Full wwPDB EM Validation Report ⓘ

Aug 23, 2026 – 10:03 am BST

PDB ID	:	7QSO / pdb_00007qso
EMDB ID	:	EMD-14140
Title	:	Bovine complex I in lipid nanodisc, State 3 (Slack)
Authors	:	Chung, I.; Bridges, H.R.; Hirst, J.
Deposited on	:	2022-01-13
Resolution	:	3.02 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:

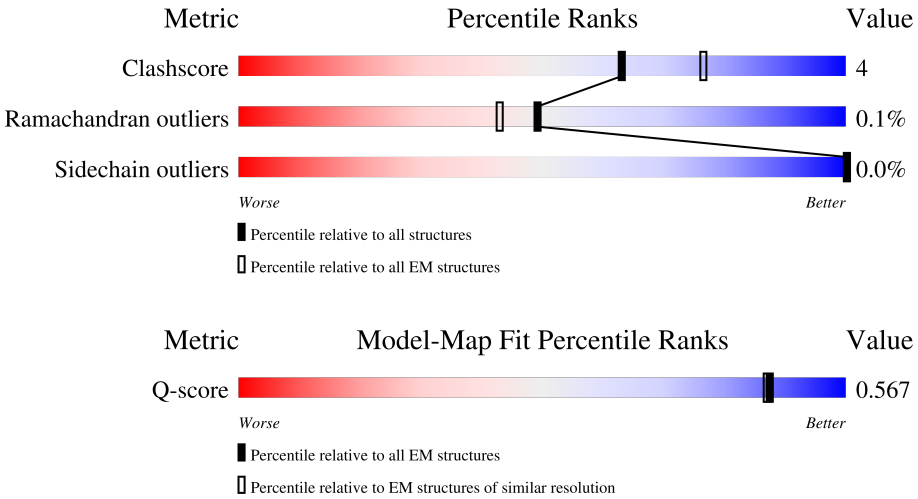
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.02 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	13913 (2.52 - 3.52)

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 <=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	7% 72% 21% 7%
2	B	216	63% 10% 27%
3	C	266	74% 5% 21%
4	D	463	75% 8% 16%

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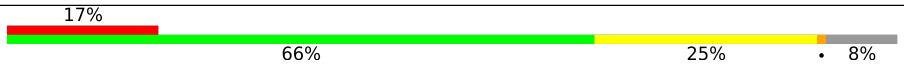
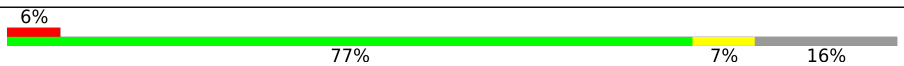
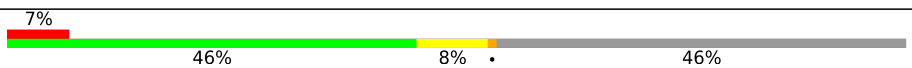
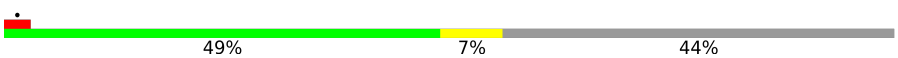
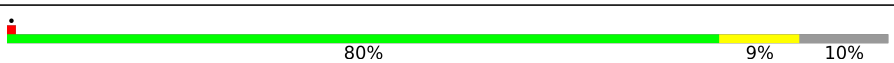
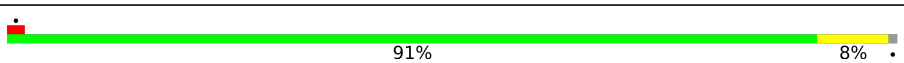
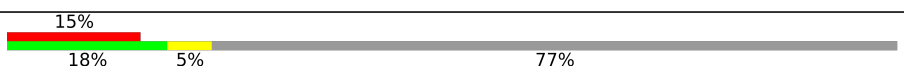
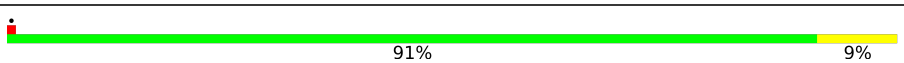
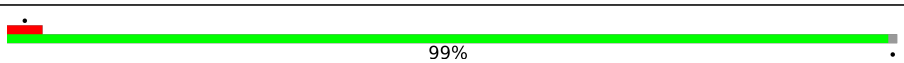
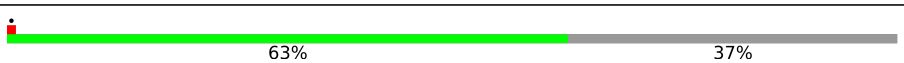
Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	

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Mol	Chain	Length	Quality of chain
29	d	120	91% 8%
30	e	106	84% 9% 7%
31	f	57	19% 89% 11%
32	g	154	54% 5% 42%
33	h	189	68% 8% 24%
34	i	127	12% 83% 16%
35	j	108	5% 57% 7% 35%
36	k	98	7% 72% 10% 17%
37	l	186	75% 9% 16%
38	m	129	14% 90% 9%
39	n	179	6% 87% 9%
40	o	137	5% 79% 9% 12%
41	p	176	90% 8%
42	q	145	95% 5%
43	r	113	82% 15%
44	s	109	39% 59%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	AME	d	1	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 66112 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
			Total	C	N	O	S		
1	A	107	864	587	125	147	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	158	1260	803	227	216	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	210	1743	1123	299	318	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	388	3110	1984	538	564	24	0	0

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	0	0
			3324	2094	594	616	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	700	Total	C	N	O	S	0	0
			5360	3356	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	0	0
			2509	1681	385	420	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	161	Total	C	N	O	S	0	0
			1226	827	173	214	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	86	Total	C	N	O	S	0	0
			647	425	96	111	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	547	Total	C	N	O	S	0	0
			4334	2880	667	746	41		

- 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	320	Total	C	N	O	S	0	0
			2560	1652	452	451	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	125	Total	C	N	O	S	0	0
			1016	641	181	191	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 subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	87	Total	C	N	O	S	0	0
			701	439	133	127	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	84	Total	C	N	O	S	0	0
			681	439	100	137	5		
20	U	88	Total	C	N	O	S	0	0
			707	454	104	144	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	113	Total	C	N	O	S	0	0
			919	595	155	166	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	115	Total	C	N	O	S	0	0
			977	625	181	167	4		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 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 subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	33	Total	C	N	O	S	0	0
			248	162	39	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	142	Total	C	N	O	S	0	0
			1157	743	202	203	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	48	Total	C	N	O	0	0
			405	268	69	68		

- 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	90	Total	C	N	O	S	0	0
			750	483	124	139	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	143	Total	C	N	O	S	0	0
			1186	776	203	205	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	70	Total	C	N	O	S	0	0
			592	387	98	106	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	127	Total	C	N	O	0	0
			1061	681	187	193		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	171	Total	C	N	O	S	0	0
			1487	952	272	256	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	120	Total	C	N	O	S	0	0
			1035	645	199	183	8		

- 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
			1455	912	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		

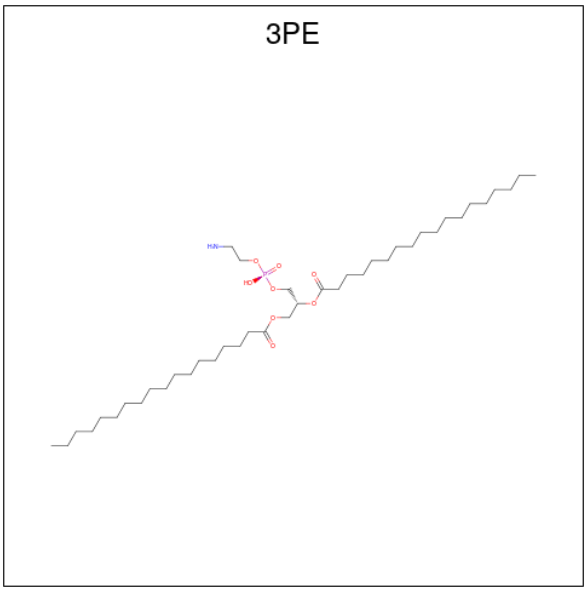
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	96	Total	C	N	O	S	0	0
			785	496	146	140	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	0	0
			380	238	67	74	1		

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
45	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
45	H	1	Total	C	N	O	P	0
			33	23	1	8	1	
45	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	I	1	Total	C	N	O	P	0
			33	23	1	8	1	
45	L	1	Total	C	N	O	P	0
			45	35	1	8	1	

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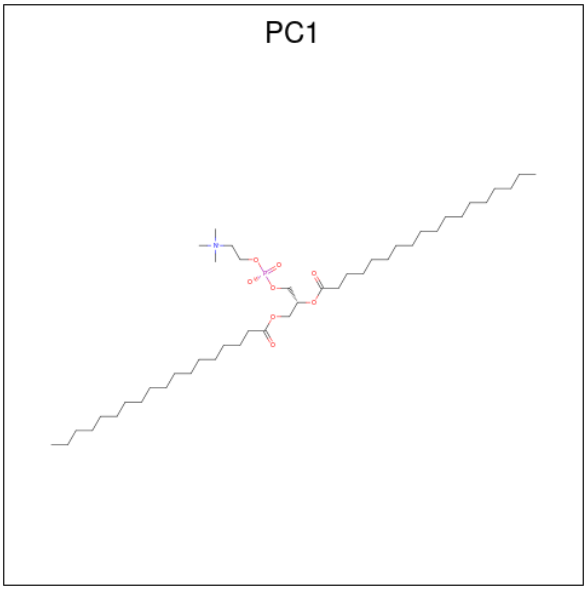
Mol	Chain	Residues	Atoms					AltConf
45	L	1	Total	C	N	O	P	0
			32	22	1	8	1	
45	M	1	Total	C	N	O	P	0
			38	28	1	8	1	
45	N	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	N	1	Total	C	N	O	P	0
			49	39	1	8	1	
45	Y	1	Total	C	N	O	P	0
			39	29	1	8	1	
45	h	1	Total	C	N	O	P	0
			32	22	1	8	1	
45	r	1	Total	C	N	O	P	0
			49	39	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	B	1	Total	C	N	O	P	0
			50	40	1	8	1	
46	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	J	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	M	1	Total	C	N	O	P	0
			46	36	1	8	1	

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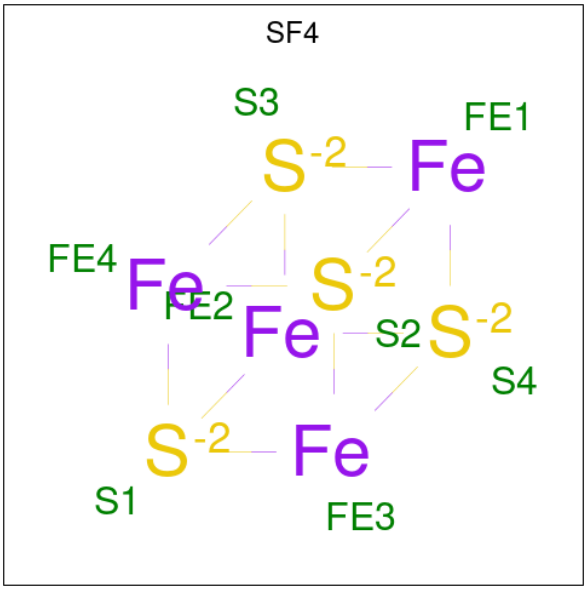
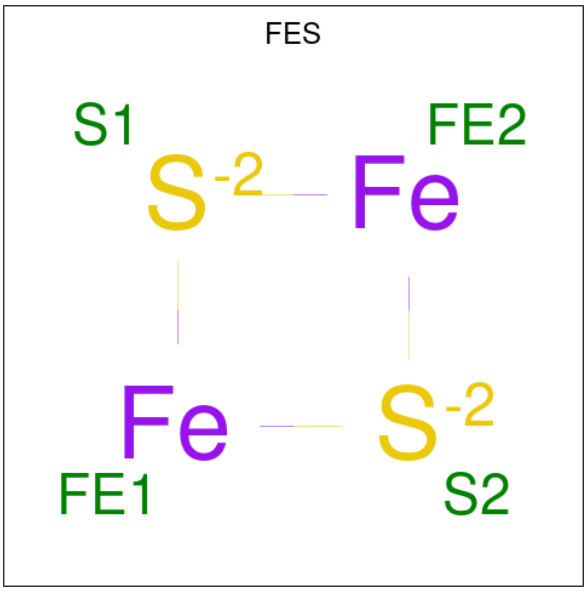
Mol	Chain	Residues	Atoms					AltConf
46	d	1	Total	C	N	O	P	0
			33	23	1	8	1	
46	q	1	Total	C	N	O	P	0
			37	27	1	8	1	

- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



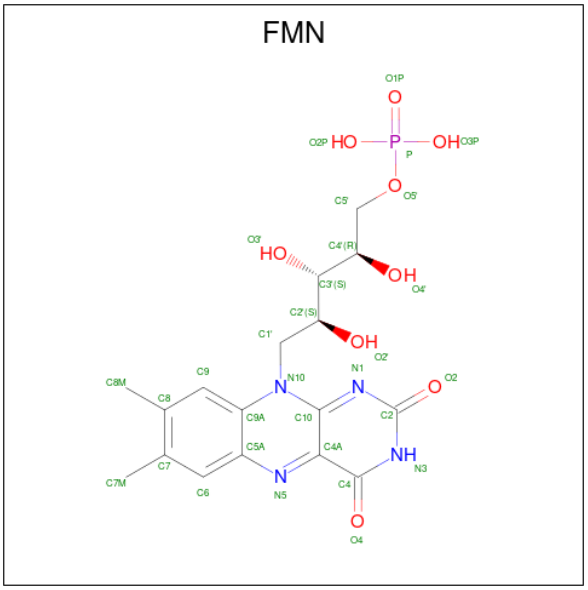
Mol	Chain	Residues	Atoms				AltConf
47	B	1	Total	Fe	S		0
			8	4	4		
47	F	1	Total	Fe	S		0
			8	4	4		
47	G	1	Total	Fe	S		0
			8	4	4		
47	G	1	Total	Fe	S		0
			8	4	4		
47	I	1	Total	Fe	S		0
			8	4	4		
47	I	1	Total	Fe	S		0
			8	4	4		

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 49 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

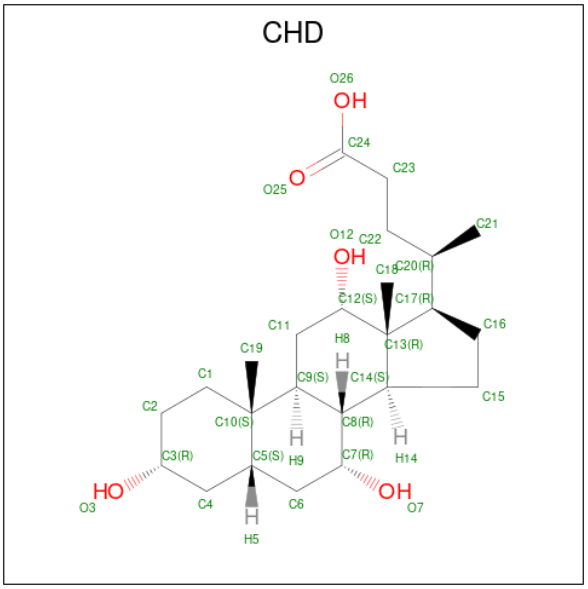


Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 50 is POTASSIUM ION (CCD ID: K) (formula: K).

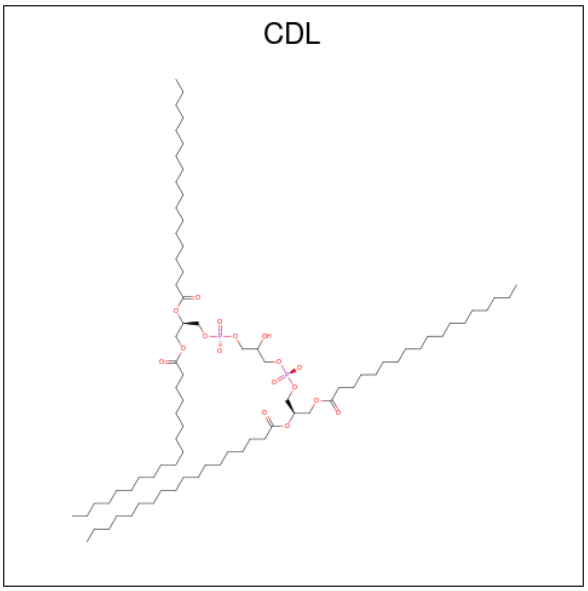
Mol	Chain	Residues	Atoms	AltConf
50	G	1	Total K 1 1	0

- Molecule 51 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



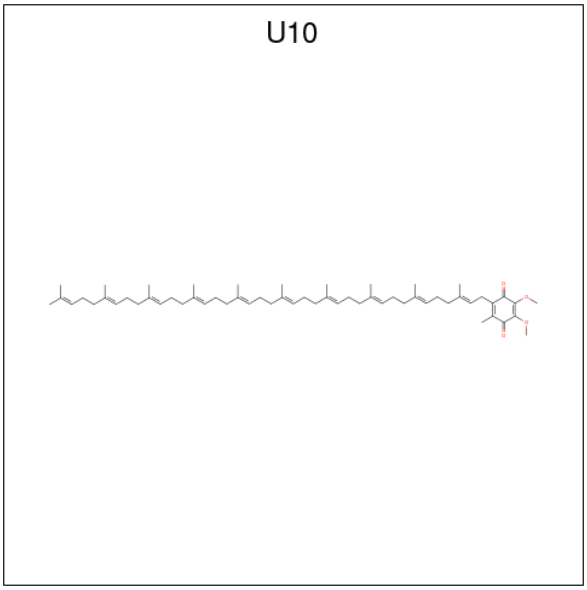
Mol	Chain	Residues	Atoms	AltConf
51	H	1	Total C O 29 24 5	0
51	L	1	Total C O 29 24 5	0

- Molecule 52 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



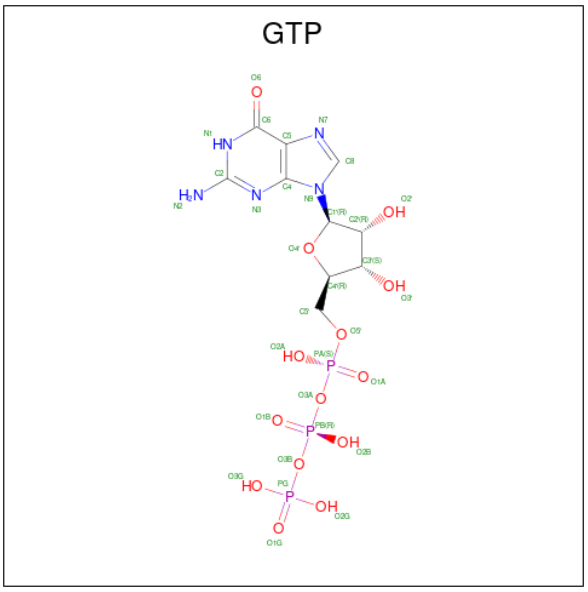
Mol	Chain	Residues	Atoms				AltConf
52	L	1	Total	C	O	P	0
			75	56	17	2	
52	N	1	Total	C	O	P	0
			73	54	17	2	
52	X	1	Total	C	O	P	0
			79	60	17	2	
52	d	1	Total	C	O	P	0
			65	46	17	2	
52	h	1	Total	C	O	P	0
			77	58	17	2	
52	r	1	Total	C	O	P	0
			60	41	17	2	

- Molecule 53 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			AltConf
53	M	1	Total	C	O	0
			63	59	4	

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

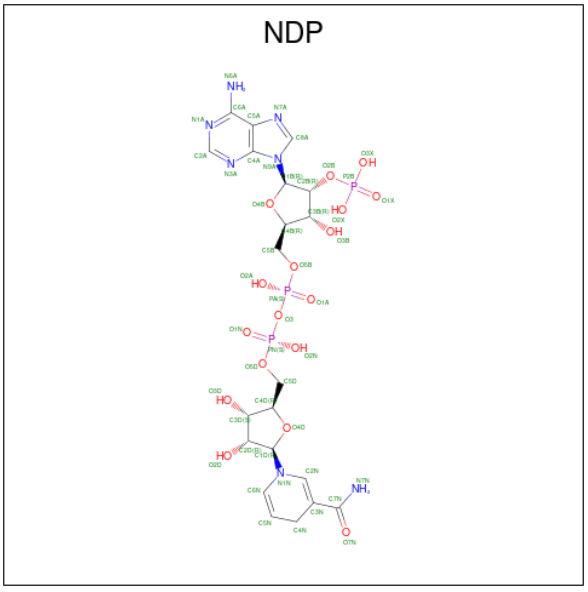


Mol	Chain	Residues	Atoms					AltConf
54	O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

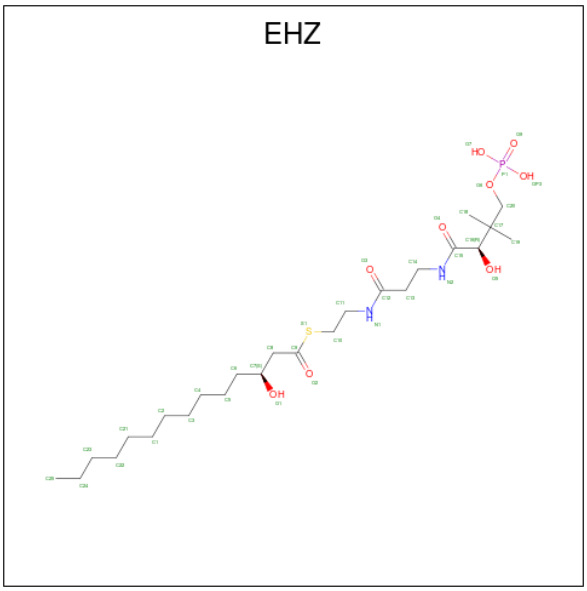


Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

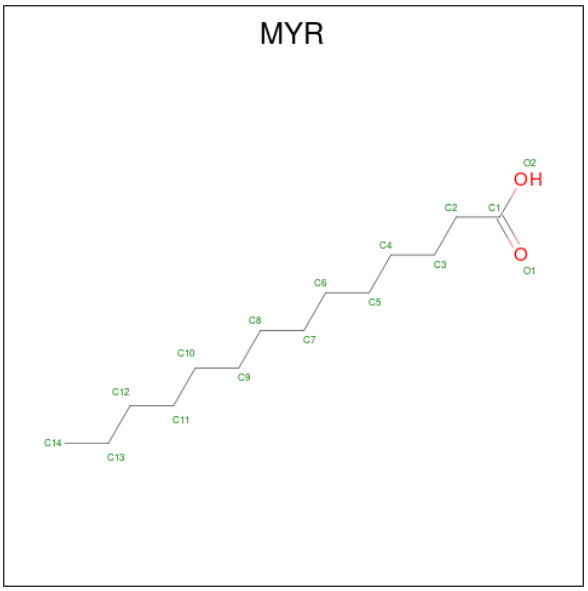
Mol	Chain	Residues	Atoms		AltConf
57	R	1	Total	Zn	0
			1	1	

- Molecule 58 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: $C_{25}H_{49}N_2O_9PS$).



Mol	Chain	Residues	Atoms						AltConf
58	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
58	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 59 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).

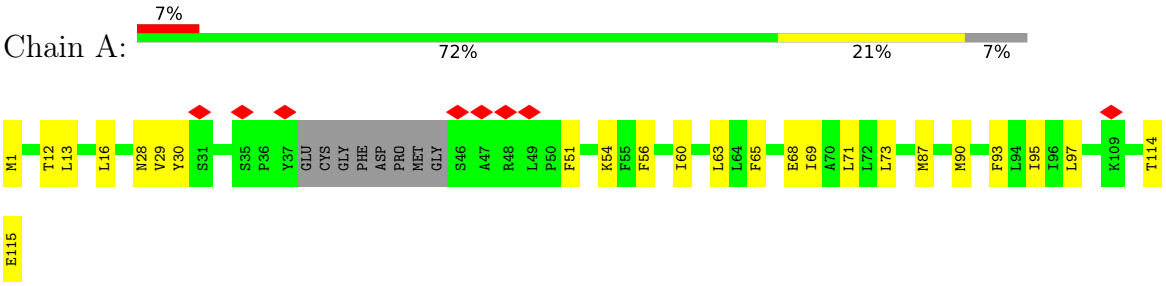


Mol	Chain	Residues	Atoms			AltConf
59	o	1	Total	C	O	0
			15	14	1	

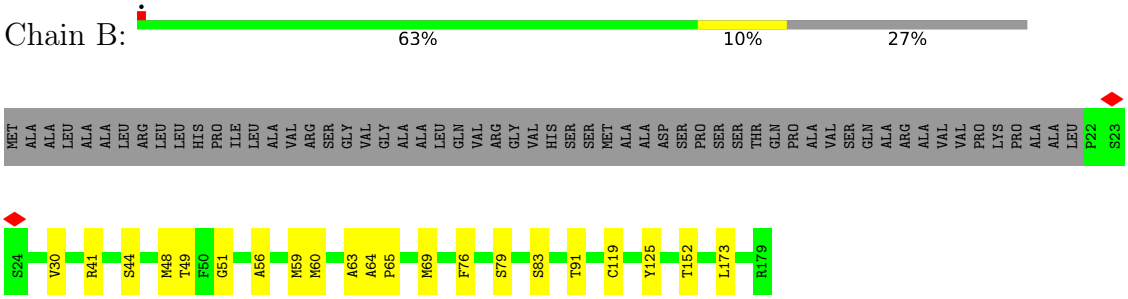
3 Residue-property plots (i)

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.

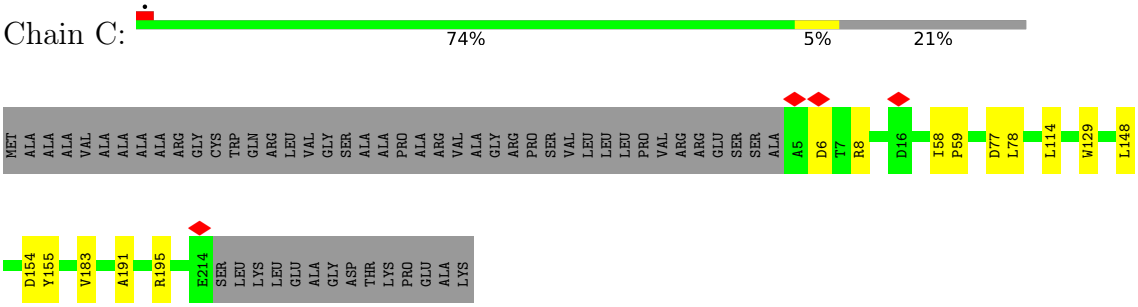
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3



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

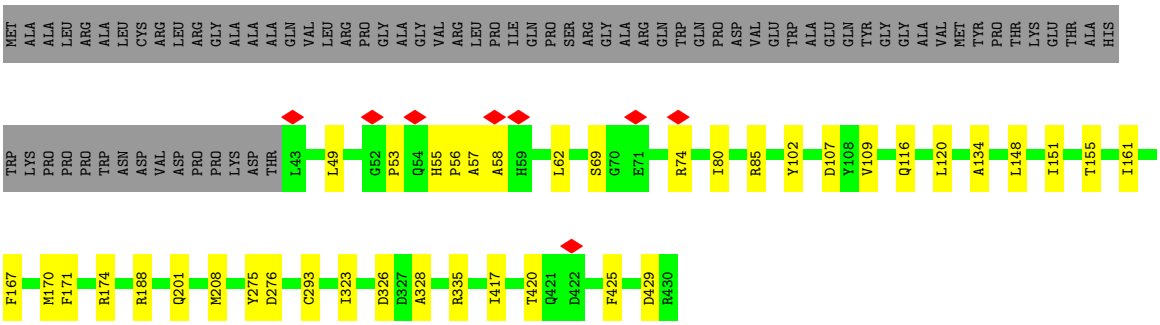


• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

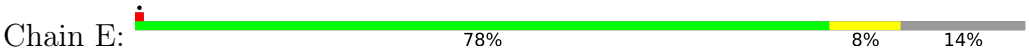


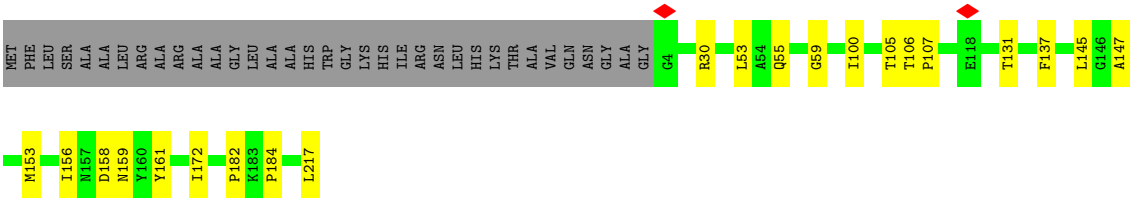
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



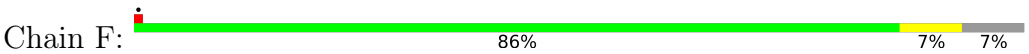


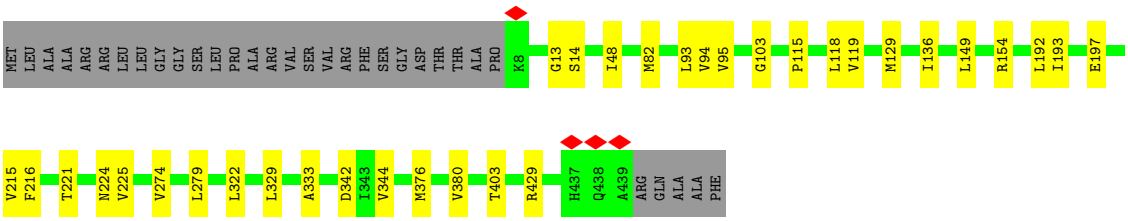
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



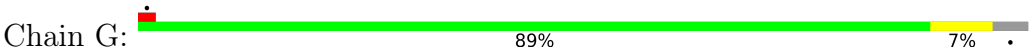


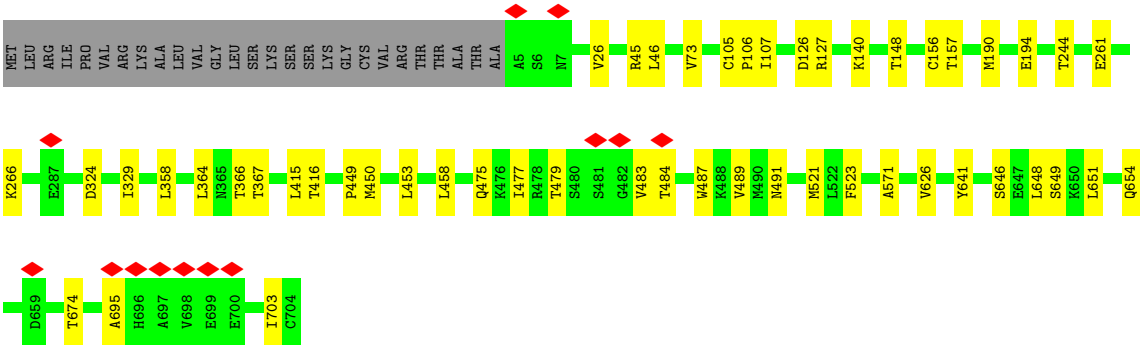
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



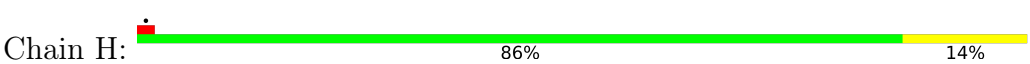


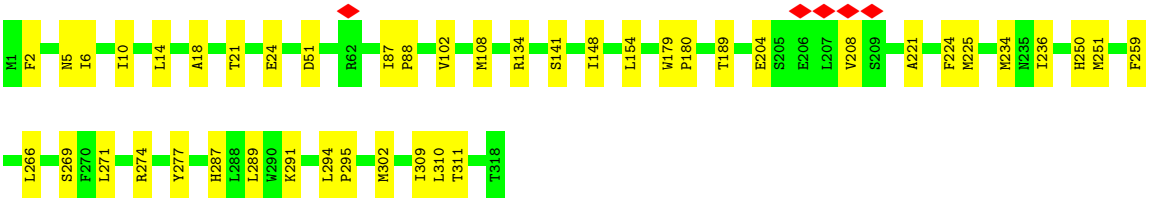
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



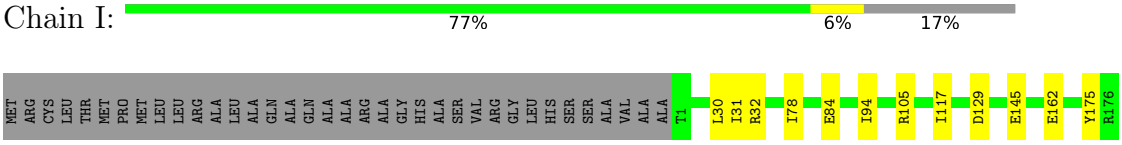


• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

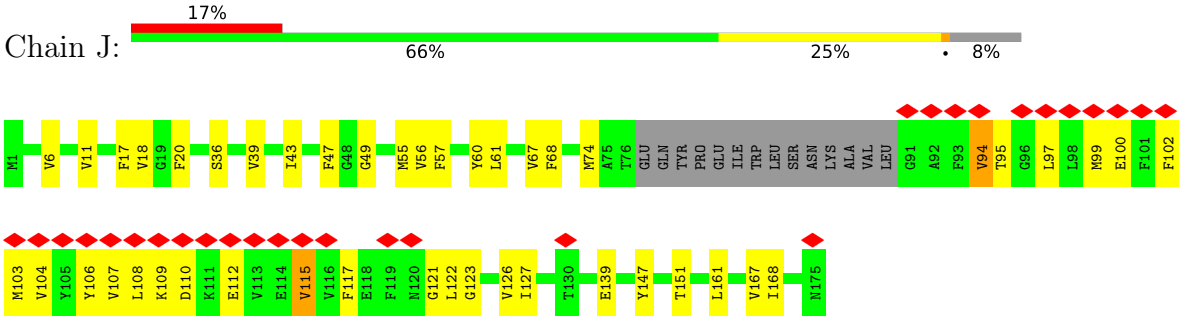




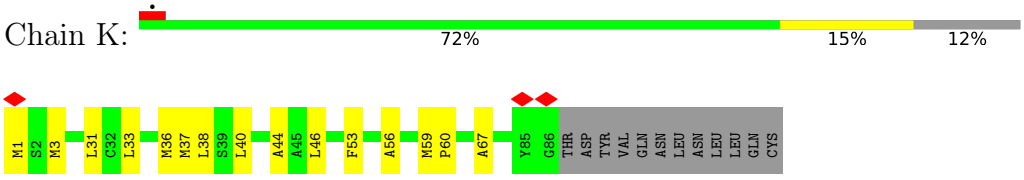
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



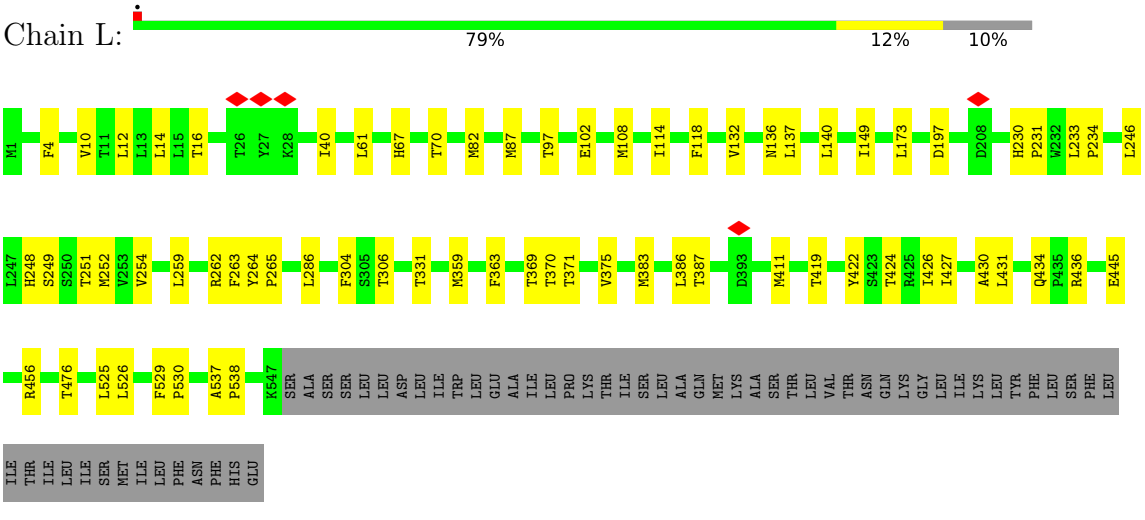
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6



• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

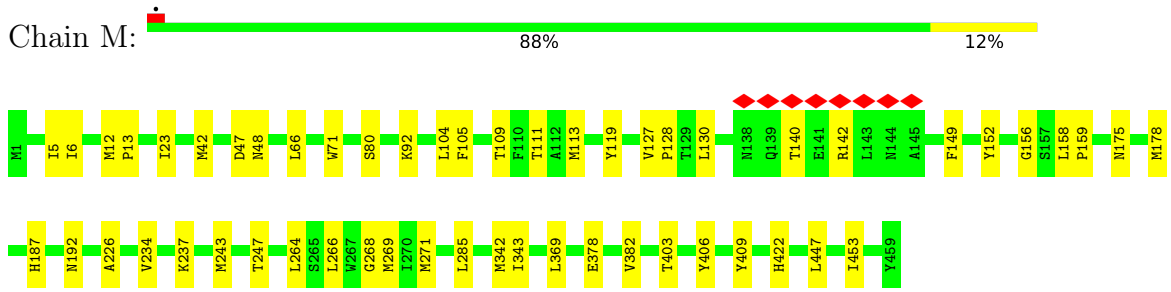


• Molecule 12: NADH-ubiquinone oxidoreductase chain 5



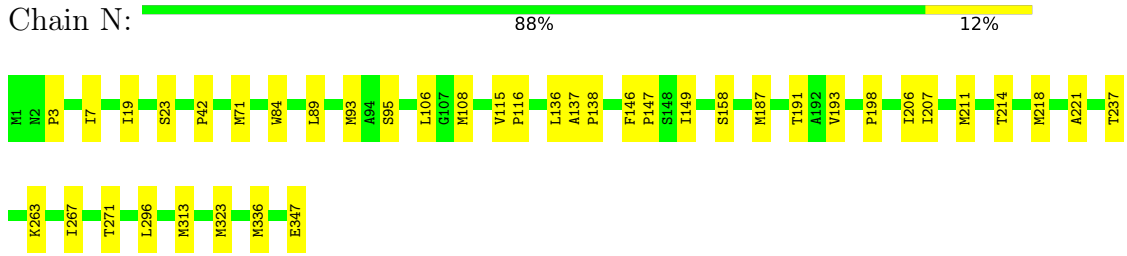
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:



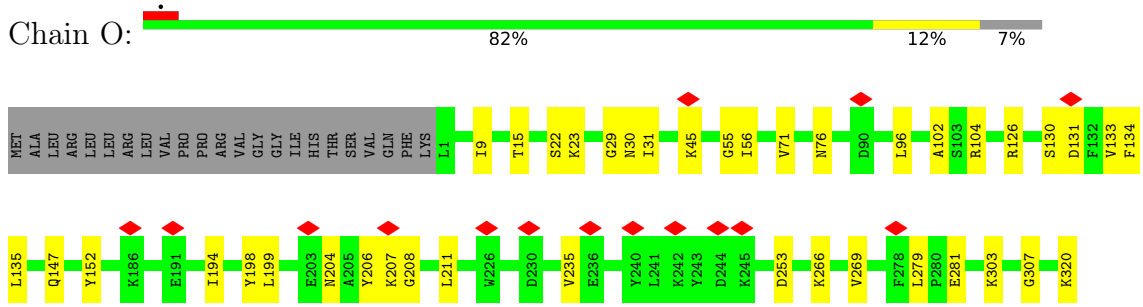
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:



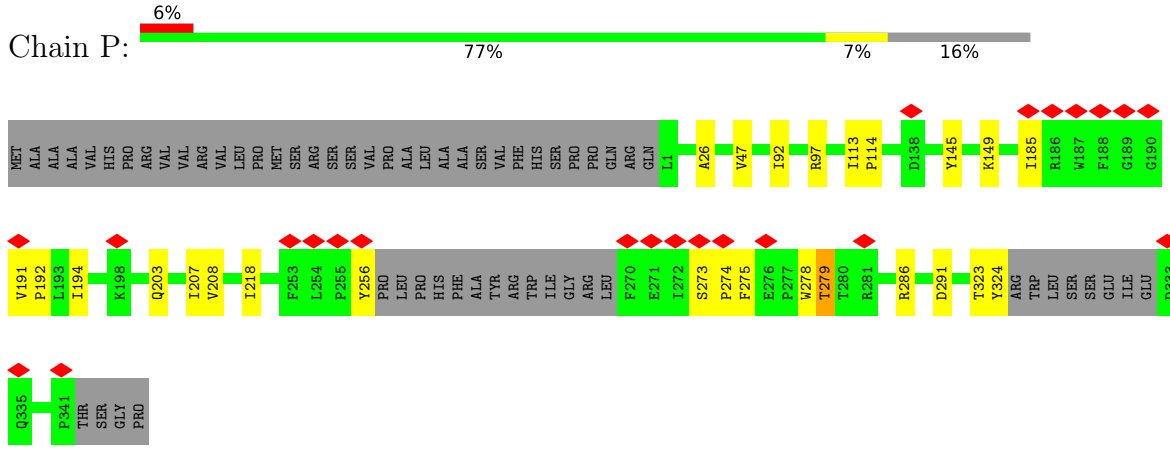
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:



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

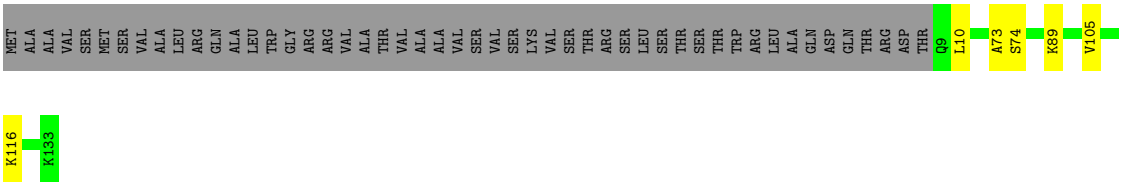
Chain P:



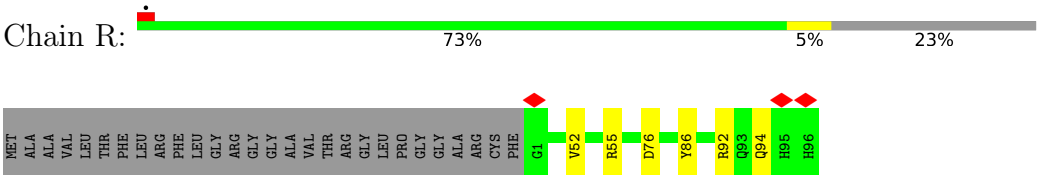
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:

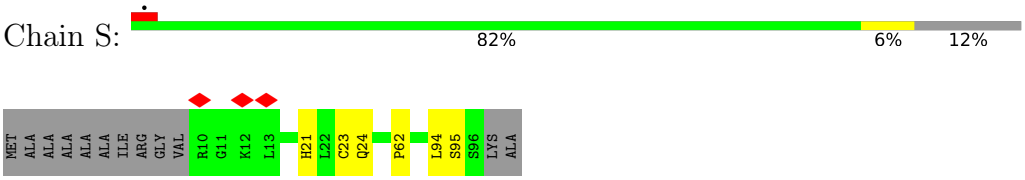




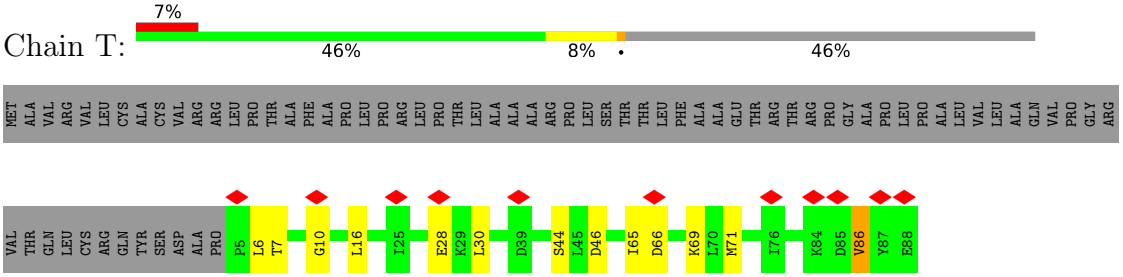
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



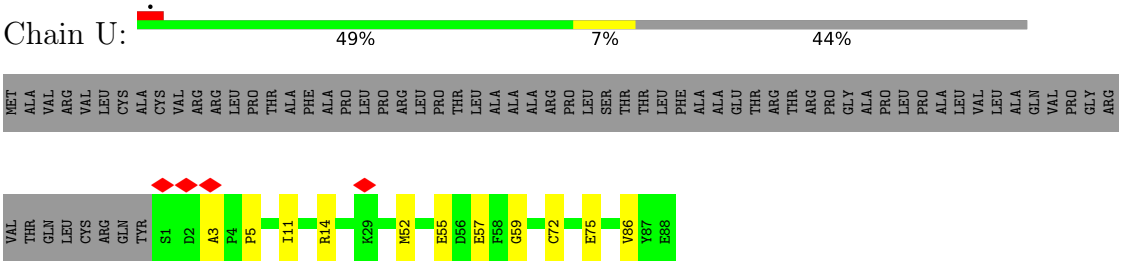
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



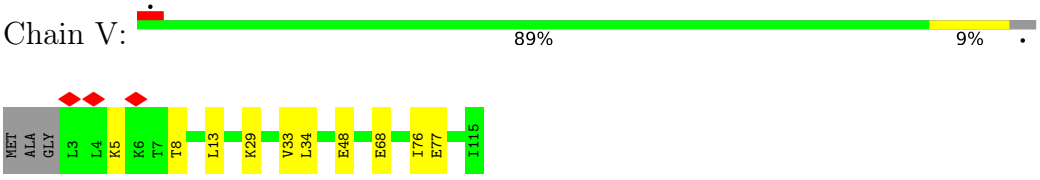
• Molecule 20: Acyl carrier protein, mitochondrial



• Molecule 20: Acyl carrier protein, mitochondrial

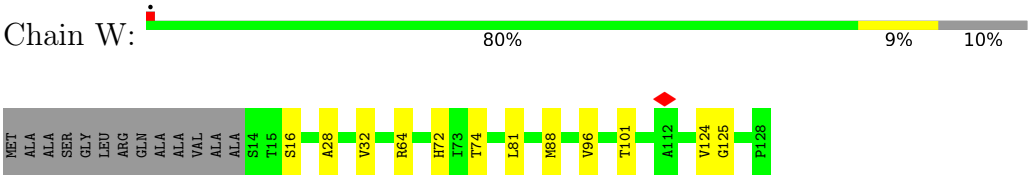


• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



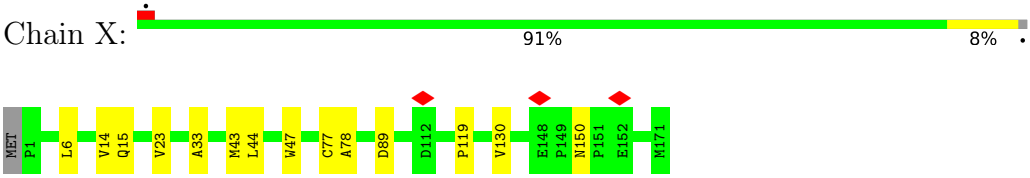
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:



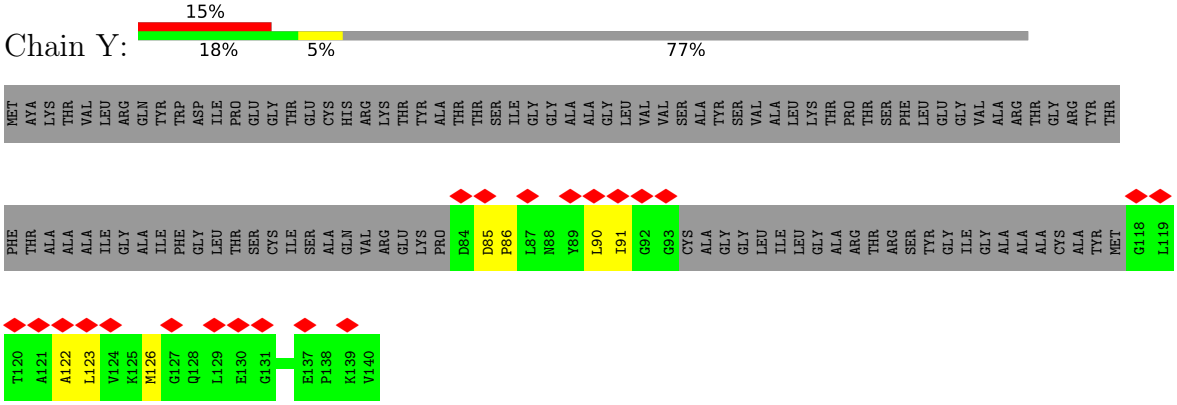
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:



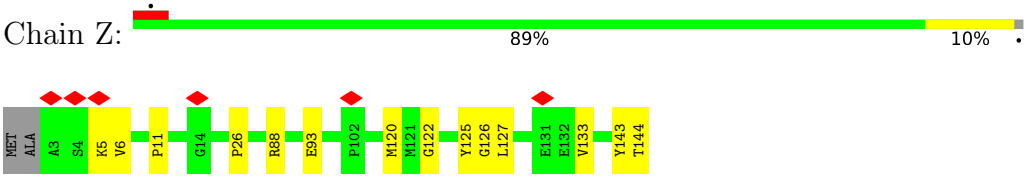
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:



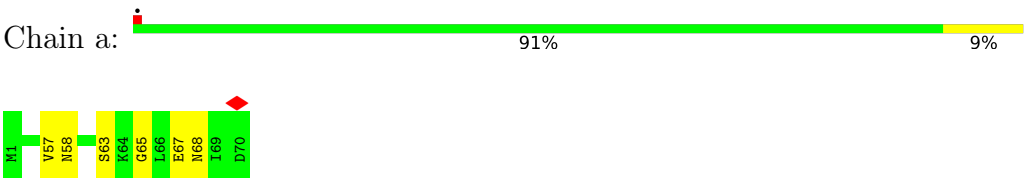
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:



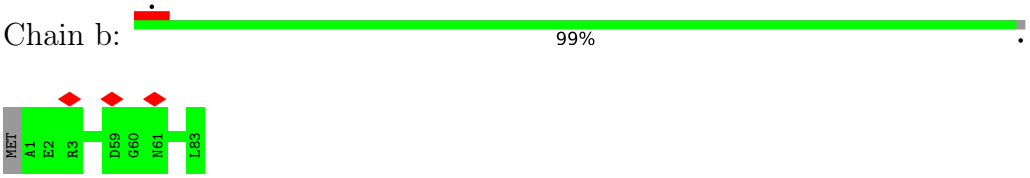
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:



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

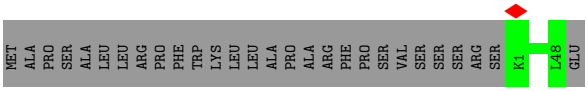
Chain b:



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

Chain c:

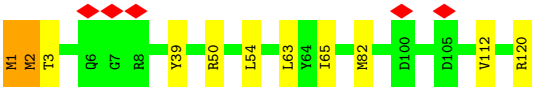




• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:

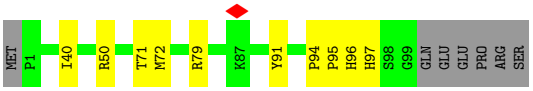




• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:

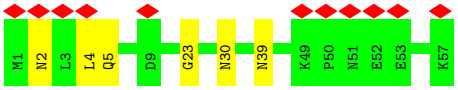




• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:





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

Chain g:



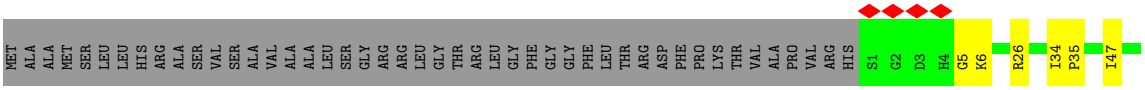


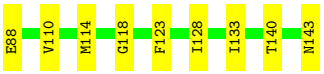


• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:



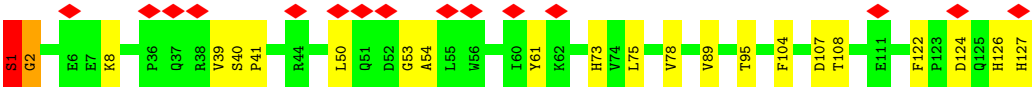




• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:

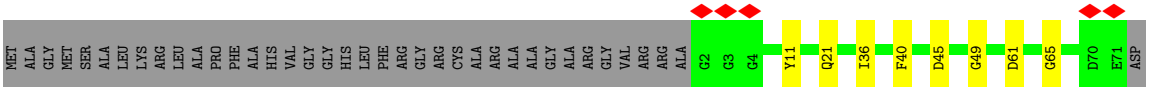




• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:





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

Chain k:

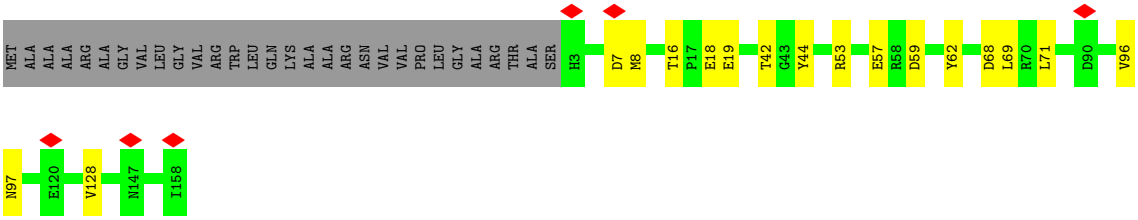




• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l:

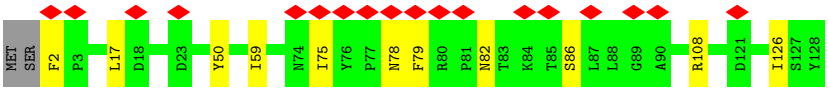




• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain m:

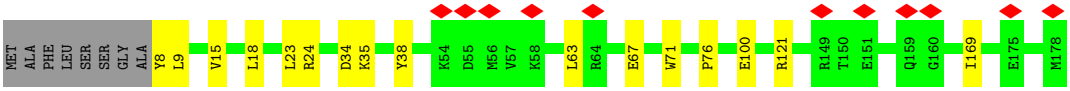




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

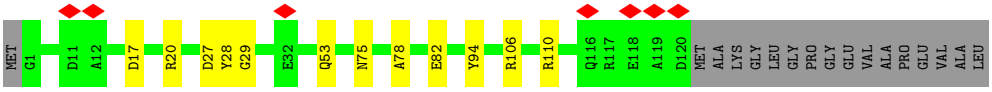
Chain n:



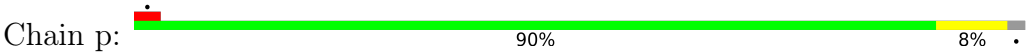


• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



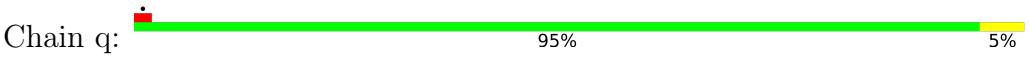


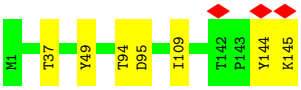
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



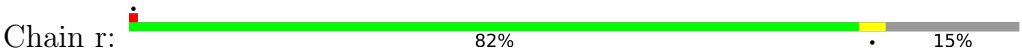


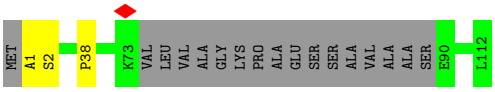
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12





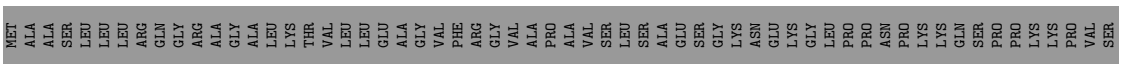
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

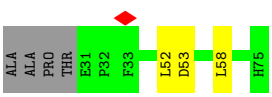




• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	22019	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 ($e^-/Å^2$)	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	34.528	Depositor
Minimum map value	-14.853	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.958	Depositor
Recommended contour level	5.5	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 (i)

5.1 Standard geometry (i)

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

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	0.24	0/876	0.31	0/1199
2	B	0.31	0/1292	0.39	0/1747
3	C	0.28	0/1794	0.32	0/2443
4	D	0.29	0/3170	0.35	0/4285
5	E	0.26	0/1699	0.32	0/2312
6	F	0.26	0/3398	0.33	0/4591
7	G	0.26	0/5450	0.33	0/7388
8	H	0.28	0/2571	0.36	0/3513
9	I	0.31	0/1445	0.36	0/1956
10	J	0.25	0/1246	0.45	2/1687 (0.1%)
11	K	0.47	0/646	0.54	1/872 (0.1%)
12	L	0.23	0/4443	0.30	0/6047
13	M	0.27	0/3738	0.33	0/5097
14	N	0.25	0/2792	0.30	0/3800
15	O	0.18	0/2651	0.27	0/3587
16	P	0.24	0/2626	0.35	0/3557
17	Q	0.27	0/1039	0.32	0/1404
18	R	0.27	0/753	0.29	0/1014
19	S	0.23	0/712	0.32	0/957
20	T	0.20	0/692	0.43	1/932 (0.1%)
20	U	0.23	0/719	0.33	0/971
21	V	0.21	0/939	0.26	0/1272
22	W	0.24	0/1001	0.30	0/1345
23	X	0.26	0/1439	0.36	0/1942
24	Y	0.12	0/252	0.25	0/340
25	Z	0.26	0/1186	0.30	0/1599
26	a	0.25	0/584	0.31	0/786
27	b	0.23	0/672	0.28	0/923
28	c	0.22	0/418	0.26	0/567
29	d	0.25	0/1018	0.30	0/1375
30	e	0.26	0/850	0.39	0/1136

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	f	0.22	0/505	0.39	0/681
32	g	0.24	0/772	0.28	0/1046
33	h	0.24	0/1221	0.31	0/1651
34	i	0.20	0/1127	0.40	1/1534 (0.1%)
35	j	0.19	0/619	0.28	0/848
36	k	0.17	0/672	0.29	0/906
37	l	0.20	0/1369	0.28	0/1873
38	m	0.20	0/1088	0.31	0/1472
39	n	0.21	0/1540	0.31	0/2085
40	o	0.27	0/1060	0.36	0/1420
41	p	0.24	0/1489	0.32	0/2008
42	q	0.26	0/1250	0.34	0/1698
43	r	0.26	0/798	0.31	0/1079
44	s	0.22	0/392	0.28	0/531
All	All	0.25	0/66013	0.33	5/89476 (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
34	i	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	K	38	LEU	N-CA-C	-5.66	105.10	112.23
10	J	94	VAL	CG1-CB-CG2	5.16	122.14	110.80
20	T	86	VAL	CG1-CB-CG2	5.15	122.14	110.80
34	i	39	VAL	CG1-CB-CG2	5.07	121.96	110.80
10	J	115	VAL	CG1-CB-CG2	5.01	121.81	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	i	1	SAC	Mainchain

5.2 Too-close contacts (i)

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	864	0	905	24	0
2	B	1260	0	1269	17	0
3	C	1743	0	1690	10	0
4	D	3110	0	3088	30	0
5	E	1659	0	1664	18	0
6	F	3324	0	3279	24	0
7	G	5360	0	5375	35	0
8	H	2509	0	2621	42	0
9	I	1414	0	1370	15	0
10	J	1226	0	1234	40	0
11	K	647	0	690	18	0
12	L	4334	0	4451	47	0
13	M	3654	0	3852	37	0
14	N	2733	0	2912	32	0
15	O	2589	0	2566	28	0
16	P	2560	0	2581	17	0
17	Q	1016	0	1014	5	0
18	R	740	0	714	4	0
19	S	701	0	717	3	0
20	T	681	0	677	10	0
20	U	707	0	700	8	0
21	V	919	0	961	5	0
22	W	977	0	994	10	0
23	X	1402	0	1379	14	0
24	Y	248	0	247	5	0
25	Z	1157	0	1156	12	0
26	a	569	0	568	5	0
27	b	651	0	662	0	0
28	c	405	0	409	0	0
29	d	999	0	988	14	0
30	e	829	0	829	10	0
31	f	492	0	501	7	0
32	g	750	0	711	7	0
33	h	1186	0	1193	14	0
34	i	1097	0	1108	15	0
35	j	592	0	528	6	0
36	k	653	0	639	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	l	1314	0	1210	11	0
38	m	1061	0	1059	12	0
39	n	1487	0	1433	12	0
40	o	1035	0	1001	8	0
41	p	1455	0	1430	13	0
42	q	1209	0	1182	5	0
43	r	785	0	795	2	0
44	s	380	0	349	3	0
45	A	124	0	176	0	0
45	H	33	0	40	0	0
45	I	84	0	122	1	0
45	L	77	0	102	1	0
45	M	38	0	50	2	0
45	N	84	0	119	2	0
45	Y	39	0	55	0	0
45	h	32	0	38	0	0
45	r	49	0	75	0	0
46	B	101	0	156	0	0
46	J	43	0	63	1	0
46	M	46	0	69	1	0
46	d	33	0	40	2	0
46	q	37	0	48	0	0
47	B	8	0	0	0	0
47	F	8	0	0	1	0
47	G	16	0	0	0	0
47	I	16	0	0	0	0
48	E	4	0	0	0	0
48	G	4	0	0	0	0
49	F	31	0	19	1	0
50	G	1	0	0	0	0
51	H	29	0	38	7	0
51	L	29	0	38	1	0
52	L	75	0	97	1	0
52	N	73	0	90	2	0
52	X	79	0	105	0	0
52	d	65	0	77	1	0
52	h	77	0	101	1	0
52	r	60	0	64	1	0
53	M	63	0	90	6	0
54	O	32	0	12	0	0
55	O	1	0	0	0	0
56	P	48	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	R	1	0	0	0	0
58	T	37	0	0	1	0
58	U	37	0	0	1	0
59	o	15	0	27	0	0
All	All	66112	0	66638	559	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 4.

All (559) 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)
23:X:43:MET:HE3	23:X:47:TRP:CZ3	2.12	0.84
38:m:82:ASN:O	38:m:86:SER:OG	1.96	0.81
7:G:366:THR:O	7:G:367:THR:OG1	1.98	0.80
12:L:251:THR:O	12:L:254:VAL:HG22	1.82	0.79
1:A:54:LYS:NZ	1:A:115:GLU:OE1	2.15	0.78
4:D:69:SER:OG	4:D:74:ARG:NE	2.17	0.78
23:X:43:MET:HE3	23:X:47:TRP:HZ3	1.48	0.78
20:T:7:THR:HG22	20:T:10:GLY:H	1.49	0.76
29:d:63:LEU:HD23	52:d:202:CDL:OA9	1.86	0.75
8:H:21:THR:HG21	51:H:701:CHD:H181	1.70	0.74
12:L:359:MET:O	12:L:436:ARG:NH2	2.21	0.74
29:d:39:TYR:HD1	29:d:65:ILE:HD11	1.54	0.72
20:U:55:GLU:OE1	39:n:24:ARG:NH1	2.24	0.71
2:B:63:ALA:HB2	2:B:69:MET:HE2	1.73	0.71
6:F:93:LEU:HD13	6:F:129:MET:HE1	1.73	0.70
15:O:104:ARG:NE	15:O:131:ASP:OD2	2.22	0.70
51:H:701:CHD:H212	51:H:701:CHD:H12	1.75	0.69
58:U:101:EHZ:O5	58:U:101:EHZ:O6	2.07	0.69
14:N:106:LEU:HD22	14:N:187:MET:HE2	1.75	0.69
1:A:71:LEU:O	10:J:147:TYR:OH	2.10	0.68
10:J:103:MET:O	10:J:107:VAL:N	2.23	0.68
19:S:23:CYS:SG	19:S:24:GLN:N	2.66	0.68
13:M:243:MET:O	13:M:247:THR:HG23	1.93	0.68
2:B:49:THR:HG21	2:B:59:MET:HG2	1.76	0.68
13:M:105:PHE:O	13:M:109:THR:OG1	2.11	0.68
15:O:303:LYS:O	29:d:50:ARG:NH2	2.28	0.67
13:M:140:THR:HG22	13:M:140:THR:O	1.94	0.67
1:A:87:MET:HE1	8:H:309:ILE:HD11	1.77	0.67
4:D:161:ILE:HG22	4:D:161:ILE:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:j:61:ASP:OD1	40:o:106:ARG:NH2	2.28	0.67
5:E:156:ILE:HD13	5:E:161:TYR:CE2	2.30	0.67
7:G:648:LEU:HD23	7:G:651:LEU:HD11	1.77	0.67
41:p:98:ASP:OD2	41:p:141:ARG:NH1	2.28	0.66
6:F:13:GLY:O	6:F:14:SER:OG	2.14	0.65
35:j:45:ASP:O	35:j:49:GLY:N	2.27	0.65
2:B:125:TYR:HB2	9:I:117:ILE:CG2	2.26	0.65
20:U:52:MET:HE1	39:n:23:LEU:HB3	1.79	0.65
32:g:101:GLU:CD	32:g:107:ILE:HD11	2.22	0.65
23:X:6:LEU:O	25:Z:88:ARG:NH2	2.28	0.64
10:J:97:LEU:HD21	10:J:99:MET:HE2	1.79	0.64
51:L:704:CHD:H212	51:L:704:CHD:H12	1.79	0.64
14:N:158:SER:OG	14:N:191:THR:OG1	2.02	0.64
5:E:30:ARG:NH1	44:s:53:ASP:OD1	2.31	0.64
7:G:364:LEU:HD12	7:G:491:ASN:HB3	1.80	0.63
7:G:646:SER:O	7:G:649:SER:OG	2.14	0.63
7:G:475:GLN:O	7:G:479:THR:HG23	1.98	0.63
12:L:434:GLN:NE2	36:k:56:PHE:O	2.31	0.63
20:T:7:THR:HG22	20:T:10:GLY:N	2.12	0.63
9:I:32:ARG:NH2	25:Z:26:PRO:O	2.31	0.63
5:E:147:ALA:HB3	5:E:153:MET:HE3	1.80	0.63
12:L:87:MET:HA	12:L:87:MET:HE2	1.79	0.63
6:F:154:ARG:HA	44:s:58:LEU:HD21	1.79	0.63
13:M:23:ILE:HD11	13:M:92:LYS:HD3	1.81	0.63
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.33	0.62
15:O:126:ARG:NH2	15:O:206:TYR:OH	2.32	0.62
5:E:105:THR:HG22	5:E:106:THR:H	1.65	0.62
17:Q:10:LEU:HD13	22:W:16:SER:OG	1.98	0.62
37:l:18:GLU:N	37:l:18:GLU:OE1	2.33	0.62
10:J:106:TYR:O	10:J:109:LYS:N	2.32	0.62
19:S:94:LEU:O	19:S:95:SER:OG	2.16	0.62
8:H:21:THR:HG21	51:H:701:CHD:C18	2.30	0.61
29:d:1:AME:C	29:d:3:THR:H	2.13	0.61
33:h:140:THR:OG1	33:h:143:ASN:ND2	2.34	0.61
14:N:214:THR:HG22	14:N:218:MET:HE2	1.83	0.61
13:M:42:MET:HE1	32:g:77:VAL:HG22	1.82	0.60
20:U:55:GLU:O	20:U:59:GLY:N	2.35	0.60
31:f:30:ASN:ND2	31:f:30:ASN:O	2.34	0.60
12:L:108:MET:O	12:L:114:ILE:HD13	2.02	0.60
10:J:110:ASP:OD1	10:J:122:LEU:HD11	2.01	0.60
13:M:23:ILE:HD11	13:M:92:LYS:CD	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:273:SER:HB2	16:P:274:PRO:HD2	1.84	0.59
23:X:89:ASP:OD2	26:a:63:SER:OG	2.13	0.59
29:d:120:ARG:O	38:m:108:ARG:NH2	2.35	0.59
3:C:195:ARG:NH1	9:I:84:GLU:OE2	2.35	0.59
10:J:94:VAL:O	10:J:95:THR:OG1	2.14	0.59
11:K:37:MET:HG3	11:K:67:ALA:CB	2.32	0.59
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.34	0.59
3:C:129:TRP:CZ3	4:D:80:ILE:HD13	2.38	0.59
7:G:140:LYS:O	7:G:148:THR:OG1	2.20	0.59
7:G:107:ILE:HG23	9:I:78:ILE:HD12	1.84	0.59
11:K:37:MET:HG3	11:K:67:ALA:HB1	1.85	0.59
14:N:237:THR:O	14:N:237:THR:HG23	2.02	0.59
41:p:43:PRO:O	41:p:47:VAL:HG23	2.02	0.59
10:J:167:VAL:HG22	14:N:42:PRO:HG3	1.85	0.59
15:O:71:VAL:HG22	15:O:76:ASN:HA	1.85	0.59
22:W:96:VAL:HG12	22:W:96:VAL:O	2.03	0.58
53:M:701:U10:H551	14:N:263:LYS:HB2	1.84	0.58
30:e:95:PRO:O	30:e:96:HIS:CD2	2.55	0.58
38:m:75:ILE:O	38:m:75:ILE:HG22	2.03	0.58
34:i:50:LEU:HD11	34:i:61:TYR:HB2	1.86	0.58
10:J:126:VAL:HG21	30:e:72:MET:SD	2.44	0.58
25:Z:93:GLU:OE1	30:e:91:TYR:OH	2.08	0.58
53:M:701:U10:H551	14:N:263:LYS:CB	2.33	0.57
23:X:43:MET:HE3	23:X:47:TRP:CH2	2.39	0.57
13:M:119:TYR:OH	53:M:701:U10:H502	2.05	0.57
13:M:266:LEU:HA	13:M:269:MET:HE2	1.85	0.57
6:F:224:ASN:ND2	49:F:501:FMN:O2	2.33	0.57
15:O:207:LYS:HA	15:O:211:LEU:HD12	1.85	0.57
35:j:61:ASP:O	35:j:65:GLY:N	2.38	0.57
15:O:15:THR:OG1	15:O:253:ASP:OD1	2.18	0.57
37:l:59:ASP:OD1	37:l:62:TYR:N	2.37	0.57
10:J:6:VAL:HG11	10:J:47:PHE:HE1	1.69	0.57
20:U:72:CYS:N	20:U:75:GLU:OE1	2.38	0.57
21:V:34:LEU:HD13	21:V:48:GLU:HG3	1.87	0.57
13:M:342:MET:HE1	13:M:409:TYR:CE2	2.39	0.56
14:N:313:MET:HE1	15:O:102:ALA:HB3	1.86	0.56
7:G:329:ILE:HD11	7:G:626:VAL:HG21	1.88	0.56
8:H:236:ILE:HG23	8:H:259:PHE:HZ	1.70	0.56
11:K:44:ALA:HB1	11:K:59:MET:HE1	1.87	0.56
23:X:150:ASN:OD1	30:e:50:ARG:NH2	2.36	0.56
25:Z:127:LEU:O	30:e:97:HIS:NE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:453:LEU:HD21	7:G:458:LEU:HD21	1.86	0.56
16:P:203:GLN:N	16:P:291:ASP:OD2	2.32	0.56
14:N:108:MET:SD	14:N:191:THR:HG21	2.46	0.56
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.88	0.56
8:H:134:ARG:NH2	8:H:204:GLU:OE1	2.39	0.56
34:i:53:GLY:O	34:i:54:ALA:HB3	2.06	0.56
4:D:167:PHE:CE1	4:D:171:PHE:CE2	2.93	0.55
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.87	0.55
32:g:111:ASN:OD1	41:p:161:ARG:NH2	2.34	0.55
34:i:1:SAC:O	34:i:2:GLY:O	2.23	0.55
40:o:17:ASP:OD2	40:o:20:ARG:N	2.35	0.55
5:E:55:GLN:O	5:E:59:GLY:N	2.36	0.55
16:P:92:ILE:HD11	16:P:218:ILE:HD11	1.87	0.55
15:O:30:ASN:OD1	15:O:31:ILE:HD12	2.06	0.55
45:M:702:3PE:O14	45:N:401:3PE:N	2.30	0.55
14:N:7:ILE:HD11	52:N:403:CDL:HB62	1.89	0.55
43:r:2:SER:O	52:r:201:CDL:O1	2.22	0.55
12:L:14:LEU:HD13	34:i:73:HIS:O	2.07	0.55
15:O:31:ILE:HD12	15:O:31:ILE:H	1.72	0.55
7:G:46:LEU:O	17:Q:116:LYS:NZ	2.37	0.55
7:G:107:ILE:CG2	9:I:78:ILE:HD12	2.37	0.55
18:R:52:VAL:O	18:R:94:GLN:N	2.37	0.55
41:p:131:PHE:O	41:p:135:VAL:HG23	2.07	0.55
45:M:702:3PE:H232	29:d:54:LEU:HD21	1.89	0.55
8:H:24:GLU:OE2	8:H:274:ARG:NH1	2.40	0.54
4:D:151:ILE:O	4:D:155:THR:OG1	2.19	0.54
13:M:149:PHE:HE2	53:M:701:U10:H8	1.73	0.54
31:f:39:ASN:N	33:h:88:GLU:OE1	2.40	0.54
34:i:89:VAL:O	34:i:95:THR:OG1	2.15	0.54
16:P:185:ILE:HD12	16:P:278:TRP:HE3	1.71	0.54
46:d:201:PC1:O13	46:d:201:PC1:H143	2.07	0.54
6:F:136:ILE:HD13	6:F:149:LEU:HD21	1.90	0.54
5:E:156:ILE:HD13	5:E:161:TYR:HE2	1.69	0.53
8:H:5:ASN:ND2	8:H:5:ASN:O	2.41	0.53
11:K:1:FME:O	11:K:3:MET:N	2.41	0.53
12:L:230:HIS:N	12:L:231:PRO:CD	2.71	0.53
14:N:267:ILE:O	14:N:271:THR:HG23	2.08	0.53
8:H:277:TYR:OH	9:I:30:LEU:O	2.21	0.53
13:M:6:ILE:HD12	31:f:23:GLY:HA2	1.90	0.53
15:O:29:GLY:O	15:O:126:ARG:NH2	2.40	0.53
21:V:68:GLU:OE1	21:V:76:ILE:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.38	0.53
34:i:108:THR:O	41:p:18:ALA:N	2.38	0.53
13:M:113:MET:HG2	13:M:175:ASN:OD1	2.09	0.53
13:M:403:THR:HA	13:M:406:TYR:CE1	2.44	0.53
4:D:335:ARG:NH2	9:I:129:ASP:OD1	2.42	0.52
12:L:411:MET:N	12:L:411:MET:HE2	2.24	0.52
1:A:73:LEU:HD13	10:J:55:MET:HE1	1.91	0.52
1:A:114:THR:HG23	8:H:287:HIS:HA	1.91	0.52
5:E:217:LEU:HD11	6:F:48:ILE:HG12	1.90	0.52
13:M:66:LEU:HD11	13:M:111:THR:CG2	2.40	0.52
4:D:134:ALA:HB2	4:D:323:ILE:O	2.09	0.52
32:g:48:ASP:OD1	32:g:49:LYS:N	2.42	0.52
6:F:344:VAL:HG12	6:F:380:VAL:HG22	1.91	0.52
6:F:197:GLU:OE2	6:F:216:PHE:N	2.41	0.52
13:M:343:ILE:HD11	37:l:69:LEU:HD21	1.91	0.52
20:T:69:LYS:O	20:T:71:MET:N	2.42	0.52
12:L:248:HIS:CD2	12:L:252:MET:HE1	2.44	0.52
7:G:45:ARG:NE	7:G:261:GLU:OE2	2.38	0.52
12:L:371:THR:O	12:L:375:VAL:HG23	2.10	0.52
12:L:426:ILE:O	12:L:430:ALA:HB3	2.10	0.52
1:A:56:PHE:HB2	10:J:74:MET:HE1	1.92	0.51
5:E:53:LEU:HD13	44:s:52:LEU:CD1	2.40	0.51
6:F:193:ILE:HG23	6:F:215:VAL:HA	1.92	0.51
15:O:133:VAL:HG11	15:O:206:TYR:CE1	2.45	0.51
25:Z:125:TYR:HB3	25:Z:133:VAL:HG22	1.92	0.51
34:i:50:LEU:HD11	34:i:61:TYR:CG	2.46	0.51
39:n:34:ASP:OD1	39:n:35:LYS:N	2.44	0.51
41:p:127:GLU:OE2	41:p:127:GLU:N	2.39	0.51
2:B:69:MET:HE3	2:B:76:PHE:HA	1.91	0.51
8:H:224:PHE:CE2	51:H:701:CHD:H193	2.45	0.51
12:L:97:THR:HG23	12:L:246:LEU:HD11	1.92	0.51
25:Z:143:TYR:O	25:Z:144:THR:C	2.53	0.51
36:k:42:ASP:OD2	36:k:45:GLY:N	2.43	0.51
4:D:171:PHE:CD1	4:D:174:ARG:HD3	2.46	0.51
29:d:112:VAL:HG21	41:p:78:GLU:OE2	2.10	0.51
3:C:191:ALA:O	17:Q:74:SER:OG	2.24	0.51
5:E:217:LEU:HD11	6:F:48:ILE:CG1	2.41	0.51
2:B:79:SER:O	2:B:83:SER:OG	2.24	0.51
20:T:28:GLU:OE1	20:T:28:GLU:N	2.43	0.51
13:M:127:VAL:HB	13:M:128:PRO:HD3	1.92	0.51
12:L:369:THR:OG1	12:L:445:GLU:OE1	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:145:TYR:CD2	16:P:286:ARG:HD3	2.46	0.51
20:T:7:THR:O	20:T:10:GLY:N	2.43	0.51
1:A:68:GLU:HG2	10:J:161:LEU:HD13	1.92	0.51
29:d:1:AME:O	33:h:123:PHE:N	2.25	0.51
3:C:183:VAL:O	22:W:101:THR:OG1	2.30	0.51
13:M:234:VAL:O	13:M:237:LYS:N	2.41	0.51
33:h:110:VAL:CG1	33:h:114:MET:HE3	2.42	0.51
1:A:13:LEU:CD2	8:H:10:ILE:HG21	2.41	0.50
8:H:102:VAL:HG11	8:H:154:LEU:HD11	1.93	0.50
16:P:97:ARG:HE	56:P:501:NDP:H8A	1.74	0.50
33:h:128:ILE:HD12	33:h:128:ILE:H	1.75	0.50
7:G:366:THR:HB	7:G:450:MET:HE3	1.92	0.50
10:J:123:GLY:O	10:J:126:VAL:HG22	2.12	0.50
25:Z:127:LEU:O	30:e:97:HIS:CD2	2.64	0.50
12:L:537:ALA:HB3	12:L:538:PRO:HD3	1.94	0.50
7:G:449:PRO:HG3	7:G:477:ILE:HG21	1.94	0.50
7:G:703:ILE:HD12	7:G:703:ILE:H	1.77	0.50
11:K:53:PHE:HD2	11:K:56:ALA:HB3	1.76	0.50
38:m:126:ILE:HD12	41:p:138:TYR:CD1	2.46	0.50
42:q:144:TYR:O	42:q:145:LYS:HE2	2.12	0.50
11:K:33:LEU:HD12	11:K:36:MET:HE3	1.94	0.49
4:D:62:LEU:HD13	4:D:425:PHE:CZ	2.47	0.49
1:A:60:ILE:HG21	10:J:168:ILE:HG21	1.95	0.49
12:L:525:LEU:HD21	39:n:76:PRO:HB3	1.95	0.49
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.46	0.49
13:M:187:HIS:O	13:M:192:ASN:ND2	2.44	0.49
25:Z:120:MET:SD	30:e:71:THR:HG21	2.52	0.49
6:F:93:LEU:HD13	6:F:129:MET:CE	2.42	0.49
6:F:115:PRO:O	6:F:119:VAL:HG23	2.12	0.49
11:K:37:MET:SD	11:K:67:ALA:CB	3.01	0.49
13:M:12:MET:HB2	13:M:13:PRO:HD3	1.94	0.49
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.94	0.49
20:U:11:ILE:HD11	20:U:86:VAL:HG21	1.93	0.49
4:D:55:HIS:NE2	4:D:57:ALA:HB2	2.28	0.49
5:E:100:ILE:HD11	5:E:137:PHE:CD1	2.48	0.49
5:E:156:ILE:HD13	5:E:161:TYR:CD2	2.48	0.49
10:J:43:ILE:HG22	11:K:46:LEU:HD11	1.95	0.49
2:B:30:VAL:HG13	2:B:173:LEU:HB3	1.94	0.49
8:H:108:MET:HE1	46:J:201:PC1:H361	1.94	0.49
10:J:97:LEU:HG	10:J:99:MET:HG2	1.94	0.49
38:m:17:LEU:HD11	39:n:71:TRP:CG	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:120:LEU:HD11	4:D:275:TYR:CD2	2.48	0.49
8:H:266:LEU:O	8:H:269:SER:OG	2.28	0.49
37:l:69:LEU:HD23	37:l:71:LEU:HD12	1.94	0.49
38:m:2:PHE:O	38:m:2:PHE:CD2	2.66	0.49
4:D:328:ALA:HB3	7:G:126:ASP:HB2	1.94	0.49
12:L:149:ILE:HG13	13:M:369:LEU:HD13	1.93	0.49
10:J:127:ILE:CD1	11:K:1:FME:HE3	2.43	0.48
12:L:102:GLU:OE2	12:L:456:ARG:NH1	2.42	0.48
2:B:51:GLY:HA2	2:B:56:ALA:HB2	1.95	0.48
4:D:417:ILE:O	4:D:420:THR:HG22	2.13	0.48
8:H:14:LEU:HD22	8:H:225:MET:HE2	1.94	0.48
8:H:221:ALA:HB1	51:H:701:CHD:H213	1.93	0.48
46:M:703:PC1:O13	46:M:703:PC1:H132	2.13	0.48
34:i:50:LEU:HD11	34:i:61:TYR:CB	2.43	0.48
1:A:51:PHE:CE1	10:J:74:MET:HE2	2.49	0.48
29:d:1:AME:C	29:d:3:THR:N	2.76	0.48
4:D:80:ILE:O	4:D:80:ILE:HG13	2.13	0.48
19:S:21:HIS:O	19:S:62:PRO:HA	2.14	0.48
2:B:64:ALA:HB1	2:B:65:PRO:HD2	1.96	0.48
38:m:126:ILE:HD12	41:p:138:TYR:HD1	1.79	0.48
23:X:77:CYS:O	23:X:77:CYS:SG	2.72	0.48
37:l:7:ASP:OD1	37:l:8:MET:N	2.46	0.48
20:T:6:LEU:HB3	20:T:86:VAL:HG12	1.96	0.48
1:A:30:TYR:OH	2:B:41:ARG:NH2	2.47	0.48
6:F:82:MET:HG3	6:F:221:THR:OG1	2.14	0.48
8:H:224:PHE:CZ	51:H:701:CHD:H193	2.48	0.48
34:i:104:PHE:N	34:i:107:ASP:OD2	2.46	0.48
1:A:90:MET:SD	10:J:151:THR:HG23	2.53	0.48
9:I:145:GLU:OE1	9:I:145:GLU:N	2.41	0.48
15:O:133:VAL:HG11	15:O:206:TYR:CD1	2.49	0.48
15:O:135:LEU:HD22	15:O:152:TYR:CG	2.49	0.47
5:E:131:THR:HG23	5:E:137:PHE:O	2.14	0.47
10:J:115:VAL:O	10:J:117:PHE:N	2.43	0.47
18:R:55:ARG:NH1	18:R:76:ASP:OD1	2.47	0.47
20:T:16:LEU:HD13	20:T:30:LEU:HD21	1.96	0.47
5:E:145:LEU:HD12	5:E:153:MET:SD	2.55	0.47
6:F:95:VAL:HG11	6:F:118:LEU:HD11	1.96	0.47
6:F:274:VAL:HG11	6:F:279:LEU:HD13	1.97	0.47
24:Y:86:PRO:O	24:Y:90:LEU:N	2.43	0.47
38:m:78:ASN:OD1	38:m:79:PHE:N	2.47	0.47
12:L:427:ILE:HG23	12:L:431:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:207:ILE:HG22	14:N:211:MET:HE2	1.96	0.47
5:E:159:ASN:HB3	5:E:184:PRO:HB3	1.97	0.47
20:U:14:ARG:NH2	20:U:57:GLU:O	2.47	0.47
10:J:108:LEU:O	10:J:109:LYS:C	2.57	0.47
52:L:702:CDL:OA9	33:h:26:ARG:NH2	2.48	0.47
13:M:422:HIS:HB2	38:m:59:ILE:HD12	1.97	0.47
14:N:89:LEU:HD12	14:N:95:SER:HA	1.97	0.47
29:d:39:TYR:CD1	29:d:65:ILE:HD11	2.43	0.47
39:n:18:LEU:HD13	39:n:67:GLU:OE1	2.15	0.47
8:H:179:TRP:N	8:H:180:PRO:CD	2.78	0.46
1:A:69:ILE:HD12	8:H:148:ILE:HG12	1.97	0.46
4:D:201:GLN:C	4:D:323:ILE:HD13	2.40	0.46
37:l:96:VAL:HG12	37:l:97:ASN:N	2.31	0.46
8:H:236:ILE:HG23	8:H:259:PHE:CZ	2.50	0.46
8:H:310:LEU:HD12	8:H:311:THR:HG23	1.98	0.46
21:V:29:LYS:O	21:V:33:VAL:HG23	2.16	0.46
21:V:8:THR:OG1	21:V:13:LEU:O	2.27	0.46
37:l:53:ARG:NE	37:l:57:GLU:OE1	2.49	0.46
6:F:322:LEU:HD12	6:F:329:LEU:HA	1.96	0.46
10:J:68:PHE:CE2	11:K:31:LEU:HD21	2.51	0.46
12:L:419:THR:HA	12:L:422:TYR:CE1	2.51	0.46
39:n:100:GLU:OE1	39:n:121:ARG:NH1	2.42	0.46
12:L:114:ILE:HD11	12:L:118:PHE:HE1	1.81	0.46
13:M:152:TYR:O	13:M:156:GLY:N	2.48	0.46
14:N:347:GLU:HB2	29:d:82:MET:HE2	1.98	0.46
15:O:133:VAL:HG23	15:O:134:PHE:N	2.31	0.46
10:J:18:VAL:HG21	10:J:100:GLU:HG2	1.98	0.46
13:M:130:LEU:HD21	13:M:149:PHE:CZ	2.51	0.46
17:Q:89:LYS:HD3	17:Q:105:VAL:HG11	1.97	0.46
18:R:52:VAL:HG22	18:R:92:ARG:O	2.16	0.46
7:G:521:MET:HE2	7:G:523:PHE:CZ	2.51	0.45
14:N:115:VAL:HB	14:N:116:PRO:HD3	1.98	0.45
15:O:45:LYS:CB	15:O:235:VAL:HG21	2.46	0.45
1:A:114:THR:HG21	8:H:291:LYS:HE3	1.96	0.45
2:B:125:TYR:HB2	9:I:117:ILE:HG21	1.98	0.45
2:B:125:TYR:CE2	4:D:102:TYR:CD1	3.04	0.45
7:G:190:MET:HG3	7:G:695:ALA:HB1	1.98	0.45
7:G:244:THR:HB	17:Q:73:ALA:HB2	1.98	0.45
10:J:167:VAL:HG13	14:N:42:PRO:HG3	1.98	0.45
15:O:147:GLN:OE1	15:O:147:GLN:N	2.45	0.45
1:A:13:LEU:HD22	8:H:10:ILE:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:289:LEU:C	8:H:289:LEU:HD23	2.41	0.45
12:L:383:MET:HB3	12:L:386:LEU:HD12	1.98	0.45
37:l:42:THR:HG21	37:l:44:TYR:CE2	2.51	0.45
39:n:169:ILE:HD12	39:n:169:ILE:H	1.81	0.45
4:D:208:MET:HE1	25:Z:11:PRO:HD3	1.98	0.45
15:O:45:LYS:HB3	15:O:235:VAL:HG21	1.99	0.45
20:U:75:GLU:OE2	34:i:8:LYS:NZ	2.49	0.45
39:n:8:TYR:O	39:n:9:LEU:CB	2.64	0.45
6:F:376:MET:O	6:F:380:VAL:HG23	2.17	0.45
16:P:274:PRO:O	16:P:275:PHE:HB2	2.15	0.45
23:X:44:LEU:HD22	23:X:130:VAL:HG13	1.98	0.45
34:i:126:HIS:O	34:i:127:HIS:C	2.59	0.45
35:j:11:TYR:HB2	36:k:13:MET:HE3	1.99	0.45
35:j:36:ILE:CG2	35:j:40:PHE:HE2	2.29	0.45
26:a:57:VAL:O	26:a:58:ASN:HB3	2.17	0.45
13:M:285:LEU:HD23	13:M:285:LEU:C	2.42	0.45
15:O:266:LYS:O	15:O:269:VAL:HG22	2.15	0.45
22:W:124:VAL:HG23	22:W:125:GLY:N	2.32	0.45
11:K:40:LEU:HD13	14:N:71:MET:HG3	1.99	0.45
12:L:249:SER:HA	12:L:306:THR:HG21	1.99	0.45
12:L:331:THR:HB	12:L:387:THR:HG22	1.99	0.45
7:G:475:GLN:NE2	7:G:479:THR:HG21	2.31	0.45
9:I:105:ARG:NH2	18:R:86:TYR:O	2.50	0.45
13:M:5:ILE:HG23	13:M:104:LEU:HD11	1.99	0.45
30:e:94:PRO:O	30:e:96:HIS:O	2.35	0.45
40:o:27:ASP:O	40:o:29:GLY:N	2.50	0.45
4:D:161:ILE:O	4:D:161:ILE:CG2	2.63	0.45
8:H:87:ILE:HG12	8:H:88:PRO:HD3	1.98	0.45
10:J:126:VAL:O	25:Z:122:GLY:N	2.49	0.45
36:k:23:ILE:O	36:k:26:THR:OG1	2.25	0.45
12:L:248:HIS:HD2	12:L:252:MET:HE1	1.81	0.44
4:D:49:LEU:C	4:D:49:LEU:HD23	2.42	0.44
4:D:148:LEU:HD23	4:D:174:ARG:HG2	1.98	0.44
7:G:266:LYS:NZ	7:G:674:THR:OG1	2.45	0.44
8:H:189:THR:HG22	8:H:234:MET:HE2	1.99	0.44
10:J:126:VAL:HG23	10:J:127:ILE:HG23	1.99	0.44
12:L:137:LEU:HD21	12:L:263:PHE:HZ	1.82	0.44
12:L:359:MET:O	12:L:436:ARG:CZ	2.66	0.44
15:O:279:LEU:HD23	15:O:281:GLU:H	1.82	0.44
31:f:2:ASN:OD1	31:f:2:ASN:O	2.35	0.44
13:M:42:MET:HE1	32:g:77:VAL:CG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:m:75:ILE:O	38:m:75:ILE:CG2	2.66	0.44
1:A:95:ILE:HG21	8:H:302:MET:HG3	1.98	0.44
15:O:130:SER:O	15:O:133:VAL:HG22	2.17	0.44
31:f:4:LEU:H	31:f:4:LEU:HD12	1.82	0.44
1:A:12:THR:O	1:A:16:LEU:HD23	2.17	0.44
3:C:148:LEU:O	22:W:88:MET:HE2	2.18	0.44
16:P:323:THR:HG22	16:P:324:TYR:HD1	1.83	0.44
20:U:3:ALA:C	20:U:5:PRO:HD3	2.43	0.44
23:X:33:ALA:HB2	23:X:119:PRO:HG3	1.99	0.44
7:G:449:PRO:O	7:G:487:TRP:NE1	2.36	0.44
8:H:208:VAL:O	8:H:208:VAL:HG13	2.17	0.44
12:L:40:ILE:HD12	12:L:40:ILE:H	1.82	0.44
12:L:476:THR:HG22	40:o:53:GLN:NE2	2.32	0.44
12:L:529:PHE:HB3	12:L:530:PRO:HD3	2.00	0.44
24:Y:123:LEU:HD23	24:Y:126:MET:CE	2.47	0.44
30:e:40:ILE:HB	33:h:133:ILE:HD11	1.99	0.44
12:L:132:VAL:O	12:L:262:ARG:NH1	2.43	0.44
13:M:271:MET:HE2	13:M:271:MET:HA	2.00	0.44
34:i:53:GLY:O	34:i:54:ALA:CB	2.66	0.44
2:B:44:SER:OG	8:H:51:ASP:OD1	2.26	0.44
26:a:67:GLU:OE1	26:a:67:GLU:N	2.44	0.44
41:p:105:ILE:HG13	41:p:134:VAL:HG21	2.00	0.44
4:D:151:ILE:HG23	4:D:170:MET:HB3	2.00	0.44
6:F:94:VAL:HG11	6:F:192:LEU:HD22	2.00	0.44
16:P:149:LYS:NZ	56:P:501:NDP:O2D	2.41	0.44
20:T:6:LEU:HD13	20:T:86:VAL:HA	2.00	0.44
23:X:43:MET:O	23:X:47:TRP:HE3	2.01	0.44
52:h:201:CDL:H592	41:p:47:VAL:HG21	1.99	0.44
39:n:15:VAL:HG22	39:n:63:LEU:HD13	2.00	0.44
16:P:26:ALA:HB3	16:P:47:VAL:HG13	1.99	0.43
23:X:14:VAL:HG22	23:X:15:GLN:H	1.83	0.43
12:L:136:ASN:HB3	12:L:197:ASP:OD1	2.17	0.43
16:P:185:ILE:HD12	16:P:278:TRP:CE3	2.50	0.43
58:T:101:EHZ:O3	22:W:32:VAL:HG21	2.18	0.43
4:D:293:CYS:SG	4:D:420:THR:HG21	2.58	0.43
9:I:162:GLU:HB3	42:q:109:ILE:HG12	2.00	0.43
13:M:47:ASP:OD1	13:M:48:ASN:N	2.51	0.43
14:N:136:LEU:HD11	52:N:403:CDL:H212	2.00	0.43
14:N:296:LEU:C	14:N:296:LEU:HD23	2.43	0.43
15:O:204:ASN:O	15:O:208:GLY:N	2.51	0.43
38:m:50:TYR:HA	38:m:59:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:141:SER:O	8:H:289:LEU:HD11	2.17	0.43
16:P:113:ILE:HB	16:P:114:PRO:HD3	2.00	0.43
6:F:192:LEU:HD23	6:F:192:LEU:O	2.18	0.43
10:J:17:PHE:HA	10:J:20:PHE:CE1	2.53	0.43
12:L:12:LEU:O	12:L:16:THR:HG23	2.18	0.43
14:N:193:VAL:O	14:N:193:VAL:HG22	2.18	0.43
25:Z:5:LYS:O	25:Z:6:VAL:C	2.60	0.43
33:h:114:MET:O	33:h:118:GLY:N	2.41	0.43
2:B:64:ALA:HB1	2:B:65:PRO:CD	2.48	0.43
8:H:18:ALA:O	8:H:21:THR:OG1	2.36	0.43
10:J:122:LEU:HD13	30:e:79:ARG:HH12	1.82	0.43
11:K:53:PHE:CE2	11:K:56:ALA:HB2	2.53	0.43
33:h:6:LYS:HD2	33:h:6:LYS:O	2.19	0.43
3:C:154:ASP:OD1	3:C:155:TYR:N	2.52	0.43
12:L:173:LEU:HD23	45:L:701:3PE:C24	2.48	0.43
13:M:378:GLU:O	13:M:382:VAL:HG23	2.19	0.43
14:N:206:ILE:HD11	46:d:201:PC1:H351	2.01	0.43
33:h:47:ILE:HD12	33:h:47:ILE:H	1.83	0.43
34:i:40:SER:OG	34:i:41:PRO:HD2	2.18	0.43
3:C:6:ASP:OD2	3:C:8:ARG:HG3	2.18	0.43
9:I:84:GLU:HB2	9:I:94:ILE:HD12	2.00	0.43
53:M:701:U10:H4M2	53:M:701:U10:H3M3	2.01	0.43
15:O:307:GLY:O	15:O:320:LYS:NZ	2.42	0.43
42:q:145:LYS:HE2	42:q:145:LYS:HA	2.00	0.43
10:J:102:PHE:C	10:J:104:VAL:H	2.26	0.43
11:K:37:MET:HE3	11:K:37:MET:HB3	1.94	0.43
12:L:264:TYR:N	12:L:265:PRO:CD	2.82	0.43
21:V:5:LYS:NZ	21:V:77:GLU:OE2	2.34	0.43
40:o:82:GLU:OE1	40:o:82:GLU:N	2.49	0.43
5:E:172:ILE:HG23	5:E:182:PRO:HG2	2.01	0.43
7:G:654:GLN:OE1	7:G:654:GLN:N	2.52	0.43
14:N:146:PHE:HA	14:N:149:ILE:HD12	2.01	0.43
2:B:91:THR:HA	2:B:119:CYS:HB3	2.01	0.42
7:G:358:LEU:HD23	7:G:641:TYR:HB2	2.02	0.42
8:H:87:ILE:N	8:H:88:PRO:CD	2.82	0.42
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.01	0.42
11:K:53:PHE:CD2	11:K:56:ALA:HB3	2.53	0.42
16:P:194:ILE:O	16:P:256:TYR:CE2	2.72	0.42
22:W:28:ALA:O	22:W:32:VAL:HG23	2.19	0.42
23:X:44:LEU:HD22	23:X:130:VAL:CG1	2.49	0.42
37:l:68:ASP:N	37:l:68:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:ILE:HB	3:C:59:PRO:HD3	2.01	0.42
4:D:326:ASP:OD1	7:G:127:ARG:NH2	2.52	0.42
12:L:363:PHE:CD2	12:L:370:THR:HG21	2.54	0.42
2:B:60:MET:SD	4:D:58:ALA:HB3	2.60	0.42
5:E:105:THR:HG22	5:E:106:THR:N	2.31	0.42
5:E:106:THR:HB	5:E:107:PRO:HD3	2.00	0.42
10:J:11:VAL:HG21	10:J:106:TYR:OH	2.20	0.42
15:O:22:SER:O	15:O:23:LYS:HE2	2.20	0.42
22:W:72:HIS:O	22:W:74:THR:HG23	2.19	0.42
10:J:57:PHE:CD1	10:J:61:LEU:HD12	2.54	0.42
12:L:4:PHE:HD2	12:L:61:LEU:HD12	1.85	0.42
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.55	0.42
13:M:266:LEU:HD23	13:M:269:MET:HE2	2.01	0.42
14:N:19:ILE:O	14:N:23:SER:OG	2.29	0.42
7:G:415:LEU:O	7:G:416:THR:OG1	2.31	0.42
12:L:445:GLU:OE2	35:j:21:GLN:NE2	2.53	0.42
2:B:152:THR:HG22	4:D:188:ARG:HD3	2.02	0.42
3:C:114:LEU:CD2	22:W:81:LEU:HD12	2.49	0.42
8:H:134:ARG:NH1	8:H:208:VAL:HG11	2.34	0.42
8:H:250:HIS:O	8:H:251:MET:HE2	2.19	0.42
10:J:109:LYS:O	10:J:110:ASP:HB2	2.20	0.42
15:O:194:ILE:HD11	15:O:198:TYR:HD2	1.84	0.42
33:h:5:GLY:O	33:h:6:LYS:HG3	2.20	0.42
33:h:110:VAL:HG12	33:h:114:MET:HE3	2.02	0.42
36:k:14:GLU:O	36:k:14:GLU:HG2	2.18	0.42
40:o:75:ASN:OD1	40:o:78:ALA:N	2.53	0.42
42:q:94:THR:OG1	42:q:95:ASP:N	2.53	0.42
6:F:342:ASP:OD1	6:F:429:ARG:NH1	2.53	0.42
6:F:403:THR:HB	47:F:502:SF4:S4	2.60	0.42
11:K:59:MET:HE2	14:N:84:TRP:HH2	1.85	0.42
29:d:1:AME:HG1	29:d:2:MET:N	2.34	0.42
33:h:34:ILE:HB	33:h:35:PRO:HD3	2.00	0.42
36:k:31:VAL:HG13	39:n:38:TYR:HB2	2.01	0.42
12:L:82:MET:HE3	12:L:87:MET:HE3	2.01	0.42
14:N:336:MET:CE	45:N:402:3PE:H2I3	2.50	0.42
3:C:77:ASP:OD1	3:C:78:LEU:N	2.53	0.42
25:Z:122:GLY:O	25:Z:126:GLY:CA	2.68	0.42
4:D:107:ASP:OD1	4:D:109:VAL:HG22	2.20	0.41
7:G:483:VAL:HG12	7:G:484:THR:N	2.35	0.41
11:K:59:MET:HB3	11:K:60:PRO:HD3	2.02	0.41
14:N:221:ALA:HB2	14:N:323:MET:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:91:ILE:H	24:Y:91:ILE:HD12	1.85	0.41
42:q:37:THR:O	42:q:49:TYR:HA	2.20	0.41
1:A:93:PHE:CZ	1:A:97:LEU:HD11	2.55	0.41
6:F:103:GLY:O	6:F:333:ALA:HB1	2.20	0.41
6:F:322:LEU:HD12	6:F:329:LEU:CA	2.50	0.41
12:L:424:THR:O	12:L:427:ILE:N	2.53	0.41
16:P:191:VAL:CG1	16:P:192:PRO:HD2	2.50	0.41
37:l:16:THR:HG23	37:l:19:GLU:H	1.84	0.41
1:A:28:ASN:C	1:A:29:VAL:HG22	2.45	0.41
1:A:65:PHE:O	1:A:69:ILE:HG12	2.21	0.41
10:J:49:GLY:HA2	10:J:139:GLU:OE1	2.20	0.41
10:J:103:MET:O	10:J:107:VAL:HG23	2.20	0.41
37:l:128:VAL:HG11	40:o:94:TYR:CZ	2.55	0.41
7:G:106:PRO:HB2	9:I:78:ILE:HD11	2.02	0.41
7:G:489:VAL:O	7:G:491:ASN:ND2	2.53	0.41
10:J:56:VAL:O	10:J:60:TYR:HB3	2.21	0.41
31:f:2:ASN:OD1	31:f:4:LEU:O	2.39	0.41
2:B:48:MET:CE	4:D:53:PRO:HA	2.51	0.41
6:F:118:LEU:HD13	6:F:225:VAL:HG13	2.01	0.41
7:G:194:GLU:OE1	7:G:194:GLU:N	2.38	0.41
9:I:175:TYR:CZ	43:r:38:PRO:HG3	2.55	0.41
10:J:117:PHE:CZ	14:N:93:MET:HG2	2.55	0.41
10:J:167:VAL:HG22	14:N:42:PRO:CG	2.49	0.41
12:L:10:VAL:O	12:L:14:LEU:N	2.46	0.41
13:M:447:LEU:CD2	13:M:453:ILE:HD11	2.51	0.41
16:P:207:ILE:HG23	16:P:208:VAL:N	2.35	0.41
34:i:122:PHE:C	34:i:124:ASP:H	2.29	0.41
39:n:8:TYR:O	39:n:9:LEU:HB2	2.20	0.41
11:K:53:PHE:CD2	11:K:56:ALA:CB	3.04	0.41
14:N:198:PRO:HD2	29:d:1:AME:OT	2.20	0.41
16:P:185:ILE:HG21	16:P:279:THR:OG1	2.21	0.41
24:Y:85:ASP:HB2	24:Y:86:PRO:HD2	2.03	0.41
40:o:28:TYR:OH	40:o:110:ARG:NH1	2.54	0.41
8:H:224:PHE:CE1	51:H:701:CHD:H182	2.55	0.41
9:I:31:ILE:HD11	45:I:201:3PE:H2C2	2.03	0.41
13:M:80:SER:OG	13:M:226:ALA:HB2	2.21	0.41
14:N:146:PHE:N	14:N:147:PRO:CD	2.84	0.41
15:O:194:ILE:HD13	15:O:199:LEU:HD21	2.01	0.41
1:A:114:THR:HG23	8:H:287:HIS:CA	2.51	0.41
4:D:55:HIS:HB2	4:D:56:PRO:CD	2.51	0.41
8:H:189:THR:HG22	8:H:234:MET:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:55:GLY:O	15:O:56:ILE:C	2.64	0.41
15:O:96:LEU:C	15:O:96:LEU:HD23	2.46	0.41
29:d:1:AME:HG2	33:h:123:PHE:CE2	2.55	0.41
1:A:114:THR:HG21	8:H:291:LYS:CE	2.50	0.41
7:G:105:CYS:HB2	7:G:106:PRO:HD3	2.03	0.41
8:H:24:GLU:HA	8:H:271:LEU:HD13	2.03	0.41
11:K:37:MET:SD	11:K:67:ALA:HB1	2.61	0.41
12:L:140:LEU:HD21	12:L:259:LEU:CD1	2.51	0.41
13:M:175:ASN:HD22	13:M:178:MET:HG2	1.86	0.41
53:M:701:U10:H401	53:M:701:U10:C43	2.49	0.41
20:T:65:ILE:HG23	20:T:66:ASP:N	2.35	0.41
4:D:80:ILE:O	4:D:429:ASP:OD1	2.39	0.41
14:N:3:PRO:HB2	15:O:9:ILE:HD11	2.02	0.41
16:P:145:TYR:HB3	16:P:286:ARG:HD3	2.03	0.41
32:g:101:GLU:OE2	41:p:130:GLN:NE2	2.46	0.41
1:A:63:LEU:HB2	10:J:67:VAL:HG21	2.02	0.40
26:a:68:ASN:OD1	26:a:68:ASN:O	2.39	0.40
36:k:21:TRP:HB3	36:k:49:ALA:HB3	2.03	0.40
8:H:87:ILE:CG1	8:H:88:PRO:HD3	2.51	0.40
12:L:149:ILE:CG1	13:M:369:LEU:HD13	2.51	0.40
12:L:286:LEU:HD13	12:L:411:MET:SD	2.61	0.40
20:T:46:ASP:OD1	22:W:64:ARG:NH2	2.50	0.40
24:Y:86:PRO:HB2	24:Y:122:ALA:HB1	2.02	0.40
31:f:4:LEU:O	31:f:5:GLN:CB	2.69	0.40
7:G:26:VAL:HG22	7:G:73:VAL:HG12	2.03	0.40
10:J:36:SER:HA	10:J:39:VAL:HG22	2.03	0.40
10:J:112:GLU:HG3	10:J:121:GLY:N	2.35	0.40
12:L:233:LEU:HB3	12:L:234:PRO:HD3	2.02	0.40
13:M:158:LEU:HB3	13:M:159:PRO:HD3	2.03	0.40
13:M:264:LEU:O	13:M:268:GLY:N	2.54	0.40
23:X:77:CYS:O	23:X:78:ALA:C	2.65	0.40
34:i:75:LEU:O	34:i:78:VAL:HG12	2.20	0.40
1:A:114:THR:O	1:A:115:GLU:C	2.63	0.40
5:E:217:LEU:C	5:E:217:LEU:HD23	2.46	0.40
7:G:156:CYS:O	7:G:157:THR:OG1	2.31	0.40
13:M:71:TRP:CZ3	32:g:69:VAL:HG11	2.57	0.40
23:X:23:VAL:HG21	26:a:65:GLY:HA2	2.04	0.40
38:m:126:ILE:CG1	41:p:135:VAL:HG13	2.52	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	103/115 (90%)	97 (94%)	6 (6%)	0	100	100
2	B	156/216 (72%)	149 (96%)	7 (4%)	0	100	100
3	C	208/266 (78%)	202 (97%)	6 (3%)	0	100	100
4	D	385/463 (83%)	368 (96%)	17 (4%)	0	100	100
5	E	212/249 (85%)	204 (96%)	7 (3%)	1 (0%)	24	59
6	F	430/464 (93%)	410 (95%)	20 (5%)	0	100	100
7	G	698/727 (96%)	676 (97%)	22 (3%)	0	100	100
8	H	316/318 (99%)	301 (95%)	15 (5%)	0	100	100
9	I	174/212 (82%)	170 (98%)	4 (2%)	0	100	100
10	J	157/175 (90%)	144 (92%)	13 (8%)	0	100	100
11	K	84/98 (86%)	82 (98%)	2 (2%)	0	100	100
12	L	545/606 (90%)	515 (94%)	30 (6%)	0	100	100
13	M	457/459 (100%)	449 (98%)	7 (2%)	1 (0%)	43	75
14	N	345/347 (99%)	336 (97%)	9 (3%)	0	100	100
15	O	318/343 (93%)	309 (97%)	9 (3%)	0	100	100
16	P	314/380 (83%)	299 (95%)	14 (4%)	1 (0%)	36	68
17	Q	123/175 (70%)	122 (99%)	1 (1%)	0	100	100
18	R	94/124 (76%)	89 (95%)	5 (5%)	0	100	100
19	S	85/99 (86%)	84 (99%)	1 (1%)	0	100	100
20	T	82/156 (53%)	78 (95%)	4 (5%)	0	100	100
20	U	86/156 (55%)	81 (94%)	5 (6%)	0	100	100
21	V	111/116 (96%)	107 (96%)	4 (4%)	0	100	100
22	W	113/128 (88%)	108 (96%)	5 (4%)	0	100	100
23	X	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
24	Y	29/141 (21%)	26 (90%)	3 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Z	140/144 (97%)	136 (97%)	4 (3%)	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	46/76 (60%)	45 (98%)	1 (2%)	0	100	100
29	d	118/120 (98%)	116 (98%)	1 (1%)	1 (1%)	16	48
30	e	97/106 (92%)	93 (96%)	4 (4%)	0	100	100
31	f	55/57 (96%)	53 (96%)	2 (4%)	0	100	100
32	g	88/154 (57%)	84 (96%)	4 (4%)	0	100	100
33	h	141/189 (75%)	137 (97%)	4 (3%)	0	100	100
34	i	125/127 (98%)	119 (95%)	5 (4%)	1 (1%)	16	48
35	j	68/108 (63%)	66 (97%)	2 (3%)	0	100	100
36	k	79/98 (81%)	79 (100%)	0	0	100	100
37	l	154/186 (83%)	144 (94%)	10 (6%)	0	100	100
38	m	125/129 (97%)	115 (92%)	10 (8%)	0	100	100
39	n	169/179 (94%)	161 (95%)	8 (5%)	0	100	100
40	o	118/137 (86%)	114 (97%)	4 (3%)	0	100	100
41	p	171/176 (97%)	166 (97%)	5 (3%)	0	100	100
42	q	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
43	r	92/113 (81%)	87 (95%)	5 (5%)	0	100	100
44	s	43/109 (39%)	41 (95%)	2 (5%)	0	100	100
All	All	7915/9212 (86%)	7613 (96%)	297 (4%)	5 (0%)	49	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	158	ASP
34	i	2	GLY
13	M	142	ARG
16	P	279	THR
29	d	2	MET

5.3.2 Protein sidechains (i)

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	94/100 (94%)	94 (100%)	0	100	100
2	B	134/175 (77%)	134 (100%)	0	100	100
3	C	190/228 (83%)	190 (100%)	0	100	100
4	D	334/392 (85%)	334 (100%)	0	100	100
5	E	183/205 (89%)	183 (100%)	0	100	100
6	F	345/368 (94%)	345 (100%)	0	100	100
7	G	586/608 (96%)	586 (100%)	0	100	100
8	H	274/274 (100%)	274 (100%)	0	100	100
9	I	151/175 (86%)	151 (100%)	0	100	100
10	J	128/141 (91%)	128 (100%)	0	100	100
11	K	73/85 (86%)	73 (100%)	0	100	100
12	L	479/533 (90%)	479 (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	276/327 (84%)	276 (100%)	0	100	100
17	Q	112/153 (73%)	112 (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	78/135 (58%)	77 (99%)	1 (1%)	61	80
20	U	81/135 (60%)	81 (100%)	0	100	100
21	V	101/102 (99%)	101 (100%)	0	100	100
22	W	108/114 (95%)	108 (100%)	0	100	100
23	X	154/155 (99%)	154 (100%)	0	100	100
24	Y	25/102 (24%)	25 (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	44/68 (65%)	44 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	81/131 (62%)	81 (100%)	0	100	100
33	h	124/158 (78%)	124 (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	113/115 (98%)	113 (100%)	0	100	100
39	n	156/161 (97%)	156 (100%)	0	100	100
40	o	109/120 (91%)	109 (100%)	0	100	100
41	p	156/157 (99%)	156 (100%)	0	100	100
42	q	131/131 (100%)	131 (100%)	0	100	100
43	r	86/97 (89%)	86 (100%)	0	100	100
44	s	44/92 (48%)	44 (100%)	0	100	100
All	All	6998/7892 (89%)	6997 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	T	44	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	94	ASN
3	C	88	ASN
4	D	200	HIS
5	E	99	HIS
5	E	150	ASN
6	F	257	ASN
6	F	421	HIS
7	G	100	ASN
7	G	141	ASN

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Mol	Chain	Res	Type
7	G	182	GLN
7	G	402	ASN
7	G	665	GLN
8	H	47	GLN
8	H	194	ASN
8	H	235	ASN
9	I	144	HIS
11	K	52	HIS
12	L	192	ASN
12	L	514	HIS
12	L	541	ASN
13	M	51	ASN
13	M	144	ASN
13	M	338	HIS
13	M	399	ASN
14	N	36	ASN
14	N	120	GLN
14	N	134	GLN
15	O	72	GLN
18	R	47	GLN
18	R	51	GLN
18	R	96	HIS
19	S	47	ASN
21	V	72	GLN
23	X	15	GLN
23	X	162	HIS
28	c	35	HIS
29	d	88	HIS
31	f	5	GLN
32	g	45	HIS
32	g	103	HIS
34	i	82	HIS
34	i	127	HIS
39	n	140	GLN
40	o	53	GLN
44	s	43	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

11 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	$\#\|Z\| > 2$
1	FME	A	1	1	8,9,10	0.96	1 (12%)	7,9,11	0.76	0
11	FME	K	1	11	8,9,10	0.92	0	7,9,11	0.97	0
4	2MR	D	85	4	10,12,13	0.51	0	5,13,15	1.26	1 (20%)
14	FME	N	1	14	8,9,10	0.96	0	7,9,11	0.85	0
43	AYA	r	1	43	6,7,8	1.25	1 (16%)	5,8,10	1.39	1 (20%)
29	AME	d	1	29	9,10,11	1.42	2 (22%)	9,11,13	2.55	2 (22%)
10	FME	J	1	10	8,9,10	0.91	0	7,9,11	0.90	0
8	FME	H	1	8	8,9,10	0.98	0	7,9,11	0.88	0
12	FME	L	1	12	8,9,10	0.96	0	7,9,11	0.91	0
13	FME	M	1	13	8,9,10	0.96	0	7,9,11	0.80	0
34	SAC	i	1	34	7,8,9	1.84	1 (14%)	8,9,11	1.62	1 (12%)

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
1	FME	A	1	1	-	1/7/9/11	-
11	FME	K	1	11	-	3/7/9/11	-
4	2MR	D	85	4	-	3/10/13/15	-
14	FME	N	1	14	-	2/7/9/11	-
43	AYA	r	1	43	-	0/4/6/8	-
29	AME	d	1	29	-	4/9/10/12	-
10	FME	J	1	10	-	5/7/9/11	-
8	FME	H	1	8	-	0/7/9/11	-
12	FME	L	1	12	-	5/7/9/11	-
13	FME	M	1	13	-	1/7/9/11	-
34	SAC	i	1	34	-	4/7/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	i	1	SAC	O-C	4.22	1.36	1.19
29	d	1	AME	CT1-N	3.12	1.45	1.34
43	r	1	AYA	CA-N	-2.45	1.44	1.46
29	d	1	AME	OT-CT1	-2.14	1.18	1.23
1	A	1	FME	CA-N	-2.00	1.43	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	d	1	AME	C-CA-N	-6.48	98.04	109.73
34	i	1	SAC	O-C-CA	-3.99	114.33	124.78
29	d	1	AME	CE-SD-CG	2.99	110.66	100.40
43	r	1	AYA	CB-CA-N	2.82	112.75	109.61
4	D	85	2MR	NE-CZ-NH2	-2.64	117.06	119.48

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
4	D	85	2MR	O-C-CA-CB
4	D	85	2MR	NE-CZ-NH2-CQ2
4	D	85	2MR	NH1-CZ-NH2-CQ2
10	J	1	FME	O1-CN-N-CA
10	J	1	FME	CB-CA-N-CN
10	J	1	FME	C-CA-CB-CG
11	K	1	FME	O1-CN-N-CA
11	K	1	FME	C-CA-CB-CG
12	L	1	FME	O1-CN-N-CA
14	N	1	FME	O1-CN-N-CA
29	d	1	AME	N-CA-CB-CG
29	d	1	AME	CB-CA-N-CT1
12	L	1	FME	CA-CB-CG-SD
10	J	1	FME	N-CA-CB-CG
29	d	1	AME	CB-CG-SD-CE
34	i	1	SAC	N-CA-CB-OG
13	M	1	FME	C-CA-CB-CG
29	d	1	AME	C-CA-CB-CG
34	i	1	SAC	C-CA-CB-OG
11	K	1	FME	N-CA-CB-CG
34	i	1	SAC	C-CA-N-C1A

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Mol	Chain	Res	Type	Atoms
34	i	1	SAC	CB-CA-N-C1A
12	L	1	FME	CB-CG-SD-CE
14	N	1	FME	CB-CA-N-CN
12	L	1	FME	N-CA-CB-CG
10	J	1	FME	CB-CG-SD-CE
12	L	1	FME	CB-CA-N-CN

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	1	FME	2	0
29	d	1	AME	6	0
34	i	1	SAC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 46 ligands modelled in this entry, 3 are monoatomic - leaving 43 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	$\#\|Z\| > 2$
58	EHZ	U	101	20	29,36,37	1.69	5 (17%)	35,44,47	1.35	3 (8%)
53	U10	M	701	-	63,63,63	2.68	17 (26%)	76,79,79	1.97	22 (28%)
46	PC1	B	301	-	49,49,53	0.98	4 (8%)	55,57,61	0.94	2 (3%)
52	CDL	L	702	-	74,74,99	1.01	8 (10%)	80,86,111	1.12	4 (5%)
51	CHD	L	704	-	32,32,32	3.19	10 (31%)	51,51,51	2.31	20 (39%)
45	3PE	N	402	-	48,48,50	0.87	3 (6%)	51,53,55	1.09	2 (3%)
45	3PE	I	201	-	50,50,50	0.86	3 (6%)	53,55,55	1.10	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	3PE	r	202	-	48,48,50	0.87	4 (8%)	51,53,55	1.09	2 (3%)
45	3PE	I	204	-	32,32,50	1.06	4 (12%)	35,37,55	1.11	2 (5%)
45	3PE	L	701	-	44,44,50	0.91	3 (6%)	47,49,55	1.10	2 (4%)
45	3PE	H	702	-	32,32,50	1.05	4 (12%)	35,37,55	1.24	2 (5%)
47	SF4	G	801	7	0,12,12	-	-	-		
48	FES	E	301	5	0,4,4	-	-	-		
49	FMN	F	501	-	33,33,33	1.12	2 (6%)	48,50,50	1.25	6 (12%)
45	3PE	A	203	-	38,38,50	0.97	4 (10%)	41,43,55	1.13	2 (4%)
58	EHZ	T	101	20	29,36,37	1.76	5 (17%)	35,44,47	1.52	5 (14%)
52	CDL	N	403	-	72,72,99	1.03	7 (9%)	78,84,111	1.09	4 (5%)
59	MYR	o	201	40	14,14,15	0.96	0	13,13,15	0.68	0
45	3PE	Y	601	-	38,38,50	0.99	4 (10%)	41,43,55	1.12	2 (4%)
52	CDL	r	201	-	59,59,99	1.11	7 (11%)	65,71,111	1.17	4 (6%)
48	FES	G	803	7	0,4,4	-	-	-		
46	PC1	M	703	-	45,45,53	1.00	3 (6%)	51,53,61	1.04	2 (3%)
46	PC1	q	701	-	36,36,53	1.13	4 (11%)	42,44,61	1.07	2 (4%)
45	3PE	A	201	-	41,41,50	0.94	4 (9%)	44,46,55	1.14	2 (4%)
54	GTP	O	401	55	30,34,34	3.06	11 (36%)	46,54,54	2.01	16 (34%)
47	SF4	B	302	2	0,12,12	-	-	-		
45	3PE	L	703	-	31,31,50	1.07	3 (9%)	34,36,55	1.17	2 (5%)
45	3PE	A	202	-	42,42,50	0.92	4 (9%)	45,47,55	1.13	2 (4%)
47	SF4	I	202	9	0,12,12	-	-	-		
46	PC1	d	201	-	32,32,53	1.22	4 (12%)	38,40,61	1.13	2 (5%)
47	SF4	G	802	7	0,12,12	-	-	-		
51	CHD	H	701	-	32,32,32	3.22	10 (31%)	51,51,51	2.58	21 (41%)
47	SF4	I	203	9	0,12,12	-	-	-		
47	SF4	F	502	6	0,12,12	-	-	-		
45	3PE	M	702	-	37,37,50	0.99	4 (10%)	40,42,55	1.05	2 (5%)
52	CDL	h	201	-	76,76,99	0.99	8 (10%)	82,88,111	1.19	5 (6%)
45	3PE	N	401	-	34,34,50	1.02	4 (11%)	37,39,55	1.06	2 (5%)
46	PC1	B	303	-	50,50,53	0.97	4 (8%)	56,58,61	1.03	2 (3%)
45	3PE	h	202	-	31,31,50	1.08	4 (12%)	34,36,55	1.05	2 (5%)
46	PC1	J	201	-	42,42,53	1.05	4 (9%)	48,50,61	1.03	2 (4%)
52	CDL	d	202	-	64,64,99	1.06	8 (12%)	70,76,111	1.13	4 (5%)
52	CDL	X	201	-	78,78,99	0.98	8 (10%)	84,90,111	1.11	4 (4%)
56	NDP	P	501	-	49,52,52	2.16	6 (12%)	66,80,80	1.61	12 (18%)

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
58	EHZ	U	101	20	-	15/42/44/45	-
53	U10	M	701	-	-	28/63/87/87	0/1/1/1
46	PC1	B	301	-	-	18/53/53/57	-
52	CDL	L	702	-	-	43/85/85/110	-
51	CHD	L	704	-	-	4/9/74/74	0/4/4/4
45	3PE	N	402	-	-	25/52/52/54	-
45	3PE	I	201	-	-	26/54/54/54	-
45	3PE	r	202	-	-	32/52/52/54	-
45	3PE	I	204	-	-	13/36/36/54	-
45	3PE	L	701	-	-	27/48/48/54	-
45	3PE	H	702	-	-	17/36/36/54	-
49	FMN	F	501	-	-	5/18/18/18	0/3/3/3
47	SF4	G	801	7	-	-	0/6/5/5
48	FES	E	301	5	-	-	0/1/1/1
45	3PE	A	203	-	-	20/42/42/54	-
58	EHZ	T	101	20	-	14/42/44/45	-
52	CDL	N	403	-	-	35/83/83/110	-
59	MYR	o	201	40	-	8/11/12/13	-
45	3PE	Y	601	-	-	14/42/42/54	-
52	CDL	r	201	-	-	28/70/70/110	-
48	FES	G	803	7	-	-	0/1/1/1
46	PC1	M	703	-	-	14/49/49/57	-
46	PC1	q	701	-	-	19/40/40/57	-
45	3PE	A	201	-	-	17/45/45/54	-
54	GTP	O	401	55	-	6/22/38/38	0/3/3/3
47	SF4	B	302	2	-	-	0/6/5/5
45	3PE	L	703	-	-	20/35/35/54	-
45	3PE	A	202	-	-	20/46/46/54	-
47	SF4	I	202	9	-	-	0/6/5/5
46	PC1	d	201	-	-	14/36/36/57	-
51	CHD	H	701	-	-	1/9/74/74	0/4/4/4
47	SF4	G	802	7	-	-	0/6/5/5
47	SF4	I	203	9	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	SF4	F	502	6	-	-	0/6/5/5
45	3PE	M	702	-	-	24/41/41/54	-
52	CDL	h	201	-	-	36/87/87/110	-
45	3PE	N	401	-	-	15/38/38/54	-
46	PC1	B	303	-	-	16/54/54/57	-
45	3PE	h	202	-	-	23/35/35/54	-
46	PC1	J	201	-	-	16/46/46/57	-
52	CDL	d	202	-	-	34/75/75/110	-
52	CDL	X	201	-	-	47/89/89/110	-
56	NDP	P	501	-	-	6/34/77/77	0/5/5/5

All (187) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	P2B-O2B	12.06	1.82	1.59
54	O	401	GTP	O6-C6	8.68	1.40	1.23
51	L	704	CHD	C11-C12	8.67	1.67	1.53
51	H	701	CHD	C11-C12	8.67	1.67	1.53
51	H	701	CHD	C16-C15	7.02	1.73	1.54
51	L	704	CHD	C16-C15	7.00	1.73	1.54
54	O	401	GTP	C5-N7	6.90	1.52	1.39
53	M	701	U10	C18-C19	6.26	1.48	1.33
53	M	701	U10	C28-C29	6.07	1.47	1.33
53	M	701	U10	C13-C14	6.06	1.47	1.33
51	H	701	CHD	C13-C17	5.96	1.65	1.55
53	M	701	U10	C8-C9	5.93	1.47	1.33
58	T	101	EHZ	C15-N2	5.91	1.46	1.33
53	M	701	U10	C23-C24	5.90	1.47	1.33
53	M	701	U10	C43-C44	5.84	1.47	1.33
53	M	701	U10	C38-C39	5.82	1.47	1.33
53	M	701	U10	C33-C34	5.73	1.46	1.33
53	M	701	U10	C48-C49	5.69	1.46	1.33
51	H	701	CHD	C8-C9	5.65	1.64	1.53
53	M	701	U10	O3-C3	-5.59	1.23	1.36
51	L	704	CHD	C13-C17	5.57	1.65	1.55
51	H	701	CHD	O12-C12	-5.55	1.34	1.43
51	L	704	CHD	C20-C17	-5.54	1.44	1.54
53	M	701	U10	O4-C4	-5.52	1.23	1.36
51	L	704	CHD	C8-C9	5.41	1.64	1.53
51	L	704	CHD	O12-C12	-5.35	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	T	101	EHZ	C12-N1	5.34	1.45	1.33
58	U	101	EHZ	C12-N1	5.32	1.45	1.33
58	U	101	EHZ	C15-N2	5.23	1.45	1.33
53	M	701	U10	C53-C54	5.19	1.47	1.32
51	H	701	CHD	C20-C17	-5.08	1.45	1.54
54	O	401	GTP	C2-N1	4.87	1.49	1.37
54	O	401	GTP	C2-N3	4.74	1.44	1.33
54	O	401	GTP	C2-N2	4.68	1.45	1.34
51	H	701	CHD	C6-C5	4.64	1.61	1.53
51	L	704	CHD	C6-C5	4.57	1.61	1.53
54	O	401	GTP	C8-N9	-4.35	1.27	1.37
51	L	704	CHD	C15-C14	4.03	1.62	1.54
51	H	701	CHD	C15-C14	3.94	1.62	1.54
51	L	704	CHD	C6-C7	3.83	1.59	1.52
54	O	401	GTP	C4-N9	-3.82	1.28	1.38
51	H	701	CHD	C6-C7	3.72	1.59	1.52
56	P	501	NDP	PN-O5D	3.71	1.74	1.59
49	F	501	FMN	C4A-N5	3.65	1.37	1.30
53	M	701	U10	C3-C2	-3.33	1.39	1.48
56	P	501	NDP	O2B-C2B	-3.26	1.32	1.44
53	M	701	U10	C4-C5	-3.22	1.39	1.48
54	O	401	GTP	O4'-C1'	2.84	1.48	1.42
52	N	403	CDL	OB6-CB4	-2.82	1.39	1.46
45	Y	601	3PE	O21-C2	-2.77	1.39	1.46
45	L	701	3PE	O21-C2	-2.76	1.39	1.46
52	r	201	CDL	OA6-CA4	-2.74	1.39	1.46
52	L	702	CDL	OB6-CB4	-2.73	1.39	1.46
52	d	202	CDL	OA6-CA4	-2.72	1.39	1.46
46	B	303	PC1	O21-C2	-2.70	1.39	1.46
45	I	201	3PE	O21-C2	-2.70	1.39	1.46
46	d	201	PC1	O21-C2	-2.68	1.39	1.46
52	h	201	CDL	OB6-CB4	-2.68	1.39	1.46
52	X	201	CDL	OB6-CB4	-2.68	1.39	1.46
46	B	301	PC1	O21-C2	-2.67	1.39	1.46
52	h	201	CDL	OA6-CA4	-2.66	1.39	1.46
46	M	703	PC1	O21-C2	-2.65	1.40	1.46
52	r	201	CDL	OB6-CB4	-2.64	1.40	1.46
52	L	702	CDL	OA8-CA7	2.63	1.41	1.33
45	L	703	3PE	O21-C2	-2.62	1.40	1.46
45	N	402	3PE	O21-C2	-2.62	1.40	1.46
52	X	201	CDL	OA6-CA4	-2.61	1.40	1.46
52	L	702	CDL	OA6-CA4	-2.61	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	M	701	U10	C6-C5	-2.60	1.39	1.46
45	A	202	3PE	O21-C2	-2.60	1.40	1.46
51	L	704	CHD	C13-C12	-2.57	1.50	1.54
46	q	701	PC1	O21-C2	-2.56	1.40	1.46
45	M	702	3PE	O21-C2	-2.55	1.40	1.46
45	I	204	3PE	O21-C2	-2.54	1.40	1.46
46	J	201	PC1	O21-C2	-2.51	1.40	1.46
52	N	403	CDL	OA6-CA4	-2.51	1.40	1.46
52	X	201	CDL	OA8-CA7	2.50	1.40	1.33
45	A	201	3PE	O21-C2	-2.49	1.40	1.46
52	d	202	CDL	OB8-CB7	2.48	1.40	1.33
46	d	201	PC1	O31-C31	2.48	1.40	1.33
52	X	201	CDL	OB8-CB7	2.47	1.40	1.33
45	N	402	3PE	O31-C31	2.47	1.40	1.33
45	A	203	3PE	O31-C31	2.47	1.40	1.33
52	N	403	CDL	OB8-CB7	2.47	1.40	1.33
45	H	702	3PE	O31-C31	2.45	1.40	1.33
52	d	202	CDL	OA8-CA7	2.44	1.40	1.33
52	L	702	CDL	OB8-CB7	2.44	1.40	1.33
46	J	201	PC1	O31-C3	-2.44	1.39	1.45
52	r	201	CDL	OB8-CB7	2.42	1.40	1.33
52	h	201	CDL	OA8-CA7	2.42	1.40	1.33
58	U	101	EHZ	O4-C15	-2.42	1.18	1.23
45	h	202	3PE	O21-C2	-2.41	1.40	1.46
45	h	202	3PE	O31-C31	2.41	1.40	1.33
45	H	702	3PE	O21-C2	-2.41	1.40	1.46
58	T	101	EHZ	O4-C15	-2.40	1.18	1.23
45	Y	601	3PE	O31-C31	2.40	1.40	1.33
52	h	201	CDL	OB8-CB7	2.40	1.40	1.33
52	d	202	CDL	OB6-CB4	-2.38	1.40	1.46
46	B	303	PC1	O31-C3	-2.38	1.39	1.45
52	N	403	CDL	OA8-CA7	2.37	1.40	1.33
46	B	301	PC1	O31-C3	-2.35	1.39	1.45
45	I	201	3PE	O31-C3	-2.35	1.39	1.45
45	A	203	3PE	O21-C21	2.34	1.40	1.34
45	r	202	3PE	O31-C31	2.34	1.40	1.33
45	A	201	3PE	O31-C31	2.33	1.40	1.33
58	T	101	EHZ	C9-S1	2.32	1.81	1.76
58	U	101	EHZ	C9-S1	2.32	1.81	1.76
46	q	701	PC1	O31-C31	2.32	1.40	1.33
45	L	703	3PE	O31-C31	2.31	1.40	1.33
45	N	401	3PE	O31-C31	2.31	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	O4B-C4B	-2.31	1.39	1.45
45	I	204	3PE	O31-C3	-2.31	1.39	1.45
45	N	401	3PE	O21-C2	-2.30	1.40	1.46
45	N	401	3PE	O21-C21	2.30	1.40	1.34
45	A	203	3PE	O21-C2	-2.30	1.40	1.46
45	M	702	3PE	O31-C31	2.30	1.40	1.33
45	A	202	3PE	O31-C31	2.29	1.40	1.33
45	I	204	3PE	O31-C31	2.29	1.40	1.33
52	r	201	CDL	OA8-CA6	-2.28	1.39	1.45
46	M	703	PC1	O31-C3	-2.28	1.39	1.45
52	N	403	CDL	OA6-CA5	2.28	1.40	1.34
45	L	701	3PE	O31-C3	-2.27	1.40	1.45
45	h	202	3PE	O21-C21	2.26	1.40	1.34
46	J	201	PC1	O31-C31	2.26	1.39	1.33
54	O	401	GTP	C2'-C3'	-2.25	1.47	1.53
52	d	202	CDL	OB6-CB5	2.25	1.40	1.34
53	M	701	U10	C6-C1	2.24	1.39	1.35
52	r	201	CDL	OA8-CA7	2.23	1.39	1.33
45	L	703	3PE	O31-C3	-2.22	1.40	1.45
45	I	201	3PE	O31-C31	2.22	1.39	1.33
52	N	403	CDL	OA8-CA6	-2.22	1.40	1.45
58	T	101	EHZ	O3-C12	-2.21	1.18	1.23
49	F	501	FMN	C10-N1	2.21	1.37	1.33
46	q	701	PC1	O31-C3	-2.20	1.40	1.45
58	U	101	EHZ	O3-C12	-2.20	1.18	1.23
46	q	701	PC1	O21-C21	2.20	1.40	1.34
45	r	202	3PE	O21-C2	-2.20	1.41	1.46
46	B	303	PC1	O31-C31	2.20	1.39	1.33
45	A	202	3PE	O31-C3	-2.20	1.40	1.45
54	O	401	GTP	PG-O3G	-2.20	1.46	1.54
45	L	701	3PE	O31-C31	2.19	1.39	1.33
45	Y	601	3PE	O31-C3	-2.19	1.40	1.45
56	P	501	NDP	O3D-C3D	-2.19	1.37	1.43
46	B	301	PC1	O21-C21	2.19	1.40	1.34
45	r	202	3PE	O31-C3	-2.18	1.40	1.45
45	N	401	3PE	O31-C3	-2.18	1.40	1.45
54	O	401	GTP	PG-O2G	-2.18	1.46	1.54
52	X	201	CDL	OB8-CB6	-2.17	1.40	1.45
45	I	204	3PE	O21-C21	2.16	1.40	1.34
46	B	301	PC1	O31-C31	2.16	1.39	1.33
52	r	201	CDL	OB8-CB6	-2.16	1.40	1.45
46	M	703	PC1	O31-C31	2.15	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	L	702	CDL	OA6-CA5	2.15	1.40	1.34
46	J	201	PC1	O21-C21	2.14	1.40	1.34
52	h	201	CDL	OA6-CA5	2.14	1.40	1.34
52	N	403	CDL	OB8-CB6	-2.14	1.40	1.45
53	M	701	U10	C1-C2	-2.13	1.39	1.47
52	d	202	CDL	OA8-CA6	-2.12	1.40	1.45
52	L	702	CDL	OB8-CB6	-2.12	1.40	1.45
52	h	201	CDL	OB8-CB6	-2.12	1.40	1.45
45	A	201	3PE	O21-C21	2.12	1.40	1.34
45	r	202	3PE	O21-C21	2.11	1.40	1.34
46	d	201	PC1	O31-C3	-2.11	1.40	1.45
52	X	201	CDL	OB6-CB5	2.10	1.40	1.34
52	X	201	CDL	OA8-CA6	-2.10	1.40	1.45
52	h	201	CDL	OA8-CA6	-2.10	1.40	1.45
45	H	702	3PE	O21-C21	2.09	1.40	1.34
45	M	702	3PE	O21-C21	2.09	1.40	1.34
45	h	202	3PE	O31-C3	-2.09	1.40	1.45
45	A	201	3PE	O31-C3	-2.09	1.40	1.45
45	M	702	3PE	O31-C3	-2.09	1.40	1.45
52	r	201	CDL	OA6-CA5	2.07	1.40	1.34
56	P	501	NDP	O5D-C5D	-2.07	1.36	1.44
52	d	202	CDL	OB8-CB6	-2.06	1.40	1.45
45	N	402	3PE	O31-C3	-2.05	1.40	1.45
45	A	202	3PE	O21-C21	2.05	1.40	1.34
46	d	201	PC1	O21-C21	2.05	1.40	1.34
45	H	702	3PE	O31-C3	-2.03	1.40	1.45
51	H	701	CHD	C13-C12	-2.03	1.51	1.54
52	X	201	CDL	OA6-CA5	2.03	1.40	1.34
52	d	202	CDL	OA6-CA5	2.02	1.40	1.34
52	L	702	CDL	OA8-CA6	-2.02	1.40	1.45
45	Y	601	3PE	O21-C21	2.02	1.40	1.34
52	h	201	CDL	OB6-CB5	2.02	1.40	1.34
46	B	303	PC1	O21-C21	2.01	1.40	1.34
45	A	203	3PE	O31-C3	-2.00	1.40	1.45
52	L	702	CDL	OB6-CB5	2.00	1.40	1.34

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	O	401	GTP	C8-N9-C4	7.30	119.95	106.05
56	P	501	NDP	PN-O3-PA	-7.08	108.53	132.83
51	H	701	CHD	C17-C13-C12	6.37	123.48	117.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	L	704	CHD	C17-C13-C12	5.81	122.97	117.67
53	M	701	U10	C40-C39-C41	5.63	124.75	115.27
51	H	701	CHD	C17-C13-C14	5.57	105.71	100.09
58	T	101	EHZ	C8-C9-S1	5.55	120.50	113.63
51	L	704	CHD	C14-C8-C9	5.24	116.91	109.71
51	H	701	CHD	C1-C10-C5	5.05	115.24	107.77
58	U	101	EHZ	C8-C9-S1	5.05	119.88	113.63
51	H	701	CHD	C4-C5-C10	4.97	117.93	112.66
45	A	201	3PE	O21-C21-C22	4.59	121.40	111.50
51	H	701	CHD	C18-C13-C12	-4.55	104.44	109.07
51	L	704	CHD	C17-C13-C14	4.52	104.65	100.09
51	H	701	CHD	C18-C13-C17	-4.46	104.23	111.21
52	L	702	CDL	OA6-CA5-C11	4.38	120.95	111.50
45	r	202	3PE	O21-C21-C22	4.37	120.91	111.50
45	A	202	3PE	O21-C21-C22	4.33	120.83	111.50
53	M	701	U10	C15-C14-C16	4.30	122.51	115.27
51	H	701	CHD	C14-C13-C12	4.28	111.38	107.40
52	h	201	CDL	OB6-CB5-C51	4.27	120.71	111.50
52	X	201	CDL	OA6-CA5-C11	4.26	120.68	111.50
58	T	101	EHZ	C16-C15-N2	4.24	125.01	116.58
45	H	702	3PE	O21-C21-C22	4.19	120.53	111.50
52	X	201	CDL	OB6-CB5-C51	4.18	120.51	111.50
53	M	701	U10	C25-C24-C26	4.12	122.21	115.27
46	q	701	PC1	O21-C21-C22	4.11	120.37	111.50
45	N	402	3PE	O21-C21-C22	4.10	120.33	111.50
45	M	702	3PE	O21-C21-C22	4.09	120.32	111.50
51	H	701	CHD	C13-C17-C20	-4.08	114.62	119.50
51	L	704	CHD	C9-C8-C7	-4.08	107.00	111.88
46	d	201	PC1	O21-C21-C22	4.07	120.28	111.50
51	L	704	CHD	C1-C10-C5	4.07	113.78	107.77
45	I	201	3PE	O21-C21-C22	4.04	120.20	111.50
46	M	703	PC1	O21-C21-C22	4.04	120.20	111.50
45	A	203	3PE	O21-C21-C22	4.02	120.16	111.50
46	B	303	PC1	O21-C21-C22	4.00	120.12	111.50
52	r	201	CDL	OB6-CB5-C51	3.99	120.09	111.50
52	d	202	CDL	OA6-CA5-C11	3.98	120.08	111.50
52	h	201	CDL	OA6-CA5-C11	3.95	120.02	111.50
52	N	403	CDL	OA6-CA5-C11	3.92	119.95	111.50
46	J	201	PC1	O21-C21-C22	3.87	119.85	111.50
45	L	703	3PE	O21-C21-C22	3.87	119.84	111.50
53	M	701	U10	C22-C23-C24	-3.86	118.36	127.66
45	I	204	3PE	O21-C21-C22	3.86	119.81	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	r	201	CDL	OA6-CA5-C11	3.85	119.81	111.50
45	Y	601	3PE	O21-C21-C22	3.80	119.69	111.50
51	H	701	CHD	C5-C4-C3	3.79	118.33	112.76
51	L	704	CHD	C13-C17-C20	-3.75	115.02	119.50
45	L	701	3PE	O21-C21-C22	3.72	119.52	111.50
45	H	702	3PE	O31-C31-C32	3.69	121.07	111.38
52	N	403	CDL	OB6-CB5-C51	3.63	119.31	111.50
45	N	401	3PE	O21-C21-C22	3.62	119.29	111.50
53	M	701	U10	C47-C48-C49	-3.59	119.02	127.66
45	h	202	3PE	O21-C21-C22	3.57	119.19	111.50
51	L	704	CHD	C18-C13-C17	-3.49	105.75	111.21
51	H	701	CHD	C5-C6-C7	-3.49	110.61	114.46
52	L	702	CDL	OB6-CB5-C51	3.48	119.00	111.50
53	M	701	U10	C27-C28-C29	-3.46	119.32	127.66
56	P	501	NDP	O2B-P2B-O1X	-3.40	96.26	109.39
49	F	501	FMN	C4-N3-C2	-3.37	119.42	125.64
51	H	701	CHD	C19-C10-C5	-3.36	104.66	110.36
53	M	701	U10	C50-C49-C51	3.36	120.93	115.27
52	d	202	CDL	OB6-CB5-C51	3.35	120.13	110.80
51	L	704	CHD	C10-C9-C8	-3.34	108.23	111.82
51	L	704	CHD	C11-C9-C8	3.33	115.75	110.88
53	M	701	U10	C7-C8-C9	-3.19	121.47	126.79
51	H	701	CHD	C18-C13-C14	-3.18	106.23	111.21
54	O	401	GTP	PB-O3B-PG	-3.16	121.97	132.83
53	M	701	U10	C37-C38-C39	-3.16	120.06	127.66
53	M	701	U10	C12-C13-C14	-3.15	120.08	127.66
53	M	701	U10	C32-C33-C34	-3.11	120.16	127.66
54	O	401	GTP	C2-N1-C6	-3.11	119.44	125.10
53	M	701	U10	C42-C43-C44	-3.09	120.22	127.66
53	M	701	U10	C45-C44-C46	3.08	120.45	115.27
51	L	704	CHD	C5-C6-C7	-3.07	111.07	114.46
53	M	701	U10	C10-C9-C11	3.05	120.40	115.27
46	B	301	PC1	O21-C21-C22	3.03	118.02	111.50
51	H	701	CHD	C9-C10-C5	3.00	112.80	108.58
54	O	401	GTP	O2G-PG-O3B	3.00	114.70	104.64
51	L	704	CHD	C18-C13-C12	-2.99	106.02	109.07
54	O	401	GTP	C3'-C2'-C1'	2.96	107.04	101.43
51	H	701	CHD	C1-C10-C9	-2.93	106.74	111.35
52	h	201	CDL	OB8-CB7-C71	2.91	121.03	111.91
46	d	201	PC1	O31-C31-C32	2.88	120.94	111.91
54	O	401	GTP	PA-O3A-PB	-2.88	122.95	132.83
53	M	701	U10	C35-C34-C36	2.87	120.10	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	M	701	U10	C52-C53-C54	-2.85	118.02	127.75
51	L	704	CHD	C19-C10-C5	-2.82	105.58	110.36
51	H	701	CHD	C4-C3-C2	2.82	113.92	110.55
56	P	501	NDP	PA-O5B-C5B	-2.81	105.20	121.68
49	F	501	FMN	C4A-C4-N3	2.80	120.30	113.19
49	F	501	FMN	O4-C4-C4A	-2.78	119.22	126.60
54	O	401	GTP	O3G-PG-O3B	2.77	113.92	104.64
45	Y	601	3PE	O31-C31-C32	2.76	120.56	111.91
51	L	704	CHD	C4-C5-C10	2.74	115.56	112.66
52	h	201	CDL	OA8-CA7-C31	2.73	120.48	111.91
45	N	402	3PE	O31-C31-C32	2.72	120.46	111.91
46	J	201	PC1	O31-C31-C32	2.71	120.42	111.91
53	M	701	U10	C1M-C1-C6	-2.70	120.00	124.40
51	L	704	CHD	C1-C10-C9	-2.69	107.12	111.35
49	F	501	FMN	C4A-C10-N10	2.69	120.41	116.48
52	L	702	CDL	OA8-CA7-C31	2.69	120.33	111.91
53	M	701	U10	C56-C54-C55	2.68	120.52	114.60
54	O	401	GTP	C4'-O4'-C1'	-2.68	103.56	109.47
52	N	403	CDL	OB8-CB7-C71	2.67	120.29	111.91
45	I	201	3PE	O31-C31-C32	2.67	120.27	111.91
56	P	501	NDP	PN-O5D-C5D	-2.66	106.09	121.68
45	A	203	3PE	O31-C31-C32	2.64	120.19	111.91
51	H	701	CHD	C6-C5-C4	-2.64	108.16	111.19
56	P	501	NDP	O4B-C4B-C3B	2.63	110.33	105.11
45	A	201	3PE	O31-C31-C32	2.63	120.16	111.91
45	L	701	3PE	O31-C31-C32	2.63	120.16	111.91
52	d	202	CDL	OB8-CB7-C71	2.62	120.12	111.91
45	N	401	3PE	O31-C31-C32	2.61	120.11	111.91
45	L	703	3PE	O31-C31-C32	2.60	120.08	111.91
51	L	704	CHD	C23-C22-C20	-2.60	109.77	114.52
45	I	204	3PE	O31-C31-C32	2.60	120.06	111.91
52	r	201	CDL	OB8-CB7-C71	2.59	120.03	111.91
51	L	704	CHD	C18-C13-C14	-2.59	107.16	111.21
45	r	202	3PE	O31-C31-C32	2.58	120.00	111.91
58	T	101	EHZ	O4-C15-N2	-2.58	117.45	122.99
56	P	501	NDP	O3X-P2B-O2X	2.57	117.44	107.64
46	B	301	PC1	O31-C31-C32	2.56	119.95	111.91
52	X	201	CDL	OB8-CB7-C71	2.56	119.95	111.91
45	h	202	3PE	O31-C31-C32	2.56	119.94	111.91
46	M	703	PC1	O31-C31-C32	2.55	119.92	111.91
51	H	701	CHD	C11-C12-C13	2.55	113.86	111.24
51	H	701	CHD	C23-C22-C20	-2.55	109.87	114.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	B	303	PC1	O31-C31-C32	2.54	119.88	111.91
52	d	202	CDL	OA8-CA7-C31	2.53	119.83	111.91
52	L	702	CDL	OB8-CB7-C71	2.52	119.82	111.91
52	N	403	CDL	OA8-CA7-C31	2.51	119.78	111.91
46	q	701	PC1	O31-C31-C32	2.50	119.75	111.91
56	P	501	NDP	N3A-C4A-N9A	2.46	131.14	127.08
51	L	704	CHD	C4-C3-C2	2.46	113.49	110.55
58	U	101	EHZ	C10-S1-C9	2.46	109.53	101.87
51	L	704	CHD	C16-C17-C20	-2.45	108.36	112.15
54	O	401	GTP	C5-C6-N1	2.44	119.38	113.19
52	h	201	CDL	CA4-OA6-CA5	-2.43	111.81	117.79
52	r	201	CDL	OA8-CA7-C31	2.40	119.45	111.91
45	A	202	3PE	O31-C31-C32	2.40	119.43	111.91
51	H	701	CHD	C14-C8-C9	2.35	112.94	109.71
45	M	702	3PE	O31-C31-C32	2.34	119.25	111.91
54	O	401	GTP	C1'-N9-C4	-2.32	119.62	126.50
52	X	201	CDL	OA8-CA7-C31	2.30	119.13	111.91
49	F	501	FMN	C4A-C10-N1	-2.27	119.46	124.73
51	H	701	CHD	C6-C5-C10	-2.27	110.25	112.66
56	P	501	NDP	C2A-N1A-C6A	-2.26	114.89	118.77
56	P	501	NDP	C5A-C4A-N3A	-2.25	123.81	126.75
54	O	401	GTP	O6-C6-C5	-2.23	120.70	126.60
54	O	401	GTP	O2A-PA-O1A	-2.22	101.25	112.24
54	O	401	GTP	C1'-N9-C8	-2.20	120.43	126.70
51	H	701	CHD	C16-C17-C20	-2.19	108.75	112.15
58	T	101	EHZ	C10-S1-C9	2.18	108.65	101.87
58	U	101	EHZ	C14-N2-C15	-2.17	118.71	122.59
53	M	701	U10	C25-C24-C23	-2.17	118.12	123.68
49	F	501	FMN	C10-C4A-N5	-2.16	120.27	124.86
56	P	501	NDP	O5D-PN-O1N	-2.15	100.65	109.07
51	L	704	CHD	C14-C13-C12	2.14	109.40	107.40
56	P	501	NDP	O2N-PN-O1N	2.13	122.79	112.24
54	O	401	GTP	C5-C4-N9	-2.12	101.79	105.63
58	T	101	EHZ	O2-C9-S1	-2.12	119.86	122.61
54	O	401	GTP	O2B-PB-O1B	-2.11	101.79	112.24
53	M	701	U10	C40-C39-C38	-2.10	118.30	123.68
53	M	701	U10	C41-C39-C38	-2.07	116.92	121.12
53	M	701	U10	C30-C29-C31	2.06	118.73	115.27
54	O	401	GTP	N9-C8-N7	-2.05	109.54	113.39
56	P	501	NDP	C5B-C4B-C3B	-2.03	107.59	115.18
51	L	704	CHD	C5-C4-C3	2.02	115.72	112.76

There are no chirality outliers.

All (700) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	3PE	O13-C11-C12-N
45	A	201	3PE	O11-C1-C2-O21
45	A	201	3PE	O22-C21-O21-C2
45	A	202	3PE	C1-O11-P-O12
45	A	202	3PE	C1-O11-P-O14
45	A	202	3PE	O13-C11-C12-N
45	A	203	3PE	C1-O11-P-O12
45	A	203	3PE	C1-O11-P-O13
45	A	203	3PE	C11-O13-P-O14
45	A	203	3PE	O13-C11-C12-N
45	A	203	3PE	C22-C21-O21-C2
45	H	702	3PE	C1-O11-P-O12
45	H	702	3PE	C1-O11-P-O14
45	H	702	3PE	C11-O13-P-O12
45	H	702	3PE	C11-O13-P-O14
45	H	702	3PE	O13-C11-C12-N
45	I	201	3PE	C11-O13-P-O12
45	I	201	3PE	C11-O13-P-O14
45	I	204	3PE	O13-C11-C12-N
45	L	701	3PE	C1-O11-P-O12
45	L	701	3PE	C1-O11-P-O14
45	L	701	3PE	C11-O13-P-O14
45	L	703	3PE	C1-O11-P-O12
45	L	703	3PE	C11-O13-P-O12
45	L	703	3PE	O13-C11-C12-N
45	M	702	3PE	C1-O11-P-O12
45	M	702	3PE	C1-O11-P-O13
45	M	702	3PE	C1-O11-P-O14
45	M	702	3PE	C11-O13-P-O12
45	M	702	3PE	O13-C11-C12-N
45	M	702	3PE	C22-C21-O21-C2
45	N	401	3PE	O22-C21-O21-C2
45	N	401	3PE	C22-C21-O21-C2
45	N	402	3PE	C1-O11-P-O12
45	N	402	3PE	O13-C11-C12-N
45	Y	601	3PE	O13-C11-C12-N
45	Y	601	3PE	O21-C2-C3-O31
45	h	202	3PE	C11-O13-P-O12
45	h	202	3PE	O13-C11-C12-N
45	r	202	3PE	C1-O11-P-O12
45	r	202	3PE	C1-O11-P-O13
45	r	202	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
45	r	202	3PE	C11-O13-P-O11
45	r	202	3PE	C11-O13-P-O14
45	r	202	3PE	C2-C1-O11-P
45	r	202	3PE	O13-C11-C12-N
45	r	202	3PE	O22-C21-O21-C2
45	r	202	3PE	C22-C21-O21-C2
46	B	303	PC1	C22-C21-O21-C2
46	J	201	PC1	C11-O13-P-O14
46	d	201	PC1	C11-O13-P-O12
46	d	201	PC1	C11-O13-P-O14
46	d	201	PC1	C11-O13-P-O11
46	q	701	PC1	C22-C21-O21-C2
49	F	501	FMN	C5'-O5'-P-O1P
49	F	501	FMN	C5'-O5'-P-O2P
49	F	501	FMN	C5'-O5'-P-O3P
52	L	702	CDL	CA4-CA3-OA5-PA1
52	L	702	CDL	CB2-OB2-PB2-OB3
52	L	702	CDL	CB2-OB2-PB2-OB4
52	L	702	CDL	CB3-OB5-PB2-OB2
52	L	702	CDL	CB3-OB5-PB2-OB3
52	N	403	CDL	CA3-OA5-PA1-OA2
52	N	403	CDL	CA3-OA5-PA1-OA3
52	N	403	CDL	CA3-OA5-PA1-OA4
52	N	403	CDL	OA6-CA4-CA6-OA8
52	N	403	CDL	CB2-OB2-PB2-OB3
52	N	403	CDL	CB2-OB2-PB2-OB5
52	N	403	CDL	CB3-OB5-PB2-OB3
52	N	403	CDL	CB3-OB5-PB2-OB4
52	X	201	CDL	CB2-OB2-PB2-OB3
52	X	201	CDL	CB3-OB5-PB2-OB4
52	X	201	CDL	OB7-CB5-OB6-CB4
52	d	202	CDL	CA3-OA5-PA1-OA3
52	d	202	CDL	C11-CA5-OA6-CA4
52	d	202	CDL	C51-CB5-OB6-CB4
52	h	201	CDL	CA3-OA5-PA1-OA3
52	h	201	CDL	CA3-OA5-PA1-OA4
52	h	201	CDL	OA5-CA3-CA4-OA6
52	h	201	CDL	C11-CA5-OA6-CA4
52	h	201	CDL	C51-CB5-OB6-CB4
52	r	201	CDL	C11-CA5-OA6-CA4
52	r	201	CDL	CB2-OB2-PB2-OB4
52	r	201	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
53	M	701	U10	C12-C13-C14-C15
53	M	701	U10	C12-C13-C14-C16
53	M	701	U10	C19-C21-C22-C23
53	M	701	U10	C22-C23-C24-C25
53	M	701	U10	C22-C23-C24-C26
53	M	701	U10	C23-C24-C26-C27
53	M	701	U10	C25-C24-C26-C27
53	M	701	U10	C27-C28-C29-C30
53	M	701	U10	C27-C28-C29-C31
53	M	701	U10	C32-C33-C34-C35
53	M	701	U10	C32-C33-C34-C36
53	M	701	U10	C37-C38-C39-C40
53	M	701	U10	C37-C38-C39-C41
53	M	701	U10	C47-C48-C49-C50
53	M	701	U10	C47-C48-C49-C51
53	M	701	U10	C52-C53-C54-C55
54	O	401	GTP	C5'-O5'-PA-O3A
54	O	401	GTP	C5'-O5'-PA-O1A
54	O	401	GTP	C5'-O5'-PA-O2A
56	P	501	NDP	O4D-C4D-C5D-O5D
58	T	101	EHZ	O1-C7-C8-C9
58	T	101	EHZ	C12-C13-C14-N2
58	T	101	EHZ	C16-C15-N2-C14
58	T	101	EHZ	C16-C17-C20-O6
58	U	101	EHZ	C6-C7-C8-C9
58	U	101	EHZ	C12-C13-C14-N2
58	U	101	EHZ	O2-C9-S1-C10
58	U	101	EHZ	C8-C9-S1-C10
52	L	702	CDL	OA9-CA7-OA8-CA6
45	N	401	3PE	C32-C31-O31-C3
52	L	702	CDL	C31-CA7-OA8-CA6
53	M	701	U10	C52-C53-C54-C56
45	A	201	3PE	O32-C31-O31-C3
45	A	203	3PE	O32-C31-O31-C3
45	H	702	3PE	O32-C31-O31-C3
45	N	401	3PE	O32-C31-O31-C3
45	N	402	3PE	O32-C31-O31-C3
46	J	201	PC1	O32-C31-O31-C3
46	d	201	PC1	O32-C31-O31-C3
46	q	701	PC1	O32-C31-O31-C3
52	N	403	CDL	OA9-CA7-OA8-CA6
45	A	203	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
45	M	702	3PE	O22-C21-O21-C2
46	B	303	PC1	O22-C21-O21-C2
46	q	701	PC1	O22-C21-O21-C2
52	d	202	CDL	OA7-CA5-OA6-CA4
52	d	202	CDL	OB7-CB5-OB6-CB4
52	h	201	CDL	OB7-CB5-OB6-CB4
52	r	201	CDL	OA7-CA5-OA6-CA4
45	A	201	3PE	C32-C31-O31-C3
45	A	203	3PE	C32-C31-O31-C3
45	H	702	3PE	C32-C31-O31-C3
45	h	202	3PE	C32-C31-O31-C3
45	r	202	3PE	C32-C31-O31-C3
46	d	201	PC1	C32-C31-O31-C3
46	q	701	PC1	C32-C31-O31-C3
52	N	403	CDL	C31-CA7-OA8-CA6
45	A	201	3PE	C22-C21-O21-C2
52	X	201	CDL	C51-CB5-OB6-CB4
45	L	701	3PE	O32-C31-O31-C3
45	L	703	3PE	O32-C31-O31-C3
51	H	701	CHD	C20-C22-C23-C24
45	N	402	3PE	C32-C31-O31-C3
46	J	201	PC1	C32-C31-O31-C3
52	h	201	CDL	OA7-CA5-OA6-CA4
45	h	202	3PE	O32-C31-O31-C3
45	r	202	3PE	O32-C31-O31-C3
45	L	701	3PE	C32-C31-O31-C3
45	L	703	3PE	C32-C31-O31-C3
52	X	201	CDL	C31-CA7-OA8-CA6
46	B	301	PC1	O32-C31-O31-C3
58	T	101	EHZ	O4-C15-N2-C14
52	N	403	CDL	C51-CB5-OB6-CB4
56	P	501	NDP	C3D-C4D-C5D-O5D
51	L	704	CHD	C17-C20-C22-C23
46	B	301	PC1	C32-C31-O31-C3
52	L	702	CDL	C1-CB2-OB2-PB2
53	M	701	U10	C40-C39-C41-C42
53	M	701	U10	C38-C39-C41-C42
51	L	704	CHD	C21-C20-C22-C23
52	X	201	CDL	OA9-CA7-OA8-CA6
52	L	702	CDL	CB2-C1-CA2-OA2
52	N	403	CDL	OB7-CB5-OB6-CB4
45	I	204	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
46	B	303	PC1	C32-C31-O31-C3
46	M	703	PC1	C32-C31-O31-C3
52	d	202	CDL	C71-CB7-OB8-CB6
56	P	501	NDP	O4D-C1D-N1N-C6N
52	h	201	CDL	OB5-CB3-CB4-OB6
52	L	702	CDL	O1-C1-CA2-OA2
46	M	703	PC1	O21-C2-C3-O31
45	I	204	3PE	O32-C31-O31-C3
46	B	303	PC1	O32-C31-O31-C3
45	I	201	3PE	C22-C21-O21-C2
45	r	202	3PE	C31-C32-C33-C34
46	M	703	PC1	O32-C31-O31-C3
52	X	201	CDL	C71-CB7-OB8-CB6
45	h	202	3PE	C31-C32-C33-C34
52	N	403	CDL	CA7-C31-C32-C33
52	X	201	CDL	CA7-C31-C32-C33
45	N	402	3PE	C21-C22-C23-C24
52	N	403	CDL	CA5-C11-C12-C13
52	X	201	CDL	CA5-C11-C12-C13
52	r	201	CDL	CA5-C11-C12-C13
46	d	201	PC1	C21-C22-C23-C24
52	L	702	CDL	CB5-C51-C52-C53
52	r	201	CDL	CB5-C51-C52-C53
52	d	202	CDL	OB9-CB7-OB8-CB6
53	M	701	U10	C9-C11-C12-C13
45	N	401	3PE	C22-C23-C24-C25
45	M	702	3PE	C31-C32-C33-C34
52	L	702	CDL	CA7-C31-C32-C33
45	A	202	3PE	C1-O11-P-O13
45	A	203	3PE	C11-O13-P-O11
45	H	702	3PE	C1-O11-P-O13
45	H	702	3PE	C11-O13-P-O11
45	I	201	3PE	C1-O11-P-O13
45	I	201	3PE	C11-O13-P-O11
45	L	701	3PE	C1-O11-P-O13
45	L	703	3PE	C1-O11-P-O13
45	L	703	3PE	C11-O13-P-O11
45	M	702	3PE	C11-O13-P-O11
45	N	402	3PE	C1-O11-P-O13
45	h	202	3PE	C11-O13-P-O11
46	B	301	PC1	C11-O13-P-O11
46	B	303	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
52	L	702	CDL	CB2-OB2-PB2-OB5
52	N	403	CDL	CB3-OB5-PB2-OB2
52	X	201	CDL	CB3-OB5-PB2-OB2
52	d	202	CDL	CA3-OA5-PA1-OA2
52	d	202	CDL	CB2-OB2-PB2-OB5
52	h	201	CDL	CA3-OA5-PA1-OA2
52	r	201	CDL	CB3-OB5-PB2-OB2
45	I	201	3PE	O22-C21-O21-C2
52	L	702	CDL	C71-CB7-OB8-CB6
45	L	701	3PE	C22-C21-O21-C2
45	A	203	3PE	C24-C25-C26-C27
45	M	702	3PE	C23-C24-C25-C26
45	r	202	3PE	C3B-C3C-C3D-C3E
46	M	703	PC1	C2A-C2B-C2C-C2D
46	M	703	PC1	C34-C35-C36-C37
52	N	403	CDL	C12-C13-C14-C15
52	X	201	CDL	C62-C63-C64-C65
52	X	201	CDL	OB9-CB7-OB8-CB6
58	T	101	EHZ	C18-C17-C20-O6
58	T	101	EHZ	C19-C17-C20-O6
45	L	701	3PE	O22-C21-O21-C2
45	I	201	3PE	C3E-C3F-C3G-C3H
45	h	202	3PE	C28-C29-C2A-C2B
52	L	702	CDL	C32-C33-C34-C35
52	L	702	CDL	CB4-CB3-OB5-PB2
45	N	402	3PE	C37-C38-C39-C3A
46	M	703	PC1	C36-C37-C38-C39
52	X	201	CDL	O1-C1-CA2-OA2
52	X	201	CDL	O1-C1-CB2-OB2
45	N	402	3PE	C27-C28-C29-C2A
45	r	202	3PE	C2E-C2F-C2G-C2H
52	h	201	CDL	C31-CA7-OA8-CA6
45	H	702	3PE	C22-C23-C24-C25
46	M	703	PC1	C23-C24-C25-C26
52	L	702	CDL	C57-C58-C59-C60
52	h	201	CDL	C11-C12-C13-C14
52	r	201	CDL	C31-C32-C33-C34
52	N	403	CDL	CB7-C71-C72-C73
45	Y	601	3PE	C26-C27-C28-C29
46	B	303	PC1	C37-C38-C39-C3A
52	L	702	CDL	C42-C43-C44-C45
45	I	201	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
45	I	204	3PE	C22-C21-O21-C2
45	I	201	3PE	C29-C2A-C2B-C2C
45	r	202	3PE	C23-C24-C25-C26
58	U	101	EHZ	C2-C3-C4-C5
53	M	701	U10	C29-C31-C32-C33
45	L	701	3PE	C27-C28-C29-C2A
45	N	401	3PE	C28-C29-C2A-C2B
45	M	702	3PE	C34-C35-C36-C37
52	L	702	CDL	C41-C42-C43-C44
52	N	403	CDL	C55-C56-C57-C58
45	N	402	3PE	C2E-C2F-C2G-C2H
46	M	703	PC1	C28-C29-C2A-C2B
45	M	702	3PE	C26-C27-C28-C29
52	L	702	CDL	C37-C38-C39-C40
45	r	202	3PE	C29-C2A-C2B-C2C
52	d	202	CDL	C33-C34-C35-C36
59	o	201	MYR	C3-C4-C5-C6
45	I	204	3PE	O22-C21-O21-C2
52	N	403	CDL	C34-C35-C36-C37
52	h	201	CDL	C12-C13-C14-C15
45	M	702	3PE	C29-C2A-C2B-C2C
45	r	202	3PE	C38-C39-C3A-C3B
52	L	702	CDL	OB9-CB7-OB8-CB6
52	X	201	CDL	CB2-C1-CA2-OA2
45	A	201	3PE	C32-C33-C34-C35
52	d	202	CDL	C1-CB2-OB2-PB2
45	L	701	3PE	C35-C36-C37-C38
45	r	202	3PE	C36-C37-C38-C39
46	B	303	PC1	C31-C32-C33-C34
45	N	402	3PE	C22-C21-O21-C2
45	h	202	3PE	C23-C24-C25-C26
46	q	701	PC1	C34-C35-C36-C37
52	h	201	CDL	OA9-CA7-OA8-CA6
45	r	202	3PE	C27-C28-C29-C2A
46	q	701	PC1	C22-C23-C24-C25
52	h	201	CDL	C56-C57-C58-C59
52	L	702	CDL	OB7-CB5-OB6-CB4
45	I	201	3PE	C32-C31-O31-C3
45	N	402	3PE	C3B-C3C-C3D-C3E
45	I	204	3PE	C23-C24-C25-C26
45	I	204	3PE	C25-C26-C27-C28
45	L	703	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
46	J	201	PC1	C23-C24-C25-C26
45	Y	601	3PE	C22-C21-O21-C2
46	J	201	PC1	C22-C21-O21-C2
52	L	702	CDL	C11-CA5-OA6-CA4
52	L	702	CDL	C51-CB5-OB6-CB4
52	L	702	CDL	OA5-CA3-CA4-OA6
45	Y	601	3PE	O22-C21-O21-C2
46	J	201	PC1	O22-C21-O21-C2
52	L	702	CDL	OA7-CA5-OA6-CA4
45	L	701	3PE	C2A-C2B-C2C-C2D
45	A	202	3PE	O21-C2-C3-O31
45	L	701	3PE	C25-C26-C27-C28
58	U	101	EHZ	C1-C2-C3-C4
53	M	701	U10	C28-C29-C31-C32
45	A	202	3PE	C28-C29-C2A-C2B
45	I	204	3PE	C33-C34-C35-C36
45	N	402	3PE	O22-C21-O21-C2
45	A	202	3PE	C35-C36-C37-C38
46	q	701	PC1	C11-O13-P-O11
46	q	701	PC1	C1-O11-P-O13
52	X	201	CDL	CB2-OB2-PB2-OB5
52	d	202	CDL	CA2-OA2-PA1-OA5
45	I	201	3PE	C39-C3A-C3B-C3C
59	o	201	MYR	C2-C3-C4-C5
45	I	201	3PE	O32-C31-O31-C3
52	h	201	CDL	OB5-CB3-CB4-CB6
45	r	202	3PE	C32-C33-C34-C35
46	J	201	PC1	C29-C2A-C2B-C2C
45	N	402	3PE	C32-C33-C34-C35
46	B	303	PC1	C26-C27-C28-C29
52	X	201	CDL	C54-C55-C56-C57
52	X	201	CDL	C59-C60-C61-C62
45	I	201	3PE	C38-C39-C3A-C3B
46	d	201	PC1	C1-C2-C3-O31
52	L	702	CDL	CB3-CB4-CB6-OB8
52	N	403	CDL	CA3-CA4-CA6-OA8
52	N	403	CDL	C19-C20-C21-C22
52	N	403	CDL	CB3-CB4-CB6-OB8
52	r	201	CDL	CA3-CA4-CA6-OA8
45	I	201	3PE	C31-C32-C33-C34
52	X	201	CDL	C19-C20-C21-C22
52	X	201	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
45	N	402	3PE	C3D-C3E-C3F-C3G
52	N	403	CDL	C14-C15-C16-C17
45	L	703	3PE	C22-C21-O21-C2
53	M	701	U10	C30-C29-C31-C32
52	h	201	CDL	CB5-C51-C52-C53
45	h	202	3PE	C25-C26-C27-C28
45	r	202	3PE	C1-C2-O21-C21
52	N	403	CDL	C33-C34-C35-C36
45	M	702	3PE	C32-C31-O31-C3
52	X	201	CDL	C17-C18-C19-C20
59	o	201	MYR	C11-C12-C13-C14
45	I	201	3PE	C35-C36-C37-C38
45	A	201	3PE	C2C-C2D-C2E-C2F
52	X	201	CDL	C74-C75-C76-C77
46	J	201	PC1	C2E-C2F-C2G-C2H
53	M	701	U10	C35-C34-C36-C37
46	J	201	PC1	C2B-C2C-C2D-C2E
53	M	701	U10	C33-C34-C36-C37
45	L	701	3PE	C28-C29-C2A-C2B
58	T	101	EHZ	C5-C6-C7-C8
52	X	201	CDL	C12-C13-C14-C15
45	A	203	3PE	C35-C36-C37-C38
45	L	701	3PE	O11-C1-C2-C3
45	L	703	3PE	O11-C1-C2-C3
45	M	702	3PE	O11-C1-C2-C3
45	Y	601	3PE	O11-C1-C2-C3
46	B	301	PC1	O11-C1-C2-C3
52	L	702	CDL	OA5-CA3-CA4-CA6
45	N	401	3PE	O13-C11-C12-N
52	N	403	CDL	C18-C19-C20-C21
53	M	701	U10	C15-C14-C16-C17
52	r	201	CDL	O1-C1-CA2-OA2
52	X	201	CDL	C11-CA5-OA6-CA4
52	r	201	CDL	C32-C31-CA7-OA8
45	L	701	3PE	C2-C1-O11-P
46	B	301	PC1	C29-C2A-C2B-C2C
52	N	403	CDL	C31-C32-C33-C34
52	d	202	CDL	C41-C42-C43-C44
52	d	202	CDL	C76-C77-C78-C79
45	L	703	3PE	C25-C26-C27-C28
52	X	201	CDL	C21-C22-C23-C24
52	d	202	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
45	A	202	3PE	C1-C2-C3-O31
45	H	702	3PE	C1-C2-C3-O31
45	M	702	3PE	C1-C2-C3-O31
46	J	201	PC1	C1-C2-C3-O31
46	M	703	PC1	C1-C2-C3-O31
46	B	303	PC1	C3B-C3C-C3D-C3E
45	I	204	3PE	C11-O13-P-O11
45	L	701	3PE	C11-O13-P-O11
45	N	402	3PE	C26-C27-C28-C29
52	X	201	CDL	C58-C59-C60-C61
45	A	203	3PE	O11-C1-C2-O21
52	L	702	CDL	OB5-CB3-CB4-OB6
52	r	201	CDL	OB5-CB3-CB4-OB6
45	M	702	3PE	O32-C31-O31-C3
45	h	202	3PE	C24-C25-C26-C27
52	d	202	CDL	C42-C43-C44-C45
52	h	201	CDL	C55-C56-C57-C58
45	L	701	3PE	C3D-C3E-C3F-C3G
58	U	101	EHZ	C5-C6-C7-O1
46	B	301	PC1	O21-C2-C3-O31
52	N	403	CDL	OB6-CB4-CB6-OB8
46	B	301	PC1	C26-C27-C28-C29
46	J	201	PC1	C22-C23-C24-C25
52	h	201	CDL	C22-C23-C24-C25
45	L	703	3PE	O22-C21-O21-C2
46	B	301	PC1	C34-C35-C36-C37
45	h	202	3PE	C2-C1-O11-P
46	M	703	PC1	C2-C1-O11-P
52	X	201	CDL	CA4-CA3-OA5-PA1
58	T	101	EHZ	C21-C22-C23-C24
58	T	101	EHZ	O2-C9-S1-C10
52	h	201	CDL	C53-C54-C55-C56
45	A	201	3PE	O11-C1-C2-C3
45	A	202	3PE	O11-C1-C2-C3
52	L	702	CDL	OB5-CB3-CB4-CB6
52	h	201	CDL	OA5-CA3-CA4-CA6
52	d	202	CDL	O1-C1-CA2-OA2
46	B	301	PC1	C3C-C3D-C3E-C3F
46	B	303	PC1	C39-C3A-C3B-C3C
46	M	703	PC1	C2C-C2D-C2E-C2F
45	r	202	3PE	C3C-C3D-C3E-C3F
45	I	201	3PE	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
52	L	702	CDL	C36-C37-C38-C39
58	U	101	EHZ	C21-C22-C23-C24
59	o	201	MYR	C10-C11-C12-C13
45	A	203	3PE	C23-C24-C25-C26
59	o	201	MYR	C7-C8-C9-C10
49	F	501	FMN	O2'-C2'-C3'-C4'
53	M	701	U10	C5-C4-O4-C4M
45	L	701	3PE	C1-C2-C3-O31
46	q	701	PC1	C1-C2-C3-O31
45	L	703	3PE	C29-C2A-C2B-C2C
45	A	202	3PE	O11-C1-C2-O21
45	L	701	3PE	O11-C1-C2-O21
45	Y	601	3PE	O11-C1-C2-O21
52	d	202	CDL	OB5-CB3-CB4-OB6
46	B	301	PC1	C33-C34-C35-C36
52	X	201	CDL	OA7-CA5-OA6-CA4
58	U	101	EHZ	O1-C7-C8-C9
52	X	201	CDL	C51-C52-C53-C54
45	H	702	3PE	O21-C2-C3-O31
46	J	201	PC1	O21-C2-C3-O31
46	d	201	PC1	O21-C2-C3-O31
46	q	701	PC1	O21-C2-C3-O31
52	L	702	CDL	OB6-CB4-CB6-OB8
52	r	201	CDL	OA6-CA4-CA6-OA8
52	N	403	CDL	C71-CB7-OB8-CB6
46	J	201	PC1	C28-C29-C2A-C2B
52	X	201	CDL	C71-C72-C73-C74
52	X	201	CDL	C72-C73-C74-C75
45	L	701	3PE	C37-C38-C39-C3A
59	o	201	MYR	C9-C10-C11-C12
52	h	201	CDL	C71-CB7-OB8-CB6
45	A	202	3PE	C11-O13-P-O11
52	L	702	CDL	CA2-OA2-PA1-OA5
45	H	702	3PE	C29-C2A-C2B-C2C
52	X	201	CDL	C20-C21-C22-C23
52	d	202	CDL	CB4-CB3-OB5-PB2
45	r	202	3PE	C35-C36-C37-C38
45	A	201	3PE	C1-O11-P-O14
45	A	203	3PE	C1-O11-P-O14
45	I	201	3PE	C1-O11-P-O14
45	L	703	3PE	C1-O11-P-O14
45	L	703	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
45	M	702	3PE	C11-O13-P-O14
45	N	402	3PE	C1-O11-P-O14
45	N	402	3PE	C11-O13-P-O12
45	h	202	3PE	C11-O13-P-O14
46	B	301	PC1	C11-O13-P-O12
46	B	303	PC1	C11-O13-P-O14
46	q	701	PC1	C11-O13-P-O12
46	q	701	PC1	C11-O13-P-O14
52	L	702	CDL	CA2-OA2-PA1-OA3
52	L	702	CDL	CA2-OA2-PA1-OA4
52	X	201	CDL	CA3-OA5-PA1-OA4
52	X	201	CDL	CB2-OB2-PB2-OB4
52	X	201	CDL	CB3-OB5-PB2-OB3
52	d	202	CDL	CA2-OA2-PA1-OA4
52	d	202	CDL	CB2-OB2-PB2-OB4
52	d	202	CDL	CB3-OB5-PB2-OB3
52	r	201	CDL	CB2-OB2-PB2-OB3
52	r	201	CDL	CB3-OB5-PB2-OB3
52	r	201	CDL	CB3-OB5-PB2-OB4
58	T	101	EHZ	C6-C7-C8-C9
45	I	201	3PE	C24-C25-C26-C27
45	A	203	3PE	O11-C1-C2-C3
45	A	203	3PE	C31-C32-C33-C34
45	A	202	3PE	C12-C11-O13-P
45	M	702	3PE	C12-C11-O13-P
46	B	301	PC1	C12-C11-O13-P
52	N	403	CDL	OB9-CB7-OB8-CB6
45	I	204	3PE	O11-C1-C2-O21
45	L	703	3PE	O11-C1-C2-O21
45	M	702	3PE	O11-C1-C2-O21
45	h	202	3PE	O11-C1-C2-O21
46	B	301	PC1	O11-C1-C2-O21
45	H	702	3PE	O31-C31-C32-C33
45	r	202	3PE	C39-C3A-C3B-C3C
45	I	201	3PE	C36-C37-C38-C39
45	A	201	3PE	C35-C36-C37-C38
45	Y	601	3PE	C1-C2-C3-O31
46	B	301	PC1	O13-C11-C12-N
46	M	703	PC1	C2B-C2C-C2D-C2E
46	d	201	PC1	C33-C34-C35-C36
46	q	701	PC1	O13-C11-C12-N
58	U	101	EHZ	C16-C17-C20-O6

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Mol	Chain	Res	Type	Atoms
52	h	201	CDL	OB9-CB7-OB8-CB6
46	q	701	PC1	C25-C26-C27-C28
53	M	701	U10	C13-C14-C16-C17
54	O	401	GTP	PG-O3B-PB-O3A
52	r	201	CDL	C14-C15-C16-C17
46	B	303	PC1	C35-C36-C37-C38
46	q	701	PC1	C23-C24-C25-C26
52	d	202	CDL	C38-C39-C40-C41
46	J	201	PC1	C33-C34-C35-C36
56	P	501	NDP	O4B-C4B-C5B-O5B
46	M	703	PC1	C32-C33-C34-C35
58	T	101	EHZ	C5-C6-C7-O1
46	M	703	PC1	C24-C25-C26-C27
58	U	101	EHZ	C18-C17-C20-O6
45	A	202	3PE	C31-C32-C33-C34
46	B	303	PC1	C33-C34-C35-C36
45	Y	601	3PE	O21-C21-C22-C23
45	h	202	3PE	O11-C1-C2-C3
52	d	202	CDL	CA2-C1-CB2-OB2
45	I	201	3PE	C32-C33-C34-C35
52	X	201	CDL	C53-C54-C55-C56
52	h	201	CDL	C31-C32-C33-C34
45	L	703	3PE	O21-C21-C22-C23
45	N	402	3PE	C11-O13-P-O11
45	Y	601	3PE	C1-O11-P-O13
45	h	202	3PE	C1-O11-P-O13
52	r	201	CDL	CA3-OA5-PA1-OA2
52	h	201	CDL	C20-C21-C22-C23
45	A	203	3PE	C26-C27-C28-C29
46	B	301	PC1	C38-C39-C3A-C3B
45	N	401	3PE	C1-C2-C3-O31
46	B	303	PC1	C3E-C3F-C3G-C3H
56	P	501	NDP	PN-O3-PA-O1A
45	L	701	3PE	C29-C2A-C2B-C2C
45	A	201	3PE	C27-C28-C29-C2A
45	h	202	3PE	C26-C27-C28-C29
46	B	303	PC1	C25-C26-C27-C28
52	X	201	CDL	C60-C61-C62-C63
46	q	701	PC1	C32-C33-C34-C35
59	o	201	MYR	C6-C7-C8-C9
52	h	201	CDL	C18-C19-C20-C21
45	A	203	3PE	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
45	A	202	3PE	C25-C26-C27-C28
45	I	201	3PE	C2C-C2D-C2E-C2F
52	r	201	CDL	C13-C14-C15-C16
45	A	202	3PE	C33-C34-C35-C36
52	d	202	CDL	C74-C75-C76-C77
45	H	702	3PE	O32-C31-C32-C33
45	M	702	3PE	C28-C29-C2A-C2B
52	L	702	CDL	C1-CA2-OA2-PA1
52	N	403	CDL	C1-CA2-OA2-PA1
52	N	403	CDL	C39-C40-C41-C42
58	U	101	EHZ	S1-C10-C11-N1
49	F	501	FMN	O2'-C2'-C3'-O3'
45	L	703	3PE	C28-C29-C2A-C2B
45	r	202	3PE	C33-C34-C35-C36
45	h	202	3PE	C32-C33-C34-C35
52	L	702	CDL	C14-C15-C16-C17
45	h	202	3PE	C1-C2-C3-O31
58	U	101	EHZ	C19-C17-C20-O6
45	L	701	3PE	C34-C35-C36-C37
46	q	701	PC1	C24-C25-C26-C27
52	N	403	CDL	O1-C1-CA2-OA2
45	I	201	3PE	C3C-C3D-C3E-C3F
52	N	403	CDL	C38-C39-C40-C41
58	U	101	EHZ	C7-C8-C9-O2
45	N	401	3PE	C32-C33-C34-C35
45	L	701	3PE	C3-C2-O21-C21
45	N	402	3PE	C1-C2-O21-C21
52	d	202	CDL	CB6-CB4-OB6-CB5
52	h	201	CDL	CB6-CB4-OB6-CB5
52	h	201	CDL	C51-C52-C53-C54
45	Y	601	3PE	C24-C25-C26-C27
52	X	201	CDL	OB5-CB3-CB4-OB6
45	M	702	3PE	C27-C28-C29-C2A
52	L	702	CDL	C40-C41-C42-C43
52	L	702	CDL	C55-C56-C57-C58
45	L	701	3PE	C3A-C3B-C3C-C3D
58	U	101	EHZ	C11-C10-S1-C9
45	M	702	3PE	O21-C2-C3-O31
52	r	201	CDL	OB6-CB4-CB6-OB8
45	N	402	3PE	C2D-C2E-C2F-C2G
46	B	301	PC1	C28-C29-C2A-C2B
52	N	403	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
52	h	201	CDL	C57-C58-C59-C60
52	r	201	CDL	OB9-CB7-OB8-CB6
54	O	401	GTP	PB-O3A-PA-O1A
52	N	403	CDL	C52-C51-CB5-OB6
45	A	202	3PE	C23-C24-C25-C26
52	X	201	CDL	C61-C62-C63-C64
46	q	701	PC1	C36-C37-C38-C39
51	L	704	CHD	C22-C23-C24-O26
52	X	201	CDL	C13-C14-C15-C16
45	I	201	3PE	O11-C1-C2-O21
52	d	202	CDL	OB5-CB3-CB4-CB6
52	r	201	CDL	OB5-CB3-CB4-CB6
45	I	201	3PE	O13-C11-C12-N
45	A	201	3PE	O21-C21-C22-C23
52	X	201	CDL	CA2-C1-CB2-OB2
45	L	701	3PE	O21-C2-C3-O31
52	d	202	CDL	OA6-CA4-CA6-OA8
52	r	201	CDL	C15-C16-C17-C18
52	h	201	CDL	CA5-C11-C12-C13
52	r	201	CDL	C71-CB7-OB8-CB6
52	X	201	CDL	CA3-OA5-PA1-OA2
52	X	201	CDL	C64-C65-C66-C67
51	L	704	CHD	C22-C23-C24-O25
45	N	402	3PE	C29-C2A-C2B-C2C
45	L	703	3PE	C32-C33-C34-C35
45	N	401	3PE	C33-C34-C35-C36
45	A	201	3PE	C34-C35-C36-C37
45	A	202	3PE	C21-C22-C23-C24
52	X	201	CDL	C32-C31-CA7-OA8
52	r	201	CDL	C52-C51-CB5-OB6
45	A	201	3PE	C24-C25-C26-C27
45	A	203	3PE	O31-C31-C32-C33
52	d	202	CDL	CA3-CA4-CA6-OA8
46	J	201	PC1	O11-C1-C2-O21
52	d	202	CDL	C31-C32-C33-C34
59	o	201	MYR	C5-C6-C7-C8
45	h	202	3PE	O21-C21-C22-C23
52	h	201	CDL	C52-C51-CB5-OB6
52	r	201	CDL	C32-C31-CA7-OA9
52	L	702	CDL	CA2-C1-CB2-OB2
46	B	301	PC1	C24-C25-C26-C27
52	L	702	CDL	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
45	I	204	3PE	C28-C29-C2A-C2B
45	A	202	3PE	C36-C37-C38-C39
45	I	201	3PE	O11-C1-C2-C3
45	N	402	3PE	O21-C21-C22-C23
45	A	201	3PE	O21-C2-C3-O31
45	L	703	3PE	O21-C2-C3-O31
45	H	702	3PE	O21-C21-C22-C23
45	h	202	3PE	O31-C31-C32-C33
45	r	202	3PE	O21-C21-C22-C23
52	h	201	CDL	C32-C31-CA7-OA8
46	d	201	PC1	C36-C37-C38-C39
45	r	202	3PE	C2C-C2D-C2E-C2F
52	h	201	CDL	CB4-CB3-OB5-PB2
45	r	202	3PE	C37-C38-C39-C3A
54	O	401	GTP	PG-O3B-PB-O1B
56	P	501	NDP	PN-O3-PA-O2A
45	N	401	3PE	C2A-C2B-C2C-C2D
52	d	202	CDL	C71-C72-C73-C74
45	r	202	3PE	C2F-C2G-C2H-C2I
52	X	201	CDL	C32-C31-CA7-OA9
46	B	301	PC1	C1-C2-C3-O31
52	h	201	CDL	C14-C15-C16-C17
46	d	201	PC1	O22-C21-O21-C2
45	N	401	3PE	C2-C1-O11-P
45	h	202	3PE	O32-C31-C32-C33
45	r	202	3PE	O22-C21-C22-C23
45	A	201	3PE	C28-C29-C2A-C2B
45	A	202	3PE	C11-O13-P-O14
45	I	204	3PE	C11-O13-P-O12
45	N	401	3PE	C1-O11-P-O14
45	N	401	3PE	C11-O13-P-O14
45	Y	601	3PE	C1-O11-P-O14
45	h	202	3PE	C1-O11-P-O14
46	B	303	PC1	C1-O11-P-O14
46	d	201	PC1	C1-O11-P-O12
52	d	202	CDL	CA2-OA2-PA1-OA3
52	d	202	CDL	CB2-OB2-PB2-OB3
52	h	201	CDL	CB3-OB5-PB2-OB3
45	I	204	3PE	O11-C1-C2-C3
52	r	201	CDL	OA5-CA3-CA4-CA6
45	h	202	3PE	O22-C21-C22-C23
52	h	201	CDL	C52-C51-CB5-OB7

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Mol	Chain	Res	Type	Atoms
52	r	201	CDL	C52-C51-CB5-OB7
52	X	201	CDL	C52-C51-CB5-OB6
45	A	203	3PE	O32-C31-C32-C33
45	N	402	3PE	O22-C21-C22-C23
45	L	701	3PE	C2B-C2C-C2D-C2E
45	A	202	3PE	C2C-C2D-C2E-C2F
45	N	401	3PE	C29-C2A-C2B-C2C
46	J	201	PC1	C24-C25-C26-C27
45	I	201	3PE	C12-C11-O13-P
45	N	402	3PE	C12-C11-O13-P
45	N	402	3PE	C3-C2-O21-C21
45	r	202	3PE	C12-C11-O13-P
52	L	702	CDL	CB6-CB4-OB6-CB5
52	L	702	CDL	C61-C62-C63-C64
45	r	202	3PE	O31-C31-C32-C33
45	Y	601	3PE	C29-C2A-C2B-C2C
45	H	702	3PE	O22-C21-C22-C23
45	L	701	3PE	C24-C25-C26-C27
46	d	201	PC1	O31-C31-C32-C33
52	h	201	CDL	C32-C31-CA7-OA9
52	d	202	CDL	OA5-CA3-CA4-OA6
58	T	101	EHZ	S1-C10-C11-N1
46	q	701	PC1	O21-C21-C22-C23
45	M	702	3PE	C36-C37-C38-C39
45	Y	601	3PE	C32-C33-C34-C35
46	d	201	PC1	O21-C21-C22-C23
58	T	101	EHZ	C10-C11-N1-C12
52	X	201	CDL	C52-C51-CB5-OB7

There are no ring outliers.

21 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	U	101	EHZ	1	0
53	M	701	U10	6	0
52	L	702	CDL	1	0
51	L	704	CHD	1	0
45	N	402	3PE	1	0
45	I	201	3PE	1	0
45	L	701	3PE	1	0
49	F	501	FMN	1	0
58	T	101	EHZ	1	0

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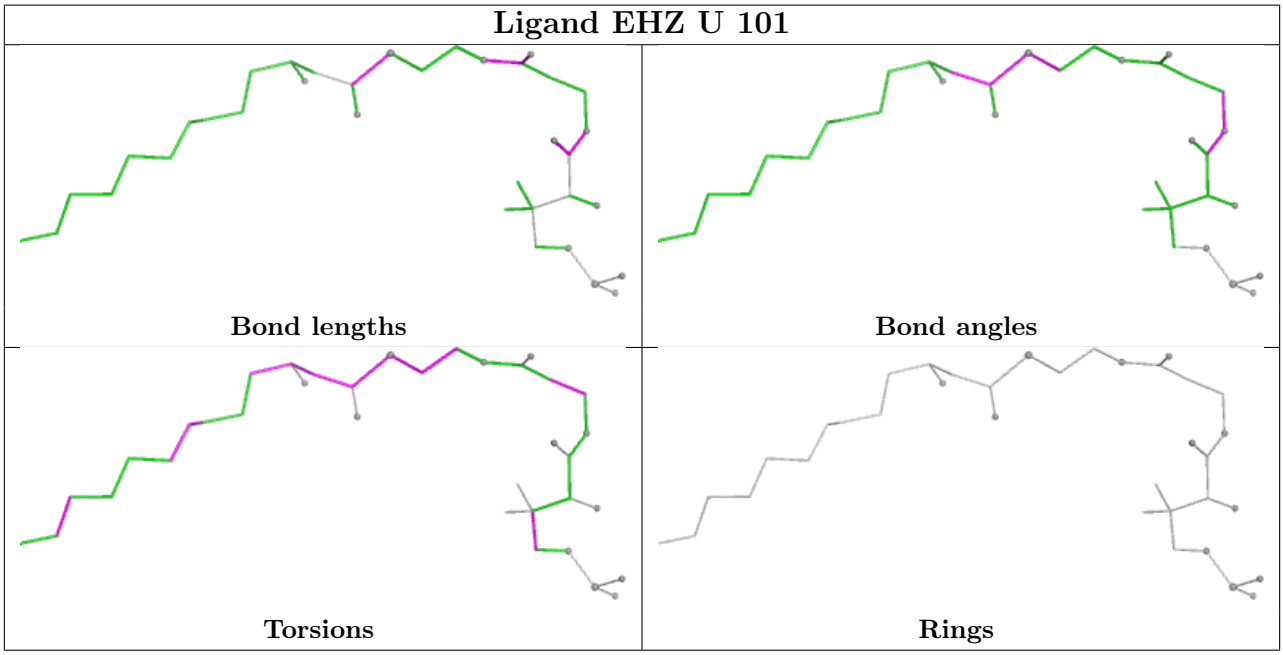
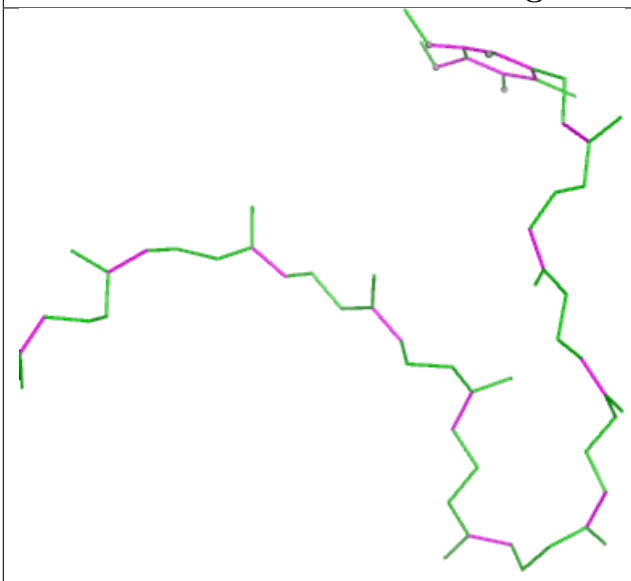
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	N	403	CDL	2	0
52	r	201	CDL	1	0
46	M	703	PC1	1	0
46	d	201	PC1	2	0
51	H	701	CHD	7	0
47	F	502	SF4	1	0
45	M	702	3PE	2	0
52	h	201	CDL	1	0
45	N	401	3PE	1	0
46	J	201	PC1	1	0
52	d	202	CDL	1	0
56	P	501	NDP	2	0

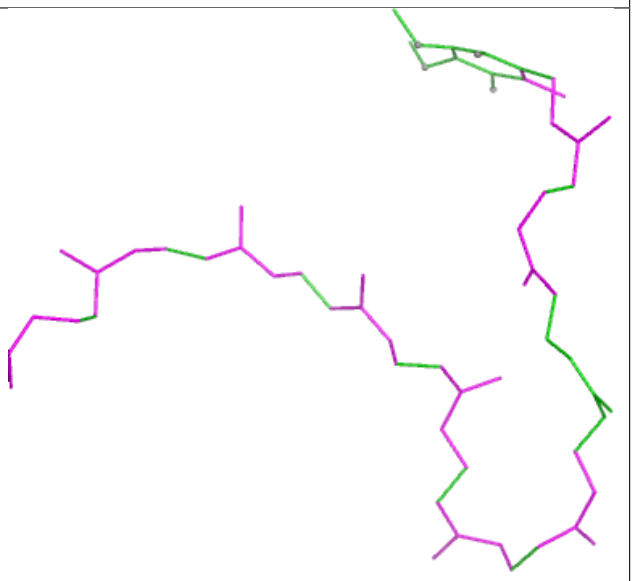
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



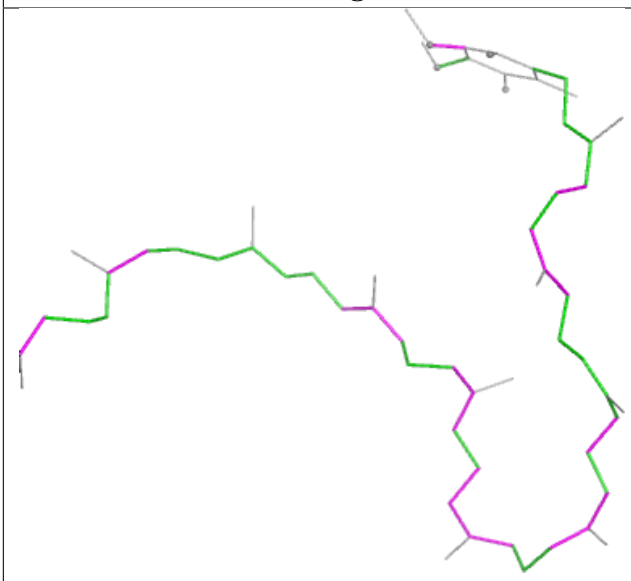
Ligand U10 M 701



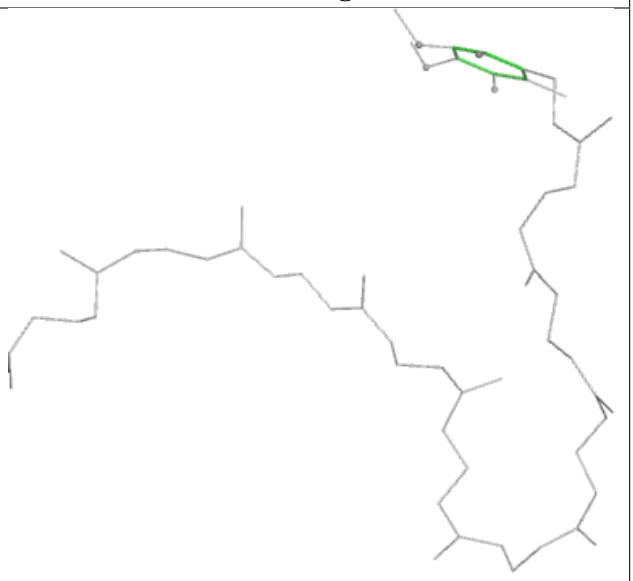
Bond lengths



Bond angles

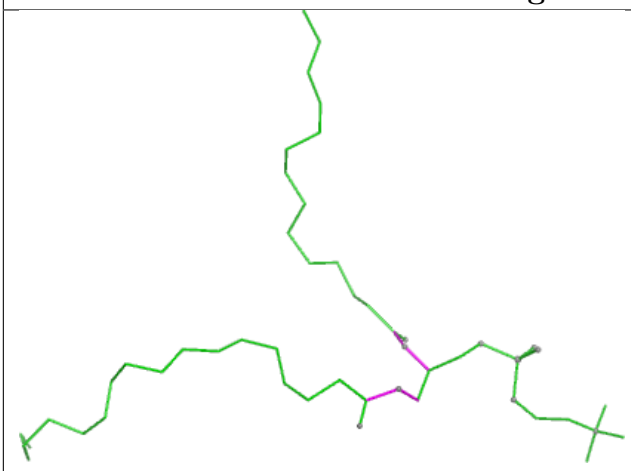


Torsions

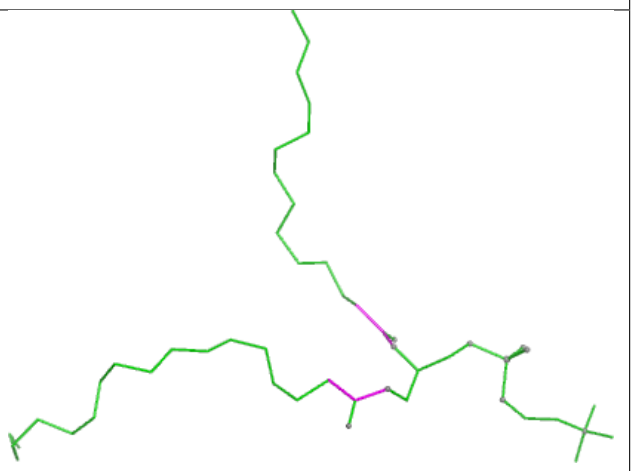


Rings

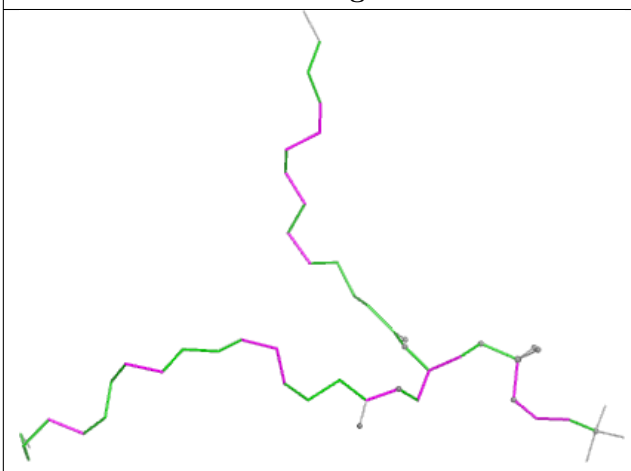
Ligand PC1 B 301



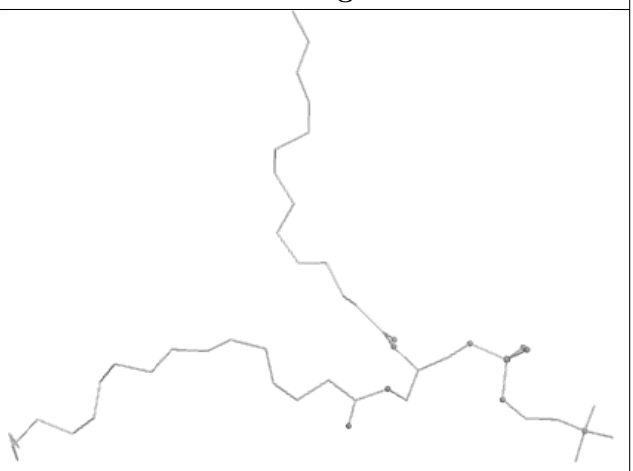
Bond lengths



Bond angles

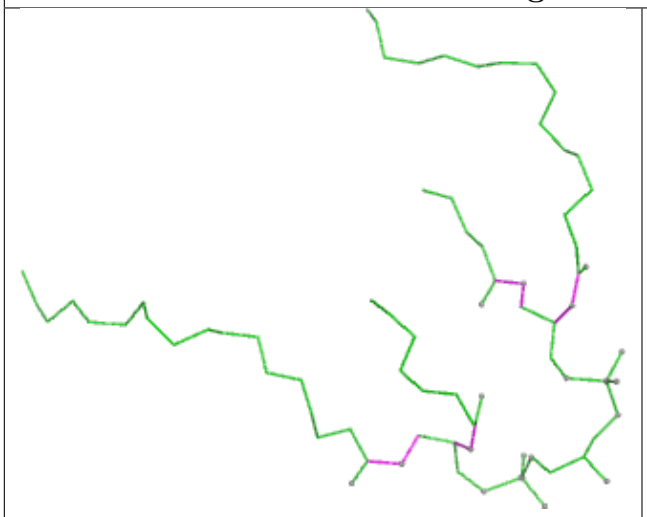


Torsions

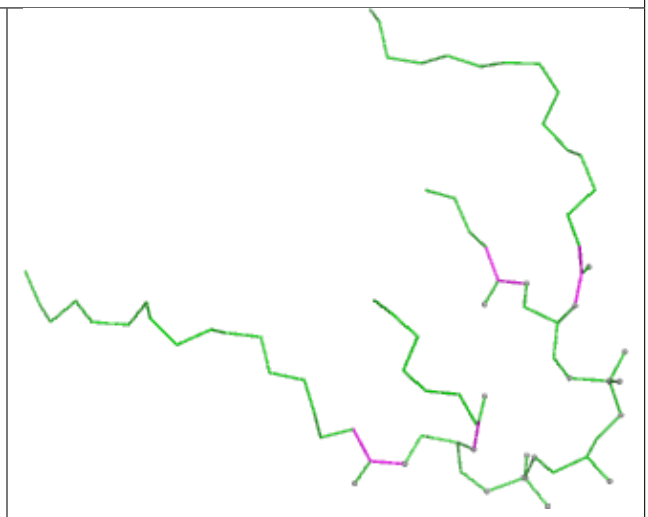


Rings

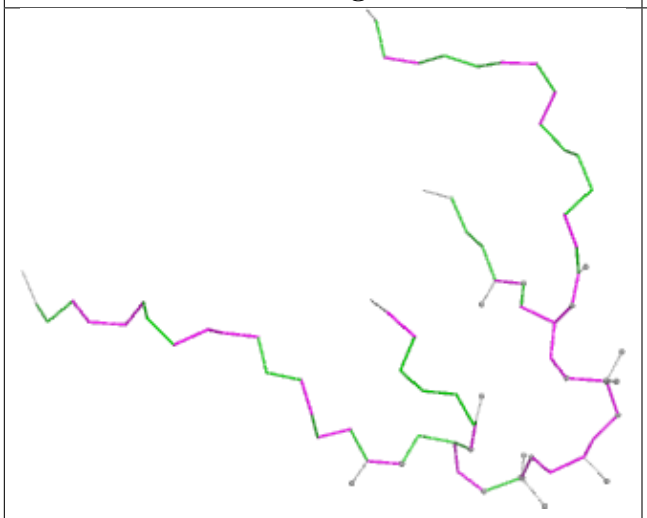
Ligand CDL L 702



Bond lengths



Bond angles

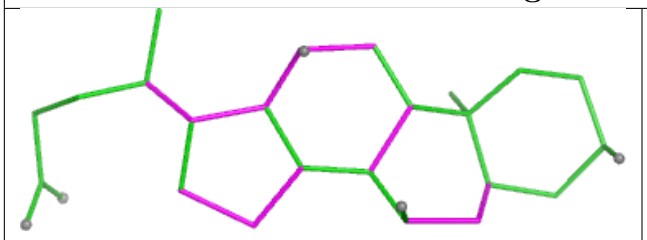


Torsions

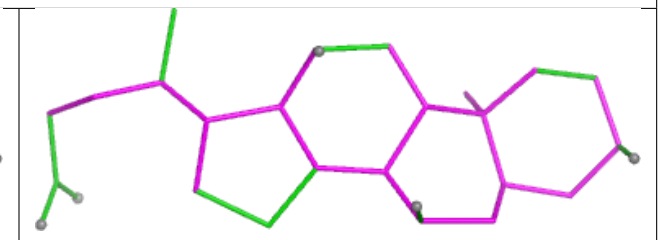


Rings

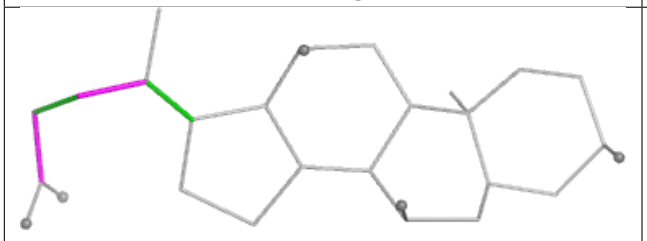
Ligand CHD L 704



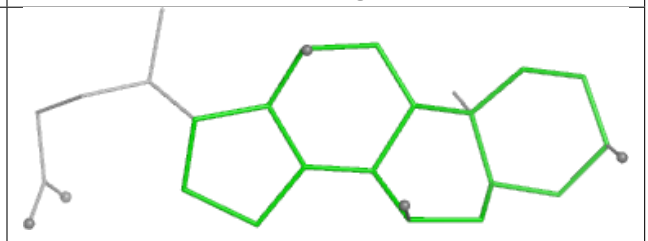
Bond lengths



Bond angles

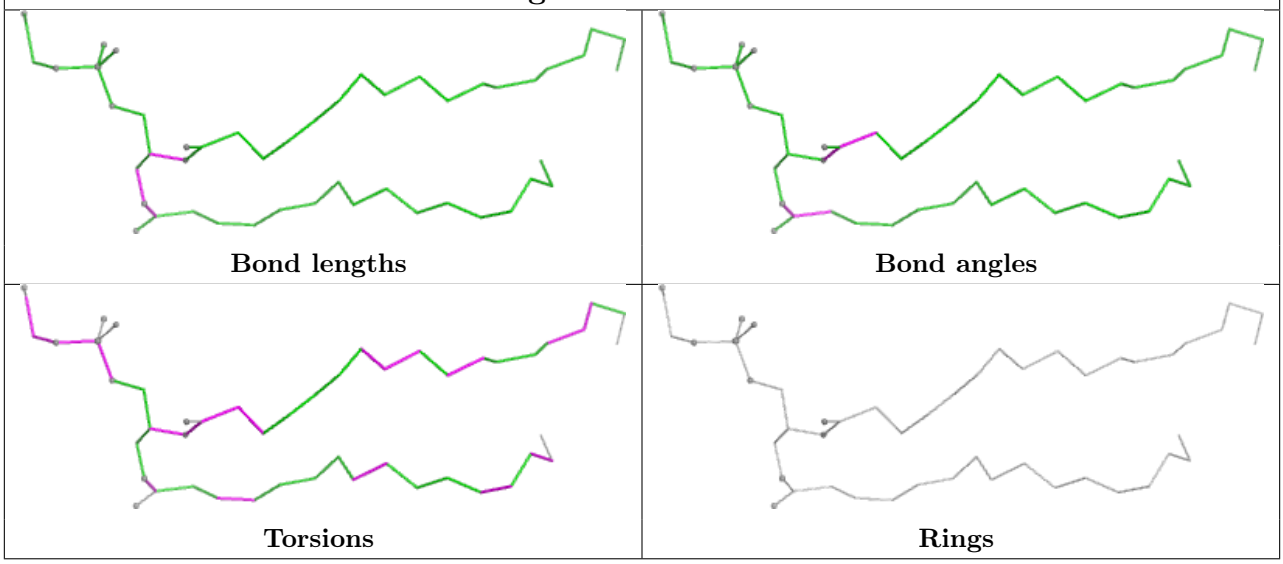


Torsions

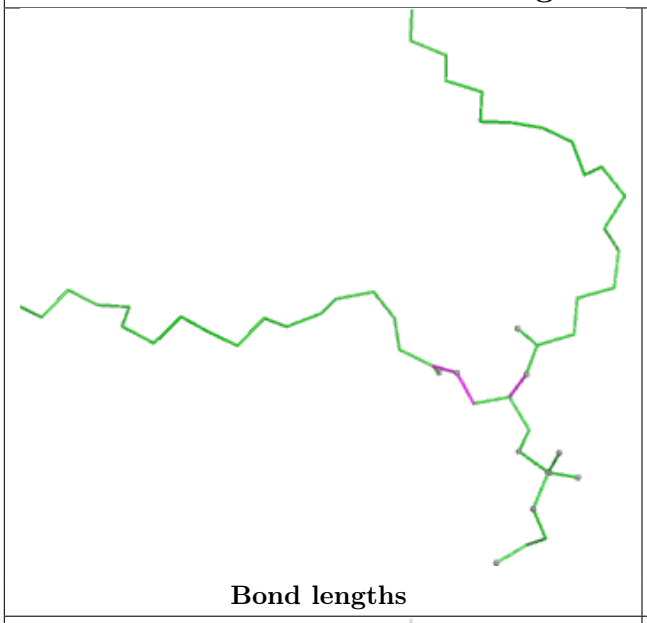


Rings

Ligand 3PE N 402



Ligand 3PE I 201



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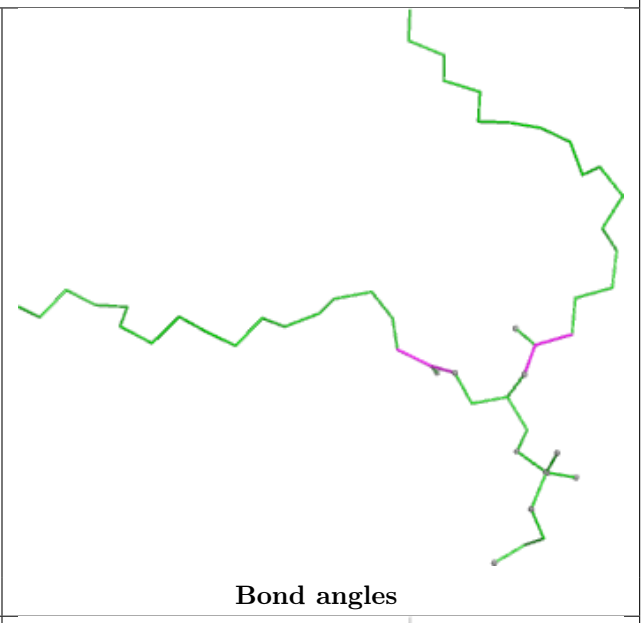
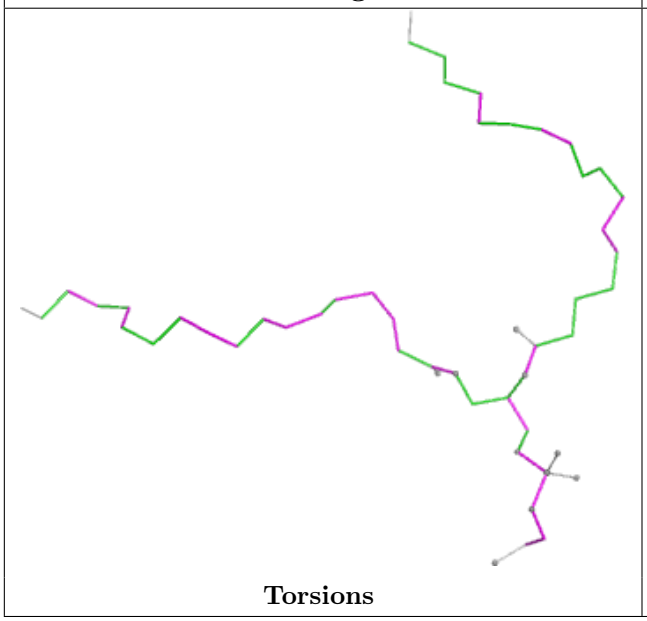


Bond angles



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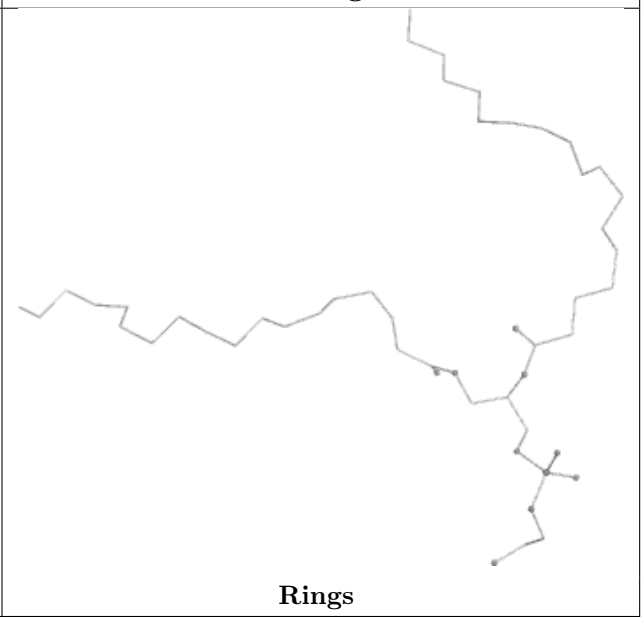

Rings

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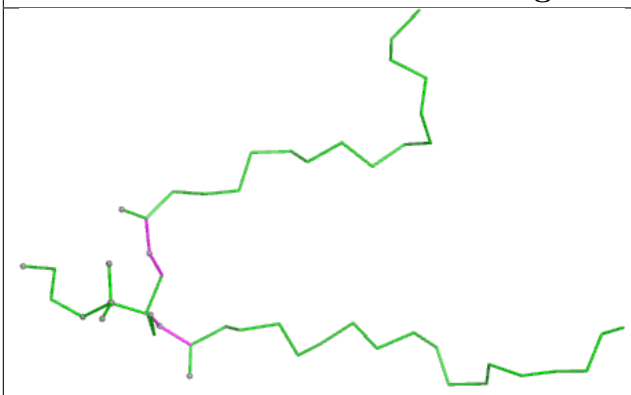

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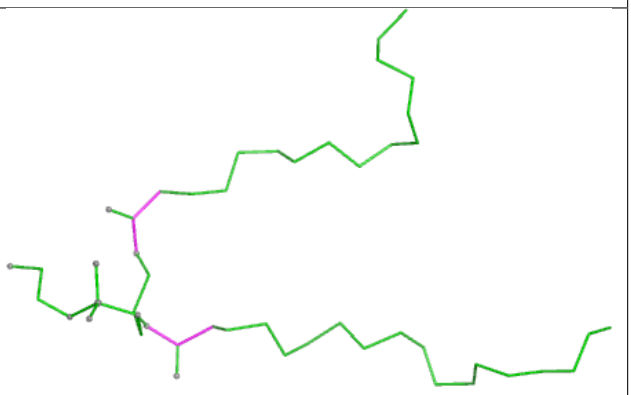
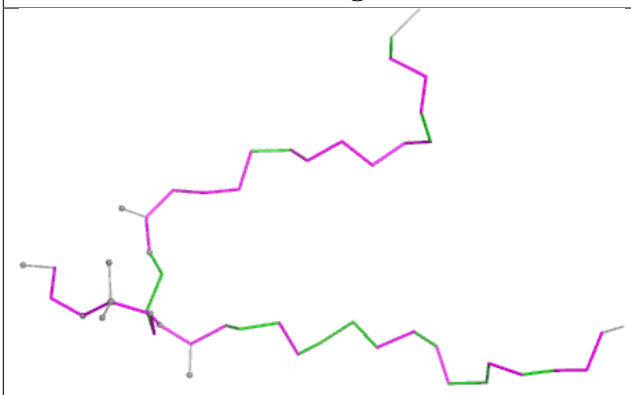


Bond angles

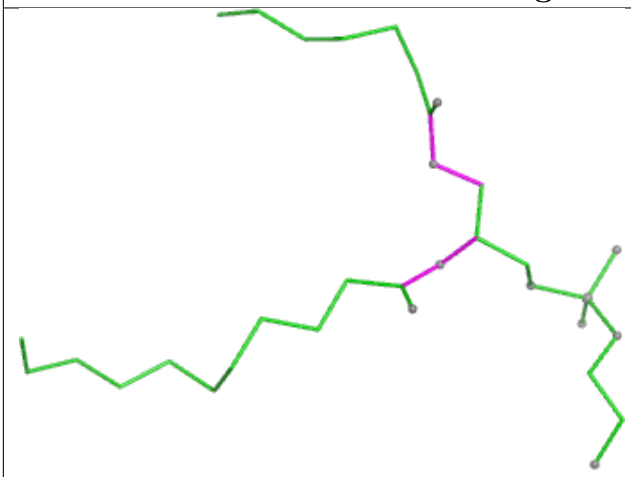


Torsions



Rings

Ligand 3PE I 204



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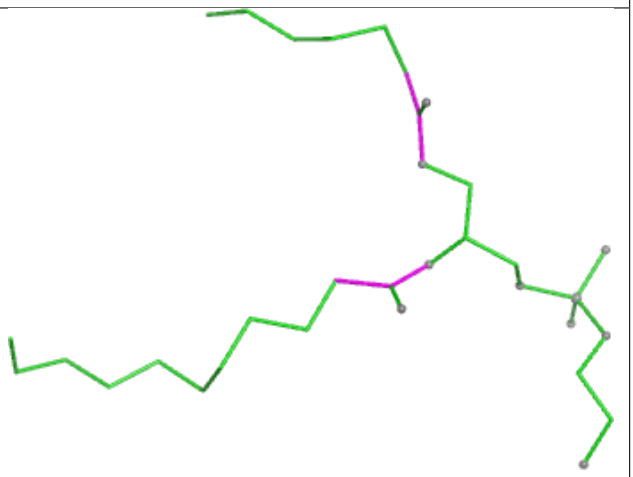

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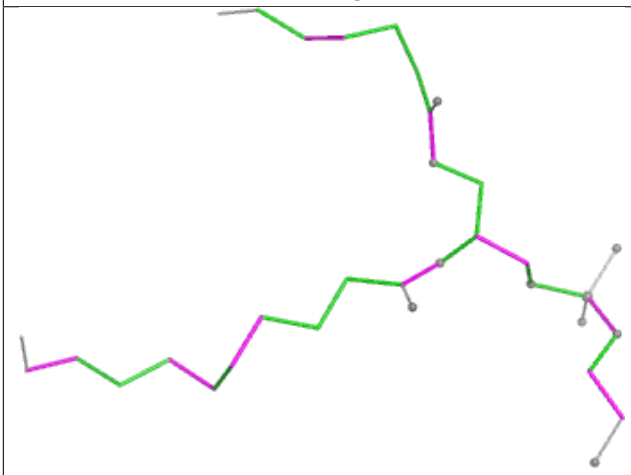

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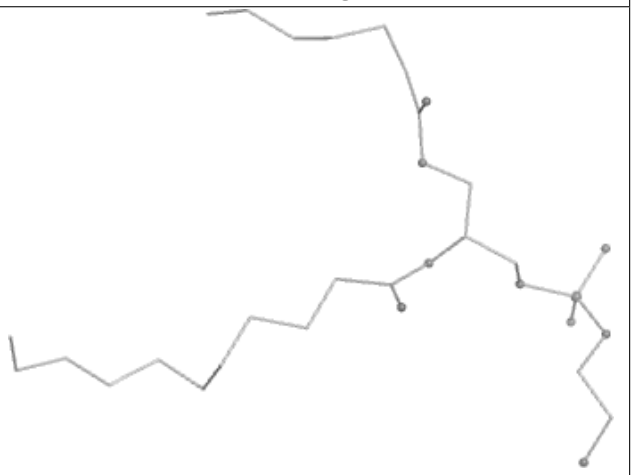
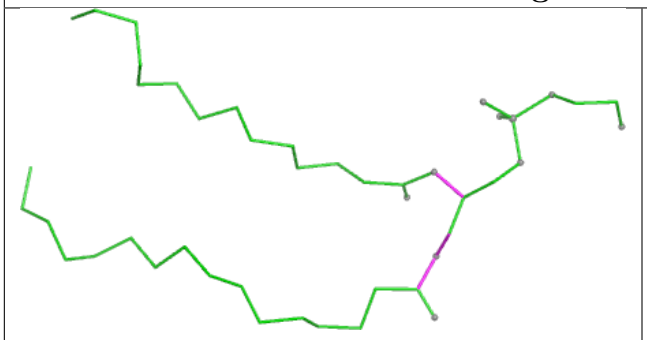


Rings

Ligand 3PE L 701



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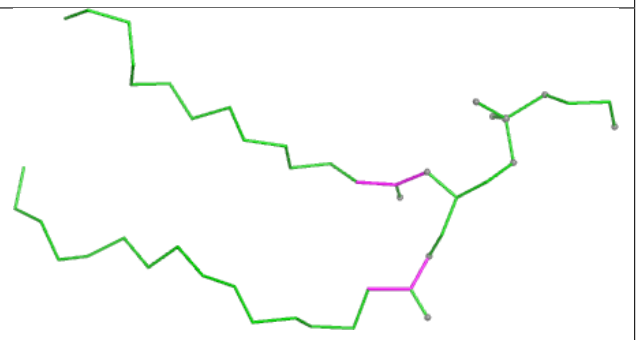
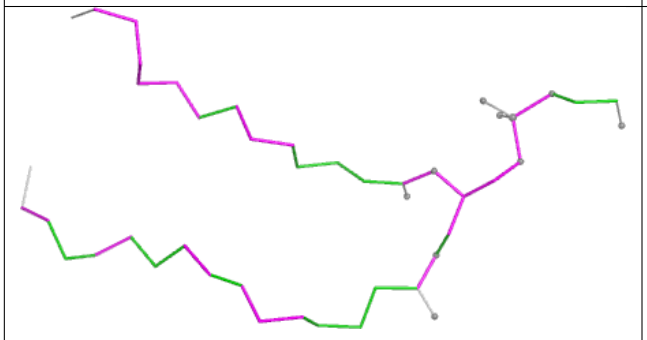


Bond angles



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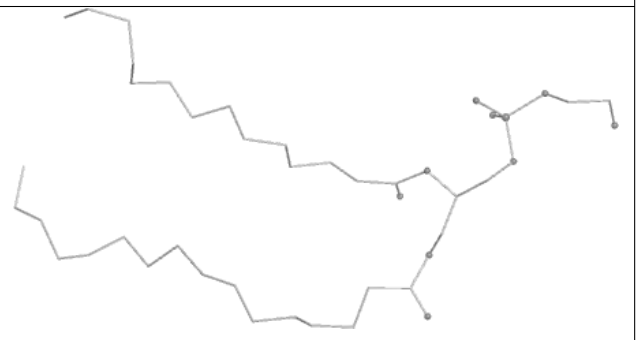
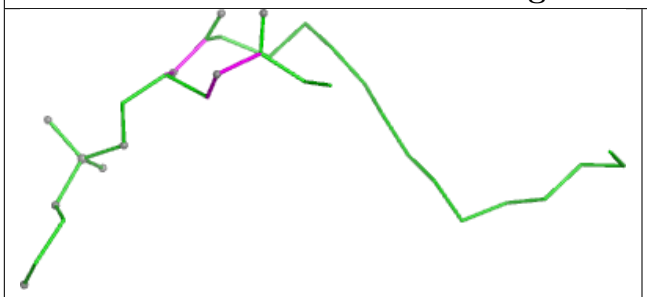
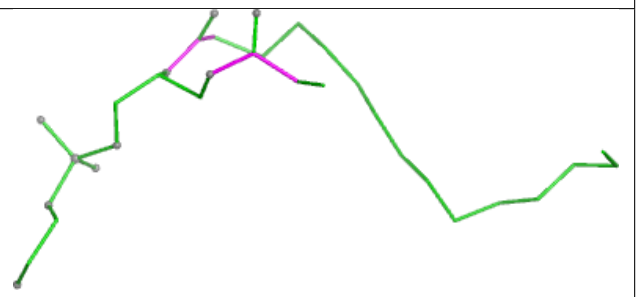


Rings

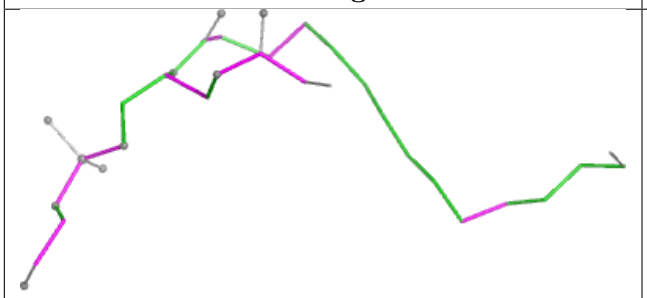
Ligand 3PE H 702



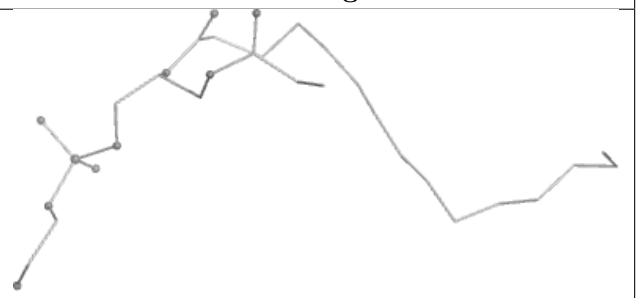
Bond lengths



Bond angles

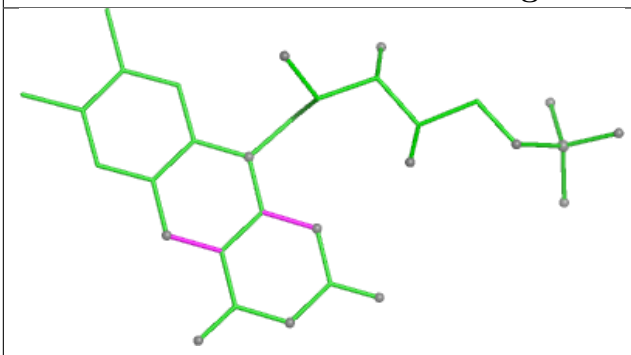


Torsions



Rings

Ligand FMN F 501



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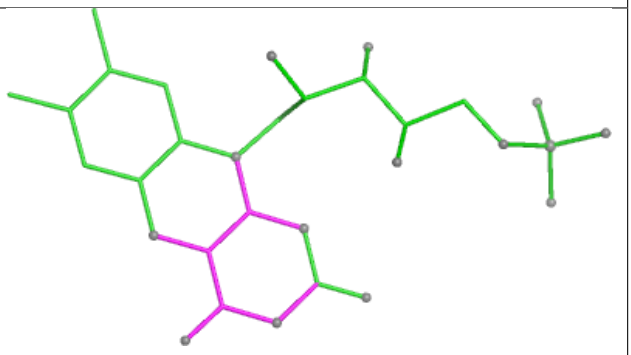

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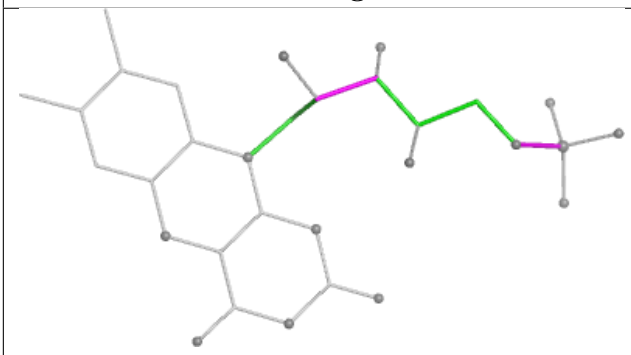

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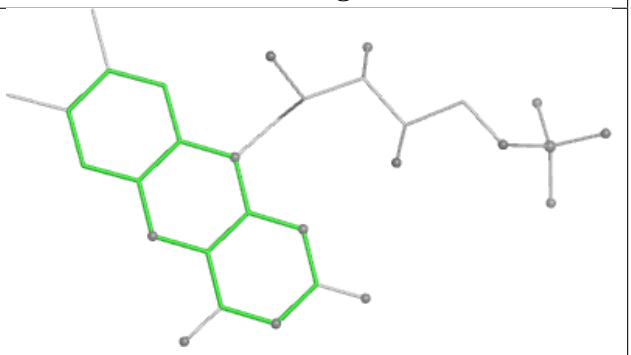
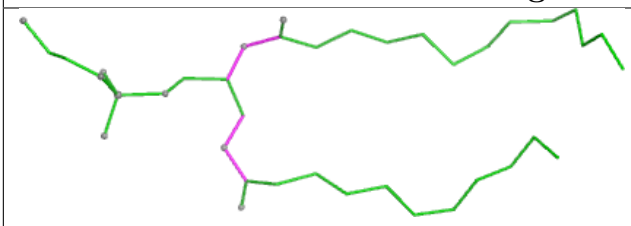


Rings

Ligand 3PE A 203



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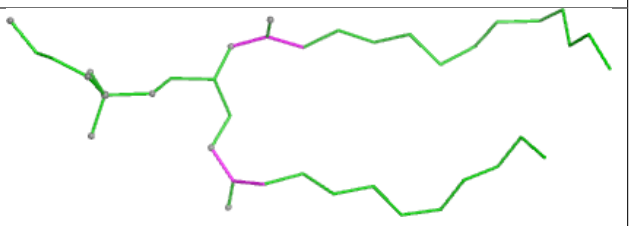

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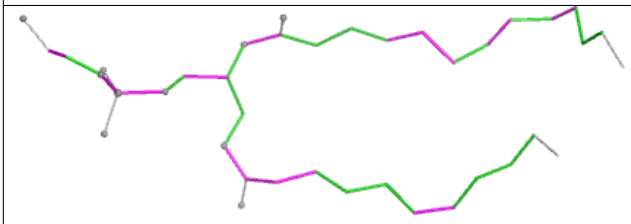

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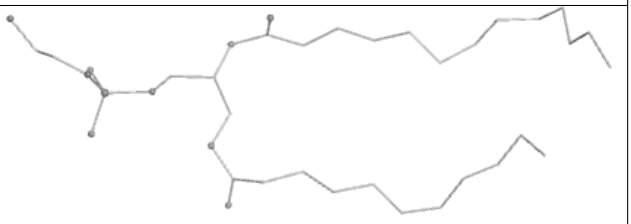
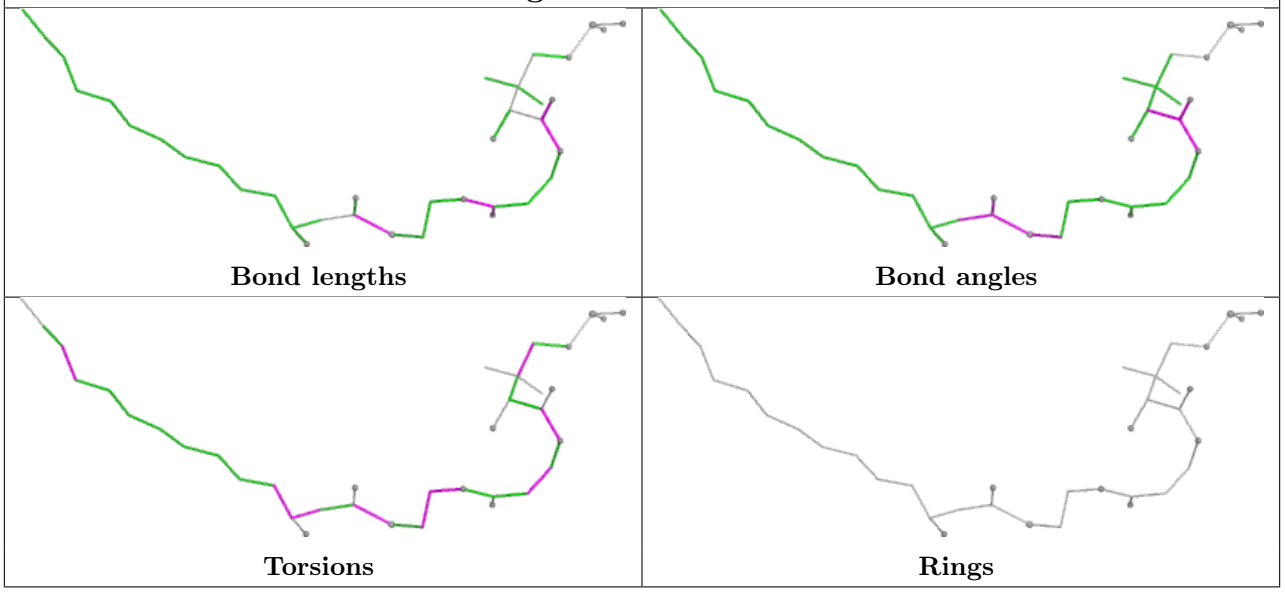


Rings

Ligand EHZ T 101



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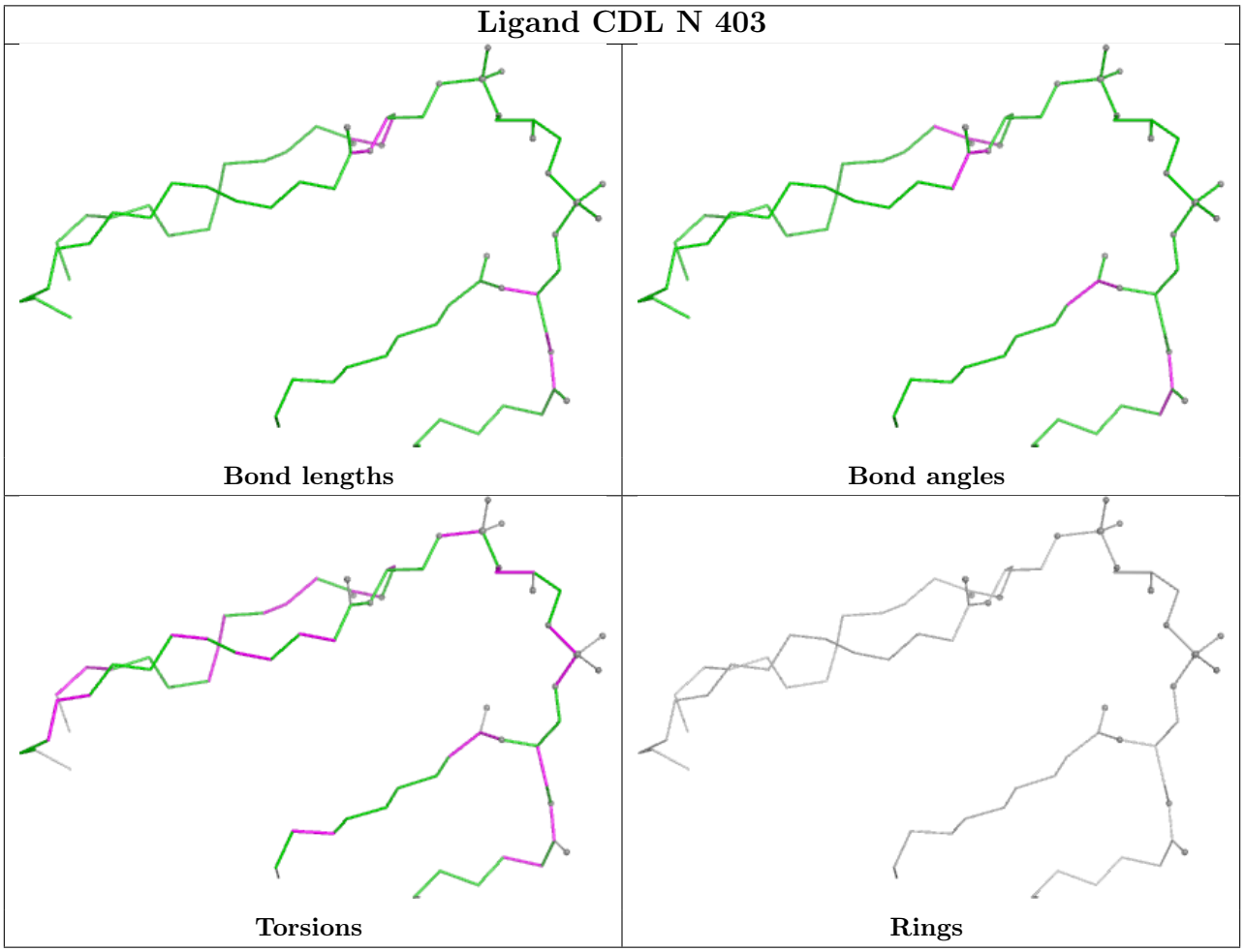

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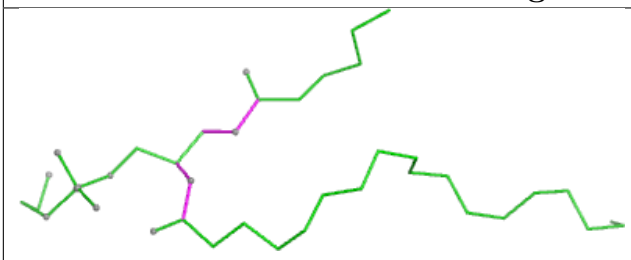

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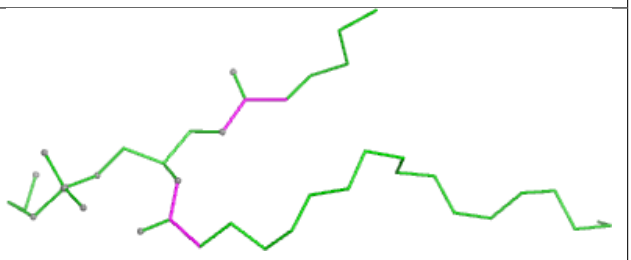

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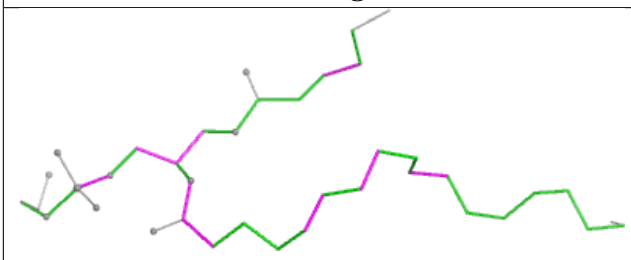

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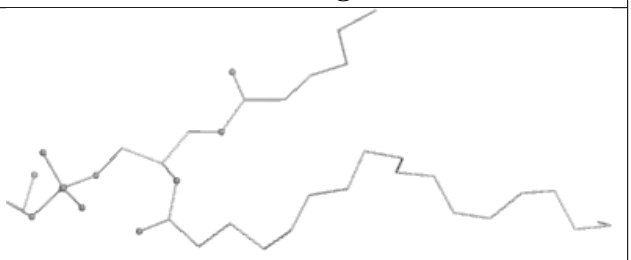
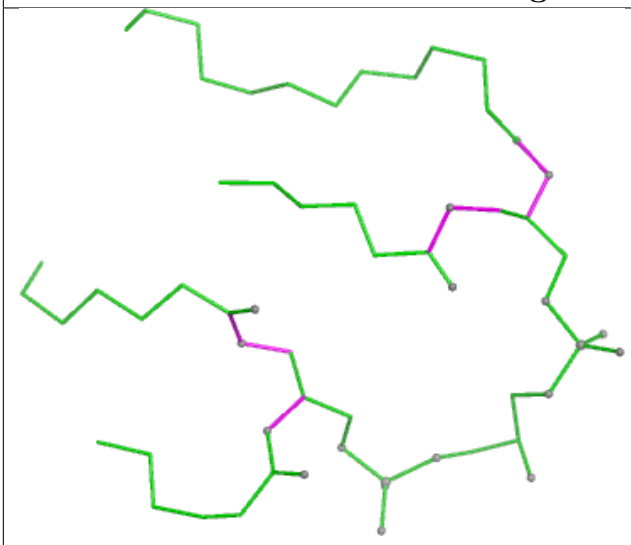


Rings

Ligand CDL r 201



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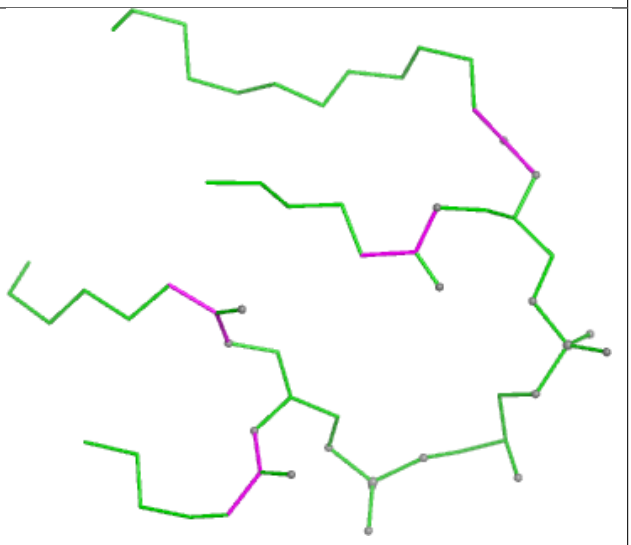

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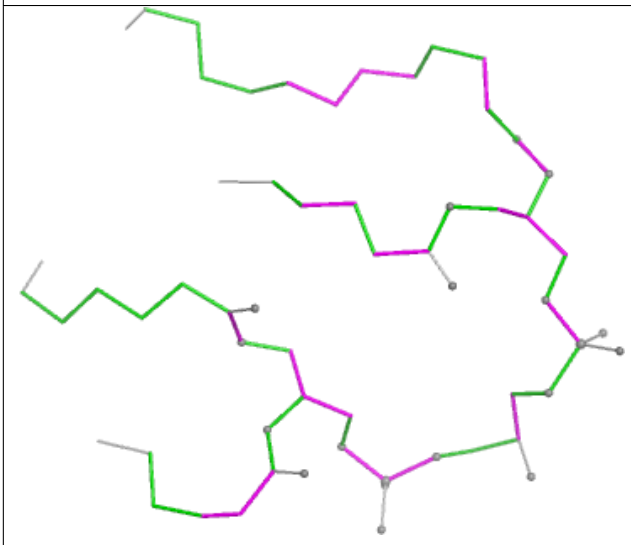

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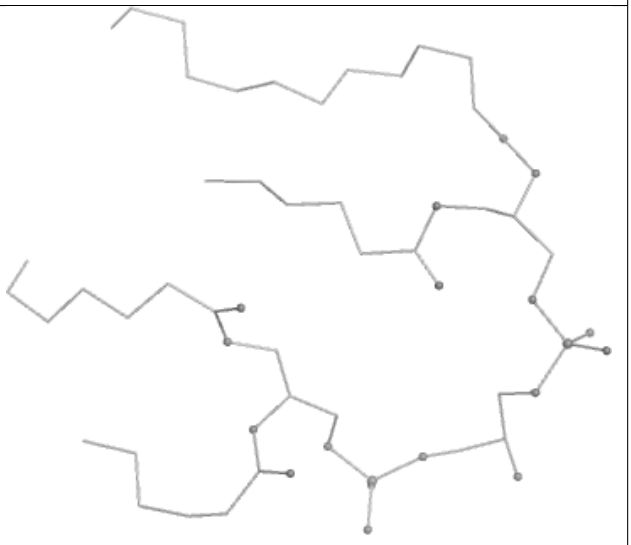
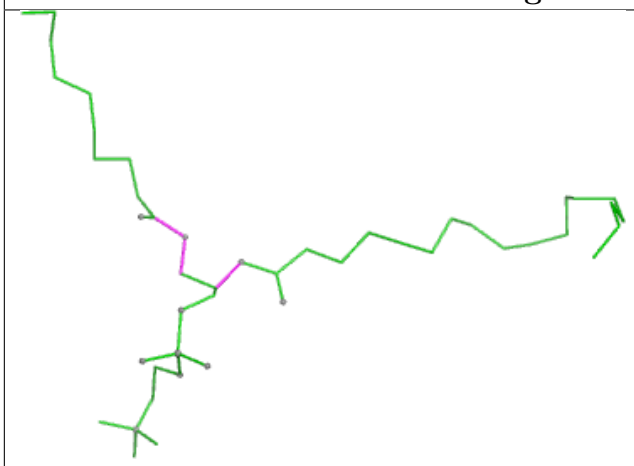


Rings

Ligand PC1 M 703



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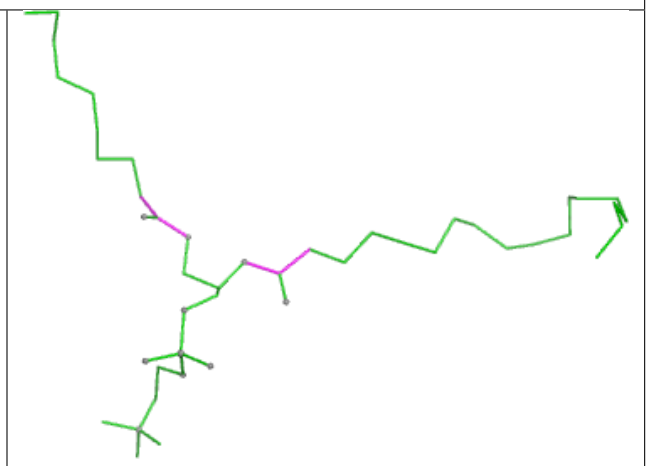

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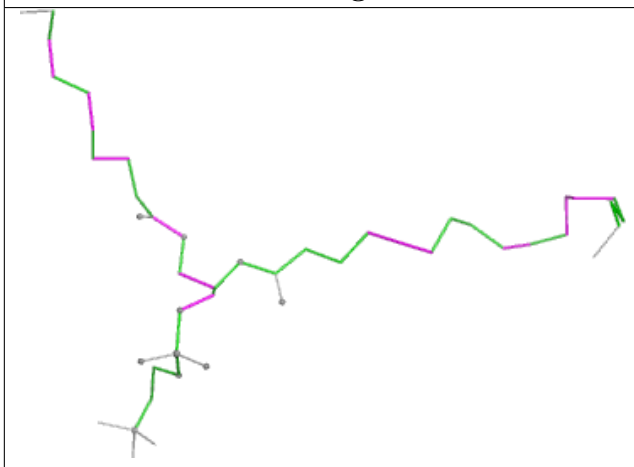

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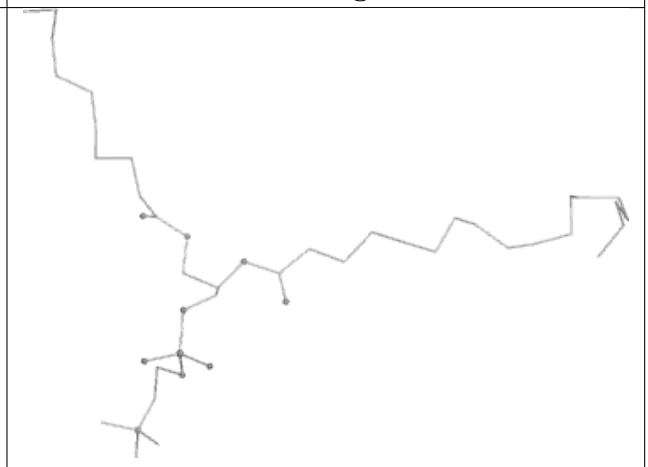
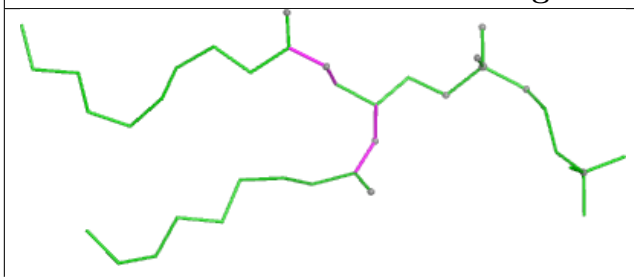


Rings

Ligand PC1 q 701



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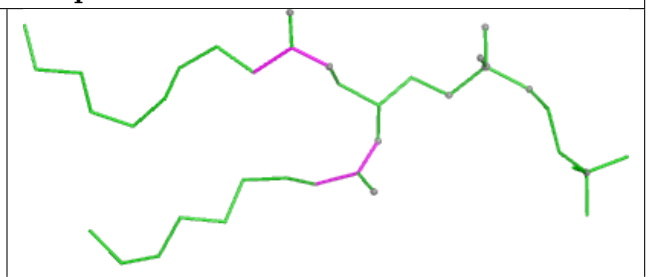
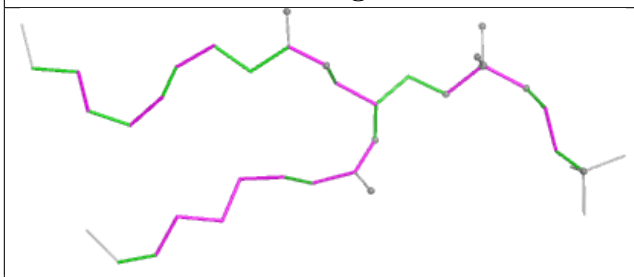


Bond angles



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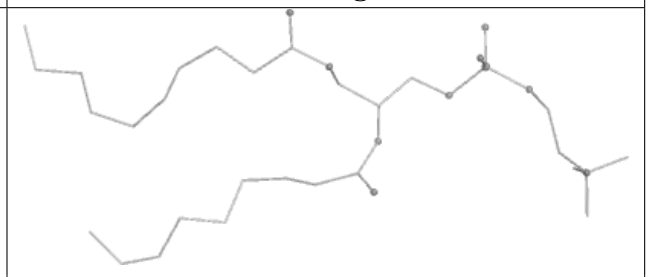
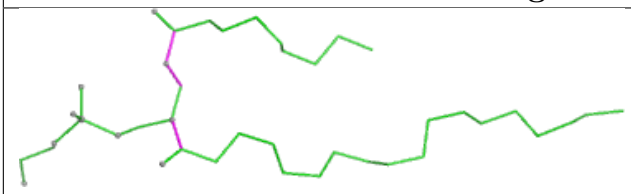


Rings

Ligand 3PE A 201



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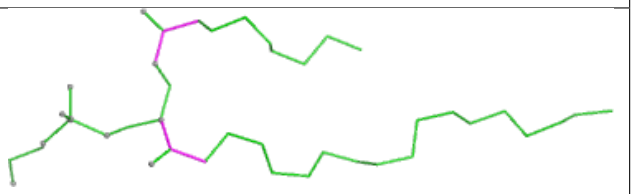

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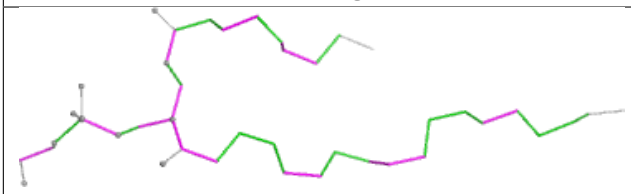

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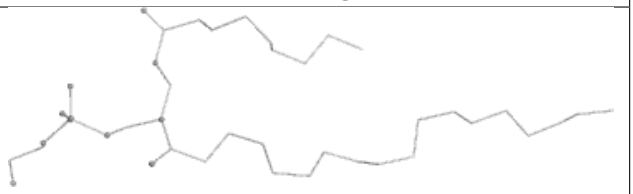
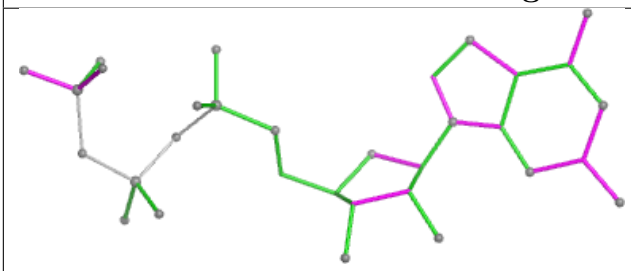


Rings

Ligand GTP O 401



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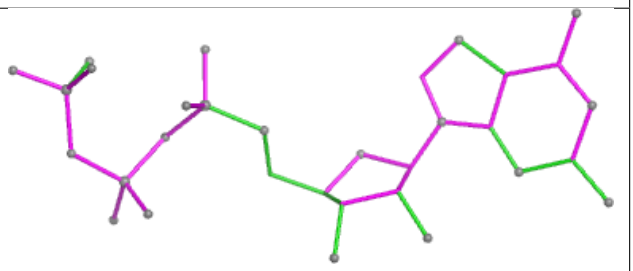
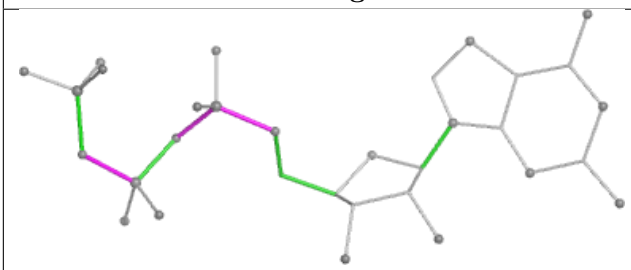


Bond angles



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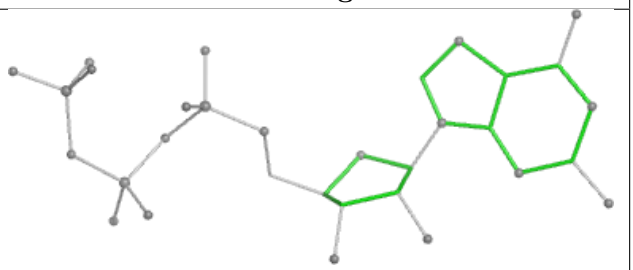
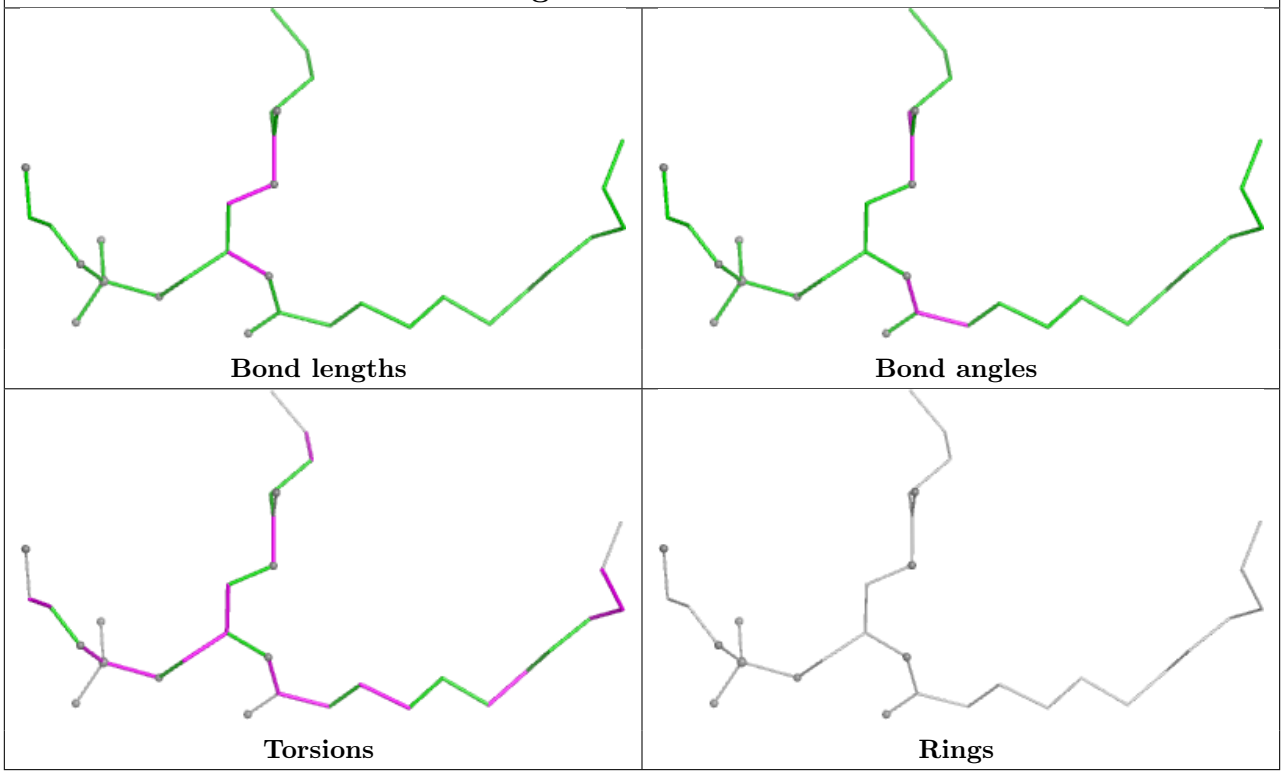
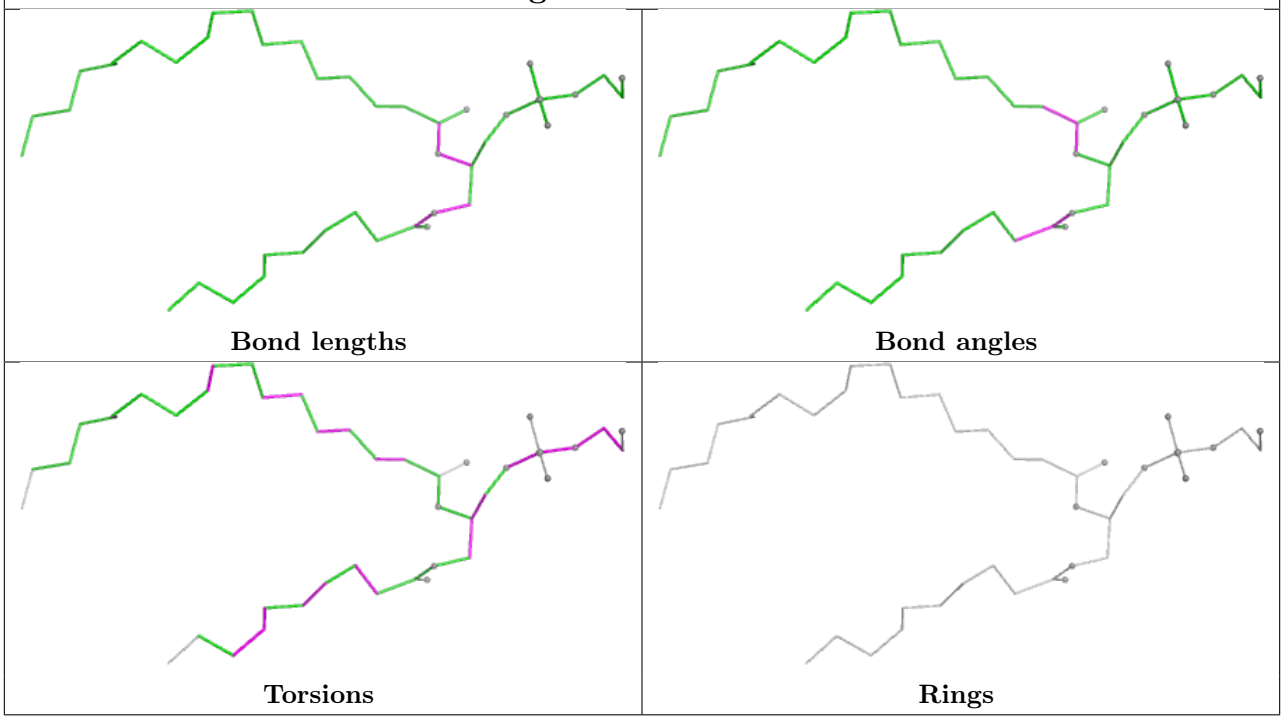


Rings

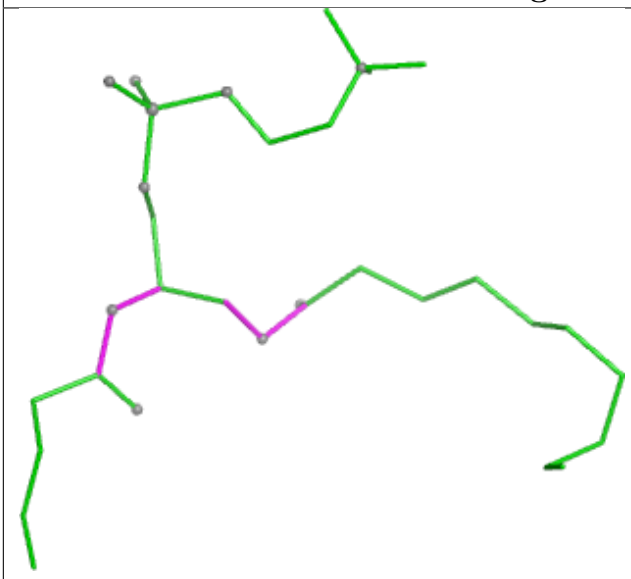
Ligand 3PE L 703



Ligand 3PE A 202



Ligand PC1 d 201



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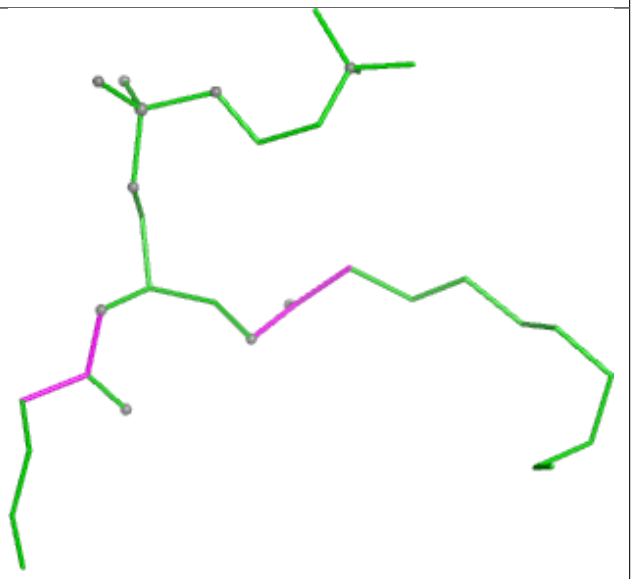
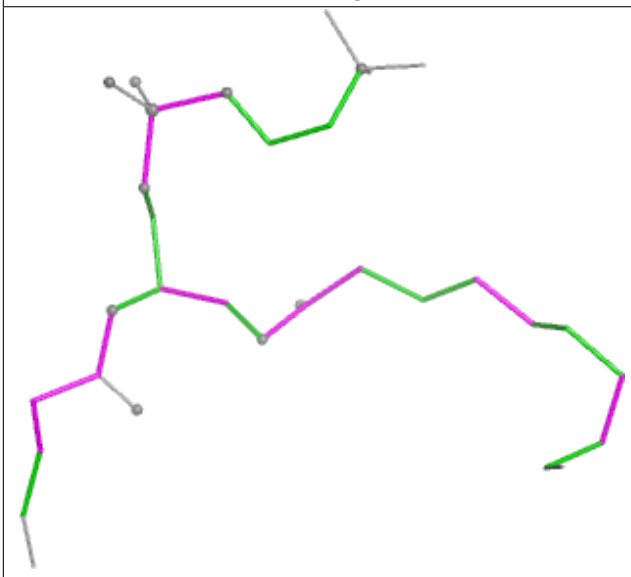


Bond angles



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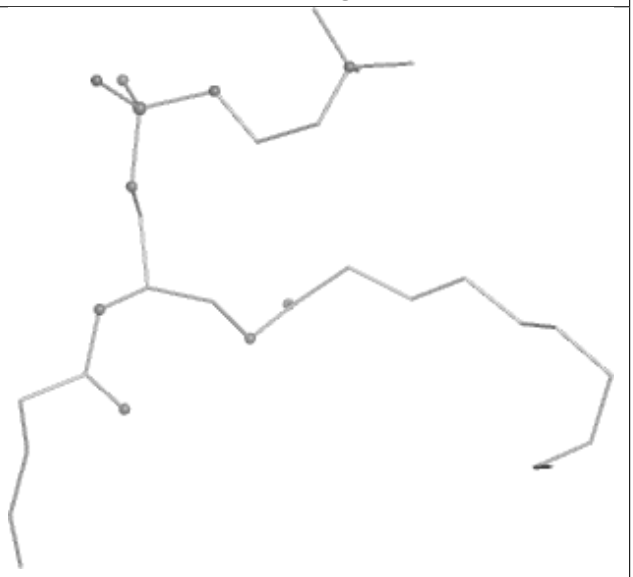
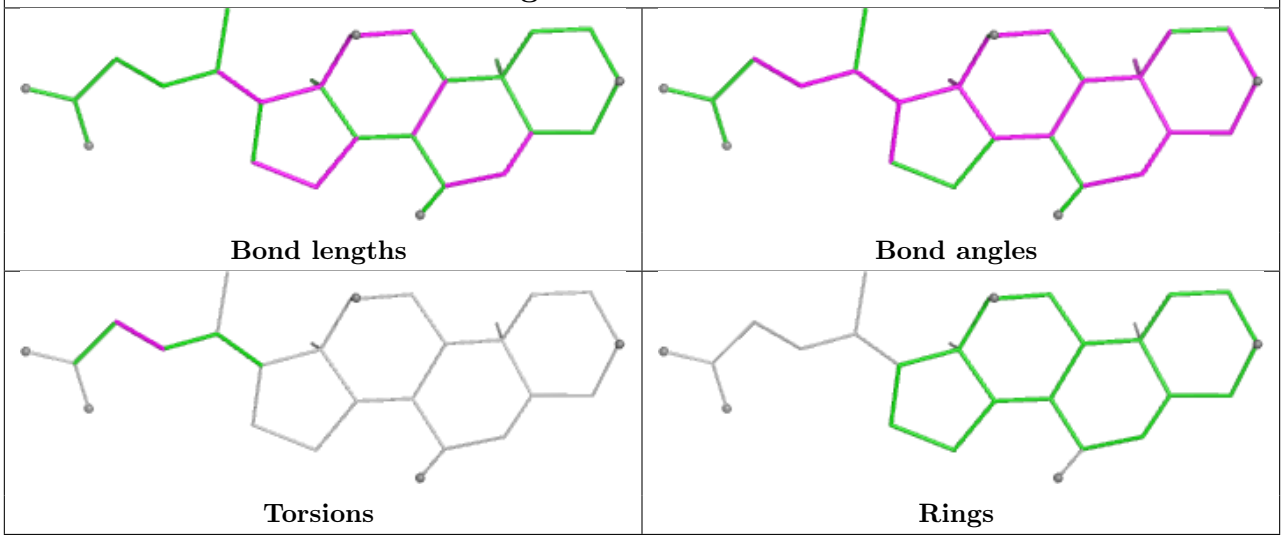


Rings

Ligand CHD H 701



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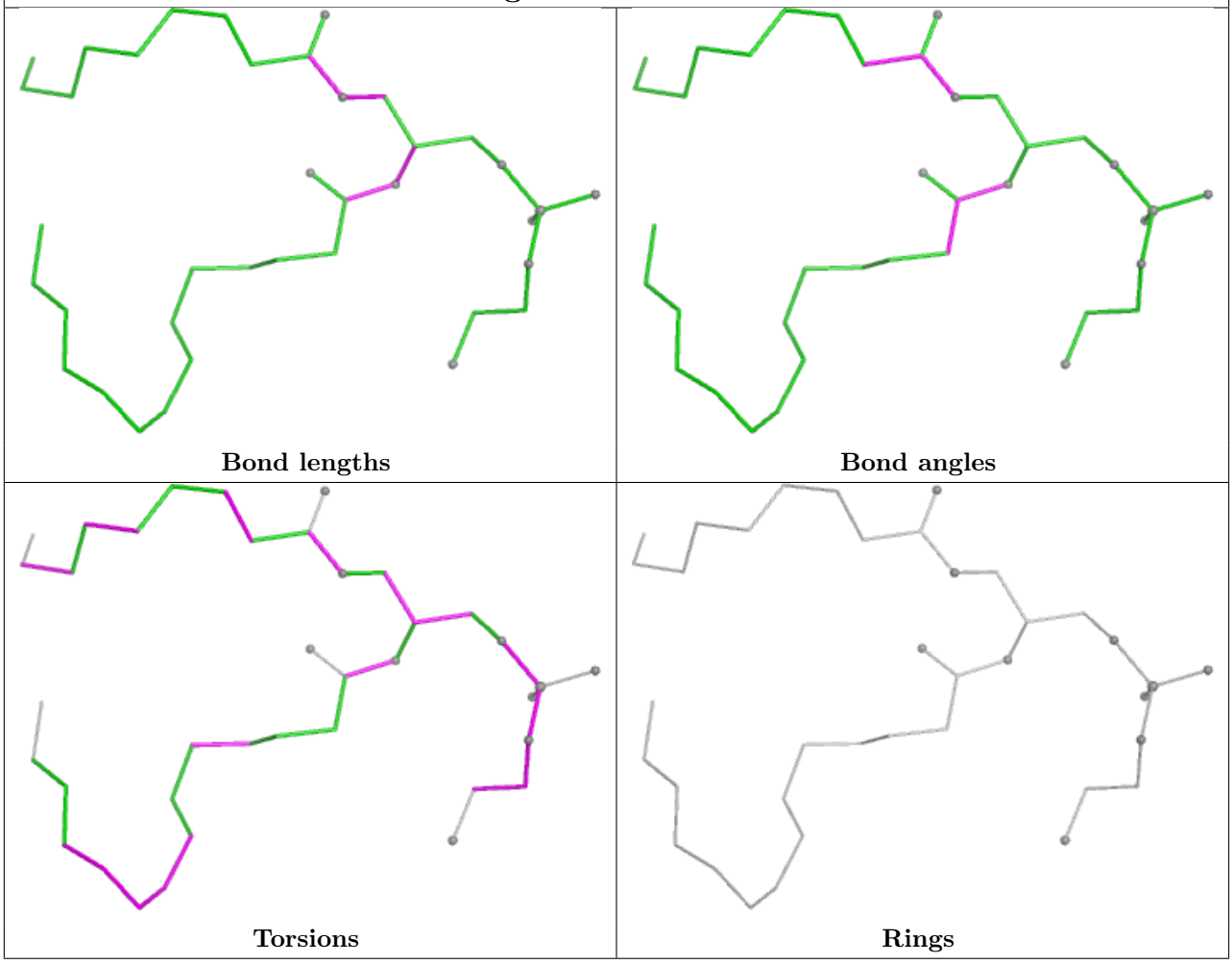
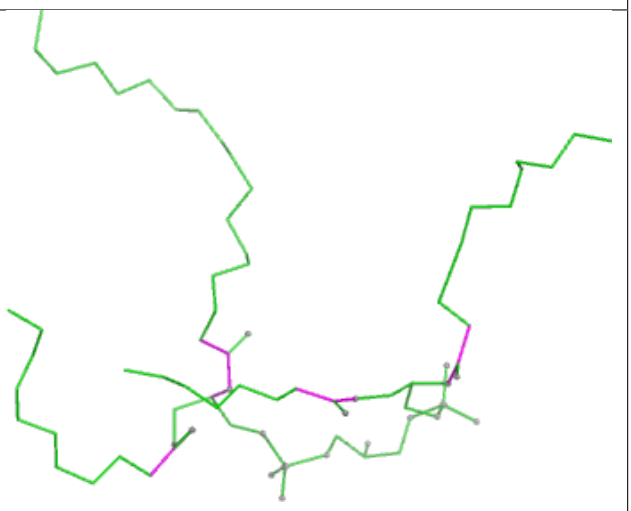


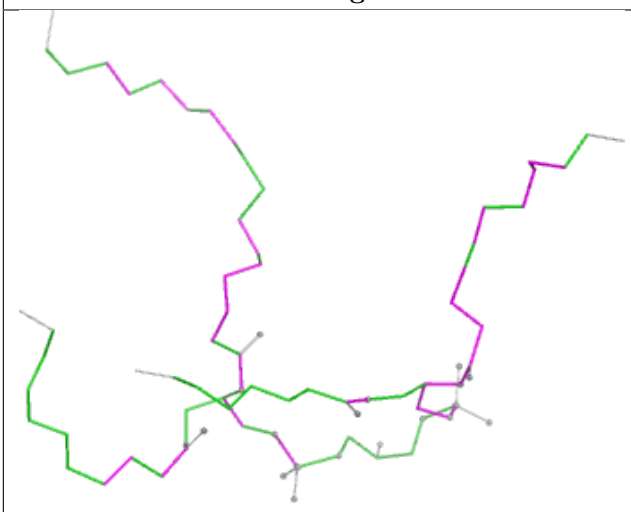
Ligand CDL h 201



Bond lengths



Bond angles



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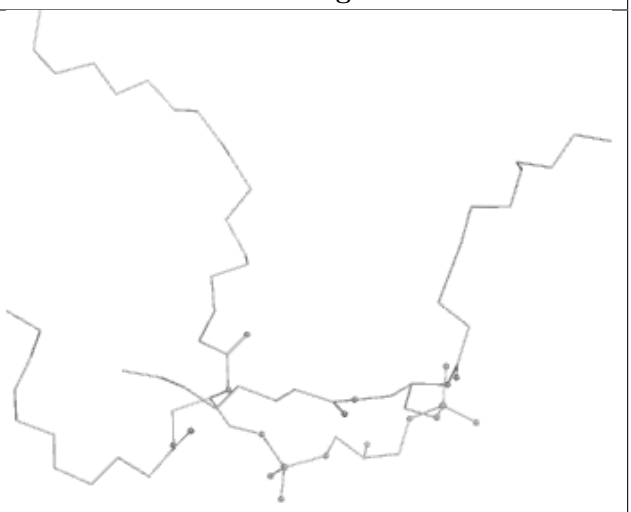

Rings

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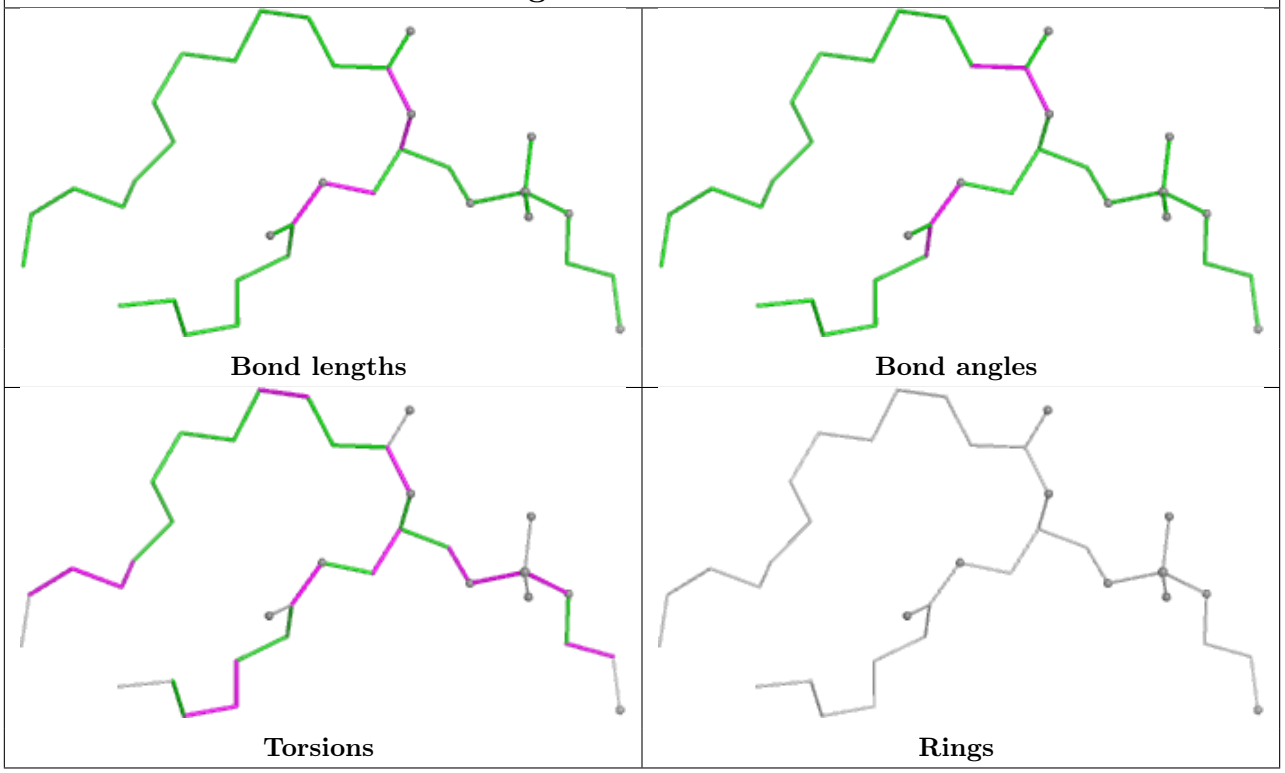
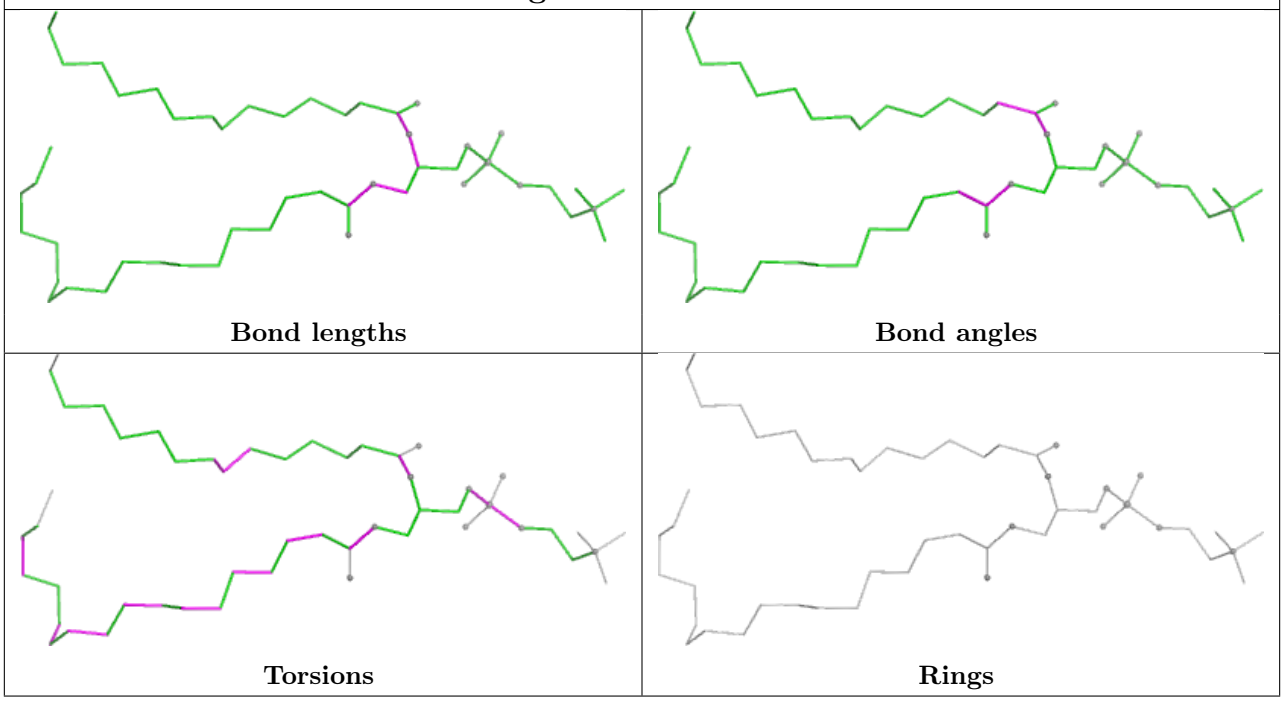


Ligand PC1 B 303



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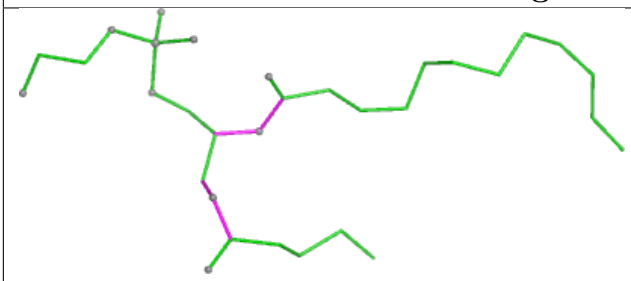

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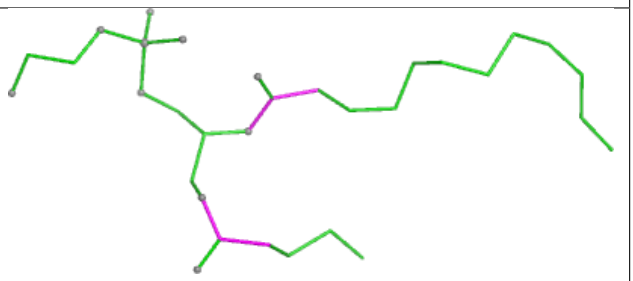
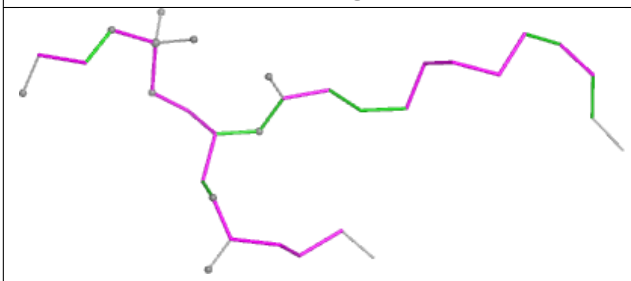


Bond angles



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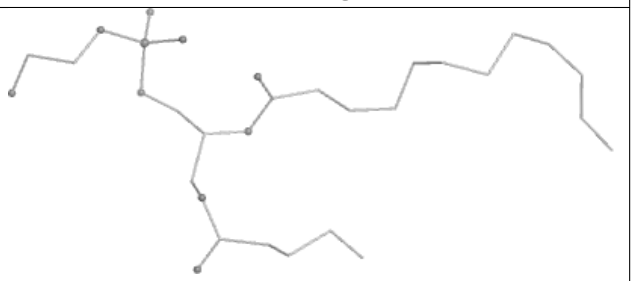
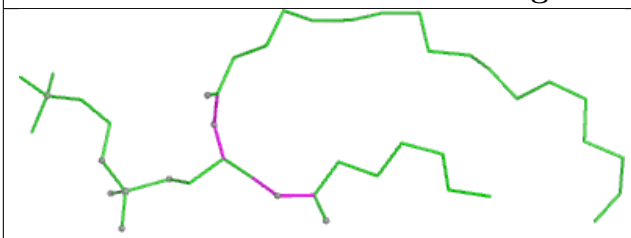


Rings

Ligand PC1 J 201



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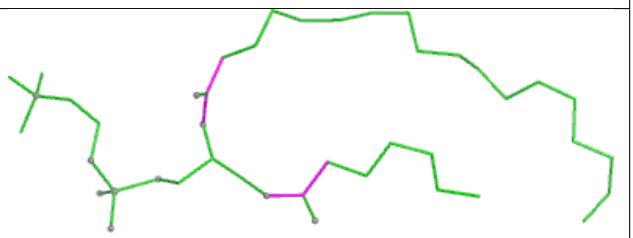
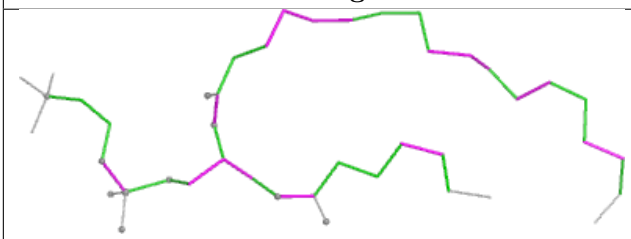


Bond angles



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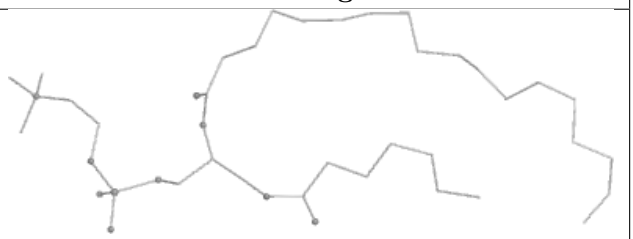
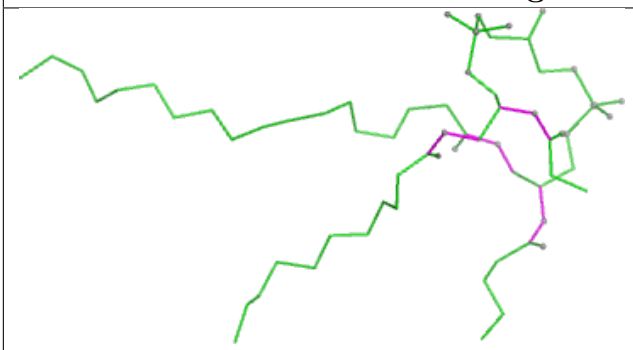
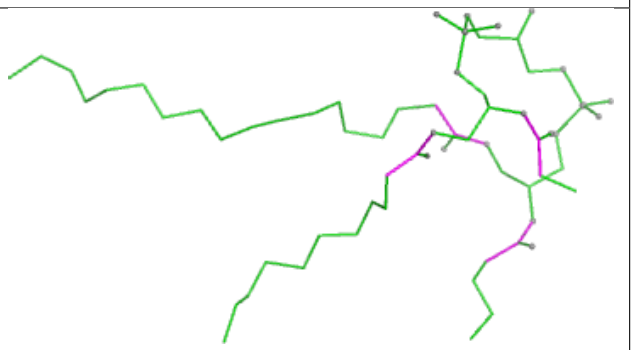


Rings

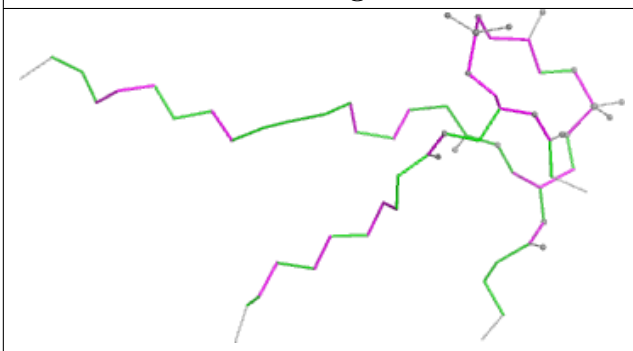
Ligand CDL d 202



Bond lengths



Bond angles

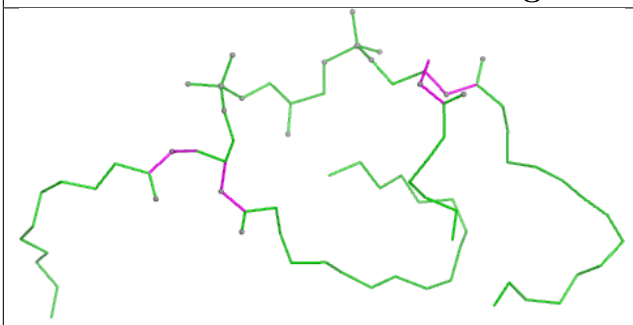


Torsions



Rings

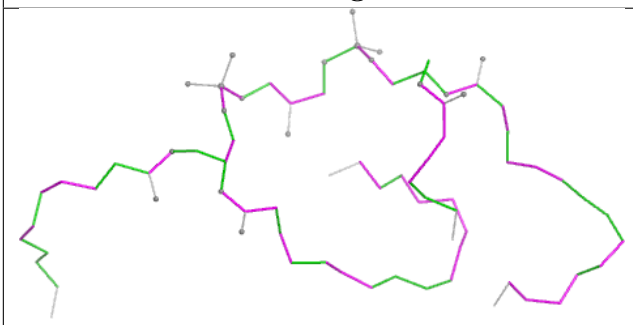
Ligand CDL X 201



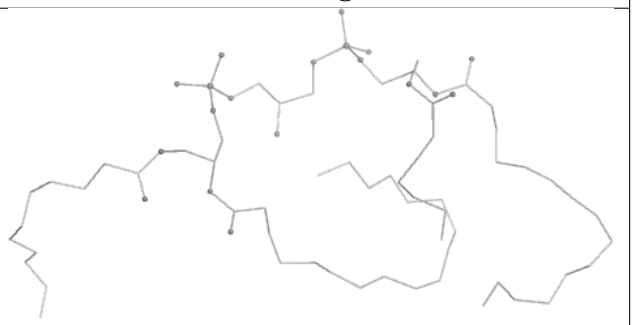
Bond lengths



Bond angles

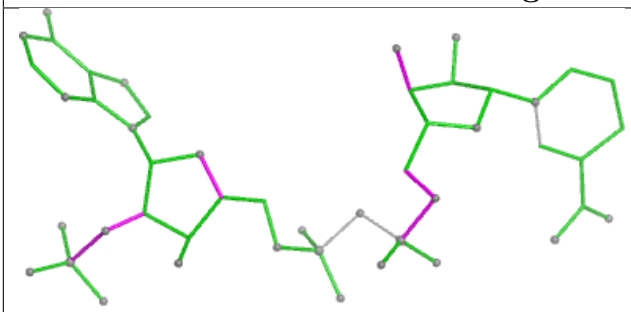


Torsions

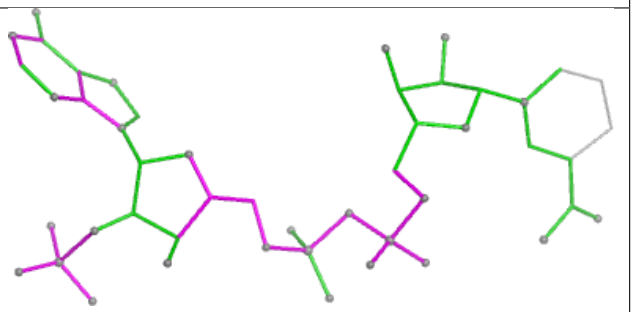


Rings

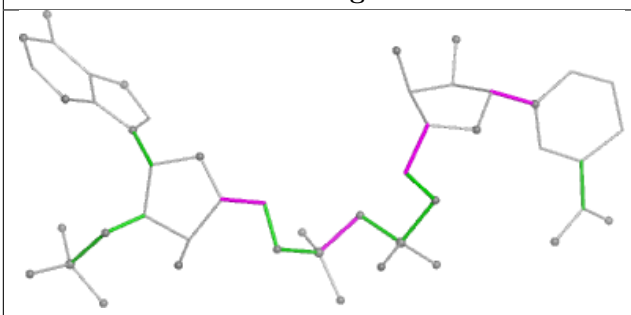
Ligand NDP P 501



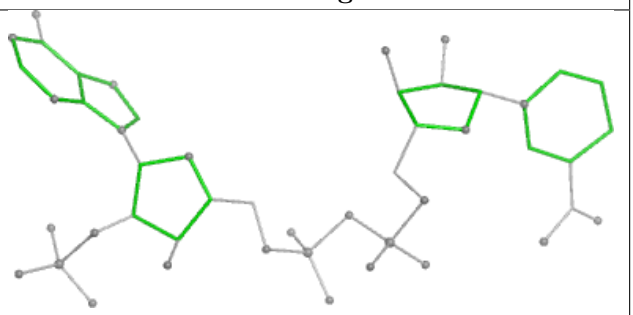
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

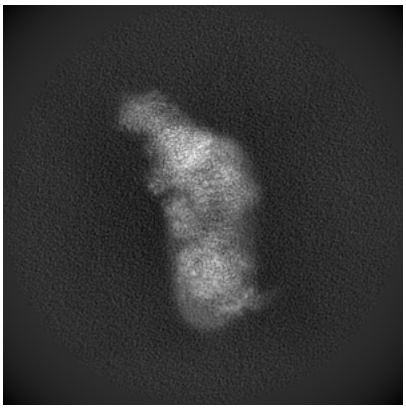
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14140. These allow visual inspection of the internal detail of the map and identification of artifacts.

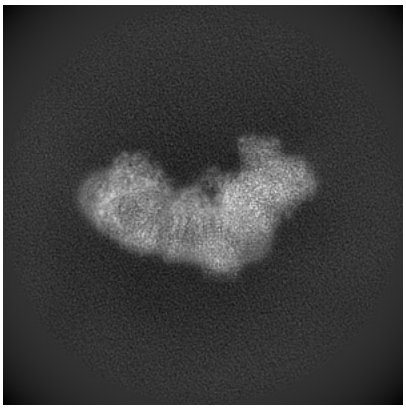
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

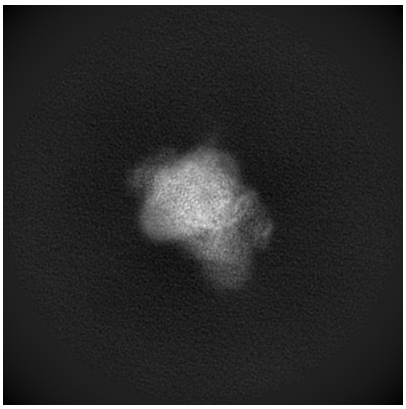
6.1.1 Primary map



X

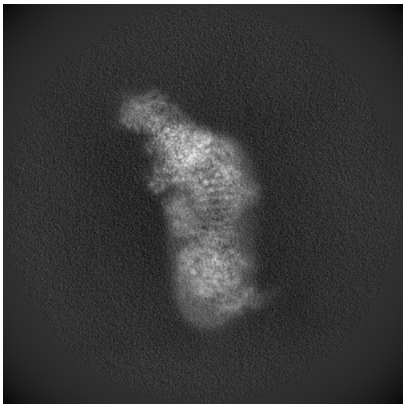


Y

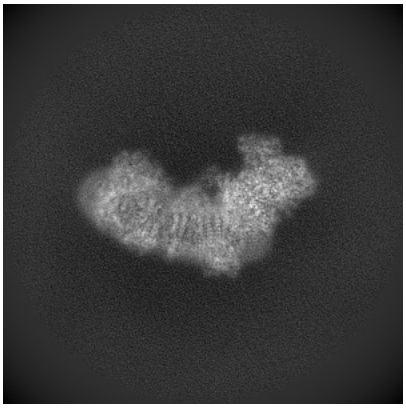


Z

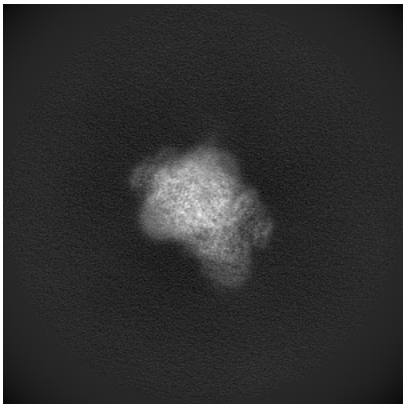
6.1.2 Raw map



X



Y

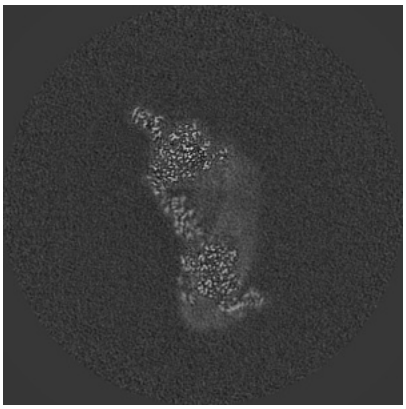


Z

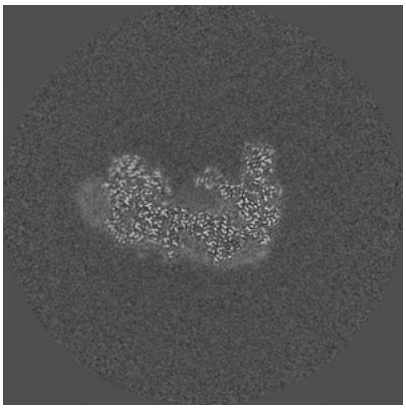
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

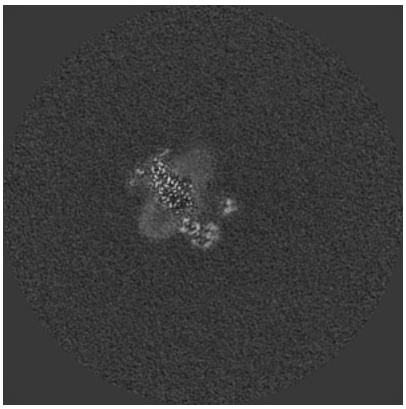
6.2.1 Primary map



X Index: 320

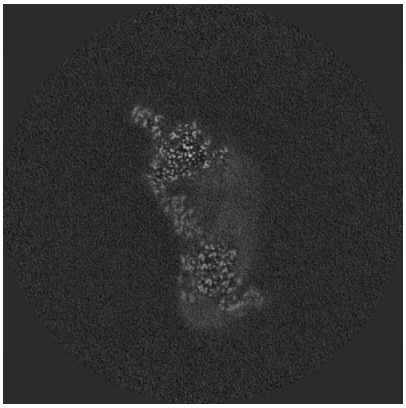


Y Index: 320

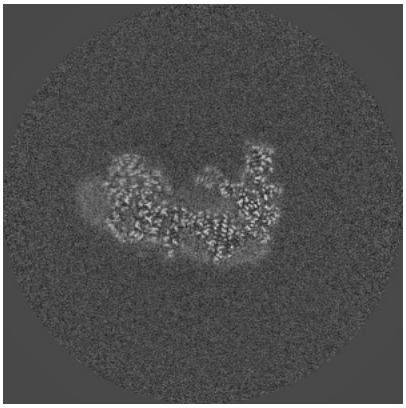


Z Index: 320

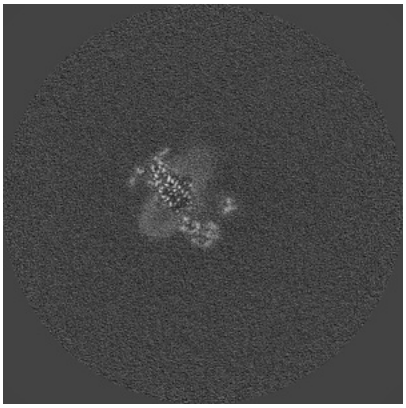
6.2.2 Raw map



X Index: 320



Y Index: 320

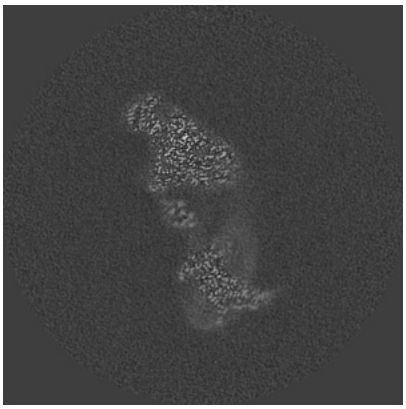


Z Index: 320

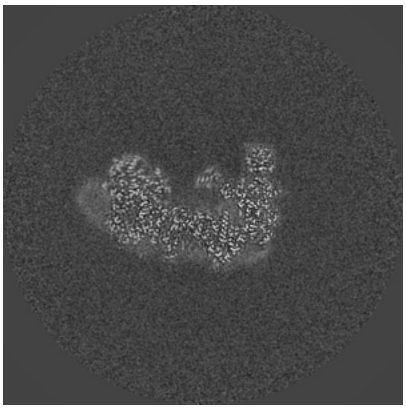
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

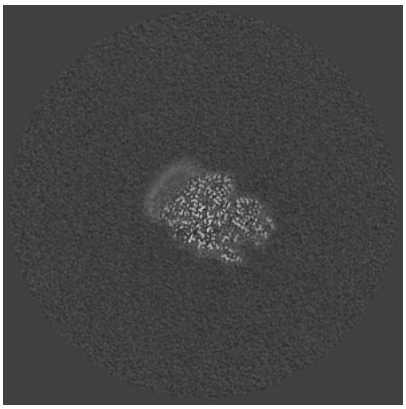
6.3.1 Primary map



X Index: 334

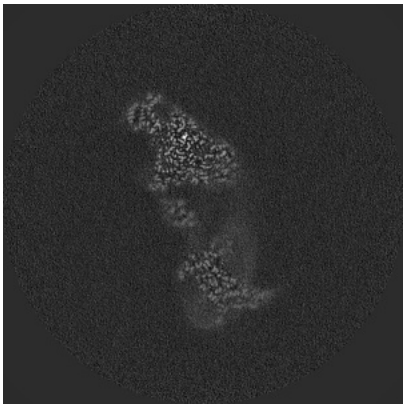


Y Index: 322

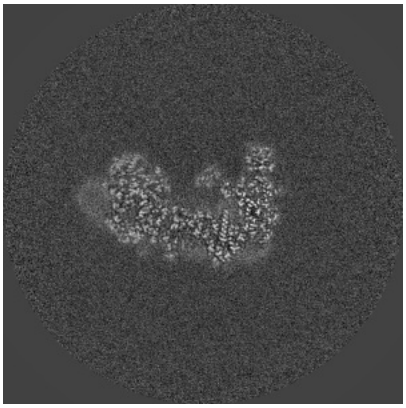


Z Index: 405

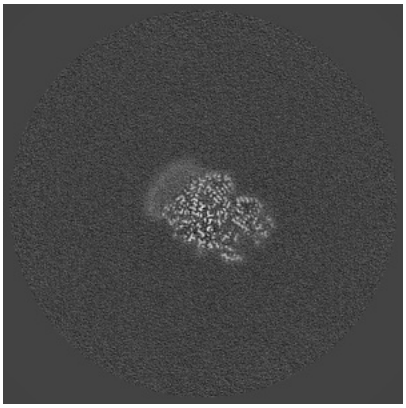
6.3.2 Raw map



X Index: 334



Y Index: 322

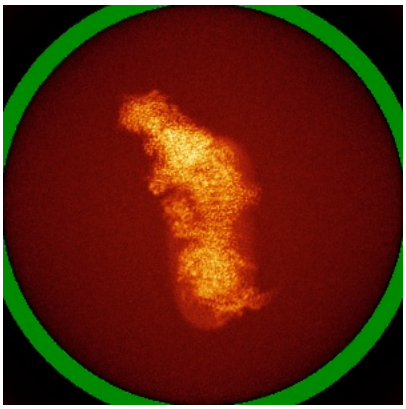


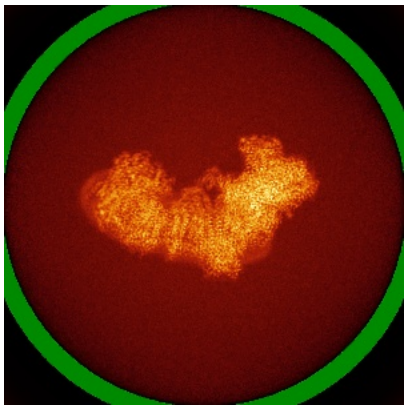
Z Index: 405

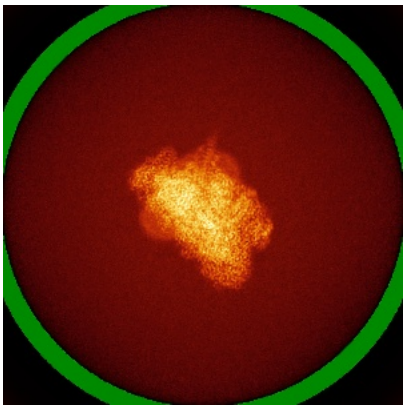
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

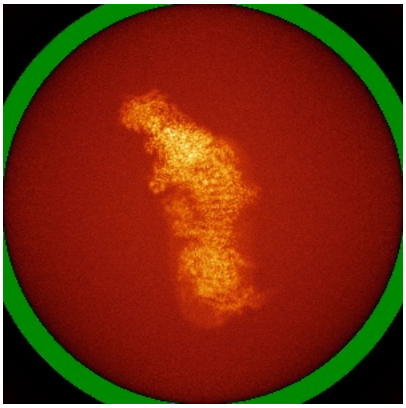
6.4.1 Primary map

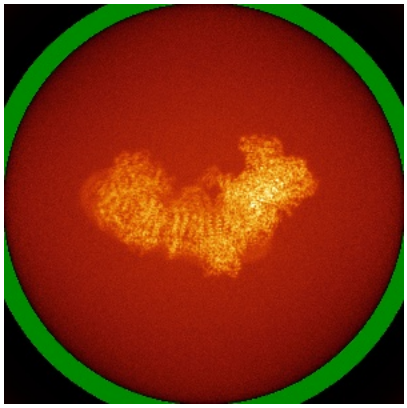

X

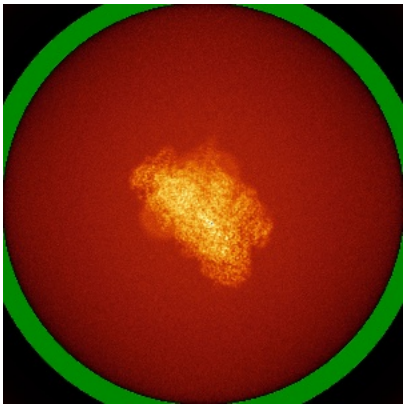

Y


Z

6.4.2 Raw map


X

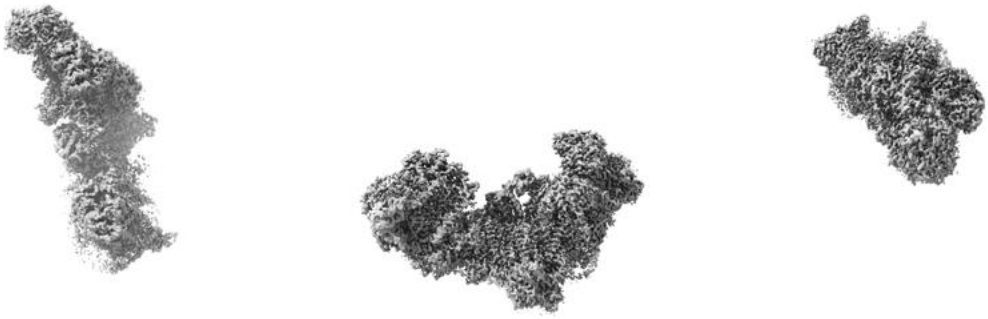

Y


Z

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

6.5 Orthogonal surface views (i)

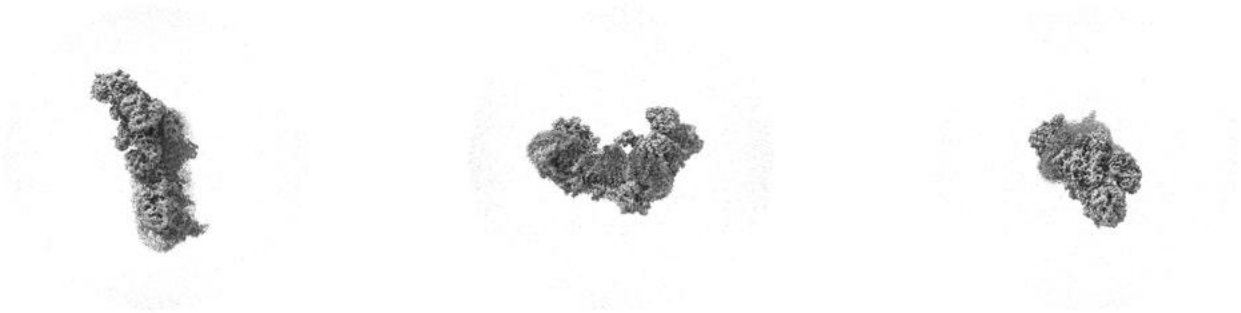
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 5.5. 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



X Y Z

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.

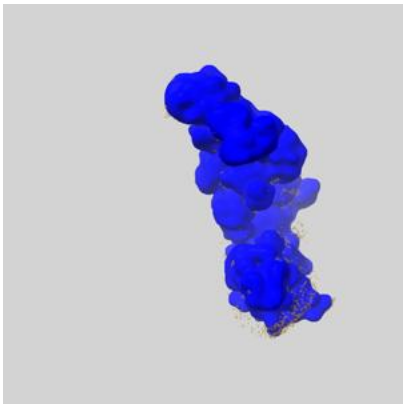
6.6 Mask visualisation

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

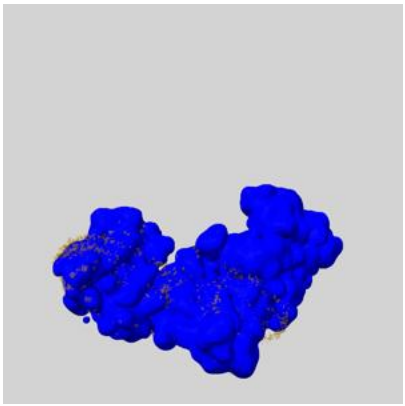
A mask typically either:

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

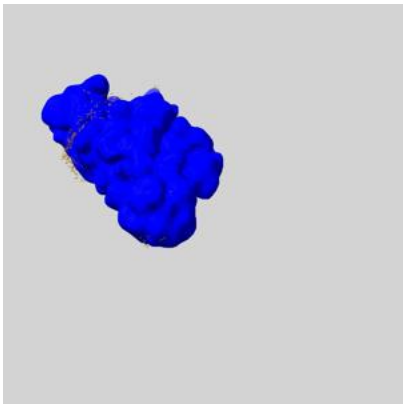
6.6.1 emd_14140_msk_1.map



X



Y

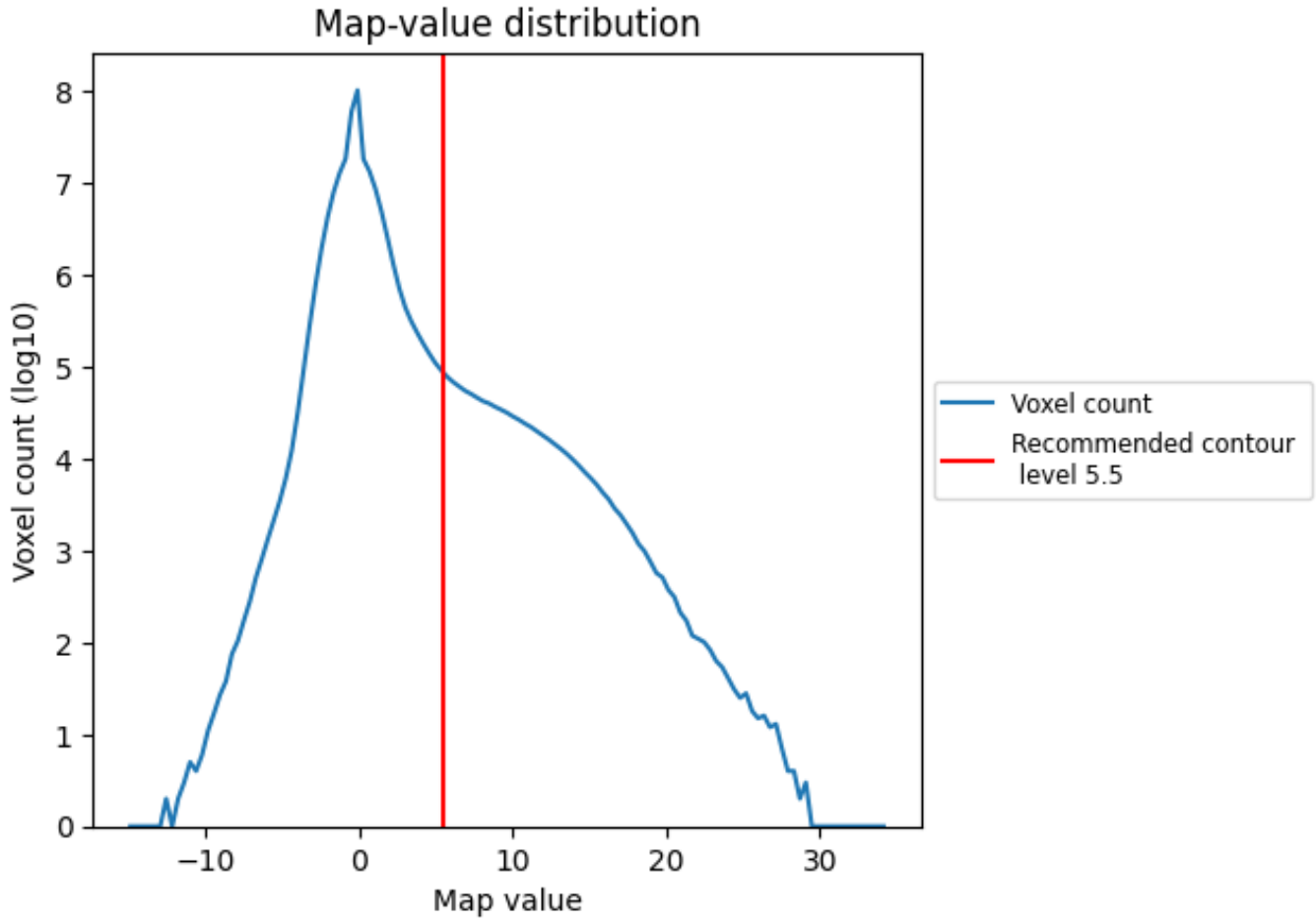


Z

7 Map analysis

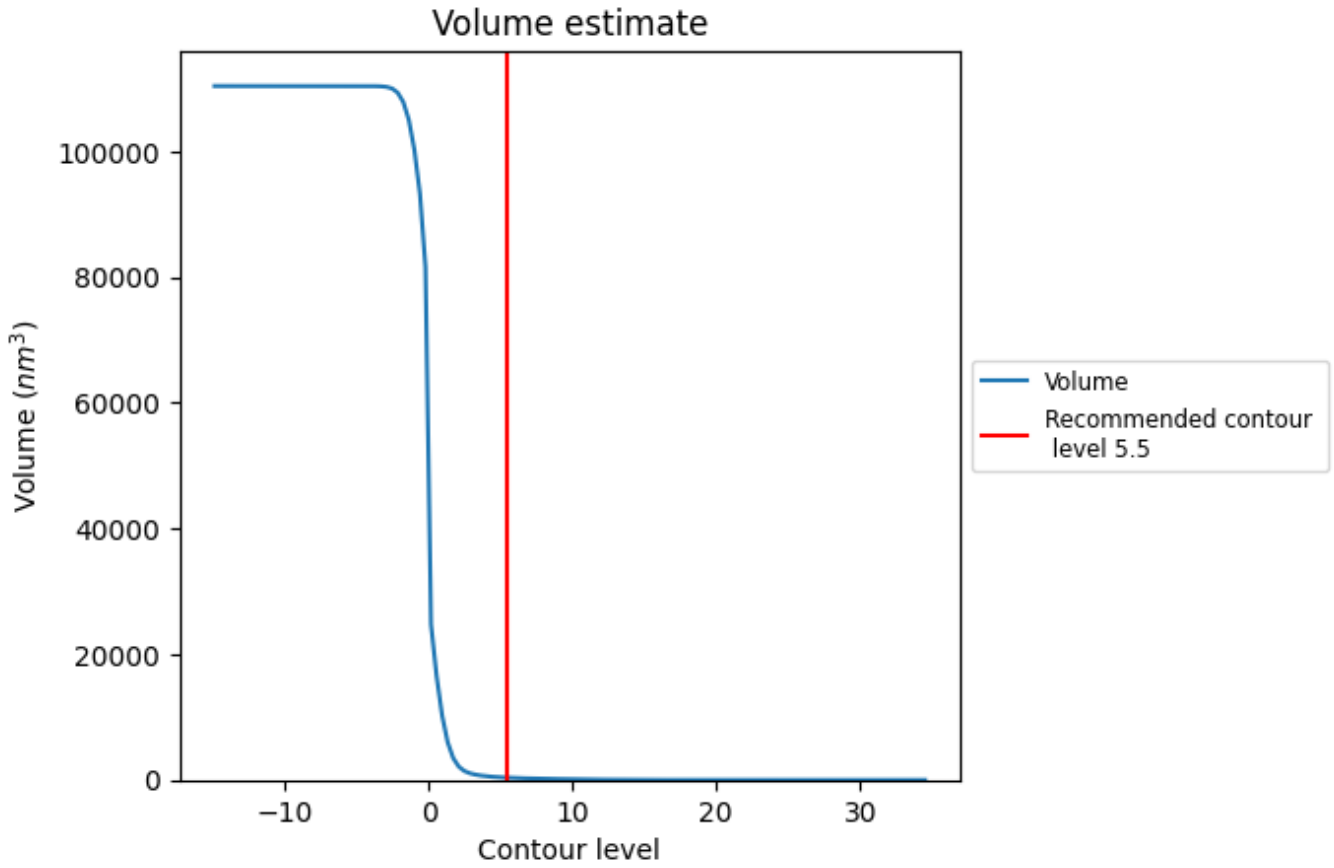
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

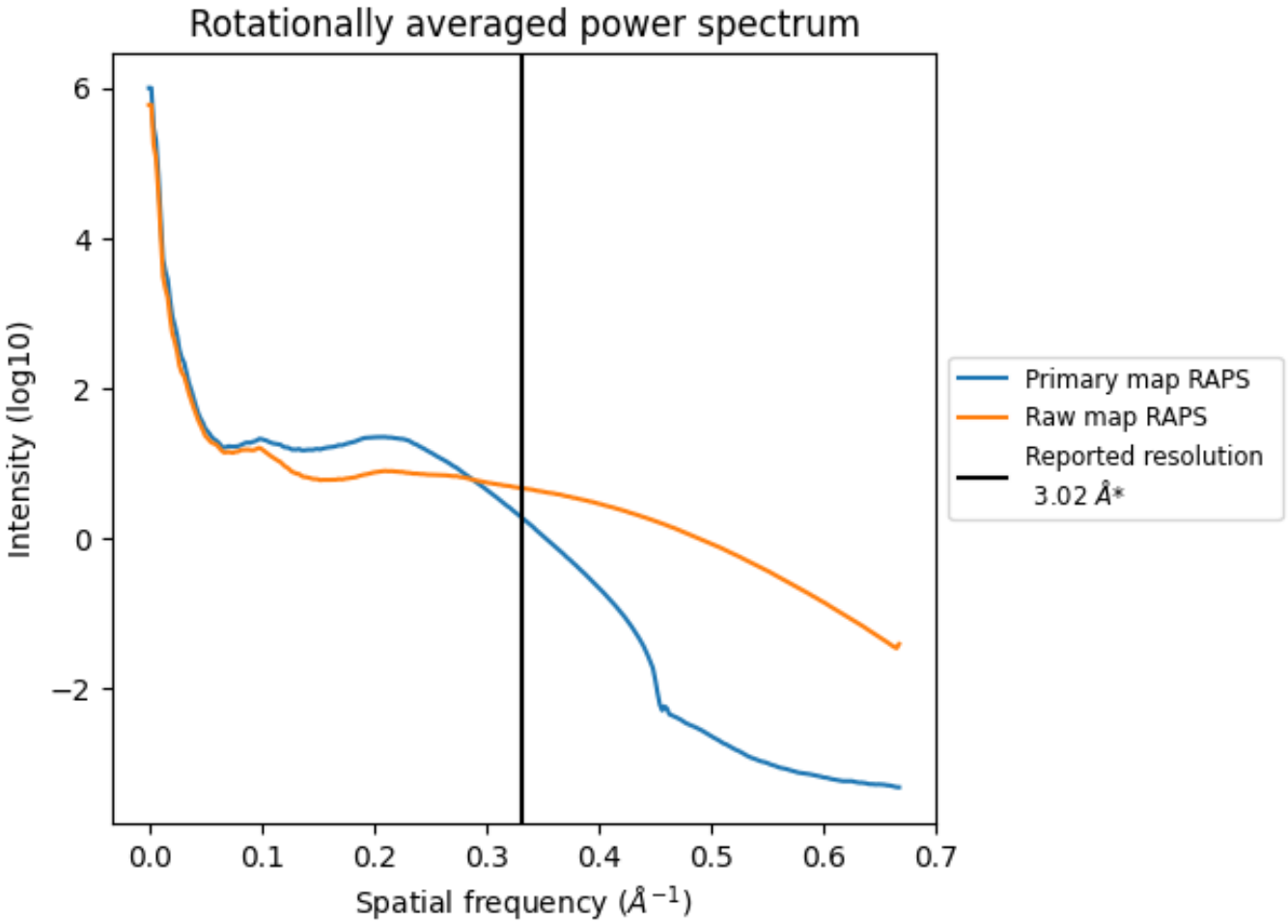
7.2 Volume estimate



The volume at the recommended contour level is 362 nm^3; this corresponds to an approximate mass of 327 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)

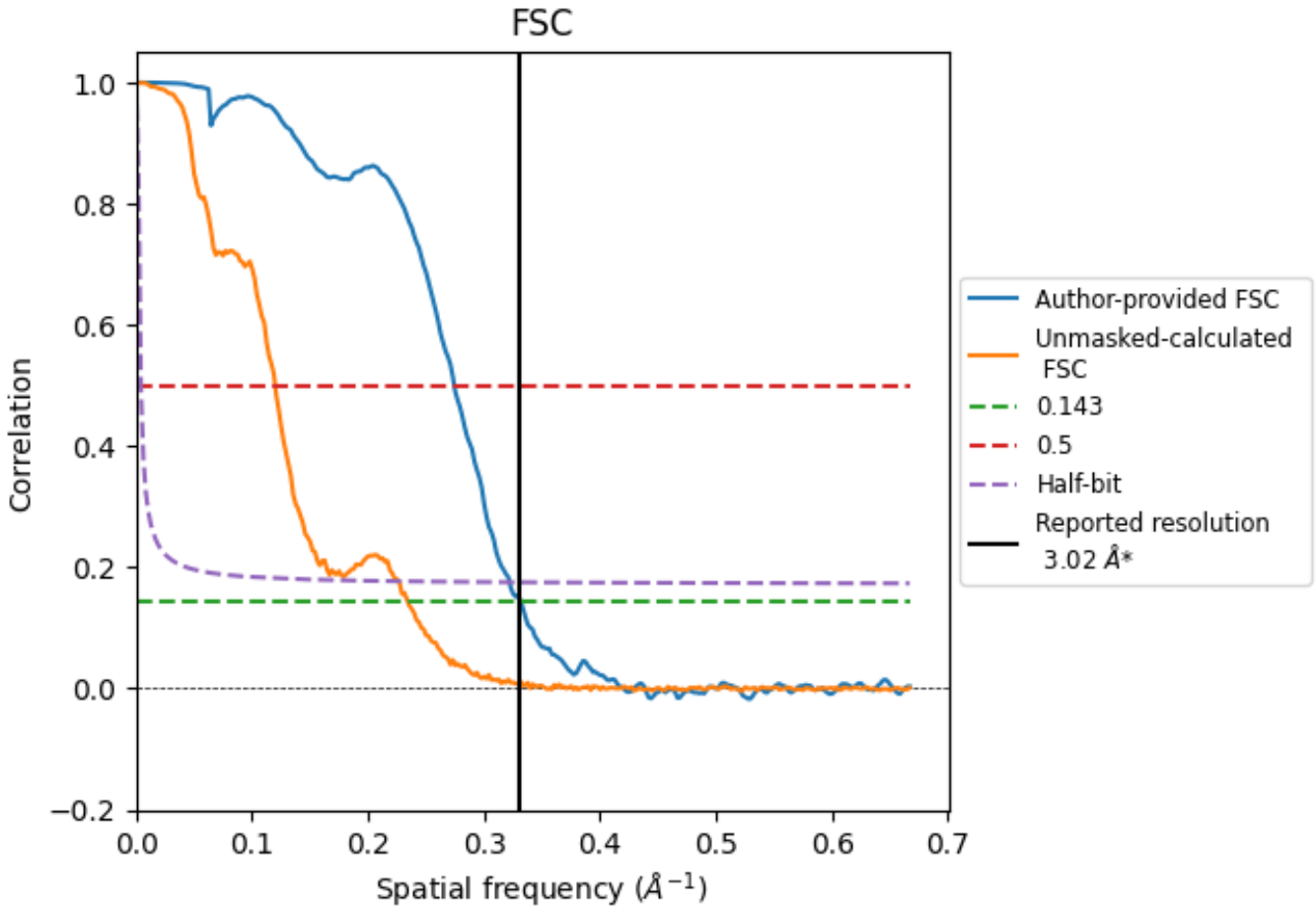


*Reported resolution corresponds to spatial frequency of 0.331 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.331 $Å^{-1}$

8.2 Resolution estimates (i)

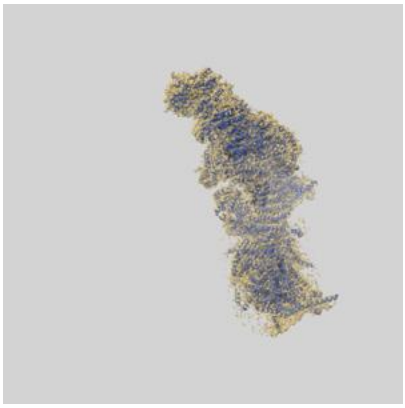
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.01	3.65	3.11
Unmasked-calculated*	4.27	8.34	4.42

*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 4.27 differs from the reported value 3.02 by more than 10 %

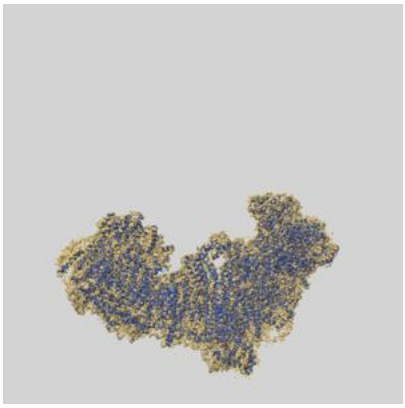
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14140 and PDB model 7QSO. Per-residue inclusion information can be found in section 3 on page 21.

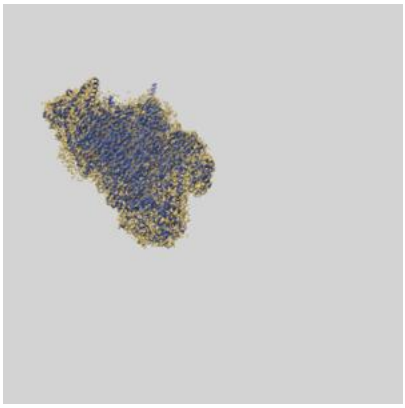
9.1 Map-model overlay



X



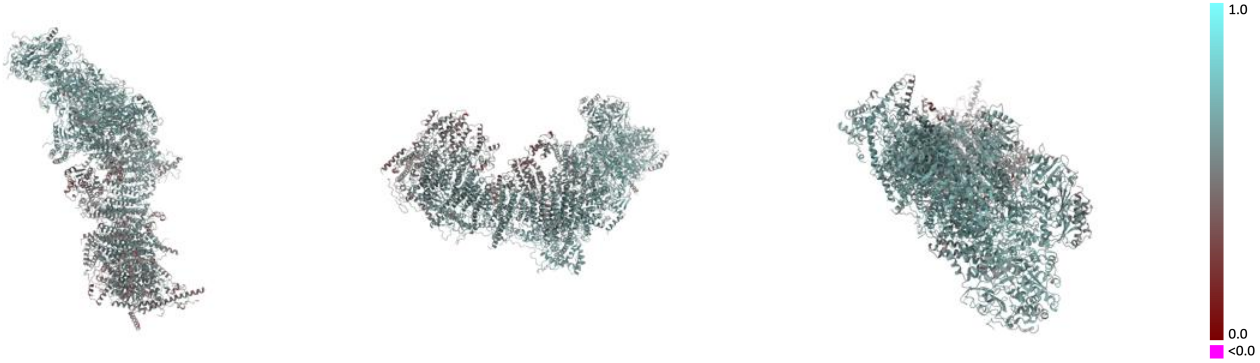
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.5 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.

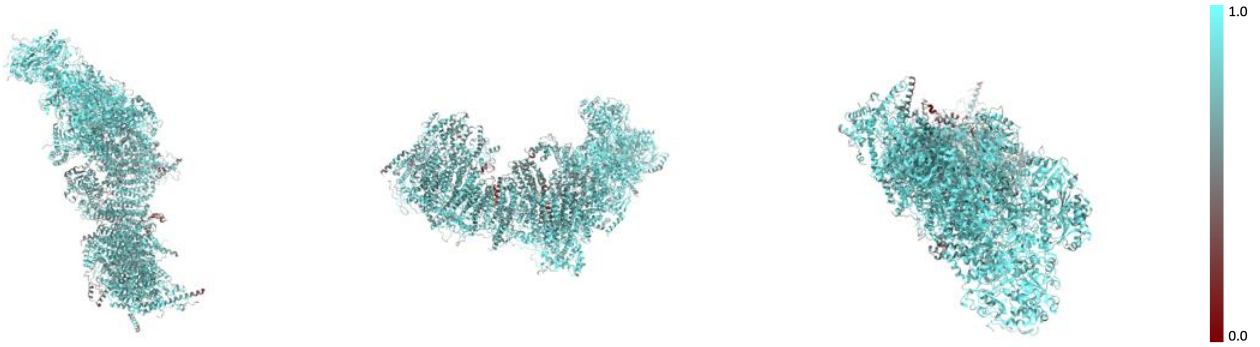
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

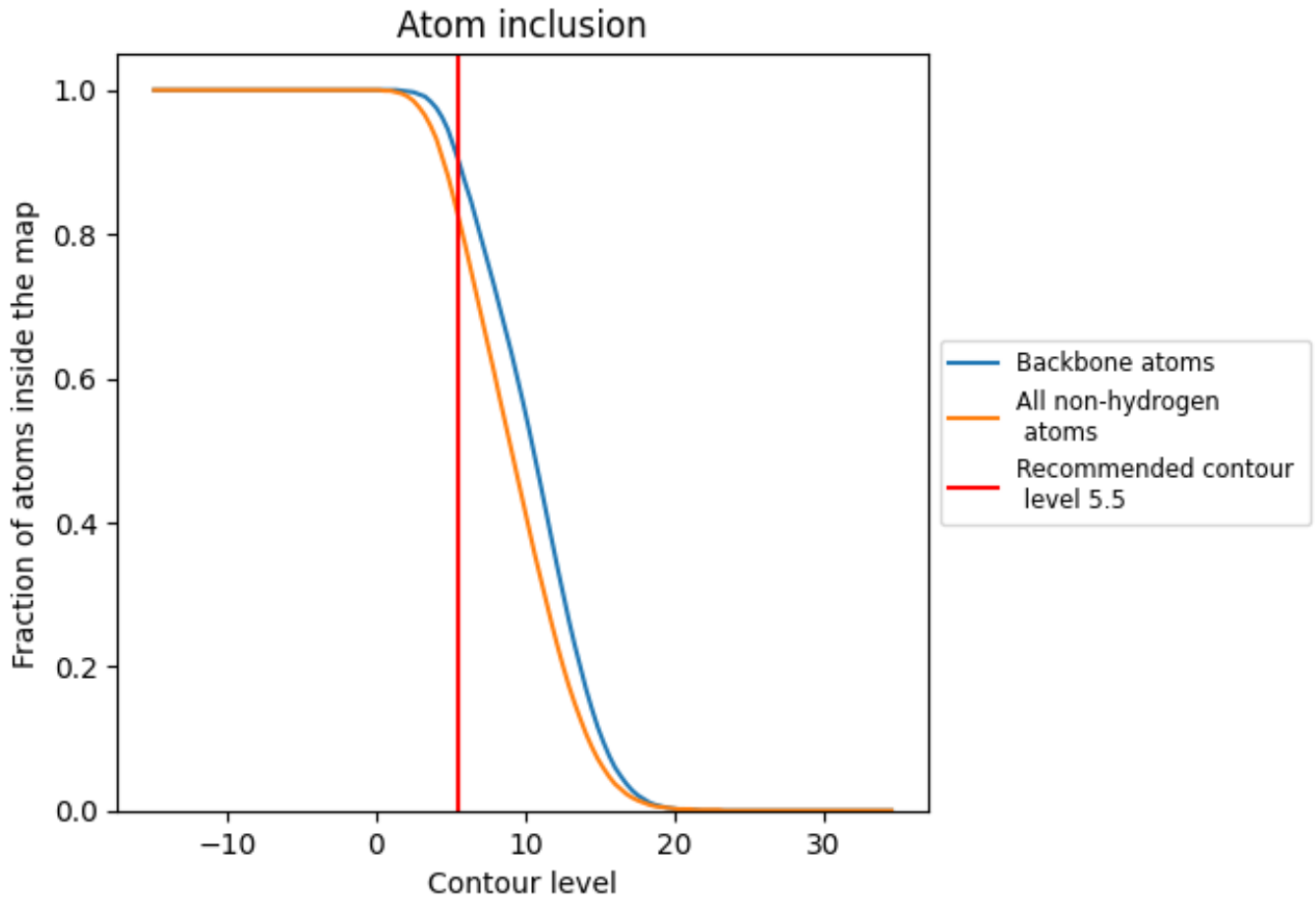
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (5.5).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 83% 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 (5.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8260	0.5670
A	0.7670	0.5830
B	0.9200	0.6370
C	0.9240	0.6340
D	0.9180	0.6320
E	0.8640	0.5710
F	0.8990	0.5960
G	0.8880	0.6060
H	0.8900	0.6160
I	0.9490	0.6570
J	0.7120	0.5390
K	0.8130	0.5810
L	0.8010	0.5440
M	0.8620	0.5910
N	0.8590	0.5930
O	0.6930	0.4570
P	0.7930	0.5550
Q	0.8950	0.6150
R	0.8730	0.6040
S	0.7970	0.5330
T	0.6220	0.4430
U	0.6800	0.4430
V	0.7880	0.5590
W	0.8370	0.5730
X	0.8300	0.5850
Y	0.3840	0.4450
Z	0.8540	0.5950
a	0.9130	0.6090
b	0.8040	0.5750
c	0.7550	0.5210
d	0.8220	0.5770
e	0.7980	0.5630
f	0.6830	0.5200
g	0.8000	0.5570
h	0.8090	0.5760



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Chain	Atom inclusion	Q-score
i	0.6920	0.4680
j	0.7470	0.4660
k	0.7000	0.4220
l	0.7750	0.4970
m	0.6940	0.4900
n	0.7650	0.4830
o	0.7370	0.4540
p	0.8030	0.5420
q	0.8870	0.6120
r	0.8400	0.6000
s	0.8540	0.5750