1.39	1.45
53	O	401	GTP	C2'-C3'	-2.40	1.46	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	m	401	3PE	O31-C31	2.40	1.40	1.33
45	L	704	3PE	O31-C31	2.40	1.40	1.33
45	A	201	3PE	O31-C31	2.39	1.40	1.33
45	Y	803	3PE	O31-C31	2.39	1.40	1.33
52	N	402	CDL	OB8-CB7	2.38	1.40	1.33
52	d	203	CDL	OB8-CB7	2.38	1.40	1.33
45	Y	804	3PE	O31-C31	2.38	1.40	1.33
45	Y	801	3PE	O21-C2	-2.38	1.41	1.46
45	M	903	3PE	O31-C31	2.38	1.40	1.33
46	g	201	PC1	O31-C3	-2.38	1.39	1.45
52	N	402	CDL	OA8-CA7	2.37	1.40	1.33
46	A	204	PC1	O31-C31	2.36	1.40	1.33
45	Y	805	3PE	O31-C31	2.36	1.40	1.33
45	m	402	3PE	O31-C31	2.36	1.40	1.33
52	N	402	CDL	OB6-CB5	2.36	1.40	1.35
45	M	902	3PE	O31-C3	-2.36	1.39	1.45
45	P	502	3PE	O21-C21	2.35	1.40	1.34
45	P	502	3PE	O21-C2	-2.35	1.41	1.46
52	X	201	CDL	OB6-CB5	2.35	1.40	1.34
45	L	701	3PE	O31-C3	-2.35	1.39	1.45
45	L	703	3PE	O31-C31	2.35	1.40	1.33
46	A	203	PC1	O31-C31	2.34	1.40	1.33
46	q	202	PC1	O21-C2	-2.34	1.41	1.46
45	d	201	3PE	O31-C31	2.34	1.40	1.33
46	A	202	PC1	O31-C3	-2.34	1.39	1.45
46	Y	806	PC1	O31-C31	2.34	1.40	1.33
45	M	902	3PE	O31-C31	2.34	1.40	1.33
45	Y	802	3PE	O31-C31	2.33	1.40	1.33
58	i	201	CHD	C13-C12	-2.32	1.51	1.54
45	L	704	3PE	O31-C3	-2.32	1.40	1.45
46	q	201	PC1	O31-C3	-2.32	1.40	1.45
46	q	201	PC1	O31-C31	2.32	1.40	1.33
45	N	401	3PE	O31-C31	2.31	1.40	1.33
45	Y	801	3PE	O21-C21	2.31	1.40	1.34
45	M	901	3PE	O31-C3	-2.31	1.40	1.45
52	d	203	CDL	OB8-CB6	-2.30	1.40	1.45
45	M	901	3PE	O31-C31	2.30	1.40	1.33
46	A	204	PC1	O31-C3	-2.29	1.40	1.45
53	O	401	GTP	PG-O3G	-2.29	1.46	1.54
57	U	101	EHZ	C9-S1	2.28	1.81	1.76
46	A	204	PC1	O21-C21	2.28	1.40	1.34
45	Y	803	3PE	O31-C3	-2.27	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	L	701	3PE	O31-C31	2.26	1.40	1.33
46	Y	806	PC1	O31-C3	-2.26	1.40	1.45
52	h	201	CDL	OB8-CB7	2.26	1.39	1.33
53	O	401	GTP	PG-O2G	-2.25	1.46	1.54
46	g	201	PC1	O31-C31	2.25	1.39	1.33
52	r	201	CDL	OA8-CA6	-2.24	1.40	1.45
57	T	101	EHZ	C9-S1	2.24	1.81	1.76
52	H	602	CDL	OA8-CA6	-2.24	1.40	1.45
52	X	201	CDL	OB6-CB4	-2.24	1.41	1.46
45	M	903	3PE	O31-C3	-2.24	1.40	1.45
52	L	702	CDL	OA8-CA6	-2.23	1.40	1.45
45	H	601	3PE	O31-C3	-2.23	1.40	1.45
45	L	703	3PE	O31-C3	-2.23	1.40	1.45
46	A	203	PC1	O31-C3	-2.23	1.40	1.45
46	Y	806	PC1	O21-C21	2.23	1.40	1.34
46	A	202	PC1	O31-C31	2.23	1.39	1.33
46	I	204	PC1	O31-C3	-2.22	1.40	1.45
52	N	402	CDL	OA8-CA6	-2.22	1.40	1.45
45	Y	805	3PE	O31-C3	-2.22	1.40	1.45
46	q	202	PC1	O21-C21	2.22	1.40	1.34
46	d	202	PC1	O31-C3	-2.21	1.40	1.45
48	D	701	U10	C1-C2	-2.20	1.39	1.47
45	N	401	3PE	O31-C3	-2.20	1.40	1.45
45	Y	804	3PE	O31-C3	-2.20	1.40	1.45
45	d	201	3PE	O21-C21	2.20	1.40	1.34
52	h	201	CDL	OA8-CA6	-2.19	1.40	1.45
45	Y	802	3PE	O31-C3	-2.19	1.40	1.45
55	P	501	NDP	C5A-C4A	2.19	1.43	1.39
45	Y	804	3PE	O21-C21	2.19	1.40	1.34
45	m	401	3PE	O21-C21	2.18	1.40	1.34
45	m	401	3PE	O31-C3	-2.18	1.40	1.45
46	I	201	PC1	O31-C3	-2.18	1.40	1.45
45	d	201	3PE	O31-C3	-2.17	1.40	1.45
45	m	402	3PE	O31-C3	-2.17	1.40	1.45
45	H	601	3PE	O21-C21	2.17	1.40	1.34
45	K	101	3PE	O31-C31	2.17	1.39	1.33
52	d	203	CDL	OB6-CB5	2.17	1.40	1.34
46	M	904	PC1	O21-C21	2.16	1.40	1.34
46	B	202	PC1	O31-C3	-2.16	1.40	1.45
52	N	402	CDL	OB8-CB6	-2.16	1.40	1.45
52	r	201	CDL	OB8-CB6	-2.16	1.40	1.45
45	Y	801	3PE	O31-C3	-2.16	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	M	903	3PE	O21-C21	2.16	1.40	1.34
45	A	201	3PE	O31-C3	-2.15	1.40	1.45
52	L	702	CDL	OB8-CB6	-2.14	1.40	1.45
45	P	502	3PE	O31-C3	-2.14	1.40	1.45
46	A	202	PC1	O21-C21	2.14	1.40	1.34
46	h	202	PC1	O31-C3	-2.13	1.40	1.45
52	N	402	CDL	OA6-CA5	2.13	1.40	1.34
52	d	203	CDL	OA6-CA5	2.12	1.40	1.34
46	q	201	PC1	O21-C21	2.12	1.40	1.34
46	I	201	PC1	O21-C21	2.11	1.40	1.34
45	Y	803	3PE	O21-C21	2.11	1.40	1.34
46	q	202	PC1	O31-C3	-2.11	1.40	1.45
45	M	901	3PE	O21-C21	2.11	1.40	1.34
45	M	902	3PE	O21-C21	2.11	1.40	1.34
46	M	904	PC1	O31-C3	-2.10	1.40	1.45
45	L	701	3PE	O21-C21	2.10	1.40	1.34
46	A	203	PC1	O21-C21	2.10	1.40	1.34
45	L	703	3PE	O21-C21	2.09	1.40	1.34
52	r	201	CDL	OB6-CB5	2.09	1.40	1.34
55	P	501	NDP	O5D-C5D	-2.09	1.36	1.44
45	m	402	3PE	O21-C21	2.09	1.40	1.34
52	L	702	CDL	OB6-CB5	2.09	1.40	1.34
45	Y	802	3PE	O21-C21	2.09	1.40	1.34
46	d	202	PC1	O21-C21	2.08	1.40	1.34
52	r	201	CDL	OA6-CA5	2.07	1.40	1.34
46	h	202	PC1	O21-C21	2.06	1.40	1.34
52	X	201	CDL	OB8-CB6	-2.06	1.40	1.45
52	h	201	CDL	OA6-CA5	2.06	1.40	1.34
45	A	201	3PE	O21-C21	2.06	1.40	1.34
52	H	602	CDL	OA6-CA5	2.06	1.40	1.34
52	X	201	CDL	OA8-CA6	-2.05	1.40	1.45
52	H	602	CDL	OB6-CB5	2.05	1.40	1.34
45	N	401	3PE	O21-C21	2.05	1.40	1.34
46	g	201	PC1	O21-C21	2.05	1.40	1.34
45	Y	805	3PE	O21-C21	2.05	1.40	1.34
46	B	202	PC1	O21-C21	2.05	1.40	1.34
52	H	602	CDL	OB8-CB6	-2.04	1.40	1.45
52	L	702	CDL	OA6-CA5	2.04	1.40	1.34
45	L	704	3PE	O21-C21	2.04	1.40	1.34
45	K	101	3PE	O21-C21	2.04	1.40	1.34
46	I	204	PC1	O21-C21	2.02	1.40	1.34
52	h	201	CDL	OB6-CB5	2.02	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	A	204	PC1	C12-N	-2.01	1.45	1.51
52	X	201	CDL	OA6-CA5	2.00	1.39	1.34
55	P	501	NDP	O4B-C4B	-2.00	1.40	1.45

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	T	101	EHZ	C14-N2-C15	10.06	140.61	122.55
58	i	201	CHD	C4-C5-C10	10.05	123.36	112.66
57	U	101	EHZ	C14-N2-C15	10.03	140.56	122.55
57	T	101	EHZ	C11-N1-C12	8.53	138.71	122.82
57	U	101	EHZ	C11-N1-C12	8.48	138.61	122.82
58	i	201	CHD	C10-C9-C8	7.76	120.49	111.84
53	O	401	GTP	C8-N9-C4	7.41	119.91	106.03
58	i	201	CHD	C14-C8-C9	6.56	118.91	109.75
58	i	201	CHD	C9-C8-C7	6.30	119.79	111.86
57	T	101	EHZ	C8-C9-S1	6.07	121.22	113.56
57	U	101	EHZ	C8-C9-S1	6.07	121.21	113.56
58	i	201	CHD	C17-C13-C12	6.06	123.12	117.67
52	N	402	CDL	OB6-CB5-C51	5.10	120.19	111.09
58	i	201	CHD	C14-C13-C12	5.02	112.00	107.42
55	P	501	NDP	P2B-O2B-C2B	-4.97	110.17	123.43
58	i	201	CHD	C1-C10-C5	4.93	114.83	107.75
58	i	201	CHD	C11-C9-C10	4.88	118.66	113.70
58	i	201	CHD	C6-C5-C10	4.87	117.84	112.66
48	D	701	U10	C17-C18-C19	-4.85	116.52	127.62
45	P	502	3PE	O21-C21-C22	4.82	121.90	111.48
48	D	701	U10	C10-C9-C11	4.74	123.45	115.23
48	D	701	U10	C7-C8-C9	-4.67	118.78	126.83
58	i	201	CHD	C14-C8-C7	4.54	117.88	111.85
58	i	201	CHD	C11-C9-C8	4.52	117.58	110.89
46	A	204	PC1	O21-C21-C22	4.41	121.03	111.48
58	i	201	CHD	C18-C13-C12	-4.38	104.67	109.06
48	D	701	U10	C32-C33-C34	-4.31	117.77	127.62
45	m	402	3PE	O21-C21-C22	4.30	120.79	111.48
46	q	202	PC1	O21-C21-C22	4.13	120.42	111.48
45	H	601	3PE	O21-C21-C22	4.12	120.39	111.48
46	h	202	PC1	O21-C21-C22	4.10	120.35	111.48
45	K	101	3PE	O21-C21-C22	4.09	120.33	111.48
45	Y	803	3PE	O21-C21-C22	4.01	120.16	111.48
45	L	701	3PE	O21-C21-C22	3.98	120.10	111.48
46	A	203	PC1	O21-C21-C22	3.97	120.08	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	D	701	U10	C30-C29-C31	3.97	122.12	115.23
45	m	401	3PE	O21-C21-C22	3.96	120.06	111.48
52	N	402	CDL	OA6-CA5-C11	3.96	120.05	111.48
45	d	201	3PE	O21-C21-C22	3.95	120.02	111.48
45	N	401	3PE	O21-C21-C22	3.93	119.97	111.48
45	Y	805	3PE	O21-C21-C22	3.92	119.97	111.48
52	d	203	CDL	OA6-CA5-C11	3.89	119.89	111.48
52	L	702	CDL	OB6-CB5-C51	3.88	119.88	111.48
46	M	904	PC1	O21-C21-C22	3.88	119.86	111.48
45	M	903	3PE	O21-C21-C22	3.85	119.81	111.48
46	A	202	PC1	O21-C21-C22	3.84	119.80	111.48
52	H	602	CDL	OB6-CB5-C51	3.83	119.76	111.48
45	A	201	3PE	O21-C21-C22	3.82	119.75	111.48
46	d	202	PC1	O21-C21-C22	3.82	119.75	111.48
46	q	201	PC1	O21-C21-C22	3.81	119.73	111.48
52	X	201	CDL	OB6-CB5-C51	3.79	119.68	111.48
58	i	201	CHD	C13-C17-C20	-3.78	114.90	119.48
46	I	201	PC1	O21-C21-C22	3.77	119.63	111.48
48	D	701	U10	C42-C43-C44	-3.76	119.01	127.62
45	L	703	3PE	O21-C21-C22	3.76	119.62	111.48
45	L	704	3PE	O21-C21-C22	3.74	119.58	111.48
46	g	201	PC1	O21-C21-C22	3.74	119.58	111.48
52	H	602	CDL	OA6-CA5-C11	3.74	119.57	111.48
52	X	201	CDL	OA6-CA5-C11	3.73	119.55	111.48
48	D	701	U10	C35-C34-C36	3.72	121.69	115.23
46	I	204	PC1	O21-C21-C22	3.71	119.50	111.48
46	B	202	PC1	O21-C21-C22	3.70	119.50	111.48
52	h	201	CDL	OB6-CB5-C51	3.69	119.47	111.48
52	r	201	CDL	OB6-CB5-C51	3.68	119.44	111.48
52	h	201	CDL	OA6-CA5-C11	3.67	119.43	111.48
48	D	701	U10	C27-C28-C29	-3.65	119.27	127.62
45	Y	802	3PE	O21-C21-C22	3.64	119.35	111.48
52	r	201	CDL	OA6-CA5-C11	3.63	119.34	111.48
46	Y	806	PC1	O21-C21-C22	3.62	119.30	111.48
45	M	901	3PE	O21-C21-C22	3.61	119.28	111.48
45	Y	801	3PE	O21-C21-C22	3.58	119.23	111.48
55	P	501	NDP	O2B-P2B-O1X	-3.55	96.70	109.33
45	Y	804	3PE	O21-C21-C22	3.52	119.10	111.48
55	P	501	NDP	O3-PA-O1A	-3.51	100.15	110.70
58	i	201	CHD	C6-C5-C4	3.48	115.20	111.23
45	M	902	3PE	O21-C21-C22	3.42	118.88	111.48
48	D	701	U10	C22-C23-C24	-3.38	119.89	127.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	i	201	CHD	C18-C13-C14	-3.36	105.93	111.20
50	F	501	FMN	C4-N3-C2	-3.34	119.71	125.64
58	i	201	CHD	C17-C13-C14	3.34	103.46	100.11
52	L	702	CDL	OA6-CA5-C11	3.28	118.57	111.48
48	D	701	U10	C45-C44-C46	3.23	120.84	115.23
53	O	401	GTP	C2-N1-C6	-3.15	119.39	125.11
55	P	501	NDP	PA-O5B-C5B	-3.04	103.90	121.35
45	P	502	3PE	O31-C31-C32	3.02	121.05	111.83
58	i	201	CHD	C18-C13-C17	-3.02	106.47	111.20
45	m	402	3PE	O31-C31-C32	3.02	121.04	111.83
48	D	701	U10	C25-C24-C26	3.00	120.43	115.23
55	P	501	NDP	PN-O5D-C5D	-2.98	104.27	121.35
48	D	701	U10	C12-C13-C14	-2.94	120.90	127.62
46	d	202	PC1	O31-C31-C32	2.94	120.79	111.83
58	i	201	CHD	C23-C22-C20	-2.93	108.99	114.46
52	r	201	CDL	OA8-CA7-C31	2.89	120.64	111.83
53	O	401	GTP	O2G-PG-O3B	2.87	114.27	104.64
52	H	602	CDL	OB8-CB7-C71	2.86	120.57	111.83
52	N	402	CDL	OA8-CA7-C31	2.85	120.53	111.83
45	Y	804	3PE	O31-C31-C32	2.80	120.36	111.83
53	O	401	GTP	O3G-PG-O3B	2.78	113.97	104.64
46	h	202	PC1	O31-C31-C32	2.78	120.31	111.83
57	U	101	EHZ	O2-C9-S1	-2.78	119.15	122.68
45	m	401	3PE	O31-C31-C32	2.77	120.28	111.83
57	T	101	EHZ	O2-C9-S1	-2.74	119.19	122.68
57	T	101	EHZ	C10-S1-C9	2.74	109.95	101.84
45	M	902	3PE	O31-C31-C32	2.74	120.20	111.83
50	F	501	FMN	C4A-C10-N10	2.74	120.40	116.48
57	U	101	EHZ	C10-S1-C9	2.74	109.93	101.84
46	M	904	PC1	O31-C31-C32	2.73	120.15	111.83
46	I	204	PC1	O31-C31-C32	2.71	120.10	111.83
45	N	401	3PE	O31-C31-C32	2.71	120.09	111.83
46	g	201	PC1	O31-C31-C32	2.71	120.08	111.83
52	N	402	CDL	OB8-CB7-C71	2.70	120.07	111.83
50	F	501	FMN	C4A-C4-N3	2.70	120.12	113.25
45	Y	805	3PE	O31-C31-C32	2.69	120.03	111.83
55	P	501	NDP	O2N-PN-O3	2.69	114.53	107.27
45	Y	801	3PE	O31-C31-C32	2.69	120.03	111.83
45	L	704	3PE	O31-C31-C32	2.69	120.02	111.83
53	O	401	GTP	C3'-C2'-C1'	2.68	106.53	101.46
46	A	204	PC1	O31-C31-C32	2.68	120.00	111.83
46	q	201	PC1	O31-C31-C32	2.67	119.98	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	M	903	3PE	O31-C31-C32	2.67	119.97	111.83
48	D	701	U10	C20-C19-C21	2.67	119.86	115.23
45	A	201	3PE	O31-C31-C32	2.65	119.92	111.83
46	A	202	PC1	O31-C31-C32	2.65	119.90	111.83
57	T	101	EHZ	O2-C9-C8	-2.64	119.58	123.74
46	A	203	PC1	O31-C31-C32	2.64	119.87	111.83
45	Y	803	3PE	O31-C31-C32	2.62	119.84	111.83
52	H	602	CDL	OA8-CA7-C31	2.62	119.81	111.83
55	P	501	NDP	C2A-N1A-C6A	-2.61	114.44	118.73
57	U	101	EHZ	O2-C9-C8	-2.61	119.64	123.74
55	P	501	NDP	N3A-C4A-N9A	2.60	131.59	127.17
46	B	202	PC1	O31-C31-C32	2.59	119.75	111.83
45	L	701	3PE	O31-C31-C32	2.59	119.74	111.83
52	r	201	CDL	OB8-CB7-C71	2.59	119.74	111.83
53	O	401	GTP	C2'-C3'-C4'	2.59	107.61	102.61
45	H	601	3PE	O31-C31-C32	2.59	119.72	111.83
58	i	201	CHD	C9-C11-C12	-2.58	110.92	114.29
55	P	501	NDP	O3X-P2B-O2X	2.57	117.45	107.80
52	X	201	CDL	OB8-CB7-C71	2.55	119.62	111.83
52	h	201	CDL	OA8-CA7-C31	2.55	119.61	111.83
45	K	101	3PE	O31-C31-C32	2.55	119.61	111.83
52	L	702	CDL	OB8-CB7-C71	2.55	119.61	111.83
52	d	203	CDL	OB6-CB5-C51	2.55	120.29	110.93
45	Y	802	3PE	O31-C31-C32	2.54	119.59	111.83
46	q	202	PC1	O31-C31-C32	2.54	119.57	111.83
45	d	201	3PE	O31-C31-C32	2.53	119.55	111.83
48	D	701	U10	C7-C6-C5	-2.53	115.58	118.52
45	M	901	3PE	O31-C31-C32	2.52	119.52	111.83
50	F	501	FMN	O4-C4-C4A	-2.49	119.96	126.53
58	i	201	CHD	C15-C14-C8	2.48	121.76	118.36
52	L	702	CDL	OA8-CA7-C31	2.48	119.40	111.83
48	D	701	U10	C56-C54-C55	2.47	120.28	114.59
52	d	203	CDL	OA8-CA7-C31	2.47	119.36	111.83
53	O	401	GTP	C1'-N9-C8	-2.46	119.74	126.73
53	O	401	GTP	O2A-PA-O1A	-2.45	101.05	112.44
52	d	203	CDL	OB8-CB7-C71	2.44	119.28	111.83
46	Y	806	PC1	O31-C31-C32	2.43	119.25	111.83
55	P	501	NDP	O2N-PN-O1N	2.41	123.65	112.44
45	L	703	3PE	O31-C31-C32	2.41	119.18	111.83
46	Z	201	PC1	O12-P-O13	-2.39	96.72	107.57
53	O	401	GTP	O2B-PB-O1B	-2.39	101.35	112.44
48	D	701	U10	C52-C53-C54	-2.38	119.70	127.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	I	201	PC1	O31-C31-C32	2.38	119.09	111.83
52	X	201	CDL	OA8-CA7-C31	2.38	119.09	111.83
58	i	201	CHD	C21-C20-C22	-2.38	106.66	110.34
48	D	701	U10	C47-C48-C49	-2.37	122.20	127.62
57	U	101	EHZ	C13-C14-N2	-2.37	106.96	112.00
52	h	201	CDL	OB8-CB7-C71	2.36	119.03	111.83
57	T	101	EHZ	C13-C14-N2	-2.35	106.99	112.00
53	O	401	GTP	C5-C6-N1	2.35	119.23	113.25
58	i	201	CHD	C16-C17-C20	-2.34	108.64	112.18
53	O	401	GTP	O6-C6-C5	-2.33	120.37	126.53
55	P	501	NDP	C5A-C4A-N3A	-2.32	123.52	126.72
50	F	501	FMN	C10-C4A-N5	-2.31	120.10	124.81
48	D	701	U10	C1M-C1-C6	-2.29	120.69	124.45
48	D	701	U10	C37-C38-C39	-2.26	122.46	127.62
53	O	401	GTP	C5-C4-N9	-2.24	101.64	105.66
55	P	501	NDP	O3X-P2B-O2B	-2.24	97.14	105.85
58	i	201	CHD	C1-C10-C9	-2.19	107.93	111.34
46	Z	201	PC1	O13-P-O14	2.17	117.55	108.94
58	i	201	CHD	C19-C10-C5	-2.17	106.80	110.44
48	D	701	U10	C15-C14-C16	2.16	118.98	115.23
45	K	101	3PE	C2-O21-C21	-2.16	112.63	117.80
48	D	701	U10	C11-C9-C8	-2.15	116.34	121.17
55	P	501	NDP	O5D-PN-O1N	-2.15	100.43	108.94
50	F	501	FMN	C4A-C10-N1	-2.11	119.42	124.59
57	T	101	EHZ	C13-C12-N1	2.10	120.17	116.34
57	U	101	EHZ	C13-C12-N1	2.10	120.17	116.34
55	P	501	NDP	O7N-C7N-C3N	2.09	124.83	120.90
55	P	501	NDP	O4B-C4B-C3B	2.08	109.28	105.15
53	O	401	GTP	C1'-N9-C4	-2.08	120.34	126.49
58	i	201	CHD	C11-C12-C13	2.06	113.36	111.26
53	O	401	GTP	N9-C8-N7	-2.06	109.58	113.40
53	O	401	GTP	C8-N7-C5	-2.02	100.66	104.26

There are no chirality outliers.

All (910) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C1-O11-P-O12
45	A	201	3PE	C1-O11-P-O13
45	A	201	3PE	C1-O11-P-O14
45	A	201	3PE	C11-O13-P-O11
45	A	201	3PE	C11-O13-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C11-O13-P-O14
45	H	601	3PE	C1-O11-P-O12
45	H	601	3PE	C1-O11-P-O13
45	H	601	3PE	O13-C11-C12-N
45	H	601	3PE	O22-C21-O21-C2
45	H	601	3PE	C22-C21-O21-C2
45	K	101	3PE	C1-O11-P-O14
45	K	101	3PE	O13-C11-C12-N
45	L	701	3PE	C1-O11-P-O13
45	L	701	3PE	C1-O11-P-O14
45	L	701	3PE	C11-O13-P-O11
45	L	701	3PE	C11-O13-P-O12
45	L	701	3PE	C22-C21-O21-C2
45	L	703	3PE	C1-O11-P-O12
45	L	703	3PE	C1-O11-P-O13
45	L	703	3PE	C11-O13-P-O11
45	L	703	3PE	C11-O13-P-O12
45	L	703	3PE	C11-O13-P-O14
45	L	703	3PE	O13-C11-C12-N
45	L	704	3PE	C1-O11-P-O14
45	L	704	3PE	C11-O13-P-O11
45	L	704	3PE	C11-O13-P-O14
45	L	704	3PE	O22-C21-O21-C2
45	M	901	3PE	C11-O13-P-O12
45	M	901	3PE	C11-O13-P-O14
45	M	901	3PE	O13-C11-C12-N
45	M	902	3PE	C1-O11-P-O12
45	M	902	3PE	C1-O11-P-O13
45	M	902	3PE	C11-O13-P-O11
45	M	902	3PE	C11-O13-P-O12
45	M	903	3PE	O13-C11-C12-N
45	M	903	3PE	O32-C31-O31-C3
45	N	401	3PE	C11-O13-P-O11
45	N	401	3PE	C11-O13-P-O14
45	N	401	3PE	O13-C11-C12-N
45	N	401	3PE	C22-C21-O21-C2
45	P	502	3PE	C1-O11-P-O13
45	P	502	3PE	C11-O13-P-O11
45	P	502	3PE	C11-O13-P-O12
45	P	502	3PE	C22-C21-O21-C2
45	Y	801	3PE	C11-O13-P-O11
45	Y	801	3PE	C11-O13-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	Y	801	3PE	C11-O13-P-O14
45	Y	801	3PE	O13-C11-C12-N
45	Y	802	3PE	C11-O13-P-O11
45	Y	802	3PE	C11-O13-P-O14
45	Y	802	3PE	C12-C11-O13-P
45	Y	803	3PE	O22-C21-O21-C2
45	Y	805	3PE	C11-O13-P-O12
45	Y	805	3PE	C11-O13-P-O14
45	Y	805	3PE	O13-C11-C12-N
45	Y	805	3PE	O22-C21-O21-C2
45	Y	805	3PE	C22-C21-O21-C2
45	d	201	3PE	C11-O13-P-O11
45	d	201	3PE	C11-O13-P-O12
45	d	201	3PE	C11-O13-P-O14
45	m	401	3PE	C11-O13-P-O14
45	m	401	3PE	O13-C11-C12-N
45	m	402	3PE	C1-O11-P-O12
45	m	402	3PE	C1-O11-P-O13
45	m	402	3PE	C1-O11-P-O14
45	m	402	3PE	C22-C21-O21-C2
46	A	202	PC1	C11-O13-P-O12
46	A	202	PC1	C11-O13-P-O14
46	A	202	PC1	C11-O13-P-O11
46	A	202	PC1	O13-C11-C12-N
46	A	203	PC1	C11-O13-P-O14
46	A	203	PC1	C11-O13-P-O11
46	A	203	PC1	C1-O11-P-O12
46	A	203	PC1	C1-O11-P-O14
46	A	203	PC1	C1-O11-P-O13
46	A	203	PC1	O22-C21-O21-C2
46	A	203	PC1	C22-C21-O21-C2
46	A	204	PC1	O13-C11-C12-N
46	A	204	PC1	C2-C1-O11-P
46	A	204	PC1	O22-C21-O21-C2
46	B	202	PC1	O21-C2-C3-O31
46	I	201	PC1	C11-O13-P-O11
46	I	201	PC1	C1-O11-P-O12
46	I	201	PC1	C1-O11-P-O14
46	I	204	PC1	C11-O13-P-O12
46	I	204	PC1	C11-O13-P-O14
46	I	204	PC1	C1-O11-P-O12
46	I	204	PC1	C1-O11-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	I	204	PC1	C1-O11-P-O13
46	I	204	PC1	O21-C2-C3-O31
46	M	904	PC1	C11-O13-P-O12
46	M	904	PC1	C1-O11-P-O12
46	M	904	PC1	C1-O11-P-O14
46	M	904	PC1	C1-O11-P-O13
46	M	904	PC1	O22-C21-O21-C2
46	M	904	PC1	C22-C21-O21-C2
46	Y	806	PC1	C11-O13-P-O12
46	Y	806	PC1	C11-O13-P-O11
46	Y	806	PC1	O13-C11-C12-N
46	Z	201	PC1	C1-O11-P-O14
46	Z	201	PC1	C1-O11-P-O13
46	d	202	PC1	C1-O11-P-O12
46	d	202	PC1	C1-O11-P-O14
46	d	202	PC1	C1-O11-P-O13
46	d	202	PC1	C22-C21-O21-C2
46	d	202	PC1	C32-C31-O31-C3
46	g	201	PC1	C11-O13-P-O14
46	g	201	PC1	C11-O13-P-O11
46	g	201	PC1	C1-O11-P-O12
46	g	201	PC1	C1-O11-P-O14
46	h	202	PC1	C11-O13-P-O12
46	h	202	PC1	C11-O13-P-O11
46	h	202	PC1	C1-O11-P-O14
46	h	202	PC1	C1-O11-P-O13
46	h	202	PC1	O13-C11-C12-N
46	h	202	PC1	C2-C1-O11-P
46	q	201	PC1	C11-O13-P-O12
46	q	201	PC1	C11-O13-P-O11
46	q	201	PC1	C22-C21-O21-C2
46	q	202	PC1	C1-O11-P-O13
46	q	202	PC1	O13-C11-C12-N
46	q	202	PC1	C22-C21-O21-C2
48	D	701	U10	C7-C8-C9-C10
48	D	701	U10	C11-C12-C13-C14
48	D	701	U10	C12-C13-C14-C15
48	D	701	U10	C12-C13-C14-C16
48	D	701	U10	C17-C18-C19-C20
48	D	701	U10	C17-C18-C19-C21
48	D	701	U10	C22-C23-C24-C25
48	D	701	U10	C22-C23-C24-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	D	701	U10	C27-C28-C29-C30
48	D	701	U10	C27-C28-C29-C31
48	D	701	U10	C32-C33-C34-C35
48	D	701	U10	C32-C33-C34-C36
48	D	701	U10	C42-C43-C44-C45
48	D	701	U10	C42-C43-C44-C46
48	D	701	U10	C52-C53-C54-C55
52	H	602	CDL	CA2-OA2-PA1-OA3
52	H	602	CDL	CA3-OA5-PA1-OA2
52	H	602	CDL	CA3-OA5-PA1-OA3
52	H	602	CDL	CA3-OA5-PA1-OA4
52	H	602	CDL	C11-CA5-OA6-CA4
52	H	602	CDL	OB7-CB5-OB6-CB4
52	L	702	CDL	OA6-CA4-CA6-OA8
52	N	402	CDL	C1-CA2-OA2-PA1
52	N	402	CDL	CA2-OA2-PA1-OA5
52	N	402	CDL	CA3-OA5-PA1-OA2
52	N	402	CDL	CA3-OA5-PA1-OA3
52	N	402	CDL	CA3-OA5-PA1-OA4
52	N	402	CDL	C11-CA5-OA6-CA4
52	N	402	CDL	CB3-OB5-PB2-OB3
52	N	402	CDL	OB7-CB5-OB6-CB4
52	N	402	CDL	C51-CB5-OB6-CB4
52	X	201	CDL	CA2-OA2-PA1-OA4
52	X	201	CDL	CA2-OA2-PA1-OA5
52	X	201	CDL	CB3-OB5-PB2-OB2
52	X	201	CDL	CB3-OB5-PB2-OB3
52	X	201	CDL	CB3-OB5-PB2-OB4
52	d	203	CDL	CB2-OB2-PB2-OB4
52	d	203	CDL	CB2-OB2-PB2-OB5
52	d	203	CDL	OB7-CB5-OB6-CB4
52	h	201	CDL	CB2-OB2-PB2-OB3
52	h	201	CDL	CB2-OB2-PB2-OB5
52	h	201	CDL	OB7-CB5-OB6-CB4
52	r	201	CDL	CB2-C1-CA2-OA2
52	r	201	CDL	C11-CA5-OA6-CA4
52	r	201	CDL	CB3-OB5-PB2-OB2
52	r	201	CDL	CB3-OB5-PB2-OB3
53	O	401	GTP	C5'-O5'-PA-O3A
53	O	401	GTP	C5'-O5'-PA-O1A
53	O	401	GTP	C5'-O5'-PA-O2A
57	T	101	EHZ	C10-C11-N1-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
57	T	101	EHZ	C15-C16-C17-C18
57	T	101	EHZ	C15-C16-C17-C19
57	T	101	EHZ	C15-C16-C17-C20
57	T	101	EHZ	O2-C9-S1-C10
57	T	101	EHZ	C8-C9-S1-C10
57	U	101	EHZ	C10-C11-N1-C12
57	U	101	EHZ	C15-C16-C17-C18
57	U	101	EHZ	C15-C16-C17-C19
57	U	101	EHZ	C15-C16-C17-C20
57	U	101	EHZ	O2-C9-S1-C10
57	U	101	EHZ	C8-C9-S1-C10
59	o	201	MYR	O1-C1-C2-C3
45	P	502	3PE	O32-C31-O31-C3
45	Y	804	3PE	O32-C31-O31-C3
46	d	202	PC1	O32-C31-O31-C3
52	N	402	CDL	OA9-CA7-OA8-CA6
48	D	701	U10	C52-C53-C54-C56
45	P	502	3PE	C32-C31-O31-C3
45	Y	801	3PE	C32-C31-O31-C3
45	L	701	3PE	O32-C31-O31-C3
45	L	704	3PE	O32-C31-O31-C3
45	N	401	3PE	O32-C31-O31-C3
45	Y	801	3PE	O32-C31-O31-C3
45	Y	805	3PE	O32-C31-O31-C3
45	d	201	3PE	O32-C31-O31-C3
45	m	402	3PE	O32-C31-O31-C3
46	B	202	PC1	O32-C31-O31-C3
46	Y	806	PC1	O32-C31-O31-C3
46	h	202	PC1	O32-C31-O31-C3
52	L	702	CDL	OA9-CA7-OA8-CA6
45	N	401	3PE	O22-C21-O21-C2
45	P	502	3PE	O22-C21-O21-C2
45	m	402	3PE	O22-C21-O21-C2
46	d	202	PC1	O22-C21-O21-C2
46	q	201	PC1	O22-C21-O21-C2
46	q	202	PC1	O22-C21-O21-C2
52	H	602	CDL	OA7-CA5-OA6-CA4
52	N	402	CDL	OA7-CA5-OA6-CA4
45	M	903	3PE	C32-C31-O31-C3
45	Y	804	3PE	C32-C31-O31-C3
45	m	402	3PE	C32-C31-O31-C3
46	Y	806	PC1	C32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	h	202	PC1	C32-C31-O31-C3
52	N	402	CDL	C31-CA7-OA8-CA6
45	L	704	3PE	C22-C21-O21-C2
45	Y	803	3PE	C22-C21-O21-C2
46	A	204	PC1	C22-C21-O21-C2
52	H	602	CDL	C51-CB5-OB6-CB4
52	d	203	CDL	C51-CB5-OB6-CB4
52	h	201	CDL	C51-CB5-OB6-CB4
48	D	701	U10	C12-C11-C9-C10
48	D	701	U10	C30-C29-C31-C32
48	D	701	U10	C12-C11-C9-C8
48	D	701	U10	C28-C29-C31-C32
45	L	701	3PE	C32-C31-O31-C3
45	L	704	3PE	C32-C31-O31-C3
45	N	401	3PE	C32-C31-O31-C3
45	Y	805	3PE	C32-C31-O31-C3
45	d	201	3PE	C32-C31-O31-C3
46	A	202	PC1	C32-C31-O31-C3
46	A	204	PC1	C32-C31-O31-C3
46	B	202	PC1	C32-C31-O31-C3
52	L	702	CDL	C31-CA7-OA8-CA6
48	D	701	U10	C7-C8-C9-C11
46	A	204	PC1	O32-C31-O31-C3
45	L	701	3PE	O22-C21-O21-C2
52	r	201	CDL	OA7-CA5-OA6-CA4
52	L	702	CDL	O1-C1-CA2-OA2
52	N	402	CDL	O1-C1-CB2-OB2
52	r	201	CDL	O1-C1-CA2-OA2
46	g	201	PC1	C32-C31-O31-C3
45	m	401	3PE	C22-C21-O21-C2
46	g	201	PC1	O32-C31-O31-C3
46	A	202	PC1	O32-C31-O31-C3
46	q	202	PC1	C2-C1-O11-P
52	H	602	CDL	C1-CA2-OA2-PA1
45	m	401	3PE	O22-C21-O21-C2
52	L	702	CDL	CB2-C1-CA2-OA2
52	N	402	CDL	CA2-C1-CB2-OB2
52	h	201	CDL	CB2-C1-CA2-OA2
45	A	201	3PE	C32-C31-O31-C3
45	Y	802	3PE	C32-C31-O31-C3
46	A	203	PC1	C32-C31-O31-C3
46	I	204	PC1	C32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	N	402	CDL	C71-CB7-OB8-CB6
52	h	201	CDL	C71-CB7-OB8-CB6
46	Z	201	PC1	C11-C12-N-C13
46	Z	201	PC1	C11-C12-N-C15
46	A	203	PC1	O32-C31-O31-C3
52	h	201	CDL	OB9-CB7-OB8-CB6
52	d	203	CDL	OB5-CB3-CB4-OB6
46	I	204	PC1	C22-C21-O21-C2
46	q	201	PC1	C31-C32-C33-C34
52	L	702	CDL	CA5-C11-C12-C13
46	I	204	PC1	O32-C31-O31-C3
52	r	201	CDL	CA5-C11-C12-C13
45	K	101	3PE	C31-C32-C33-C34
46	I	204	PC1	C31-C32-C33-C34
46	q	202	PC1	C31-C32-C33-C34
45	A	201	3PE	O32-C31-O31-C3
52	X	201	CDL	CA5-C11-C12-C13
52	h	201	CDL	CB5-C51-C52-C53
45	Y	802	3PE	O32-C31-O31-C3
52	h	201	CDL	O1-C1-CA2-OA2
52	N	402	CDL	OB9-CB7-OB8-CB6
45	N	401	3PE	C2C-C2D-C2E-C2F
45	K	101	3PE	C32-C31-O31-C3
45	K	101	3PE	C22-C21-O21-C2
46	A	202	PC1	C22-C21-O21-C2
52	X	201	CDL	C11-CA5-OA6-CA4
45	Y	802	3PE	C31-C32-C33-C34
45	K	101	3PE	O22-C21-O21-C2
46	A	202	PC1	O22-C21-O21-C2
46	I	204	PC1	O22-C21-O21-C2
52	X	201	CDL	OA7-CA5-OA6-CA4
52	X	201	CDL	OB7-CB5-OB6-CB4
46	q	201	PC1	C32-C31-O31-C3
46	I	201	PC1	C22-C21-O21-C2
52	X	201	CDL	C51-CB5-OB6-CB4
48	D	701	U10	C39-C41-C42-C43
52	d	203	CDL	O1-C1-CA2-OA2
45	N	401	3PE	C3-C2-O21-C21
52	H	602	CDL	CA3-CA4-OA6-CA5
52	L	702	CDL	C11-CA5-OA6-CA4
45	m	401	3PE	C32-C31-O31-C3
46	Z	201	PC1	C11-C12-N-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	M	903	3PE	C21-C22-C23-C24
46	q	201	PC1	O32-C31-O31-C3
46	h	202	PC1	C2B-C2C-C2D-C2E
52	r	201	CDL	C53-C54-C55-C56
45	M	901	3PE	C37-C38-C39-C3A
45	d	201	3PE	C26-C27-C28-C29
45	m	401	3PE	C24-C25-C26-C27
45	L	703	3PE	C21-C22-C23-C24
45	Y	803	3PE	C31-C32-C33-C34
45	K	101	3PE	C29-C2A-C2B-C2C
45	d	201	3PE	C33-C34-C35-C36
46	I	201	PC1	C3E-C3F-C3G-C3H
52	h	201	CDL	C12-C13-C14-C15
45	N	401	3PE	C23-C24-C25-C26
45	m	401	3PE	C36-C37-C38-C39
45	m	401	3PE	C39-C3A-C3B-C3C
52	X	201	CDL	C12-C13-C14-C15
52	h	201	CDL	C58-C59-C60-C61
59	o	201	MYR	C2-C3-C4-C5
46	I	201	PC1	O22-C21-O21-C2
52	L	702	CDL	OA7-CA5-OA6-CA4
45	L	703	3PE	C35-C36-C37-C38
45	N	401	3PE	C2D-C2E-C2F-C2G
45	m	402	3PE	C29-C2A-C2B-C2C
52	L	702	CDL	C36-C37-C38-C39
52	L	702	CDL	C40-C41-C42-C43
52	N	402	CDL	C12-C13-C14-C15
45	A	201	3PE	C21-C22-C23-C24
45	m	401	3PE	C21-C22-C23-C24
45	Y	802	3PE	C26-C27-C28-C29
45	m	401	3PE	C3D-C3E-C3F-C3G
46	Z	201	PC1	C38-C39-C3A-C3B
45	K	101	3PE	O32-C31-O31-C3
45	M	902	3PE	C39-C3A-C3B-C3C
46	A	203	PC1	C35-C36-C37-C38
52	h	201	CDL	C15-C16-C17-C18
45	m	401	3PE	C2C-C2D-C2E-C2F
55	P	501	NDP	O4B-C4B-C5B-O5B
45	M	902	3PE	C24-C25-C26-C27
45	Y	804	3PE	C35-C36-C37-C38
46	M	904	PC1	C32-C33-C34-C35
52	X	201	CDL	C62-C63-C64-C65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	h	201	CDL	C74-C75-C76-C77
45	d	201	3PE	C35-C36-C37-C38
52	r	201	CDL	CA3-CA4-CA6-OA8
46	Z	201	PC1	C27-C28-C29-C2A
52	L	702	CDL	C63-C64-C65-C66
45	M	901	3PE	C31-C32-C33-C34
45	L	703	3PE	C39-C3A-C3B-C3C
45	M	901	3PE	C27-C28-C29-C2A
45	d	201	3PE	C27-C28-C29-C2A
46	Y	806	PC1	C35-C36-C37-C38
52	L	702	CDL	C57-C58-C59-C60
52	X	201	CDL	C19-C20-C21-C22
52	X	201	CDL	C57-C58-C59-C60
45	H	601	3PE	C2C-C2D-C2E-C2F
45	K	101	3PE	C38-C39-C3A-C3B
45	L	704	3PE	C24-C25-C26-C27
52	X	201	CDL	C23-C24-C25-C26
59	o	201	MYR	C5-C6-C7-C8
45	P	502	3PE	C23-C24-C25-C26
45	Y	801	3PE	C22-C23-C24-C25
46	q	202	PC1	C39-C3A-C3B-C3C
45	Y	801	3PE	C22-C21-O21-C2
45	Y	802	3PE	C22-C21-O21-C2
52	d	203	CDL	C11-CA5-OA6-CA4
45	M	902	3PE	C22-C23-C24-C25
45	Y	801	3PE	C35-C36-C37-C38
46	I	204	PC1	C25-C26-C27-C28
45	m	401	3PE	O32-C31-O31-C3
45	N	401	3PE	C34-C35-C36-C37
52	H	602	CDL	C31-CA7-OA8-CA6
52	d	203	CDL	C35-C36-C37-C38
45	Y	801	3PE	C33-C34-C35-C36
45	L	701	3PE	C22-C23-C24-C25
45	M	901	3PE	C34-C35-C36-C37
45	M	901	3PE	C33-C34-C35-C36
52	X	201	CDL	C59-C60-C61-C62
45	A	201	3PE	C22-C21-O21-C2
45	M	901	3PE	C22-C21-O21-C2
46	h	202	PC1	C22-C21-O21-C2
52	h	201	CDL	C11-CA5-OA6-CA4
45	Y	803	3PE	C21-C22-C23-C24
45	A	201	3PE	O22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	X	201	CDL	C15-C16-C17-C18
46	h	202	PC1	C2E-C2F-C2G-C2H
46	q	202	PC1	C28-C29-C2A-C2B
55	P	501	NDP	O4D-C4D-C5D-O5D
45	A	201	3PE	C2E-C2F-C2G-C2H
45	d	201	3PE	C3A-C3B-C3C-C3D
45	L	703	3PE	C33-C34-C35-C36
52	N	402	CDL	CB4-CB6-OB8-CB7
46	h	202	PC1	C34-C35-C36-C37
45	L	701	3PE	C23-C24-C25-C26
52	d	203	CDL	C33-C34-C35-C36
52	L	702	CDL	C52-C53-C54-C55
46	Z	201	PC1	C31-C32-C33-C34
45	Y	804	3PE	C33-C34-C35-C36
52	d	203	CDL	C72-C73-C74-C75
46	A	202	PC1	O11-C1-C2-O21
52	r	201	CDL	C72-C73-C74-C75
45	K	101	3PE	C34-C35-C36-C37
45	K	101	3PE	C32-C33-C34-C35
46	M	904	PC1	C24-C25-C26-C27
52	N	402	CDL	CA5-C11-C12-C13
45	Y	803	3PE	C23-C24-C25-C26
45	K	101	3PE	O21-C2-C3-O31
46	Y	806	PC1	O21-C2-C3-O31
52	H	602	CDL	OA6-CA4-CA6-OA8
52	N	402	CDL	OA6-CA4-CA6-OA8
52	d	203	CDL	C42-C43-C44-C45
46	B	202	PC1	C3B-C3C-C3D-C3E
46	I	201	PC1	C32-C33-C34-C35
46	I	204	PC1	C38-C39-C3A-C3B
52	h	201	CDL	OA7-CA5-OA6-CA4
52	L	702	CDL	C32-C33-C34-C35
52	X	201	CDL	C35-C36-C37-C38
46	g	201	PC1	C2A-C2B-C2C-C2D
45	M	901	3PE	C2B-C2C-C2D-C2E
45	d	201	3PE	C31-C32-C33-C34
45	P	502	3PE	C33-C34-C35-C36
57	T	101	EHZ	C21-C22-C23-C24
46	I	201	PC1	C38-C39-C3A-C3B
52	N	402	CDL	C20-C21-C22-C23
57	U	101	EHZ	C21-C22-C23-C24
52	N	402	CDL	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	m	402	3PE	O11-C1-C2-C3
52	L	702	CDL	OB5-CB3-CB4-CB6
52	d	203	CDL	OB5-CB3-CB4-CB6
45	Y	801	3PE	O22-C21-O21-C2
45	Y	802	3PE	O22-C21-O21-C2
52	d	203	CDL	OA7-CA5-OA6-CA4
52	H	602	CDL	OA9-CA7-OA8-CA6
52	H	602	CDL	CA7-C31-C32-C33
45	L	701	3PE	C37-C38-C39-C3A
46	g	201	PC1	C23-C24-C25-C26
45	N	401	3PE	C25-C26-C27-C28
52	r	201	CDL	C13-C14-C15-C16
45	K	101	3PE	C1-C2-C3-O31
45	M	901	3PE	C1-C2-C3-O31
45	M	902	3PE	C1-C2-C3-O31
45	M	903	3PE	C1-C2-C3-O31
45	d	201	3PE	C1-C2-C3-O31
46	B	202	PC1	C1-C2-C3-O31
46	d	202	PC1	C1-C2-C3-O31
46	h	202	PC1	C1-C2-C3-O31
52	H	602	CDL	CA3-CA4-CA6-OA8
52	L	702	CDL	CA3-CA4-CA6-OA8
52	h	201	CDL	CA3-CA4-CA6-OA8
46	Y	806	PC1	C28-C29-C2A-C2B
46	d	202	PC1	C33-C34-C35-C36
46	B	202	PC1	C27-C28-C29-C2A
46	g	201	PC1	C26-C27-C28-C29
52	d	203	CDL	CA5-C11-C12-C13
46	h	202	PC1	C25-C26-C27-C28
45	K	101	3PE	C22-C23-C24-C25
45	Y	801	3PE	C32-C33-C34-C35
46	q	201	PC1	C23-C24-C25-C26
45	L	704	3PE	C37-C38-C39-C3A
58	i	201	CHD	C21-C20-C22-C23
45	P	502	3PE	C1-C2-O21-C21
45	Y	803	3PE	C3-C2-O21-C21
52	X	201	CDL	CB6-CB4-OB6-CB5
45	m	402	3PE	C32-C33-C34-C35
46	I	204	PC1	C26-C27-C28-C29
52	L	702	CDL	C60-C61-C62-C63
57	T	101	EHZ	C2-C3-C4-C5
52	N	402	CDL	OA5-CA3-CA4-OA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	m	402	3PE	C34-C35-C36-C37
57	U	101	EHZ	C2-C3-C4-C5
45	H	601	3PE	C32-C31-O31-C3
46	Z	201	PC1	C32-C31-O31-C3
52	N	402	CDL	C19-C20-C21-C22
46	q	202	PC1	C36-C37-C38-C39
46	A	204	PC1	C33-C34-C35-C36
45	P	502	3PE	C36-C37-C38-C39
52	L	702	CDL	C59-C60-C61-C62
52	N	402	CDL	C13-C14-C15-C16
52	h	201	CDL	OB6-CB4-CB6-OB8
46	Y	806	PC1	C26-C27-C28-C29
45	m	402	3PE	C26-C27-C28-C29
45	N	401	3PE	C36-C37-C38-C39
52	h	201	CDL	C76-C77-C78-C79
48	D	701	U10	C19-C21-C22-C23
45	N	401	3PE	C37-C38-C39-C3A
46	h	202	PC1	C29-C2A-C2B-C2C
45	L	704	3PE	C33-C34-C35-C36
46	I	201	PC1	C2B-C2C-C2D-C2E
46	Y	806	PC1	C23-C24-C25-C26
46	q	202	PC1	C35-C36-C37-C38
45	N	401	3PE	C21-C22-C23-C24
57	T	101	EHZ	O4-C15-C16-C17
57	U	101	EHZ	O4-C15-C16-C17
45	A	201	3PE	C28-C29-C2A-C2B
45	M	901	3PE	O22-C21-O21-C2
45	M	903	3PE	C2-C1-O11-P
45	M	903	3PE	C38-C39-C3A-C3B
46	h	202	PC1	C32-C33-C34-C35
52	H	602	CDL	C71-CB7-OB8-CB6
45	L	701	3PE	C3A-C3B-C3C-C3D
45	Y	801	3PE	O11-C1-C2-C3
46	A	202	PC1	O11-C1-C2-C3
52	X	201	CDL	OB5-CB3-CB4-CB6
46	I	204	PC1	C33-C34-C35-C36
46	h	202	PC1	O22-C21-O21-C2
57	T	101	EHZ	N2-C15-C16-C17
57	U	101	EHZ	N2-C15-C16-C17
45	L	703	3PE	C34-C35-C36-C37
52	N	402	CDL	C38-C39-C40-C41
52	h	201	CDL	C40-C41-C42-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	M	901	3PE	C32-C31-O31-C3
52	L	702	CDL	C35-C36-C37-C38
45	L	703	3PE	C23-C24-C25-C26
46	M	904	PC1	C23-C24-C25-C26
45	m	402	3PE	C24-C25-C26-C27
45	m	402	3PE	C2F-C2G-C2H-C2I
52	X	201	CDL	C55-C56-C57-C58
45	Y	801	3PE	C1-C2-C3-O31
46	Y	806	PC1	C1-C2-C3-O31
45	H	601	3PE	C32-C33-C34-C35
59	o	201	MYR	C7-C8-C9-C10
45	M	903	3PE	C31-C32-C33-C34
45	P	502	3PE	C31-C32-C33-C34
52	N	402	CDL	C31-C32-C33-C34
45	Y	805	3PE	O11-C1-C2-O21
45	m	402	3PE	O11-C1-C2-O21
52	X	201	CDL	OB5-CB3-CB4-OB6
45	M	902	3PE	C37-C38-C39-C3A
45	H	601	3PE	O32-C31-O31-C3
46	h	202	PC1	C26-C27-C28-C29
59	o	201	MYR	C3-C4-C5-C6
45	M	902	3PE	O21-C2-C3-O31
45	Y	801	3PE	O21-C2-C3-O31
45	d	201	3PE	O21-C2-C3-O31
46	h	202	PC1	O21-C2-C3-O31
52	h	201	CDL	OA6-CA4-CA6-OA8
52	N	402	CDL	C21-C22-C23-C24
46	M	904	PC1	C22-C23-C24-C25
45	d	201	3PE	C21-C22-C23-C24
52	L	702	CDL	C15-C16-C17-C18
46	h	202	PC1	C22-C23-C24-C25
46	h	202	PC1	C33-C34-C35-C36
45	m	402	3PE	C25-C26-C27-C28
46	q	201	PC1	C27-C28-C29-C2A
52	h	201	CDL	C53-C54-C55-C56
45	m	401	3PE	O11-C1-C2-C3
46	g	201	PC1	O11-C1-C2-C3
52	N	402	CDL	OA5-CA3-CA4-CA6
45	M	901	3PE	O32-C31-O31-C3
46	Z	201	PC1	C21-C22-C23-C24
52	h	201	CDL	CB7-C71-C72-C73
52	h	201	CDL	C39-C40-C41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	M	901	3PE	C2A-C2B-C2C-C2D
52	H	602	CDL	CA5-C11-C12-C13
45	Y	803	3PE	C25-C26-C27-C28
46	Z	201	PC1	O32-C31-O31-C3
52	H	602	CDL	OB9-CB7-OB8-CB6
45	m	402	3PE	C2C-C2D-C2E-C2F
45	d	201	3PE	C3D-C3E-C3F-C3G
45	L	701	3PE	O11-C1-C2-O21
45	Y	801	3PE	O11-C1-C2-O21
45	m	401	3PE	O11-C1-C2-O21
52	r	201	CDL	OA5-CA3-CA4-OA6
45	H	601	3PE	C1-C2-C3-O31
46	A	203	PC1	C1-C2-C3-O31
46	I	204	PC1	C1-C2-C3-O31
52	N	402	CDL	CA3-CA4-CA6-OA8
45	L	703	3PE	C22-C21-O21-C2
52	N	402	CDL	C16-C17-C18-C19
46	Z	201	PC1	C33-C34-C35-C36
52	r	201	CDL	C51-C52-C53-C54
45	A	201	3PE	C12-C11-O13-P
45	L	704	3PE	C12-C11-O13-P
45	M	902	3PE	C12-C11-O13-P
45	Y	801	3PE	C12-C11-O13-P
46	A	202	PC1	C12-C11-O13-P
46	I	201	PC1	C12-C11-O13-P
45	H	601	3PE	C29-C2A-C2B-C2C
45	M	901	3PE	O21-C2-C3-O31
46	d	202	PC1	O21-C2-C3-O31
46	Y	806	PC1	C31-C32-C33-C34
46	g	201	PC1	C2B-C2C-C2D-C2E
45	L	704	3PE	C2D-C2E-C2F-C2G
45	m	401	3PE	C26-C27-C28-C29
55	P	501	NDP	O4D-C1D-N1N-C6N
55	P	501	NDP	C3B-C4B-C5B-O5B
52	N	402	CDL	CA4-CA3-OA5-PA1
45	M	901	3PE	C28-C29-C2A-C2B
46	A	203	PC1	O13-C11-C12-N
46	I	201	PC1	O13-C11-C12-N
45	A	201	3PE	C37-C38-C39-C3A
45	M	902	3PE	C31-C32-C33-C34
45	N	401	3PE	C3C-C3D-C3E-C3F
46	I	201	PC1	C3B-C3C-C3D-C3E

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	m	402	3PE	C23-C24-C25-C26
45	K	101	3PE	C36-C37-C38-C39
46	A	202	PC1	C33-C34-C35-C36
45	M	901	3PE	C3B-C3C-C3D-C3E
45	A	201	3PE	C2A-C2B-C2C-C2D
45	d	201	3PE	C37-C38-C39-C3A
45	H	601	3PE	O11-C1-C2-C3
45	L	701	3PE	O11-C1-C2-C3
45	Y	805	3PE	O11-C1-C2-C3
52	r	201	CDL	OA5-CA3-CA4-CA6
58	i	201	CHD	C17-C20-C22-C23
45	P	502	3PE	O21-C21-C22-C23
46	M	904	PC1	C2-C1-O11-P
46	q	201	PC1	C2-C1-O11-P
52	X	201	CDL	C1-CA2-OA2-PA1
45	L	703	3PE	O22-C21-O21-C2
45	H	601	3PE	O11-C1-C2-O21
46	g	201	PC1	O11-C1-C2-O21
52	L	702	CDL	OB5-CB3-CB4-OB6
45	N	401	3PE	C28-C29-C2A-C2B
45	H	601	3PE	O21-C2-C3-O31
45	M	903	3PE	O21-C2-C3-O31
52	r	201	CDL	OA6-CA4-CA6-OA8
45	M	903	3PE	C3C-C3D-C3E-C3F
52	h	201	CDL	CB3-CB4-CB6-OB8
52	X	201	CDL	C60-C61-C62-C63
46	g	201	PC1	C32-C33-C34-C35
45	M	903	3PE	C36-C37-C38-C39
45	m	402	3PE	C2A-C2B-C2C-C2D
46	B	202	PC1	C31-C32-C33-C34
45	Y	804	3PE	C38-C39-C3A-C3B
52	H	602	CDL	C51-C52-C53-C54
45	A	201	3PE	C35-C36-C37-C38
45	H	601	3PE	C1-O11-P-O14
45	K	101	3PE	C1-O11-P-O12
45	K	101	3PE	C1-O11-P-O13
45	L	701	3PE	C1-O11-P-O12
45	M	901	3PE	C11-O13-P-O11
45	M	903	3PE	C1-O11-P-O14
45	N	401	3PE	C1-O11-P-O12
45	N	401	3PE	C1-O11-P-O13
45	N	401	3PE	C11-O13-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	P	502	3PE	C11-O13-P-O14
45	Y	803	3PE	C1-O11-P-O14
45	Y	804	3PE	C1-O11-P-O14
45	Y	804	3PE	C11-O13-P-O11
45	Y	804	3PE	C11-O13-P-O12
45	Y	804	3PE	C11-O13-P-O14
45	Y	805	3PE	C11-O13-P-O11
45	d	201	3PE	C1-O11-P-O14
45	m	401	3PE	C1-O11-P-O12
45	m	401	3PE	C1-O11-P-O13
45	m	401	3PE	C1-O11-P-O14
45	m	402	3PE	O13-C11-C12-N
46	A	202	PC1	C1-O11-P-O14
46	B	202	PC1	C11-O13-P-O14
46	I	201	PC1	C11-O13-P-O14
46	I	201	PC1	C1-O11-P-O13
46	I	204	PC1	C11-O13-P-O11
46	M	904	PC1	C11-O13-P-O11
46	Y	806	PC1	C11-O13-P-O14
46	Z	201	PC1	C1-O11-P-O12
46	d	202	PC1	C11-O13-P-O12
46	d	202	PC1	C11-O13-P-O14
46	d	202	PC1	C11-O13-P-O11
46	g	201	PC1	C11-O13-P-O12
46	g	201	PC1	C1-O11-P-O13
46	q	201	PC1	C11-O13-P-O14
46	q	202	PC1	C1-O11-P-O12
52	H	602	CDL	CB3-OB5-PB2-OB3
52	X	201	CDL	CB2-OB2-PB2-OB4
52	X	201	CDL	CB2-OB2-PB2-OB5
52	d	203	CDL	CB2-OB2-PB2-OB3
52	d	203	CDL	CB3-OB5-PB2-OB4
52	h	201	CDL	CB3-OB5-PB2-OB2
52	h	201	CDL	CB3-OB5-PB2-OB3
52	h	201	CDL	CB3-OB5-PB2-OB4
55	P	501	NDP	C5B-O5B-PA-O1A
55	P	501	NDP	C5B-O5B-PA-O3
45	L	704	3PE	C34-C35-C36-C37
45	N	401	3PE	C32-C33-C34-C35
45	Y	801	3PE	C36-C37-C38-C39
45	m	401	3PE	C32-C33-C34-C35
45	Y	804	3PE	C22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	Y	802	3PE	C2-C1-O11-P
52	H	602	CDL	CB4-CB3-OB5-PB2
52	X	201	CDL	C1-CB2-OB2-PB2
52	d	203	CDL	C1-CB2-OB2-PB2
52	d	203	CDL	CB4-CB3-OB5-PB2
52	r	201	CDL	CA4-CA3-OA5-PA1
52	N	402	CDL	C32-C31-CA7-OA8
45	L	703	3PE	C37-C38-C39-C3A
45	M	902	3PE	C36-C37-C38-C39
46	A	204	PC1	C21-C22-C23-C24
45	Y	804	3PE	C3-C2-O21-C21
46	A	204	PC1	C3-C2-O21-C21
52	d	203	CDL	C31-C32-C33-C34
45	A	201	3PE	C31-C32-C33-C34
46	M	904	PC1	O11-C1-C2-O21
45	A	201	3PE	C32-C33-C34-C35
45	L	701	3PE	C36-C37-C38-C39
52	L	702	CDL	C31-C32-C33-C34
45	M	901	3PE	C2E-C2F-C2G-C2H
46	Y	806	PC1	C38-C39-C3A-C3B
46	A	202	PC1	C27-C28-C29-C2A
52	X	201	CDL	C20-C21-C22-C23
52	X	201	CDL	C52-C53-C54-C55
45	Y	804	3PE	O22-C21-O21-C2
46	I	204	PC1	C22-C23-C24-C25
46	A	203	PC1	O21-C2-C3-O31
45	m	402	3PE	O31-C31-C32-C33
45	L	701	3PE	C39-C3A-C3B-C3C
46	Z	201	PC1	C32-C33-C34-C35
46	A	202	PC1	C24-C25-C26-C27
52	H	602	CDL	C72-C71-CB7-OB8
45	L	703	3PE	C32-C31-O31-C3
52	r	201	CDL	C72-C71-CB7-OB8
52	X	201	CDL	C18-C19-C20-C21
52	X	201	CDL	C39-C40-C41-C42
46	Y	806	PC1	C36-C37-C38-C39
46	M	904	PC1	O32-C31-O31-C3
46	q	201	PC1	C32-C33-C34-C35
46	M	904	PC1	C32-C31-O31-C3
45	L	703	3PE	O32-C31-O31-C3
46	A	204	PC1	O11-C1-C2-O21
52	L	702	CDL	OA5-CA3-CA4-OA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	N	402	CDL	C11-C12-C13-C14
45	A	201	3PE	C2C-C2D-C2E-C2F
45	N	401	3PE	C3F-C3G-C3H-C3I
45	L	703	3PE	O21-C2-C3-O31
46	d	202	PC1	C36-C37-C38-C39
48	D	701	U10	C20-C19-C21-C22
45	L	701	3PE	C29-C2A-C2B-C2C
52	H	602	CDL	C32-C33-C34-C35
52	L	702	CDL	CB4-CB6-OB8-CB7
45	M	903	3PE	C26-C27-C28-C29
52	X	201	CDL	C33-C34-C35-C36
52	h	201	CDL	C1-CA2-OA2-PA1
45	L	701	3PE	C25-C26-C27-C28
45	L	703	3PE	C36-C37-C38-C39
45	H	601	3PE	C28-C29-C2A-C2B
45	M	902	3PE	C2E-C2F-C2G-C2H
45	Y	801	3PE	C1-C2-O21-C21
46	q	202	PC1	C3-C2-O21-C21
52	H	602	CDL	CB6-CB4-OB6-CB5
45	M	903	3PE	C24-C25-C26-C27
45	Y	802	3PE	C2E-C2F-C2G-C2H
52	H	602	CDL	OB5-CB3-CB4-OB6
52	r	201	CDL	OB5-CB3-CB4-OB6
45	K	101	3PE	C3B-C3C-C3D-C3E
52	L	702	CDL	C58-C59-C60-C61
52	r	201	CDL	C1-CB2-OB2-PB2
46	q	202	PC1	C2B-C2C-C2D-C2E
46	M	904	PC1	C25-C26-C27-C28
52	N	402	CDL	C37-C38-C39-C40
52	X	201	CDL	C43-C44-C45-C46
52	L	702	CDL	C54-C55-C56-C57
45	M	902	3PE	C29-C2A-C2B-C2C
52	N	402	CDL	C39-C40-C41-C42
46	I	201	PC1	C37-C38-C39-C3A
46	B	202	PC1	O21-C21-C22-C23
48	D	701	U10	C18-C19-C21-C22
46	B	202	PC1	C24-C25-C26-C27
52	X	201	CDL	CB7-C71-C72-C73
45	d	201	3PE	C39-C3A-C3B-C3C
48	D	701	U10	C26-C27-C28-C29
45	M	901	3PE	C2D-C2E-C2F-C2G
45	Y	803	3PE	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	N	401	3PE	C3A-C3B-C3C-C3D
48	D	701	U10	C25-C24-C26-C27
45	A	201	3PE	C2-C1-O11-P
45	Y	801	3PE	C2-C1-O11-P
45	L	701	3PE	C2A-C2B-C2C-C2D
52	r	201	CDL	C18-C19-C20-C21
45	H	601	3PE	C22-C23-C24-C25
45	Y	802	3PE	C2C-C2D-C2E-C2F
45	M	903	3PE	C34-C35-C36-C37
48	D	701	U10	C23-C24-C26-C27
52	L	702	CDL	C39-C40-C41-C42
52	X	201	CDL	C41-C42-C43-C44
45	A	201	3PE	O21-C21-C22-C23
45	K	101	3PE	O21-C21-C22-C23
46	I	201	PC1	C26-C27-C28-C29
52	h	201	CDL	C32-C33-C34-C35
53	O	401	GTP	C4'-C5'-O5'-PA
45	A	201	3PE	C23-C24-C25-C26
45	m	402	3PE	C2D-C2E-C2F-C2G
46	A	202	PC1	C22-C23-C24-C25
45	H	601	3PE	C2D-C2E-C2F-C2G
52	H	602	CDL	CB5-C51-C52-C53
45	N	401	3PE	C3E-C3F-C3G-C3H
45	m	402	3PE	C22-C23-C24-C25
52	h	201	CDL	C38-C39-C40-C41
45	M	903	3PE	C33-C34-C35-C36
52	X	201	CDL	C32-C33-C34-C35
45	Y	801	3PE	C3-C2-O21-C21
46	q	202	PC1	C1-C2-O21-C21
46	Z	201	PC1	C22-C23-C24-C25
45	m	401	3PE	C33-C34-C35-C36
46	I	201	PC1	C23-C24-C25-C26
45	L	701	3PE	C32-C33-C34-C35
46	A	202	PC1	C2-C1-O11-P
45	N	401	3PE	C22-C23-C24-C25
52	X	201	CDL	CA2-C1-CB2-OB2
45	Y	802	3PE	O11-C1-C2-O21
52	N	402	CDL	OB5-CB3-CB4-OB6
45	L	704	3PE	C26-C27-C28-C29
45	M	903	3PE	C2D-C2E-C2F-C2G
46	q	202	PC1	C24-C25-C26-C27
46	A	204	PC1	C12-C11-O13-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	h	202	PC1	C12-C11-O13-P
45	d	201	3PE	C29-C2A-C2B-C2C
45	m	401	3PE	O31-C31-C32-C33
52	X	201	CDL	C64-C65-C66-C67
45	M	902	3PE	C34-C35-C36-C37
45	d	201	3PE	O21-C21-C22-C23
45	Y	802	3PE	O11-C1-C2-C3
46	M	904	PC1	O11-C1-C2-C3
52	d	203	CDL	OA5-CA3-CA4-CA6
45	N	401	3PE	O21-C21-C22-C23
45	N	401	3PE	C2B-C2C-C2D-C2E
46	A	202	PC1	C34-C35-C36-C37
45	m	402	3PE	C27-C28-C29-C2A
45	m	402	3PE	C2E-C2F-C2G-C2H
45	Y	802	3PE	O21-C21-C22-C23
45	Y	804	3PE	O21-C21-C22-C23
52	X	201	CDL	C12-C11-CA5-OA6
46	q	202	PC1	C34-C35-C36-C37
48	D	701	U10	C35-C34-C36-C37
52	X	201	CDL	C72-C71-CB7-OB8
45	m	401	3PE	C37-C38-C39-C3A
46	A	202	PC1	O31-C31-C32-C33
46	d	202	PC1	C35-C36-C37-C38
46	B	202	PC1	C32-C33-C34-C35
52	L	702	CDL	C72-C71-CB7-OB8
46	I	201	PC1	O11-C1-C2-O21
59	o	201	MYR	C1-C2-C3-C4
46	d	202	PC1	O21-C21-C22-C23
46	Z	201	PC1	C29-C2A-C2B-C2C
45	Y	802	3PE	C24-C25-C26-C27
46	h	202	PC1	C37-C38-C39-C3A
45	m	402	3PE	C33-C34-C35-C36
45	L	703	3PE	C3F-C3G-C3H-C3I
45	Y	802	3PE	O31-C31-C32-C33
52	X	201	CDL	C51-C52-C53-C54
45	L	703	3PE	C1-C2-C3-O31
48	D	701	U10	C34-C36-C37-C38
46	q	201	PC1	C38-C39-C3A-C3B
45	L	704	3PE	C28-C29-C2A-C2B
46	A	203	PC1	O21-C21-C22-C23
46	q	202	PC1	O31-C31-C32-C33
45	K	101	3PE	O31-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	M	903	3PE	C25-C26-C27-C28
45	Y	804	3PE	C31-C32-C33-C34
57	T	101	EHZ	C4-C5-C6-C7
57	U	101	EHZ	C4-C5-C6-C7
45	M	901	3PE	O21-C21-C22-C23
46	I	201	PC1	O31-C31-C32-C33
50	F	501	FMN	N10-C1'-C2'-O2'
52	d	203	CDL	CB2-C1-CA2-OA2
45	Y	801	3PE	O21-C21-C22-C23
46	Y	806	PC1	C39-C3A-C3B-C3C
55	P	501	NDP	C3D-C4D-C5D-O5D
45	M	902	3PE	O22-C21-O21-C2
45	Y	802	3PE	O22-C21-C22-C23
52	L	702	CDL	C13-C14-C15-C16
45	Y	801	3PE	C31-C32-C33-C34
45	P	502	3PE	O22-C21-C22-C23
45	Y	802	3PE	O32-C31-C32-C33
45	H	601	3PE	O31-C31-C32-C33
45	Y	801	3PE	O31-C31-C32-C33
45	Y	802	3PE	C28-C29-C2A-C2B
52	L	702	CDL	C72-C71-CB7-OB9
46	d	202	PC1	C37-C38-C39-C3A
45	M	902	3PE	C35-C36-C37-C38
46	q	202	PC1	O21-C21-C22-C23
45	N	401	3PE	O22-C21-C22-C23
52	X	201	CDL	C72-C71-CB7-OB9
45	K	101	3PE	C3D-C3E-C3F-C3G
46	Z	201	PC1	C37-C38-C39-C3A
46	A	202	PC1	O32-C31-C32-C33
45	M	903	3PE	C2A-C2B-C2C-C2D
45	K	101	3PE	O32-C31-C32-C33
45	M	901	3PE	O22-C21-C22-C23
52	X	201	CDL	C12-C11-CA5-OA7
46	q	201	PC1	O21-C21-C22-C23
45	Y	804	3PE	O22-C21-C22-C23
45	d	201	3PE	O22-C21-C22-C23
46	I	201	PC1	O32-C31-C32-C33
52	X	201	CDL	C63-C64-C65-C66
45	Y	802	3PE	C2A-C2B-C2C-C2D
52	H	602	CDL	C52-C51-CB5-OB6
45	N	401	3PE	C2A-C2B-C2C-C2D
46	A	203	PC1	O22-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
57	U	101	EHZ	C22-C23-C24-C25
57	T	101	EHZ	C22-C23-C24-C25
45	m	401	3PE	O32-C31-C32-C33
46	M	904	PC1	O31-C31-C32-C33
45	A	201	3PE	C34-C35-C36-C37
46	h	202	PC1	C2C-C2D-C2E-C2F
50	F	501	FMN	C4'-C5'-O5'-P
46	d	202	PC1	O22-C21-C22-C23
45	Y	804	3PE	C21-C22-C23-C24
46	A	202	PC1	O21-C21-C22-C23
52	L	702	CDL	OA5-CA3-CA4-CA6
46	A	204	PC1	O21-C21-C22-C23
52	h	201	CDL	C32-C31-CA7-OA8
45	P	502	3PE	C35-C36-C37-C38
57	U	101	EHZ	C3-C4-C5-C6
45	M	903	3PE	C2C-C2D-C2E-C2F
53	O	401	GTP	PA-O3A-PB-O2B
46	g	201	PC1	C2F-C2G-C2H-C2I
57	T	101	EHZ	C3-C4-C5-C6
45	Y	801	3PE	O32-C31-C32-C33
46	A	202	PC1	O22-C21-C22-C23
46	q	202	PC1	O32-C31-C32-C33
52	H	602	CDL	C52-C51-CB5-OB7

There are no ring outliers.

23 monomers are involved in 41 short contacts:

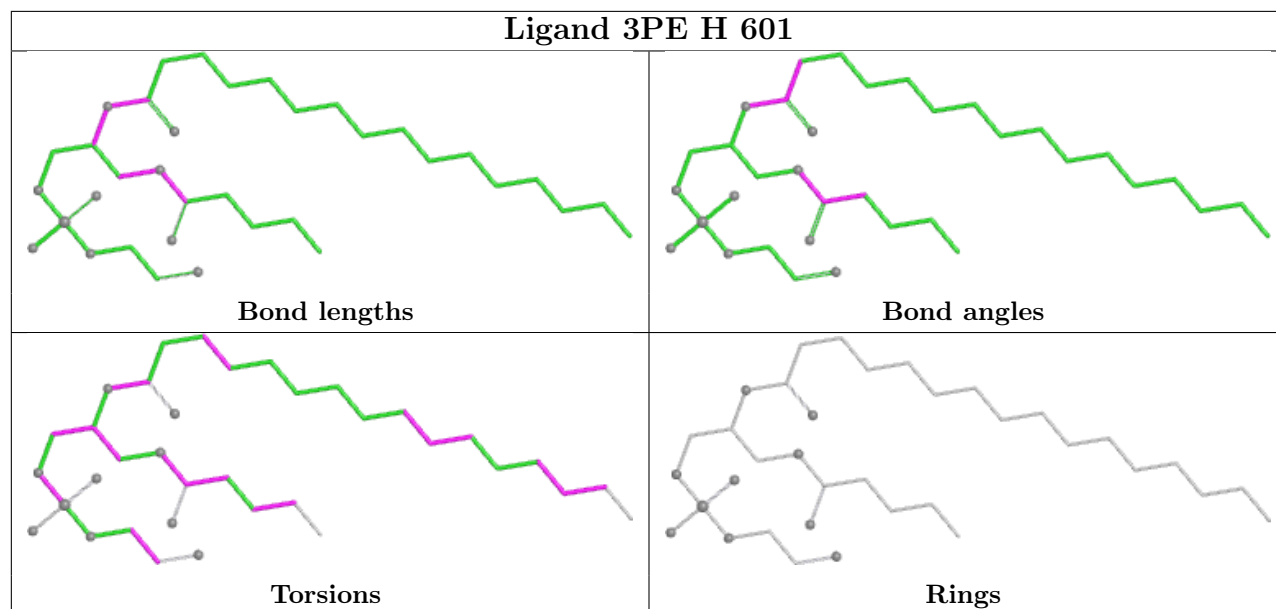
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	X	201	CDL	1	0
46	A	202	PC1	1	0
47	B	201	SF4	1	0
53	O	401	GTP	1	0
45	m	401	3PE	1	0
46	q	201	PC1	1	0
57	U	101	EHZ	2	0
58	i	201	CHD	1	0
57	T	101	EHZ	2	0
45	L	701	3PE	1	0
45	m	402	3PE	1	0
45	M	903	3PE	1	0
45	L	704	3PE	1	0
55	P	501	NDP	3	0

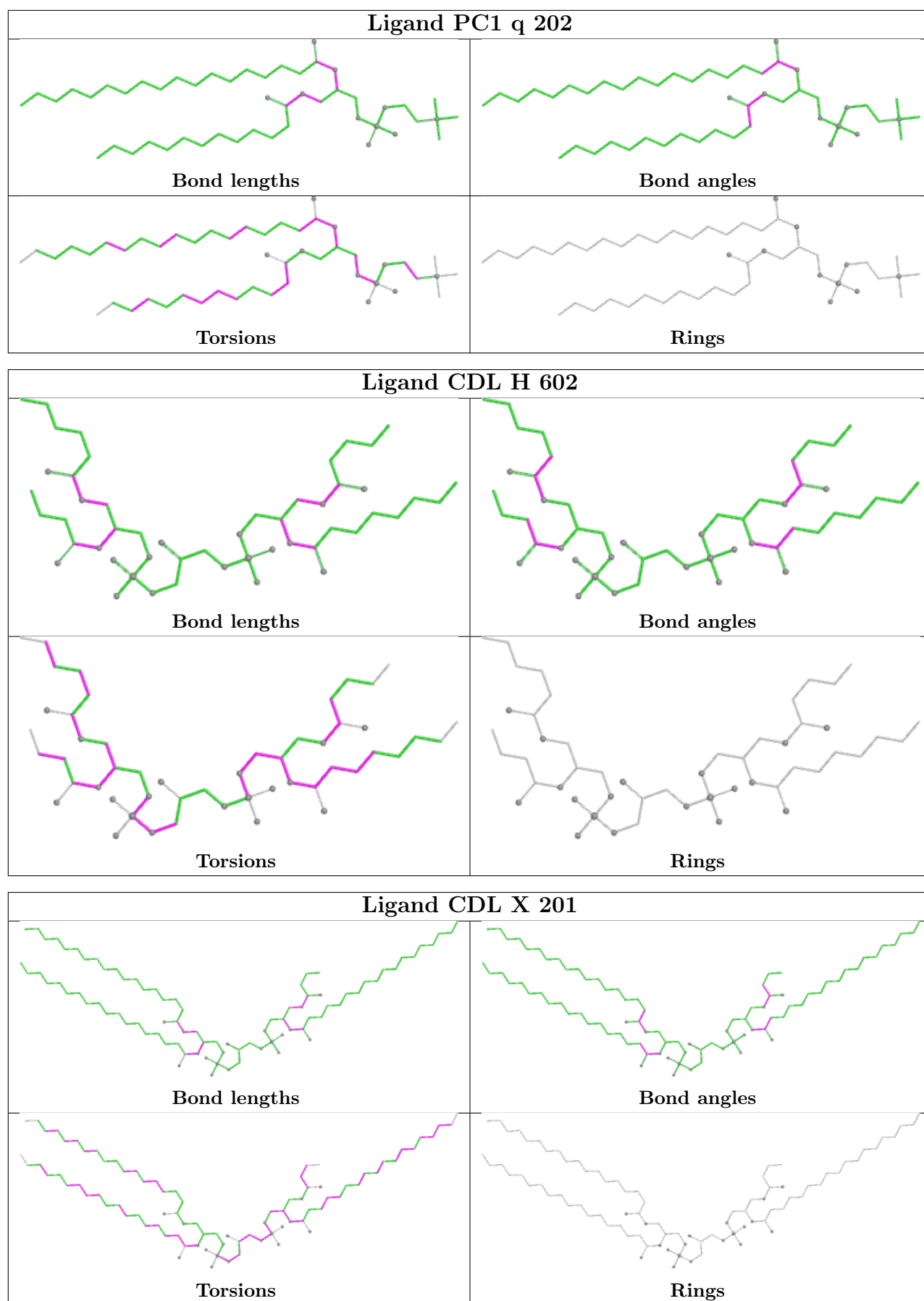
Continued on next page...

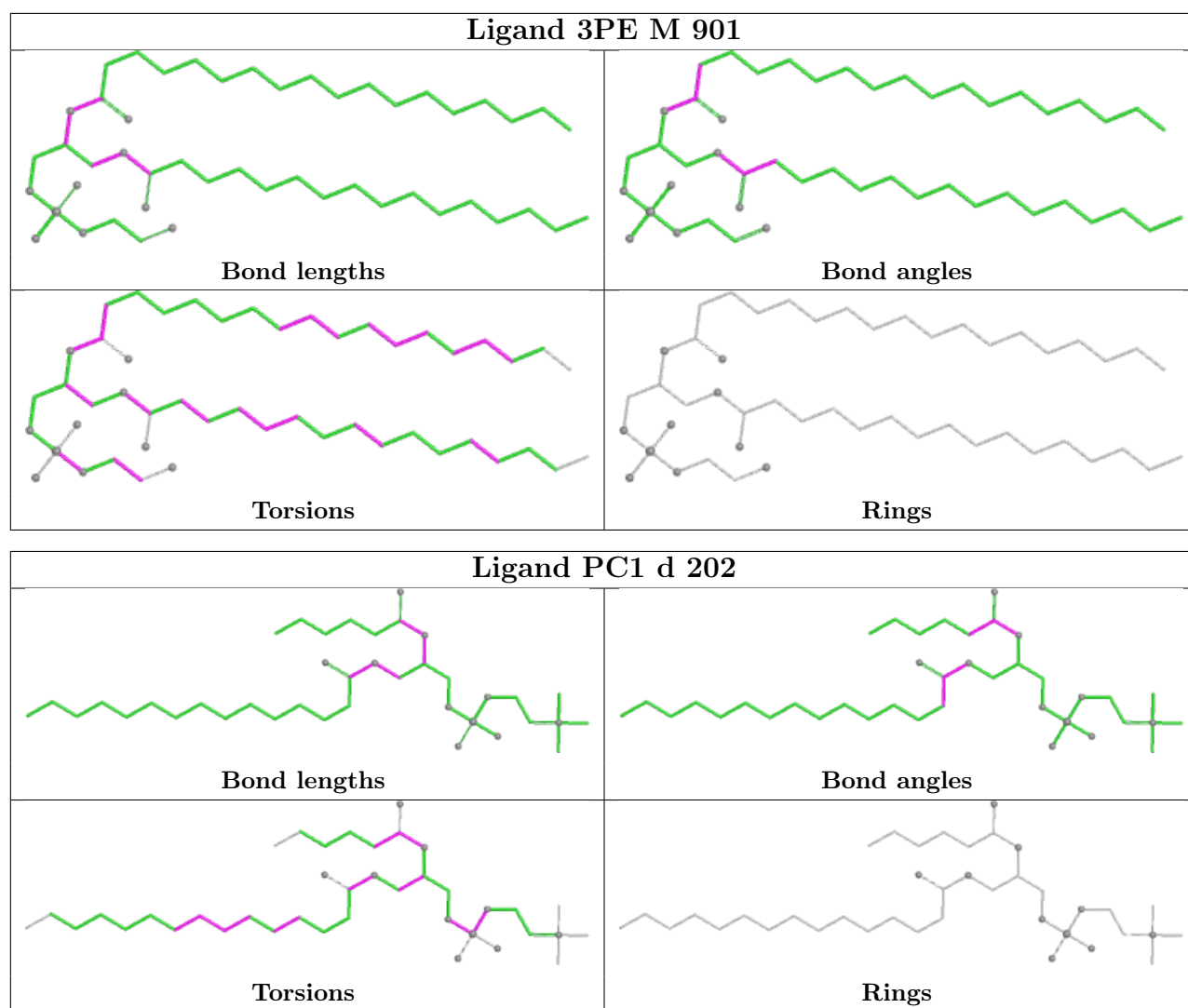
Continued from previous page...

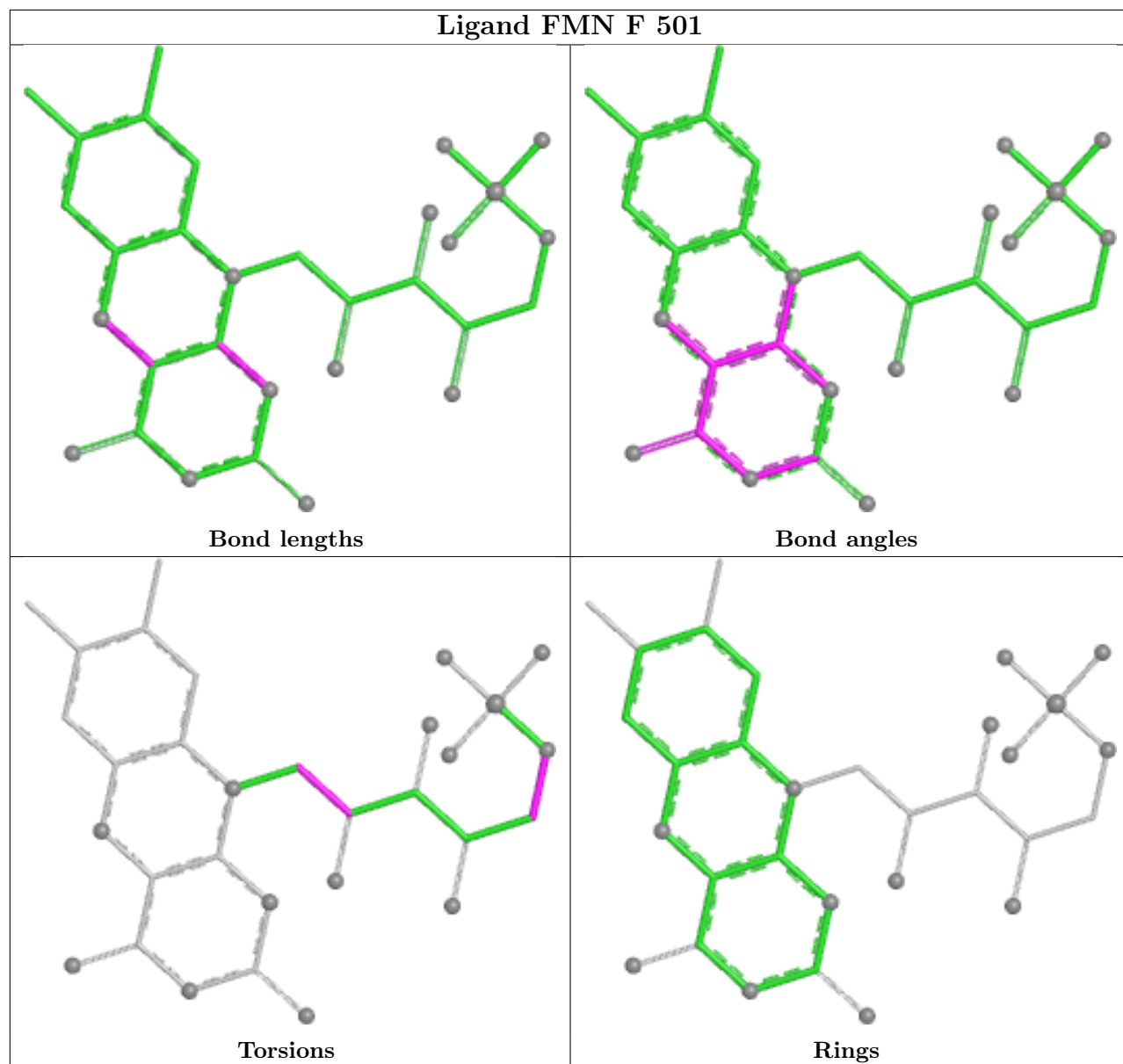
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	Y	803	3PE	1	0
52	d	203	CDL	2	0
46	Z	201	PC1	7	0
46	h	202	PC1	1	0
45	M	902	3PE	1	0
46	I	201	PC1	1	0
48	D	701	U10	2	0
52	h	201	CDL	1	0
45	N	401	3PE	7	0

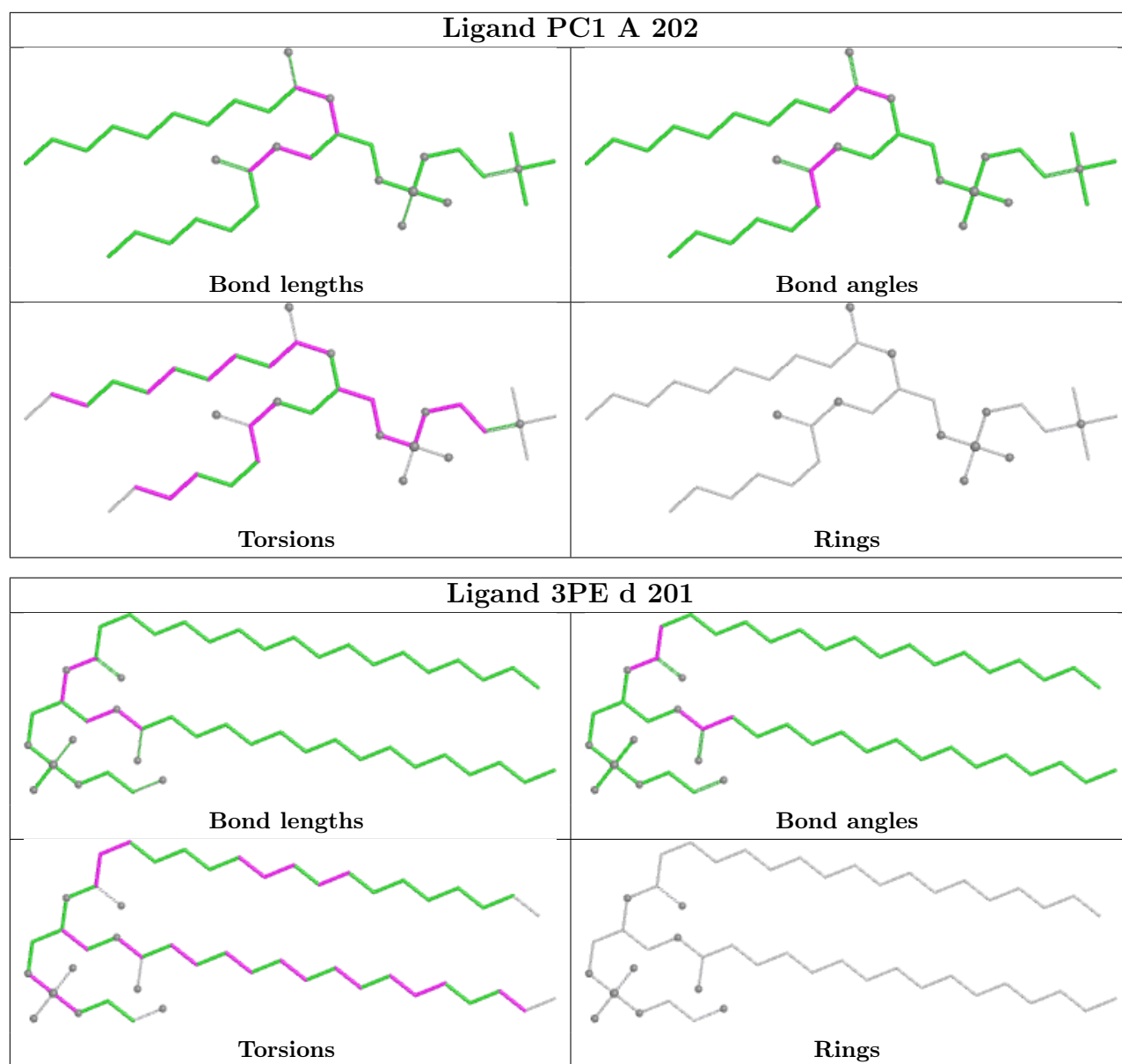
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

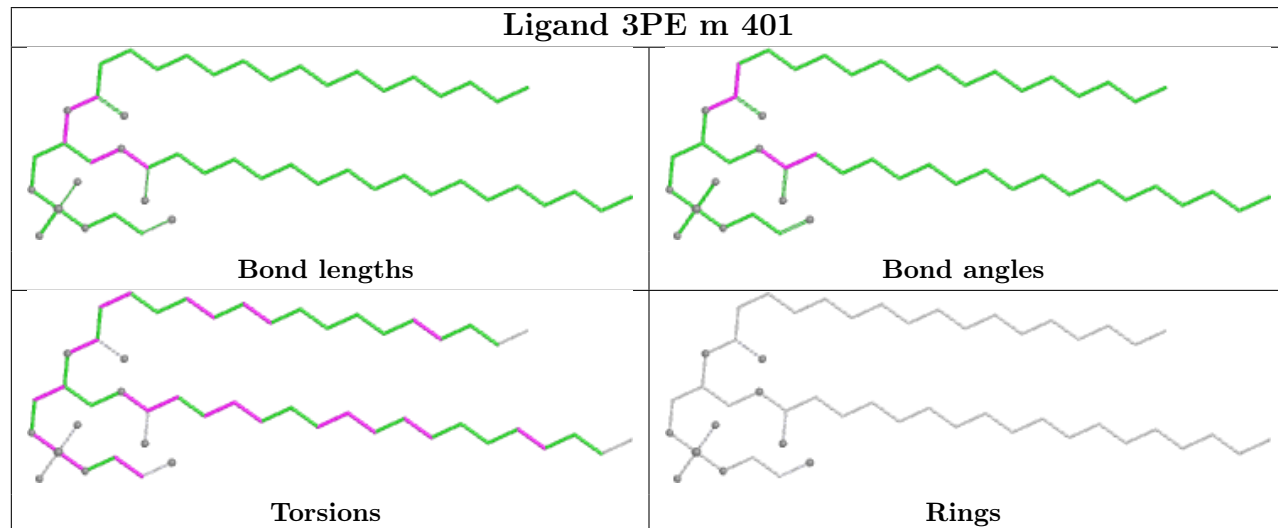
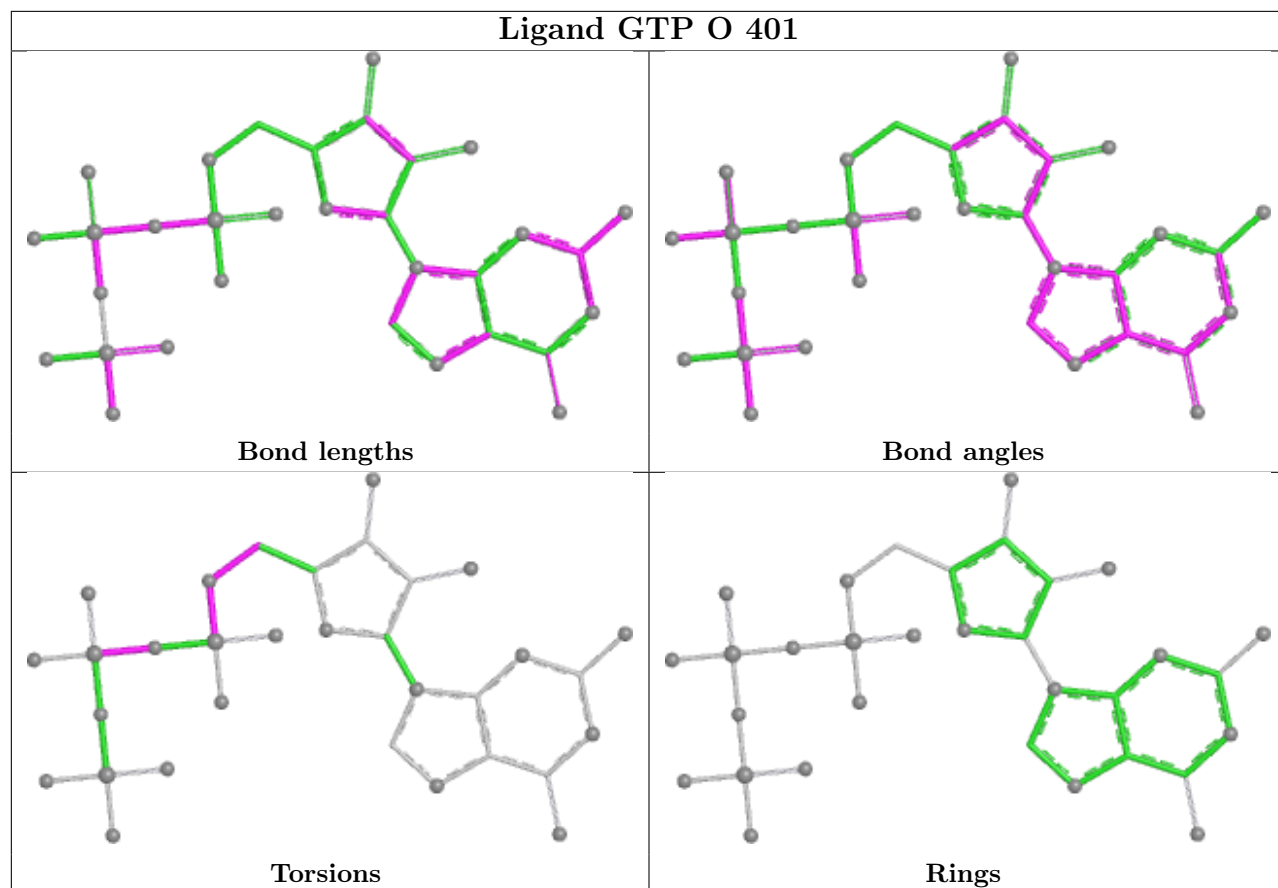


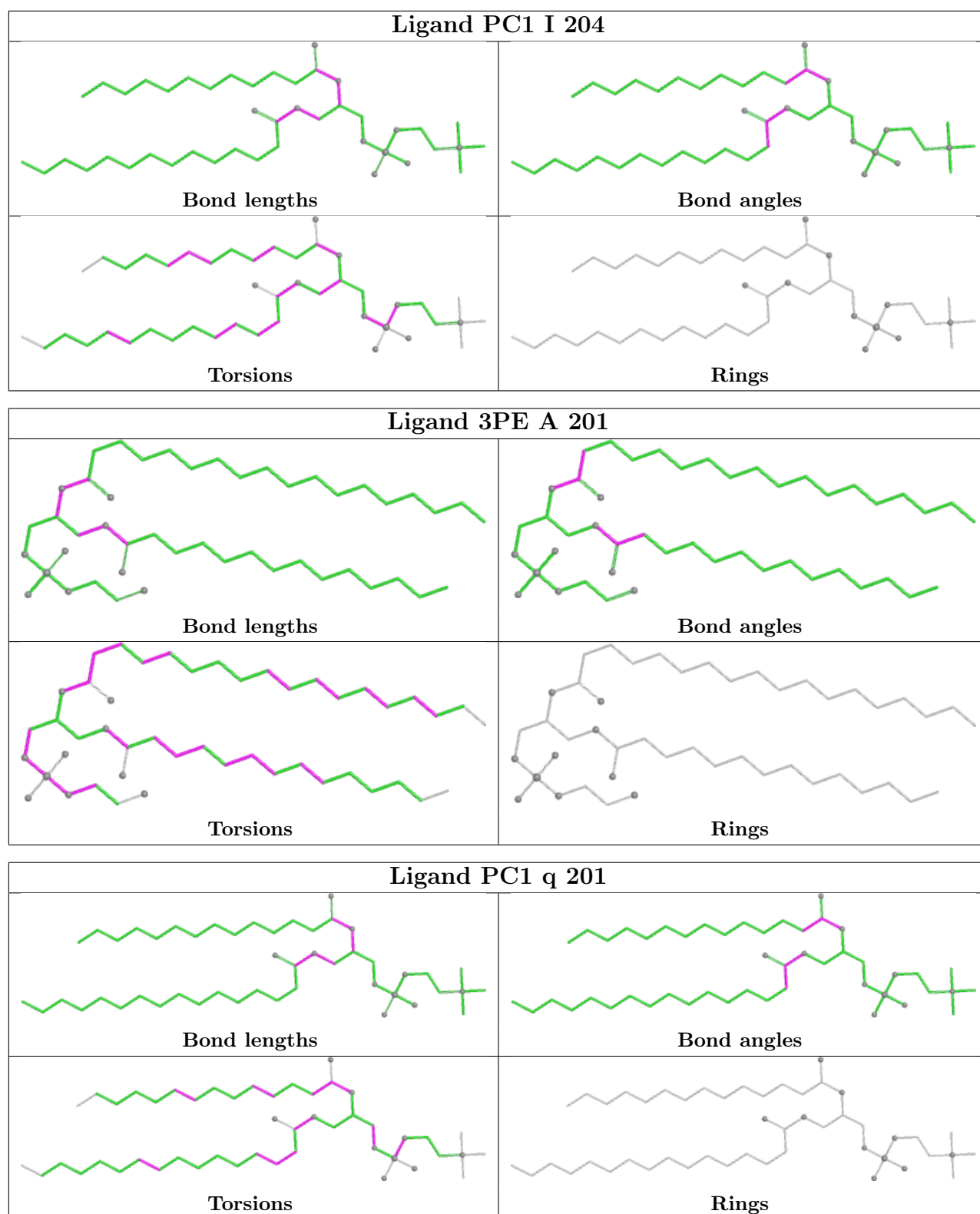


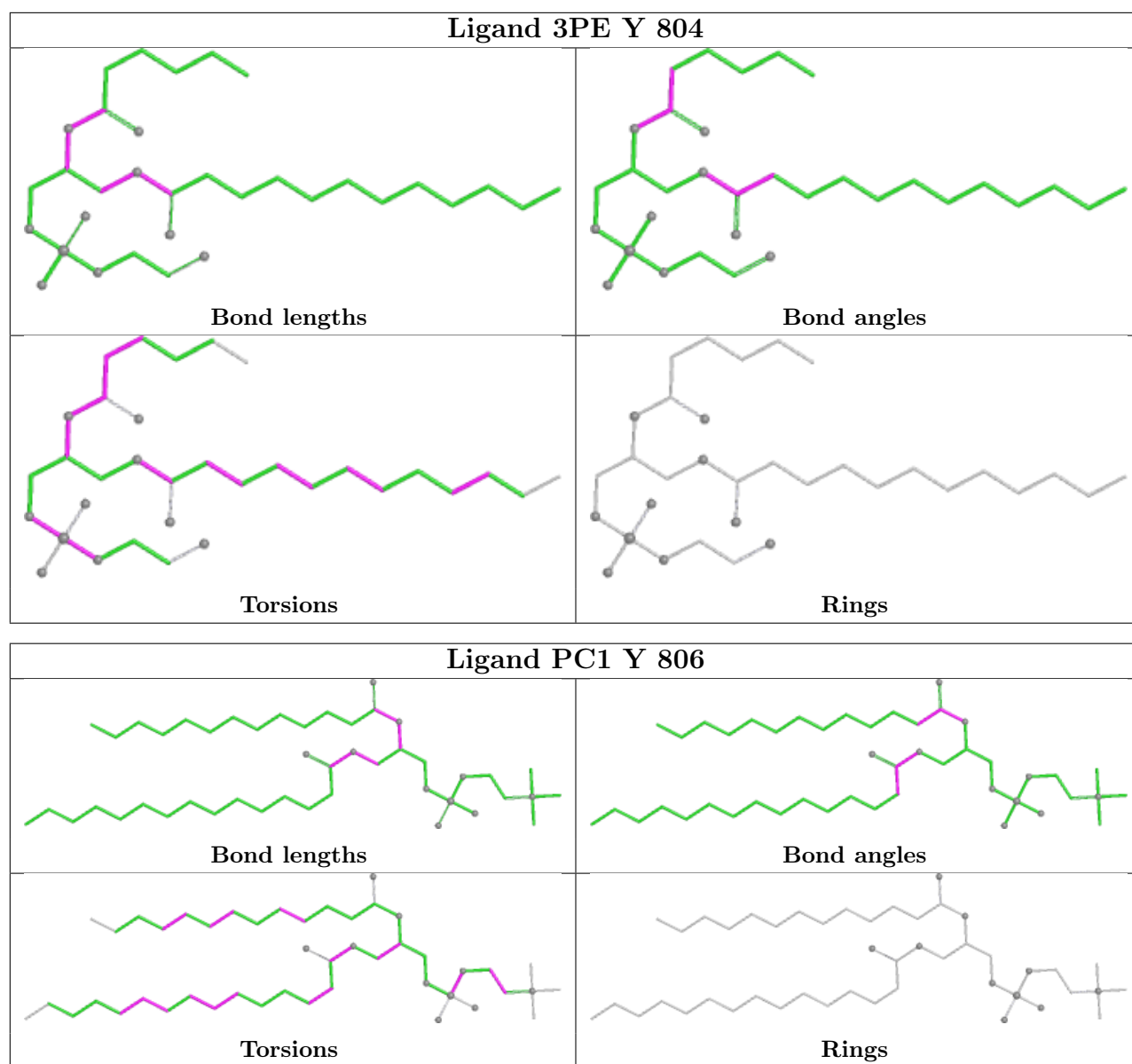


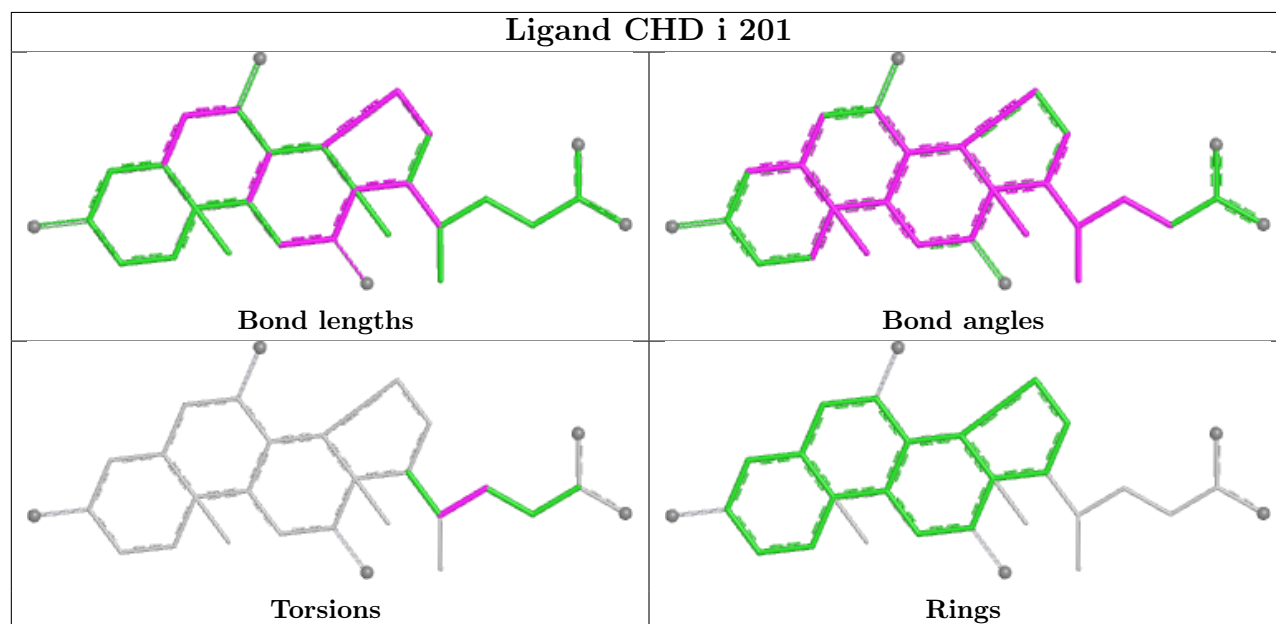
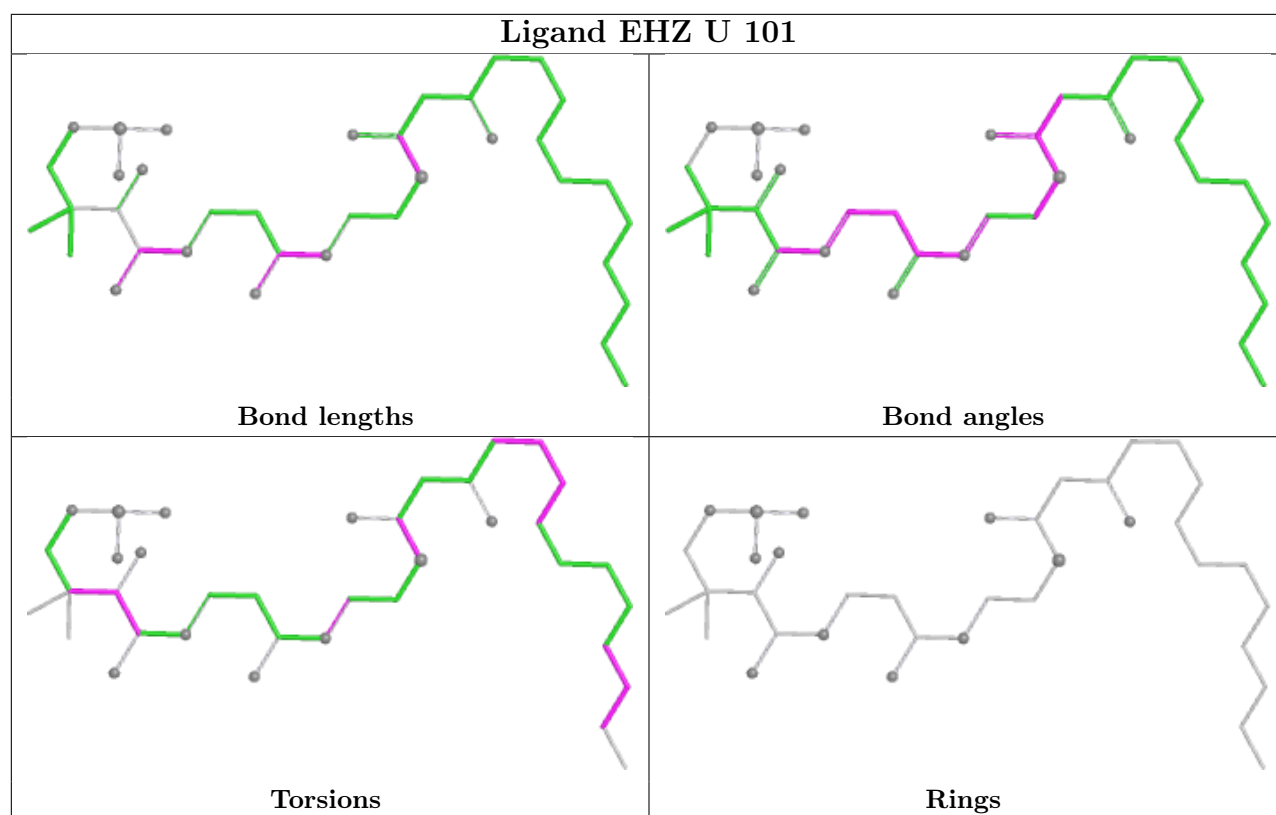


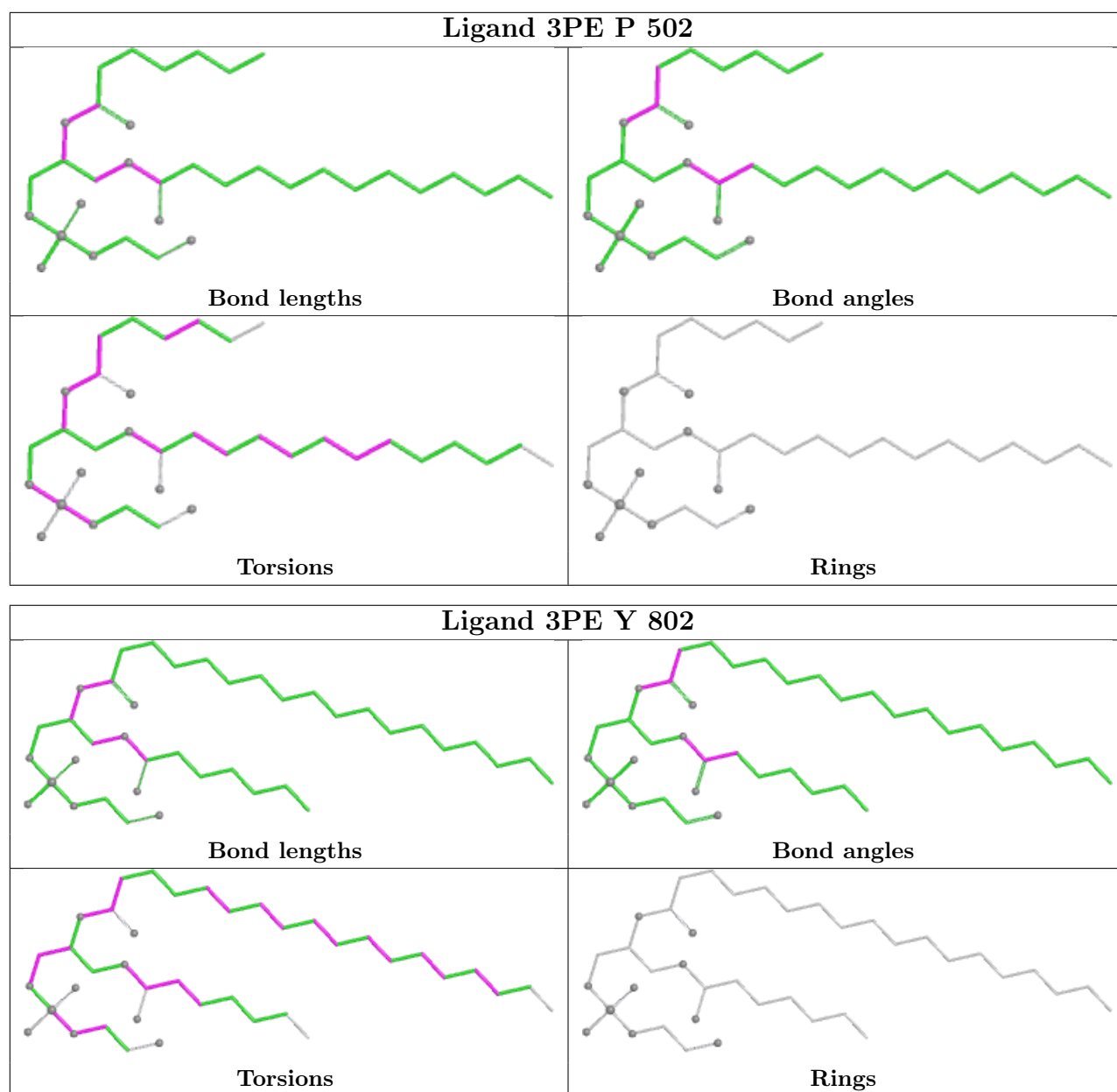


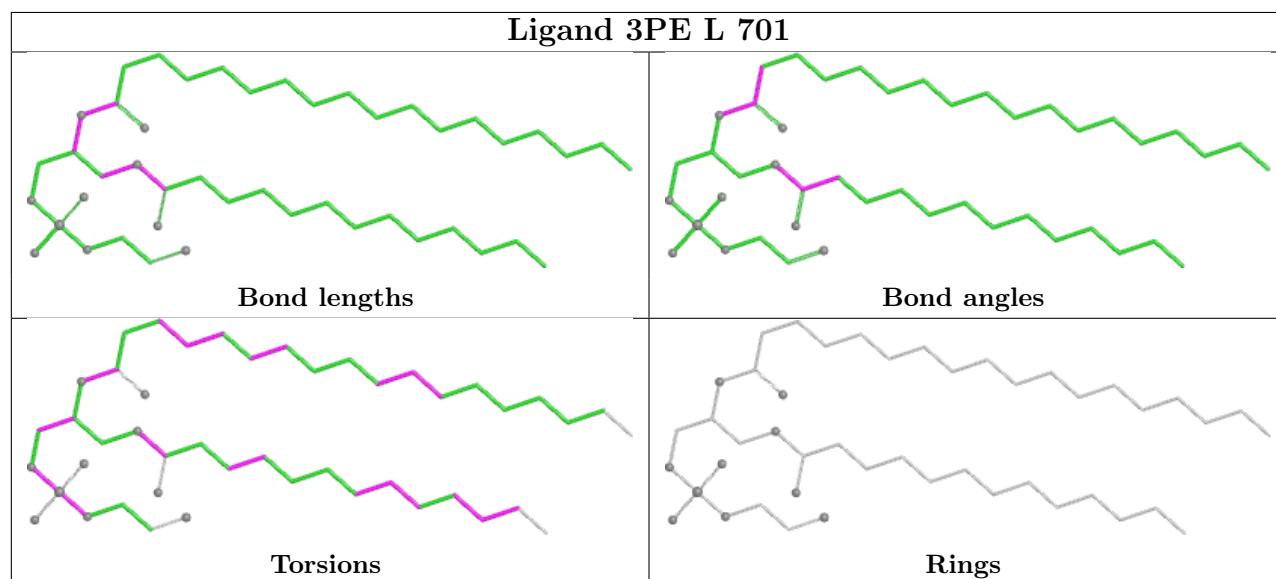
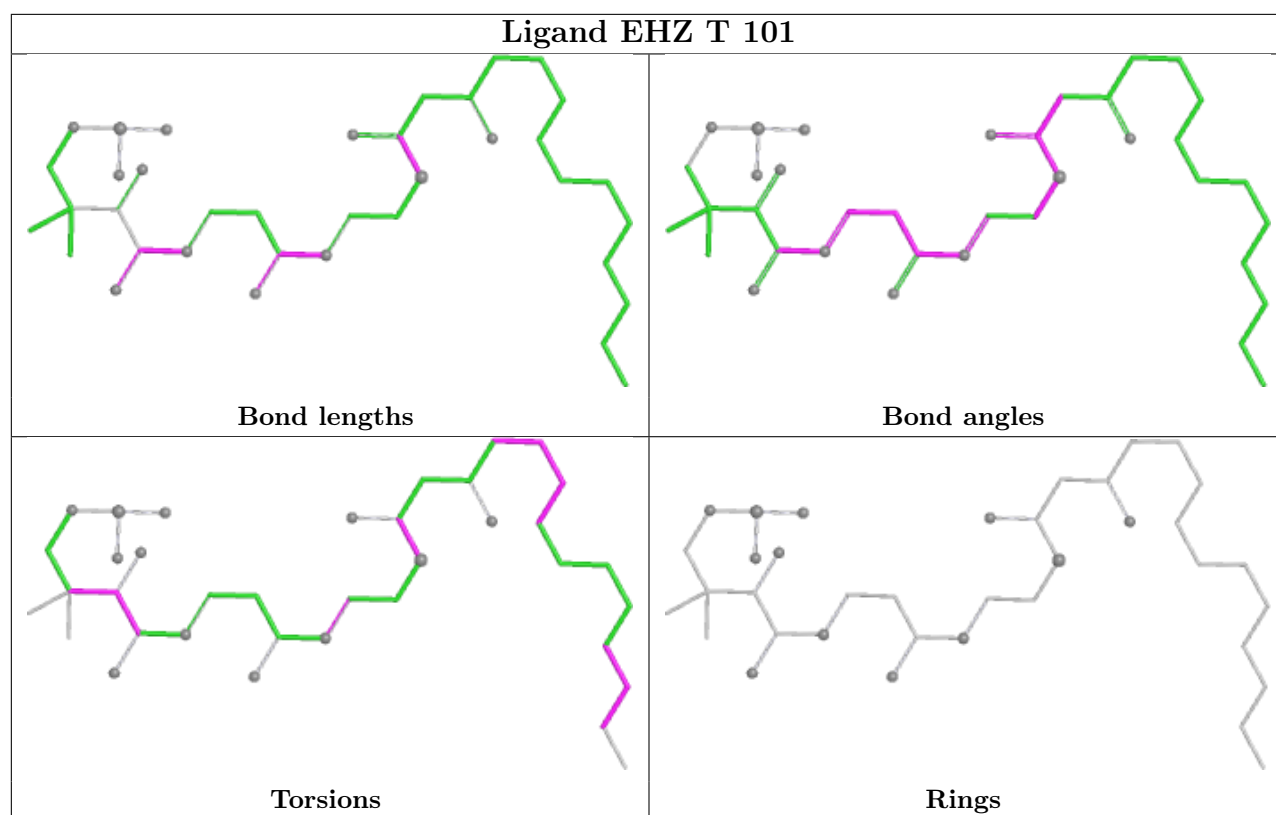


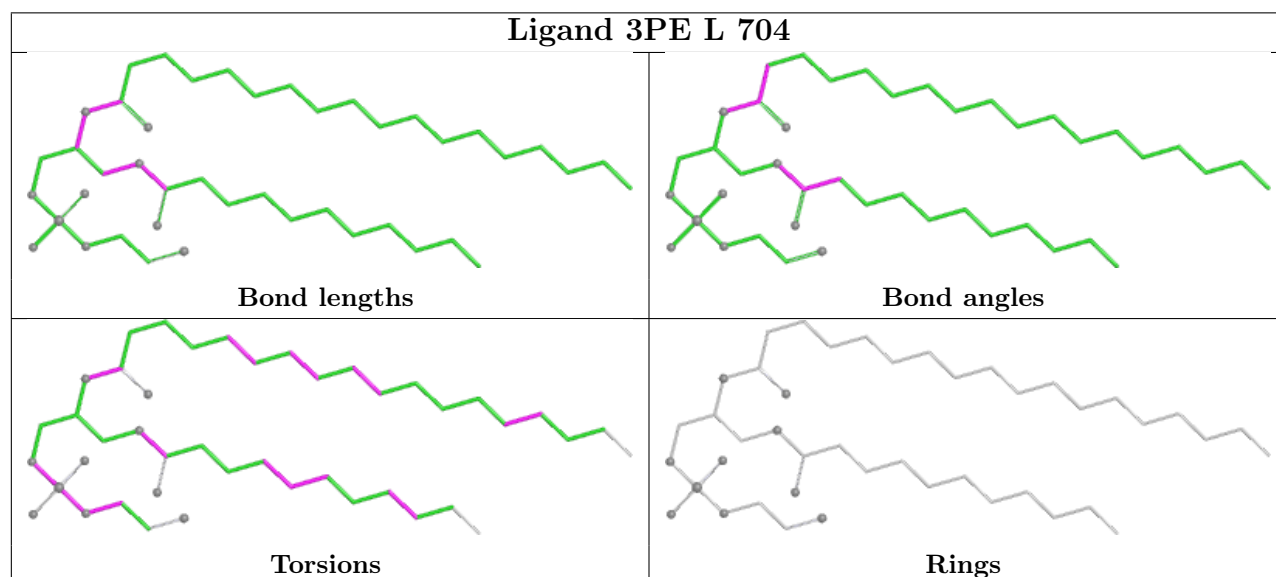
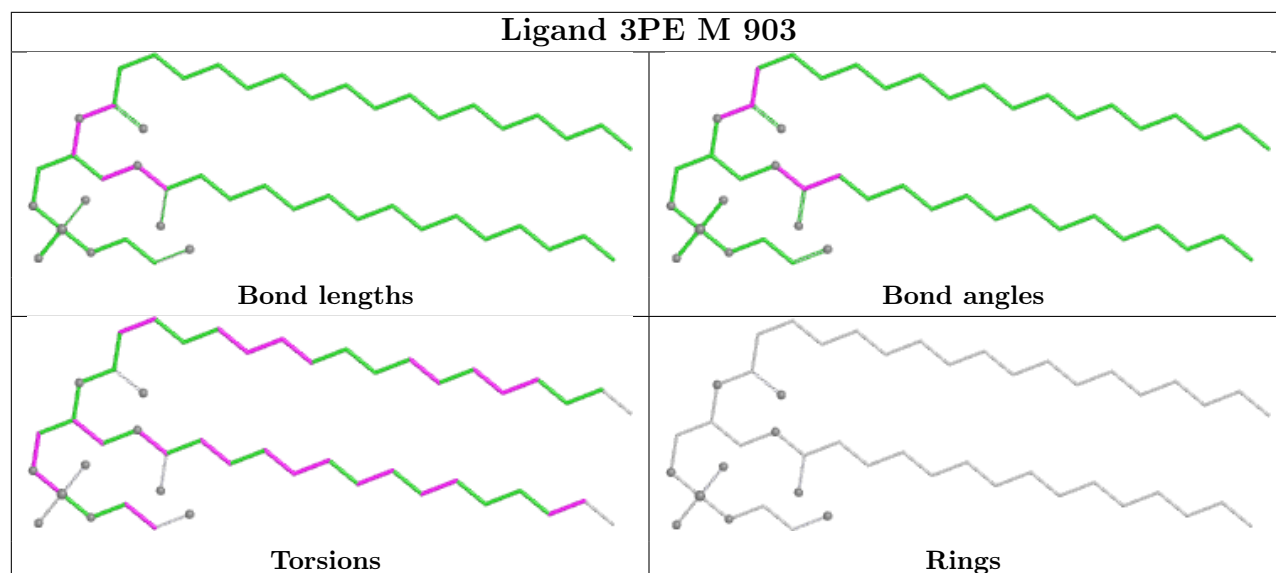
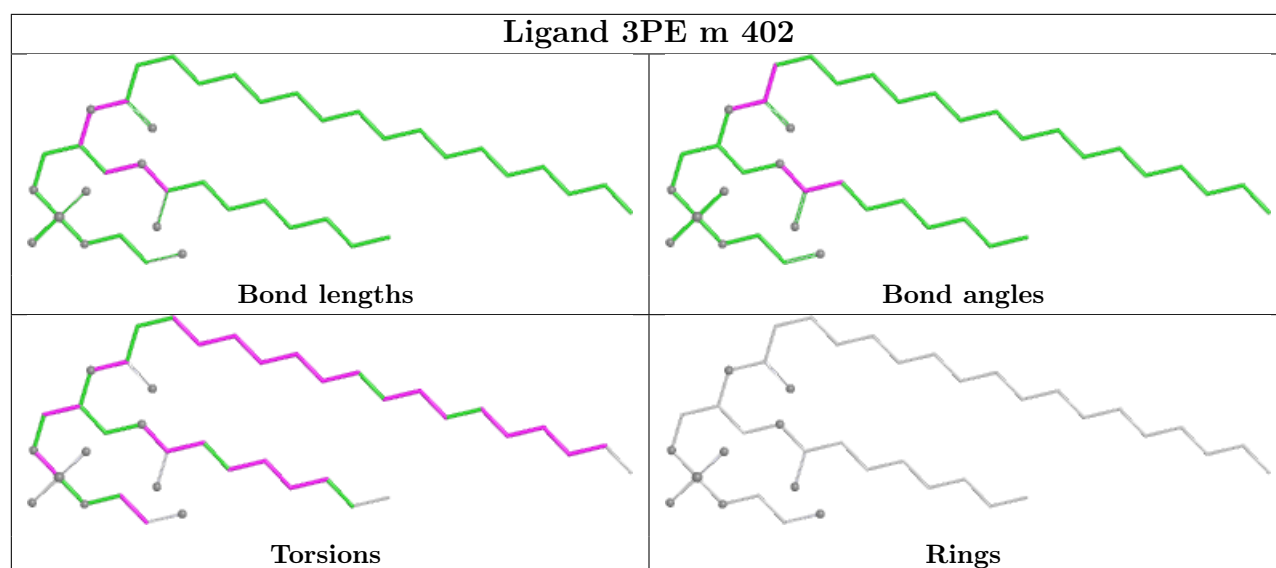


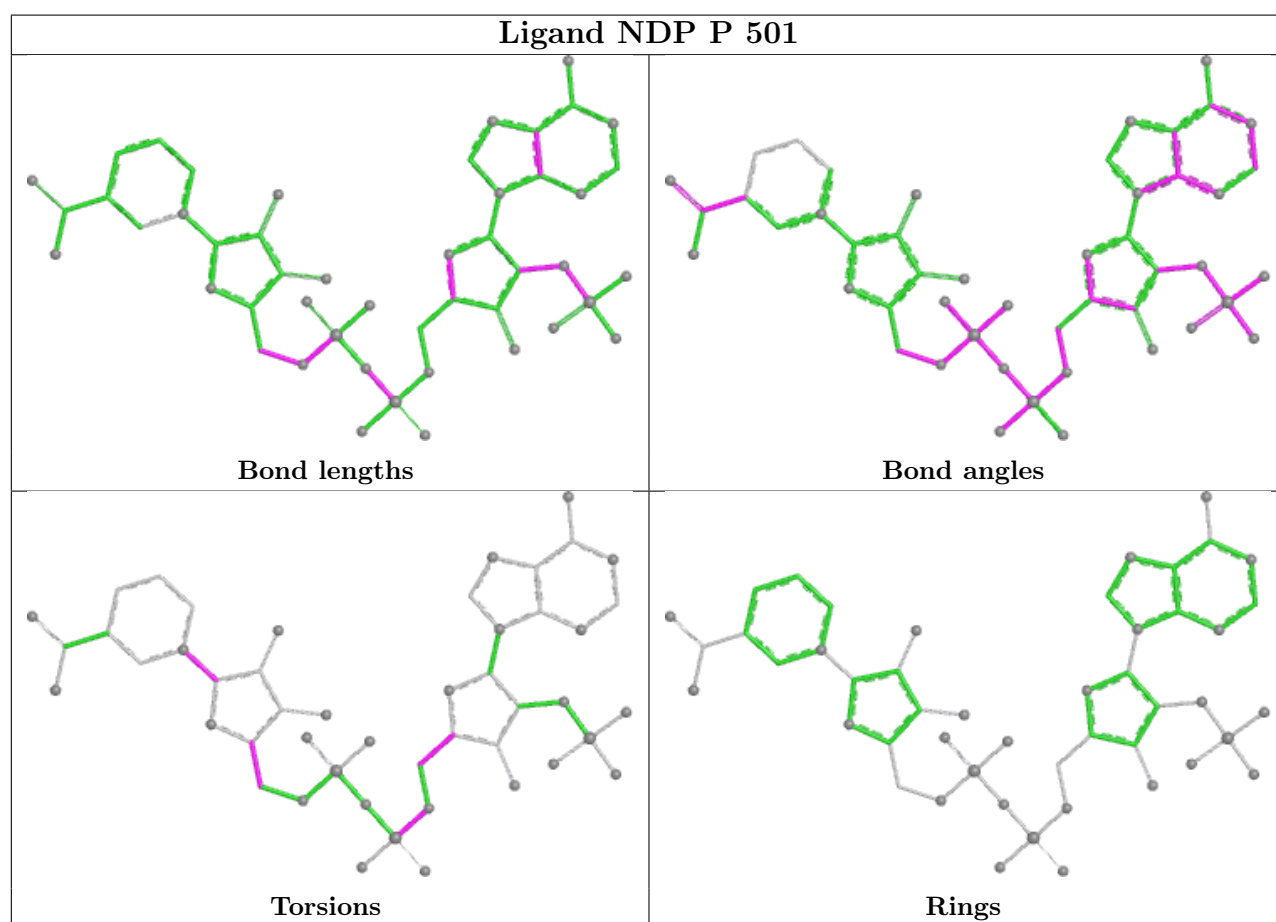
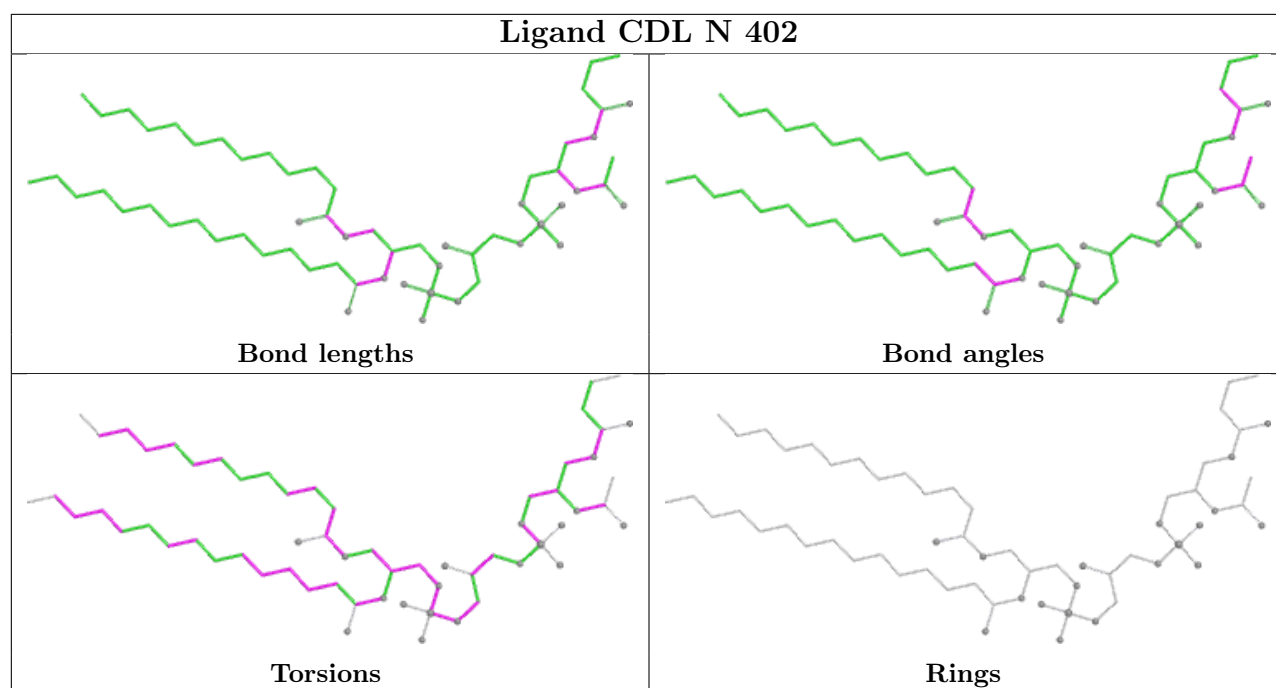


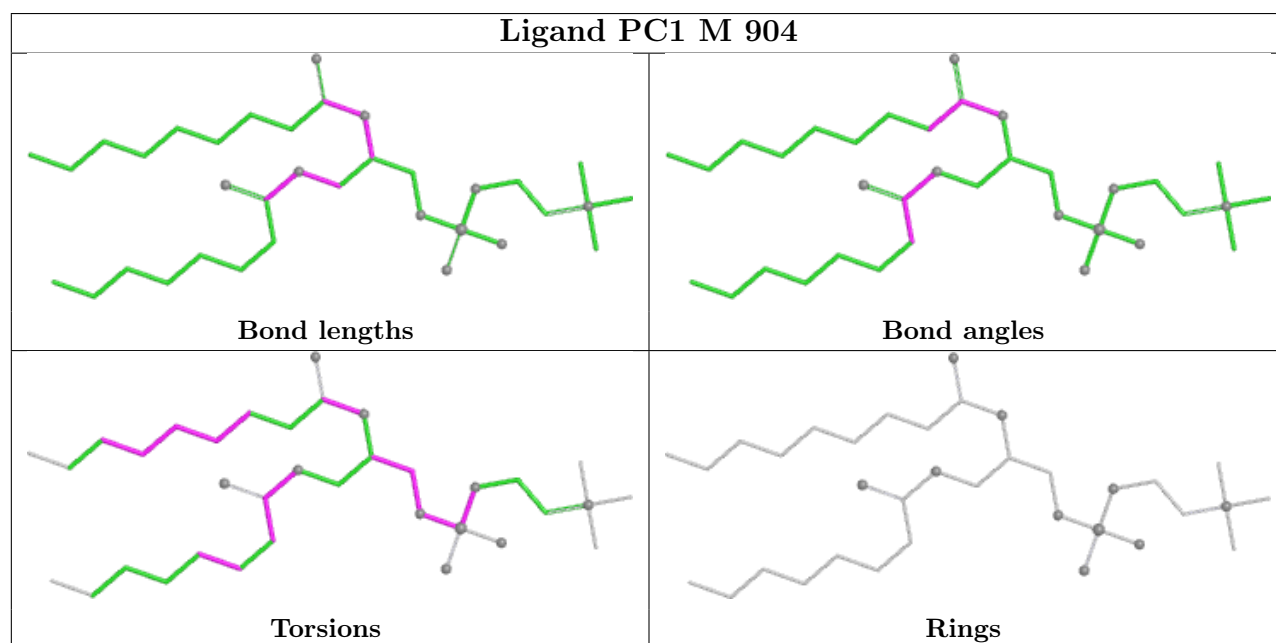
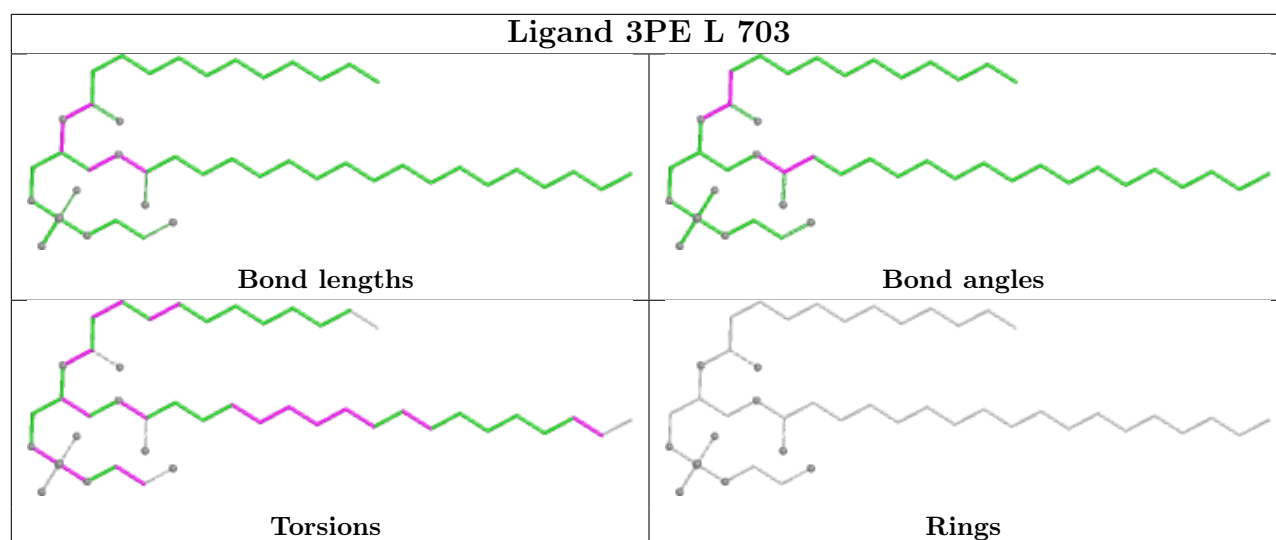


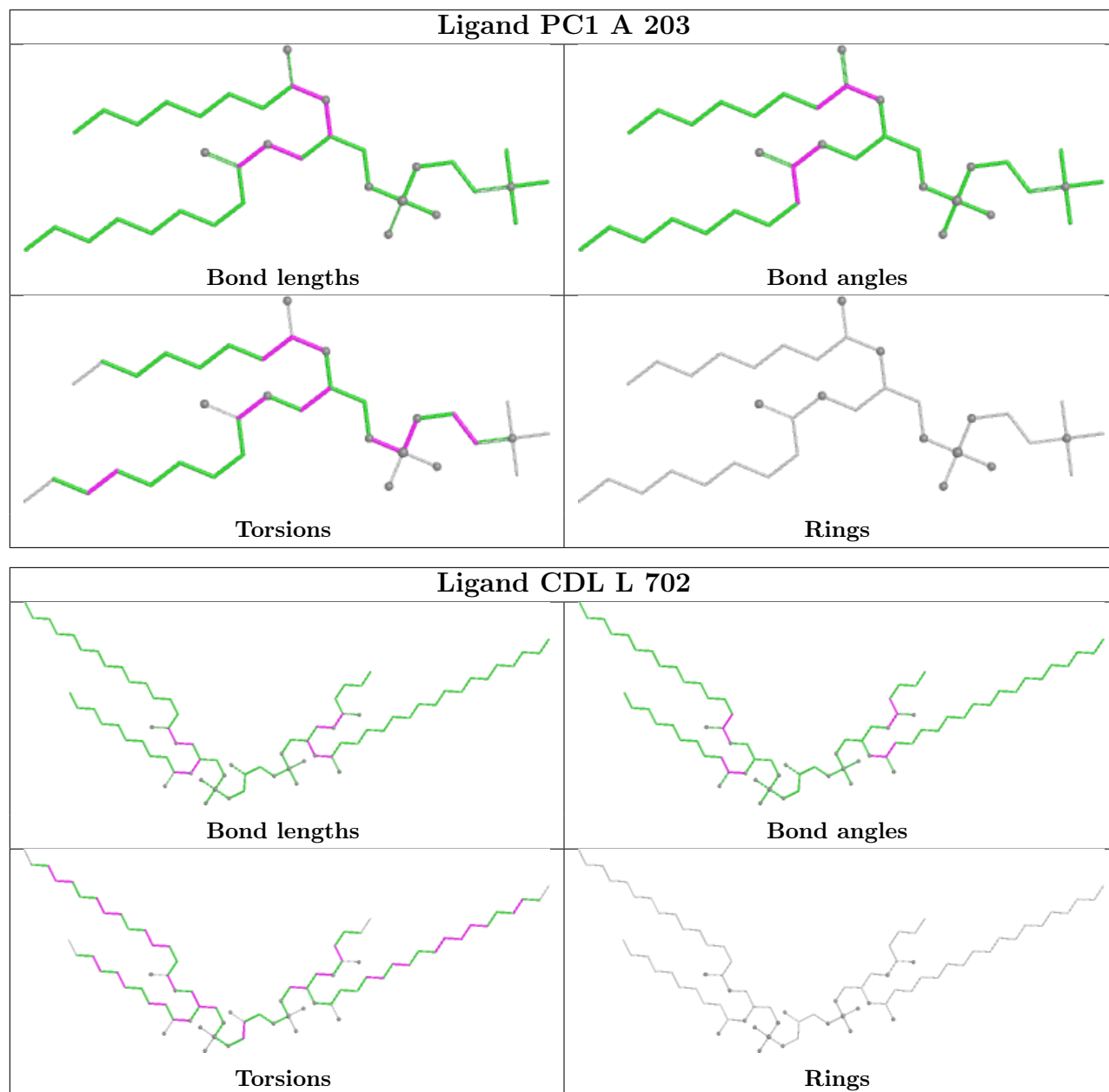


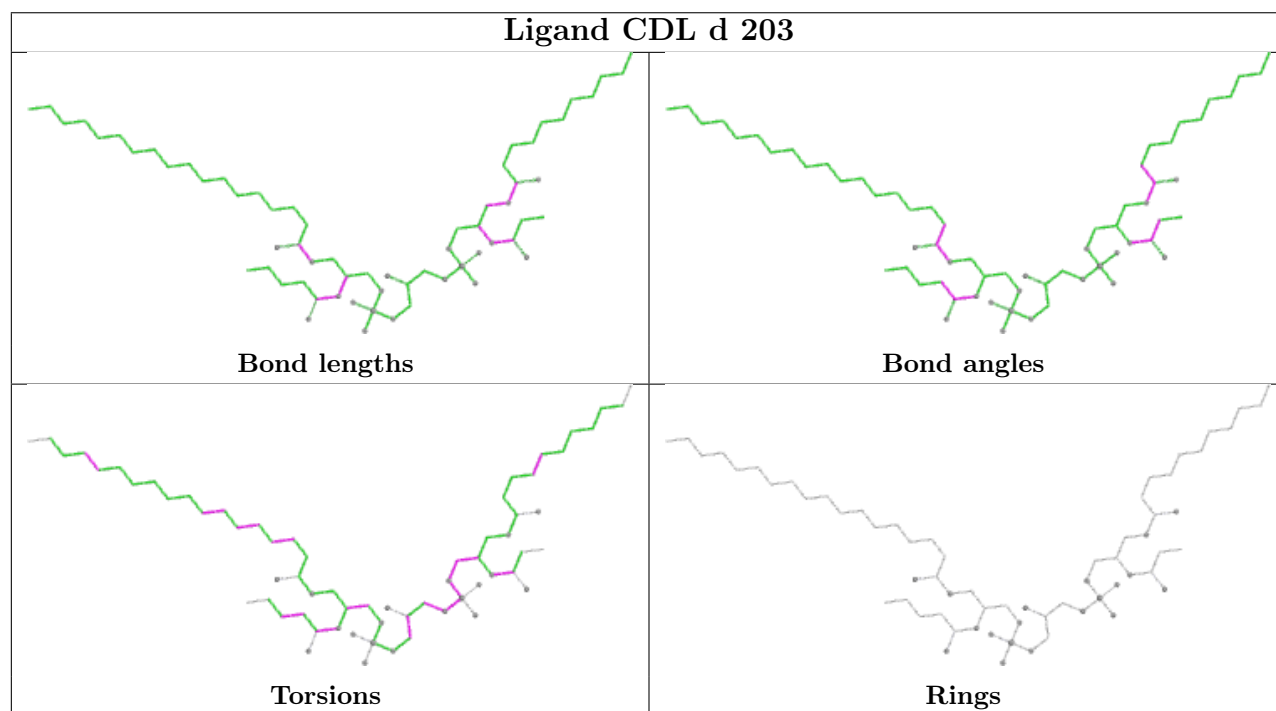
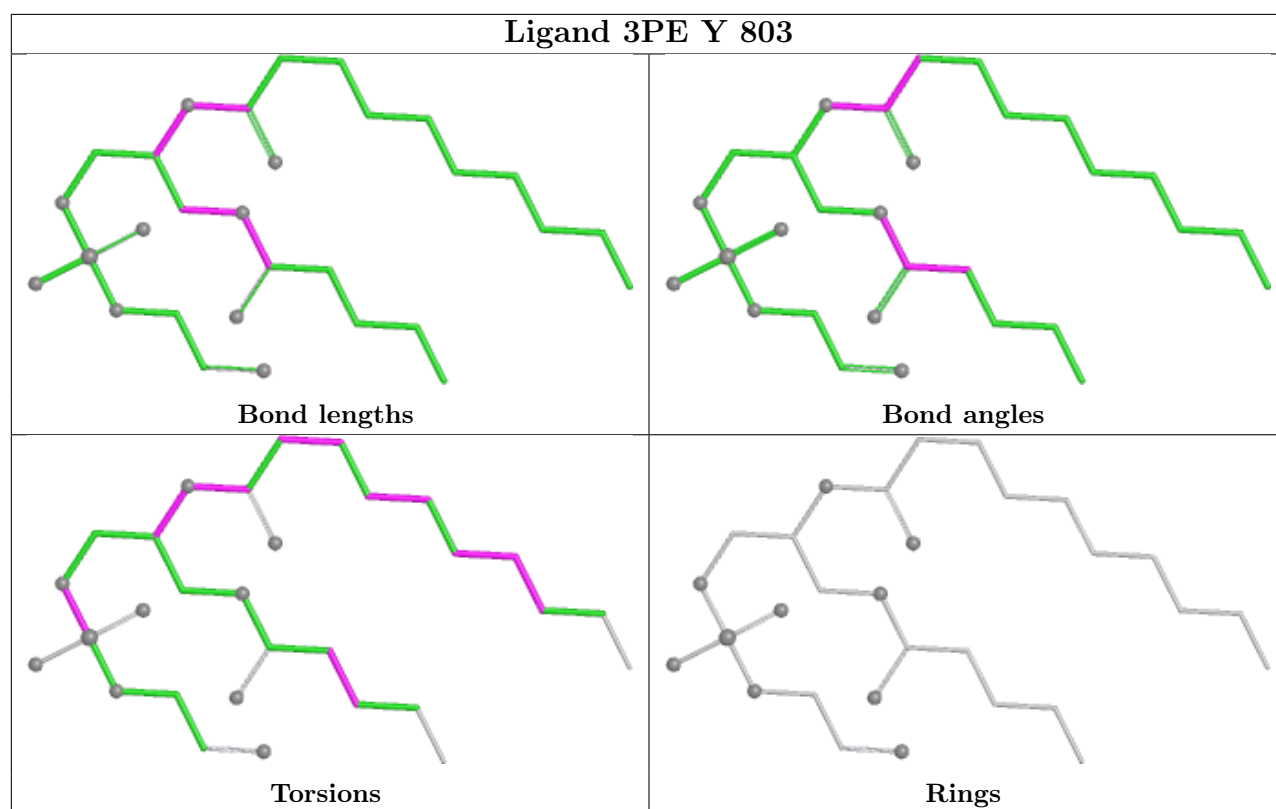


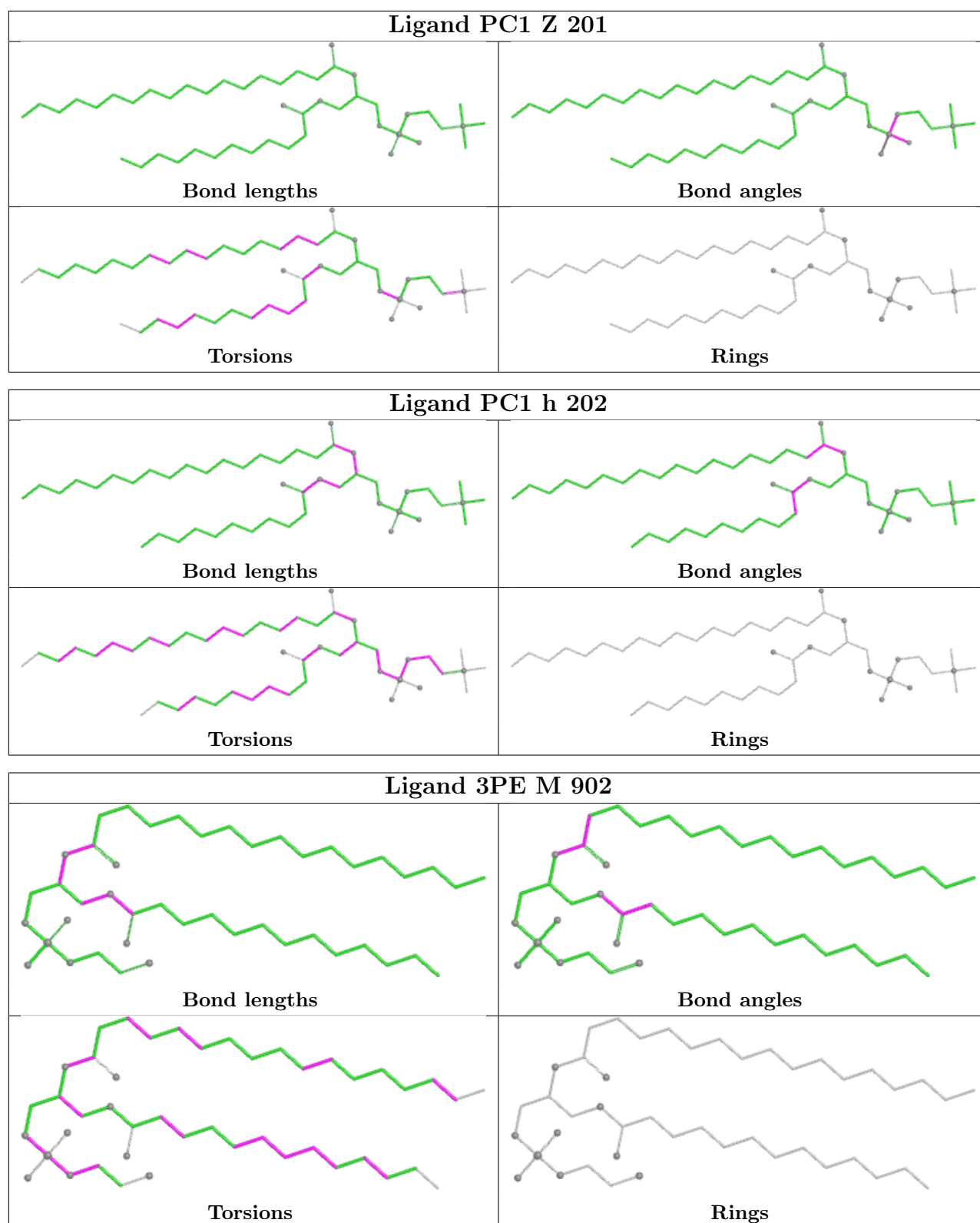


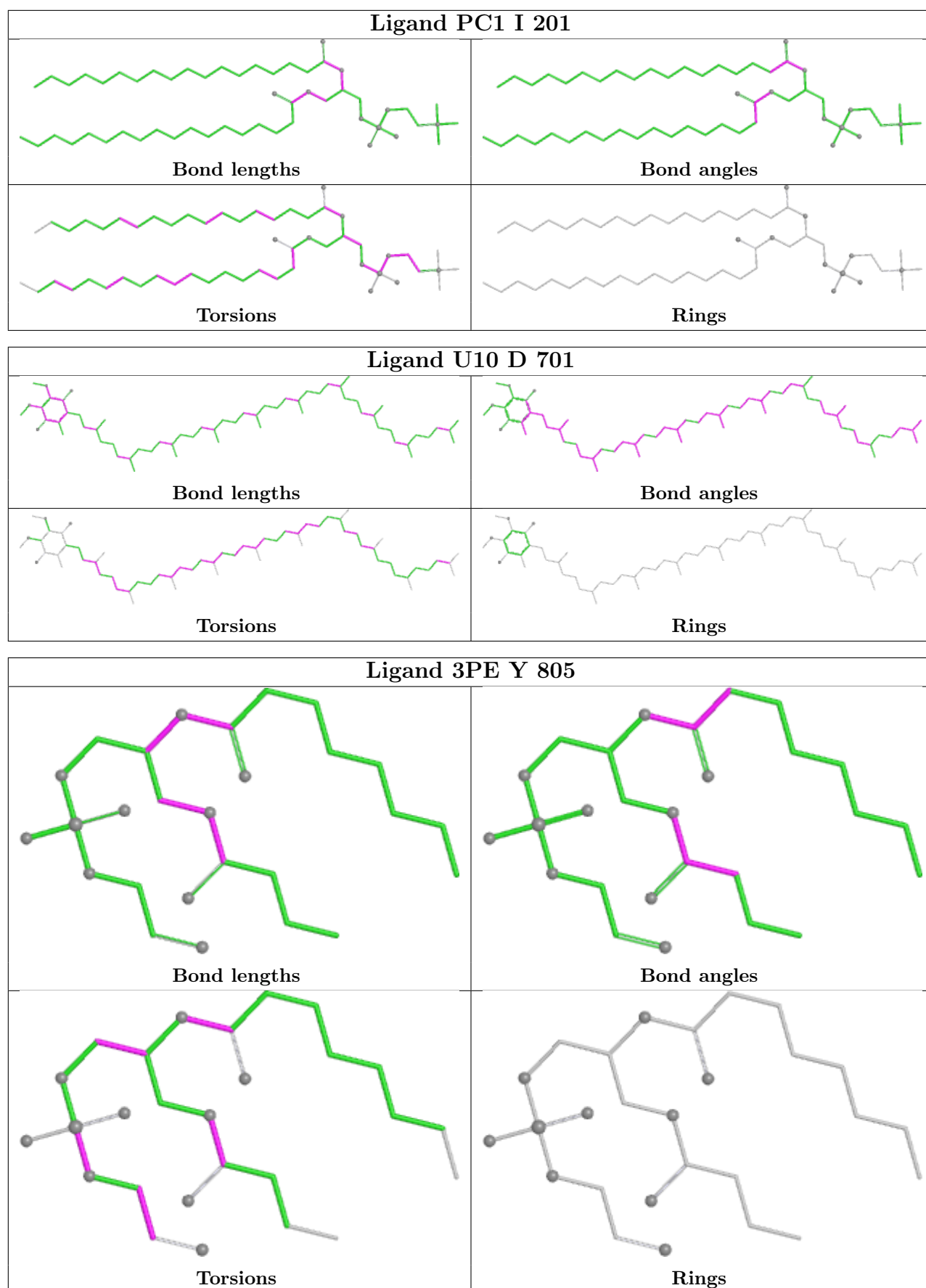


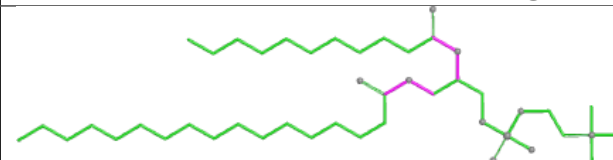
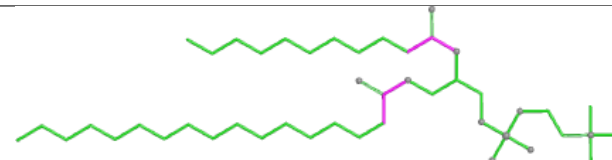
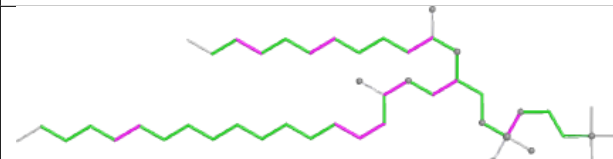
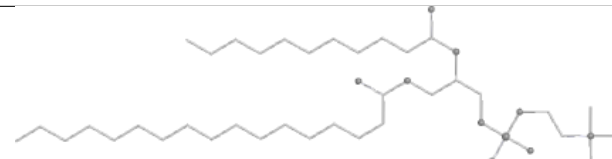


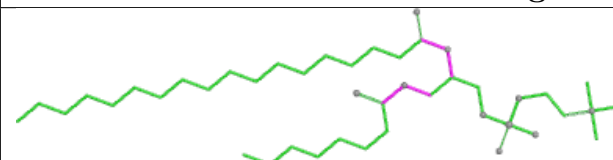
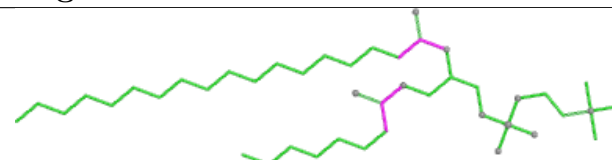
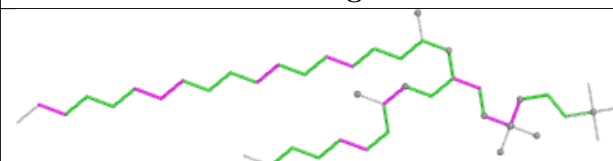
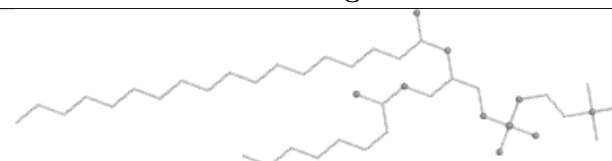


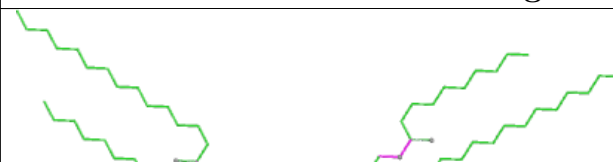
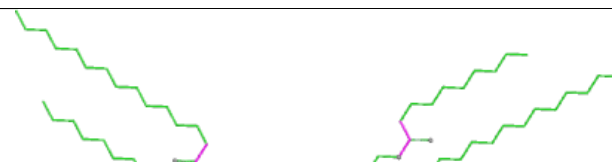
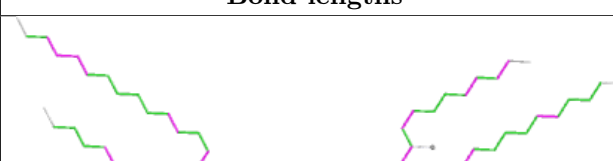


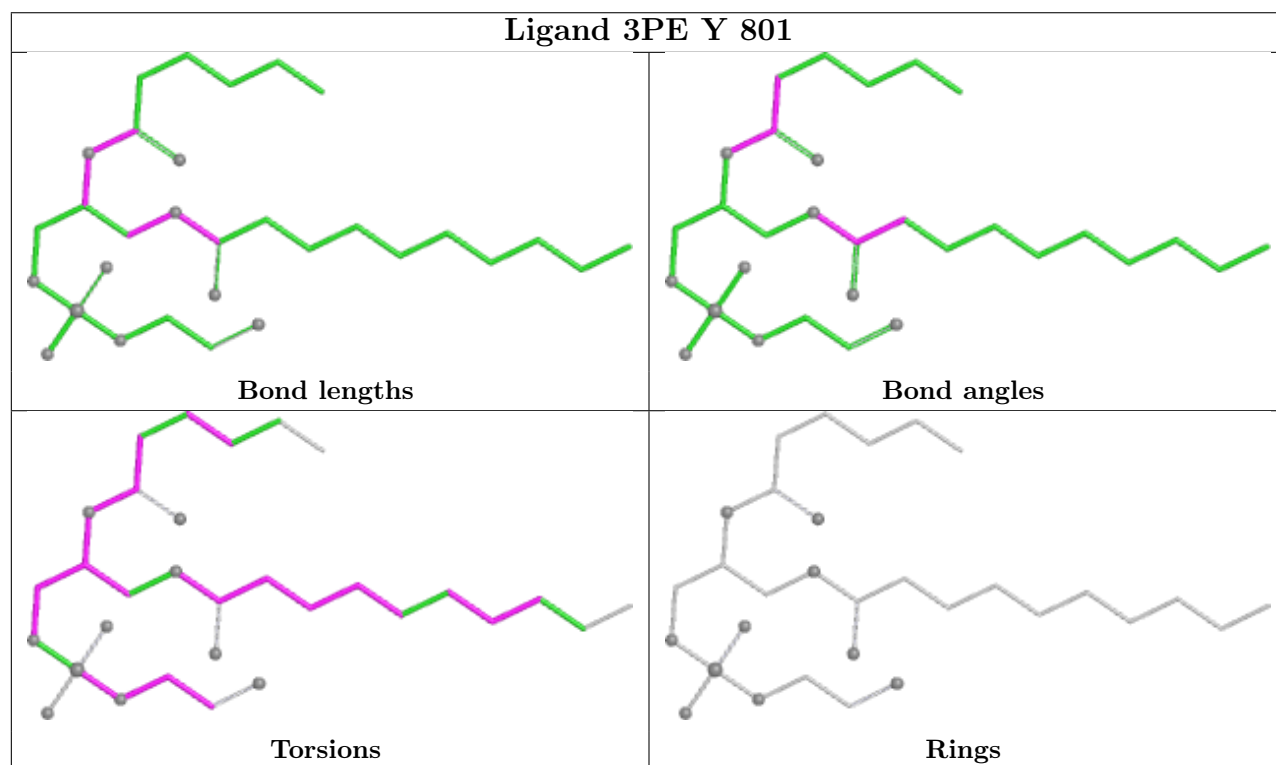
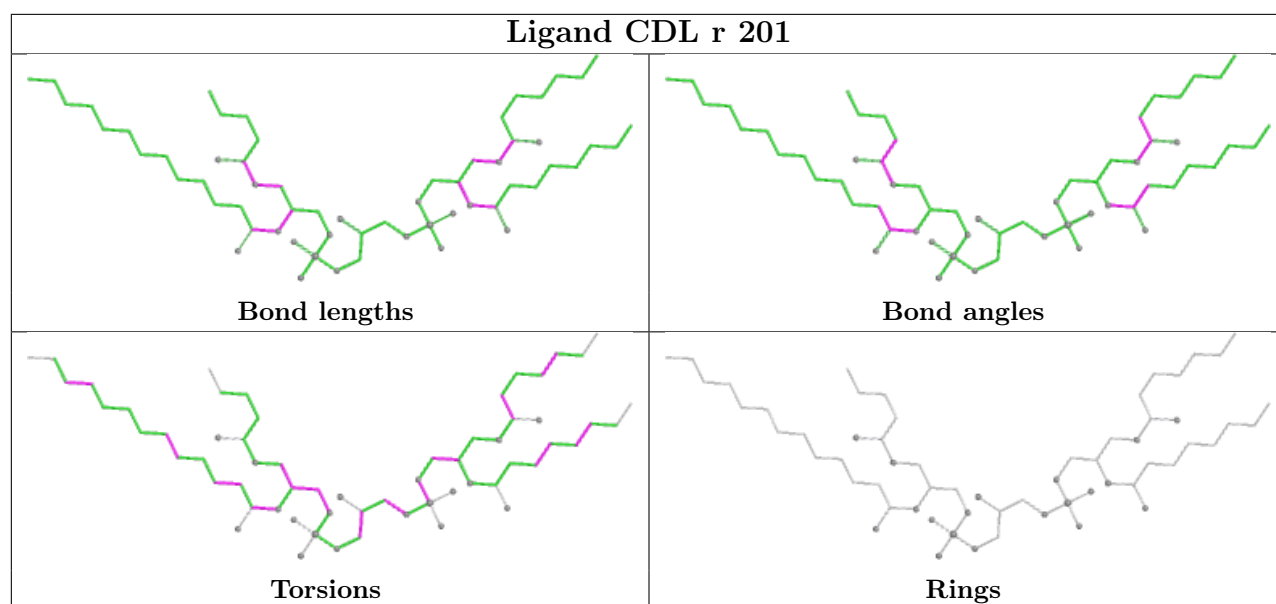


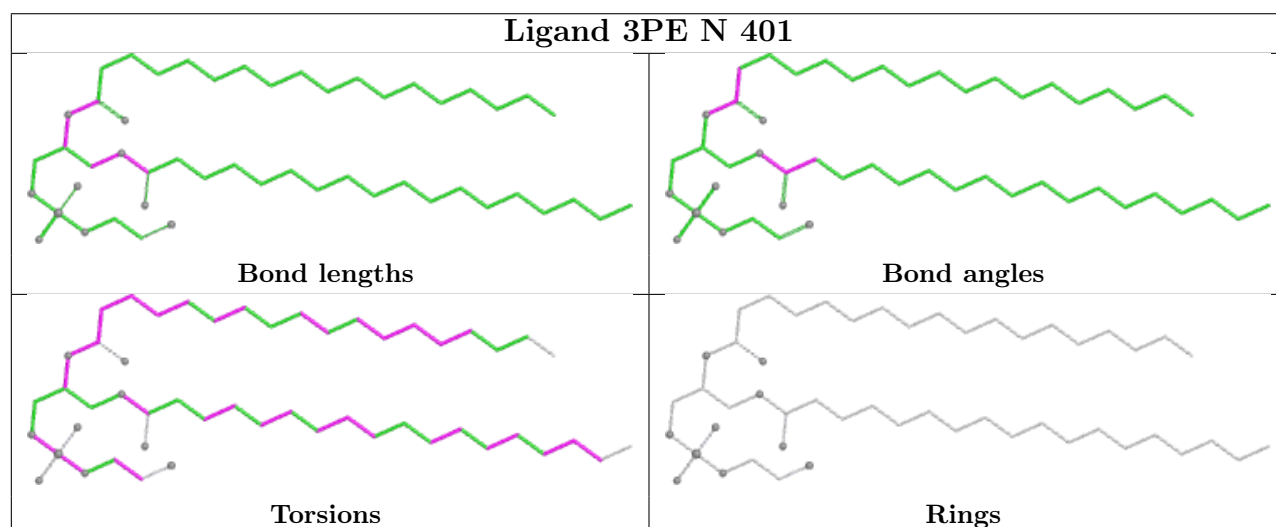
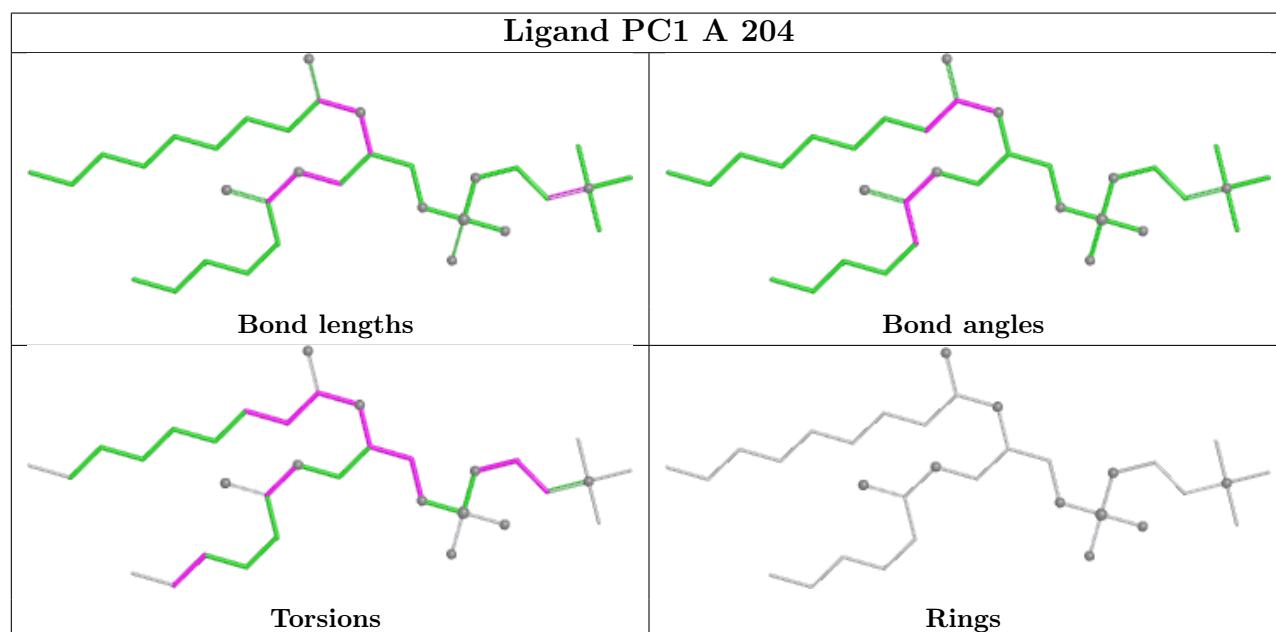
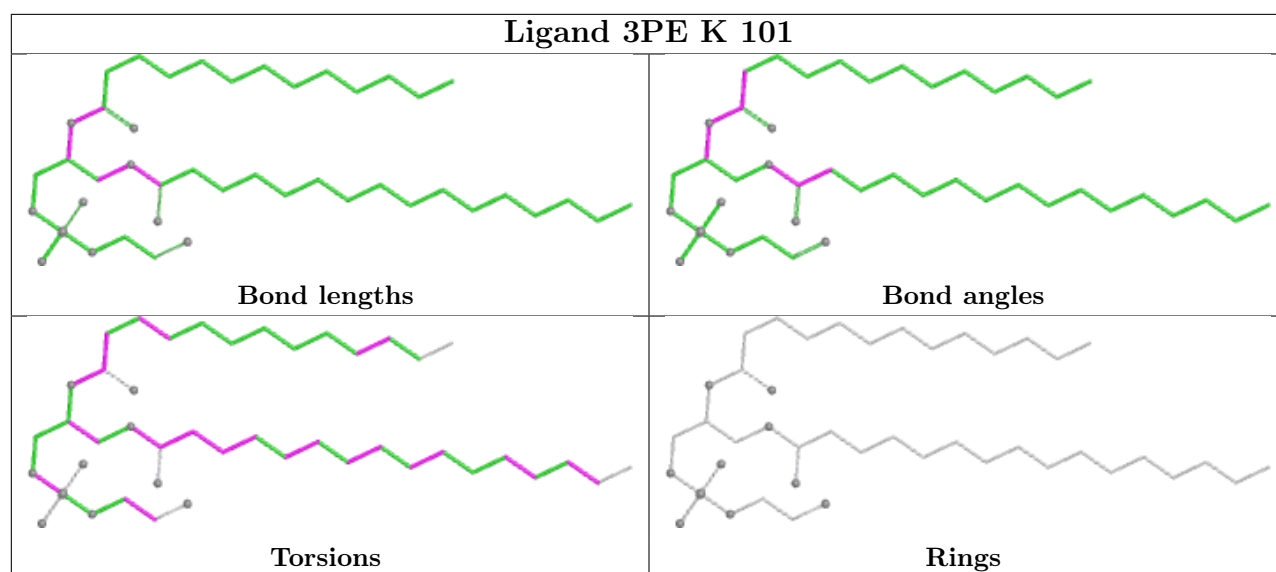


Ligand PC1 B 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PC1 g 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CDL h 201	
	
Bond lengths	Bond angles
	
Torsions	Rings





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

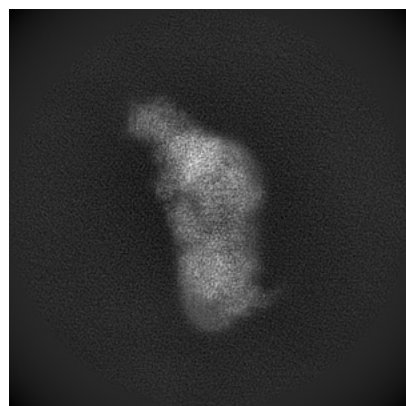
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14132. These allow visual inspection of the internal detail of the map and identification of artifacts.

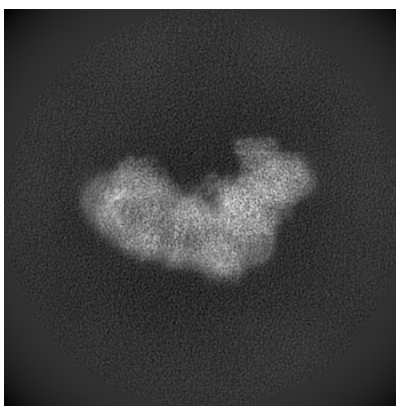
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

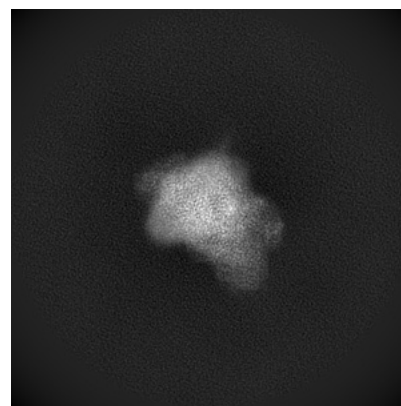
6.1.1 Primary map



X

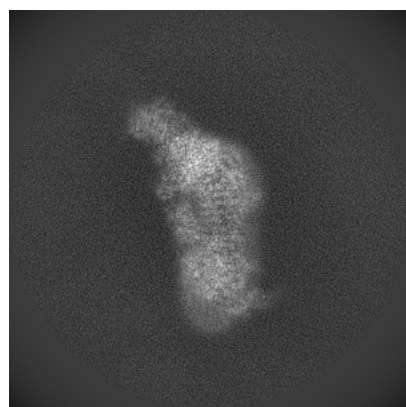


Y

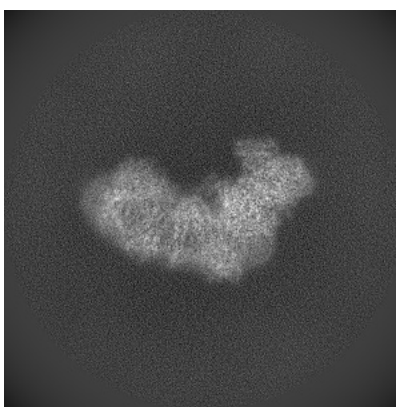


Z

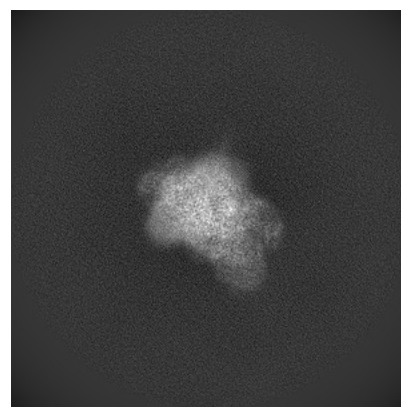
6.1.2 Raw map



X



Y

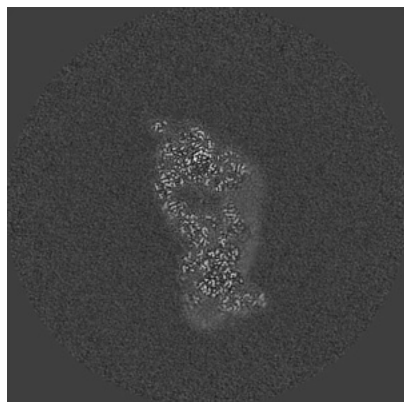


Z

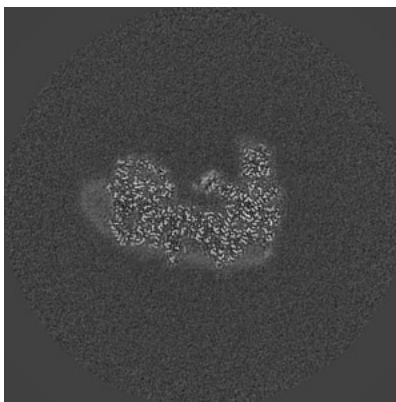
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

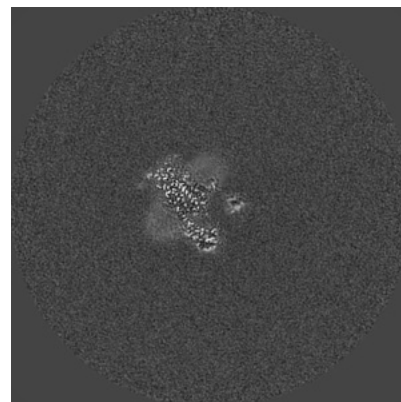
6.2.1 Primary map



X Index: 320

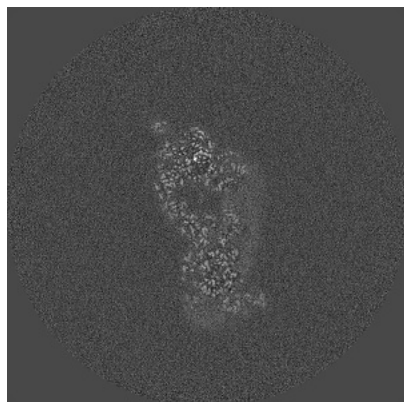


Y Index: 320

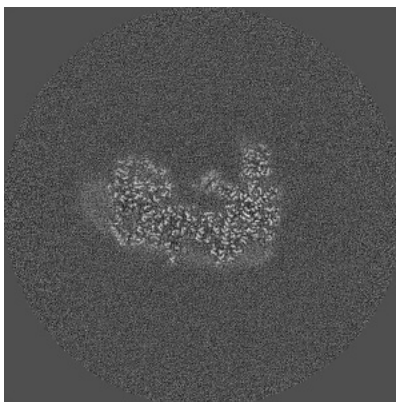


Z Index: 320

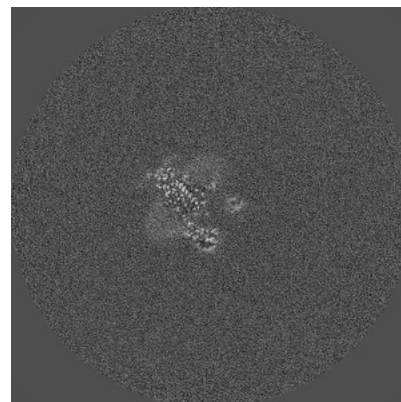
6.2.2 Raw map



X Index: 320



Y Index: 320

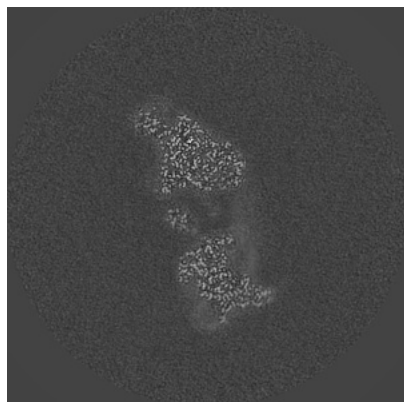


Z Index: 320

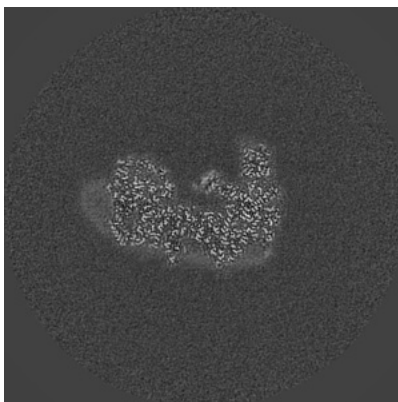
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

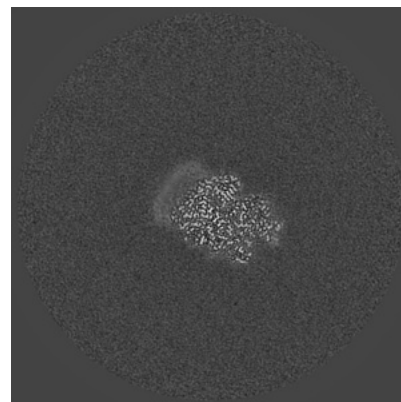
6.3.1 Primary map



X Index: 339

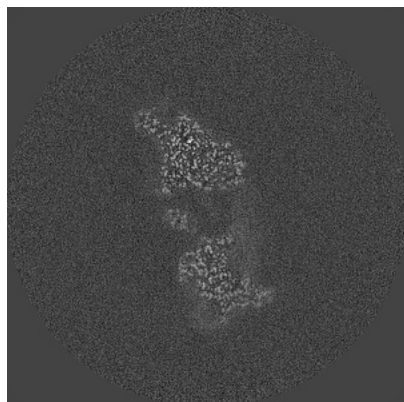


Y Index: 320

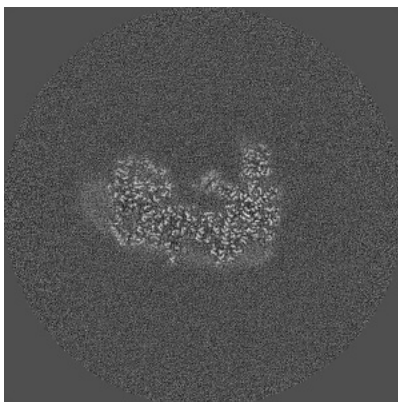


Z Index: 405

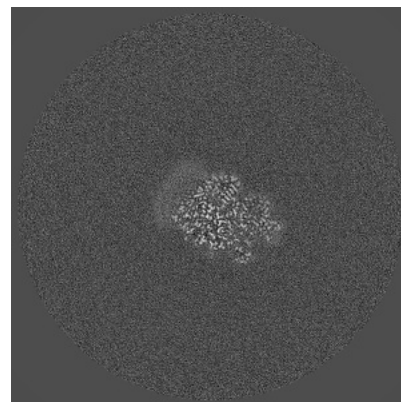
6.3.2 Raw map



X Index: 339



Y Index: 320

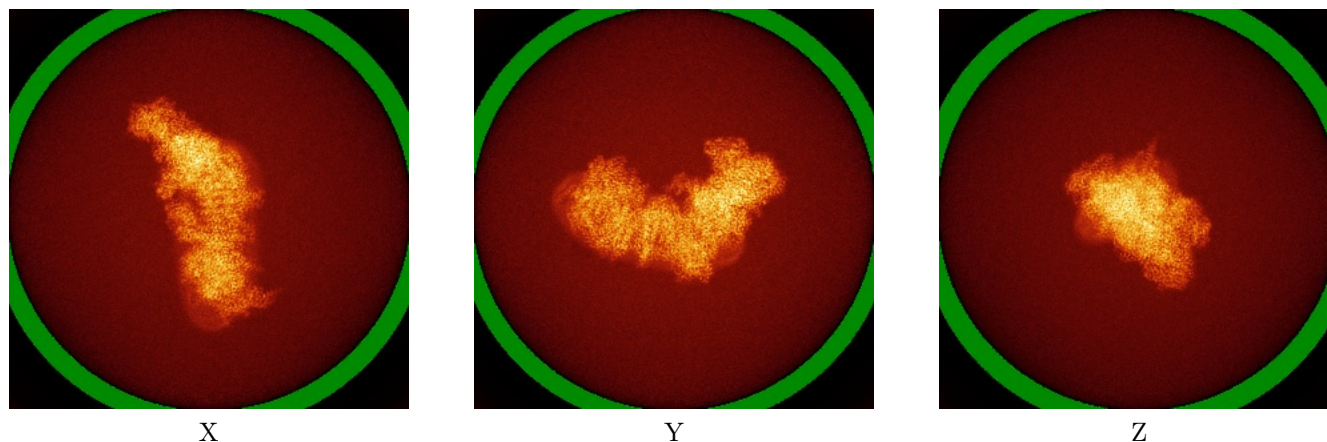


Z Index: 404

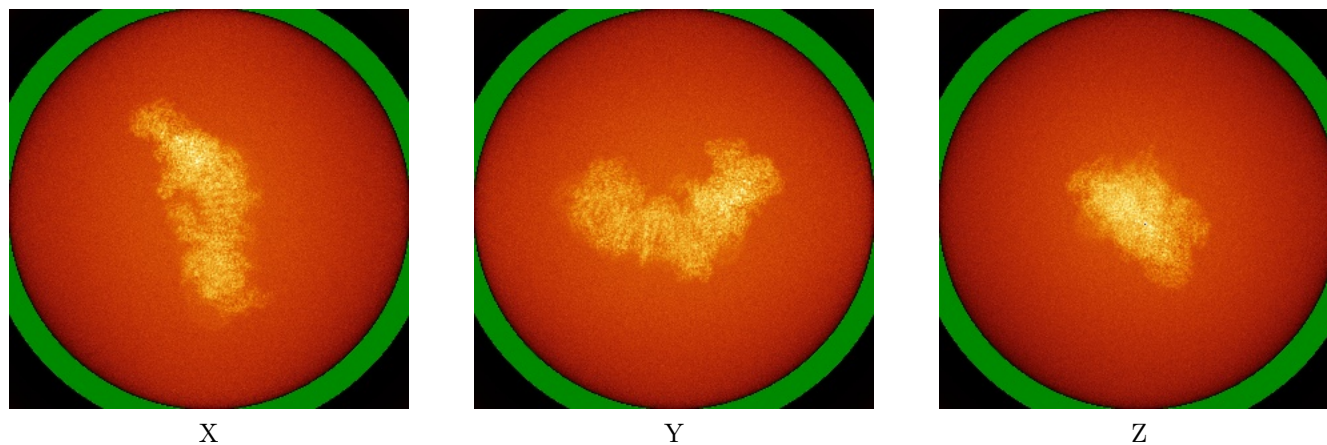
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



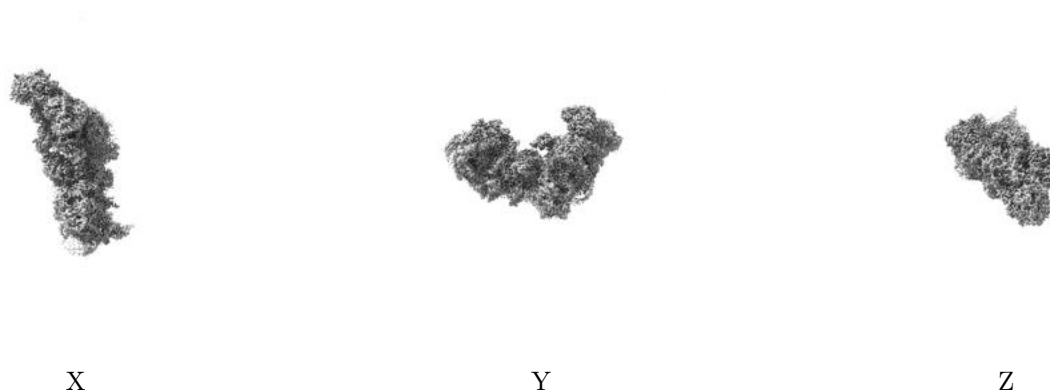
6.4.2 Raw map



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.

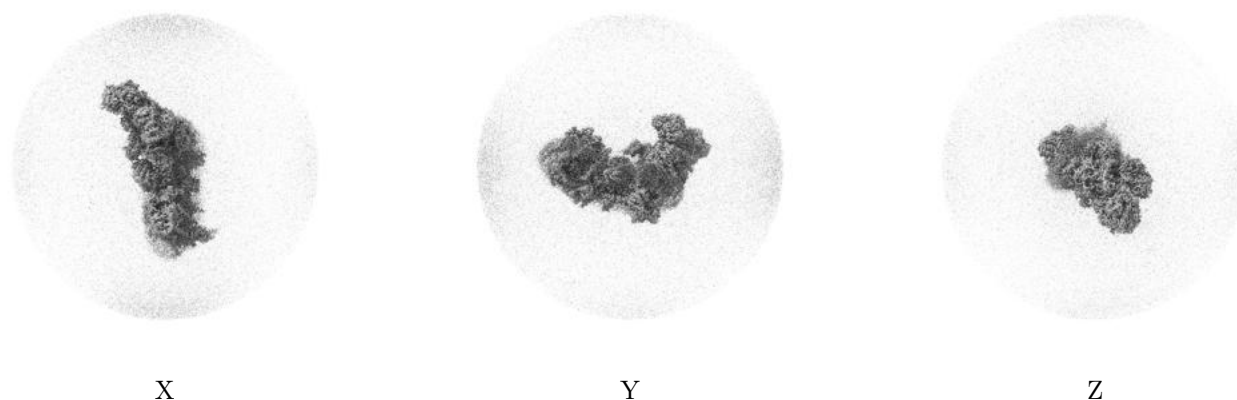
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

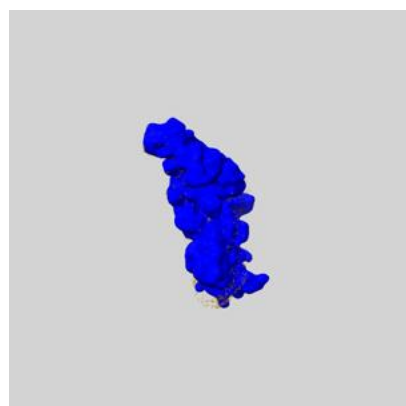
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

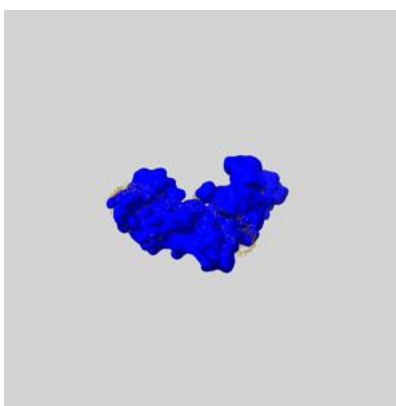
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

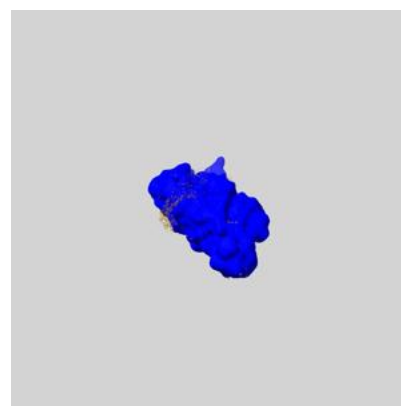
6.6.1 emd_14132_msk_1.map [i](#)



X



Y

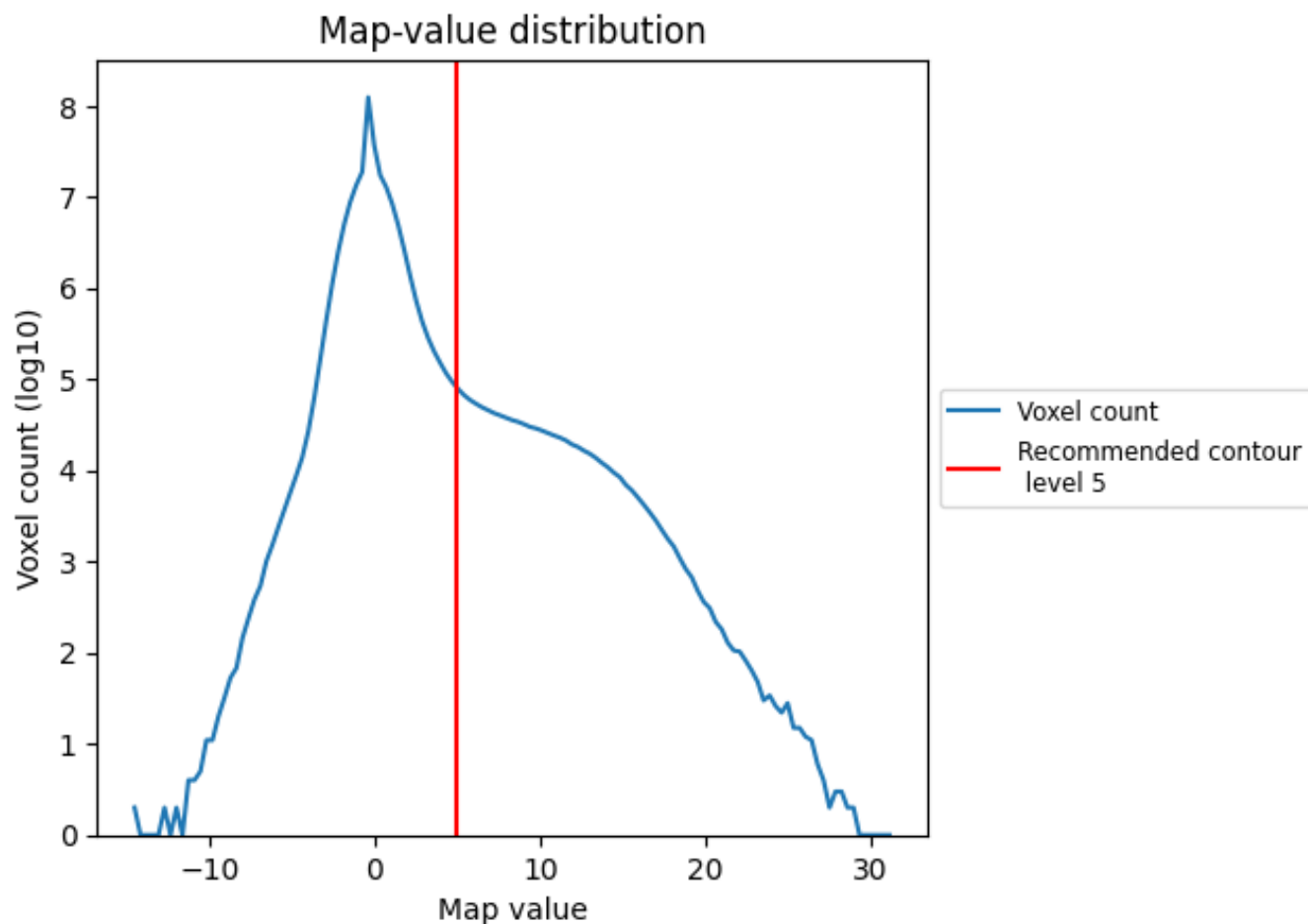


Z

7 Map analysis [i](#)

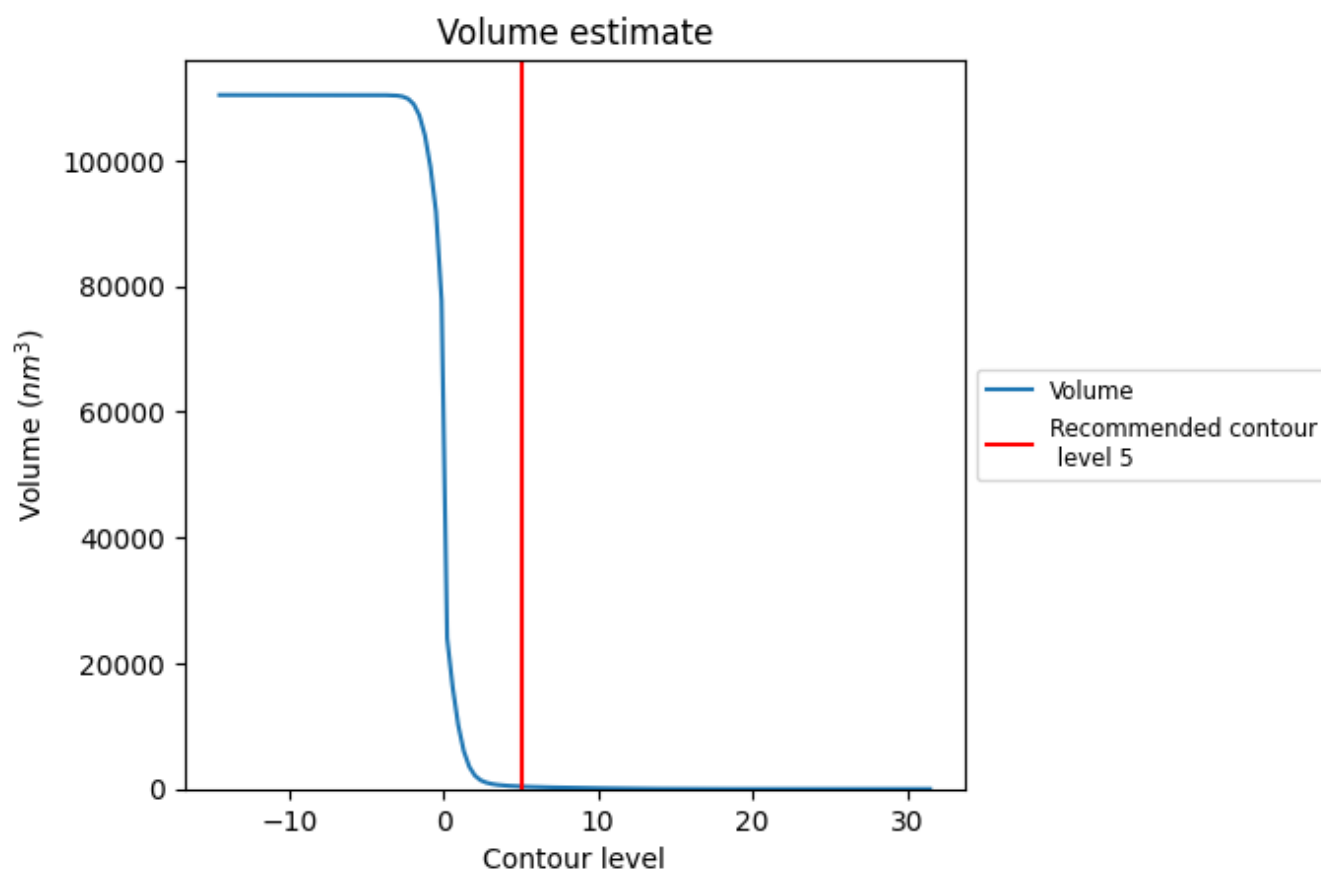
This section contains the results of statistical analysis of the map.

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.

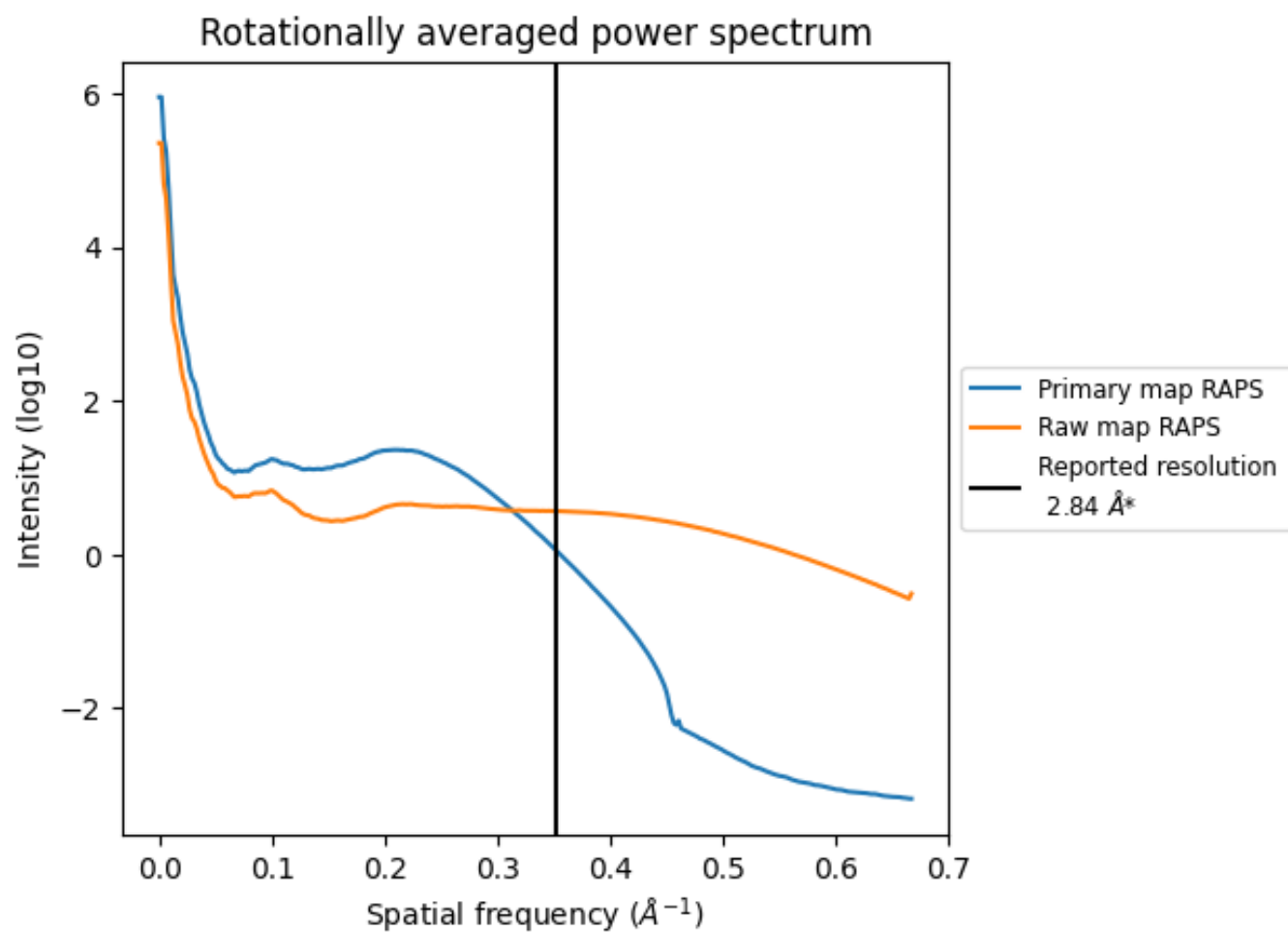
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 393 nm^3 ; this corresponds to an approximate mass of 355 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

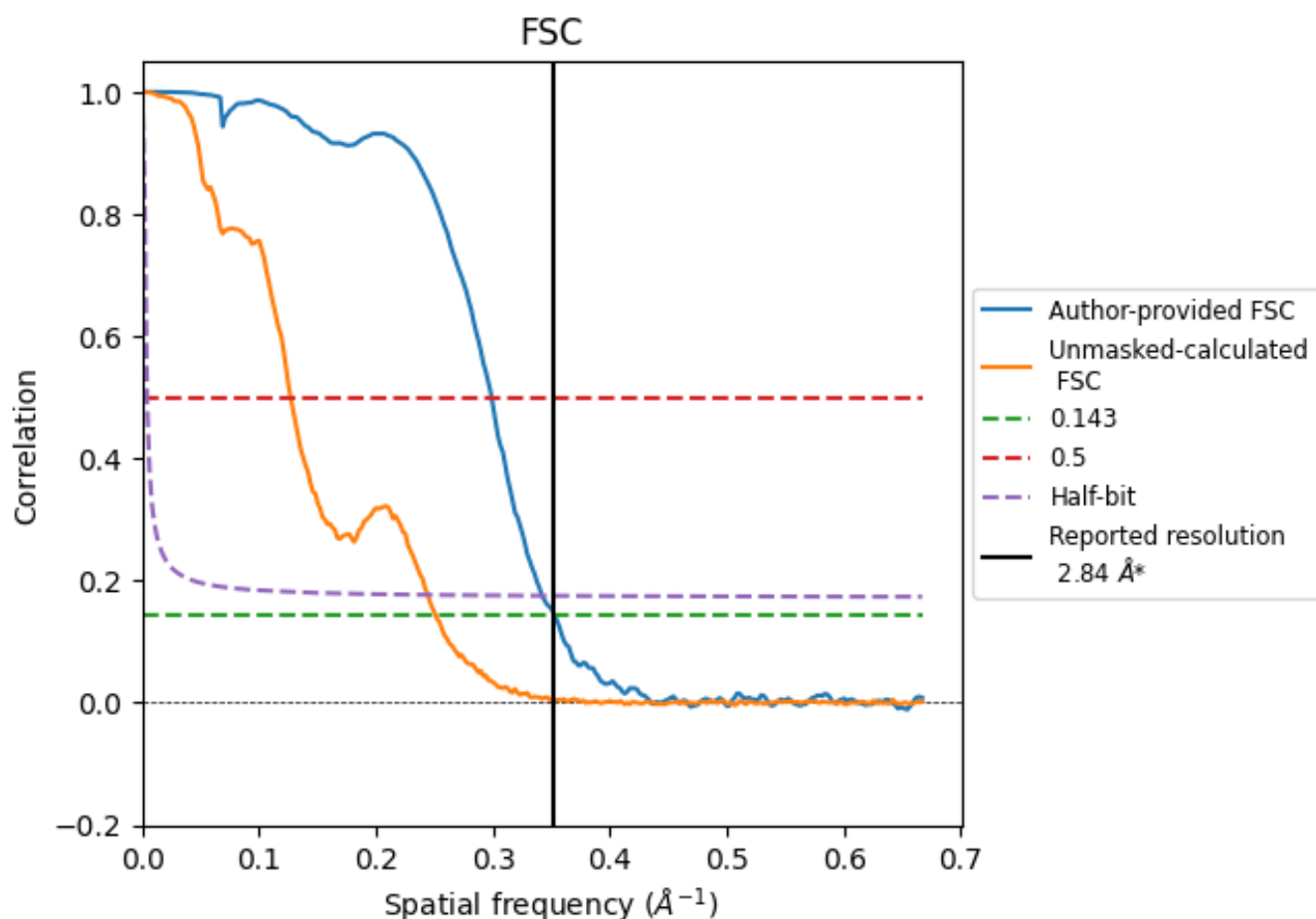


*Reported resolution corresponds to spatial frequency of 0.352 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.352 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

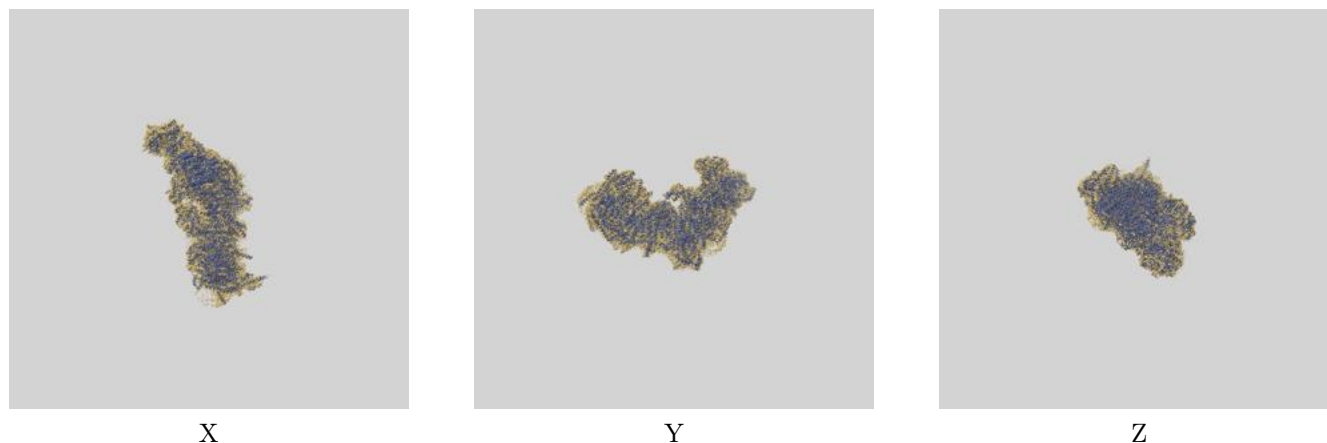
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.84	3.35	2.92
Unmasked-calculated*	3.98	7.88	4.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 2.84 by more than 10 %

9 Map-model fit [i](#)

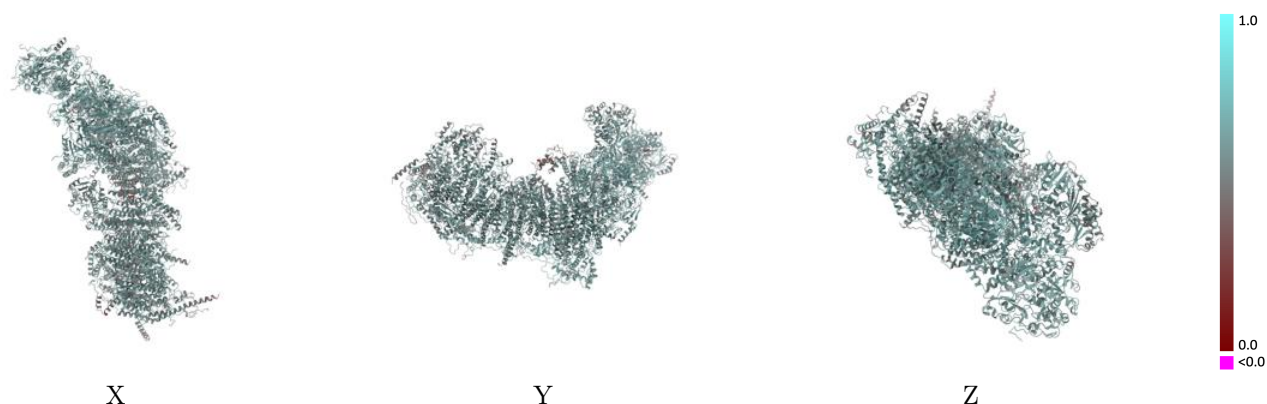
This section contains information regarding the fit between EMDB map EMD-14132 and PDB model 7QSK. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



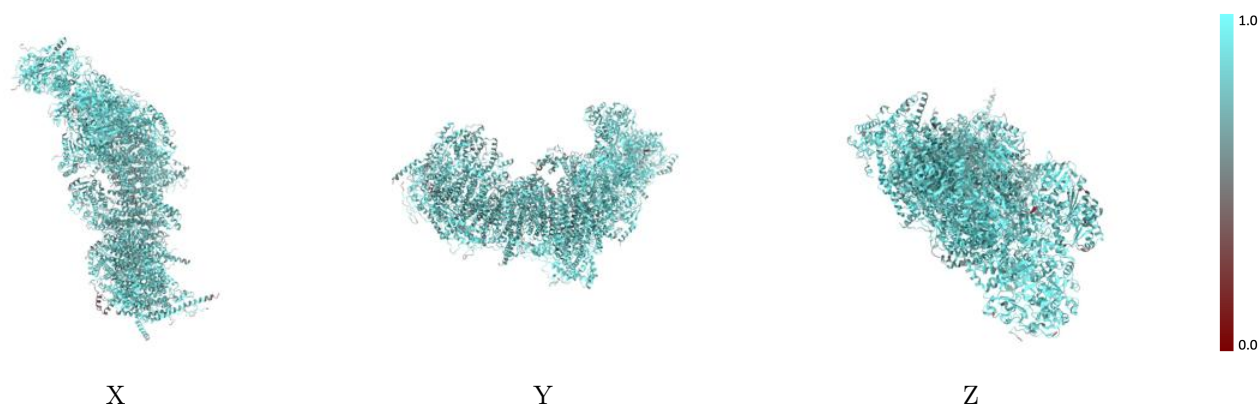
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



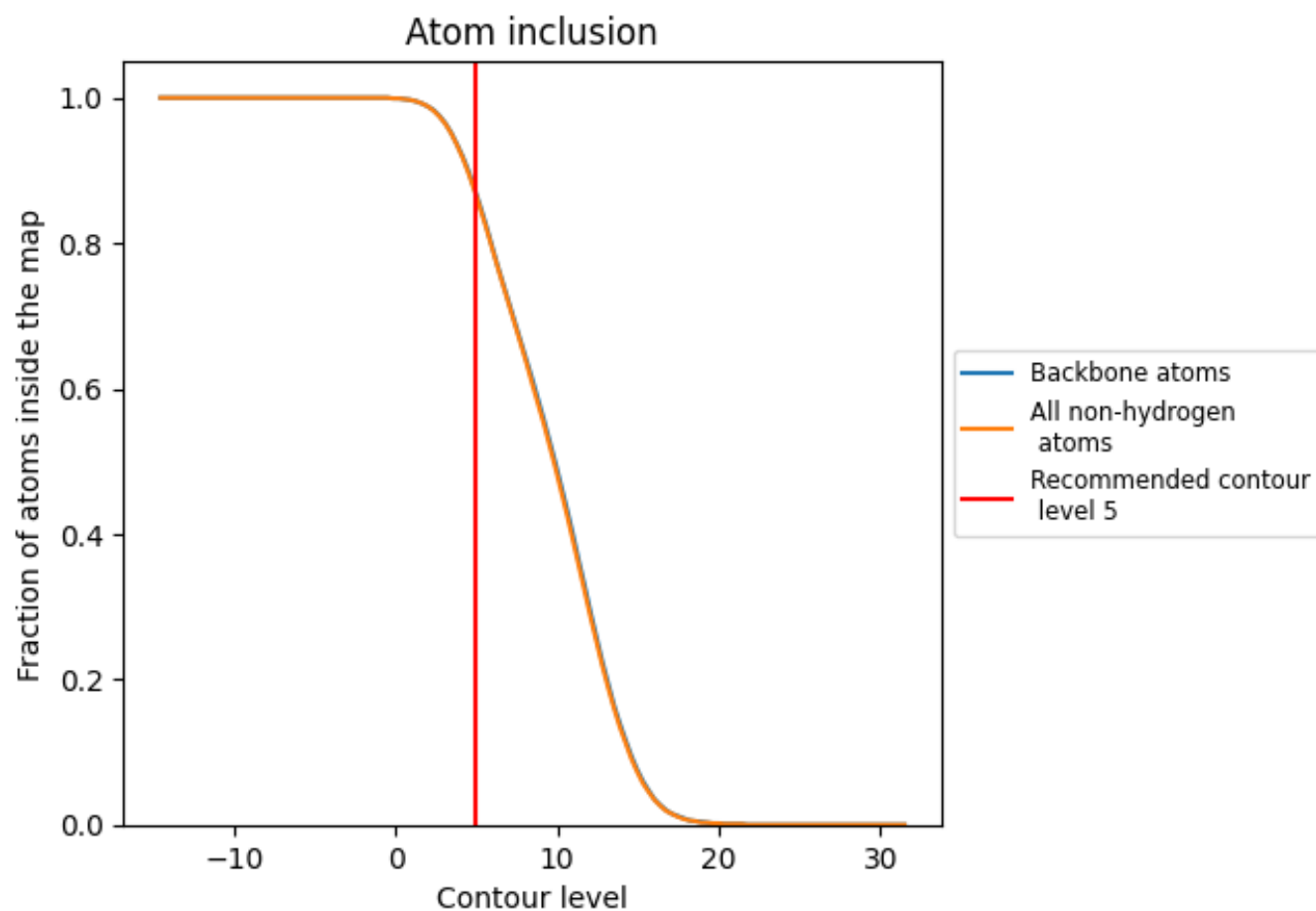
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8660	 0.5980
A	 0.8670	 0.6110
B	 0.9500	 0.6440
C	 0.9250	 0.6380
D	 0.9250	 0.6350
E	 0.8710	 0.5840
F	 0.8980	 0.6010
G	 0.8870	 0.6060
H	 0.9230	 0.6320
I	 0.9440	 0.6500
J	 0.8680	 0.6000
K	 0.8930	 0.6180
L	 0.8660	 0.5970
M	 0.9150	 0.6240
N	 0.9380	 0.6310
O	 0.8430	 0.5820
P	 0.8740	 0.6050
Q	 0.8850	 0.6200
R	 0.8740	 0.6160
S	 0.7970	 0.5480
T	 0.6220	 0.4120
U	 0.7490	 0.5180
V	 0.8190	 0.5940
W	 0.8460	 0.5990
X	 0.8530	 0.5890
Y	 0.7890	 0.5670
Z	 0.8800	 0.6000
a	 0.9220	 0.6080
b	 0.8270	 0.5760
c	 0.7950	 0.5620
d	 0.8470	 0.5960
e	 0.8520	 0.5890
f	 0.7100	 0.5210
g	 0.8230	 0.5720
h	 0.8820	 0.6080



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.7080	 0.5220
j	 0.7970	 0.5410
k	 0.7770	 0.5260
l	 0.8440	 0.5760
m	 0.8010	 0.5730
n	 0.8210	 0.5760
o	 0.7840	 0.5240
p	 0.8440	 0.5760
q	 0.8720	 0.6130
r	 0.8780	 0.5970
s	 0.8490	 0.5760