Full wwPDB EM Validation Report ⓘ

May 10, 2026 – 01:16 AM JST

PDB ID	:	9W2U / pdb_00009w2u
EMDB ID	:	EMD-65580
Title	:	Cryo-EM structure of complex I on the bovine heart submitochondrial particles, open
Authors	:	Nakano, A.; Masuya, T.; Akisada, S.; Ishikawa-Fukuda, M.; Mitsuoka, K.; Miyoshi, H.; Murai, M.; Yokoyama, K.
Deposited on	:	2025-07-28
Resolution	:	2.60 Å(reported)
Based on initial model	:	7QSK

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

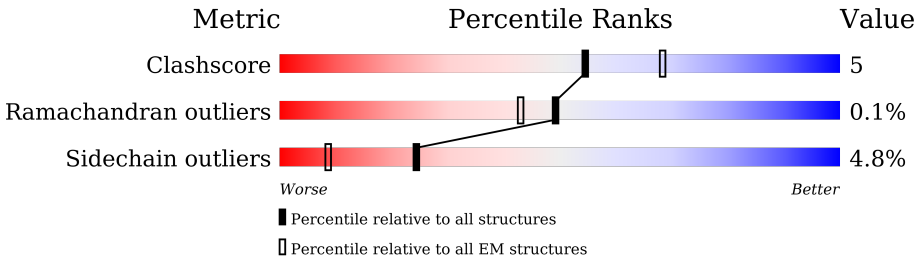
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.49

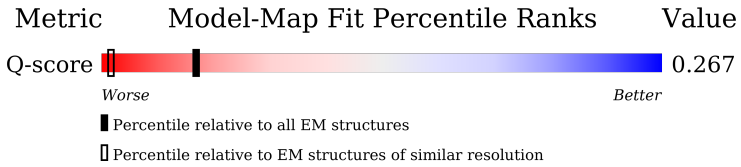
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	8728 (2.10 - 3.10)

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	J	175	25% 79% 15% • 5%
2	A	114	35% 66% 11% • 21%
3	B	155	17% 85% 14% ••
4	C	209	25% 87% 12%

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Mol	Chain	Length	Quality of chain
5	D	430	21% 84% 12%
6	E	214	12% 85% 14%
7	F	432	18% 88% 11%
8	G	699	13% 84% 15%
9	H	317	33% 79% 13% 7%
10	I	176	15% 89% 11%
11	K	97	24% 87% 13%
12	L	605	88% 11%
13	M	458	7% 88% 12%
14	N	346	19% 82% 17%
15	O	320	48% 90% 9%
16	P	342	29% 83% 16%
17	Q	129	18% 81% 18%
18	R	96	11% 92% 7%
19	S	87	26% 75% 22%
20	T	85	44% 68% 27% 5%
21	U	86	10% 72% 26%
22	V	115	44% 75% 24%
23	W	115	27% 83% 17%
24	X	171	41% 86% 12%
25	t	141	9% 77% 18%
26	Z	141	35% 86% 13%
27	a	70	31% 79% 21%
28	b	83	57% 88% 12%
29	c	49	51% 80% 20%

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Mol	Chain	Length	Quality of chain
30	d	119	35% 86% 13%
31	e	99	27% 82% 17%
32	f	57	35% 74% 26%
33	g	100	25% 85% 15%
34	h	138	22% 90% 9%
35	u	128	28% 77% 23%
36	j	71	18% 79% 18%
37	k	81	22% 78% 22%
38	l	156	10% 82% 17%
39	m	128	11% 85% 12%
40	n	172	17% 87% 13%
41	o	122	9% 77% 23%
42	p	173	12% 88% 10%
43	q	145	15% 90% 10%
44	v	113	26% 72% 13% 15%
45	s	45	16% 84% 16%

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
48	SF4	F	502	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 68035 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 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	J	167	1269	854	181	222	12	0	0

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	90	724	499	102	119	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	ALA	THR	conflict	UNP Q8WAB4

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

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

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	416	Total	C	N	O	S	0	0
			3362	2150	577	610	25		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

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

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	432	Total	C	N	O	S	1	0
			3336	2102	597	617	20		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

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

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	294	Total	C	N	O	S	0	0
			2338	1577	360	379	22		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	97	Total	C	N	O	S	0	0
			735	480	111	129	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	605	Total	C	N	O	S	0	0
			4792	3189	736	825	42		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	458	Total	C	N	O	S	0	0
			3644	2430	569	607	38		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	346	Total	C	N	O	S	0	0
			2723	1811	415	455	42		

- 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	conflict	UNP P34942

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	85	Total	C	N	O	S	0	0
			688	444	101	138	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	9	GLU	ASP	conflict	UNP Q9CR21

- Molecule 21 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	86	Total	C	N	O	S	0	0
			693	447	102	139	5		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

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

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

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

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	t	141	Total	C	N	O	S	0	0
			1030	657	176	191	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
t	0	ACE	-	acetylation	UNP Q8HXG6

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

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

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

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

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	119	Total	C	N	O	S	0	0
			988	643	171	170	4		

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

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

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

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

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

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

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	u	128	Total	C	N	O	S	0	0
			1097	722	191	183	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	0	ACE	-	acetylation	UNP Q02367

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

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

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

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

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

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

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	v	96	Total	C	N	O	S	0	0
			776	490	144	139	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	0	ACE	-	acetylation	UNP Q05752

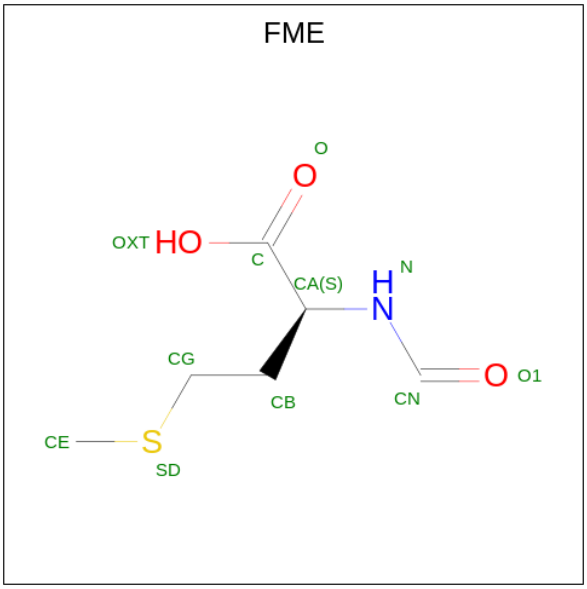
- Molecule 45 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

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

There is a discrepancy between the modelled and reference sequences:

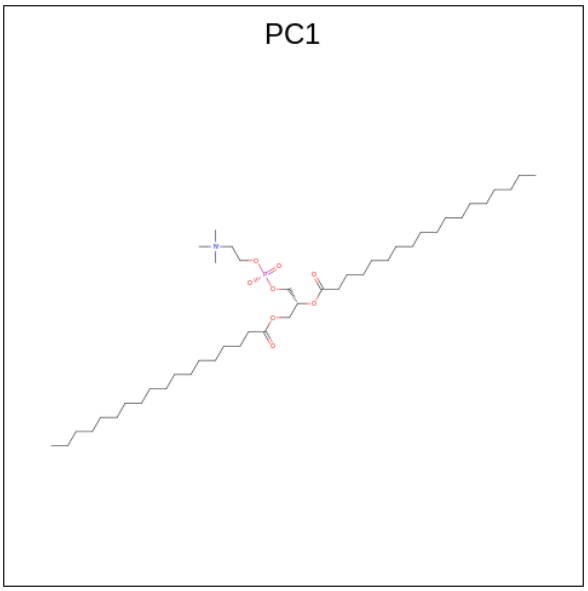
Chain	Residue	Modelled	Actual	Comment	Reference
s	57	ASP	GLU	conflict	UNP P56181

- Molecule 46 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$) (labeled as "Ligand of Interest" by depositor).



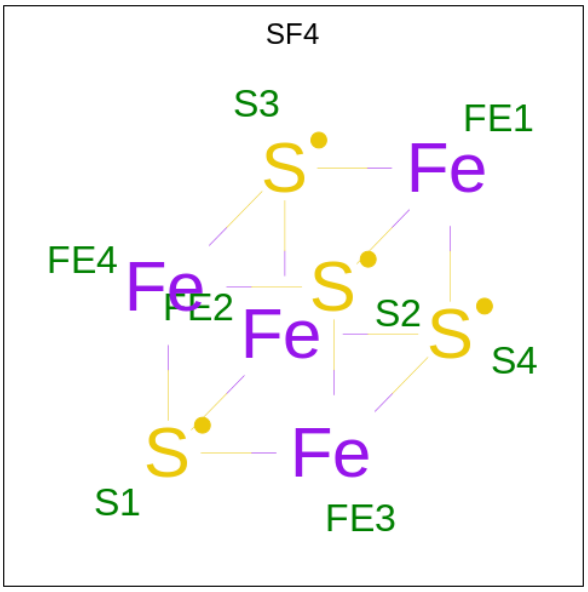
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	S	0
			10	6	1	2	1	
46	H	1	Total	C	N	O	S	0
			10	6	1	2	1	
46	K	1	Total	C	N	O	S	0
			10	6	1	2	1	
46	L	1	Total	C	N	O	S	0
			10	6	1	2	1	
46	M	1	Total	C	N	O	S	0
			10	6	1	2	1	
46	N	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 47 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



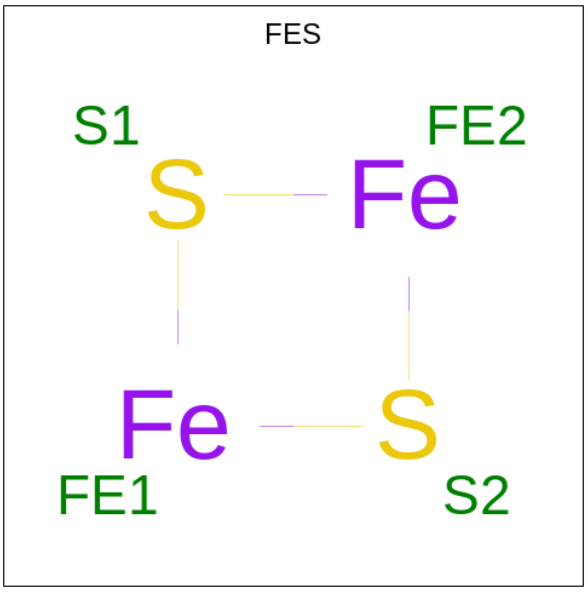
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
47	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
47	B	1	Total	C	N	O	P	0
			48	38	1	8	1	
47	H	1	Total	C	N	O	P	0
			48	38	1	8	1	
47	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
47	L	1	Total	C	N	O	P	0
			44	34	1	8	1	
47	M	1	Total	C	N	O	P	0
			35	25	1	8	1	
47	Z	1	Total	C	N	O	P	0
			44	34	1	8	1	
47	d	1	Total	C	N	O	P	0
			39	29	1	8	1	
47	h	1	Total	C	N	O	P	0
			47	37	1	8	1	
47	m	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 48 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



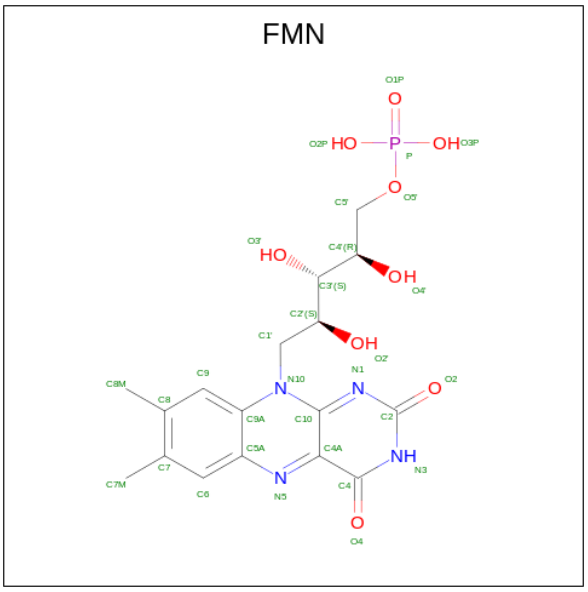
Mol	Chain	Residues	Atoms	AltConf
48	B	1	Total Fe S 8 4 4	0
48	F	1	Total Fe S 8 4 4	0
48	G	1	Total Fe S 8 4 4	0
48	G	1	Total Fe S 8 4 4	0
48	I	1	Total Fe S 8 4 4	0
48	I	1	Total Fe S 8 4 4	0

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



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

- Molecule 50 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).

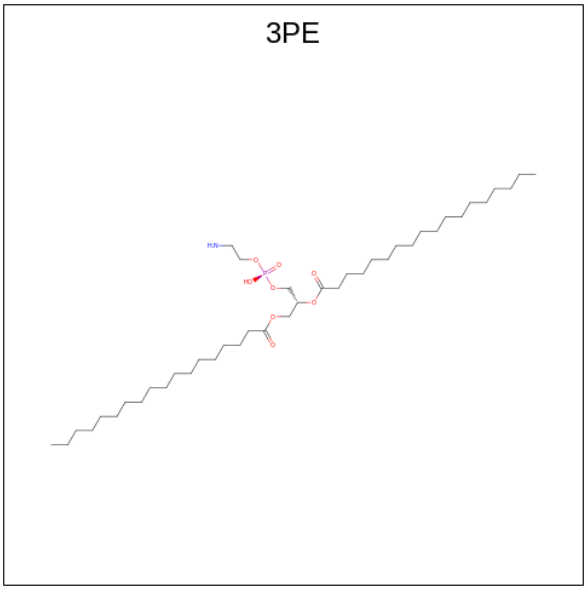


Mol	Chain	Residues	Atoms					AltConf
50	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

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

- Molecule 52 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



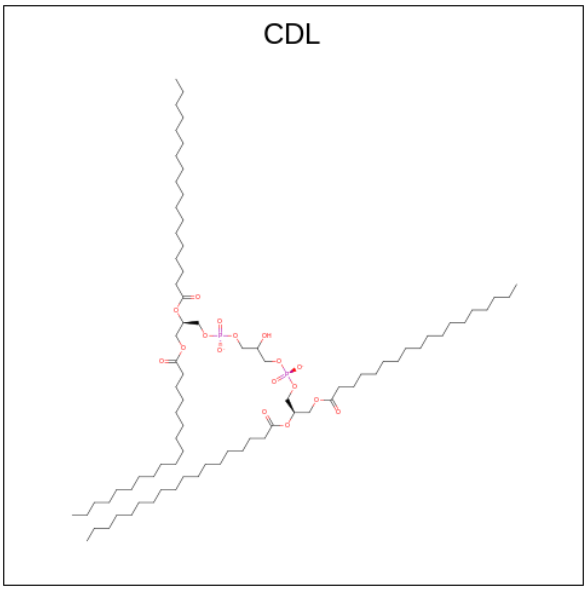
Mol	Chain	Residues	Atoms	AltConf
52	H	1	Total C N O P 36 26 1 8 1	0
52	K	1	Total C N O P 44 34 1 8 1	0
52	L	1	Total C N O P 46 36 1 8 1	0
52	L	1	Total C N O P 49 39 1 8 1	0
52	M	1	Total C N O P 45 35 1 8 1	0
52	M	1	Total C N O P 51 41 1 8 1	0
52	M	1	Total C N O P 50 40 1 8 1	0
52	O	1	Total C N O P 48 38 1 8 1	0
52	t	1	Total C N O P 31 21 1 8 1	0

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Mol	Chain	Residues	Atoms					AltConf
52	t	1	Total	C	N	O	P	0
			40	30	1	8	1	
52	t	1	Total	C	N	O	P	0
			30	20	1	8	1	
52	t	1	Total	C	N	O	P	0
			33	23	1	8	1	
52	t	1	Total	C	N	O	P	0
			27	17	1	8	1	
52	b	1	Total	C	N	O	P	0
			47	37	1	8	1	
52	d	1	Total	C	N	O	P	0
			49	39	1	8	1	
52	u	1	Total	C	N	O	P	0
			45	35	1	8	1	
52	j	1	Total	C	N	O	P	0
			44	34	1	8	1	
52	m	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 53 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



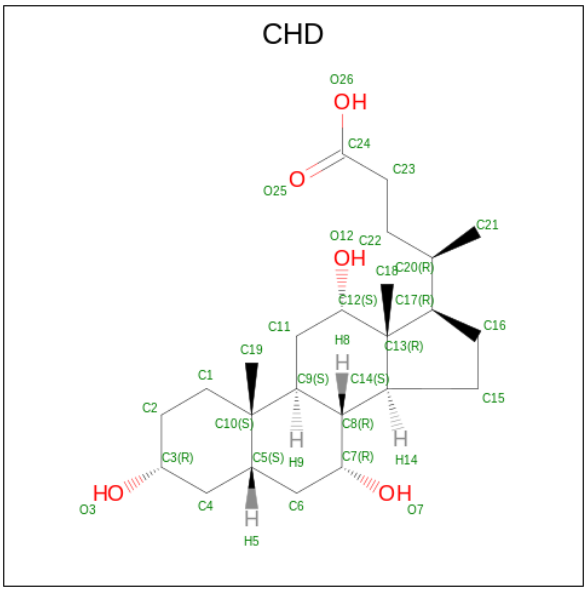
Mol	Chain	Residues	Atoms				AltConf
53	L	1	Total	C	O	P	0
			76	57	17	2	
53	O	1	Total	C	O	P	0
			62	43	17	2	

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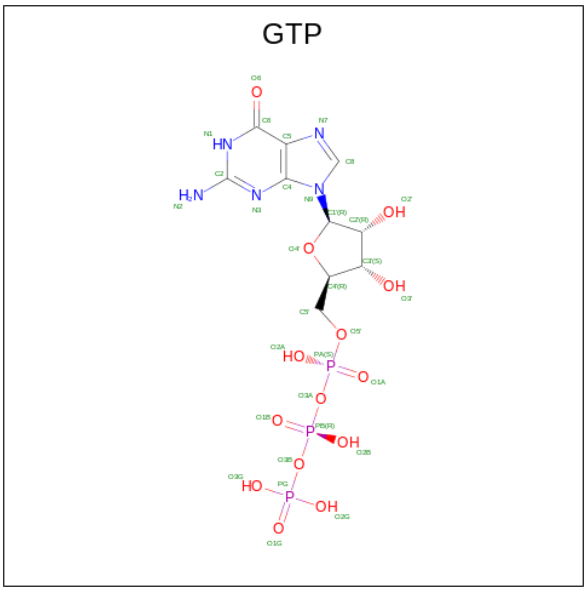
Mol	Chain	Residues	Atoms				AltConf
53	d	1	Total	C	O	P	0
			86	67	17	2	
53	d	1	Total	C	O	P	0
			65	46	17	2	
53	h	1	Total	C	O	P	0
			80	61	17	2	
53	v	1	Total	C	O	P	0
			61	42	17	2	

- Molecule 54 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 55 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).

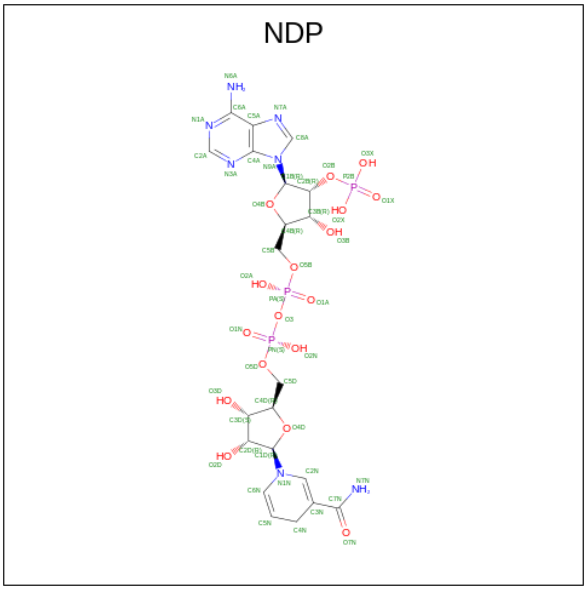


Mol	Chain	Residues	Atoms					AltConf
55	O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 57 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

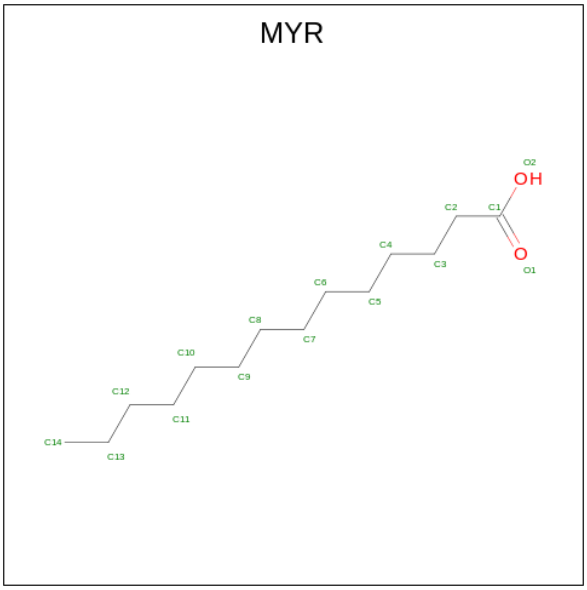


Mol	Chain	Residues	Atoms					AltConf
57	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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



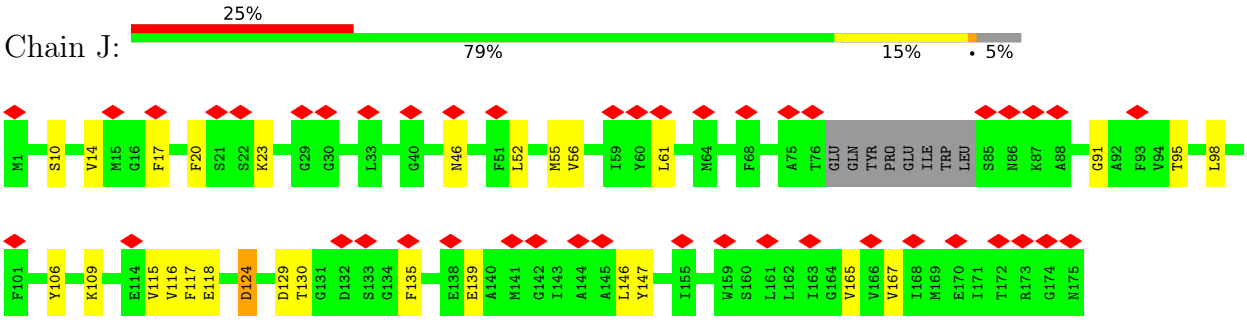
Mol	Chain	Residues	Atoms			AltConf
59	o	1	Total	C	O	0
			15	14	1	

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.

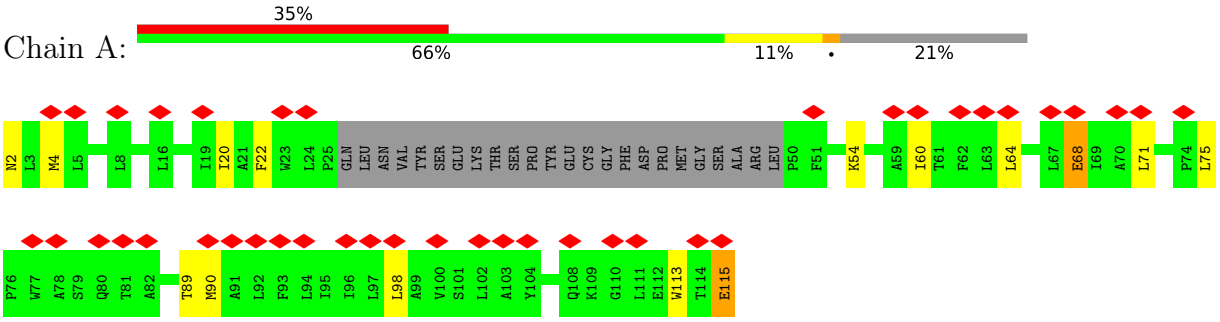
• Molecule 1: NADH-ubiquinone oxidoreductase chain 6

Chain J:



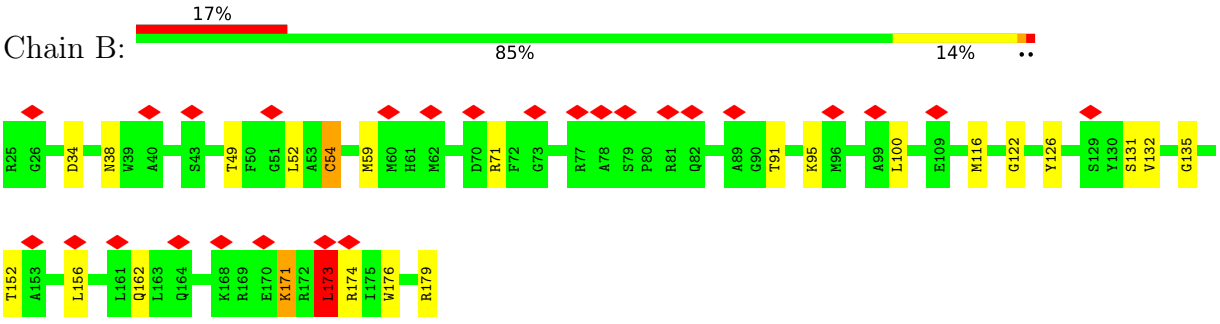
• Molecule 2: NADH-ubiquinone oxidoreductase chain 3

Chain A:



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

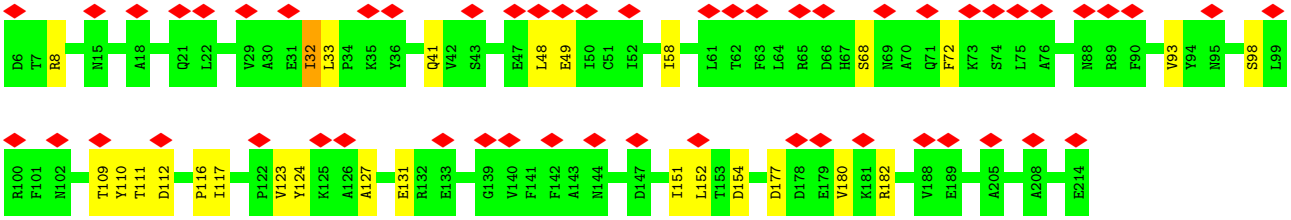
Chain B:



• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:

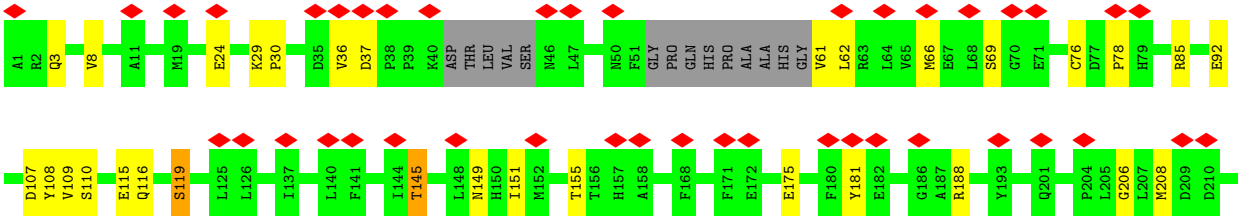




• Molecule 5: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D:

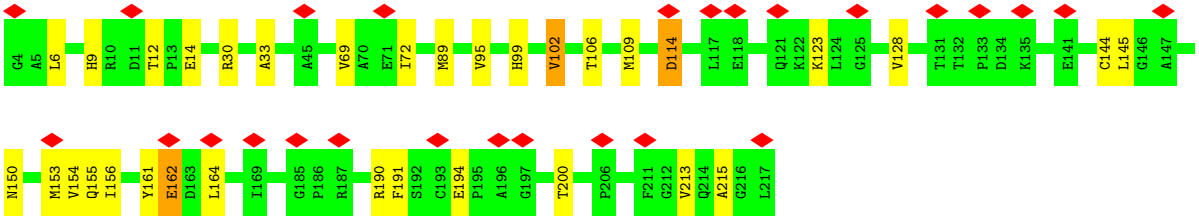




• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

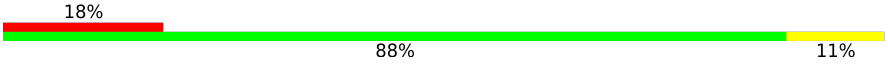
Chain E:

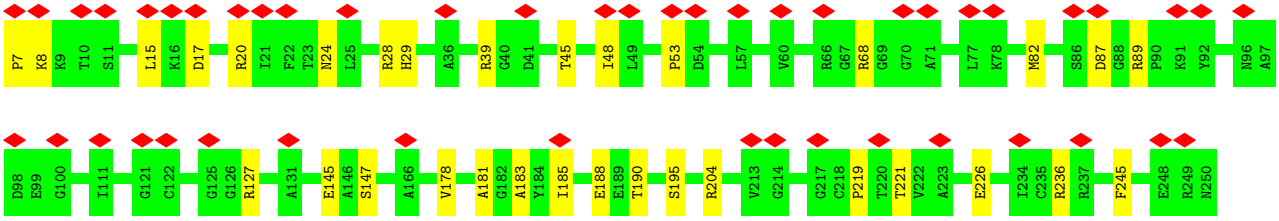


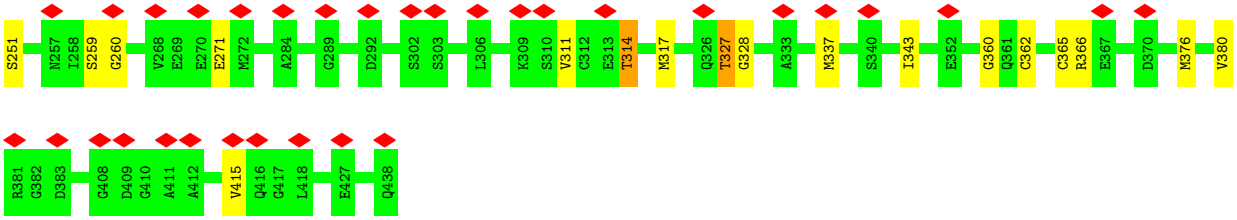


• Molecule 7: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

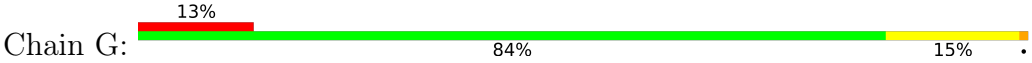
Chain F:

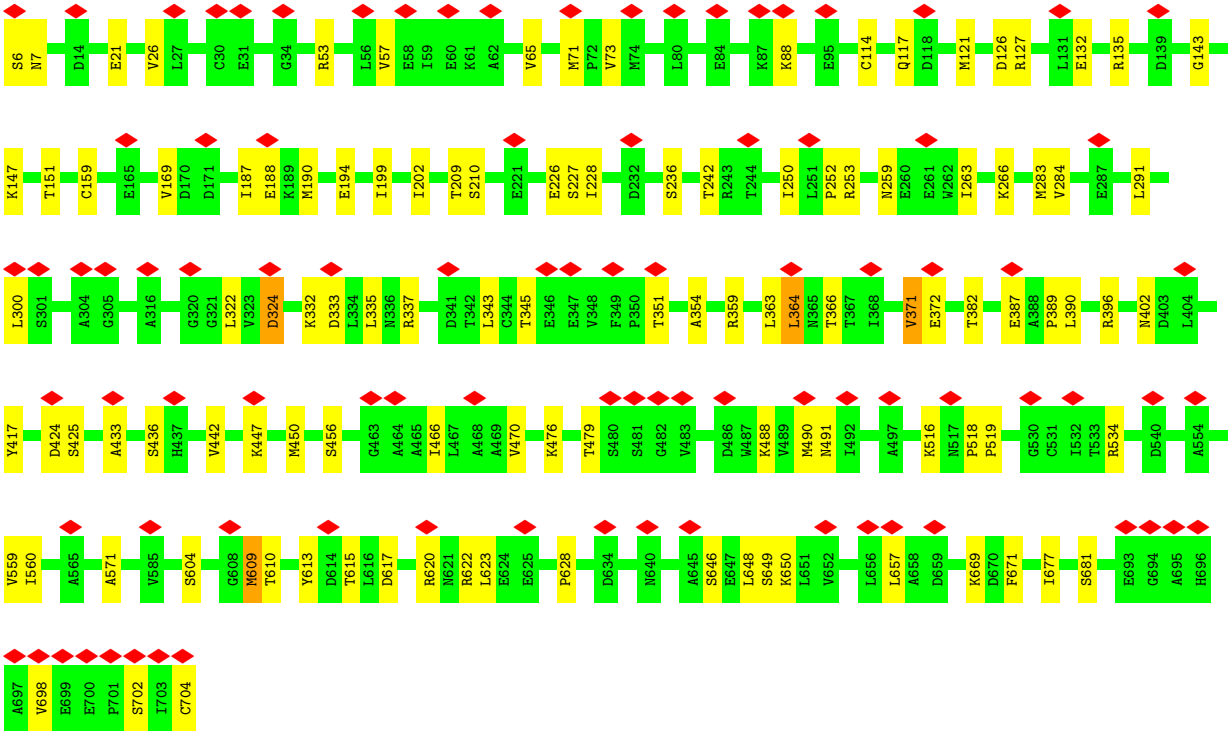




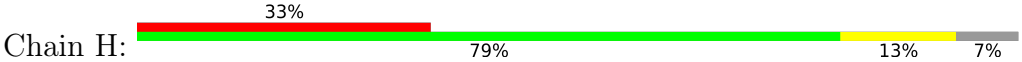


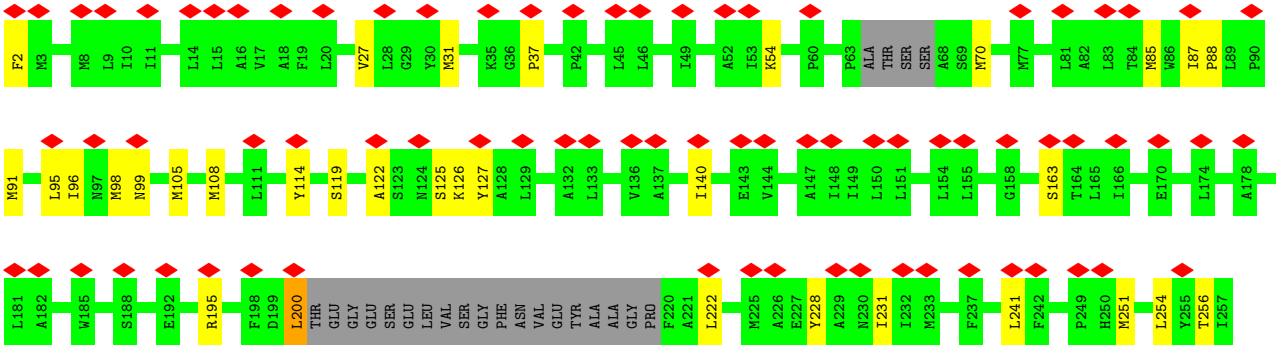
• Molecule 8: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

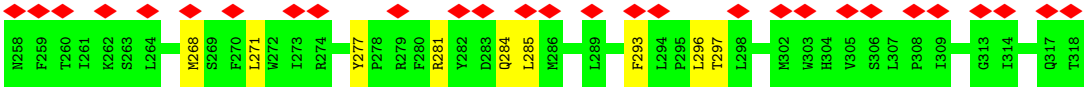




• Molecule 9: NADH-ubiquinone oxidoreductase chain 1

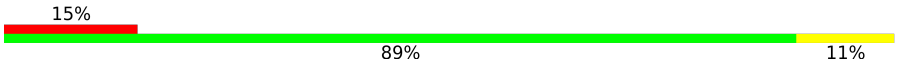


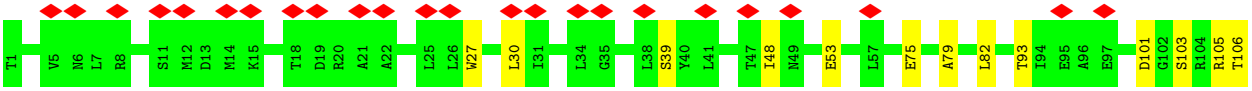


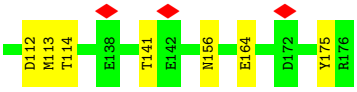


• Molecule 10: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:



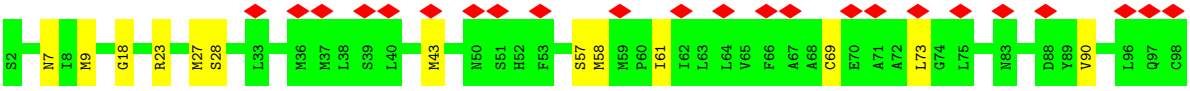




• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:

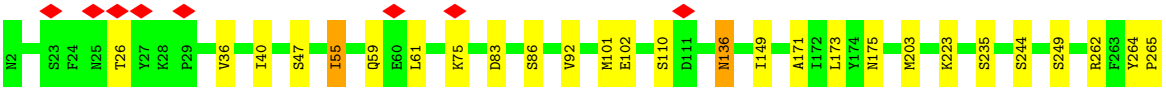


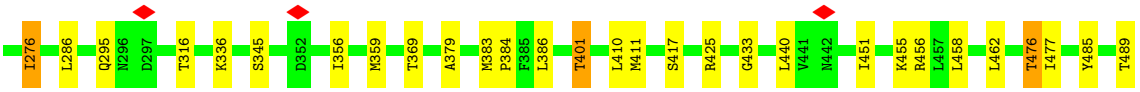


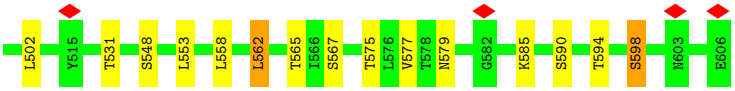
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:





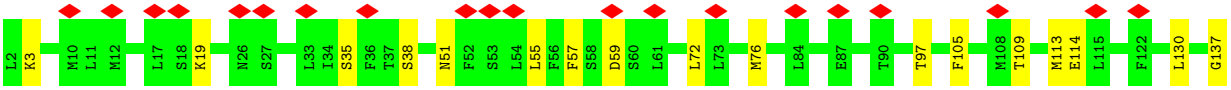




• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:

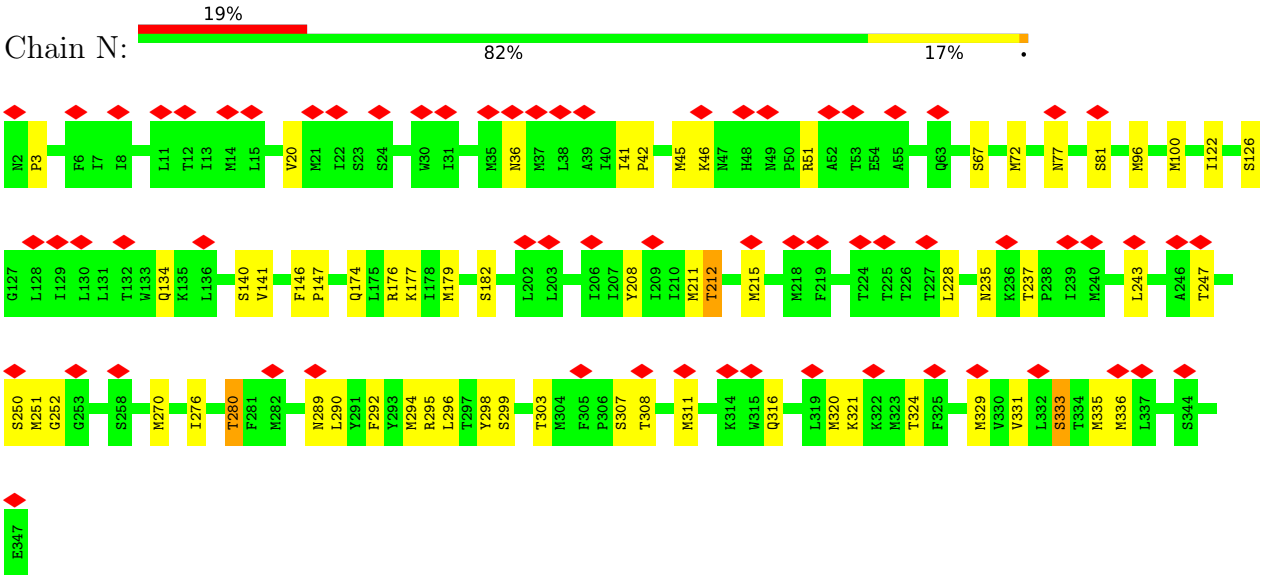








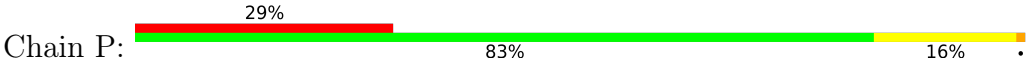
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

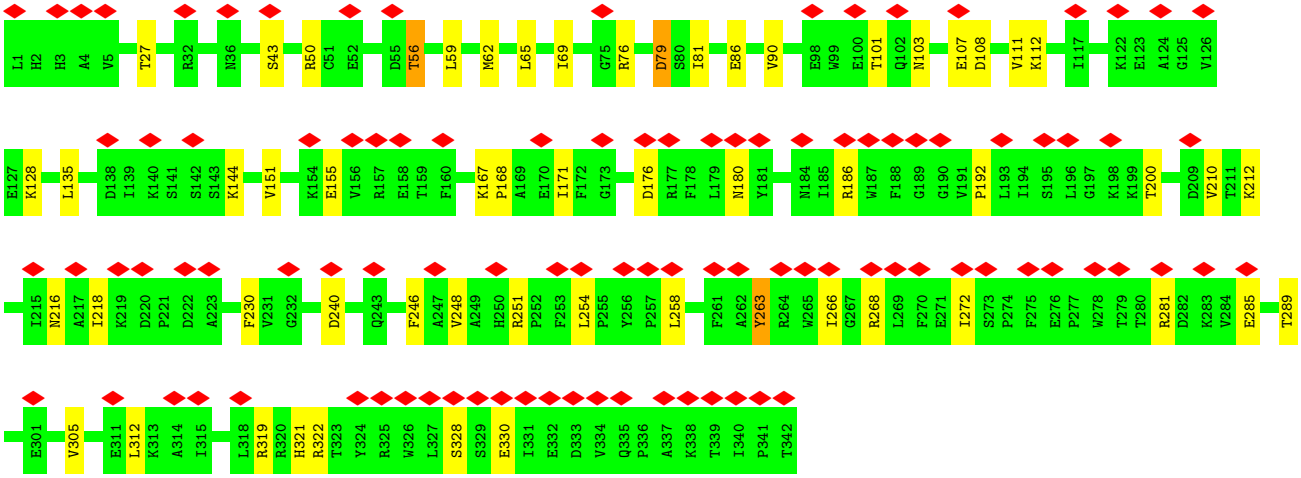


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



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

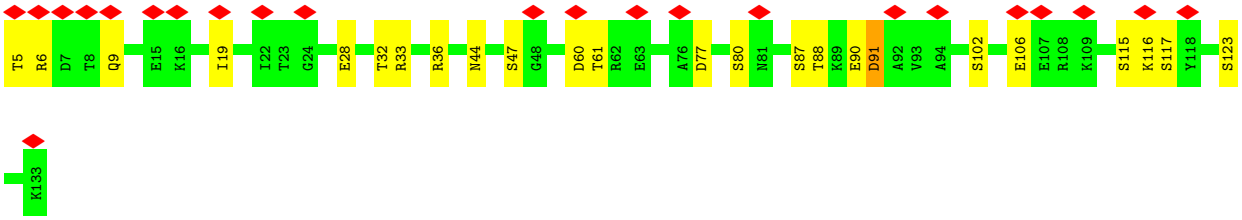




• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

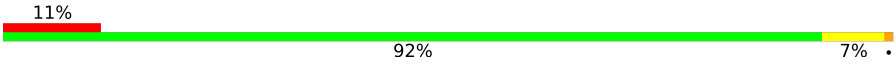
Chain Q:

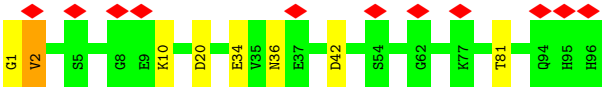




• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:

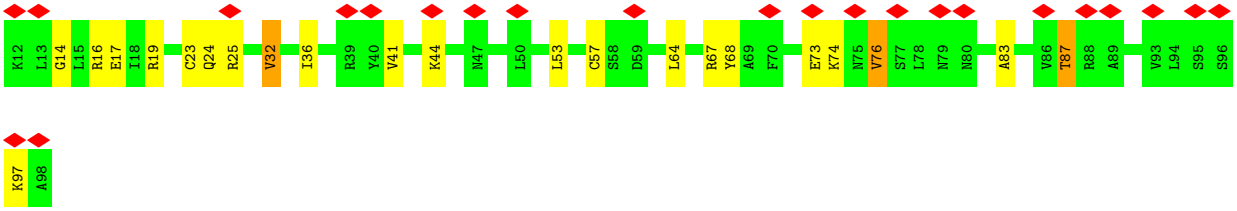




• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:

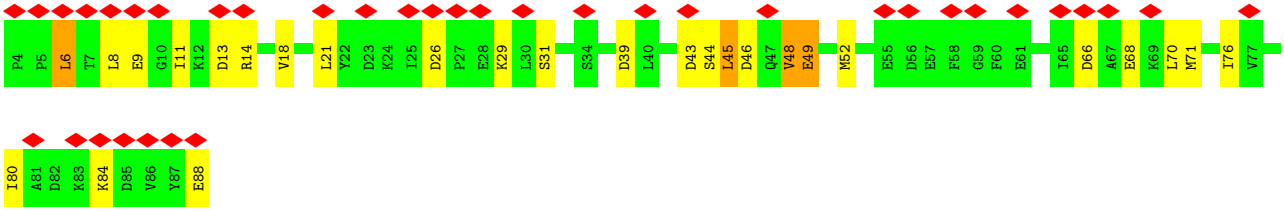




• Molecule 20: Acyl carrier protein, mitochondrial

Chain T:

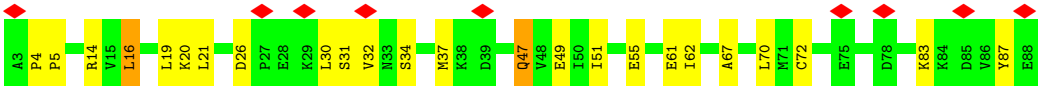




• Molecule 21: Acyl carrier protein, mitochondrial

Chain U:

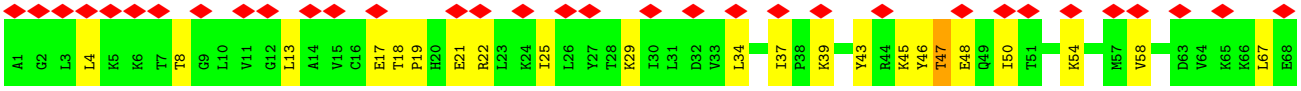


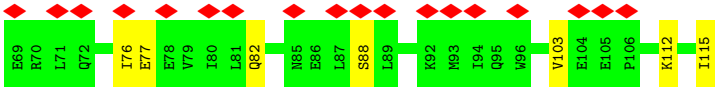


• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:



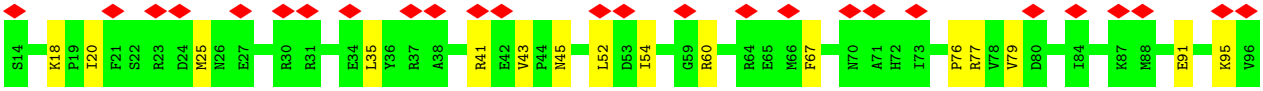


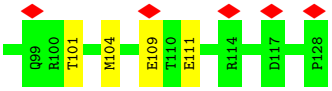


• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:



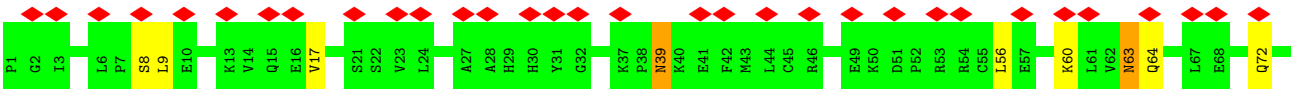


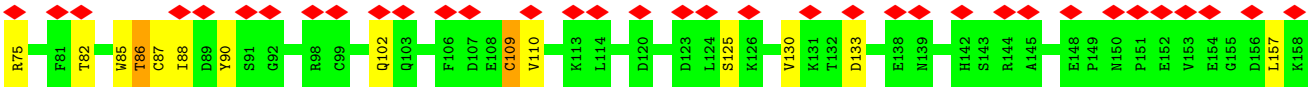


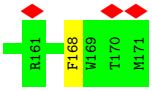
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:





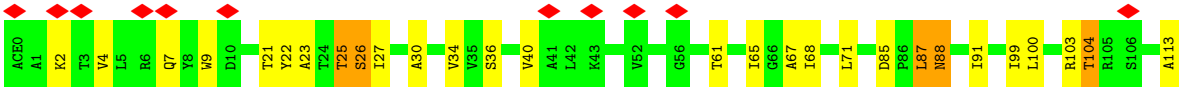


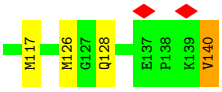


• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain t:



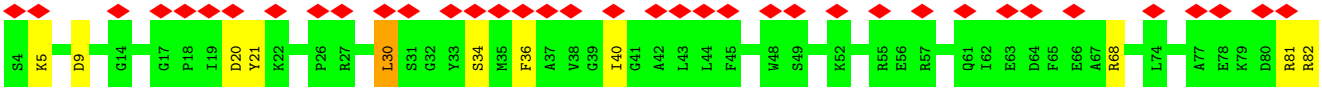


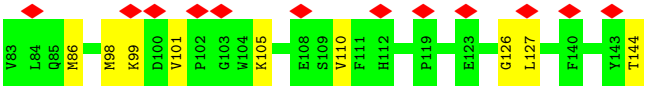


• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:



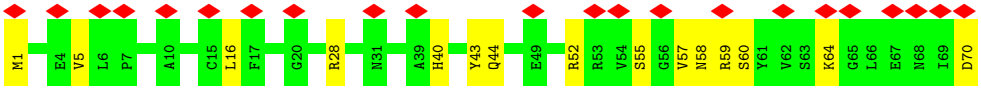




• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:

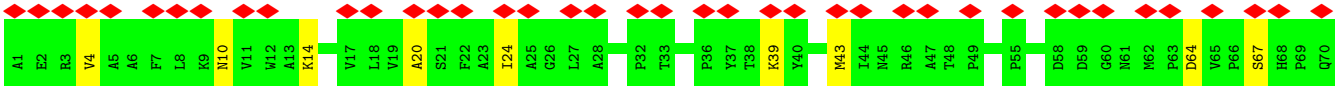


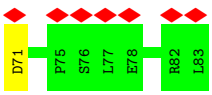


• Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:

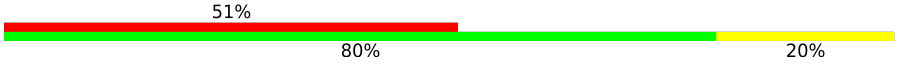


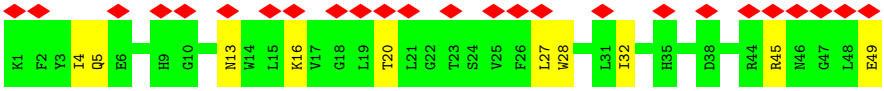




• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

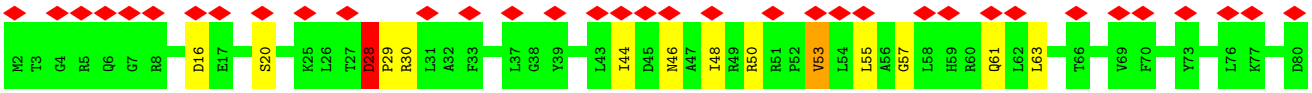
Chain c:

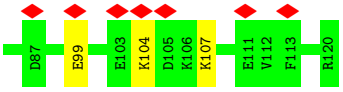




• Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

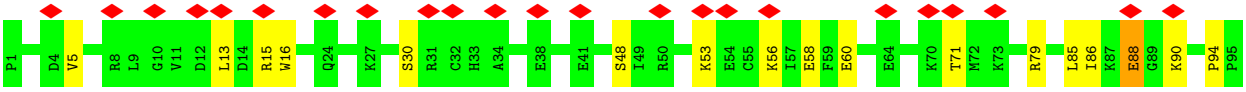






• Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

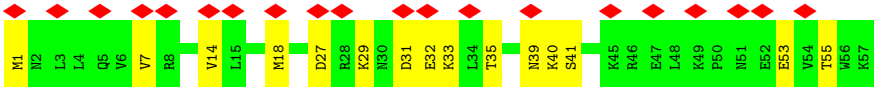






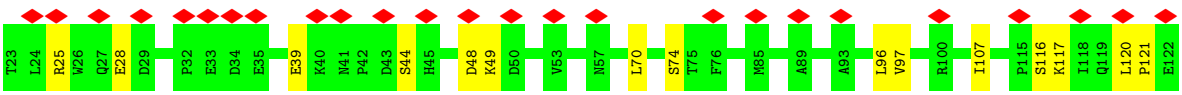
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



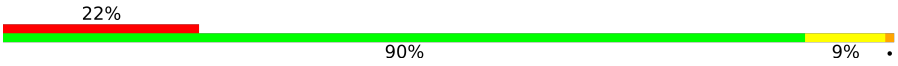


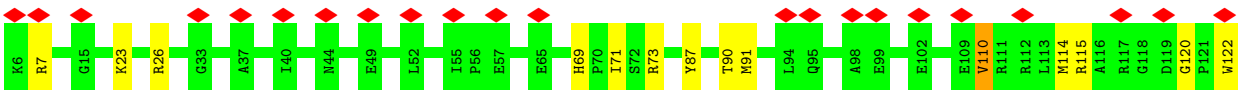
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

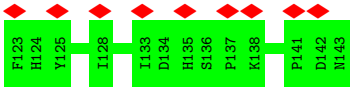




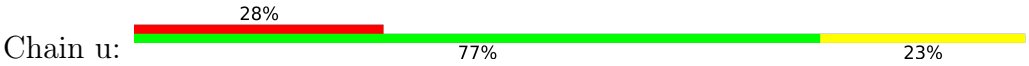
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

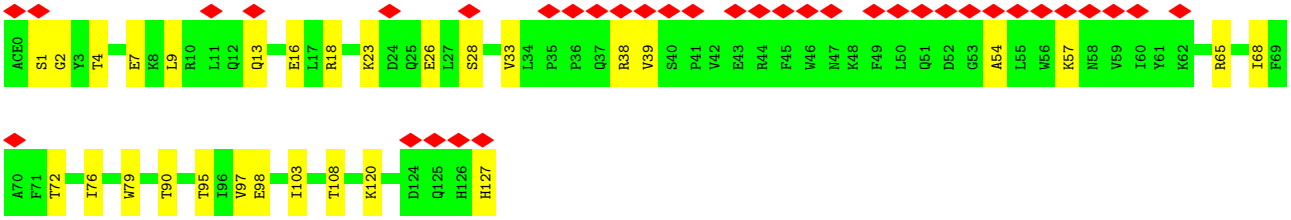




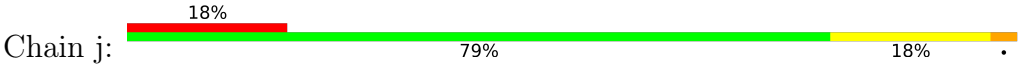


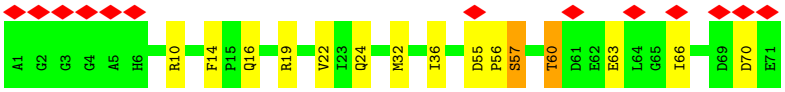
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



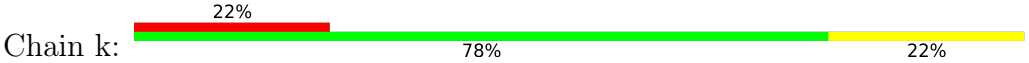


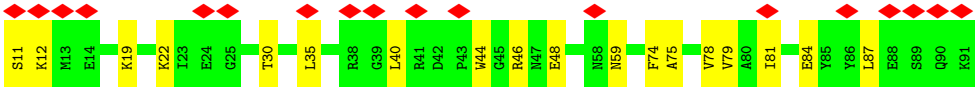
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



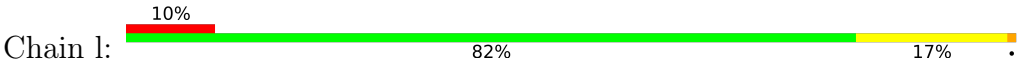


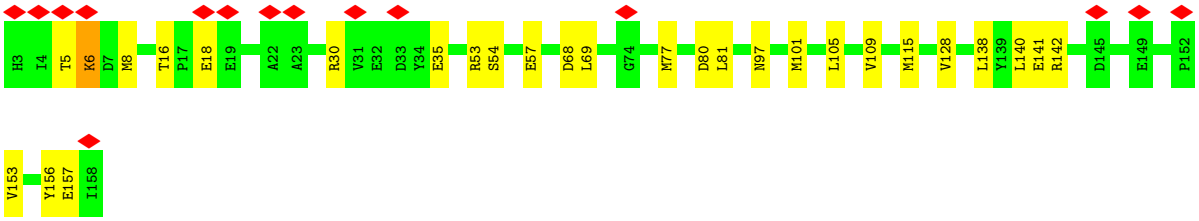
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



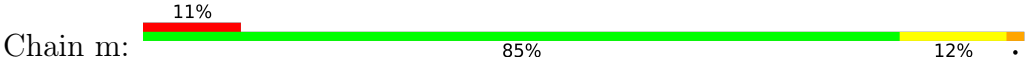


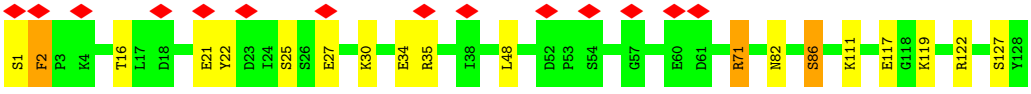
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial





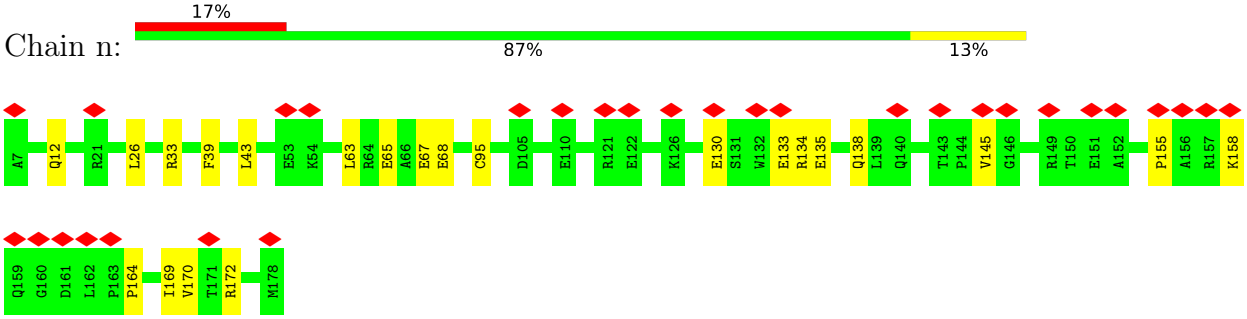
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4





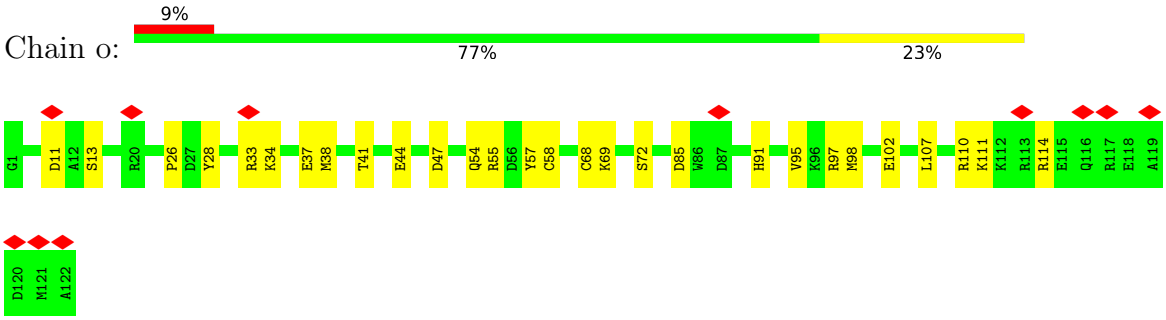
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n:



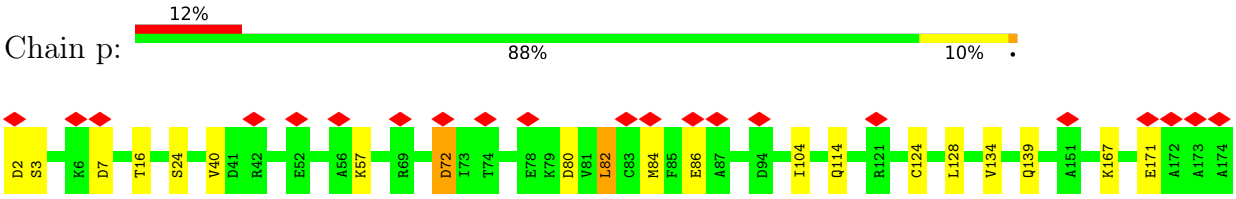
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:



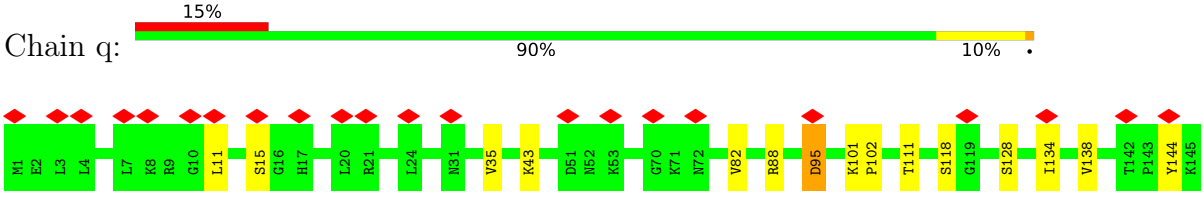
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p:



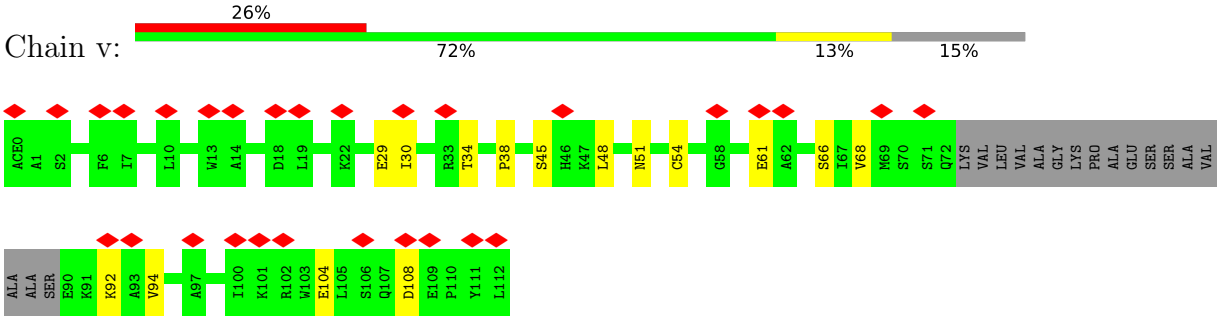
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:



• Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

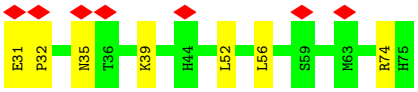
Chain v:



• Molecule 45: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	252601	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.020	Depositor
Minimum map value	-0.612	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	654.0, 654.0, 654.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	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: 2MR, 3PE, FME, MG, ACE, CHD, NDP, CDL, ZN, FES, GTP, PC1, FMN, SF4, K, MYR

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	J	0.18	0/1289	0.42	0/1745
2	A	0.16	0/743	0.37	0/1017
3	B	0.19	0/1272	0.42	1/1720 (0.1%)
4	C	0.14	0/1789	0.29	0/2436
5	D	0.16	0/3434	0.34	0/4648
6	E	0.13	0/1699	0.35	0/2312
7	F	0.13	0/3412	0.32	0/4610
8	G	0.14	0/5457	0.33	0/7397
9	H	0.17	0/2405	0.38	0/3283
10	I	0.16	0/1445	0.30	0/1956
11	K	0.15	0/745	0.36	0/1008
12	L	0.14	0/4920	0.34	0/6694
13	M	0.16	0/3738	0.31	0/5097
14	N	0.17	0/2792	0.34	0/3800
15	O	0.16	0/2651	0.35	0/3587
16	P	0.16	0/2847	0.36	0/3864
17	Q	0.15	0/1072	0.37	0/1449
18	R	0.14	0/753	0.30	0/1014
19	S	0.22	0/711	0.56	0/956
20	T	0.26	0/700	0.75	3/944 (0.3%)
21	U	0.18	0/705	0.48	0/952
22	V	0.19	0/948	0.45	0/1284
23	W	0.21	0/1000	0.45	0/1344
24	X	0.14	0/1439	0.33	0/1942
25	t	0.24	0/1048	0.50	0/1423
26	Z	0.21	0/1181	0.39	0/1592
27	a	0.14	0/584	0.29	0/786
28	b	0.18	0/672	0.44	0/923
29	c	0.20	0/427	0.52	0/579
30	d	0.20	0/1018	0.38	0/1375
31	e	0.18	0/850	0.47	0/1136
32	f	0.20	0/505	0.57	0/681

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	g	0.22	0/865	0.52	0/1175
34	h	0.14	0/1188	0.28	0/1607
35	u	0.23	0/1134	0.54	0/1544
36	j	0.20	0/624	0.47	0/855
37	k	0.21	0/672	0.56	0/906
38	l	0.18	0/1369	0.46	0/1873
39	m	0.21	0/1094	0.51	0/1480
40	n	0.16	0/1545	0.40	0/2092
41	o	0.18	0/1073	0.46	0/1437
42	p	0.13	0/1486	0.31	0/2004
43	q	0.15	0/1250	0.32	0/1698
44	v	0.22	0/795	0.50	0/1077
45	s	0.16	0/403	0.35	0/545
All	All	0.17	0/67749	0.39	4/91847 (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
7	F	0	1
30	d	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	T	48	VAL	CA-C-N	-6.22	109.44	121.58
20	T	48	VAL	C-N-CA	-6.22	109.44	121.58
20	T	49	GLU	CA-CB-CG	5.77	125.64	114.10
3	B	173	LEU	CA-CB-CG	5.48	135.48	116.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	F	236	ARG	Peptide
30	d	28	ASP	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	J	1269	0	1283	19	0
2	A	724	0	766	12	0
3	B	1241	0	1251	13	0
4	C	1738	0	1685	12	0
5	D	3362	0	3314	35	0
6	E	1659	0	1664	14	0
7	F	3336	0	3286	28	0
8	G	5366	0	5378	51	0
9	H	2338	0	2466	22	0
10	I	1414	0	1370	11	0
11	K	735	0	774	8	0
12	L	4792	0	4949	31	0
13	M	3644	0	3841	33	0
14	N	2723	0	2901	34	0
15	O	2589	0	2566	24	0
16	P	2768	0	2782	32	0
17	Q	1049	0	1045	11	0
18	R	740	0	714	4	0
19	S	700	0	719	15	0
20	T	688	0	685	20	0
21	U	693	0	689	17	0
22	V	928	0	972	17	0
23	W	976	0	991	16	0
24	X	1402	0	1381	16	0
25	t	1030	0	1039	20	0
26	Z	1152	0	1151	19	0
27	a	569	0	568	8	0
28	b	651	0	662	7	0
29	c	414	0	415	7	0
30	d	988	0	975	14	0
31	e	829	0	829	10	0
32	f	492	0	501	9	0
33	g	839	0	790	11	0
34	h	1154	0	1168	11	0
35	u	1097	0	1108	18	0
36	j	597	0	536	10	0
37	k	653	0	639	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	l	1314	0	1210	20	0
39	m	1067	0	1067	17	0
40	n	1492	0	1438	12	0
41	o	1048	0	1020	22	0
42	p	1453	0	1425	12	0
43	q	1209	0	1182	4	0
44	v	776	0	782	7	0
45	s	391	0	361	5	0
46	A	10	0	10	2	0
46	H	10	0	10	1	0
46	K	10	0	10	0	0
46	L	10	0	10	1	0
46	M	10	0	10	0	0
46	N	10	0	10	1	0
47	A	35	0	44	0	0
47	B	94	0	132	4	0
47	H	48	0	73	3	0
47	I	54	0	88	2	0
47	L	44	0	65	0	0
47	M	35	0	44	1	0
47	Z	44	0	62	0	0
47	d	39	0	52	2	0
47	h	47	0	71	1	0
47	m	46	0	66	0	0
48	B	8	0	0	0	0
48	F	8	0	0	2	0
48	G	16	0	0	0	0
48	I	16	0	0	0	0
49	E	4	0	0	0	0
49	G	4	0	0	0	0
50	F	31	0	19	2	0
51	G	1	0	0	0	0
52	H	36	0	46	0	0
52	K	44	0	62	0	0
52	L	95	0	144	1	0
52	M	146	0	223	6	0
52	O	48	0	73	1	0
52	b	47	0	71	2	0
52	d	49	0	75	1	0
52	j	44	0	65	1	0
52	m	41	0	59	1	0
52	t	161	0	195	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	u	45	0	67	1	0
53	L	76	0	99	4	0
53	O	62	0	67	5	0
53	d	151	0	202	10	0
53	h	80	0	104	2	0
53	v	61	0	66	2	0
54	L	29	0	39	2	0
55	O	32	0	12	1	0
56	O	1	0	0	0	0
57	P	48	0	26	0	0
58	R	1	0	0	0	0
59	o	15	0	27	0	0
All	All	68035	0	68836	691	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 5.

All (691) 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)
12:L:383:MET:HE3	12:L:384:PRO:HD2	1.55	0.89
30:d:28:ASP:N	53:d:201:CDL:OB9	1.98	0.89
25:t:68:ILE:HD11	25:t:99:ILE:HG12	1.70	0.72
33:g:97:VAL:HG23	33:g:107:ILE:HD11	1.71	0.71
11:K:43:MET:HE1	14:N:72:MET:HE1	1.72	0.70
39:m:117:GLU:HG2	39:m:119:LYS:HZ1	1.56	0.70
41:o:26:PRO:O	41:o:33:ARG:NH2	2.25	0.70
5:D:328:ALA:HB3	8:G:126:ASP:HB2	1.74	0.69
8:G:114:CYS:HB3	8:G:117:GLN:HB2	1.74	0.69
12:L:40:ILE:HD12	12:L:101:MET:HE2	1.73	0.69
8:G:470:VAL:HG12	8:G:490:MET:HE1	1.76	0.67
19:S:23:CYS:SG	19:S:24:GLN:N	2.68	0.67
13:M:237:LYS:HD2	13:M:316:MET:HB3	1.77	0.67
16:P:192:PRO:HB2	16:P:263:TYR:HE1	1.59	0.67
5:D:29:LYS:HE2	5:D:30:PRO:HD2	1.79	0.65
37:k:35:LEU:HB3	37:k:40:LEU:HB2	1.79	0.64
39:m:117:GLU:N	39:m:117:GLU:OE2	2.31	0.64
26:Z:5:LYS:HE2	26:Z:5:LYS:HA	1.81	0.63
9:H:85:MET:HE3	9:H:108:MET:HB2	1.80	0.63
16:P:240:ASP:N	16:P:240:ASP:OD1	2.31	0.63
16:P:144:LYS:H	16:P:144:LYS:HZ3	1.44	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:90:GLU:N	17:Q:90:GLU:OE2	2.31	0.63
7:F:82:MET:SD	7:F:221:THR:OG1	2.57	0.63
9:H:251:MET:HG3	9:H:254:LEU:HD23	1.79	0.63
54:L:706:CHD:H213	35:u:65:ARG:HB3	1.80	0.63
14:N:215:MET:HE3	14:N:251:MET:HE2	1.80	0.62
31:e:58:GLU:N	31:e:58:GLU:OE1	2.32	0.62
8:G:615:THR:OG1	8:G:617:ASP:OD1	2.17	0.62
32:f:1:MET:SD	32:f:1:MET:N	2.66	0.62
1:J:23:LYS:NZ	11:K:18:GLY:O	2.32	0.62
22:V:19:PRO:HB3	22:V:76:ILE:HG21	1.80	0.62
19:S:64:LEU:HB3	19:S:76:VAL:HG13	1.81	0.62
35:u:26:GLU:N	35:u:26:GLU:OE2	2.32	0.61
33:g:48:ASP:OD1	33:g:49:LYS:N	2.33	0.61
1:J:129:ASP:OD2	1:J:130:THR:N	2.34	0.61
14:N:36:ASN:OD1	14:N:134:GLN:NE2	2.34	0.61
14:N:174:GLN:HB2	14:N:177:LYS:HG3	1.83	0.61
12:L:102:GLU:OE1	12:L:456:ARG:NH2	2.33	0.60
1:J:146:LEU:HA	11:K:58:MET:HE2	1.82	0.60
38:l:68:ASP:N	38:l:68:ASP:OD1	2.34	0.60
8:G:143:GLY:HA2	8:G:190:MET:HE2	1.84	0.60
13:M:281:ASP:HB3	13:M:284:SER:HB2	1.81	0.60
1:J:124:ASP:OD1	1:J:124:ASP:N	2.34	0.60
12:L:477:ILE:HD11	41:o:54:GLN:HA	1.82	0.60
30:d:99:GLU:OE2	30:d:99:GLU:N	2.32	0.60
14:N:179:MET:HE1	14:N:251:MET:HE1	1.84	0.60
7:F:365:CYS:HB3	48:F:502:SF4:S3	2.43	0.59
8:G:324:ASP:HB3	8:G:571:ALA:HB1	1.83	0.59
19:S:83:ALA:O	19:S:87:THR:OG1	2.19	0.59
20:T:70:LEU:HD23	20:T:76:ILE:HG12	1.83	0.59
40:n:12:GLN:OE1	40:n:12:GLN:N	2.33	0.59
41:o:85:ASP:OD1	41:o:85:ASP:N	2.35	0.59
25:t:27:ILE:HG23	52:t:804:3PE:H342	1.84	0.59
28:b:64:ASP:OD1	28:b:64:ASP:N	2.35	0.59
8:G:534:ARG:NH2	43:q:144:TYR:OH	2.36	0.59
39:m:117:GLU:O	39:m:119:LYS:NZ	2.35	0.59
24:X:90:TYR:OH	27:a:28:ARG:NH1	2.36	0.59
41:o:28:TYR:OH	41:o:111:LYS:NZ	2.36	0.59
16:P:76:ARG:NH1	16:P:108:ASP:OD2	2.35	0.58
31:e:94:PRO:HG2	31:e:97:HIS:HB2	1.85	0.58
1:J:118:GLU:N	1:J:118:GLU:OE1	2.35	0.58
9:H:2:PHE:N	46:H:401:FME:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:319:ARG:HA	16:P:322:ARG:HD3	1.85	0.58
22:V:17:GLU:OE1	22:V:17:GLU:N	2.35	0.58
40:n:135:GLU:HG2	40:n:164:PRO:HA	1.86	0.58
8:G:266:LYS:NZ	8:G:671:PHE:O	2.37	0.58
38:l:30:ARG:NH1	39:m:34:GLU:OE1	2.36	0.58
37:k:48:GLU:OE1	40:n:33:ARG:NE	2.37	0.58
12:L:562:LEU:HD22	52:L:704:3PE:H3B2	1.85	0.58
34:h:114:MET:HE2	34:h:122:TRP:H	1.68	0.58
10:I:156:ASN:ND2	18:R:34:GLU:OE1	2.36	0.58
19:S:32:VAL:O	19:S:36:ILE:HD12	2.04	0.58
24:X:82:THR:O	24:X:86:THR:OG1	2.22	0.58
29:c:28:TRP:O	29:c:32:ILE:HD12	2.03	0.58
6:E:145:LEU:HD12	6:E:153:MET:HE1	1.85	0.57
9:H:70:MET:HB2	9:H:122:ALA:HB2	1.86	0.57
25:t:113:ALA:HB1	25:t:117:MET:HE3	1.85	0.57
22:V:39:LYS:O	22:V:45:LYS:NZ	2.36	0.57
36:j:32:MET:O	36:j:36:ILE:HG13	2.05	0.57
8:G:337:ARG:HD3	8:G:609:MET:HB2	1.86	0.57
16:P:90:VAL:HG21	16:P:218:ILE:HD11	1.85	0.57
30:d:28:ASP:OD1	30:d:29:PRO:HD2	2.03	0.57
12:L:59:GLN:NE2	46:L:701:FME:O	2.37	0.57
20:T:49:GLU:HA	20:T:52:MET:HB2	1.87	0.57
8:G:490:MET:HE2	8:G:490:MET:HA	1.87	0.57
14:N:235:ASN:HD21	15:O:289:SER:HB3	1.70	0.57
13:M:243:MET:O	13:M:247:THR:OG1	2.22	0.57
5:D:261:ARG:NH2	5:D:303:GLU:OE2	2.37	0.56
47:H:403:PC1:H392	47:H:403:PC1:H2H1	1.87	0.56
12:L:433:GLY:O	37:k:59:ASN:ND2	2.37	0.56
15:O:317:ILE:HD11	30:d:55:LEU:HD23	1.88	0.56
7:F:245:PHE:HB3	7:F:271:GLU:HG3	1.86	0.56
35:u:98:GLU:N	35:u:98:GLU:OE2	2.39	0.56
8:G:226:GLU:OE1	8:G:253:ARG:NH1	2.37	0.56
17:Q:36:ARG:NE	17:Q:106:GLU:OE2	2.39	0.56
20:T:39:ASP:OD1	20:T:39:ASP:N	2.33	0.56
14:N:77:ASN:O	14:N:81:SER:OG	2.24	0.56
16:P:59:LEU:HA	16:P:62:MET:HE3	1.85	0.56
36:j:10:ARG:NH1	36:j:14:PHE:O	2.39	0.56
2:A:2:ASN:N	46:A:201:FME:O	2.38	0.56
8:G:21:GLU:OE2	8:G:21:GLU:N	2.32	0.56
53:L:703:CDL:OA9	34:h:26:ARG:NH1	2.38	0.56
20:T:8:LEU:HA	20:T:11:ILE:HB	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:43:ASP:OD2	20:T:44:SER:N	2.36	0.56
4:C:68:SER:HA	22:V:82:GLN:NE2	2.20	0.56
17:Q:5:THR:OG1	17:Q:6:ARG:N	2.34	0.56
44:v:104:GLU:OE2	44:v:104:GLU:N	2.39	0.55
8:G:194:GLU:HG3	8:G:389:PRO:HB3	1.87	0.55
30:d:29:PRO:HB2	53:d:201:CDL:H312	1.86	0.55
1:J:147:TYR:OH	2:A:71:LEU:O	2.22	0.55
9:H:96:ILE:HG23	26:Z:144:THR:HB	1.89	0.55
35:u:38:ARG:NH1	35:u:38:ARG:O	2.39	0.55
23:W:91:GLU:OE1	23:W:95:LYS:NZ	2.35	0.55
6:E:12:THR:HG22	6:E:14:GLU:H	1.70	0.55
13:M:130:LEU:HD21	14:N:294:MET:HE1	1.89	0.55
13:M:324:SER:OG	13:M:440:HIS:NE2	2.39	0.55
13:M:343:ILE:O	13:M:346:ARG:NH1	2.40	0.55
25:t:65:ILE:HG13	25:t:99:ILE:HD11	1.87	0.55
25:t:140:VAL:O	34:h:115:ARG:NH1	2.39	0.55
4:C:151:ILE:HG23	4:C:152:LEU:HG	1.89	0.55
7:F:327:THR:OG1	7:F:328:GLY:N	2.40	0.55
10:I:164:GLU:HG3	43:q:88:ARG:HG3	1.89	0.55
14:N:298:TYR:O	14:N:303:THR:OG1	2.23	0.55
22:V:43:TYR:O	22:V:47:THR:OG1	2.22	0.55
35:u:68:ILE:O	35:u:72:THR:HG22	2.07	0.54
21:U:47:GLN:NE2	21:U:70:LEU:O	2.40	0.54
23:W:111:GLU:OE2	23:W:111:GLU:N	2.29	0.54
1:J:61:LEU:O	9:H:114:TYR:OH	2.26	0.54
5:D:66:MET:HE2	5:D:66:MET:HA	1.89	0.54
10:I:27:TRP:HB3	10:I:30:LEU:HD12	1.88	0.54
21:U:49:GLU:OE1	37:k:44:TRP:NE1	2.36	0.54
3:B:131:SER:O	3:B:131:SER:OG	2.24	0.54
7:F:89:ARG:HH21	7:F:219:PRO:HD3	1.72	0.54
8:G:227:SER:OG	8:G:228:ILE:N	2.39	0.54
19:S:68:TYR:OH	19:S:74:LYS:NZ	2.40	0.54
41:o:68:CYS:O	41:o:72:SER:OG	2.24	0.54
3:B:173:LEU:HD13	47:B:202:PC1:H3C1	1.89	0.54
8:G:7:ASN:OD1	8:G:7:ASN:N	2.40	0.54
5:D:279:ASP:OD1	5:D:279:ASP:N	2.36	0.54
8:G:333:ASP:OD2	8:G:613:TYR:OH	2.26	0.54
20:T:9:GLU:HB3	20:T:88:GLU:HG2	1.90	0.54
39:m:122:ARG:O	42:p:139:GLN:NE2	2.35	0.54
32:f:39:ASN:ND2	32:f:55:THR:OG1	2.40	0.54
16:P:168:PRO:HA	16:P:230:PHE:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:16:LEU:HD21	21:U:32:VAL:HG12	1.89	0.54
30:d:57:GLY:O	30:d:61:GLN:NE2	2.41	0.54
36:j:66:ILE:HD12	36:j:66:ILE:H	1.73	0.54
3:B:34:ASP:OD2	3:B:38:ASN:ND2	2.40	0.53
25:t:85:ASP:O	25:t:88:ASN:ND2	2.42	0.53
36:j:70:ASP:HB2	41:o:114:ARG:HD2	1.89	0.53
40:n:63:LEU:O	40:n:67:GLU:HG3	2.09	0.53
15:O:280:PRO:HG3	33:g:25:ARG:HH21	1.73	0.53
16:P:107:GLU:O	16:P:111:VAL:HB	2.09	0.53
22:V:8:THR:HG21	22:V:13:LEU:HB3	1.91	0.53
24:X:85:TRP:HA	24:X:88:ILE:HG22	1.89	0.53
43:q:101:LYS:NZ	43:q:102:PRO:O	2.40	0.53
16:P:285:GLU:O	16:P:289:THR:OG1	2.25	0.53
35:u:120:LYS:NZ	41:o:37:GLU:OE2	2.41	0.53
3:B:176:TRP:HB3	47:B:202:PC1:H3E1	1.91	0.53
8:G:620:ARG:HA	8:G:623:LEU:HD12	1.91	0.53
8:G:648:LEU:HD21	19:S:44:LYS:HG2	1.90	0.53
20:T:68:GLU:OE2	20:T:68:GLU:N	2.41	0.53
13:M:51:ASN:ND2	34:h:90:THR:OG1	2.41	0.53
5:D:149:ASN:OD1	5:D:371:LYS:NZ	2.41	0.53
7:F:87:ASP:OD1	7:F:87:ASP:N	2.40	0.53
13:M:72:LEU:HB3	13:M:76:MET:HE3	1.90	0.53
14:N:307:SER:OG	14:N:308:THR:N	2.42	0.53
16:P:251:ARG:NH2	16:P:321:HIS:O	2.42	0.53
4:C:111:THR:OG1	4:C:112:ASP:N	2.43	0.52
36:j:55:ASP:OD1	36:j:57:SER:OG	2.26	0.52
5:D:8:VAL:HG11	33:g:25:ARG:HH11	1.74	0.52
6:E:102:VAL:HG13	6:E:154:VAL:HG12	1.91	0.52
12:L:440:LEU:HG	21:U:14:ARG:HH12	1.75	0.52
40:n:65:GLU:N	40:n:65:GLU:OE1	2.42	0.52
8:G:433:ALA:HB1	8:G:476:LYS:HE3	1.90	0.52
12:L:171:ALA:O	12:L:175:ASN:ND2	2.38	0.52
27:a:40:HIS:N	27:a:44:GLN:OE1	2.42	0.52
38:l:35:GLU:OE2	38:l:35:GLU:N	2.42	0.52
42:p:72:ASP:N	42:p:72:ASP:OD1	2.42	0.52
8:G:324:ASP:OD1	8:G:324:ASP:N	2.30	0.52
21:U:20:LYS:HG3	21:U:30:LEU:HD23	1.90	0.52
33:g:39:GLU:OE2	33:g:39:GLU:N	2.40	0.52
4:C:109:THR:OG1	4:C:110:TYR:N	2.43	0.52
22:V:46:TYR:O	22:V:50:ILE:HG12	2.09	0.52
17:Q:28:GLU:O	17:Q:32:THR:OG1	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:31:ASP:OD1	32:f:31:ASP:N	2.35	0.52
1:J:23:LYS:HD2	11:K:23:ARG:HB2	1.92	0.52
12:L:575:THR:O	12:L:579:ASN:ND2	2.43	0.52
24:X:133:ASP:OD1	24:X:133:ASP:N	2.41	0.52
7:F:15:LEU:HD13	7:F:271:GLU:HB2	1.92	0.52
13:M:57:PHE:HB3	13:M:113:MET:HE2	1.92	0.52
16:P:176:ASP:O	16:P:180:ASN:ND2	2.35	0.52
22:V:58:VAL:HG23	22:V:67:LEU:HD21	1.92	0.52
24:X:63:ASN:OD1	26:Z:81:ARG:NH2	2.43	0.52
8:G:359:ARG:HE	8:G:363:LEU:HD11	1.75	0.51
9:H:268:MET:HA	9:H:271:LEU:HD12	1.92	0.51
6:E:30:ARG:HD3	45:s:52:LEU:HB3	1.93	0.51
11:K:73:LEU:HD21	14:N:41:ILE:HG13	1.91	0.51
17:Q:88:THR:OG1	17:Q:91:ASP:OD1	2.25	0.51
2:A:89:THR:HG22	2:A:90:MET:HE2	1.91	0.51
10:I:75:GLU:O	10:I:105:ARG:NH1	2.44	0.51
13:M:278:ARG:NH2	38:l:80:ASP:OD1	2.40	0.51
14:N:329:MET:O	14:N:333:SER:OG	2.26	0.51
16:P:212:LYS:O	16:P:216:ASN:ND2	2.37	0.51
36:j:60:THR:OG1	36:j:63:GLU:OE1	2.24	0.51
38:l:30:ARG:HD2	39:m:34:GLU:HG2	1.93	0.51
5:D:175:GLU:OE2	5:D:188:ARG:NH2	2.41	0.51
19:S:14:GLY:HA2	19:S:97:LYS:HD2	1.91	0.51
19:S:67:ARG:HB2	19:S:73:GLU:HG2	1.91	0.51
25:t:21:THR:O	25:t:25:THR:OG1	2.28	0.51
5:D:107:ASP:OD2	5:D:110:SER:OG	2.29	0.51
16:P:268:ARG:HB2	16:P:281:ARG:HE	1.76	0.51
23:W:109:GLU:N	23:W:109:GLU:OE1	2.44	0.51
16:P:90:VAL:HG22	16:P:128:LYS:HB2	1.93	0.51
12:L:485:TYR:O	12:L:489:THR:OG1	2.26	0.51
28:b:10:ASN:HB3	28:b:14:LYS:NZ	2.26	0.51
8:G:332:LYS:HA	8:G:343:LEU:HD11	1.93	0.50
38:l:105:LEU:O	38:l:109:VAL:HG23	2.11	0.50
7:F:314:THR:O	7:F:314:THR:OG1	2.23	0.50
7:F:337:MET:HE1	7:F:343:ILE:HD13	1.92	0.50
24:X:82:THR:HA	24:X:85:TRP:CD1	2.46	0.50
25:t:61:THR:OG1	25:t:103:ARG:NH1	2.44	0.50
39:m:21:GLU:OE2	39:m:21:GLU:N	2.31	0.50
6:E:156:ILE:HB	6:E:161:TYR:HE2	1.76	0.50
10:I:27:TRP:NE1	47:I:201:PC1:O32	2.44	0.50
35:u:1:SER:OG	35:u:2:GLY:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:141:GLU:OE2	13:M:141:GLU:N	2.35	0.50
20:T:52:MET:HE3	23:W:41:ARG:HE	1.75	0.50
7:F:28:ARG:NH1	45:s:35:ASN:O	2.38	0.50
13:M:150:LEU:HD22	14:N:294:MET:HE2	1.92	0.50
53:d:201:CDL:H552	53:d:201:CDL:HA21	1.93	0.50
35:u:9:LEU:O	35:u:13:GLN:HG2	2.11	0.50
37:k:84:GLU:OE1	37:k:84:GLU:N	2.30	0.50
39:m:22:TYR:OH	40:n:67:GLU:OE1	2.30	0.50
41:o:34:LYS:N	41:o:34:LYS:HE2	2.26	0.50
8:G:147:LYS:HD2	8:G:702:SER:HB3	1.93	0.50
35:u:4:THR:OG1	35:u:7:GLU:OE1	2.23	0.50
12:L:136:ASN:OD1	12:L:136:ASN:N	2.45	0.50
39:m:34:GLU:OE2	39:m:34:GLU:N	2.30	0.50
22:V:21:GLU:OE1	22:V:21:GLU:N	2.26	0.49
29:c:16:LYS:HD2	53:d:204:CDL:HA32	1.93	0.49
53:d:201:CDL:OB2	32:f:29:LYS:NZ	2.44	0.49
2:A:4:MET:HG3	46:A:201:FME:HCN	1.94	0.49
15:O:4:GLY:O	15:O:7:ALA:N	2.39	0.49
20:T:76:ILE:O	20:T:80:ILE:HG22	2.12	0.49
23:W:25:MET:SD	23:W:25:MET:N	2.85	0.49
28:b:20:ALA:O	28:b:24:ILE:HG13	2.11	0.49
38:l:53:ARG:NH1	38:l:57:GLU:OE1	2.45	0.49
13:M:420:THR:HB	13:M:423:ILE:HG13	1.93	0.49
17:Q:33:ARG:NH1	17:Q:77:ASP:OD1	2.45	0.49
19:S:17:GLU:N	19:S:17:GLU:OE1	2.45	0.49
20:T:18:VAL:HA	20:T:21:LEU:HG	1.94	0.49
12:L:295:GLN:O	12:L:425:ARG:NH2	2.41	0.49
25:t:36:SER:O	25:t:40:VAL:HG23	2.12	0.49
38:l:5:THR:H	38:l:8:MET:HE1	1.76	0.49
13:M:59:ASP:OD2	13:M:245:ARG:NH2	2.37	0.49
30:d:29:PRO:HG2	30:d:30:ARG:HD3	1.94	0.49
39:m:82:ASN:O	39:m:86:SER:OG	2.23	0.49
24:X:60:LYS:O	24:X:64:GLN:HG2	2.13	0.49
12:L:356:ILE:HA	12:L:359:MET:HG3	1.94	0.49
40:n:133:GLU:HG2	40:n:134:ARG:HD3	1.95	0.49
53:v:201:CDL:H541	53:v:201:CDL:H722	1.95	0.49
15:O:4:GLY:O	15:O:6:LEU:N	2.46	0.49
16:P:268:ARG:HH22	16:P:272:ILE:HD13	1.78	0.49
1:J:91:GLY:O	1:J:95:THR:HG22	2.12	0.48
8:G:6:SER:OG	8:G:7:ASN:N	2.42	0.48
9:H:87:ILE:HG22	9:H:95:LEU:HD23	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:105:LYS:HB3	26:Z:105:LYS:HZ2	1.78	0.48
8:G:283:MET:HB3	8:G:291:LEU:HD22	1.94	0.48
12:L:476:THR:OG1	12:L:477:ILE:N	2.45	0.48
16:P:56:THR:O	16:P:56:THR:OG1	2.29	0.48
4:C:182:ARG:CZ	23:W:104:MET:HG3	2.42	0.48
8:G:372:GLU:O	8:G:402:ASN:ND2	2.45	0.48
20:T:66:ASP:OD2	20:T:66:ASP:N	2.46	0.48
15:O:79:LEU:HD11	55:O:403:GTP:H1'	1.96	0.48
28:b:39:LYS:O	28:b:43:MET:HG3	2.13	0.48
37:k:78:VAL:HA	37:k:81:ILE:HG22	1.94	0.48
12:L:401:THR:O	12:L:401:THR:OG1	2.31	0.48
33:g:120:LEU:HD13	33:g:121:PRO:HD2	1.96	0.48
9:H:277:TYR:HE2	47:I:201:PC1:H282	1.79	0.48
52:M:504:3PE:H2C2	52:O:401:3PE:H3D1	1.95	0.48
19:S:19:ARG:HG2	19:S:53:LEU:HD12	1.96	0.48
37:k:11:SER:OG	37:k:12:LYS:N	2.46	0.48
38:l:115:MET:HE2	38:l:115:MET:HA	1.96	0.48
41:o:38:MET:HE1	41:o:57:TYR:HA	1.94	0.48
14:N:211:MET:HE3	14:N:251:MET:HG2	1.96	0.48
34:h:114:MET:HE3	34:h:120:GLY:HA3	1.96	0.48
13:M:105:PHE:O	13:M:109:THR:OG1	2.30	0.48
14:N:208:TYR:O	14:N:212:THR:OG1	2.26	0.48
15:O:223:TYR:OH	15:O:237:ASP:OD2	2.32	0.48
21:U:26:ASP:OD1	21:U:26:ASP:N	2.47	0.48
39:m:71:ARG:HE	39:m:71:ARG:HB3	1.45	0.48
44:v:29:GLU:OE1	44:v:29:GLU:N	2.45	0.48
9:H:281:ARG:HB3	9:H:284:GLN:HG3	1.96	0.48
26:Z:82:ARG:O	26:Z:86:MET:HG3	2.13	0.48
35:u:18:ARG:HA	40:n:170:VAL:HG13	1.96	0.48
47:H:403:PC1:H2A1	47:H:403:PC1:H351	1.96	0.47
15:O:104:ARG:NE	15:O:131:ASP:OD1	2.40	0.47
5:D:145:THR:OG1	5:D:181:TYR:OH	2.31	0.47
8:G:333:ASP:OD2	8:G:622:ARG:NH1	2.47	0.47
27:a:1:MET:HB3	27:a:1:MET:HE2	1.74	0.47
30:d:44:ILE:O	30:d:48:ILE:HG23	2.14	0.47
31:e:15:ARG:HG2	31:e:15:ARG:HH11	1.79	0.47
45:s:31:GLU:HG3	45:s:32:PRO:HD3	1.96	0.47
9:H:293:PHE:O	9:H:297:THR:OG1	2.27	0.47
12:L:173:LEU:HD12	13:M:405:LEU:HD21	1.96	0.47
13:M:3:LYS:NZ	32:f:27:ASP:OD1	2.47	0.47
18:R:20:ASP:OD1	18:R:20:ASP:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:23:LYS:HG2	11:K:28:SER:HB3	1.96	0.47
6:E:69:VAL:HA	6:E:72:ILE:HG12	1.97	0.47
9:H:27:VAL:O	9:H:31:MET:HG3	2.15	0.47
12:L:36:VAL:HG12	12:L:101:MET:HE1	1.95	0.47
8:G:252:PRO:HG3	8:G:263:ILE:HG12	1.96	0.47
3:B:71:ARG:HA	9:H:37:PRO:HA	1.97	0.47
7:F:24:ASN:HB2	7:F:39:ARG:HH12	1.80	0.47
8:G:364:LEU:HG	8:G:491:ASN:HB3	1.95	0.47
8:G:396:ARG:HG3	8:G:417:TYR:HD2	1.80	0.47
14:N:311:MET:HE2	14:N:311:MET:HB2	1.83	0.47
17:Q:9:GLN:OE1	17:Q:9:GLN:N	2.38	0.47
27:a:70:ASP:OD1	27:a:70:ASP:N	2.48	0.47
53:h:201:CDL:H412	53:h:201:CDL:H381	1.58	0.47
7:F:190:THR:HB	7:F:204:ARG:H	1.80	0.47
20:T:71:MET:SD	20:T:71:MET:N	2.88	0.47
25:t:23:ALA:O	25:t:27:ILE:HG13	2.15	0.47
40:n:26:LEU:HD21	40:n:39:PHE:HB3	1.97	0.47
3:B:179:ARG:HG2	16:P:50:ARG:HH21	1.80	0.47
52:d:202:3PE:H221	47:d:203:PC1:H242	1.97	0.47
44:v:45:SER:O	44:v:51:ASN:ND2	2.44	0.47
1:J:135:PHE:HD2	26:Z:68:ARG:HD2	1.79	0.47
23:W:25:MET:HE2	23:W:25:MET:H	1.80	0.47
33:g:70:LEU:O	33:g:74:SER:OG	2.27	0.47
7:F:68:ARG:HG3	7:F:226:GLU:HG2	1.96	0.46
7:F:183:ALA:HB1	7:F:185:ILE:HG22	1.97	0.46
15:O:5:PRO:HA	15:O:8:TYR:HB3	1.97	0.46
20:T:45:LEU:HA	20:T:48:VAL:HG23	1.98	0.46
23:W:52:LEU:HD13	23:W:104:MET:HE1	1.96	0.46
14:N:252:GLY:HA3	14:N:290:LEU:HD13	1.96	0.46
25:t:87:LEU:O	25:t:91:ILE:HG13	2.16	0.46
26:Z:68:ARG:HG3	27:a:43:TYR:CE1	2.51	0.46
53:d:201:CDL:H391	53:d:201:CDL:H361	1.62	0.46
2:A:68:GLU:HG2	2:A:98:LEU:HD13	1.97	0.46
5:D:350:LYS:HB2	8:G:121:MET:HE2	1.98	0.46
14:N:122:ILE:O	14:N:176:ARG:NH1	2.49	0.46
18:R:2:VAL:HG21	18:R:10:LYS:HE3	1.97	0.46
1:J:52:LEU:O	1:J:56:VAL:HG23	2.16	0.46
5:D:381:ASP:OD1	5:D:381:ASP:N	2.48	0.46
13:M:253:MET:HE3	13:M:253:MET:HB2	1.82	0.46
28:b:10:ASN:HB3	28:b:14:LYS:HZ3	1.80	0.46
29:c:4:ILE:HG23	29:c:5:GLN:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:n:169:ILE:O	40:n:172:ARG:NH1	2.49	0.46
5:D:208:MET:HG3	26:Z:9:ASP:OD1	2.16	0.46
32:f:32:GLU:OE2	32:f:32:GLU:N	2.31	0.46
8:G:382:THR:OG1	8:G:387:GLU:OE1	2.32	0.46
12:L:55:ILE:H	12:L:55:ILE:HG12	1.30	0.46
13:M:178:MET:HB3	13:M:178:MET:HE2	1.85	0.46
26:Z:20:ASP:OD1	26:Z:20:ASP:N	2.34	0.46
1:J:165:VAL:HG12	2:A:64:LEU:HG	1.97	0.46
4:C:8:ARG:NH1	44:v:61:GLU:OE2	2.49	0.46
8:G:354:ALA:HA	8:G:648:LEU:HD23	1.98	0.46
33:g:107:ILE:HG21	42:p:134:VAL:HG22	1.97	0.46
41:o:41:THR:N	41:o:44:GLU:OE1	2.47	0.46
8:G:617:ASP:OD1	8:G:617:ASP:N	2.47	0.45
20:T:8:LEU:HD13	20:T:11:ILE:HD12	1.98	0.45
26:Z:98:MET:HE2	26:Z:98:MET:HA	1.99	0.45
10:I:101:ASP:OD2	10:I:101:ASP:N	2.35	0.45
27:a:52:ARG:NH1	27:a:58:ASN:OD1	2.40	0.45
5:D:8:VAL:HG11	33:g:25:ARG:HD3	1.98	0.45
5:D:36:VAL:HG23	5:D:37:ASP:H	1.81	0.45
5:D:424:VAL:HG23	5:D:427:GLU:HG2	1.98	0.45
7:F:48:ILE:H	7:F:48:ILE:HG13	1.64	0.45
8:G:88:LYS:HE3	8:G:88:LYS:HB3	1.75	0.45
26:Z:21:TYR:OH	44:v:108:ASP:OD1	2.35	0.45
37:k:74:PHE:O	37:k:78:VAL:HG22	2.17	0.45
3:B:171:LYS:HB2	3:B:174:ARG:HE	1.82	0.45
7:F:53:PRO:HD3	7:F:127:ARG:HH12	1.80	0.45
14:N:276:ILE:O	14:N:280:THR:OG1	2.34	0.45
22:V:25:ILE:O	22:V:29:LYS:HG3	2.17	0.45
22:V:39:LYS:HE3	22:V:39:LYS:HB3	1.58	0.45
8:G:300:LEU:HD23	8:G:300:LEU:HA	1.84	0.45
16:P:135:LEU:HA	16:P:167:LYS:HB3	1.98	0.45
20:T:84:LYS:HA	20:T:84:LYS:HD3	1.83	0.45
22:V:18:THR:O	22:V:18:THR:OG1	2.25	0.45
14:N:320:MET:HE1	14:N:321:LYS:HD3	1.99	0.45
53:O:402:CDL:H711	53:O:402:CDL:HB61	1.64	0.45
31:e:88:GLU:HB3	31:e:90:LYS:HD3	1.99	0.45
35:u:54:ALA:H	35:u:57:LYS:HG2	1.82	0.45
41:o:11:ASP:OD1	41:o:13:SER:N	2.50	0.45
5:D:66:MET:HE1	5:D:76:CYS:SG	2.57	0.45
10:I:175:TYR:CZ	44:v:38:PRO:HG3	2.52	0.45
13:M:19:LYS:HB3	13:M:19:LYS:HE2	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:u:201:3PE:H362	52:u:201:3PE:H331	1.85	0.45
6:E:89:MET:HE2	7:F:181:ALA:HA	1.99	0.45
12:L:336:LYS:HA	12:L:336:LYS:HD3	1.77	0.45
14:N:335:MET:O	14:N:336:MET:HE2	2.17	0.45
24:X:87:CYS:SG	24:X:102:GLN:NE2	2.90	0.45
38:l:156:TYR:HB2	41:o:33:ARG:HH11	1.82	0.45
7:F:28:ARG:O	7:F:29:HIS:ND1	2.50	0.45
13:M:337:ILE:HD12	13:M:344:LEU:HD23	1.99	0.45
15:O:6:LEU:H	53:O:402:CDL:CB5	2.30	0.45
19:S:17:GLU:OE2	19:S:67:ARG:NE	2.50	0.45
20:T:14:ARG:O	20:T:18:VAL:HG13	2.17	0.45
5:D:36:VAL:HG21	14:N:51:ARG:HB2	1.99	0.45
8:G:284:VAL:HG12	8:G:559:VAL:HG22	1.99	0.45
8:G:518:PRO:HA	8:G:519:PRO:HD3	1.82	0.45
53:O:402:CDL:H371	53:O:402:CDL:H181	1.99	0.45
23:W:20:ILE:HG13	23:W:77:ARG:HG2	1.98	0.45
36:j:56:PRO:HB2	41:o:102:GLU:HG3	1.98	0.45
21:U:87:TYR:CE2	35:u:23:LYS:HE2	2.51	0.44
26:Z:126:GLY:O	31:e:79:ARG:NH2	2.50	0.44
53:d:204:CDL:H321	53:d:204:CDL:H351	1.60	0.44
32:f:53:GLU:CD	32:f:53:GLU:H	2.25	0.44
38:l:77:MET:HG2	38:l:81:LEU:HD22	1.98	0.44
5:D:76:CYS:HB2	5:D:403:ASP:HA	1.99	0.44
8:G:53:ARG:HA	8:G:53:ARG:HD2	1.72	0.44
16:P:103:ASN:OD1	16:P:103:ASN:N	2.50	0.44
25:t:25:THR:HG23	25:t:67:ALA:HB2	1.98	0.44
52:j:101:3PE:H351	52:j:101:3PE:H242	1.98	0.44
38:l:97:ASN:O	38:l:101:MET:HG3	2.17	0.44
5:D:3:GLN:NE2	13:M:137:GLY:O	2.50	0.44
15:O:37:LYS:HB3	15:O:37:LYS:HE3	1.58	0.44
15:O:285:GLY:HA3	33:g:28:GLU:HG2	1.99	0.44
24:X:72:GLN:OE1	24:X:75:ARG:NH1	2.51	0.44
38:l:138:LEU:O	38:l:142:ARG:HG2	2.17	0.44
21:U:21:LEU:HD23	37:k:46:ARG:HB3	1.98	0.44
38:l:30:ARG:HD3	39:m:35:ARG:HG2	1.99	0.44
39:m:1:SER:OG	39:m:2:PHE:N	2.50	0.44
15:O:303:LYS:O	30:d:50:ARG:NH2	2.51	0.44
17:Q:91:ASP:OD1	17:Q:91:ASP:N	2.50	0.44
20:T:6:LEU:HD22	20:T:84:LYS:HG3	2.00	0.44
21:U:51:ILE:HD13	21:U:51:ILE:HA	1.85	0.44
26:Z:30:LEU:H	26:Z:30:LEU:HG	1.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:20:ILE:H	2:A:20:ILE:HG13	1.64	0.44
9:H:87:ILE:HG13	9:H:88:PRO:HD3	1.99	0.44
10:I:112:ASP:OD1	10:I:114:THR:OG1	2.34	0.44
20:T:46:ASP:HA	20:T:49:GLU:OE2	2.18	0.44
31:e:56:LYS:O	31:e:60:GLU:HG2	2.17	0.44
43:q:95:ASP:OD1	43:q:95:ASP:N	2.50	0.44
5:D:116:GLN:NE2	5:D:276:ASP:OD2	2.51	0.44
13:M:35:SER:O	13:M:38:SER:OG	2.33	0.44
16:P:79:ASP:OD1	16:P:79:ASP:N	2.51	0.44
21:U:83:LYS:HB2	21:U:83:LYS:HE2	1.56	0.44
22:V:22:ARG:HD2	22:V:22:ARG:HA	1.79	0.44
6:E:33:ALA:HB2	45:s:56:LEU:HD12	1.98	0.44
7:F:360:GLY:HA2	7:F:366:ARG:HB2	2.00	0.44
53:L:703:CDL:H581	53:L:703:CDL:H552	1.79	0.44
23:W:43:VAL:HG11	23:W:60:ARG:HG3	1.99	0.44
3:B:54:CYS:HB3	5:D:108:TYR:CG	2.52	0.44
4:C:177:ASP:HB3	4:C:180:VAL:HG22	2.00	0.44
9:H:105:MET:HB3	9:H:105:MET:HE3	1.79	0.44
12:L:264:TYR:CD2	12:L:265:PRO:HD3	2.53	0.44
53:d:201:CDL:H251	53:d:201:CDL:H432	2.00	0.44
35:u:72:THR:HA	35:u:76:ILE:HD12	2.00	0.44
47:B:202:PC1:H3B2	47:B:202:PC1:H3E2	1.85	0.43
5:D:78:PRO:HG3	5:D:402:LEU:HD23	2.00	0.43
7:F:7:PRO:HB2	7:F:8:LYS:H	1.59	0.43
1:J:115:VAL:O	1:J:117:PHE:N	2.51	0.43
47:B:202:PC1:H3G1	47:B:202:PC1:H11	2.00	0.43
8:G:71:MET:HE2	8:G:71:MET:HB2	1.75	0.43
8:G:476:LYS:O	8:G:479:THR:OG1	2.35	0.43
9:H:99:ASN:N	47:H:403:PC1:O12	2.41	0.43
16:P:107:GLU:OE2	16:P:112:LYS:NZ	2.50	0.43
2:A:115:GLU:H	2:A:115:GLU:HG2	1.36	0.43
7:F:317:MET:HE3	7:F:317:MET:HB3	1.84	0.43
21:U:55:GLU:HG2	21:U:61:GLU:HA	2.00	0.43
29:c:20:THR:HG23	30:d:63:LEU:HD22	1.99	0.43
36:j:60:THR:N	36:j:63:GLU:OE2	2.51	0.43
36:j:66:ILE:HG13	41:o:107:LEU:HD12	1.99	0.43
1:J:17:PHE:HA	1:J:20:PHE:CE2	2.53	0.43
12:L:379:ALA:HB2	12:L:386:LEU:HD23	2.01	0.43
15:O:318:TRP:H	15:O:318:TRP:CD1	2.36	0.43
16:P:151:VAL:HG12	16:P:155:GLU:OE1	2.18	0.43
17:Q:28:GLU:OE2	17:Q:28:GLU:N	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:55:GLU:HG3	21:U:62:ILE:HD12	1.99	0.43
22:V:34:LEU:HA	22:V:37:ILE:HD12	2.01	0.43
52:b:201:3PE:H122	52:b:201:3PE:H2	2.00	0.43
37:k:75:ALA:O	37:k:79:VAL:HG13	2.17	0.43
5:D:269:LEU:HB2	5:D:368:GLU:HB2	2.00	0.43
12:L:276:ILE:H	12:L:276:ILE:HG12	1.53	0.43
12:L:502:LEU:HD12	12:L:502:LEU:HA	1.91	0.43
12:L:558:LEU:HD23	12:L:558:LEU:HA	1.88	0.43
16:P:101:THR:HG22	16:P:103:ASN:H	1.84	0.43
25:t:22:TYR:O	25:t:26:SER:OG	2.37	0.43
7:F:259:SER:OG	7:F:260:GLY:N	2.51	0.43
7:F:365:CYS:HB2	48:F:502:SF4:S4	2.58	0.43
27:a:57:VAL:HG23	27:a:59:ARG:HB2	1.99	0.43
34:h:7:ARG:HE	34:h:7:ARG:HB2	1.59	0.43
35:u:16:GLU:N	35:u:16:GLU:OE2	2.51	0.43
35:u:79:TRP:HE1	42:p:40:VAL:HA	1.83	0.43
14:N:270:MET:HE2	14:N:270:MET:HB3	1.93	0.43
16:P:312:LEU:HD23	16:P:312:LEU:HA	1.90	0.43
3:B:116:MET:HE3	3:B:156:LEU:HD22	1.99	0.43
4:C:127:ALA:O	4:C:131:GLU:HG3	2.19	0.43
6:E:9:HIS:HB3	8:G:187:ILE:HG22	2.01	0.43
21:U:51:ILE:HG21	21:U:67:ALA:HB1	2.01	0.43
22:V:34:LEU:HD13	22:V:48:GLU:HG3	2.01	0.43
26:Z:99:LYS:HE3	26:Z:99:LYS:HA	2.01	0.43
38:l:6:LYS:HE3	38:l:6:LYS:HB3	1.74	0.43
52:m:202:3PE:O22	52:m:202:3PE:N	2.52	0.43
41:o:95:VAL:HA	41:o:98:MET:HG3	2.01	0.43
41:o:111:LYS:HA	41:o:111:LYS:HD3	1.78	0.43
52:M:504:3PE:H2A2	14:N:335:MET:HE2	2.01	0.43
34:h:69:HIS:CE1	34:h:71:ILE:HD12	2.53	0.43
41:o:28:TYR:HE2	41:o:110:ARG:HH21	1.66	0.43
45:s:39:LYS:HE3	45:s:39:LYS:HB2	1.85	0.43
5:D:24:GLU:OE2	5:D:24:GLU:N	2.40	0.43
50:F:501:FMN:HM83	50:F:501:FMN:HM71	1.86	0.43
12:L:203:MET:HE1	42:p:124:CYS:HB2	2.01	0.43
52:M:504:3PE:H381	52:M:504:3PE:H352	1.75	0.43
16:P:186:ARG:HG3	16:P:246:PHE:HE2	1.84	0.43
30:d:46:ASN:HB3	30:d:53:VAL:HA	2.01	0.43
39:m:27:GLU:HA	39:m:30:LYS:HD2	2.00	0.43
40:n:158:LYS:NZ	40:n:158:LYS:HB3	2.34	0.43
42:p:167:LYS:HD3	42:p:171:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:151:ILE:O	5:D:155:THR:OG1	2.31	0.42
12:L:594:THR:O	12:L:598:SER:OG	2.30	0.42
14:N:46:LYS:NZ	46:N:401:FME:O	2.52	0.42
14:N:146:PHE:CD2	14:N:147:PRO:HD3	2.54	0.42
17:Q:116:LYS:HD3	17:Q:116:LYS:HA	1.89	0.42
26:Z:127:LEU:HB2	31:e:97:HIS:CE1	2.55	0.42
35:u:7:GLU:OE1	35:u:7:GLU:N	2.31	0.42
35:u:97:VAL:HG23	42:p:114:GLN:HG2	2.01	0.42
6:E:190:ARG:NH2	6:E:194:GLU:O	2.52	0.42
13:M:191:SER:HB2	52:M:502:3PE:H2	2.01	0.42
13:M:278:ARG:HE	13:M:278:ARG:HB3	1.76	0.42
31:e:85:LEU:HD23	31:e:85:LEU:HA	1.87	0.42
32:f:32:GLU:HA	32:f:35:THR:HG23	2.01	0.42
13:M:190:TRP:CE3	25:t:126:MET:HE3	2.55	0.42
47:M:503:PC1:H232	52:M:505:3PE:H251	2.01	0.42
14:N:243:LEU:O	14:N:247:THR:HG22	2.18	0.42
22:V:21:GLU:O	22:V:25:ILE:HG23	2.19	0.42
41:o:91:HIS:O	41:o:95:VAL:HG22	2.19	0.42
53:L:703:CDL:H122	53:L:703:CDL:H151	1.64	0.42
15:O:60:ASP:OD1	15:O:60:ASP:N	2.51	0.42
53:O:402:CDL:H341	53:O:402:CDL:H312	1.84	0.42
28:b:71:ASP:OD1	28:b:71:ASP:N	2.51	0.42
34:h:73:ARG:NE	47:h:202:PC1:O14	2.43	0.42
39:m:111:LYS:HE3	39:m:111:LYS:HB3	1.78	0.42
2:A:4:MET:HG3	2:A:4:MET:H	1.61	0.42
9:H:126:LYS:HD2	9:H:127:TYR:N	2.34	0.42
13:M:403:THR:HA	13:M:406:TYR:CE2	2.55	0.42
25:t:100:LEU:O	25:t:104:THR:OG1	2.32	0.42
2:A:54:LYS:HE2	2:A:113:TRP:HA	2.01	0.42
5:D:62:LEU:HD22	5:D:425:PHE:HZ	1.84	0.42
6:E:123:LYS:HE2	6:E:123:LYS:HB2	1.69	0.42
8:G:283:MET:HB2	8:G:560:ILE:HB	2.02	0.42
9:H:98:MET:HE2	9:H:98:MET:HB2	1.80	0.42
10:I:48:ILE:O	10:I:53:GLU:HB2	2.19	0.42
24:X:109:CYS:SG	24:X:110:VAL:N	2.92	0.42
26:Z:36:PHE:O	26:Z:40:ILE:HD13	2.20	0.42
33:g:116:SER:OG	33:g:117:LYS:HD3	2.19	0.42
38:l:157:GLU:OE2	38:l:157:GLU:N	2.51	0.42
6:E:114:ASP:OD1	6:E:114:ASP:N	2.52	0.42
6:E:150:ASN:ND2	6:E:162:GLU:OE1	2.38	0.42
53:L:703:CDL:H331	53:L:703:CDL:H361	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:114:GLU:HG3	24:X:168:PHE:HB3	2.01	0.42
15:O:140:ARG:HA	15:O:140:ARG:HD3	1.86	0.42
34:h:110:VAL:O	34:h:114:MET:HB2	2.19	0.42
38:l:128:VAL:HB	41:o:97:ARG:HE	1.83	0.42
3:B:95:LYS:HD2	4:C:154:ASP:HA	2.02	0.42
8:G:628:PRO:HG2	19:S:57:CYS:HB2	2.02	0.42
13:M:164:LEU:HD23	13:M:164:LEU:HA	1.91	0.42
13:M:183:VAL:HG23	13:M:249:ILE:HG22	2.02	0.42
14:N:316:GLN:HB3	15:O:63:THR:HG21	2.02	0.42
15:O:2:GLN:OE1	15:O:2:GLN:N	2.35	0.42
15:O:4:GLY:HA2	15:O:5:PRO:HD2	1.77	0.42
19:S:25:ARG:NH1	19:S:25:ARG:HB2	2.34	0.42
21:U:19:LEU:HB3	21:U:30:LEU:HD21	2.02	0.42
23:W:35:LEU:HD23	23:W:67:PHE:CZ	2.55	0.42
24:X:157:LEU:HD12	24:X:157:LEU:HA	1.87	0.42
38:l:18:GLU:H	38:l:18:GLU:CD	2.24	0.42
5:D:115:GLU:O	5:D:119:SER:OG	2.37	0.42
8:G:132:GLU:OE1	8:G:132:GLU:N	2.53	0.42
8:G:646:SER:O	8:G:650:LYS:HG2	2.19	0.42
21:U:16:LEU:HD13	21:U:16:LEU:HA	1.84	0.42
24:X:56:LEU:HD23	24:X:56:LEU:HA	1.87	0.42
3:B:122:GLY:H	3:B:135:GLY:HA2	1.84	0.42
6:E:106:THR:HA	6:E:109:MET:HG3	2.01	0.41
15:O:49:LYS:HB3	15:O:122:VAL:HG12	2.02	0.41
21:U:4:PRO:HA	21:U:5:PRO:HD3	1.91	0.41
23:W:76:PRO:O	23:W:79:VAL:N	2.53	0.41
42:p:82:LEU:HD12	42:p:82:LEU:HA	1.83	0.41
7:F:145:GLU:N	7:F:145:GLU:OE1	2.53	0.41
8:G:199:ILE:HA	8:G:202:ILE:HG12	2.01	0.41
13:M:55:LEU:HD23	13:M:55:LEU:HA	1.94	0.41
38:l:141:GLU:HG2	41:o:55:ARG:HH11	1.85	0.41
7:F:188:GLU:OE1	7:F:190:THR:OG1	2.35	0.41
7:F:337:MET:HB2	7:F:337:MET:HE2	1.82	0.41
12:L:455:LYS:HB2	12:L:455:LYS:HE3	1.72	0.41
14:N:3:PRO:HB3	53:O:402:CDL:HB32	2.01	0.41
14:N:96:MET:SD	14:N:100:MET:HE3	2.61	0.41
15:O:10:LEU:HD12	15:O:10:LEU:HA	1.90	0.41
29:c:13:ASN:HD22	29:c:16:LYS:HE2	1.85	0.41
34:h:23:LYS:HB2	34:h:23:LYS:HE2	1.86	0.41
42:p:2:ASP:OD1	42:p:3:SER:N	2.54	0.41
42:p:80:ASP:O	42:p:84:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:v:92:LYS:HE2	44:v:92:LYS:H	1.85	0.41
1:J:14:VAL:HG21	11:K:7:ASN:ND2	2.36	0.41
1:J:167:VAL:HG13	14:N:42:PRO:HG3	2.03	0.41
2:A:54:LYS:HE3	2:A:54:LYS:HB3	1.82	0.41
5:D:92:GLU:H	5:D:92:GLU:HG3	1.67	0.41
8:G:657:LEU:HD23	8:G:657:LEU:HA	1.88	0.41
52:M:504:3PE:H2C1	14:N:335:MET:HE2	2.01	0.41
14:N:289:ASN:HA	14:N:292:PHE:CE2	2.55	0.41
19:S:16:ARG:HA	19:S:16:ARG:HD2	1.95	0.41
25:t:2:LYS:HA	25:t:2:LYS:HD2	1.89	0.41
53:d:201:CDL:H562	53:d:201:CDL:H591	1.62	0.41
3:B:49:THR:HG21	3:B:59:MET:HG2	2.01	0.41
4:C:72:PHE:O	4:C:124:TYR:OH	2.34	0.41
4:C:116:PRO:HG2	23:W:18:LYS:HE2	2.01	0.41
8:G:259:ASN:HB3	8:G:390:LEU:HD13	2.01	0.41
9:H:195:ARG:HE	9:H:195:ARG:HB3	1.67	0.41
9:H:200:LEU:HD11	9:H:285:LEU:HD21	2.03	0.41
9:H:228:TYR:HA	9:H:231:ILE:HD12	2.03	0.41
23:W:52:LEU:HD12	23:W:54:ILE:HG12	2.01	0.41
29:c:45:ARG:NH2	30:d:16:ASP:OD1	2.49	0.41
29:c:49:GLU:OE2	29:c:49:GLU:N	2.53	0.41
5:D:206:GLY:N	26:Z:9:ASP:OD2	2.50	0.41
7:F:376:MET:HE3	7:F:376:MET:HA	2.02	0.41
10:I:79:ALA:HB2	10:I:106:THR:HG23	2.03	0.41
12:L:286:LEU:HD13	12:L:411:MET:HE3	2.02	0.41
16:P:322:ARG:HH22	16:P:330:GLU:HB3	1.85	0.41
24:X:39:ASN:OD1	24:X:39:ASN:N	2.54	0.41
24:X:102:GLN:OE1	24:X:102:GLN:N	2.52	0.41
25:t:71:LEU:HD12	25:t:71:LEU:HA	1.95	0.41
26:Z:105:LYS:HB3	26:Z:105:LYS:NZ	2.35	0.41
31:e:16:TRP:H	31:e:16:TRP:CD1	2.39	0.41
53:v:201:CDL:H562	53:v:201:CDL:H531	1.77	0.41
5:D:69:SER:O	5:D:69:SER:OG	2.37	0.41
5:D:151:ILE:HD11	5:D:218:PHE:HZ	1.86	0.41
5:D:359:PRO:HA	5:D:360:PRO:HD3	1.97	0.41
8:G:447:LYS:HA	8:G:447:LYS:HD3	1.84	0.41
10:I:113:MET:HE3	10:I:113:MET:HB3	1.89	0.41
25:t:30:ALA:O	25:t:34:VAL:HG13	2.21	0.41
40:n:138:GLN:NE2	40:n:155:PRO:O	2.34	0.41
41:o:98:MET:HE2	41:o:98:MET:HB3	1.83	0.41
54:L:706:CHD:H232	54:L:706:CHD:H211	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:59:LEU:HD23	16:P:62:MET:HE3	2.03	0.41
17:Q:33:ARG:NH2	17:Q:60:ASP:OD1	2.42	0.41
18:R:1:GLY:N	18:R:42:ASP:OD2	2.54	0.41
26:Z:86:MET:HE2	26:Z:86:MET:HB3	1.87	0.41
47:d:203:PC1:H132	47:d:203:PC1:H111	1.89	0.41
1:J:109:LYS:HA	1:J:109:LYS:HD2	1.79	0.41
4:C:32:ILE:HG22	4:C:33:LEU:HG	2.01	0.41
5:D:350:LYS:HD2	5:D:350:LYS:HA	1.85	0.41
7:F:17:ASP:HA	7:F:20:ARG:HH11	1.86	0.41
11:K:27:MET:HE2	11:K:27:MET:HB2	1.87	0.41
15:O:177:PRO:O	15:O:180:GLN:HG3	2.21	0.41
16:P:258:LEU:HD23	16:P:258:LEU:HA	1.88	0.41
27:a:64:LYS:HD3	27:a:64:LYS:HA	1.94	0.41
1:J:55:MET:HE2	1:J:55:MET:HB2	1.75	0.41
9:H:200:LEU:H	9:H:200:LEU:HG	1.55	0.41
14:N:228:LEU:HD23	14:N:228:LEU:HA	1.89	0.41
16:P:263:TYR:O	16:P:266:ILE:HG13	2.21	0.41
19:S:19:ARG:NH2	19:S:73:GLU:OE1	2.54	0.41
20:T:26:ASP:OD2	20:T:29:LYS:N	2.49	0.41
24:X:9:LEU:HD23	24:X:9:LEU:HA	1.94	0.41
35:u:103:ILE:HB	41:o:47:ASP:OD2	2.21	0.41
42:p:57:LYS:HE3	42:p:57:LYS:HB2	1.89	0.41
50:F:501:FMN:H1'1	50:F:501:FMN:H9	1.86	0.40
12:L:440:LEU:HD23	12:L:440:LEU:HA	1.81	0.40
15:O:65:ASP:OD1	15:O:65:ASP:N	2.53	0.40
16:P:176:ASP:OD1	16:P:180:ASN:ND2	2.54	0.40
21:U:37:MET:H	21:U:37:MET:HG2	1.63	0.40
23:W:25:MET:H	23:W:25:MET:CE	2.34	0.40
28:b:39:LYS:H	28:b:39:LYS:HG2	1.67	0.40
30:d:104:LYS:HD2	30:d:104:LYS:C	2.47	0.40
30:d:107:LYS:HE2	30:d:107:LYS:HB3	1.96	0.40
39:m:27:GLU:H	39:m:27:GLU:CD	2.28	0.40
13:M:238:LEU:HD23	13:M:238:LEU:HA	1.91	0.40
22:V:77:GLU:OE1	22:V:77:GLU:N	2.50	0.40
32:f:18:MET:HE3	32:f:18:MET:HB3	1.92	0.40
53:h:201:CDL:H621	53:h:201:CDL:H591	1.77	0.40
8:G:371:VAL:HG22	8:G:450:MET:HE1	2.04	0.40
25:t:9:TRP:CZ3	25:t:128:GLN:HG3	2.56	0.40
31:e:53:LYS:HE2	31:e:53:LYS:HB2	1.85	0.40
36:j:19:ARG:O	36:j:22:VAL:HG22	2.20	0.40
37:k:19:LYS:O	37:k:22:LYS:NZ	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:m:48:LEU:HD23	39:m:48:LEU:HA	1.81	0.40
2:A:75:LEU:HD23	2:A:75:LEU:HA	1.85	0.40
13:M:200:MET:HE1	13:M:243:MET:HG2	2.02	0.40
15:O:37:LYS:O	15:O:41:GLU:HG3	2.21	0.40
16:P:86:GLU:H	16:P:86:GLU:HG2	1.71	0.40
20:T:52:MET:CE	23:W:41:ARG:HE	2.35	0.40
53:d:201:CDL:H201	53:d:201:CDL:H171	1.82	0.40
34:h:87:TYR:OH	42:p:86:GLU:OE1	2.34	0.40
3:B:126:TYR:O	3:B:132:VAL:HG21	2.22	0.40
5:D:292:ASP:OD1	5:D:292:ASP:N	2.51	0.40
12:L:83:ASP:OD1	12:L:262:ARG:NH1	2.55	0.40
25:t:4:VAL:HA	25:t:7:GLN:HG3	2.02	0.40
52:b:201:3PE:H2E2	52:b:201:3PE:H2B2	1.83	0.40
38:l:6:LYS:H	38:l:6:LYS:HG2	1.41	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	J	163/175 (93%)	157 (96%)	5 (3%)	1 (1%)	21 42
2	A	86/114 (75%)	84 (98%)	2 (2%)	0	100 100
3	B	153/155 (99%)	146 (95%)	7 (5%)	0	100 100
4	C	207/209 (99%)	204 (99%)	3 (1%)	0	100 100
5	D	409/430 (95%)	397 (97%)	12 (3%)	0	100 100
6	E	212/214 (99%)	201 (95%)	9 (4%)	2 (1%)	14 30
7	F	431/432 (100%)	423 (98%)	8 (2%)	0	100 100
8	G	698/699 (100%)	679 (97%)	18 (3%)	1 (0%)	48 70
9	H	288/317 (91%)	279 (97%)	9 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	I	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
11	K	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
12	L	603/605 (100%)	576 (96%)	26 (4%)	1 (0%)	43	66
13	M	456/458 (100%)	448 (98%)	8 (2%)	0	100	100
14	N	344/346 (99%)	334 (97%)	10 (3%)	0	100	100
15	O	318/320 (99%)	314 (99%)	2 (1%)	2 (1%)	21	42
16	P	341/342 (100%)	329 (96%)	12 (4%)	0	100	100
17	Q	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
18	R	94/96 (98%)	94 (100%)	0	0	100	100
19	S	85/87 (98%)	81 (95%)	4 (5%)	0	100	100
20	T	83/85 (98%)	81 (98%)	2 (2%)	0	100	100
21	U	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
22	V	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
23	W	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
24	X	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
25	t	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
26	Z	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
27	a	68/70 (97%)	68 (100%)	0	0	100	100
28	b	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
29	c	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
30	d	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
31	e	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
32	f	55/57 (96%)	51 (93%)	4 (7%)	0	100	100
33	g	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
34	h	136/138 (99%)	135 (99%)	1 (1%)	0	100	100
35	u	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
36	j	69/71 (97%)	67 (97%)	2 (3%)	0	100	100
37	k	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
38	l	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
39	m	126/128 (98%)	126 (100%)	0	0	100	100
40	n	170/172 (99%)	165 (97%)	4 (2%)	1 (1%)	21	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	o	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
42	p	171/173 (99%)	171 (100%)	0	0	100	100
43	q	143/145 (99%)	143 (100%)	0	0	100	100
44	v	92/113 (81%)	91 (99%)	1 (1%)	0	100	100
45	s	44/45 (98%)	44 (100%)	0	0	100	100
All	All	8117/8304 (98%)	7903 (97%)	206 (2%)	8 (0%)	49	70

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	O	5	PRO
8	G	188	GLU
6	E	215	ALA
12	L	562	LEU
15	O	126	ARG
6	E	213	VAL
40	n	145	VAL
1	J	116	VAL

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	J	133/141 (94%)	127 (96%)	6 (4%)	24	50
2	A	79/100 (79%)	75 (95%)	4 (5%)	21	45
3	B	131/131 (100%)	123 (94%)	8 (6%)	17	37
4	C	190/190 (100%)	181 (95%)	9 (5%)	23	48
5	D	360/370 (97%)	351 (98%)	9 (2%)	42	69
6	E	183/183 (100%)	171 (93%)	12 (7%)	15	34
7	F	347/346 (100%)	336 (97%)	11 (3%)	34	62
8	G	587/586 (100%)	548 (93%)	39 (7%)	15	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	H	257/274 (94%)	246 (96%)	11 (4%)	26 51
10	I	151/151 (100%)	146 (97%)	5 (3%)	33 61
11	K	85/85 (100%)	80 (94%)	5 (6%)	18 38
12	L	533/533 (100%)	499 (94%)	34 (6%)	16 35
13	M	412/412 (100%)	399 (97%)	13 (3%)	34 62
14	N	315/315 (100%)	298 (95%)	17 (5%)	20 42
15	O	283/283 (100%)	277 (98%)	6 (2%)	47 73
16	P	297/296 (100%)	282 (95%)	15 (5%)	21 45
17	Q	116/116 (100%)	105 (90%)	11 (10%)	8 18
18	R	79/79 (100%)	76 (96%)	3 (4%)	29 56
19	S	77/77 (100%)	73 (95%)	4 (5%)	21 44
20	T	79/79 (100%)	75 (95%)	4 (5%)	21 45
21	U	79/79 (100%)	74 (94%)	5 (6%)	16 36
22	V	101/101 (100%)	94 (93%)	7 (7%)	14 32
23	W	107/108 (99%)	105 (98%)	2 (2%)	50 75
24	X	154/154 (100%)	146 (95%)	8 (5%)	21 44
25	t	101/101 (100%)	95 (94%)	6 (6%)	18 38
26	Z	120/120 (100%)	116 (97%)	4 (3%)	33 61
27	a	59/59 (100%)	55 (93%)	4 (7%)	14 32
28	b	71/71 (100%)	69 (97%)	2 (3%)	38 66
29	c	45/45 (100%)	44 (98%)	1 (2%)	45 72
30	d	105/105 (100%)	102 (97%)	3 (3%)	37 65
31	e	89/89 (100%)	82 (92%)	7 (8%)	11 26
32	f	54/54 (100%)	49 (91%)	5 (9%)	8 18
33	g	91/91 (100%)	89 (98%)	2 (2%)	45 72
34	h	121/121 (100%)	119 (98%)	2 (2%)	53 78
35	u	121/121 (100%)	114 (94%)	7 (6%)	18 39
36	j	61/61 (100%)	57 (93%)	4 (7%)	15 34
37	k	63/63 (100%)	61 (97%)	2 (3%)	34 62
38	l	140/140 (100%)	134 (96%)	6 (4%)	26 51
39	m	114/114 (100%)	108 (95%)	6 (5%)	20 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	n	156/156 (100%)	152 (97%)	4 (3%)	40 68
41	o	110/110 (100%)	108 (98%)	2 (2%)	51 76
42	p	155/155 (100%)	148 (96%)	7 (4%)	24 50
43	q	131/131 (100%)	120 (92%)	11 (8%)	10 23
44	v	85/96 (88%)	78 (92%)	7 (8%)	10 24
45	s	45/44 (102%)	43 (96%)	2 (4%)	25 50
All	All	7172/7236 (99%)	6830 (95%)	342 (5%)	24 47

All (342) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	10	SER
1	J	46	ASN
1	J	98	LEU
1	J	106	TYR
1	J	124	ASP
1	J	139	GLU
2	A	22	PHE
2	A	60	ILE
2	A	68	GLU
2	A	115	GLU
3	B	52	LEU
3	B	54	CYS
3	B	91	THR
3	B	100	LEU
3	B	152	THR
3	B	162	GLN
3	B	171	LYS
3	B	173	LEU
4	C	32	ILE
4	C	41	GLN
4	C	48	LEU
4	C	49	GLU
4	C	58	ILE
4	C	93	VAL
4	C	98	SER
4	C	117	ILE
4	C	123	VAL
5	D	61	VAL
5	D	109	VAL

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Mol	Chain	Res	Type
5	D	119	SER
5	D	145	THR
5	D	331	SER
5	D	341	SER
5	D	344	SER
5	D	384	SER
5	D	392	LYS
6	E	6	LEU
6	E	95	VAL
6	E	99	HIS
6	E	102	VAL
6	E	114	ASP
6	E	128	VAL
6	E	144	CYS
6	E	155	GLN
6	E	162	GLU
6	E	164	LEU
6	E	191	PHE
6	E	200	THR
7	F	45	THR
7	F	147	SER
7	F	178	VAL
7	F	195	SER
7	F	251	SER
7	F	311	VAL
7	F	314	THR
7	F	327	THR
7	F	362	CYS
7	F	380	VAL
7	F	415	VAL
8	G	26	VAL
8	G	57	VAL
8	G	65	VAL
8	G	73	VAL
8	G	127	ARG
8	G	135	ARG
8	G	151	THR
8	G	159	CYS
8	G	169	VAL
8	G	209	THR
8	G	210	SER
8	G	236	SER

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Mol	Chain	Res	Type
8	G	242	THR
8	G	250	ILE
8	G	322	LEU
8	G	324	ASP
8	G	335	LEU
8	G	345	THR
8	G	351	THR
8	G	364	LEU
8	G	366	THR
8	G	371	VAL
8	G	424	ASP
8	G	425	SER
8	G	436	SER
8	G	442	VAL
8	G	456	SER
8	G	466	ILE
8	G	488	LYS
8	G	516	LYS
8	G	604	SER
8	G	609	MET
8	G	610	THR
8	G	649	SER
8	G	669	LYS
8	G	677	ILE
8	G	681	SER
8	G	698	VAL
8	G	704	CYS
9	H	54	LYS
9	H	91	MET
9	H	119	SER
9	H	125	SER
9	H	140	ILE
9	H	163	SER
9	H	200	LEU
9	H	222	LEU
9	H	241	LEU
9	H	256	THR
9	H	296	LEU
10	I	39	SER
10	I	82	LEU
10	I	93	THR
10	I	103	SER

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Mol	Chain	Res	Type
10	I	141	THR
11	K	9	MET
11	K	57	SER
11	K	61	ILE
11	K	69	CYS
11	K	90	VAL
12	L	26	THR
12	L	47	SER
12	L	55	ILE
12	L	61	LEU
12	L	75	LYS
12	L	86	SER
12	L	92	VAL
12	L	110	SER
12	L	136	ASN
12	L	149	ILE
12	L	223	LYS
12	L	235	SER
12	L	244	SER
12	L	249	SER
12	L	276	ILE
12	L	316	THR
12	L	345	SER
12	L	369	THR
12	L	401	THR
12	L	410	LEU
12	L	417	SER
12	L	451	ILE
12	L	458	LEU
12	L	462	LEU
12	L	476	THR
12	L	531	THR
12	L	548	SER
12	L	553	LEU
12	L	565	THR
12	L	567	SER
12	L	577	VAL
12	L	585	LYS
12	L	590	SER
12	L	598	SER
13	M	97	THR
13	M	167	ILE

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Mol	Chain	Res	Type
13	M	234	VAL
13	M	284	SER
13	M	324	SER
13	M	350	THR
13	M	367	LEU
13	M	373	ILE
13	M	374	ASN
13	M	385	THR
13	M	390	ASN
13	M	423	ILE
13	M	438	SER
14	N	20	VAL
14	N	45	MET
14	N	67	SER
14	N	126	SER
14	N	140	SER
14	N	141	VAL
14	N	182	SER
14	N	212	THR
14	N	237	THR
14	N	250	SER
14	N	280	THR
14	N	295	ARG
14	N	296	LEU
14	N	299	SER
14	N	324	THR
14	N	331	VAL
14	N	333	SER
15	O	10	LEU
15	O	46	LEU
15	O	79	LEU
15	O	179	VAL
15	O	195	THR
15	O	279	LEU
16	P	27	THR
16	P	43	SER
16	P	56	THR
16	P	65	LEU
16	P	69	ILE
16	P	79	ASP
16	P	81	ILE
16	P	171	ILE

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Mol	Chain	Res	Type
16	P	200	THR
16	P	210	VAL
16	P	248	VAL
16	P	254	LEU
16	P	263	TYR
16	P	305	VAL
16	P	328	SER
17	Q	19	ILE
17	Q	44	ASN
17	Q	47	SER
17	Q	61	THR
17	Q	80	SER
17	Q	87	SER
17	Q	91	ASP
17	Q	102	SER
17	Q	115	SER
17	Q	117	SER
17	Q	123	SER
18	R	2	VAL
18	R	36	ASN
18	R	81	THR
19	S	32	VAL
19	S	41	VAL
19	S	76	VAL
19	S	87	THR
20	T	6	LEU
20	T	13	ASP
20	T	31	SER
20	T	45	LEU
21	U	16	LEU
21	U	31	SER
21	U	34	SER
21	U	47	GLN
21	U	72	CYS
22	V	4	LEU
22	V	47	THR
22	V	54	LYS
22	V	88	SER
22	V	103	VAL
22	V	112	LYS
22	V	115	ILE
23	W	45	ASN

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Mol	Chain	Res	Type
23	W	101	THR
24	X	8	SER
24	X	17	VAL
24	X	39	ASN
24	X	63	ASN
24	X	86	THR
24	X	109	CYS
24	X	125	SER
24	X	130	VAL
25	t	25	THR
25	t	26	SER
25	t	87	LEU
25	t	88	ASN
25	t	104	THR
25	t	140	VAL
26	Z	30	LEU
26	Z	34	SER
26	Z	101	VAL
26	Z	110	VAL
27	a	5	VAL
27	a	16	LEU
27	a	55	SER
27	a	60	SER
28	b	4	VAL
28	b	67	SER
29	c	27	LEU
30	d	20	SER
30	d	28	ASP
30	d	53	VAL
31	e	5	VAL
31	e	13	LEU
31	e	30	SER
31	e	48	SER
31	e	71	THR
31	e	86	ILE
31	e	88	GLU
32	f	7	VAL
32	f	14	VAL
32	f	33	LYS
32	f	40	LYS
32	f	41	SER
33	g	44	SER

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Mol	Chain	Res	Type
33	g	96	LEU
34	h	91	MET
34	h	110	VAL
35	u	28	SER
35	u	33	VAL
35	u	39	VAL
35	u	90	THR
35	u	95	THR
35	u	108	THR
35	u	127	HIS
36	j	16	GLN
36	j	24	GLN
36	j	57	SER
36	j	60	THR
37	k	30	THR
37	k	87	LEU
38	l	6	LYS
38	l	16	THR
38	l	54	SER
38	l	69	LEU
38	l	140	LEU
38	l	153	VAL
39	m	2	PHE
39	m	16	THR
39	m	25	SER
39	m	71	ARG
39	m	86	SER
39	m	127	SER
40	n	43	LEU
40	n	68	GLU
40	n	95	CYS
40	n	130	GLU
41	o	58	CYS
41	o	69	LYS
42	p	7	ASP
42	p	16	THR
42	p	24	SER
42	p	72	ASP
42	p	82	LEU
42	p	104	ILE
42	p	128	LEU
43	q	11	LEU

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Mol	Chain	Res	Type
43	q	15	SER
43	q	35	VAL
43	q	43	LYS
43	q	82	VAL
43	q	95	ASP
43	q	111	THR
43	q	118	SER
43	q	128	SER
43	q	134	ILE
43	q	138	VAL
44	v	30	ILE
44	v	34	THR
44	v	48	LEU
44	v	54	CYS
44	v	66	SER
44	v	68	VAL
44	v	94	VAL
45	s	74[A]	ARG
45	s	74[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	2	ASN
2	A	10	ASN
2	A	85	ASN
3	B	162	GLN
4	C	41	GLN
5	D	5	GLN
5	D	84	HIS
5	D	135	GLN
5	D	200	HIS
6	E	112	ASN
7	F	116	HIS
7	F	398	GLN
7	F	402	HIS
8	G	28	GLN
8	G	640	ASN
9	H	124	ASN
9	H	138	GLN
9	H	248	ASN
9	H	258	ASN

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Mol	Chain	Res	Type
11	K	7	ASN
12	L	170	GLN
12	L	269	ASN
12	L	296	ASN
12	L	309	GLN
12	L	320	ASN
12	L	442	ASN
12	L	444	ASN
12	L	541	ASN
12	L	579	ASN
13	M	30	HIS
13	M	51	ASN
13	M	81	GLN
13	M	82	HIS
13	M	83	HIS
13	M	103	GLN
13	M	138	ASN
13	M	180	GLN
13	M	220	HIS
13	M	251	ASN
13	M	304	GLN
13	M	415	GLN
13	M	422	HIS
14	N	36	ASN
14	N	120	GLN
14	N	134	GLN
15	O	114	HIS
15	O	184	GLN
15	O	229	GLN
15	O	251	GLN
16	P	36	ASN
16	P	136	ASN
17	Q	99	ASN
22	V	20	HIS
22	V	75	GLN
23	W	26	ASN
23	W	126	HIS
24	X	29	HIS
29	c	35	HIS
29	c	46	ASN
30	d	117	HIS
31	e	69	GLN

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Mol	Chain	Res	Type
32	f	39	ASN
34	h	69	HIS
34	h	86	ASN
34	h	124	HIS
34	h	143	ASN
36	j	50	HIS
37	k	32	GLN
38	l	136	ASN
39	m	74	ASN
39	m	78	ASN
40	n	13	GLN
40	n	50	HIS
42	p	27	ASN
42	p	90	GLN
42	p	106	GLN
42	p	148	HIS
43	q	5	GLN
43	q	112	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 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	$\#\|Z\| > 2$
5	2MR	D	85	5	10,12,13	2.42	2 (20%)	5,13,15	0.92	0
1	FME	J	1	1	8,9,10	0.93	0	7,9,11	0.89	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	2MR	D	85	5	-	0/10/13/15	-
1	FME	J	1	1	-	3/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	85	2MR	CZ-NE	5.10	1.45	1.34
5	D	85	2MR	CZ-NH2	5.06	1.44	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	J	1	FME	N-CA-CB-CG
1	J	1	FME	CB-CA-N-CN
1	J	1	FME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 57 ligands modelled in this entry, 3 are monoatomic - leaving 54 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	$\#\|Z\|>2$
52	3PE	j	101	-	43,43,50	0.54	0	46,48,55	0.59	1 (2%)
57	NDP	P	501	-	49,52,52	2.22	5 (10%)	66,80,80	1.60	13 (19%)
48	SF4	G	802	8	0,12,12	-	-	-		
53	CDL	L	703	-	75,75,99	0.35	0	81,87,111	0.22	0
48	SF4	G	801	8	0,12,12	-	-	-		
52	3PE	u	201	-	44,44,50	0.54	0	47,49,55	0.57	1 (2%)
47	PC1	h	202	-	46,46,53	0.52	0	52,54,61	0.49	1 (1%)
46	FME	A	201	-	8,9,10	0.95	0	7,9,11	0.83	0
46	FME	M	501	-	8,9,10	0.95	0	7,9,11	0.89	0
47	PC1	H	403	-	47,47,53	0.52	0	53,55,61	0.51	1 (1%)
47	PC1	M	503	-	34,34,53	0.60	0	40,42,61	0.56	1 (2%)
52	3PE	t	805	-	26,26,50	0.68	0	29,31,55	0.67	1 (3%)
47	PC1	I	201	-	53,53,53	0.50	0	59,61,61	0.47	1 (1%)
52	3PE	H	402	-	35,35,50	0.60	0	38,40,55	0.62	1 (2%)
47	PC1	m	201	-	45,45,53	0.53	0	51,53,61	0.50	1 (1%)
52	3PE	M	502	-	44,44,50	0.54	0	47,49,55	0.58	1 (2%)
46	FME	N	401	-	8,9,10	0.96	0	7,9,11	0.89	0
46	FME	K	101	-	8,9,10	0.94	0	7,9,11	0.90	0
49	FES	G	803	8	0,4,4	-	-	-		
54	CHD	L	706	-	32,32,32	0.61	0	51,51,51	1.11	5 (9%)
48	SF4	F	502	7	0,12,12	-	-	-		
48	SF4	I	203	10	0,12,12	-	-	-		
48	SF4	I	202	10	0,12,12	-	-	-		
52	3PE	L	704	-	48,48,50	0.53	0	51,53,55	0.52	1 (1%)
52	3PE	O	401	-	47,47,50	0.53	0	50,52,55	0.55	1 (2%)
55	GTP	O	403	56	30,34,34	0.84	1 (3%)	46,54,54	1.70	11 (23%)
52	3PE	d	202	-	48,48,50	0.53	0	51,53,55	0.54	1 (1%)
52	3PE	m	202	-	40,40,50	0.57	0	43,45,55	0.57	1 (2%)
52	3PE	b	201	-	46,46,50	0.53	0	49,51,55	0.54	1 (2%)
53	CDL	h	201	-	79,79,99	0.34	0	85,91,111	0.21	0
47	PC1	Z	201	-	43,43,53	0.54	0	49,51,61	0.52	1 (2%)
52	3PE	t	801	-	30,30,50	0.62	0	33,35,55	0.81	2 (6%)
52	3PE	t	802	-	39,39,50	0.57	0	42,44,55	0.58	1 (2%)
52	3PE	t	803	-	29,29,50	0.64	0	32,34,55	0.80	2 (6%)
47	PC1	d	203	-	38,38,53	0.57	0	44,46,61	0.53	1 (2%)
52	3PE	K	102	-	43,43,50	0.55	0	46,48,55	0.56	1 (2%)
52	3PE	L	702	-	45,45,50	0.55	0	48,50,55	0.56	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
53	CDL	d	204	-	64,64,99	0.38	0	70,76,111	0.26	0
48	SF4	B	201	3	0,12,12	-	-	-		
49	FES	E	301	6	0,4,4	-	-	-		
52	3PE	M	505	-	49,49,50	0.51	0	52,54,55	0.53	1 (1%)
52	3PE	M	504	-	50,50,50	0.50	0	53,55,55	0.65	2 (3%)
53	CDL	v	201	-	60,60,99	0.39	0	66,72,111	0.24	0
52	3PE	t	804	-	32,32,50	0.61	0	35,37,55	0.75	2 (5%)
53	CDL	O	402	-	61,61,99	0.46	0	67,73,111	0.46	0
47	PC1	A	202	-	34,34,53	0.59	0	40,42,61	0.56	1 (2%)
47	PC1	L	705	-	43,43,53	0.54	0	49,51,61	0.50	1 (2%)
47	PC1	B	203	-	47,47,53	0.51	0	53,55,61	0.52	1 (1%)
47	PC1	B	202	-	45,45,53	0.53	0	51,53,61	0.63	1 (1%)
53	CDL	d	201	-	85,85,99	0.41	1 (1%)	91,97,111	0.27	0
46	FME	H	401	-	8,9,10	0.93	0	7,9,11	0.95	0
59	MYR	o	201	-	14,14,15	0.36	0	13,13,15	0.71	0
50	FMN	F	501	-	33,33,33	1.09	2 (6%)	48,50,50	1.20	7 (14%)
46	FME	L	701	-	8,9,10	0.96	0	7,9,11	0.90	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	3PE	j	101	-	-	13/47/47/54	-
57	NDP	P	501	-	-	12/34/77/77	0/5/5/5
48	SF4	G	802	8	-	-	0/6/5/5
53	CDL	L	703	-	-	50/86/86/110	-
52	3PE	u	201	-	-	22/48/48/54	-
48	SF4	G	801	8	-	-	0/6/5/5
47	PC1	h	202	-	-	22/50/50/57	-
46	FME	A	201	-	-	2/7/9/11	-
46	FME	M	501	-	-	2/7/9/11	-
47	PC1	H	403	-	-	16/51/51/57	-
47	PC1	M	503	-	-	22/38/38/57	-
52	3PE	t	805	-	-	17/30/30/54	-
47	PC1	I	201	-	-	17/57/57/57	-
52	3PE	H	402	-	-	12/39/39/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	PC1	m	201	-	-	22/49/49/57	-
52	3PE	M	502	-	-	12/48/48/54	-
46	FME	N	401	-	-	2/7/9/11	-
46	FME	K	101	-	-	2/7/9/11	-
49	FES	G	803	8	-	-	0/1/1/1
54	CHD	L	706	-	-	3/9/74/74	0/4/4/4
48	SF4	F	502	7	-	-	0/6/5/5
55	GTP	O	403	56	-	4/22/38/38	0/3/3/3
52	3PE	O	401	-	-	18/51/51/54	-
52	3PE	L	704	-	-	22/52/52/54	-
48	SF4	I	202	10	-	-	0/6/5/5
48	SF4	I	203	10	-	-	0/6/5/5
52	3PE	d	202	-	-	18/52/52/54	-
52	3PE	m	202	-	-	15/44/44/54	-
52	3PE	b	201	-	-	26/50/50/54	-
53	CDL	h	201	-	-	54/90/90/110	-
47	PC1	Z	201	-	-	16/47/47/57	-
52	3PE	t	801	-	-	15/34/34/54	-
52	3PE	t	802	-	-	17/43/43/54	-
52	3PE	t	803	-	-	21/33/33/54	-
47	PC1	d	203	-	-	11/42/42/57	-
52	3PE	K	102	-	-	14/47/47/54	-
52	3PE	L	702	-	-	22/49/49/54	-
53	CDL	d	204	-	-	42/75/75/110	-
48	SF4	B	201	3	-	-	0/6/5/5
49	FES	E	301	6	-	-	0/1/1/1
52	3PE	M	505	-	-	26/53/53/54	-
52	3PE	M	504	-	-	18/54/54/54	-
53	CDL	v	201	-	-	33/71/71/110	-
52	3PE	t	804	-	-	19/36/36/54	-
53	CDL	O	402	-	-	46/71/71/110	-
47	PC1	A	202	-	-	16/38/38/57	-
47	PC1	L	705	-	-	15/47/47/57	-
47	PC1	B	203	-	-	16/51/51/57	-
47	PC1	B	202	-	-	24/49/49/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	CDL	d	201	-	-	55/96/96/110	-
46	FME	H	401	-	-	4/7/9/11	-
59	MYR	o	201	-	-	0/11/12/13	-
50	FMN	F	501	-	-	1/18/18/18	0/3/3/3
46	FME	L	701	-	-	4/7/9/11	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	P	501	NDP	P2B-O2B	12.64	1.83	1.59
57	P	501	NDP	PN-O5D	4.15	1.76	1.59
50	F	501	FMN	C4A-N5	3.81	1.38	1.30
57	P	501	NDP	O2B-C2B	-3.00	1.33	1.44
50	F	501	FMN	C10-N1	2.49	1.38	1.33
57	P	501	NDP	C5A-C4A	2.38	1.43	1.39
53	d	201	CDL	OB8-CB6	2.34	1.50	1.45
55	O	403	GTP	C2-N3	2.14	1.38	1.33
57	P	501	NDP	C2A-N1A	2.09	1.37	1.33

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	P	501	NDP	PN-O3-PA	-6.62	110.12	132.83
55	O	403	GTP	C5-C4-N3	-4.95	120.43	128.46
55	O	403	GTP	C2-N3-C4	4.40	120.13	112.30
57	P	501	NDP	O2B-P2B-O1X	-3.39	96.29	109.39
55	O	403	GTP	N9-C4-N3	3.23	132.43	125.94
57	P	501	NDP	PA-O5B-C5B	-3.12	103.37	121.68
50	F	501	FMN	C4-N3-C2	-3.05	120.02	125.64
55	O	403	GTP	C2-N1-C6	-2.96	119.71	125.10
52	t	804	3PE	C2-O21-C21	2.92	124.99	117.79
52	t	803	3PE	C2-O21-C21	2.92	124.97	117.79
52	M	504	3PE	C2-O21-C21	2.88	124.89	117.79
52	t	801	3PE	C2-O21-C21	2.86	124.83	117.79
57	P	501	NDP	PN-O5D-C5D	-2.83	105.11	121.68
55	O	403	GTP	PB-O3B-PG	-2.80	123.21	132.83
50	F	501	FMN	C4A-C4-N3	2.72	120.09	113.19
55	O	403	GTP	N9-C8-N7	-2.71	108.29	113.39
55	O	403	GTP	C8-N7-C5	2.61	108.97	104.24
54	L	706	CHD	C2-C1-C10	2.61	117.26	112.78
55	O	403	GTP	PA-O3A-PB	-2.59	123.95	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	F	501	FMN	O4-C4-C4A	-2.55	119.84	126.60
57	P	501	NDP	O3X-P2B-O2X	2.53	117.30	107.64
55	O	403	GTP	C5-C6-N1	2.52	119.58	113.19
57	P	501	NDP	N3A-C4A-N9A	2.46	131.13	127.08
55	O	403	GTP	O6-C6-C5	-2.42	120.17	126.60
57	P	501	NDP	C2A-N1A-C6A	-2.40	114.65	118.77
50	F	501	FMN	C4A-C10-N10	2.40	119.98	116.48
52	M	504	3PE	O12-P-O14	2.39	124.05	112.24
57	P	501	NDP	O4B-C4B-C3B	2.37	109.81	105.11
52	b	201	3PE	O12-P-O14	2.37	123.97	112.24
54	L	706	CHD	C4-C5-C10	2.37	115.18	112.66
52	M	502	3PE	O12-P-O14	2.37	123.95	112.24
52	t	801	3PE	O12-P-O14	2.36	123.91	112.24
52	j	101	3PE	O12-P-O14	2.36	123.89	112.24
47	B	202	PC1	O12-P-O14	2.36	123.88	112.24
52	K	102	3PE	O12-P-O14	2.35	123.87	112.24
52	t	802	3PE	O12-P-O14	2.35	123.86	112.24
57	P	501	NDP	C5A-C4A-N3A	-2.35	123.69	126.75
52	d	202	3PE	O12-P-O14	2.35	123.84	112.24
47	Z	201	PC1	O12-P-O14	2.34	123.82	112.24
52	O	401	3PE	O12-P-O14	2.34	123.81	112.24
52	M	505	3PE	O12-P-O14	2.34	123.80	112.24
47	I	201	PC1	O12-P-O14	2.34	123.79	112.24
54	L	706	CHD	C19-C10-C1	-2.33	104.50	108.26
52	L	702	3PE	O12-P-O14	2.33	123.76	112.24
47	M	503	PC1	O12-P-O14	2.33	123.76	112.24
47	h	202	PC1	O12-P-O14	2.33	123.76	112.24
52	t	805	3PE	O12-P-O14	2.33	123.76	112.24
52	u	201	3PE	O12-P-O14	2.33	123.74	112.24
47	m	201	PC1	O12-P-O14	2.32	123.72	112.24
52	H	402	3PE	O12-P-O14	2.32	123.71	112.24
47	d	203	PC1	O12-P-O14	2.32	123.71	112.24
47	A	202	PC1	O12-P-O14	2.32	123.69	112.24
52	t	803	3PE	O12-P-O14	2.32	123.69	112.24
52	m	202	3PE	O12-P-O14	2.30	123.63	112.24
47	H	403	PC1	O12-P-O14	2.30	123.62	112.24
47	B	203	PC1	O12-P-O14	2.30	123.60	112.24
52	L	704	3PE	O12-P-O14	2.29	123.56	112.24
54	L	706	CHD	C17-C13-C14	2.28	102.39	100.09
47	L	705	PC1	O12-P-O14	2.26	123.43	112.24
57	P	501	NDP	C5B-C4B-C3B	-2.26	106.71	115.18
52	t	804	3PE	O12-P-O14	2.26	123.42	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	O	403	GTP	C3'-C2'-C1'	2.23	105.65	101.43
50	F	501	FMN	C4A-C10-N1	-2.22	119.58	124.73
50	F	501	FMN	C10-C4A-N5	-2.21	120.17	124.86
50	F	501	FMN	C9A-C5A-N5	-2.20	120.04	122.43
57	P	501	NDP	O5D-PN-O1N	-2.14	100.70	109.07
57	P	501	NDP	O2N-PN-O1N	2.11	122.67	112.24
54	L	706	CHD	C18-C13-C17	-2.10	107.93	111.21
57	P	501	NDP	C5A-C6A-N1A	2.03	121.75	117.39

There are no chirality outliers.

All (840) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	201	FME	O1-CN-N-CA
46	H	401	FME	N-CA-CB-CG
46	H	401	FME	O-C-CA-CB
46	K	101	FME	O1-CN-N-CA
46	K	101	FME	O-C-CA-CB
46	L	701	FME	O1-CN-N-CA
46	N	401	FME	O1-CN-N-CA
47	A	202	PC1	C11-O13-P-O12
47	A	202	PC1	C11-O13-P-O14
47	A	202	PC1	C1-O11-P-O14
47	A	202	PC1	C22-C21-O21-C2
47	B	202	PC1	C11-O13-P-O12
47	B	202	PC1	C11-O13-P-O11
47	B	203	PC1	O22-C21-O21-C2
47	H	403	PC1	C11-O13-P-O12
47	H	403	PC1	C1-O11-P-O14
47	I	201	PC1	C11-O13-P-O12
47	M	503	PC1	C11-O13-P-O12
47	M	503	PC1	C11-O13-P-O14
47	Z	201	PC1	C11-O13-P-O14
47	Z	201	PC1	C22-C21-O21-C2
47	d	203	PC1	C1-O11-P-O13
47	d	203	PC1	O13-C11-C12-N
47	d	203	PC1	O22-C21-O21-C2
47	h	202	PC1	C11-O13-P-O12
47	h	202	PC1	C11-O13-P-O11
47	h	202	PC1	C1-O11-P-O12
47	h	202	PC1	C1-O11-P-O14
47	h	202	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
47	m	201	PC1	C11-O13-P-O14
52	H	402	3PE	C1-O11-P-O12
52	H	402	3PE	C1-O11-P-O13
52	H	402	3PE	C1-O11-P-O14
52	K	102	3PE	C1-O11-P-O12
52	K	102	3PE	O13-C11-C12-N
52	L	702	3PE	O13-C11-C12-N
52	L	702	3PE	C22-C21-O21-C2
52	L	704	3PE	C1-O11-P-O14
52	L	704	3PE	O13-C11-C12-N
52	M	502	3PE	C1-O11-P-O12
52	M	502	3PE	C11-O13-P-O11
52	M	502	3PE	C11-O13-P-O14
52	M	505	3PE	O11-C1-C2-O21
52	M	505	3PE	C22-C21-O21-C2
52	O	401	3PE	C1-O11-P-O12
52	t	801	3PE	C1-O11-P-O13
52	t	801	3PE	C11-O13-P-O14
52	t	802	3PE	C11-O13-P-O14
52	t	802	3PE	C2-C1-O11-P
52	t	803	3PE	C1-O11-P-O14
52	t	803	3PE	C11-O13-P-O11
52	t	803	3PE	C11-O13-P-O14
52	t	803	3PE	O13-C11-C12-N
52	t	804	3PE	C1-O11-P-O12
52	t	804	3PE	C1-O11-P-O14
52	t	805	3PE	C1-O11-P-O14
52	t	805	3PE	C11-O13-P-O12
52	t	805	3PE	O22-C21-O21-C2
52	b	201	3PE	C11-O13-P-O12
52	d	202	3PE	C1-O11-P-O12
52	d	202	3PE	C1-O11-P-O13
52	d	202	3PE	C1-O11-P-O14
52	d	202	3PE	C11-O13-P-O14
52	u	201	3PE	C1-O11-P-O12
52	u	201	3PE	C1-O11-P-O13
52	u	201	3PE	C1-O11-P-O14
52	u	201	3PE	C11-O13-P-O14
52	j	101	3PE	C1-O11-P-O12
52	j	101	3PE	C1-O11-P-O13
52	j	101	3PE	C1-O11-P-O14
52	j	101	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
52	j	101	3PE	O22-C21-O21-C2
52	m	202	3PE	C11-O13-P-O11
52	m	202	3PE	C11-O13-P-O12
52	m	202	3PE	C11-O13-P-O14
53	L	703	CDL	O1-C1-CB2-OB2
53	L	703	CDL	CA2-OA2-PA1-OA3
53	L	703	CDL	CA2-OA2-PA1-OA4
53	L	703	CDL	OA6-CA4-CA6-OA8
53	L	703	CDL	CB2-OB2-PB2-OB3
53	L	703	CDL	CB2-OB2-PB2-OB4
53	O	402	CDL	CB2-C1-CA2-OA2
53	O	402	CDL	CA2-C1-CB2-OB2
53	O	402	CDL	CA2-OA2-PA1-OA3
53	O	402	CDL	CA2-OA2-PA1-OA4
53	O	402	CDL	CA3-OA5-PA1-OA2
53	O	402	CDL	CA3-OA5-PA1-OA3
53	O	402	CDL	CA3-OA5-PA1-OA4
53	O	402	CDL	C11-CA5-OA6-CA4
53	O	402	CDL	CB2-OB2-PB2-OB4
53	O	402	CDL	CB3-OB5-PB2-OB2
53	d	201	CDL	CB2-C1-CA2-OA2
53	d	201	CDL	CB2-OB2-PB2-OB3
53	d	201	CDL	CB2-OB2-PB2-OB4
53	d	201	CDL	CB2-OB2-PB2-OB5
53	d	201	CDL	CB4-CB3-OB5-PB2
53	d	201	CDL	OB7-CB5-OB6-CB4
53	d	204	CDL	CA2-OA2-PA1-OA3
53	d	204	CDL	CA2-OA2-PA1-OA4
53	d	204	CDL	CA3-OA5-PA1-OA2
53	d	204	CDL	CA3-OA5-PA1-OA3
53	d	204	CDL	CA3-OA5-PA1-OA4
53	d	204	CDL	C51-CB5-OB6-CB4
53	h	201	CDL	CB2-C1-CA2-OA2
53	h	201	CDL	CA2-OA2-PA1-OA3
53	h	201	CDL	CA2-OA2-PA1-OA4
53	h	201	CDL	CB2-OB2-PB2-OB4
53	h	201	CDL	CB3-OB5-PB2-OB2
53	h	201	CDL	CB3-OB5-PB2-OB3
53	h	201	CDL	CB3-OB5-PB2-OB4
53	h	201	CDL	C51-CB5-OB6-CB4
53	v	201	CDL	CA3-OA5-PA1-OA2
53	v	201	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
53	v	201	CDL	CB2-OB2-PB2-OB4
57	P	501	NDP	C5B-O5B-PA-O3
57	P	501	NDP	O4B-C4B-C5B-O5B
57	P	501	NDP	C3B-C4B-C5B-O5B
57	P	501	NDP	C5D-O5D-PN-O3
57	P	501	NDP	O4D-C4D-C5D-O5D
53	O	402	CDL	C51-CB5-OB6-CB4
52	H	402	3PE	O32-C31-O31-C3
53	O	402	CDL	OA9-CA7-OA8-CA6
53	O	402	CDL	OB9-CB7-OB8-CB6
47	h	202	PC1	C32-C31-O31-C3
53	O	402	CDL	C71-CB7-OB8-CB6
53	d	204	CDL	C71-CB7-OB8-CB6
47	d	203	PC1	O32-C31-O31-C3
47	h	202	PC1	O32-C31-O31-C3
52	L	704	3PE	O32-C31-O31-C3
52	O	401	3PE	O32-C31-O31-C3
52	t	801	3PE	O32-C31-O31-C3
52	t	804	3PE	O32-C31-O31-C3
52	d	202	3PE	O32-C31-O31-C3
52	m	202	3PE	O32-C31-O31-C3
53	d	204	CDL	OB9-CB7-OB8-CB6
53	O	402	CDL	OB7-CB5-OB6-CB4
47	A	202	PC1	O22-C21-O21-C2
47	Z	201	PC1	O22-C21-O21-C2
52	K	102	3PE	O22-C21-O21-C2
52	L	702	3PE	O22-C21-O21-C2
52	M	505	3PE	O22-C21-O21-C2
53	d	204	CDL	OB7-CB5-OB6-CB4
53	h	201	CDL	OB7-CB5-OB6-CB4
47	d	203	PC1	C32-C31-O31-C3
52	H	402	3PE	C32-C31-O31-C3
52	L	704	3PE	C32-C31-O31-C3
52	O	401	3PE	C32-C31-O31-C3
52	t	801	3PE	C32-C31-O31-C3
52	t	804	3PE	C32-C31-O31-C3
52	d	202	3PE	C32-C31-O31-C3
52	m	202	3PE	C32-C31-O31-C3
53	O	402	CDL	C31-CA7-OA8-CA6
47	B	203	PC1	C22-C21-O21-C2
47	d	203	PC1	C22-C21-O21-C2
52	K	102	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
52	t	805	3PE	C22-C21-O21-C2
52	j	101	3PE	C22-C21-O21-C2
53	d	201	CDL	C51-CB5-OB6-CB4
53	d	201	CDL	C71-CB7-OB8-CB6
53	O	402	CDL	C37-C38-C39-C40
53	O	402	CDL	OA7-CA5-OA6-CA4
53	O	402	CDL	O1-C1-CB2-OB2
53	h	201	CDL	O1-C1-CA2-OA2
53	v	201	CDL	O1-C1-CB2-OB2
47	M	503	PC1	C32-C31-O31-C3
53	L	703	CDL	C31-CA7-OA8-CA6
52	H	402	3PE	C22-C21-O21-C2
52	O	401	3PE	C22-C21-O21-C2
53	d	204	CDL	C38-C39-C40-C41
53	h	201	CDL	C57-C58-C59-C60
53	O	402	CDL	C17-C18-C19-C20
53	d	201	CDL	C59-C60-C61-C62
53	d	204	CDL	C32-C33-C34-C35
52	L	704	3PE	C2-C1-O11-P
53	d	201	CDL	C51-C52-C53-C54
53	d	201	CDL	C17-C18-C19-C20
47	M	503	PC1	O32-C31-O31-C3
53	L	703	CDL	OA9-CA7-OA8-CA6
53	d	201	CDL	C36-C37-C38-C39
47	m	201	PC1	C22-C21-O21-C2
53	L	703	CDL	C55-C56-C57-C58
53	L	703	CDL	CA2-C1-CB2-OB2
53	d	201	CDL	CA2-C1-CB2-OB2
53	h	201	CDL	CA2-C1-CB2-OB2
52	H	402	3PE	O22-C21-O21-C2
47	H	403	PC1	C11-C12-N-C13
52	b	201	3PE	C32-C31-O31-C3
53	L	703	CDL	C33-C34-C35-C36
53	h	201	CDL	C38-C39-C40-C41
53	h	201	CDL	C59-C60-C61-C62
53	h	201	CDL	C73-C74-C75-C76
53	h	201	CDL	OB5-CB3-CB4-OB6
53	h	201	CDL	C13-C14-C15-C16
53	d	201	CDL	O1-C1-CB2-OB2
47	B	202	PC1	O21-C2-C3-O31
53	O	402	CDL	C33-C34-C35-C36
53	d	201	CDL	C56-C57-C58-C59

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Mol	Chain	Res	Type	Atoms
53	O	402	CDL	C19-C20-C21-C22
52	O	401	3PE	O22-C21-O21-C2
53	L	703	CDL	C12-C13-C14-C15
52	K	102	3PE	C31-C32-C33-C34
53	v	201	CDL	CB7-C71-C72-C73
52	t	803	3PE	C21-C22-C23-C24
47	B	203	PC1	C21-C22-C23-C24
52	m	202	3PE	C21-C22-C23-C24
53	L	703	CDL	CB7-C71-C72-C73
53	d	204	CDL	CA5-C11-C12-C13
53	d	204	CDL	CB7-C71-C72-C73
53	h	201	CDL	CB7-C71-C72-C73
53	v	201	CDL	CA5-C11-C12-C13
53	O	402	CDL	C15-C16-C17-C18
47	H	403	PC1	C11-C12-N-C14
53	d	204	CDL	C11-CA5-OA6-CA4
52	b	201	3PE	O32-C31-O31-C3
53	d	201	CDL	OB9-CB7-OB8-CB6
53	O	402	CDL	C11-C12-C13-C14
53	d	204	CDL	O1-C1-CB2-OB2
53	h	201	CDL	O1-C1-CB2-OB2
47	m	201	PC1	O22-C21-O21-C2
47	Z	201	PC1	C32-C31-O31-C3
47	M	503	PC1	C22-C21-O21-C2
52	L	704	3PE	C35-C36-C37-C38
47	A	202	PC1	C11-O13-P-O11
47	A	202	PC1	C1-O11-P-O13
47	M	503	PC1	C11-O13-P-O11
47	Z	201	PC1	C11-O13-P-O11
47	h	202	PC1	C1-O11-P-O13
47	m	201	PC1	C11-O13-P-O11
52	K	102	3PE	C1-O11-P-O13
52	M	505	3PE	C11-O13-P-O11
52	O	401	3PE	C1-O11-P-O13
52	t	802	3PE	C1-O11-P-O13
52	t	802	3PE	C11-O13-P-O11
52	t	803	3PE	C1-O11-P-O13
52	t	804	3PE	C1-O11-P-O13
52	t	805	3PE	C11-O13-P-O11
52	b	201	3PE	C11-O13-P-O11
53	L	703	CDL	CA2-OA2-PA1-OA5
53	L	703	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
53	O	402	CDL	CA2-OA2-PA1-OA5
53	O	402	CDL	CB2-OB2-PB2-OB5
53	d	201	CDL	CB3-OB5-PB2-OB2
53	d	204	CDL	CA2-OA2-PA1-OA5
53	d	204	CDL	CB2-OB2-PB2-OB5
53	h	201	CDL	CA2-OA2-PA1-OA5
53	h	201	CDL	CB2-OB2-PB2-OB5
53	v	201	CDL	CB2-OB2-PB2-OB5
53	v	201	CDL	C31-CA7-OA8-CA6
47	I	201	PC1	C3B-C3C-C3D-C3E
53	d	204	CDL	CA2-C1-CB2-OB2
53	v	201	CDL	CA2-C1-CB2-OB2
47	M	503	PC1	O22-C21-O21-C2
53	d	204	CDL	OA7-CA5-OA6-CA4
53	h	201	CDL	C34-C35-C36-C37
47	I	201	PC1	C39-C3A-C3B-C3C
47	m	201	PC1	C26-C27-C28-C29
53	d	201	CDL	C43-C44-C45-C46
47	B	202	PC1	C33-C34-C35-C36
47	B	202	PC1	C36-C37-C38-C39
53	d	201	CDL	C38-C39-C40-C41
47	h	202	PC1	C22-C21-O21-C2
53	d	201	CDL	C11-CA5-OA6-CA4
47	B	202	PC1	C35-C36-C37-C38
47	B	202	PC1	C3D-C3E-C3F-C3G
47	h	202	PC1	C2B-C2C-C2D-C2E
47	m	201	PC1	C27-C28-C29-C2A
52	H	402	3PE	C2A-C2B-C2C-C2D
52	K	102	3PE	C32-C33-C34-C35
52	K	102	3PE	C33-C34-C35-C36
52	M	502	3PE	C2D-C2E-C2F-C2G
52	O	401	3PE	C36-C37-C38-C39
52	u	201	3PE	C3D-C3E-C3F-C3G
53	L	703	CDL	C36-C37-C38-C39
53	O	402	CDL	C32-C33-C34-C35
53	d	201	CDL	C37-C38-C39-C40
53	d	201	CDL	C60-C61-C62-C63
53	h	201	CDL	C75-C76-C77-C78
47	h	202	PC1	C2A-C2B-C2C-C2D
52	t	804	3PE	C38-C39-C3A-C3B
53	L	703	CDL	C32-C33-C34-C35
53	v	201	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
53	d	201	CDL	OA7-CA5-OA6-CA4
47	L	705	PC1	C29-C2A-C2B-C2C
47	h	202	PC1	C2E-C2F-C2G-C2H
53	d	201	CDL	C55-C56-C57-C58
53	h	201	CDL	C32-C33-C34-C35
52	K	102	3PE	C39-C3A-C3B-C3C
52	b	201	3PE	C2A-C2B-C2C-C2D
53	L	703	CDL	C57-C58-C59-C60
46	N	401	FME	N-CA-CB-CG
53	O	402	CDL	O1-C1-CA2-OA2
53	d	201	CDL	O1-C1-CA2-OA2
52	t	801	3PE	C34-C35-C36-C37
53	d	201	CDL	C19-C20-C21-C22
53	h	201	CDL	C31-C32-C33-C34
53	v	201	CDL	OA9-CA7-OA8-CA6
47	d	203	PC1	C32-C33-C34-C35
52	K	102	3PE	C29-C2A-C2B-C2C
52	j	101	3PE	C24-C25-C26-C27
53	d	201	CDL	C23-C24-C25-C26
53	d	201	CDL	C57-C58-C59-C60
52	u	201	3PE	C31-C32-C33-C34
53	L	703	CDL	CB5-C51-C52-C53
47	H	403	PC1	C33-C34-C35-C36
47	h	202	PC1	C2C-C2D-C2E-C2F
52	L	702	3PE	C29-C2A-C2B-C2C
52	M	504	3PE	C2C-C2D-C2E-C2F
53	L	703	CDL	C40-C41-C42-C43
53	d	204	CDL	C71-C72-C73-C74
53	h	201	CDL	C60-C61-C62-C63
47	h	202	PC1	O22-C21-O21-C2
47	B	203	PC1	C39-C3A-C3B-C3C
52	M	504	3PE	C2B-C2C-C2D-C2E
52	t	802	3PE	C29-C2A-C2B-C2C
52	d	202	3PE	C2E-C2F-C2G-C2H
53	v	201	CDL	C16-C17-C18-C19
47	A	202	PC1	C31-C32-C33-C34
47	Z	201	PC1	C31-C32-C33-C34
52	t	802	3PE	C31-C32-C33-C34
52	d	202	3PE	C25-C26-C27-C28
53	L	703	CDL	C62-C63-C64-C65
53	d	201	CDL	C20-C21-C22-C23
53	h	201	CDL	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
53	v	201	CDL	C72-C73-C74-C75
47	H	403	PC1	C11-C12-N-C15
52	L	702	3PE	O11-C1-C2-C3
47	Z	201	PC1	C22-C23-C24-C25
52	L	704	3PE	C23-C24-C25-C26
52	d	202	3PE	C35-C36-C37-C38
53	L	703	CDL	C51-C52-C53-C54
52	M	505	3PE	C23-C24-C25-C26
53	L	703	CDL	C54-C55-C56-C57
53	d	201	CDL	C63-C64-C65-C66
53	O	402	CDL	CA7-C31-C32-C33
53	L	703	CDL	C11-C12-C13-C14
53	L	703	CDL	C60-C61-C62-C63
52	M	505	3PE	C33-C34-C35-C36
52	M	505	3PE	C34-C35-C36-C37
53	d	201	CDL	C54-C55-C56-C57
52	K	102	3PE	C34-C35-C36-C37
52	L	702	3PE	C28-C29-C2A-C2B
53	d	204	CDL	C40-C41-C42-C43
53	d	201	CDL	C31-C32-C33-C34
53	h	201	CDL	C16-C17-C18-C19
47	I	201	PC1	C38-C39-C3A-C3B
53	O	402	CDL	C20-C21-C22-C23
47	Z	201	PC1	O32-C31-O31-C3
52	t	804	3PE	C22-C21-O21-C2
52	j	101	3PE	C33-C34-C35-C36
52	m	202	3PE	C26-C27-C28-C29
53	O	402	CDL	C13-C14-C15-C16
53	d	201	CDL	C16-C17-C18-C19
53	d	204	CDL	C75-C76-C77-C78
53	h	201	CDL	C17-C18-C19-C20
53	d	201	CDL	CB7-C71-C72-C73
52	u	201	3PE	C3C-C3D-C3E-C3F
53	d	204	CDL	C31-CA7-OA8-CA6
53	h	201	CDL	C52-C53-C54-C55
53	v	201	CDL	C11-C12-C13-C14
52	t	801	3PE	O22-C21-O21-C2
52	t	804	3PE	O22-C21-O21-C2
53	h	201	CDL	C12-C13-C14-C15
53	h	201	CDL	C37-C38-C39-C40
53	h	201	CDL	C55-C56-C57-C58
52	L	702	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
53	O	402	CDL	C35-C36-C37-C38
53	h	201	CDL	C74-C75-C76-C77
52	t	801	3PE	C22-C21-O21-C2
53	d	201	CDL	C39-C40-C41-C42
53	L	703	CDL	CA7-C31-C32-C33
52	M	502	3PE	C23-C24-C25-C26
52	M	504	3PE	O22-C21-O21-C2
52	t	803	3PE	O22-C21-O21-C2
52	t	802	3PE	C32-C31-O31-C3
47	B	202	PC1	C3A-C3B-C3C-C3D
53	d	204	CDL	C44-C45-C46-C47
52	L	702	3PE	C2D-C2E-C2F-C2G
52	t	801	3PE	C36-C37-C38-C39
53	d	201	CDL	C15-C16-C17-C18
47	M	503	PC1	C22-C23-C24-C25
52	M	505	3PE	C29-C2A-C2B-C2C
53	d	201	CDL	C40-C41-C42-C43
53	d	204	CDL	C37-C38-C39-C40
52	t	805	3PE	C24-C25-C26-C27
53	d	201	CDL	C32-C33-C34-C35
53	v	201	CDL	C17-C18-C19-C20
53	d	204	CDL	OA9-CA7-OA8-CA6
52	u	201	3PE	C32-C33-C34-C35
53	d	201	CDL	C22-C23-C24-C25
52	M	504	3PE	C22-C21-O21-C2
52	t	803	3PE	C22-C21-O21-C2
52	m	202	3PE	C22-C21-O21-C2
53	v	201	CDL	C11-CA5-OA6-CA4
47	m	201	PC1	C24-C25-C26-C27
47	m	201	PC1	C32-C33-C34-C35
52	M	505	3PE	C2A-C2B-C2C-C2D
53	d	204	CDL	C33-C34-C35-C36
53	L	703	CDL	C14-C15-C16-C17
52	m	202	3PE	O22-C21-O21-C2
52	b	201	3PE	O21-C2-C3-O31
52	L	704	3PE	C32-C33-C34-C35
47	B	203	PC1	C36-C37-C38-C39
47	L	705	PC1	C32-C31-O31-C3
52	m	202	3PE	C29-C2A-C2B-C2C
47	H	403	PC1	C11-O13-P-O11
52	t	801	3PE	C11-O13-P-O11
52	j	101	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
53	O	402	CDL	C1-CB2-OB2-PB2
52	m	202	3PE	C28-C29-C2A-C2B
52	L	704	3PE	O11-C1-C2-C3
52	M	505	3PE	O11-C1-C2-C3
52	t	802	3PE	O11-C1-C2-C3
52	t	804	3PE	O11-C1-C2-C3
52	O	401	3PE	C23-C24-C25-C26
52	t	802	3PE	O32-C31-O31-C3
47	H	403	PC1	C37-C38-C39-C3A
47	L	705	PC1	C23-C24-C25-C26
47	B	202	PC1	C1-C2-C3-O31
47	B	203	PC1	C1-C2-C3-O31
47	H	403	PC1	C27-C28-C29-C2A
47	I	201	PC1	C1-C2-C3-O31
47	M	503	PC1	C1-C2-C3-O31
47	h	202	PC1	C1-C2-C3-O31
47	h	202	PC1	C25-C26-C27-C28
52	t	801	3PE	C1-C2-C3-O31
52	b	201	3PE	C1-C2-C3-O31
52	d	202	3PE	C1-C2-C3-O31
52	u	201	3PE	C1-C2-C3-O31
53	L	703	CDL	CA3-CA4-CA6-OA8
53	h	201	CDL	CA3-CA4-CA6-OA8
53	O	402	CDL	C39-C40-C41-C42
53	L	703	CDL	C71-C72-C73-C74
53	d	201	CDL	C33-C34-C35-C36
53	d	201	CDL	C44-C45-C46-C47
53	h	201	CDL	C11-C12-C13-C14
53	h	201	CDL	C18-C19-C20-C21
52	t	804	3PE	C31-C32-C33-C34
52	u	201	3PE	C36-C37-C38-C39
53	v	201	CDL	C52-C53-C54-C55
53	L	703	CDL	C16-C17-C18-C19
47	I	201	PC1	C26-C27-C28-C29
52	b	201	3PE	C34-C35-C36-C37
53	h	201	CDL	C1-CA2-OA2-PA1
47	B	202	PC1	C3E-C3F-C3G-C3H
52	t	805	3PE	O11-C1-C2-O21
47	m	201	PC1	C28-C29-C2A-C2B
46	L	701	FME	C-CA-CB-CG
52	M	504	3PE	C31-C32-C33-C34
52	t	803	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
53	d	204	CDL	C77-C78-C79-C80
47	M	503	PC1	O21-C2-C3-O31
53	v	201	CDL	OA7-CA5-OA6-CA4
47	L	705	PC1	O32-C31-O31-C3
47	I	201	PC1	C21-C22-C23-C24
52	t	803	3PE	C25-C26-C27-C28
53	L	703	CDL	C39-C40-C41-C42
46	L	701	FME	CB-CG-SD-CE
53	d	201	CDL	CA5-C11-C12-C13
53	v	201	CDL	C51-C52-C53-C54
47	h	202	PC1	C2-C3-O31-C31
47	H	403	PC1	O11-C1-C2-C3
52	M	504	3PE	O11-C1-C2-C3
53	h	201	CDL	OB5-CB3-CB4-CB6
52	b	201	3PE	O13-C11-C12-N
53	d	204	CDL	C76-C77-C78-C79
53	L	703	CDL	C35-C36-C37-C38
52	L	702	3PE	C27-C28-C29-C2A
52	L	704	3PE	C38-C39-C3A-C3B
53	d	204	CDL	C11-C12-C13-C14
52	O	401	3PE	C2-C1-O11-P
52	L	702	3PE	C32-C31-O31-C3
53	d	201	CDL	C13-C14-C15-C16
53	h	201	CDL	C53-C54-C55-C56
47	A	202	PC1	C1-C2-C3-O31
47	m	201	PC1	C1-C2-C3-O31
52	M	504	3PE	C1-C2-C3-O31
52	M	505	3PE	C1-C2-C3-O31
52	O	401	3PE	C1-C2-C3-O31
52	t	803	3PE	C1-C2-C3-O31
52	t	804	3PE	C1-C2-C3-O31
52	j	101	3PE	C1-C2-C3-O31
53	O	402	CDL	CB3-CB4-CB6-OB8
53	d	204	CDL	CA3-CA4-CA6-OA8
53	h	201	CDL	CB3-CB4-CB6-OB8
53	v	201	CDL	CA3-CA4-CA6-OA8
52	L	704	3PE	C24-C25-C26-C27
47	h	202	PC1	C22-C23-C24-C25
52	M	502	3PE	C1-O11-P-O13
53	h	201	CDL	C61-C62-C63-C64
47	B	203	PC1	C37-C38-C39-C3A
52	t	803	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
52	b	201	3PE	C28-C29-C2A-C2B
53	d	204	CDL	C36-C37-C38-C39
53	h	201	CDL	C51-C52-C53-C54
52	L	704	3PE	O11-C1-C2-O21
52	t	802	3PE	O11-C1-C2-O21
52	t	803	3PE	O11-C1-C2-O21
53	O	402	CDL	OB5-CB3-CB4-OB6
53	v	201	CDL	C53-C54-C55-C56
47	Z	201	PC1	C38-C39-C3A-C3B
47	A	202	PC1	O21-C2-C3-O31
47	I	201	PC1	O21-C2-C3-O31
47	L	705	PC1	O21-C2-C3-O31
52	t	801	3PE	O21-C2-C3-O31
52	d	202	3PE	O21-C2-C3-O31
52	u	201	3PE	O21-C2-C3-O31
52	M	504	3PE	C33-C34-C35-C36
52	b	201	3PE	C3B-C3C-C3D-C3E
47	I	201	PC1	C3C-C3D-C3E-C3F
52	t	801	3PE	C32-C33-C34-C35
52	t	803	3PE	C2-C1-O11-P
52	t	804	3PE	C2-C1-O11-P
53	d	204	CDL	C1-CB2-OB2-PB2
53	h	201	CDL	C36-C37-C38-C39
52	O	401	3PE	C25-C26-C27-C28
57	P	501	NDP	PN-O3-PA-O5B
47	L	705	PC1	O11-C1-C2-C3
47	M	503	PC1	O11-C1-C2-C3
52	M	502	3PE	O11-C1-C2-C3
52	b	201	3PE	O11-C1-C2-C3
52	d	202	3PE	O11-C1-C2-C3
52	u	201	3PE	O11-C1-C2-C3
47	L	705	PC1	C26-C27-C28-C29
52	m	202	3PE	C2D-C2E-C2F-C2G
53	L	703	CDL	C11-CA5-OA6-CA4
55	O	403	GTP	O4'-C4'-C5'-O5'
53	L	703	CDL	C34-C35-C36-C37
53	L	703	CDL	C71-CB7-OB8-CB6
52	M	505	3PE	C35-C36-C37-C38
52	M	505	3PE	C26-C27-C28-C29
53	d	204	CDL	C42-C43-C44-C45
52	M	504	3PE	C3-C2-O21-C21
52	t	804	3PE	C3-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
53	d	201	CDL	C41-C42-C43-C44
53	O	402	CDL	CA3-CA4-CA6-OA8
53	d	201	CDL	CB3-CB4-CB6-OB8
47	A	202	PC1	C33-C34-C35-C36
52	b	201	3PE	C32-C33-C34-C35
47	H	403	PC1	O11-C1-C2-O21
47	M	503	PC1	O11-C1-C2-O21
47	Z	201	PC1	O11-C1-C2-O21
52	L	702	3PE	O11-C1-C2-O21
52	M	502	3PE	O11-C1-C2-O21
52	t	804	3PE	O11-C1-C2-O21
52	u	201	3PE	O11-C1-C2-O21
47	h	202	PC1	C28-C29-C2A-C2B
52	L	702	3PE	C39-C3A-C3B-C3C
53	O	402	CDL	C31-C32-C33-C34
53	L	703	CDL	OA7-CA5-OA6-CA4
52	L	702	3PE	O32-C31-O31-C3
52	m	202	3PE	C27-C28-C29-C2A
52	b	201	3PE	C33-C34-C35-C36
52	H	402	3PE	O21-C2-C3-O31
52	M	505	3PE	O21-C2-C3-O31
52	O	401	3PE	O21-C2-C3-O31
52	t	804	3PE	O21-C2-C3-O31
52	j	101	3PE	O21-C2-C3-O31
53	v	201	CDL	OA6-CA4-CA6-OA8
47	Z	201	PC1	C11-C12-N-C14
47	Z	201	PC1	C11-C12-N-C15
52	L	702	3PE	C23-C24-C25-C26
55	O	403	GTP	C3'-C4'-C5'-O5'
47	M	503	PC1	C21-C22-C23-C24
47	I	201	PC1	C28-C29-C2A-C2B
52	d	202	3PE	C3B-C3C-C3D-C3E
47	B	202	PC1	C23-C24-C25-C26
52	d	202	3PE	C36-C37-C38-C39
53	L	703	CDL	C63-C64-C65-C66
52	u	201	3PE	C33-C34-C35-C36
47	B	202	PC1	C27-C28-C29-C2A
53	L	703	CDL	C59-C60-C61-C62
47	m	201	PC1	C32-C31-O31-C3
53	h	201	CDL	C72-C73-C74-C75
52	d	202	3PE	C11-O13-P-O11
52	u	201	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
53	v	201	CDL	C73-C74-C75-C76
57	P	501	NDP	C2D-C1D-N1N-C6N
47	B	203	PC1	C2-C1-O11-P
52	L	702	3PE	C25-C26-C27-C28
47	A	202	PC1	C1-O11-P-O12
47	H	403	PC1	C11-O13-P-O14
47	Z	201	PC1	C11-O13-P-O12
47	Z	201	PC1	C11-C12-N-C13
47	d	203	PC1	C1-O11-P-O12
47	h	202	PC1	C11-O13-P-O14
47	m	201	PC1	C11-O13-P-O12
52	M	502	3PE	C1-O11-P-O14
52	M	505	3PE	C11-O13-P-O14
52	O	401	3PE	C1-O11-P-O14
52	t	801	3PE	C1-O11-P-O12
52	t	801	3PE	C11-O13-P-O12
52	t	802	3PE	C1-O11-P-O14
52	t	802	3PE	C11-O13-P-O12
52	t	803	3PE	C1-O11-P-O12
52	t	805	3PE	C11-O13-P-O14
52	b	201	3PE	C11-O13-P-O14
53	O	402	CDL	CB2-OB2-PB2-OB3
53	d	201	CDL	CB3-OB5-PB2-OB3
53	d	201	CDL	CB3-OB5-PB2-OB4
53	d	204	CDL	CB2-OB2-PB2-OB3
53	h	201	CDL	CB2-OB2-PB2-OB3
53	v	201	CDL	CB2-OB2-PB2-OB3
57	P	501	NDP	C5B-O5B-PA-O2A
57	P	501	NDP	C5D-O5D-PN-O1N
52	t	804	3PE	C21-C22-C23-C24
47	B	202	PC1	C32-C31-O31-C3
52	t	803	3PE	O11-C1-C2-C3
53	d	204	CDL	OA5-CA3-CA4-CA6
47	L	705	PC1	C2D-C2E-C2F-C2G
47	B	202	PC1	C39-C3A-C3B-C3C
53	L	703	CDL	OB9-CB7-OB8-CB6
47	B	202	PC1	C12-C11-O13-P
47	I	201	PC1	C12-C11-O13-P
52	M	505	3PE	C12-C11-O13-P
52	t	805	3PE	C12-C11-O13-P
52	b	201	3PE	C12-C11-O13-P
47	M	503	PC1	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
53	h	201	CDL	C56-C57-C58-C59
47	L	705	PC1	O11-C1-C2-O21
52	M	504	3PE	O11-C1-C2-O21
52	d	202	3PE	O11-C1-C2-O21
53	O	402	CDL	OA5-CA3-CA4-OA6
53	d	204	CDL	OA5-CA3-CA4-OA6
52	H	402	3PE	C22-C23-C24-C25
52	M	502	3PE	C38-C39-C3A-C3B
52	O	401	3PE	C2F-C2G-C2H-C2I
52	t	802	3PE	C34-C35-C36-C37
52	b	201	3PE	C22-C21-O21-C2
53	d	204	CDL	C72-C73-C74-C75
47	B	202	PC1	C11-C12-N-C15
47	L	705	PC1	C11-C12-N-C14
47	L	705	PC1	C11-C12-N-C15
47	M	503	PC1	C11-C12-N-C15
47	m	201	PC1	C11-C12-N-C13
52	d	202	3PE	C2A-C2B-C2C-C2D
47	A	202	PC1	O13-C11-C12-N
47	B	203	PC1	O13-C11-C12-N
47	I	201	PC1	O13-C11-C12-N
47	L	705	PC1	C1-C2-C3-O31
52	t	805	3PE	C1-C2-C3-O31
52	M	504	3PE	O21-C2-C3-O31
52	t	805	3PE	O21-C2-C3-O31
53	O	402	CDL	OA6-CA4-CA6-OA8
53	O	402	CDL	OB6-CB4-CB6-OB8
53	d	204	CDL	OA6-CA4-CA6-OA8
53	h	201	CDL	OA6-CA4-CA6-OA8
53	h	201	CDL	OB6-CB4-CB6-OB8
53	v	201	CDL	C14-C15-C16-C17
47	m	201	PC1	C29-C2A-C2B-C2C
47	B	202	PC1	C2-C1-O11-P
53	v	201	CDL	C18-C19-C20-C21
47	m	201	PC1	O32-C31-O31-C3
52	b	201	3PE	C39-C3A-C3B-C3C
52	L	702	3PE	C36-C37-C38-C39
53	d	201	CDL	C12-C13-C14-C15
47	B	202	PC1	O32-C31-O31-C3
57	P	501	NDP	O4D-C1D-N1N-C6N
52	H	402	3PE	C23-C24-C25-C26
52	M	505	3PE	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
52	j	101	3PE	C25-C26-C27-C28
52	M	504	3PE	C3B-C3C-C3D-C3E
47	B	203	PC1	C2A-C2B-C2C-C2D
52	t	804	3PE	C37-C38-C39-C3A
52	b	201	3PE	C2B-C2C-C2D-C2E
52	u	201	3PE	C35-C36-C37-C38
53	h	201	CDL	C39-C40-C41-C42
52	t	801	3PE	C3-C2-O21-C21
52	t	803	3PE	C3-C2-O21-C21
52	t	805	3PE	C3-C2-O21-C21
53	d	201	CDL	CB6-CB4-OB6-CB5
52	t	805	3PE	O11-C1-C2-C3
53	O	402	CDL	OA5-CA3-CA4-CA6
52	b	201	3PE	O22-C21-O21-C2
53	L	703	CDL	C52-C53-C54-C55
52	b	201	3PE	C31-C32-C33-C34
52	t	802	3PE	C22-C21-O21-C2
46	H	401	FME	CA-CB-CG-SD
52	M	504	3PE	C2-C1-O11-P
52	b	201	3PE	O11-C1-C2-O21
47	M	503	PC1	C11-C12-N-C14
52	t	802	3PE	O22-C21-O21-C2
46	H	401	FME	C-CA-CB-CG
46	M	501	FME	C-CA-CB-CG
52	K	102	3PE	C3B-C3C-C3D-C3E
52	M	504	3PE	C39-C3A-C3B-C3C
47	h	202	PC1	O21-C2-C3-O31
52	t	803	3PE	O21-C2-C3-O31
53	d	201	CDL	OB6-CB4-CB6-OB8
52	M	504	3PE	C3F-C3G-C3H-C3I
47	M	503	PC1	C1-O11-P-O13
52	L	704	3PE	C1-O11-P-O13
52	L	704	3PE	C11-O13-P-O11
52	M	504	3PE	C11-O13-P-O11
52	t	805	3PE	C1-O11-P-O13
53	d	204	CDL	C73-C74-C75-C76
47	I	201	PC1	C2C-C2D-C2E-C2F
52	L	702	3PE	C1-C2-C3-O31
52	K	102	3PE	C26-C27-C28-C29
52	m	202	3PE	C32-C33-C34-C35
47	B	203	PC1	C24-C25-C26-C27
47	m	201	PC1	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
52	b	201	3PE	C35-C36-C37-C38
53	O	402	CDL	C16-C17-C18-C19
52	M	505	3PE	C24-C25-C26-C27
52	t	805	3PE	O13-C11-C12-N
52	K	102	3PE	O11-C1-C2-O21
47	B	203	PC1	C38-C39-C3A-C3B
52	m	202	3PE	C2E-C2F-C2G-C2H
53	h	201	CDL	C54-C55-C56-C57
52	L	704	3PE	C39-C3A-C3B-C3C
53	O	402	CDL	C36-C37-C38-C39
53	v	201	CDL	OB6-CB4-CB6-OB8
52	b	201	3PE	C23-C24-C25-C26
53	d	201	CDL	C72-C71-CB7-OB9
47	B	203	PC1	C26-C27-C28-C29
47	B	203	PC1	C27-C28-C29-C2A
53	L	703	CDL	C13-C14-C15-C16
52	M	505	3PE	C3B-C3C-C3D-C3E
53	L	703	CDL	C38-C39-C40-C41
53	L	703	CDL	C37-C38-C39-C40
54	L	706	CHD	C20-C22-C23-C24
52	u	201	3PE	C3B-C3C-C3D-C3E
54	L	706	CHD	C22-C23-C24-O25
53	v	201	CDL	C19-C20-C21-C22
47	B	202	PC1	C11-C12-N-C14
47	L	705	PC1	C11-C12-N-C13
47	M	503	PC1	C11-C12-N-C13
47	I	201	PC1	C23-C24-C25-C26
47	I	201	PC1	C11-O13-P-O11
57	P	501	NDP	C2D-C1D-N1N-C2N
53	d	201	CDL	CA4-CA3-OA5-PA1
47	B	202	PC1	C3B-C3C-C3D-C3E
52	t	803	3PE	C32-C33-C34-C35
52	t	804	3PE	C34-C35-C36-C37
46	L	701	FME	N-CA-CB-CG
52	M	505	3PE	C3E-C3F-C3G-C3H
52	M	505	3PE	C28-C29-C2A-C2B
52	u	201	3PE	C39-C3A-C3B-C3C
53	h	201	CDL	C76-C77-C78-C79
47	B	202	PC1	C37-C38-C39-C3A
47	m	201	PC1	C34-C35-C36-C37
47	B	203	PC1	O21-C2-C3-O31
47	L	705	PC1	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
47	m	201	PC1	C31-C32-C33-C34
54	L	706	CHD	C22-C23-C24-O26
52	L	704	3PE	C3D-C3E-C3F-C3G
47	m	201	PC1	C11-C12-N-C14
52	u	201	3PE	C32-C31-O31-C3
52	u	201	3PE	O32-C31-O31-C3
53	L	703	CDL	OB5-CB3-CB4-CB6
53	d	201	CDL	C72-C71-CB7-OB8
47	Z	201	PC1	O21-C2-C3-O31
47	Z	201	PC1	C37-C38-C39-C3A
52	M	504	3PE	C35-C36-C37-C38
52	O	401	3PE	C2C-C2D-C2E-C2F
52	H	402	3PE	C27-C28-C29-C2A
47	B	202	PC1	C11-C12-N-C13
47	M	503	PC1	C33-C34-C35-C36
52	L	704	3PE	C28-C29-C2A-C2B
53	d	204	CDL	O1-C1-CA2-OA2
52	t	805	3PE	C1-C2-O21-C21
53	d	201	CDL	CB3-CB4-OB6-CB5
47	I	201	PC1	C31-C32-C33-C34
52	M	502	3PE	C3A-C3B-C3C-C3D
47	A	202	PC1	C35-C36-C37-C38
57	P	501	NDP	O4D-C1D-N1N-C2N
52	L	702	3PE	C21-C22-C23-C24
52	M	505	3PE	O21-C21-C22-C23
47	B	202	PC1	O11-C1-C2-O21
53	L	703	CDL	OB5-CB3-CB4-OB6
47	H	403	PC1	O21-C21-C22-C23
52	O	401	3PE	O31-C31-C32-C33
47	h	202	PC1	C27-C28-C29-C2A
52	d	202	3PE	C3D-C3E-C3F-C3G
46	M	501	FME	N-CA-CB-CG
52	b	201	3PE	C3A-C3B-C3C-C3D
53	v	201	CDL	OB7-CB5-OB6-CB4
47	A	202	PC1	O21-C21-C22-C23
47	M	503	PC1	O31-C31-C32-C33
52	M	505	3PE	O31-C31-C32-C33
53	v	201	CDL	C72-C71-CB7-OB8
52	L	704	3PE	C2A-C2B-C2C-C2D
47	H	403	PC1	O21-C2-C3-O31
53	L	703	CDL	OB6-CB4-CB6-OB8
47	d	203	PC1	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
47	m	201	PC1	O31-C31-C32-C33
47	m	201	PC1	C11-C12-N-C15
52	t	802	3PE	C2A-C2B-C2C-C2D
53	L	703	CDL	C32-C31-CA7-OA8
53	v	201	CDL	C52-C51-CB5-OB6
52	t	803	3PE	O21-C21-C22-C23
55	O	403	GTP	PB-O3A-PA-O2A
47	B	203	PC1	C23-C24-C25-C26
52	O	401	3PE	O32-C31-C32-C33
47	H	403	PC1	O22-C21-C22-C23
53	d	204	CDL	CB3-CB4-CB6-OB8
53	h	201	CDL	C33-C34-C35-C36
52	L	704	3PE	C27-C28-C29-C2A
52	M	505	3PE	O22-C21-C22-C23
53	v	201	CDL	C52-C51-CB5-OB7
52	M	505	3PE	C22-C23-C24-C25
47	I	201	PC1	C11-O13-P-O14
47	M	503	PC1	C1-O11-P-O14
47	d	203	PC1	C11-O13-P-O14
52	L	702	3PE	C1-O11-P-O14
52	L	702	3PE	C11-O13-P-O12
52	L	704	3PE	C1-O11-P-O12
52	L	704	3PE	C11-O13-P-O14
53	L	703	CDL	CB3-OB5-PB2-OB3
55	O	403	GTP	C5'-O5'-PA-O1A
47	L	705	PC1	C31-C32-C33-C34
52	L	702	3PE	C2C-C2D-C2E-C2F
47	A	202	PC1	O22-C21-C22-C23
53	O	402	CDL	OB5-CB3-CB4-CB6
52	u	201	3PE	C38-C39-C3A-C3B
52	t	803	3PE	O22-C21-C22-C23
46	A	201	FME	CB-CA-N-CN
52	t	802	3PE	C12-C11-O13-P
53	L	703	CDL	C32-C31-CA7-OA9
47	d	203	PC1	O22-C21-C22-C23
52	M	504	3PE	O31-C31-C32-C33
47	H	403	PC1	C2B-C2C-C2D-C2E
52	u	201	3PE	C27-C28-C29-C2A
53	d	201	CDL	C52-C51-CB5-OB6
53	h	201	CDL	C72-C71-CB7-OB8
50	F	501	FMN	N10-C1'-C2'-O2'
52	O	401	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
47	m	201	PC1	O32-C31-C32-C33
52	M	502	3PE	C2B-C2C-C2D-C2E
52	t	805	3PE	C21-C22-C23-C24
52	L	702	3PE	C26-C27-C28-C29
52	L	704	3PE	C37-C38-C39-C3A
52	b	201	3PE	C27-C28-C29-C2A
52	j	101	3PE	C2F-C2G-C2H-C2I
47	M	503	PC1	O32-C31-C32-C33
52	M	505	3PE	O32-C31-C32-C33
53	v	201	CDL	C72-C71-CB7-OB9
47	B	202	PC1	C34-C35-C36-C37
53	L	703	CDL	C12-C11-CA5-OA6
52	t	804	3PE	C32-C33-C34-C35

There are no ring outliers.

31 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	j	101	3PE	1	0
53	L	703	CDL	4	0
52	u	201	3PE	1	0
47	h	202	PC1	1	0
46	A	201	FME	2	0
47	H	403	PC1	3	0
47	M	503	PC1	1	0
47	I	201	PC1	2	0
52	M	502	3PE	1	0
46	N	401	FME	1	0
54	L	706	CHD	2	0
48	F	502	SF4	2	0
52	L	704	3PE	1	0
52	O	401	3PE	1	0
55	O	403	GTP	1	0
52	d	202	3PE	1	0
52	m	202	3PE	1	0
52	b	201	3PE	2	0
53	h	201	CDL	2	0
47	d	203	PC1	2	0
53	d	204	CDL	2	0
52	M	505	3PE	1	0
52	M	504	3PE	4	0
53	v	201	CDL	2	0

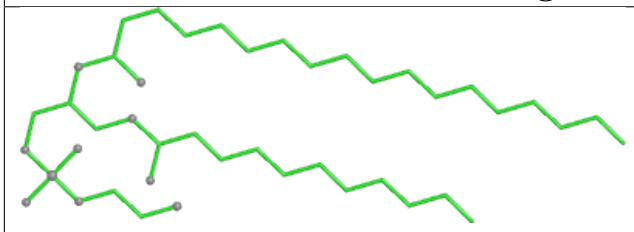
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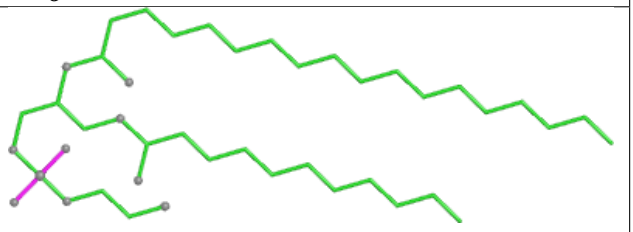
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	t	804	3PE	1	0
53	O	402	CDL	5	0
47	B	202	PC1	4	0
53	d	201	CDL	8	0
46	H	401	FME	1	0
50	F	501	FMN	2	0
46	L	701	FME	1	0

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.

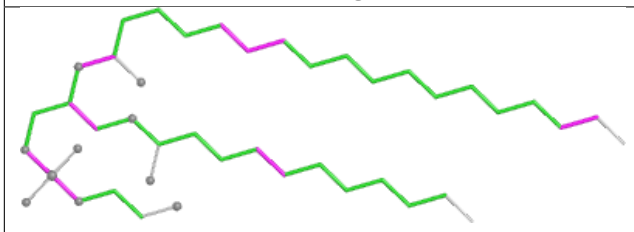
Ligand 3PE j 101



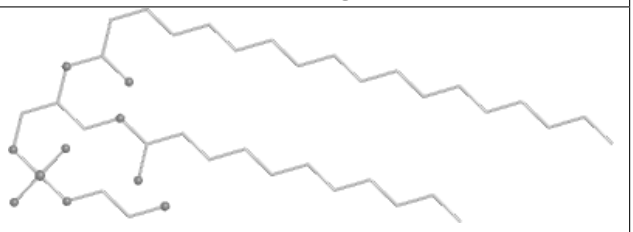
Bond lengths



Bond angles

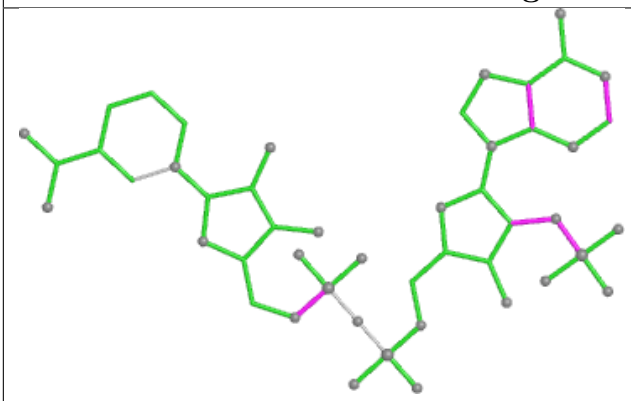


Torsions

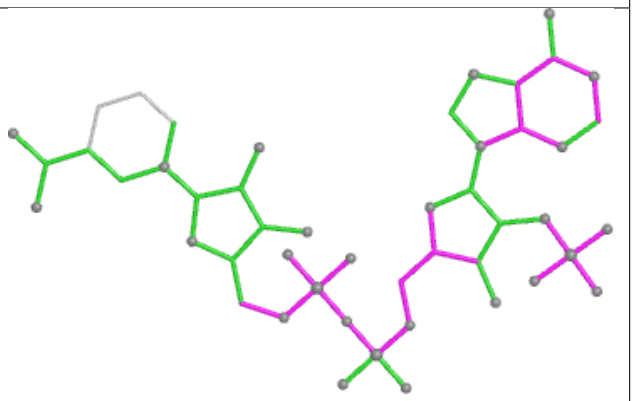


Rings

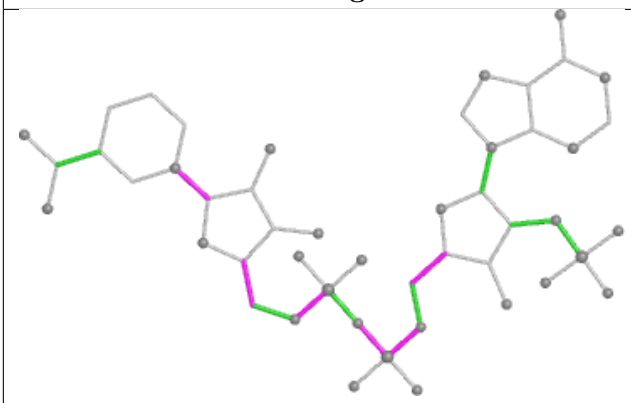
Ligand NDP P 501



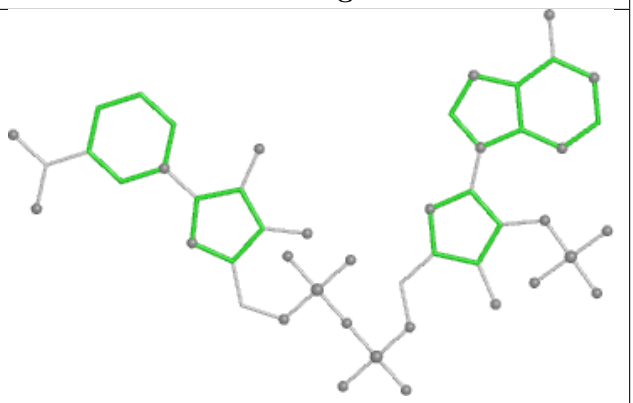
Bond lengths



Bond angles

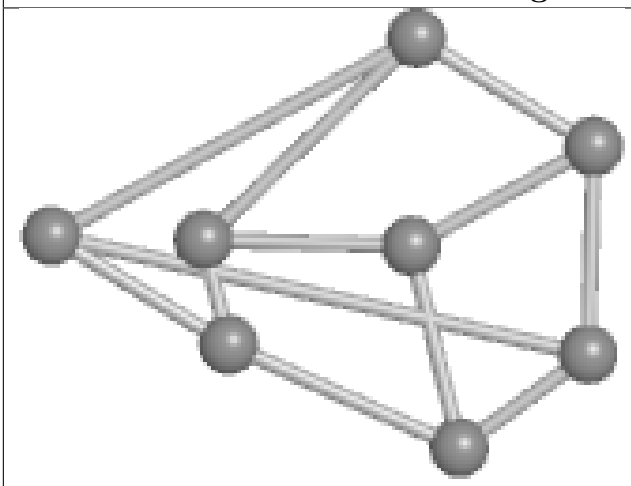


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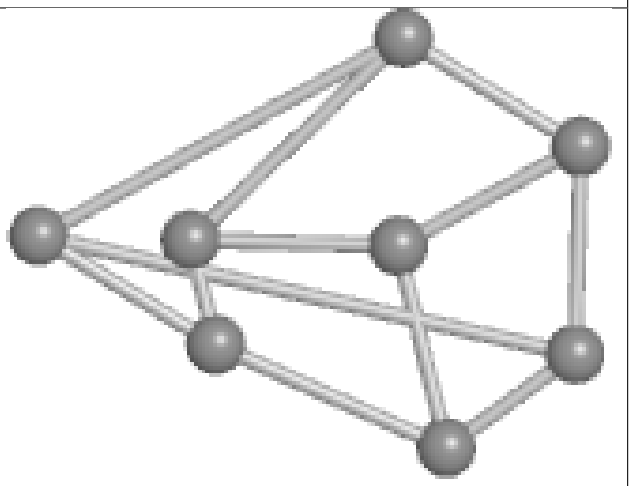


Rings

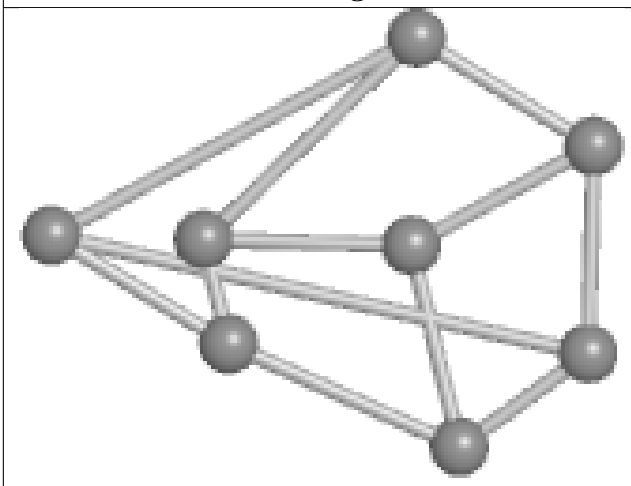
Ligand SF4 G 802



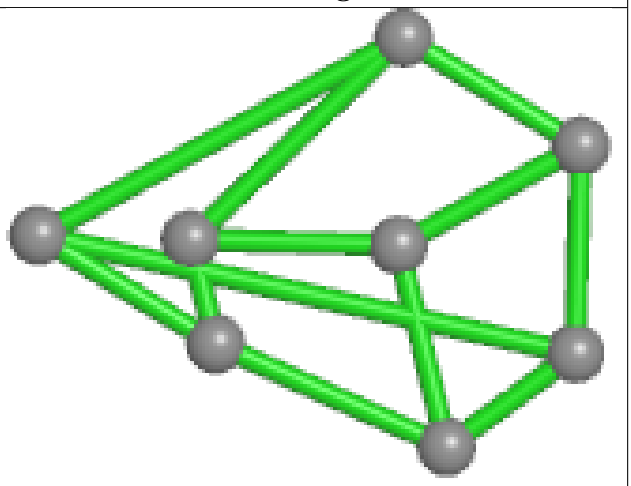
Bond lengths



Bond angles

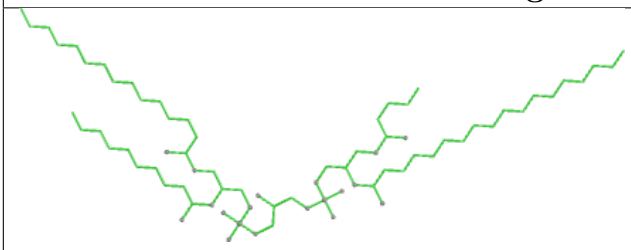


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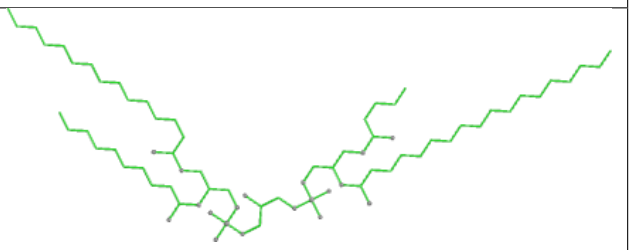


Rings

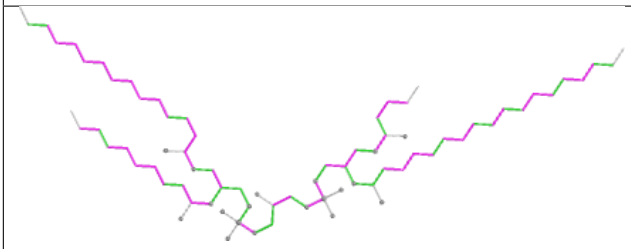
Ligand CDL L 703



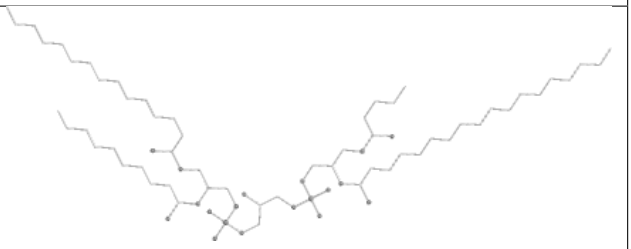
Bond lengths



Bond angles

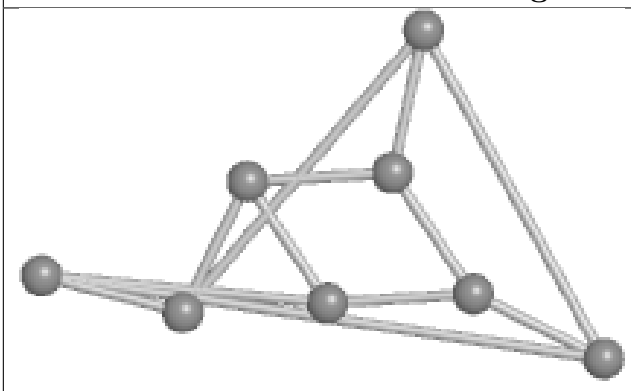


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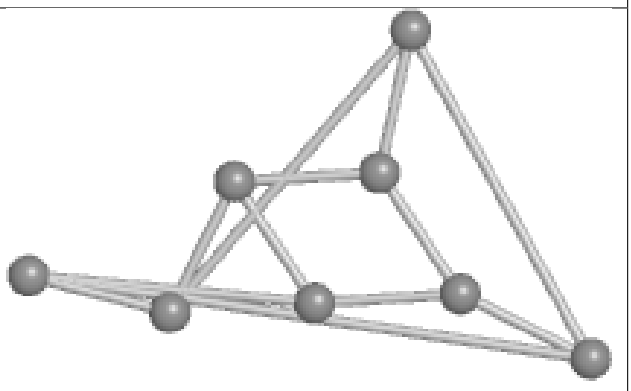


Rings

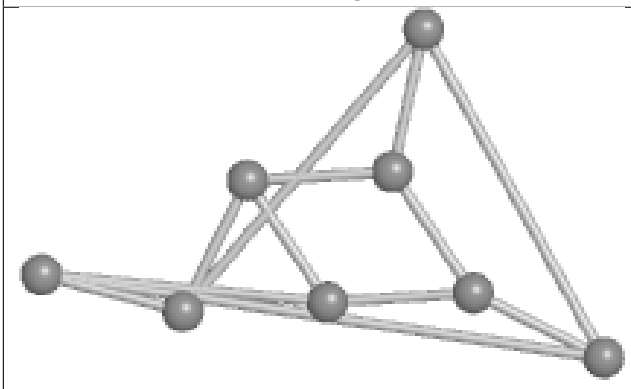
Ligand SF4 G 801



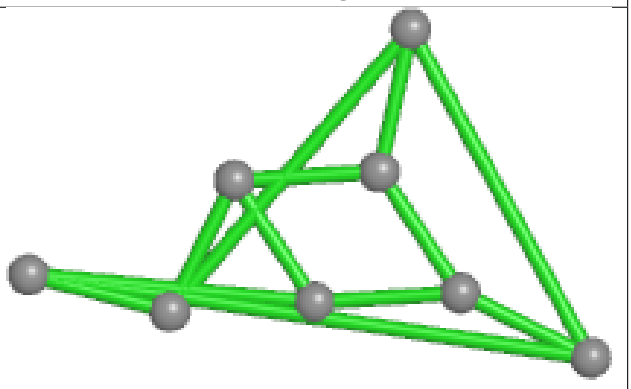
Bond lengths



Bond angles

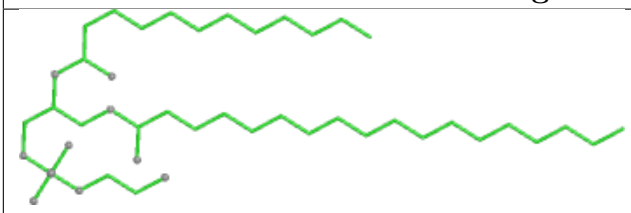


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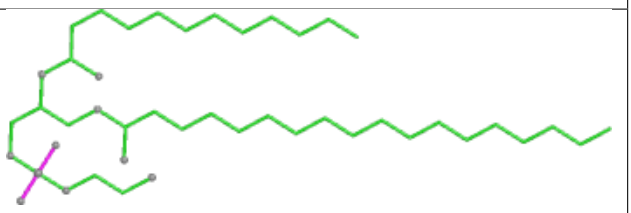


Rings

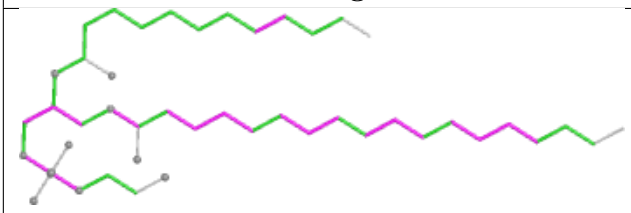
Ligand 3PE u 201



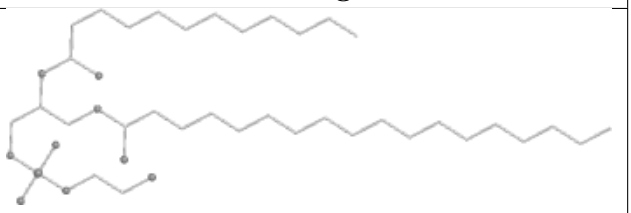
Bond lengths



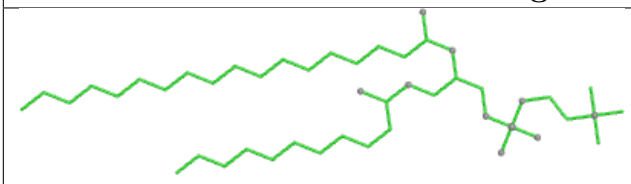
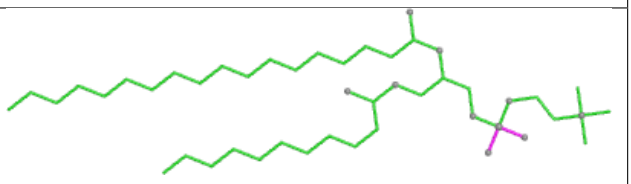
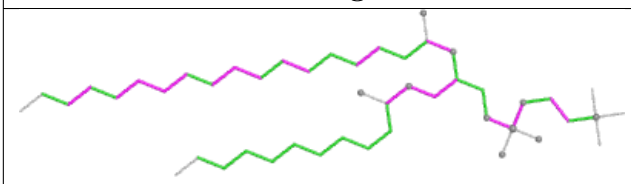
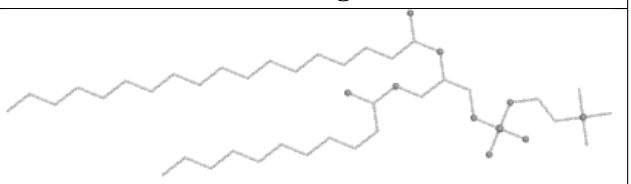
Bond angles

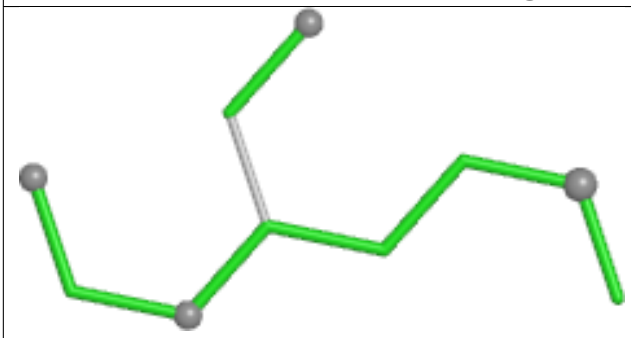
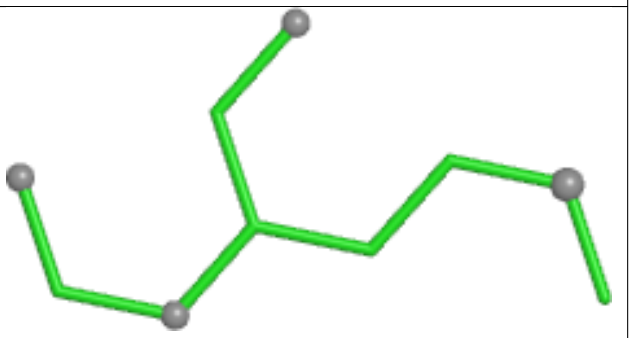
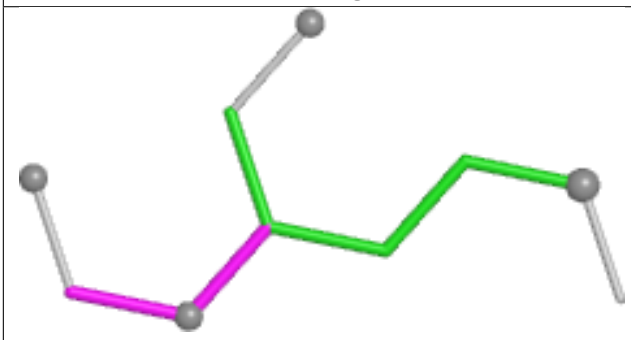
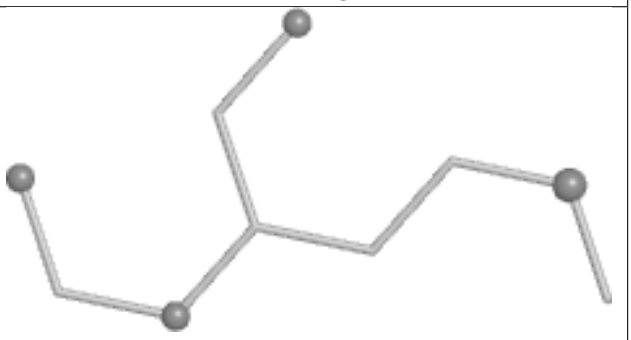


Torsions

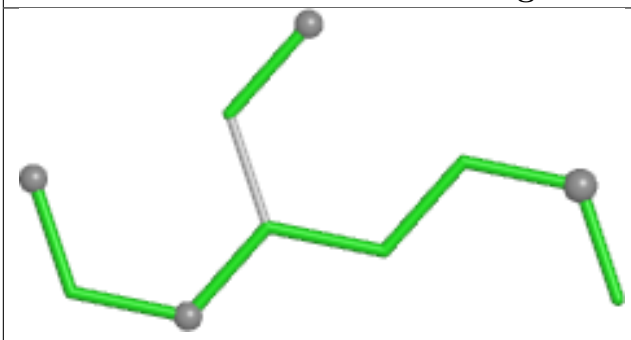


Rings

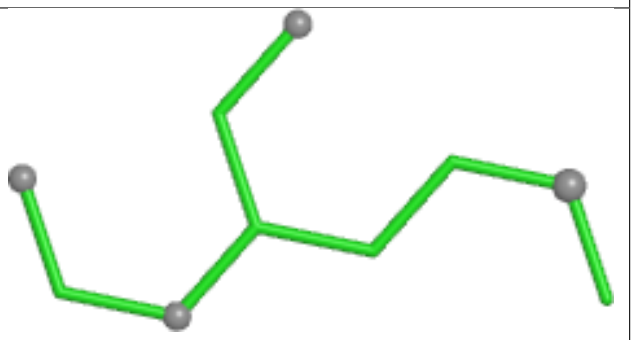
Ligand PC1 h 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FME A 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

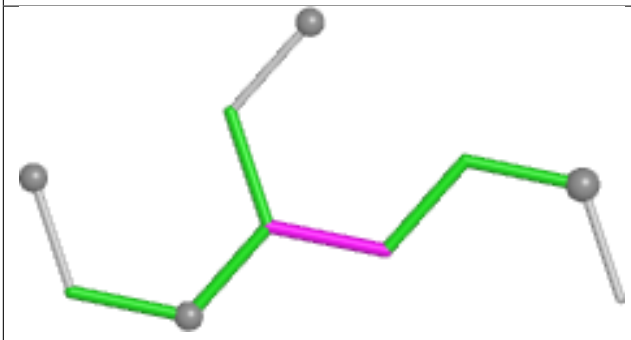
Ligand FME M 501



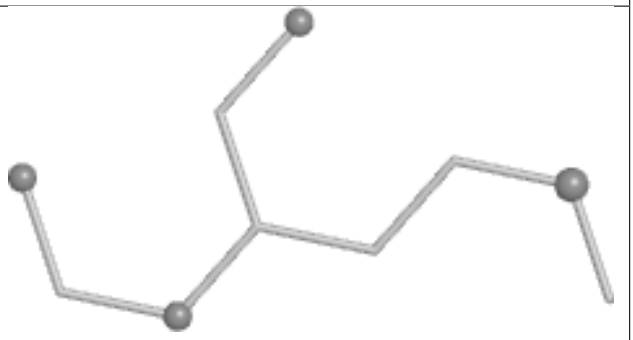
Bond lengths



Bond angles

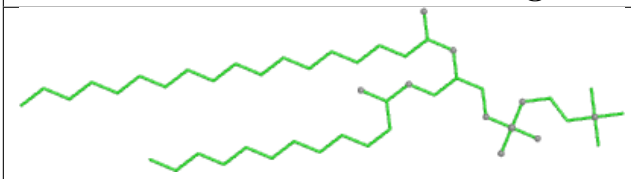


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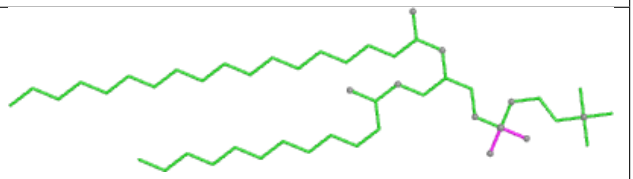


Rings

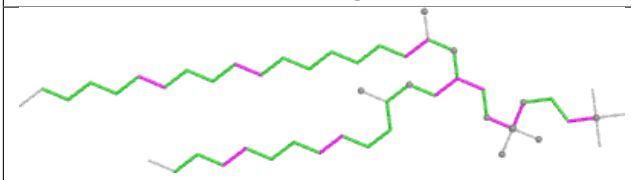
Ligand PC1 H 403



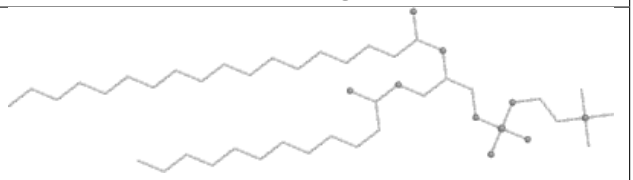
Bond lengths



Bond angles

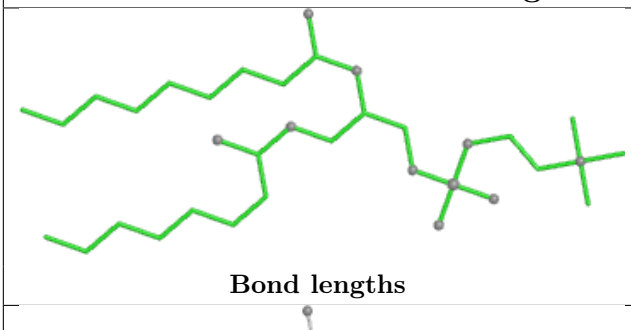


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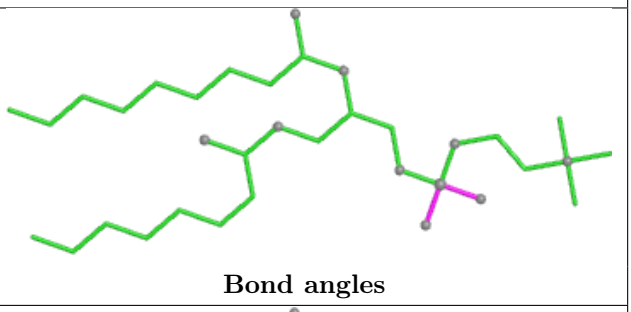


Rings

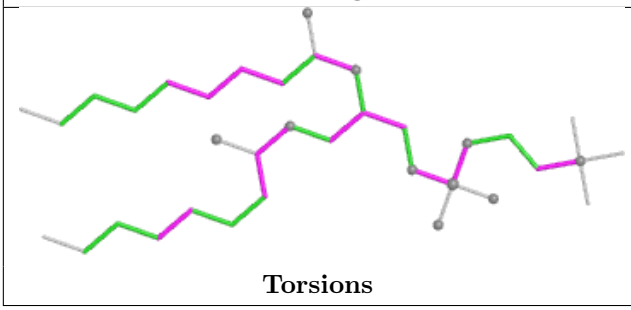
Ligand PC1 M 503



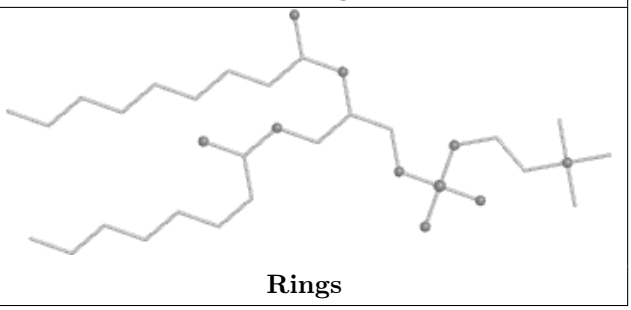
Bond lengths



Bond angles

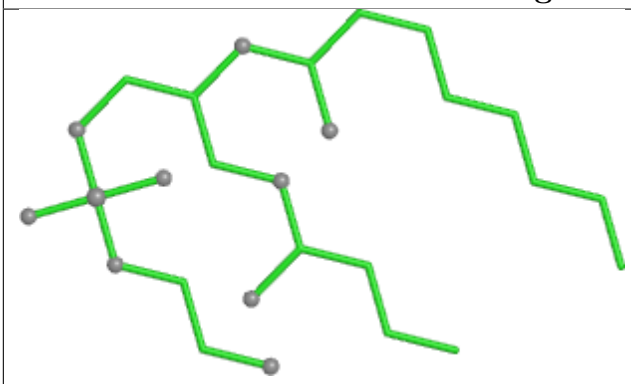


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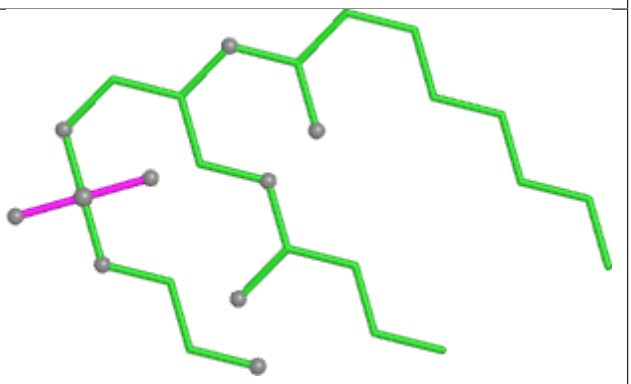


Rings

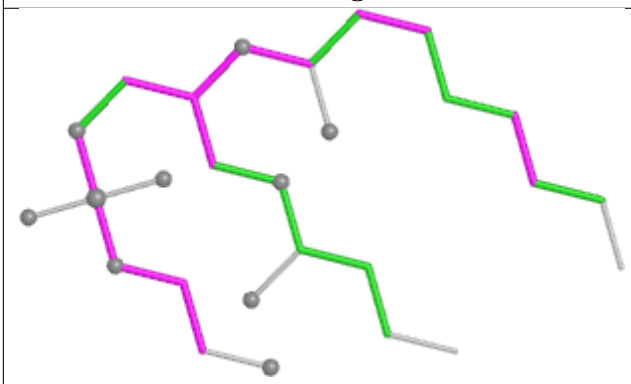
Ligand 3PE t 805



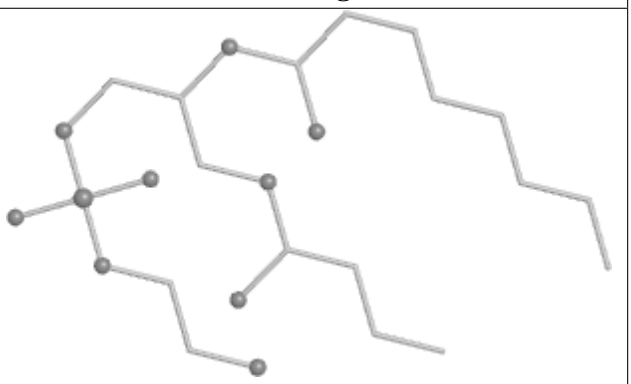
Bond lengths



Bond angles

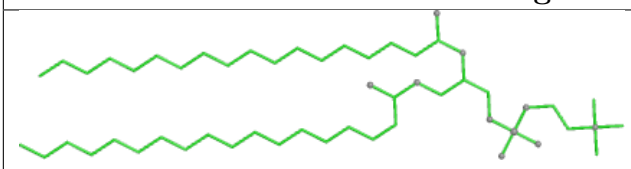


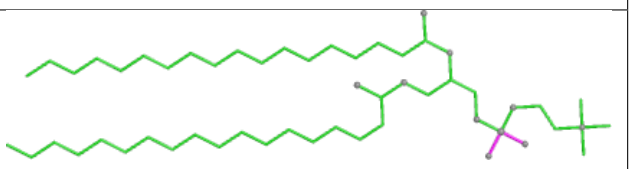
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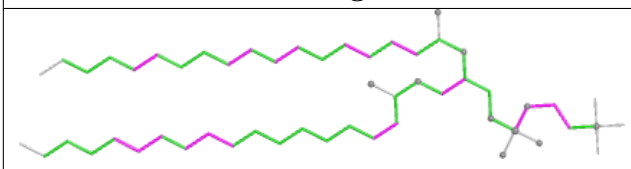


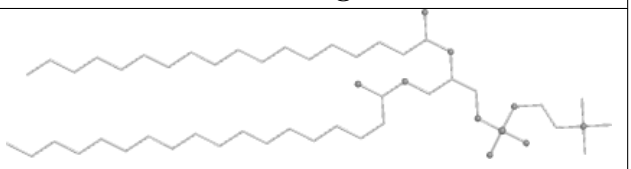
Rings

Ligand PC1 I 201

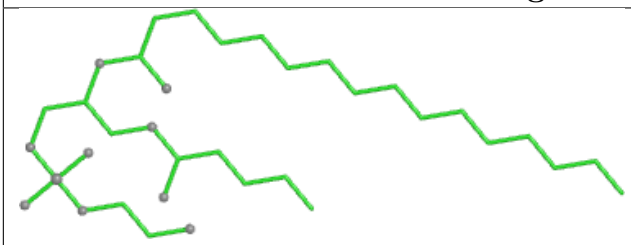

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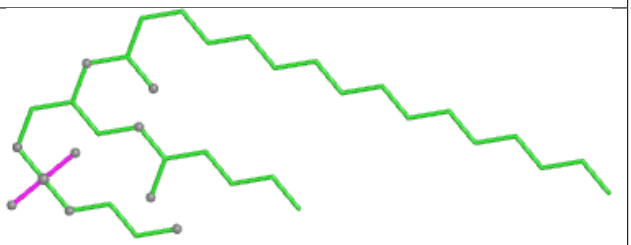

Bond angles

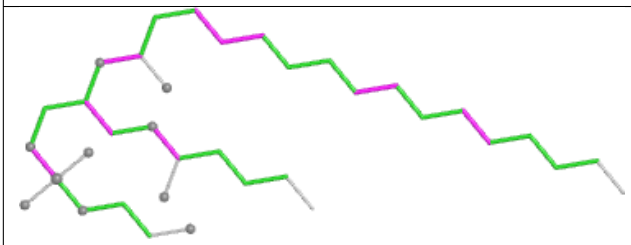

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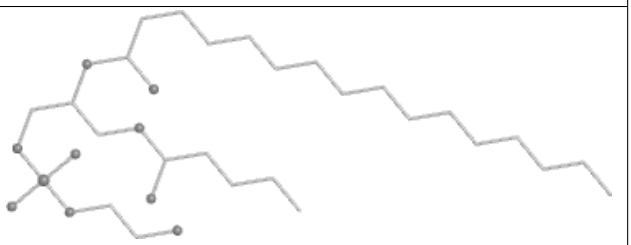

Rings

Ligand 3PE H 402

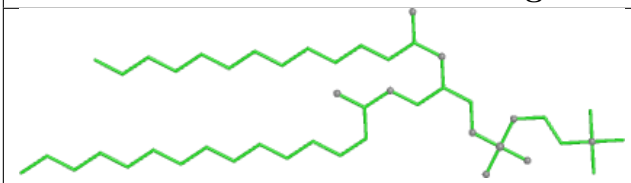

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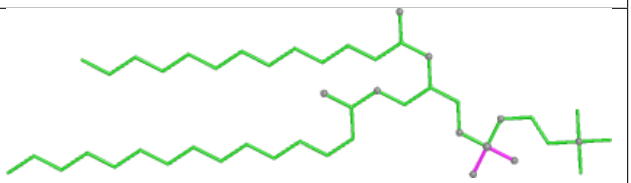

Bond angles

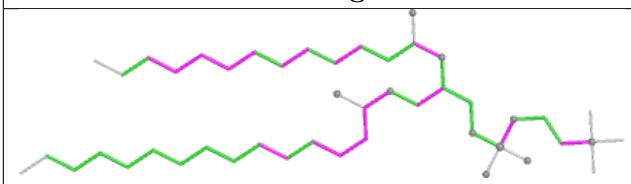

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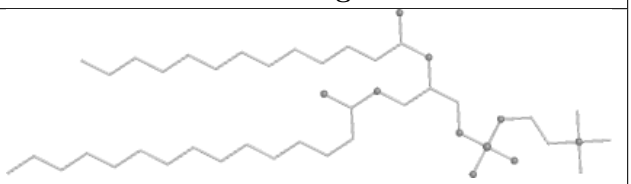

Rings

Ligand PC1 m 201

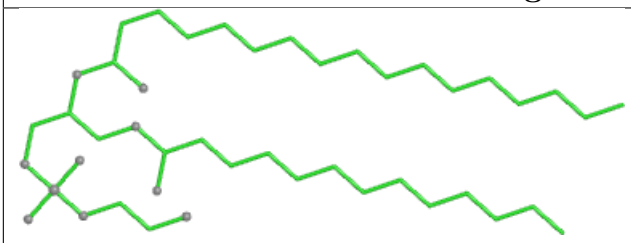

Bond lengths


Bond angles

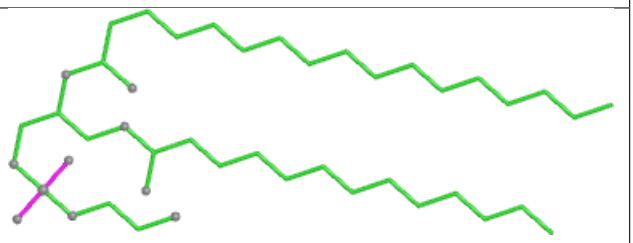

Torsions


Rings

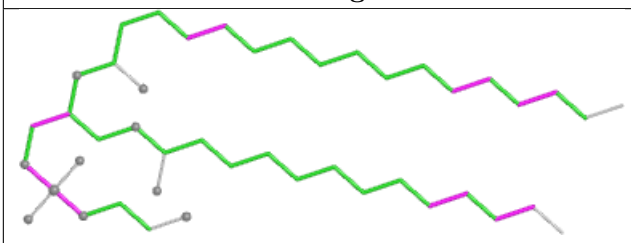
Ligand 3PE M 502



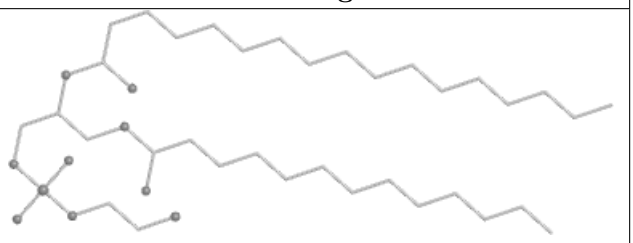
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Bond angles

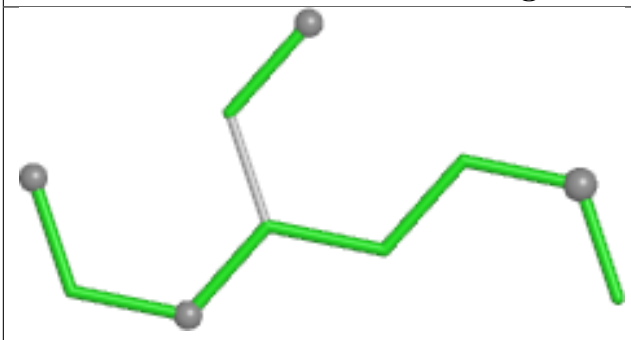


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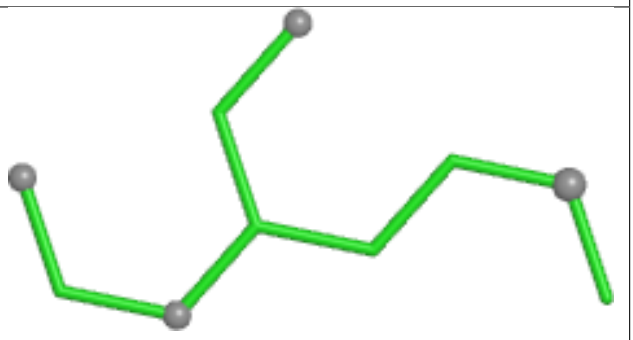


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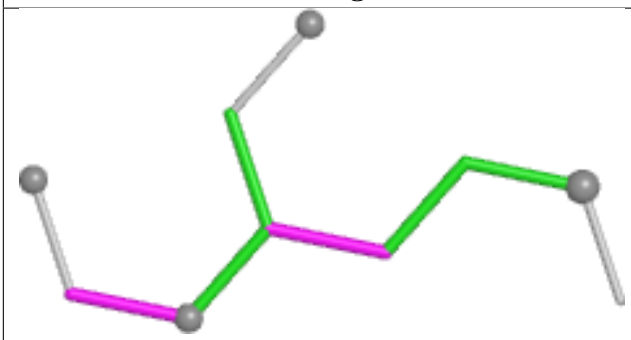
Ligand FME N 401



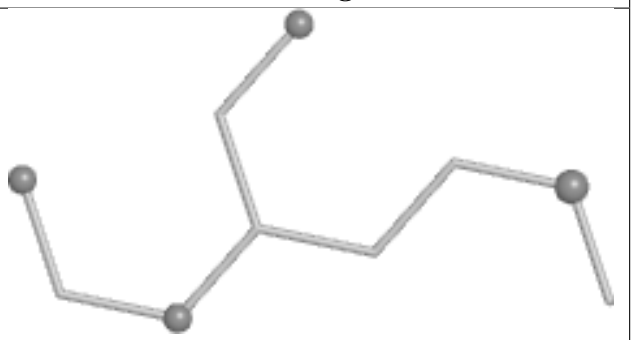
Bond lengths



Bond angles

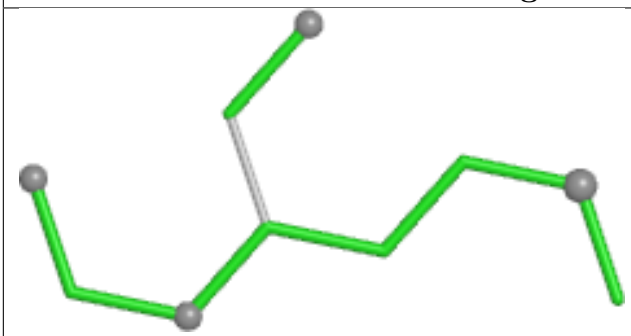


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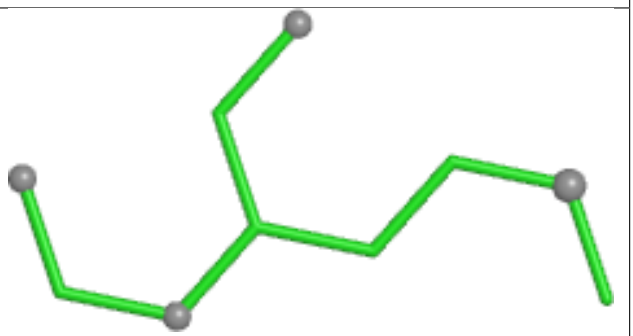


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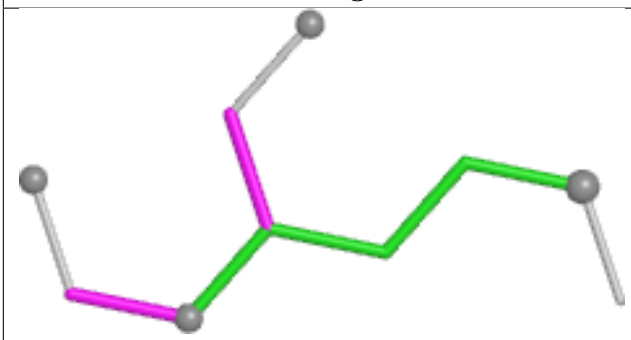
Ligand FME K 101



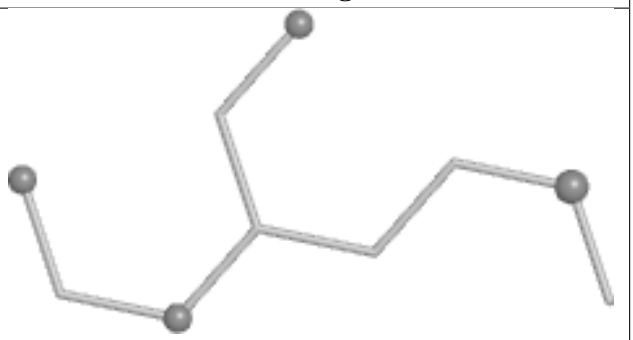
Bond lengths



Bond angles

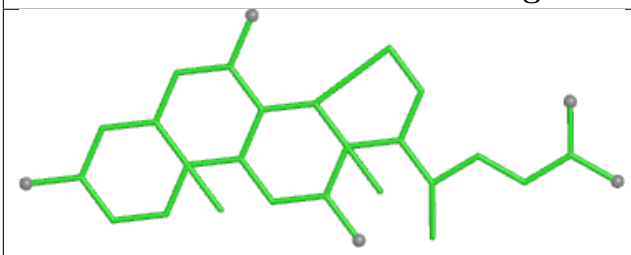


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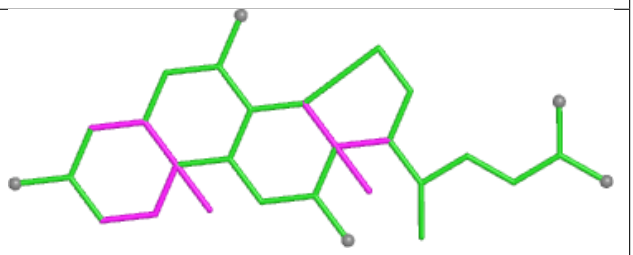


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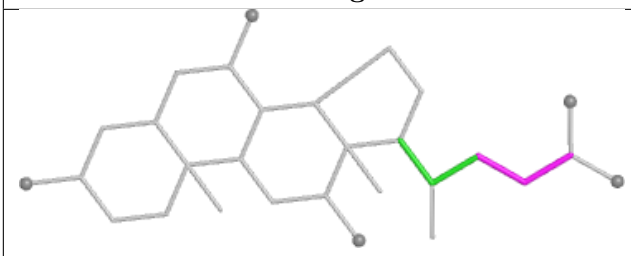
Ligand CHD L 706



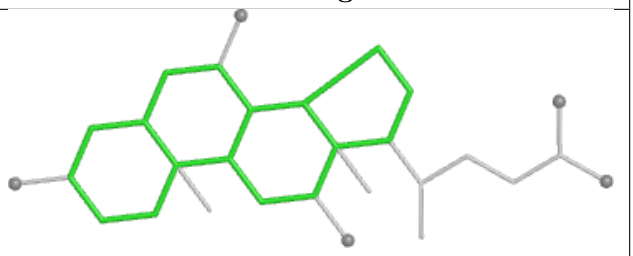
Bond lengths



Bond angles

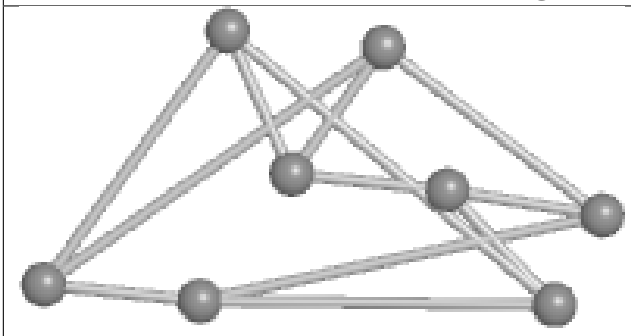


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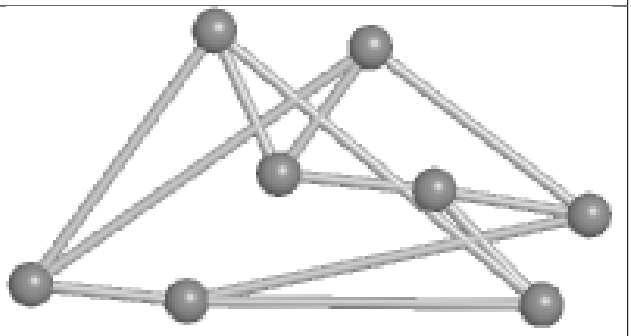


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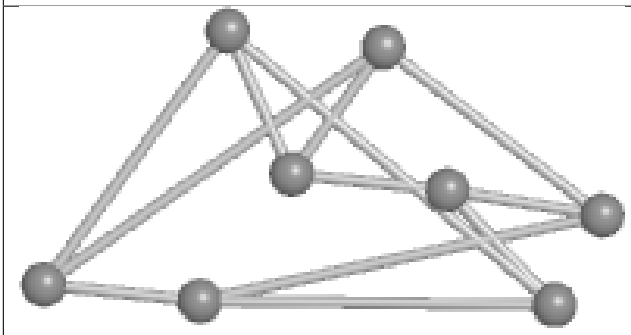
Ligand SF4 F 502



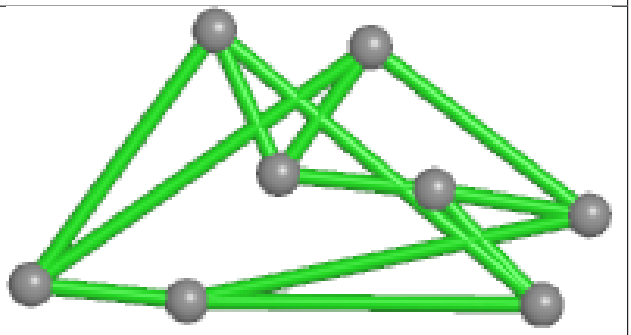
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Bond angles

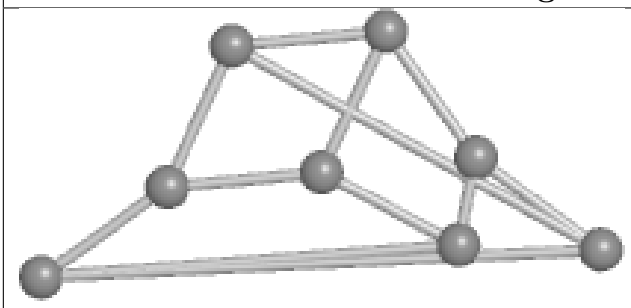


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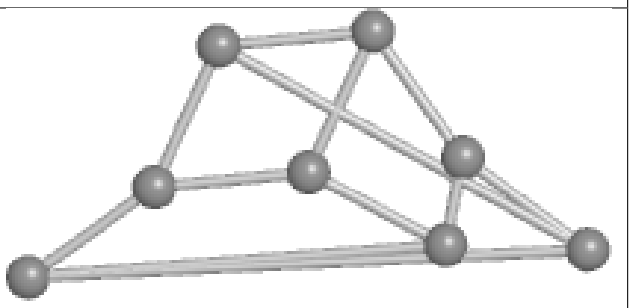


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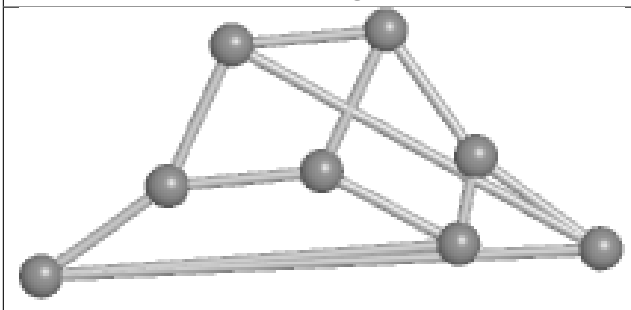
Ligand SF4 I 203



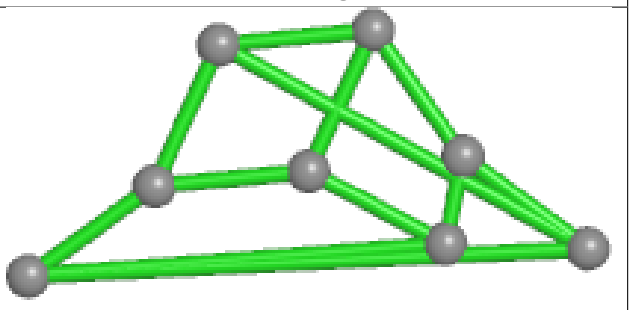
Bond lengths



Bond angles

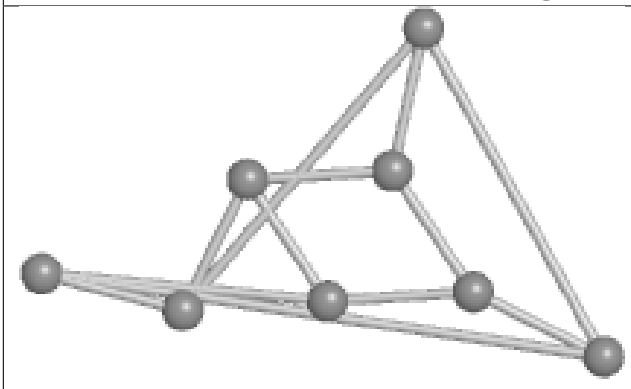


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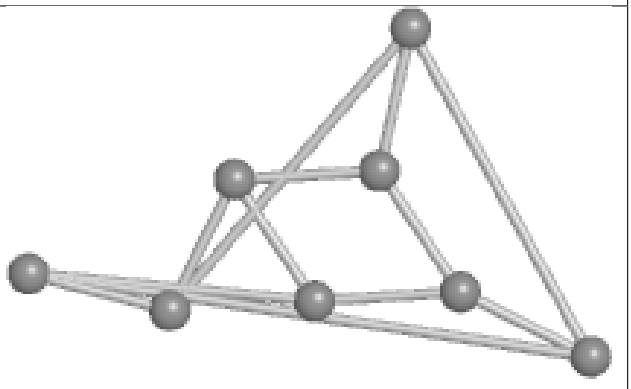


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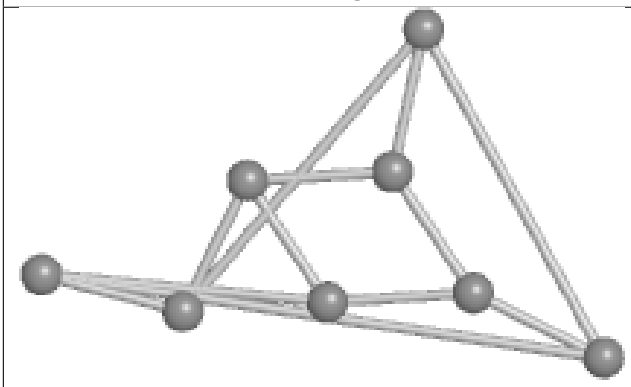
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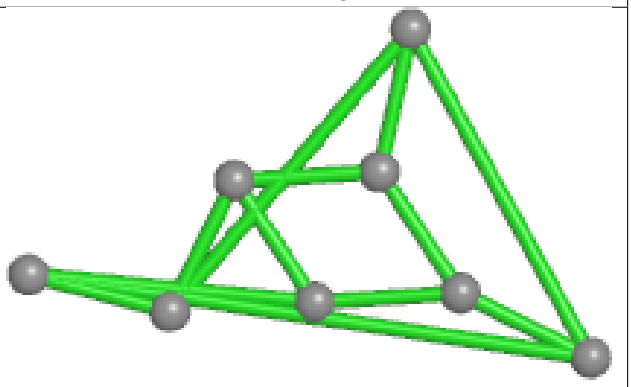
Bond lengths



Bond angles

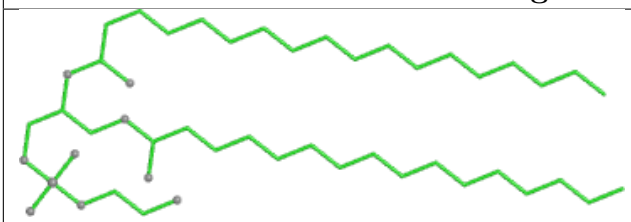


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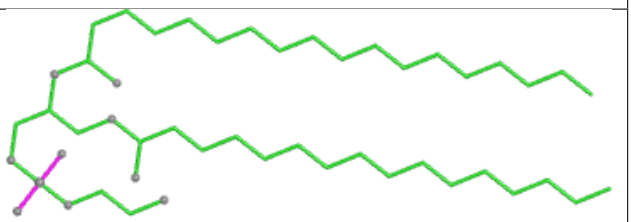


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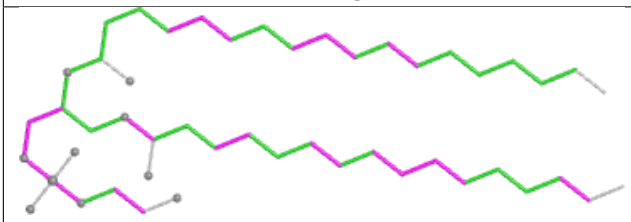
Ligand 3PE L 704



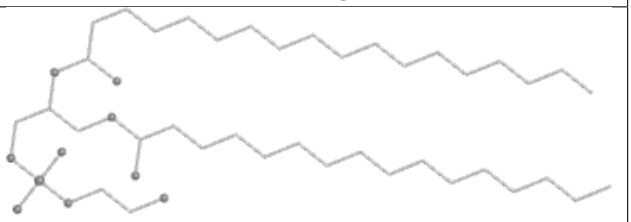
Bond lengths



Bond angles

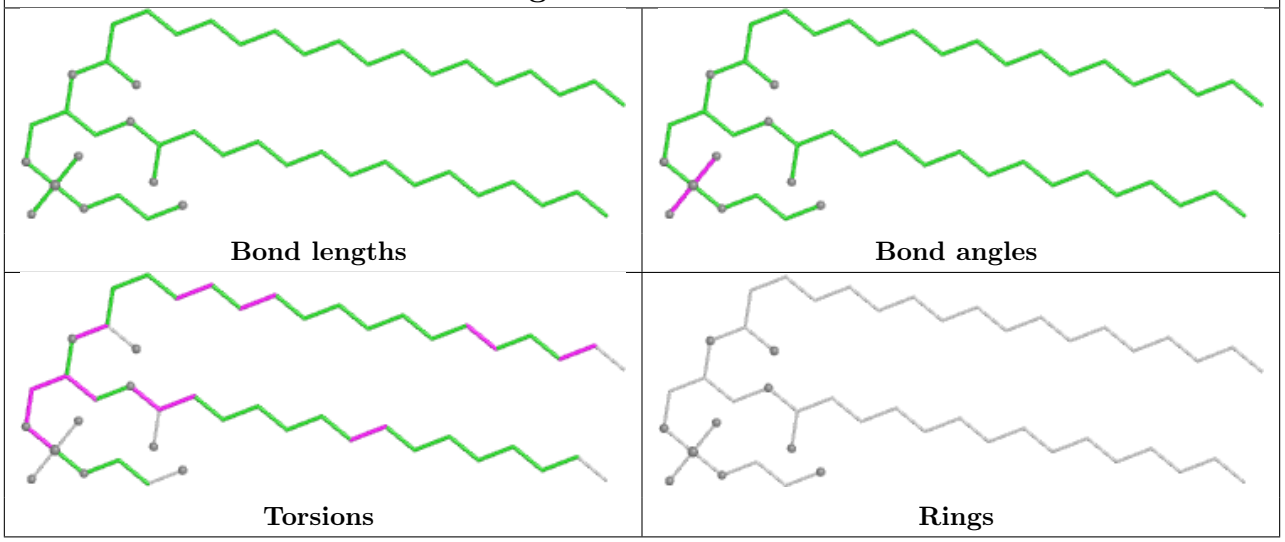


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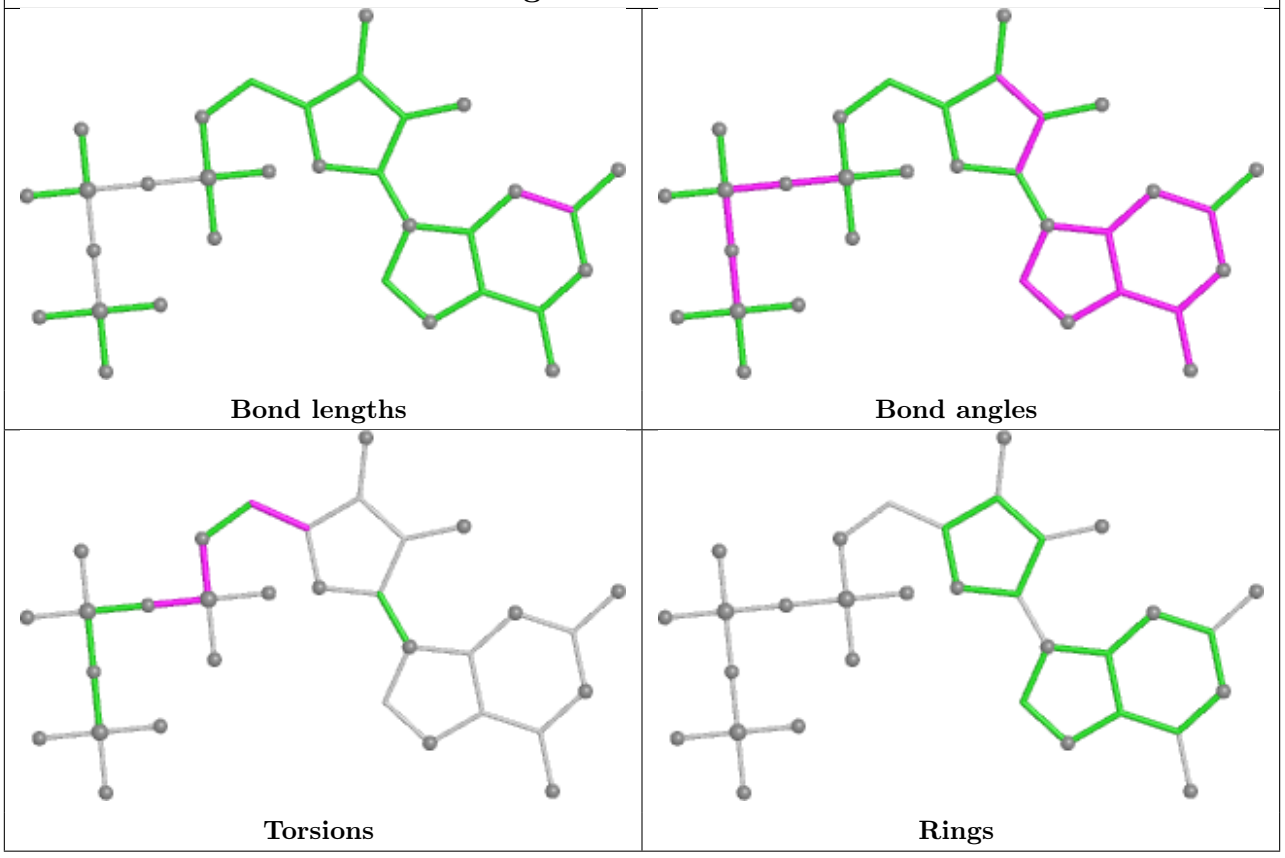


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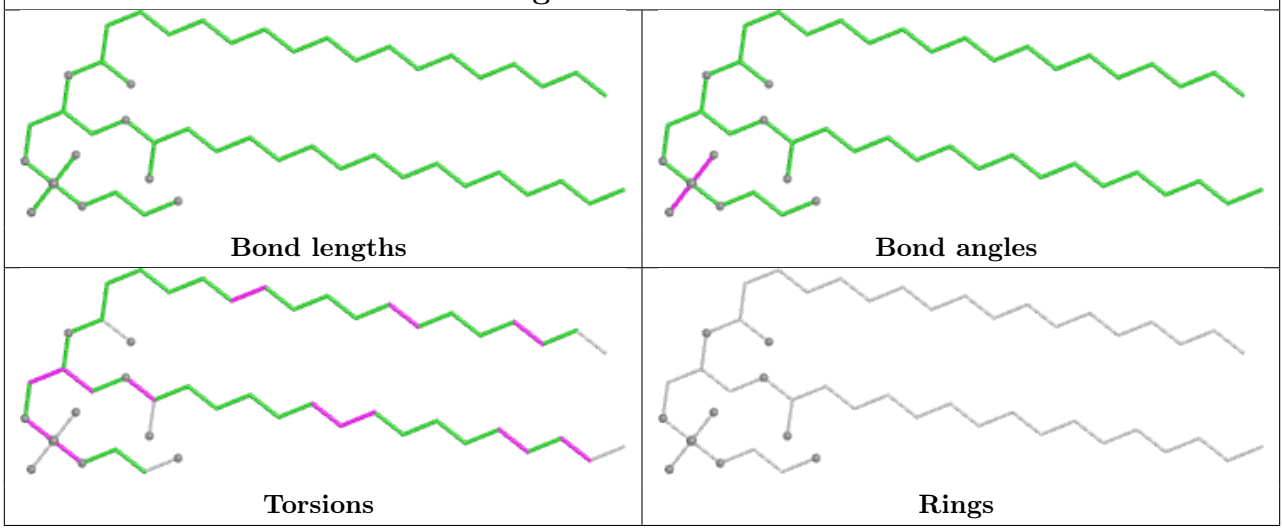
Ligand 3PE O 401



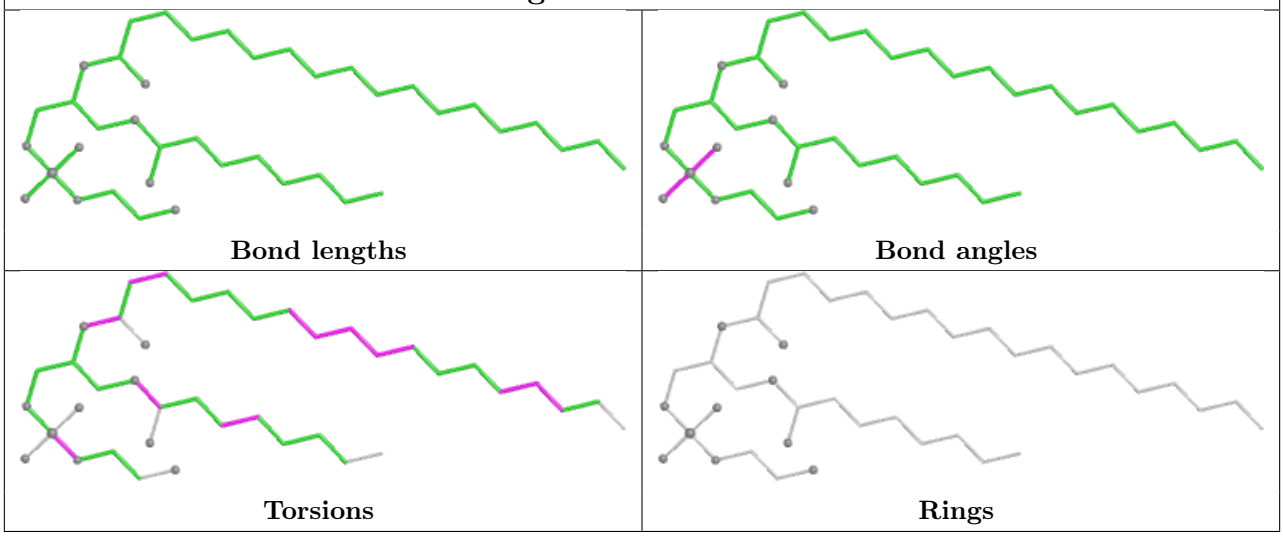
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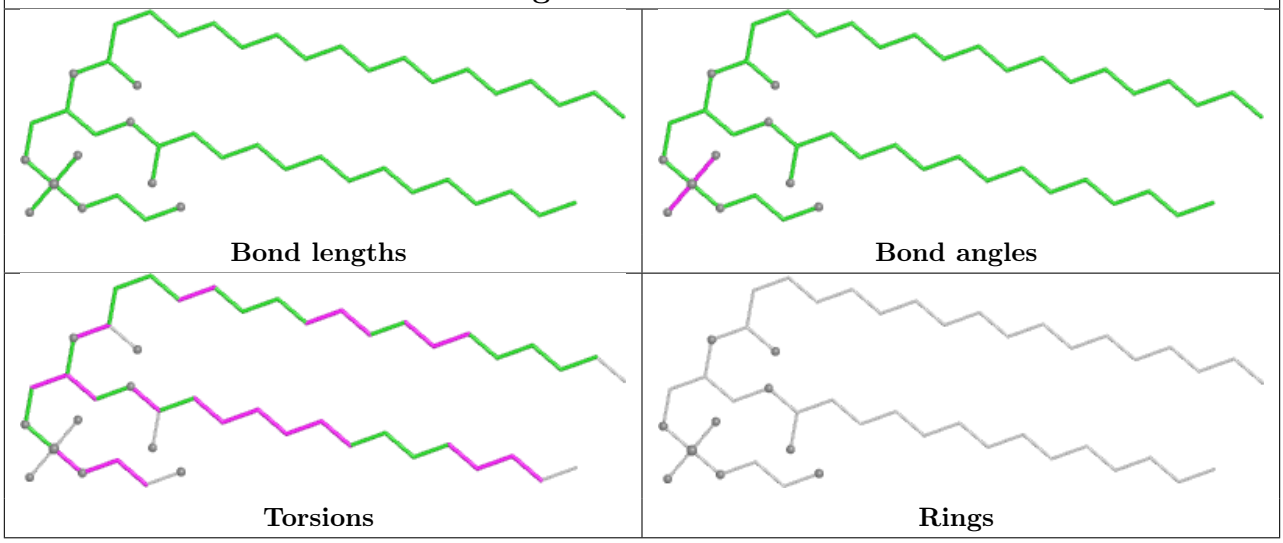
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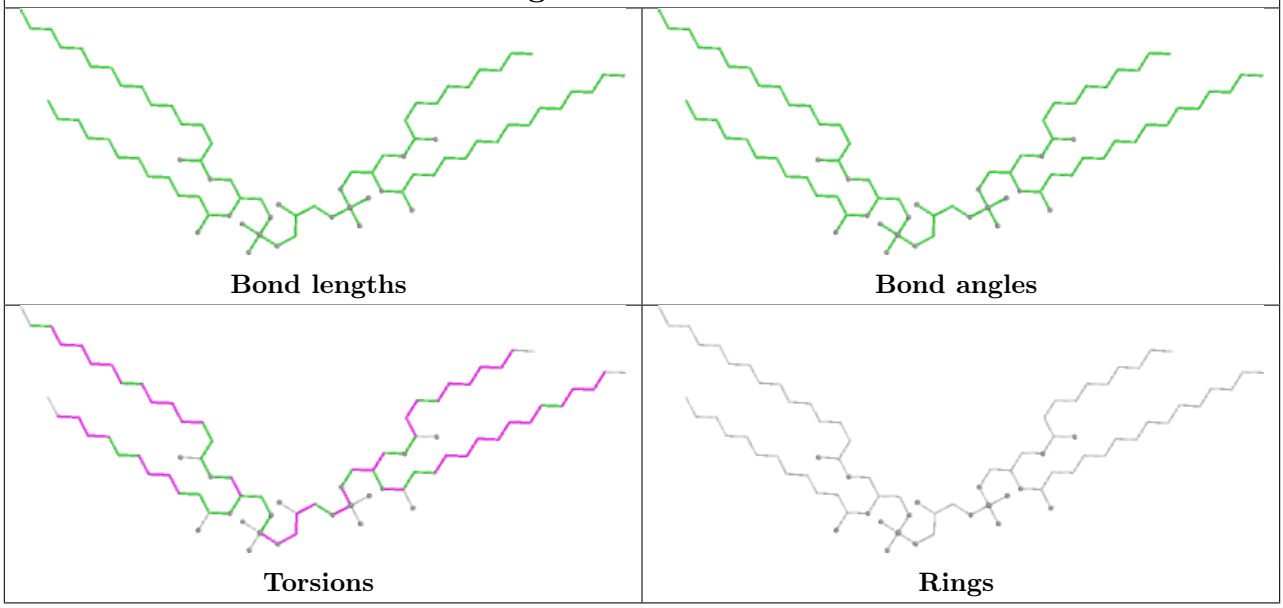
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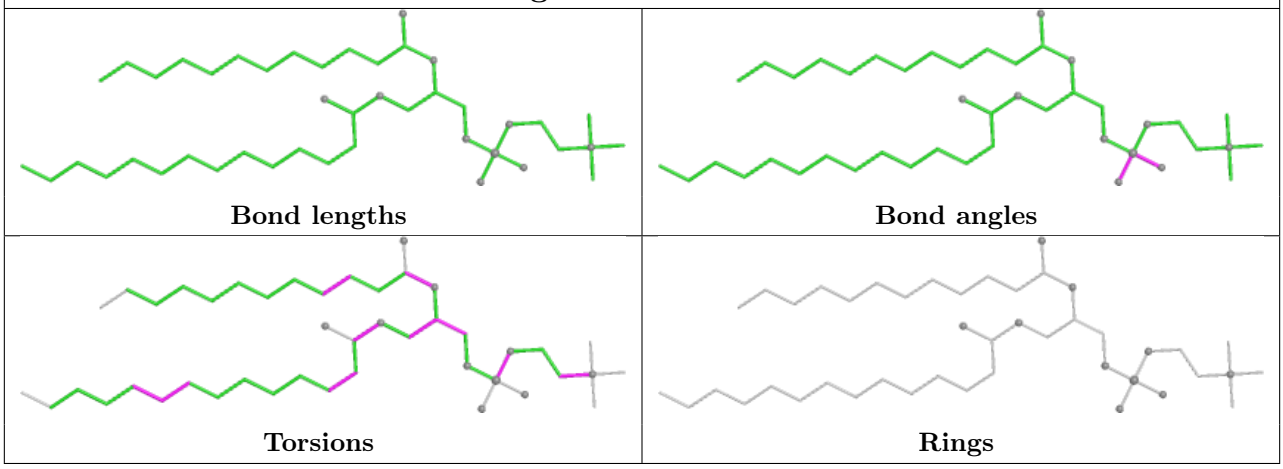
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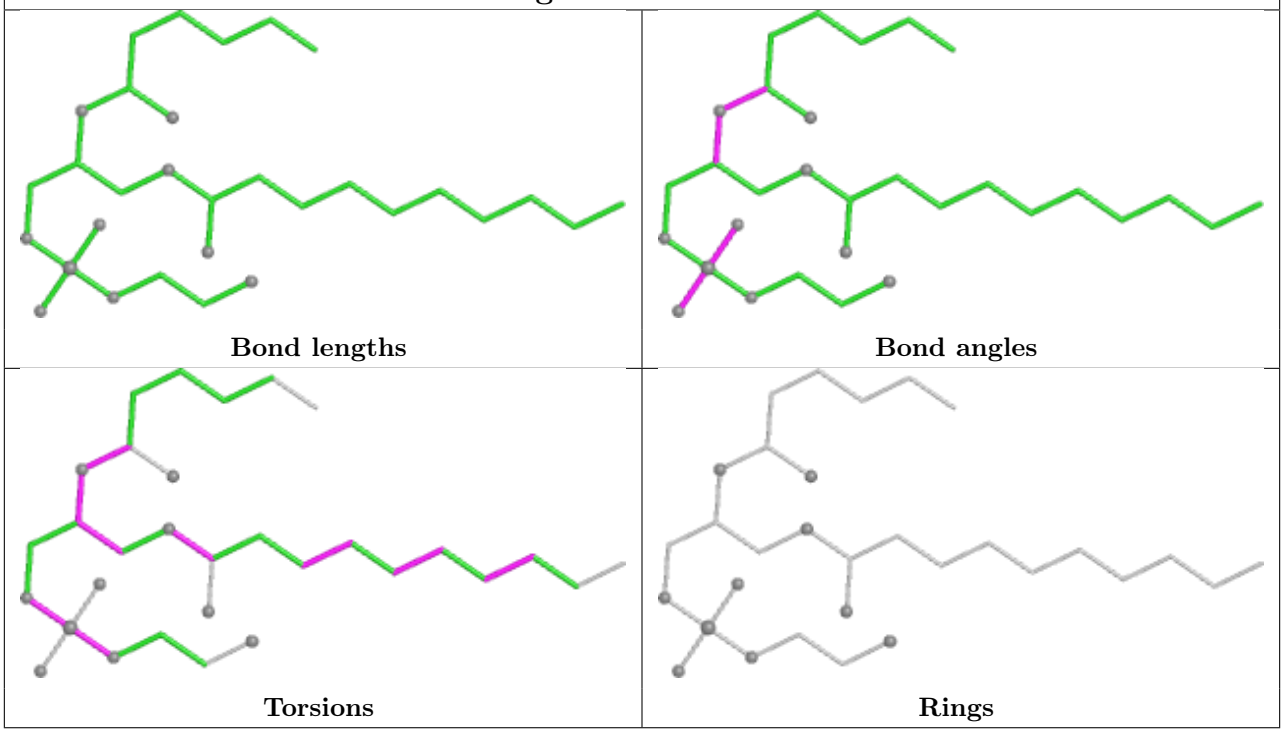
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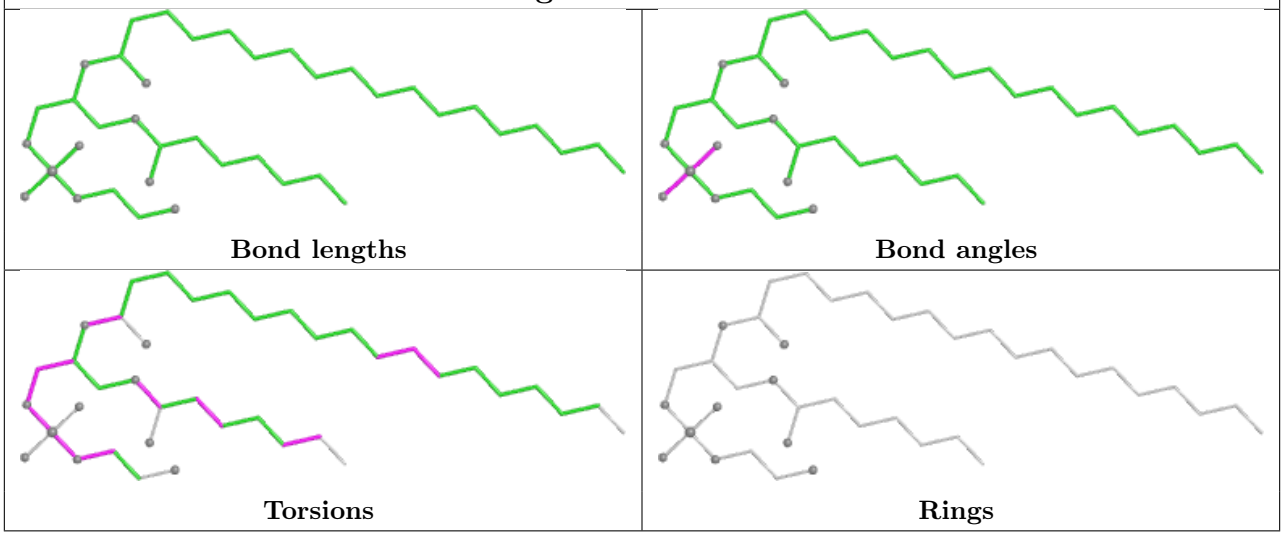
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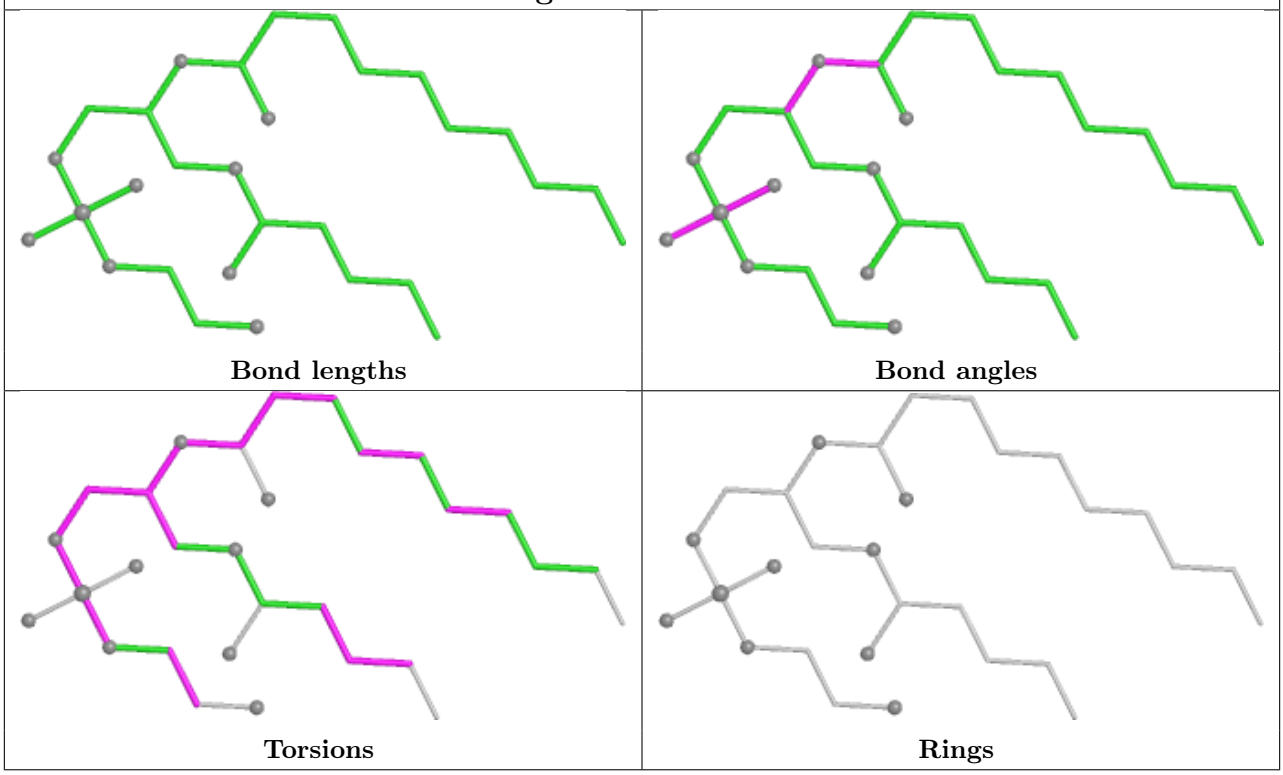
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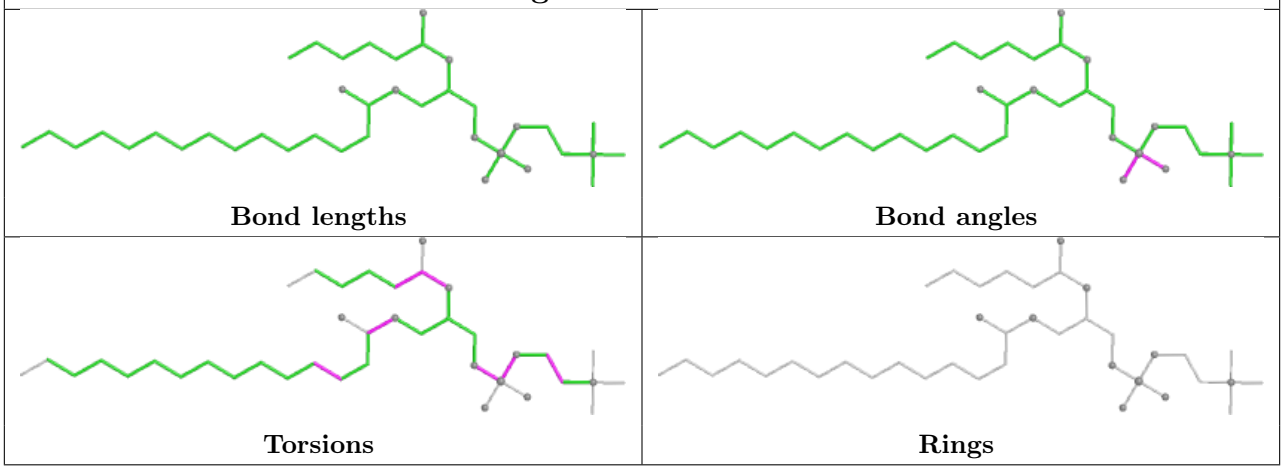
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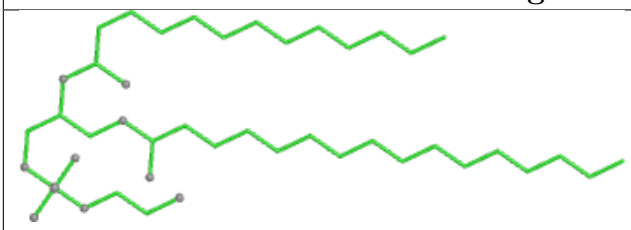
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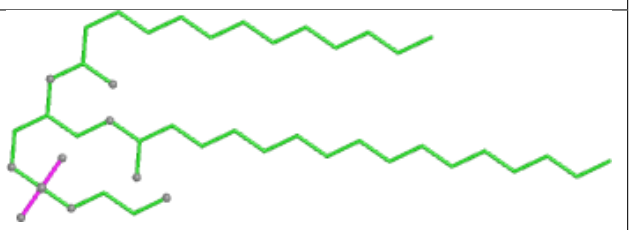
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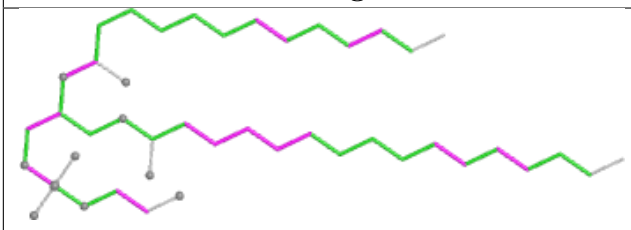
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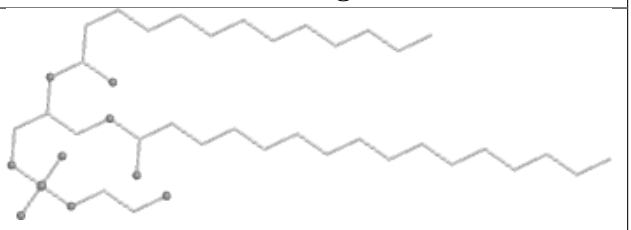
Bond lengths



Bond angles

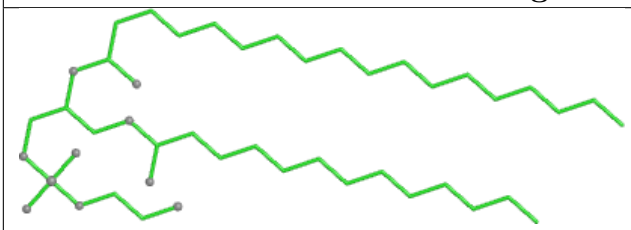


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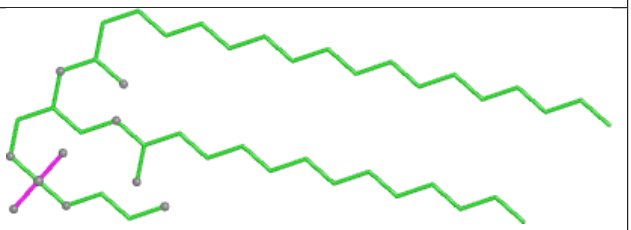


Rings

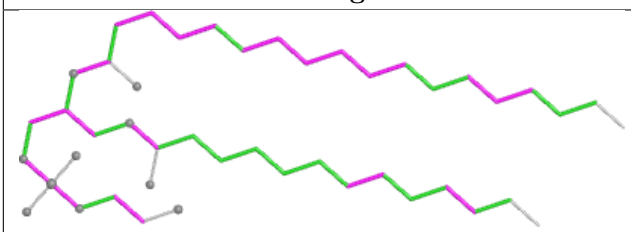
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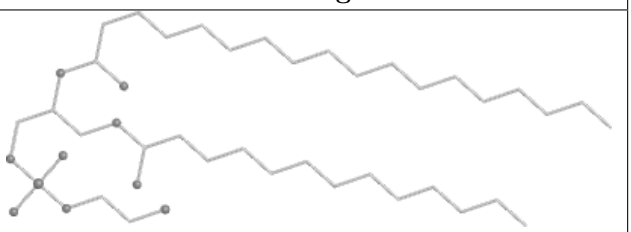
Bond lengths



Bond angles

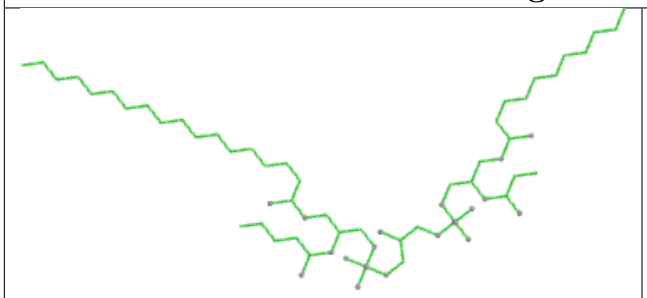


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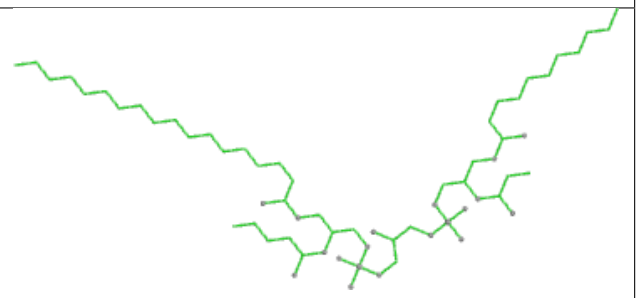


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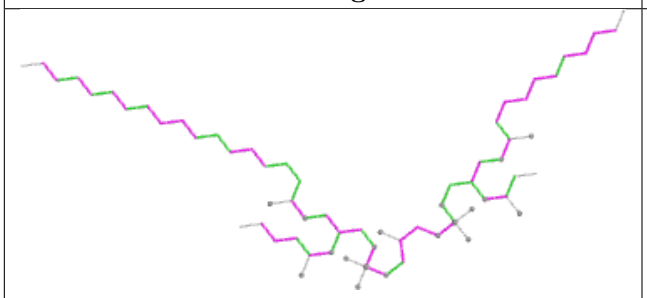
Ligand CDL d 204



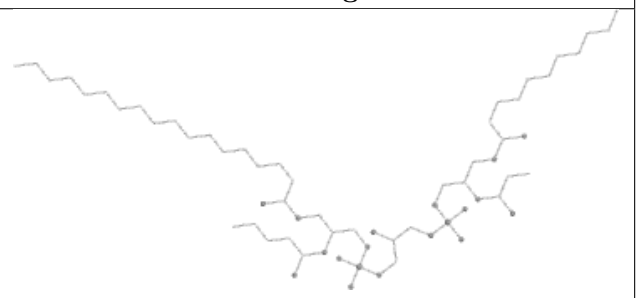
Bond lengths



Bond angles

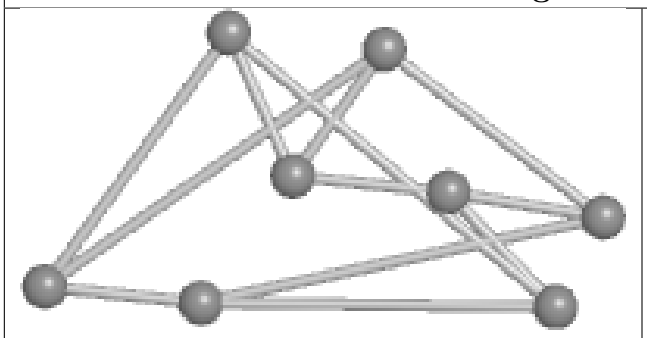


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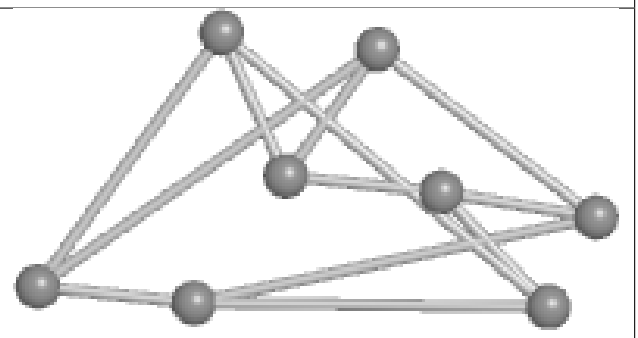


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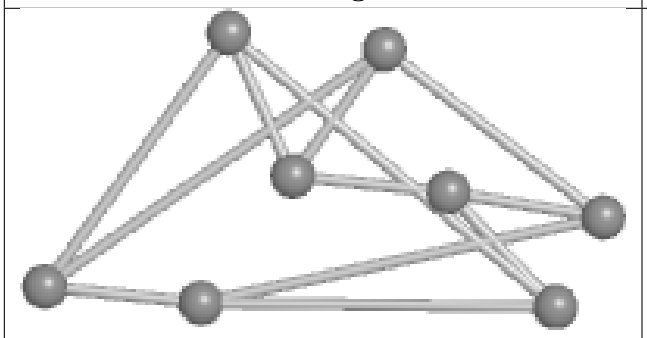
Ligand SF4 B 201



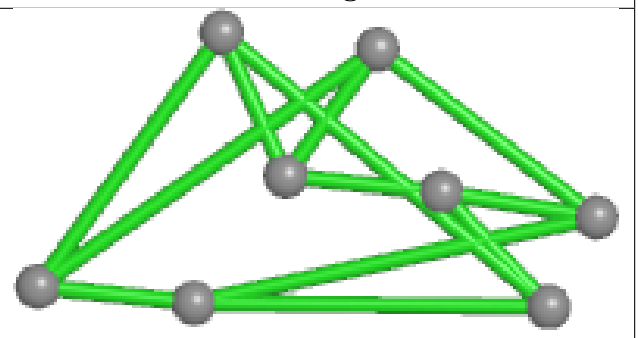
Bond lengths



Bond angles

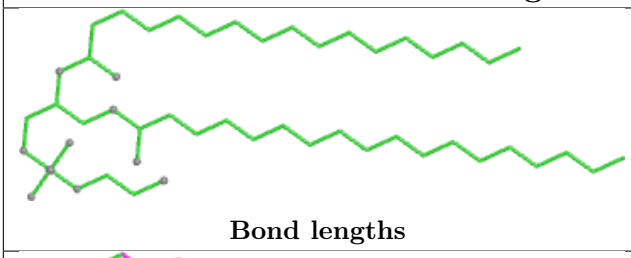


Torsions

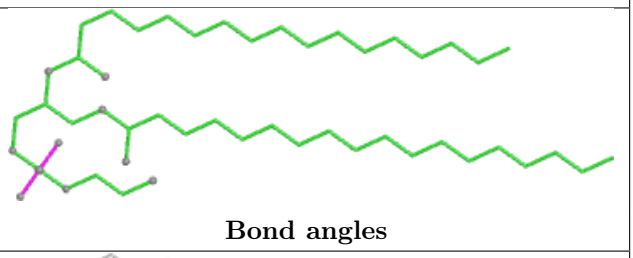


Rings

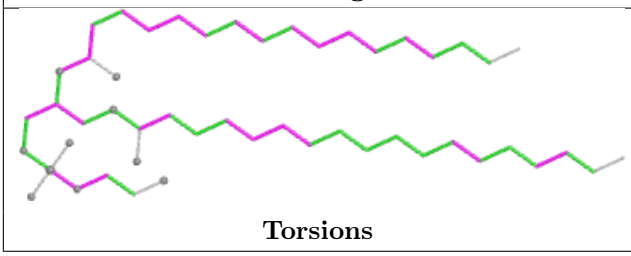
Ligand 3PE M 505



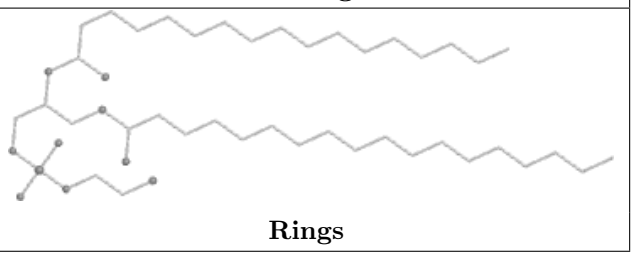
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Bond angles

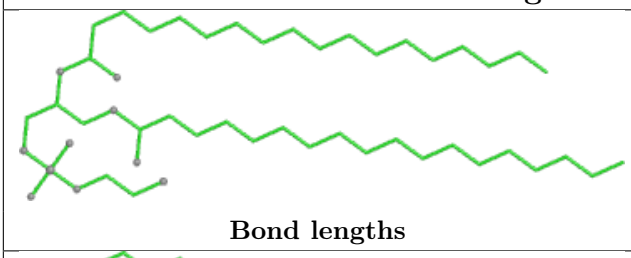


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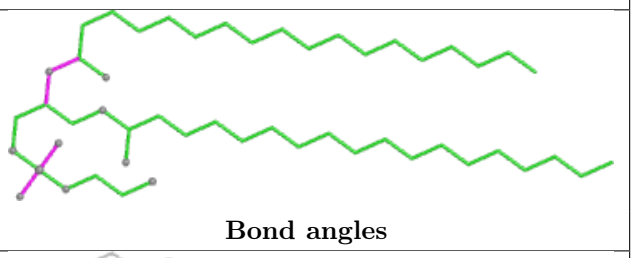


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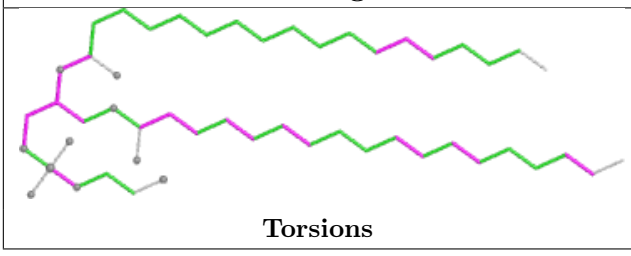
Ligand 3PE M 504



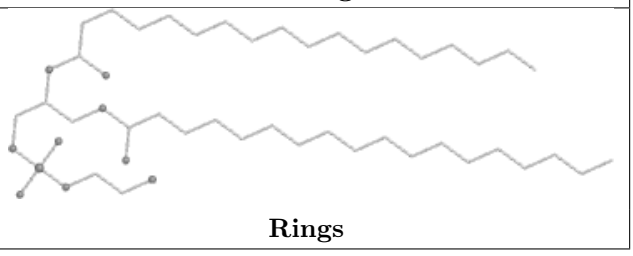
Bond lengths



Bond angles

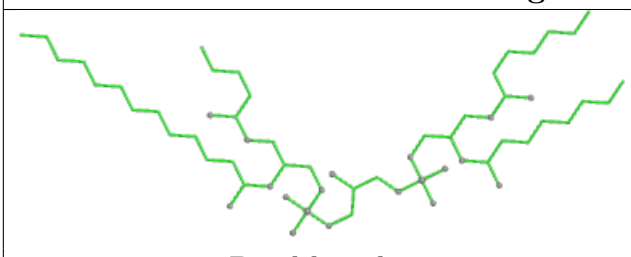


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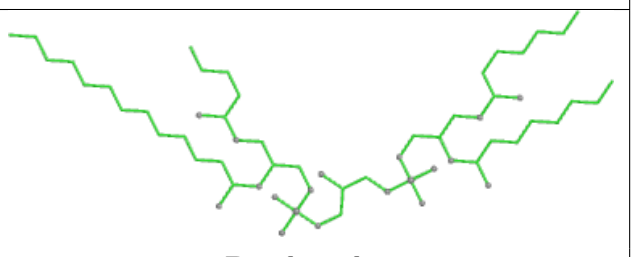


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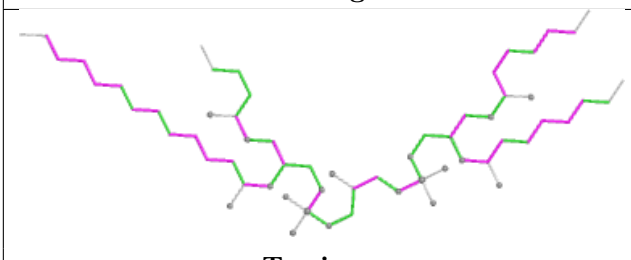
Ligand CDL v 201



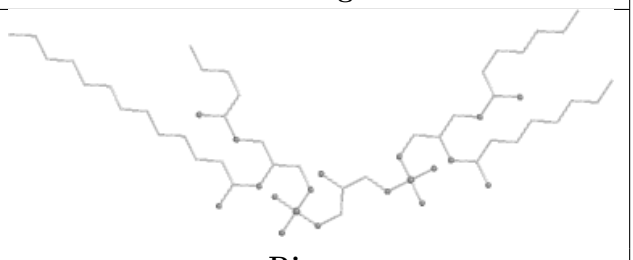
Bond lengths



Bond angles

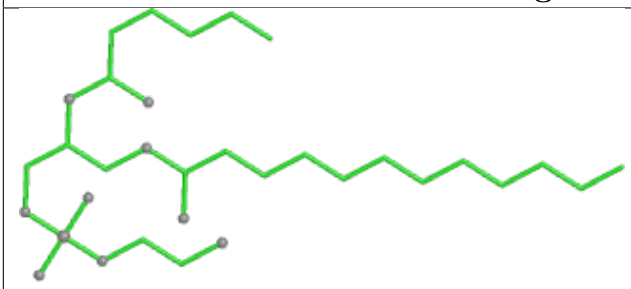


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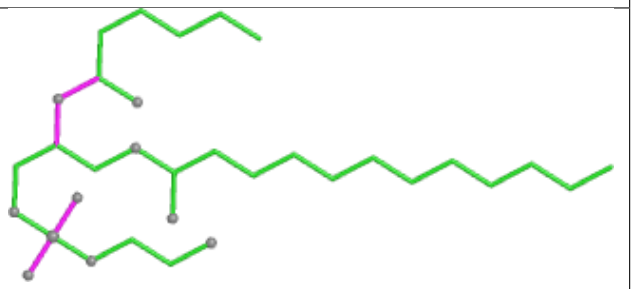


Rings

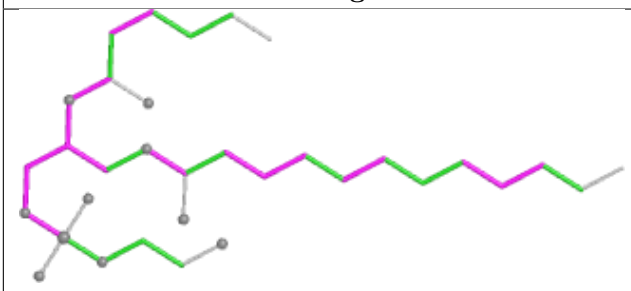
Ligand 3PE t 804



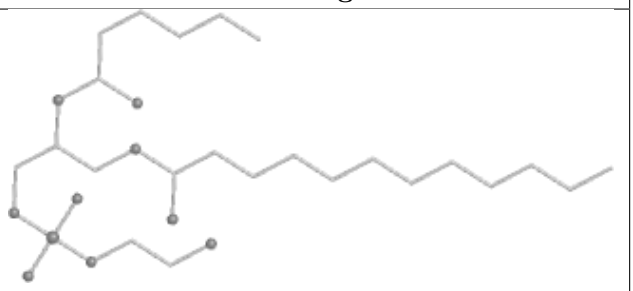
Bond lengths



Bond angles

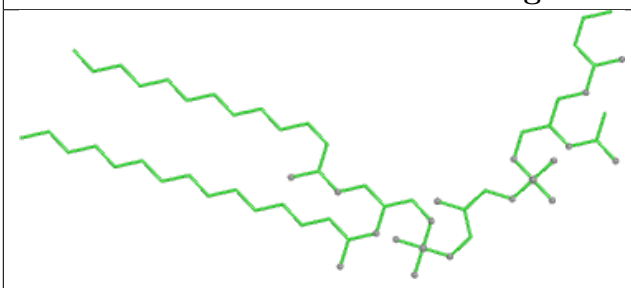


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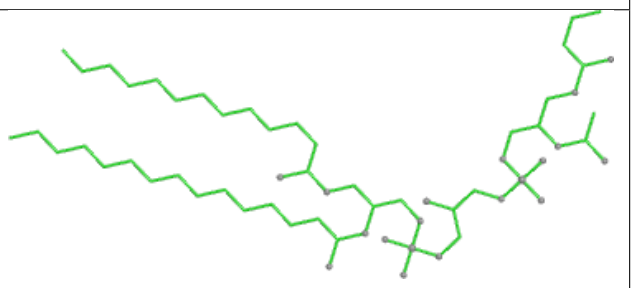


Rings

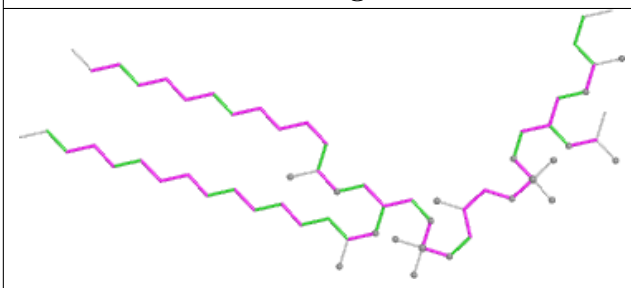
Ligand CDL O 402



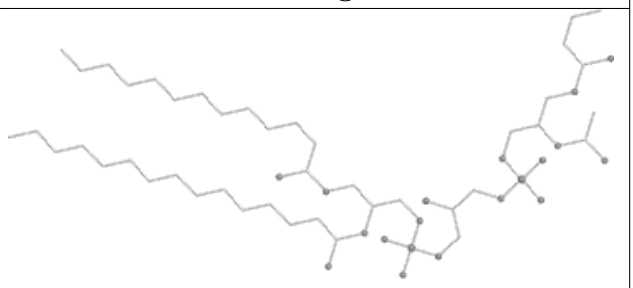
Bond lengths



Bond angles

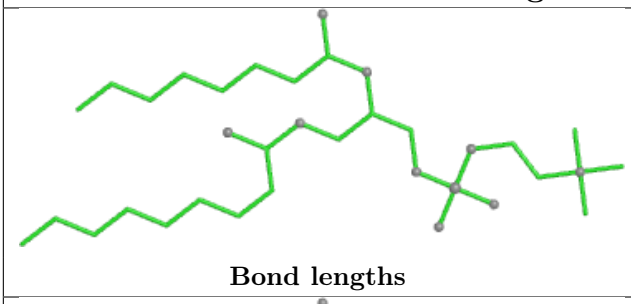


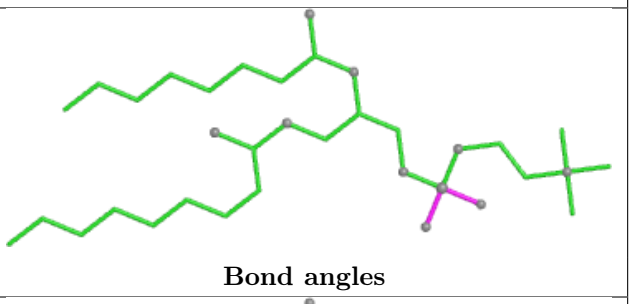
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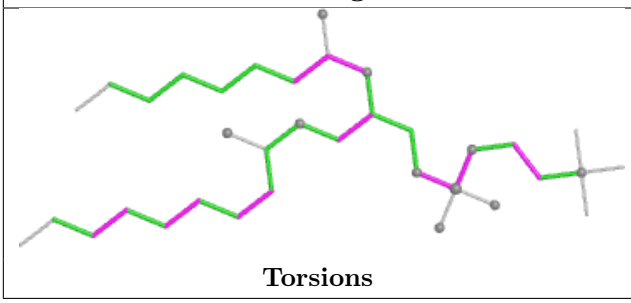


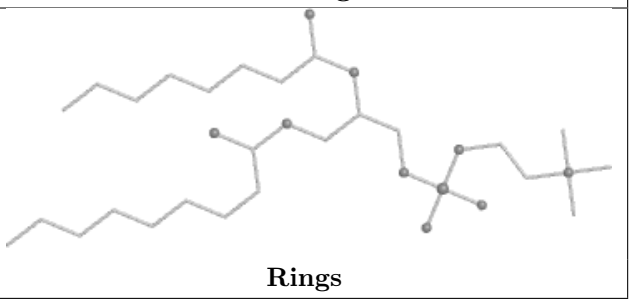
Rings

Ligand PC1 A 202

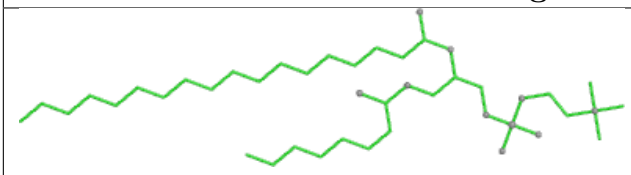

Bond lengths

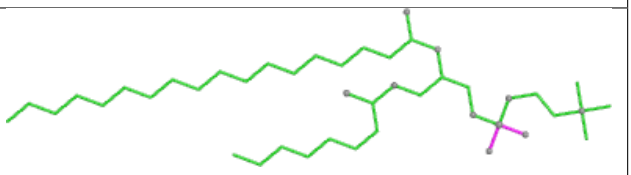

Bond angles

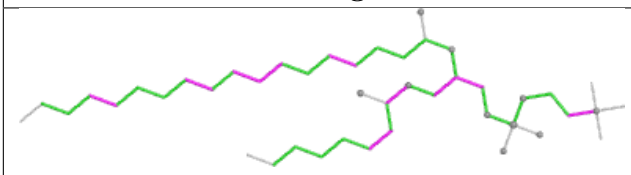

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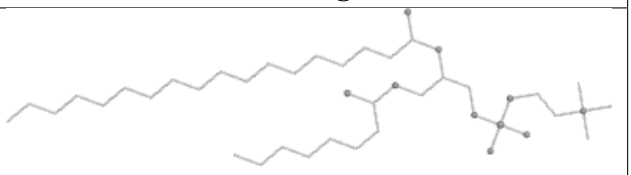

Rings

Ligand PC1 L 705

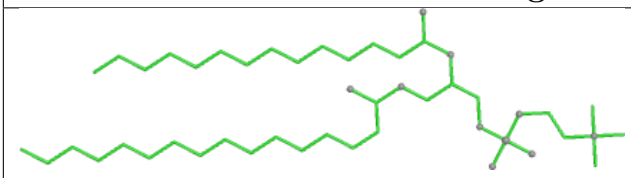

Bond lengths

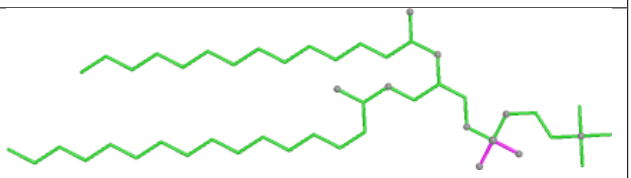

Bond angles

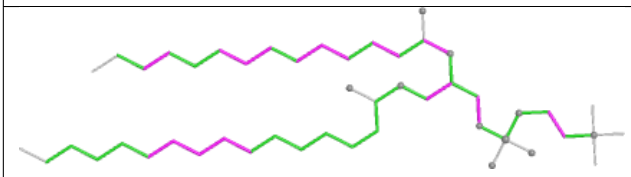

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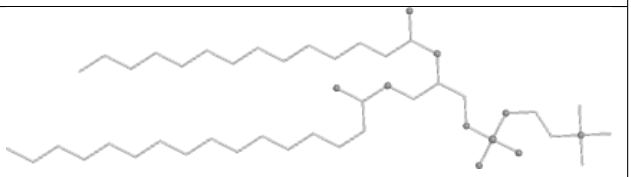

Rings

Ligand PC1 B 203

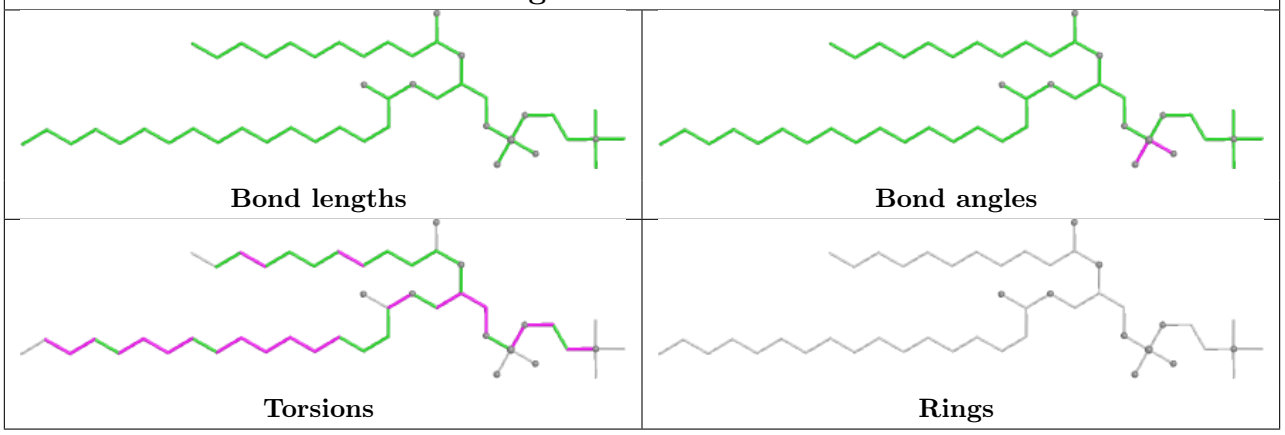

Bond lengths


Bond angles

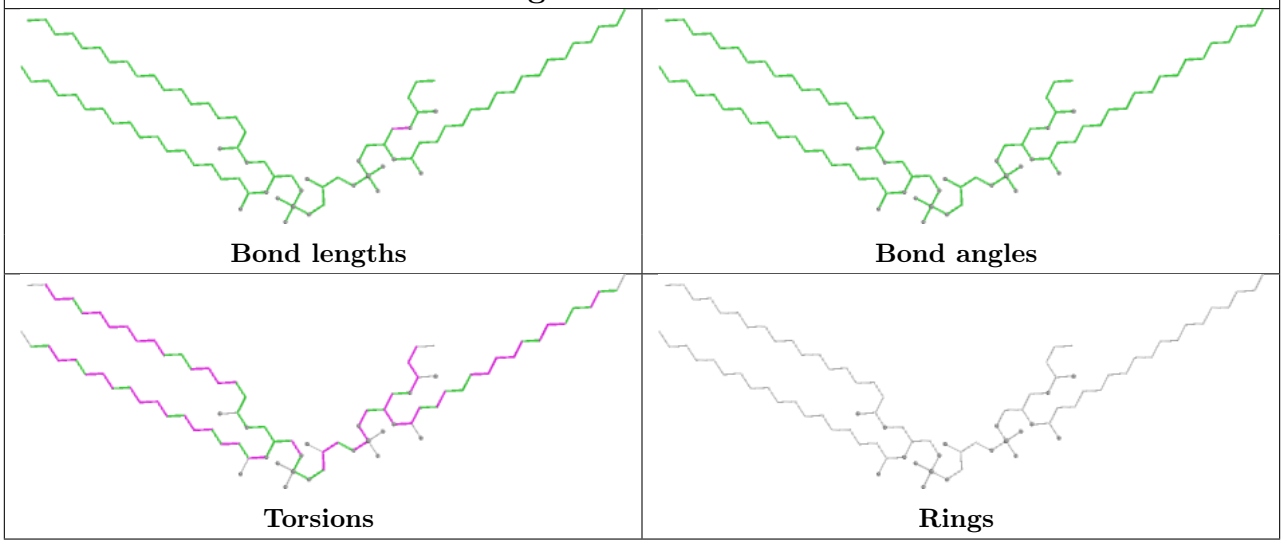

Torsions


Rings

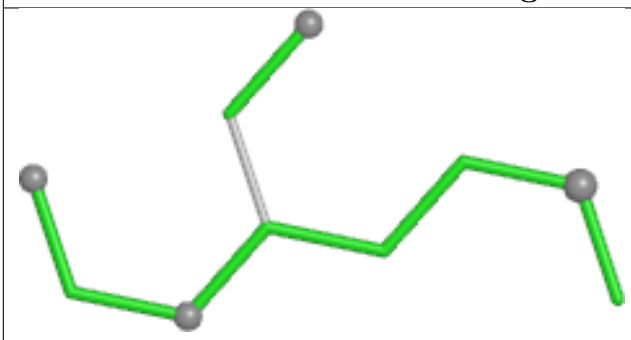
Ligand PC1 B 202



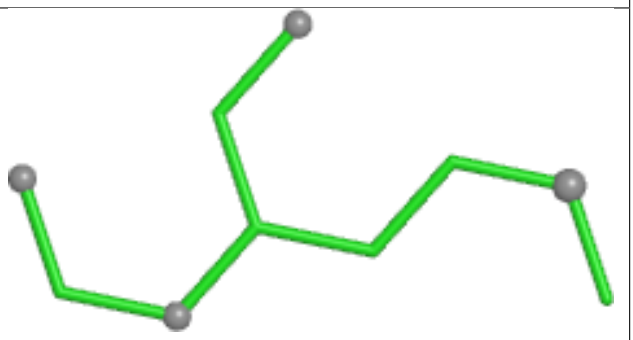
Ligand CDL d 201



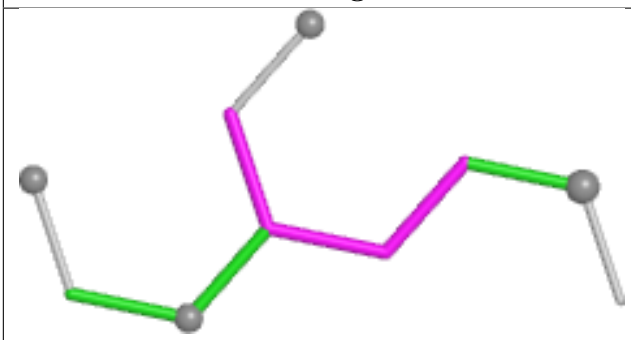
Ligand FME H 401



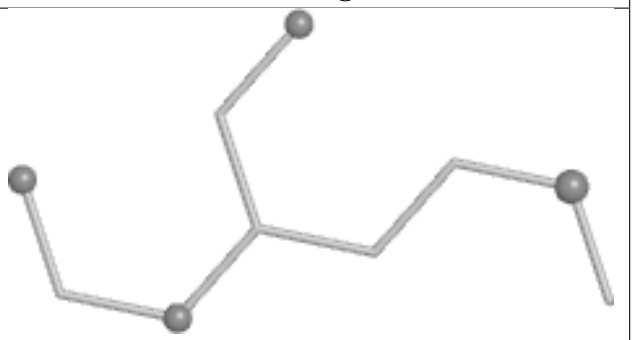
Bond lengths



Bond angles

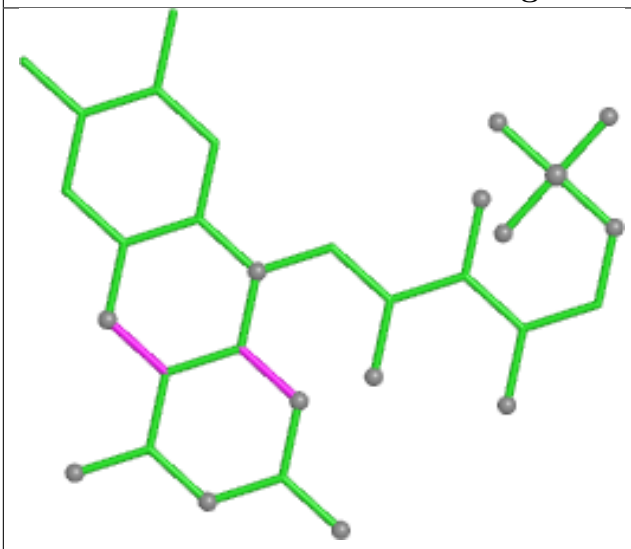


Torsions

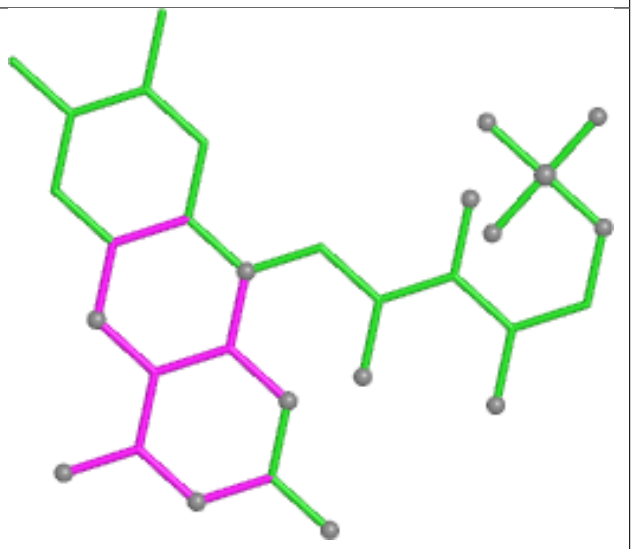


Rings

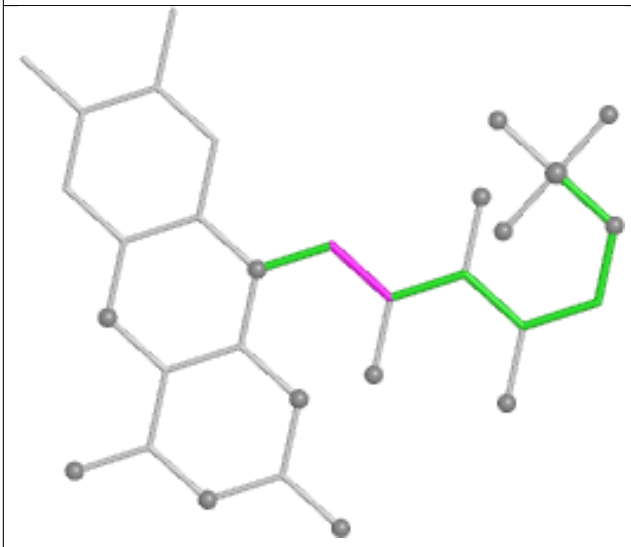
Ligand FMN F 501



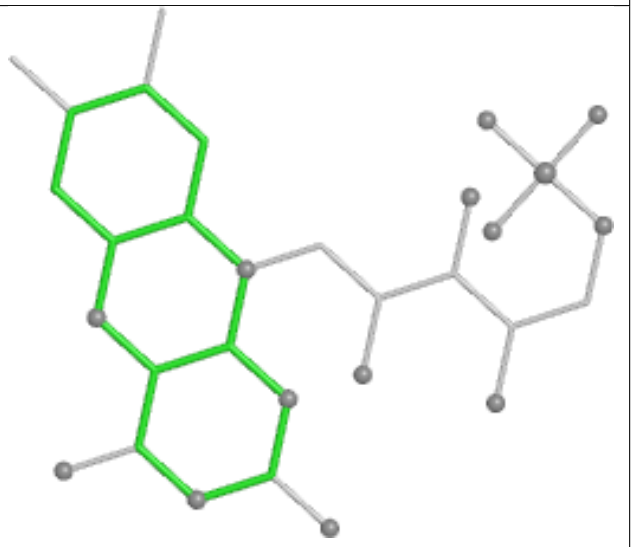
Bond lengths



Bond angles

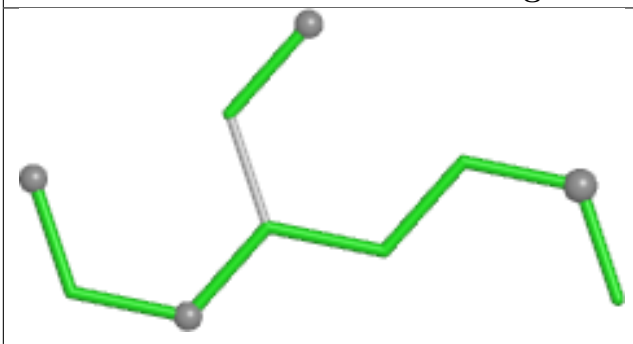


Torsions

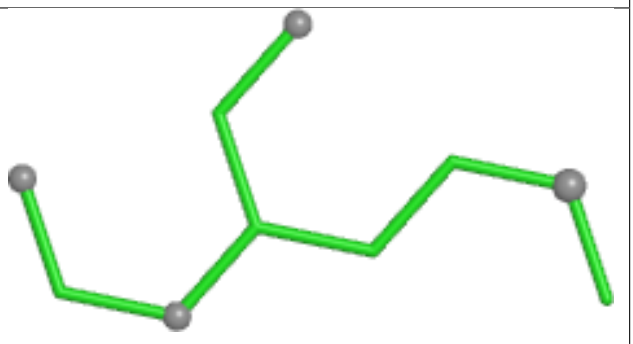


Rings

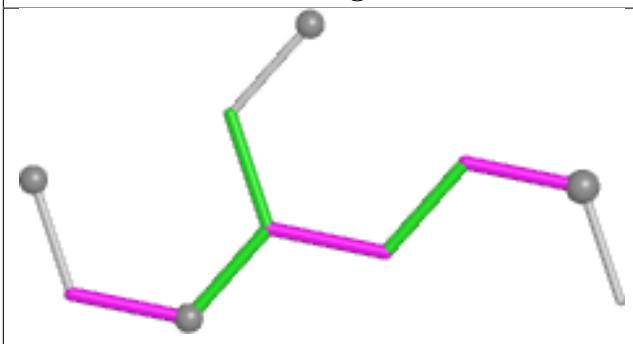
Ligand FME L 701



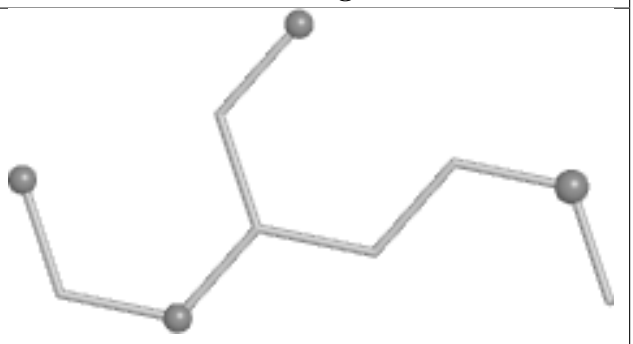
Bond lengths



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.

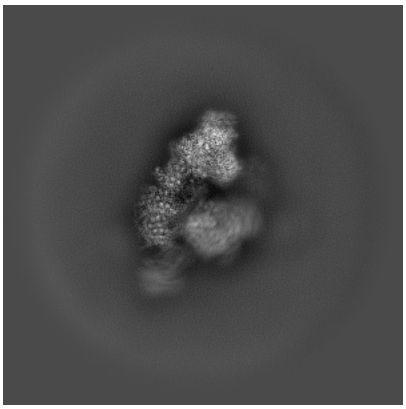
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-65580. These allow visual inspection of the internal detail of the map and identification of artifacts.

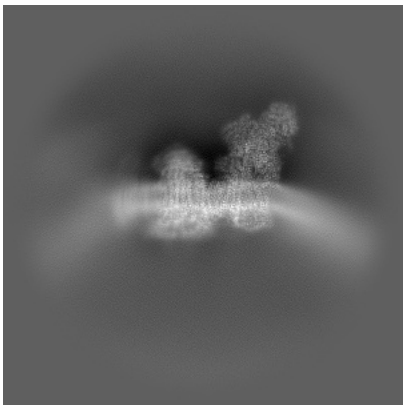
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

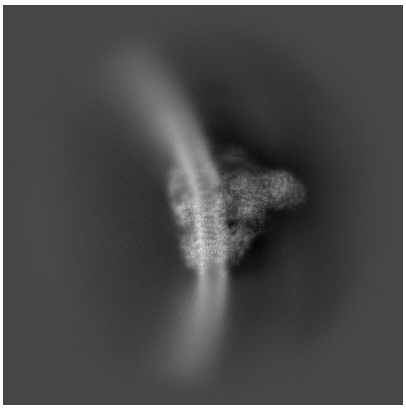
6.1.1 Primary map



X

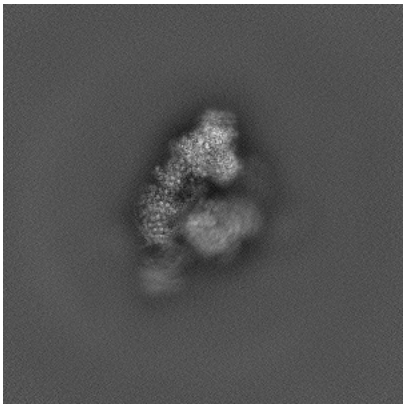


Y

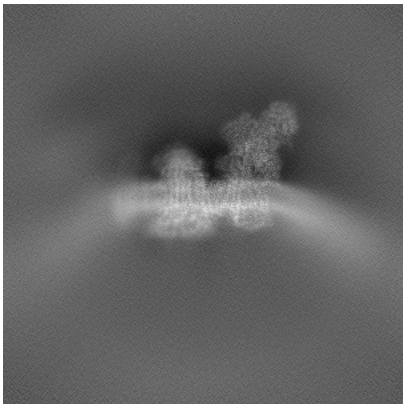


Z

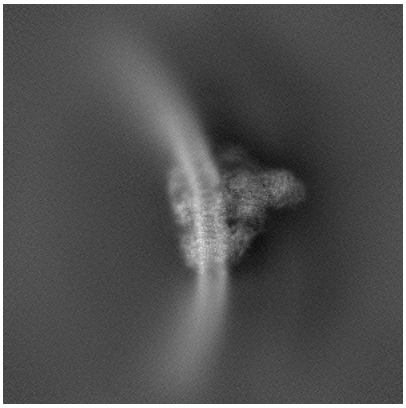
6.1.2 Raw map



X



Y

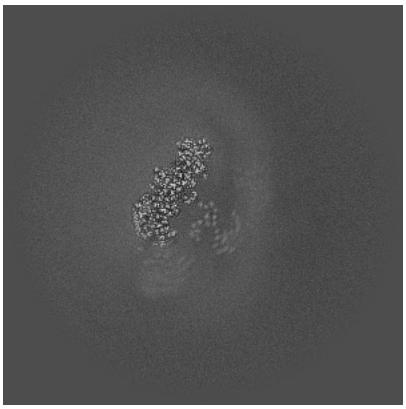


Z

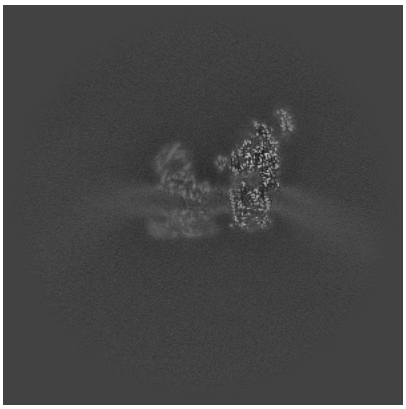
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

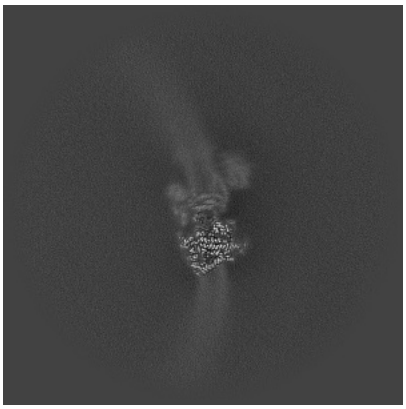
6.2.1 Primary map



X Index: 300

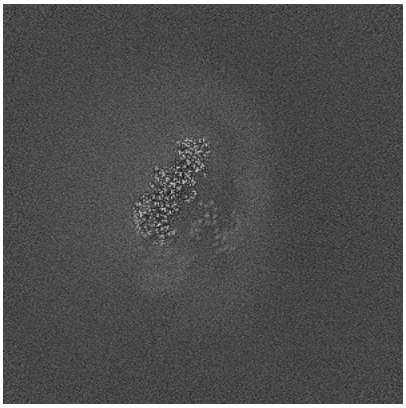


Y Index: 300

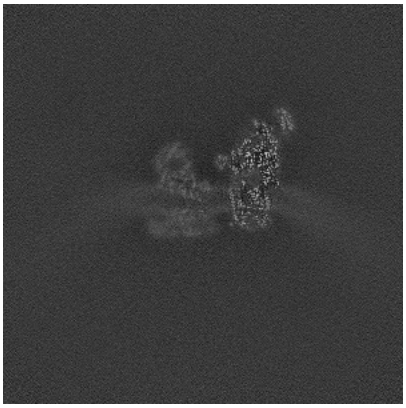


Z Index: 300

6.2.2 Raw map



X Index: 300



Y Index: 300

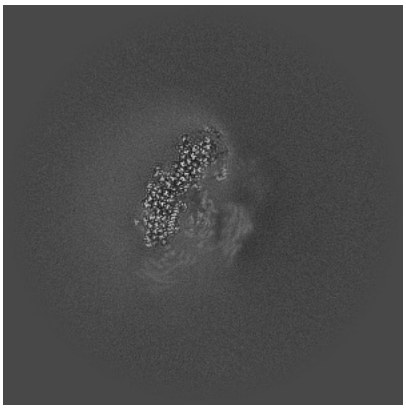


Z Index: 300

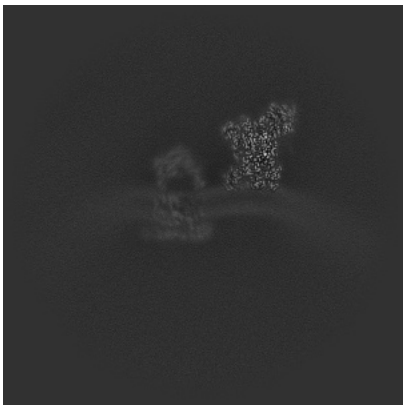
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

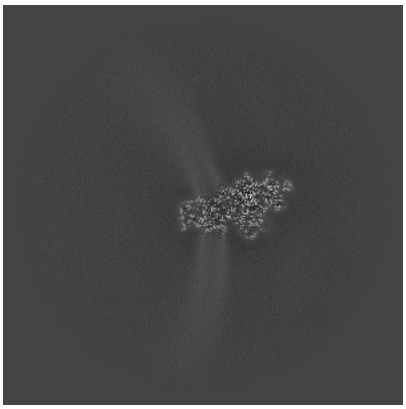
6.3.1 Primary map



X Index: 322

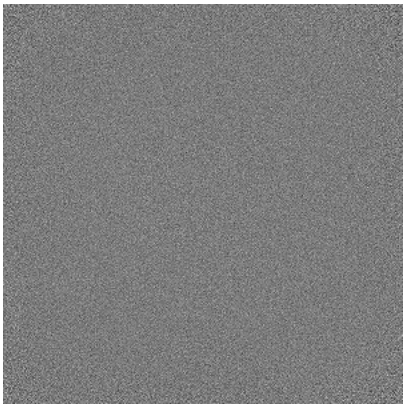


Y Index: 323

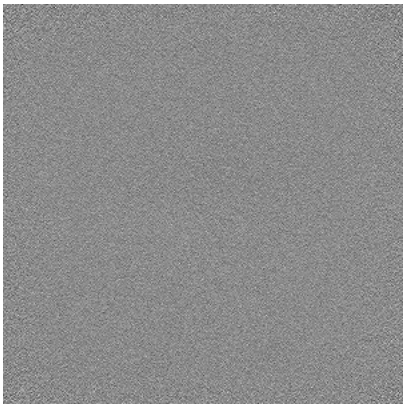


Z Index: 386

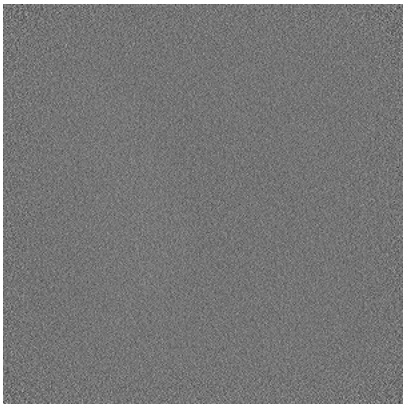
6.3.2 Raw map



X Index: 0



Y Index: 0

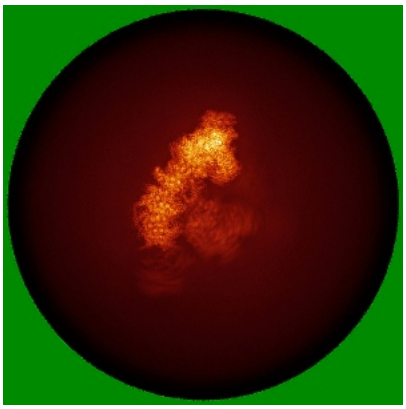


Z Index: 0

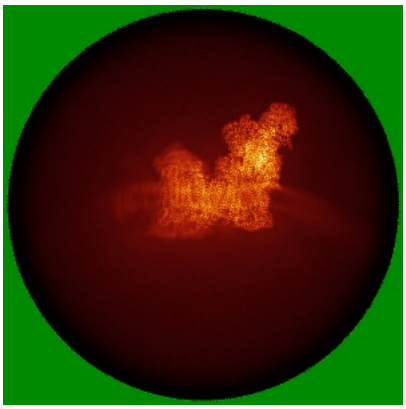
The images above show the largest variance slices of the map in three orthogonal directions.

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

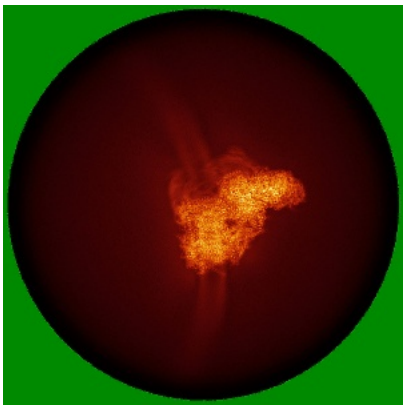
6.4.1 Primary map



X

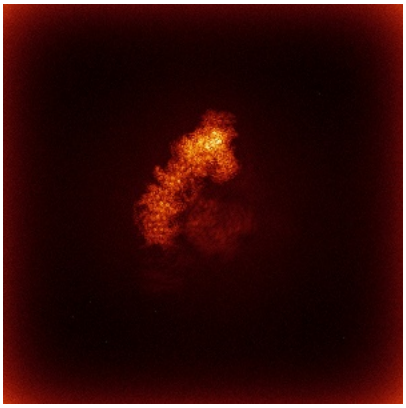


Y

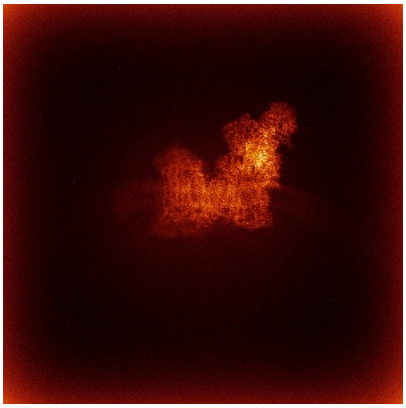


Z

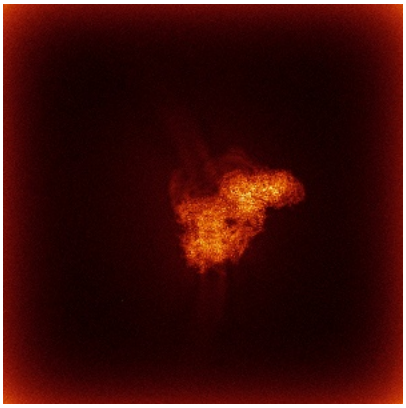
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

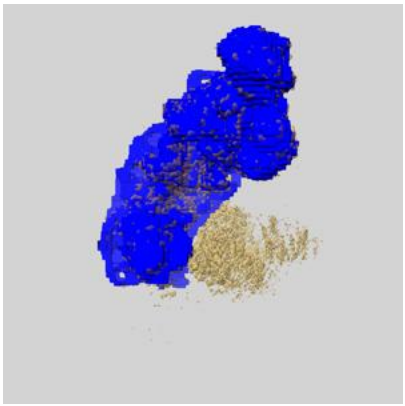
6.6 Mask visualisation (i)

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

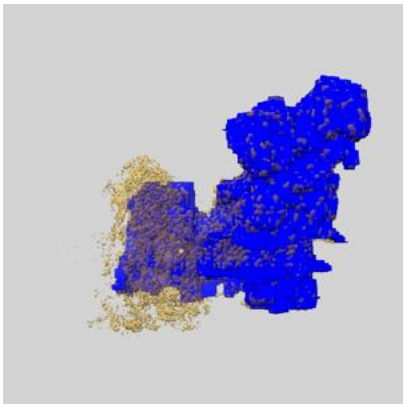
A mask typically either:

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

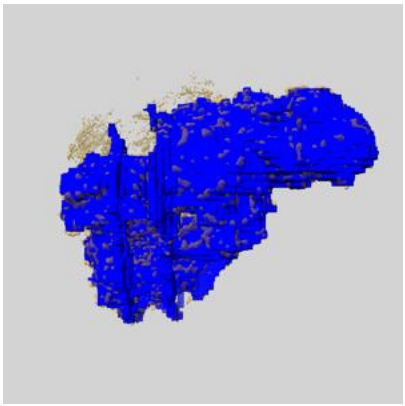
6.6.1 emd_65580_msk_1.map (i)



X



Y

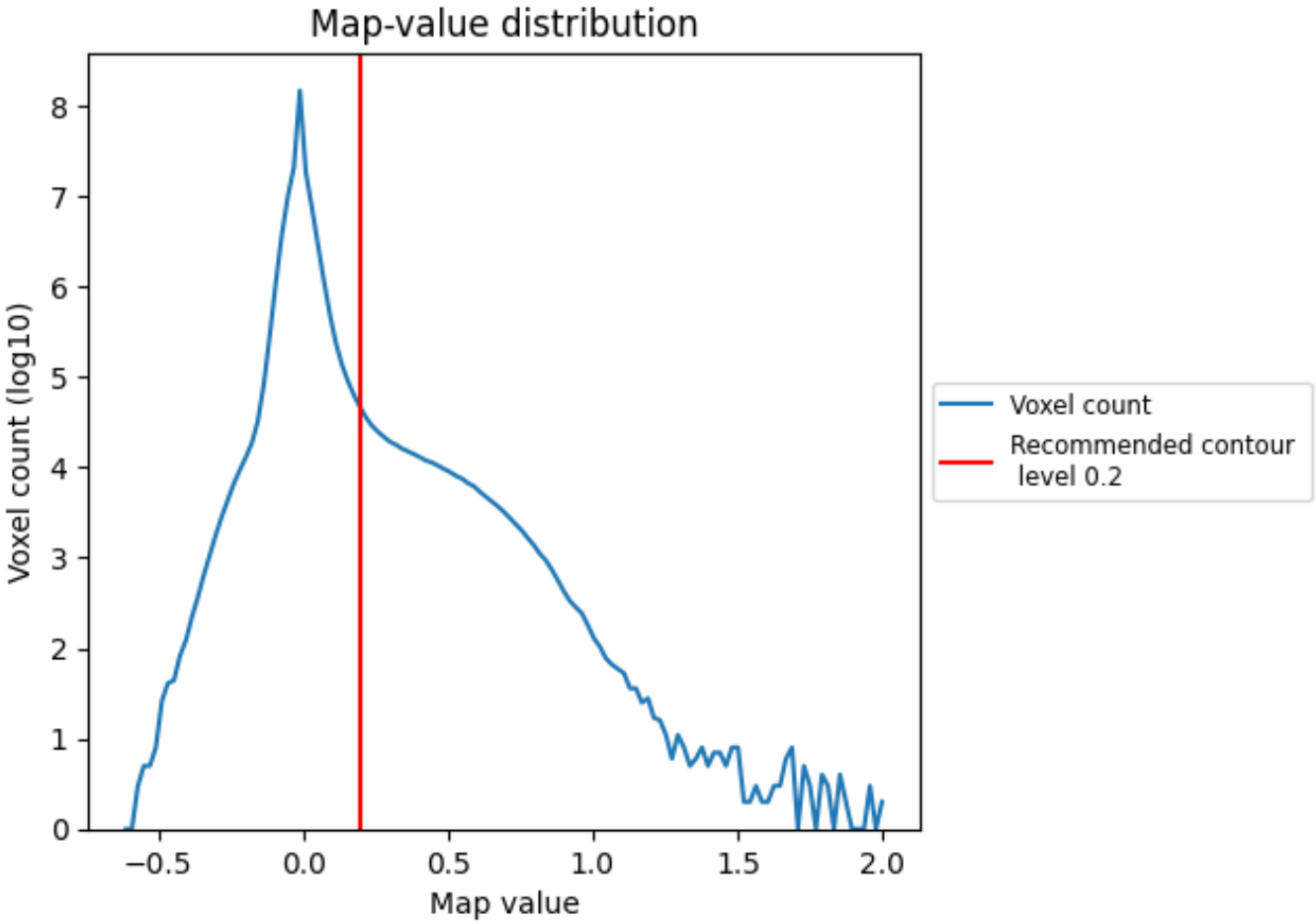


Z

7 Map analysis

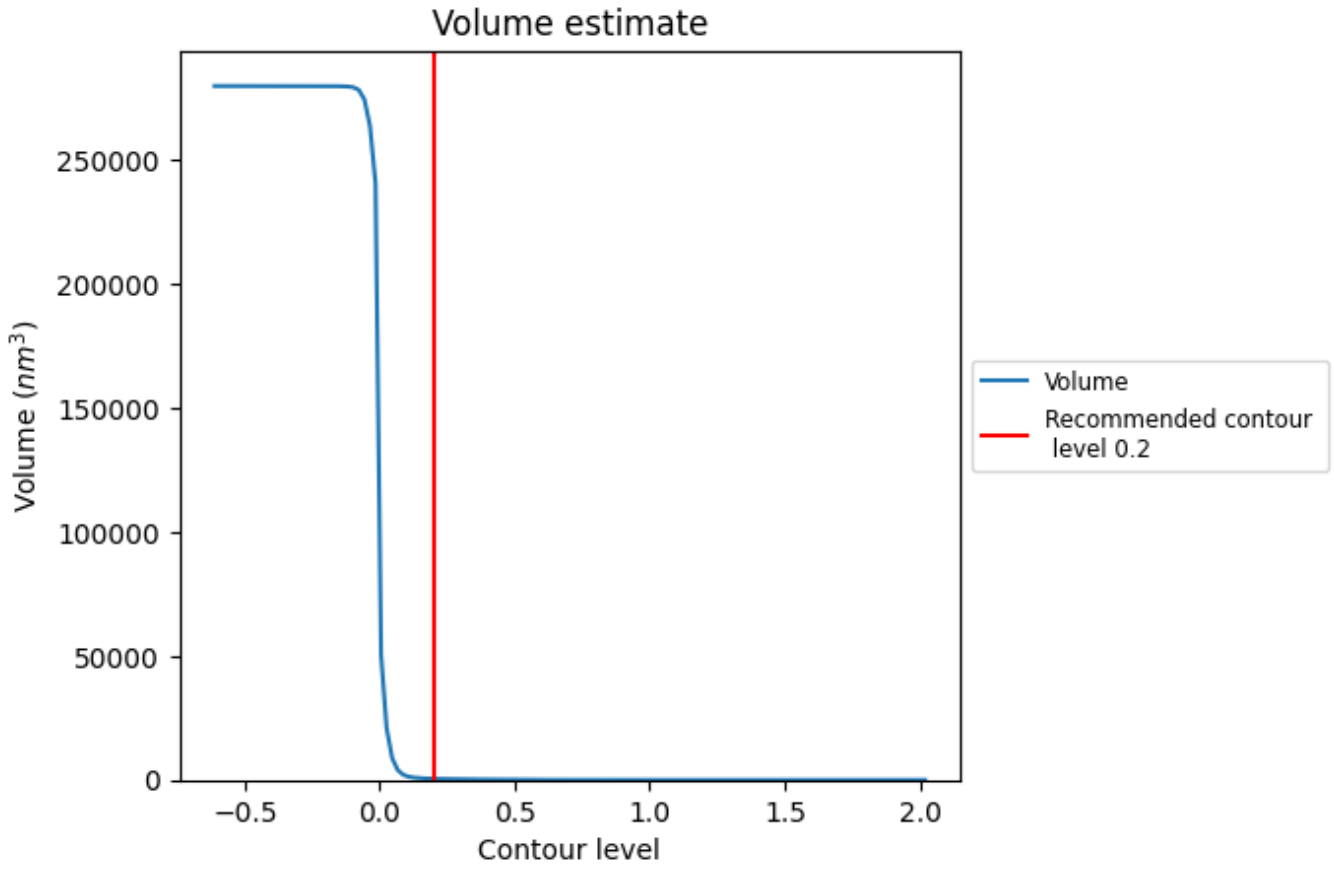
This section contains the results of statistical analysis of the map.

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.

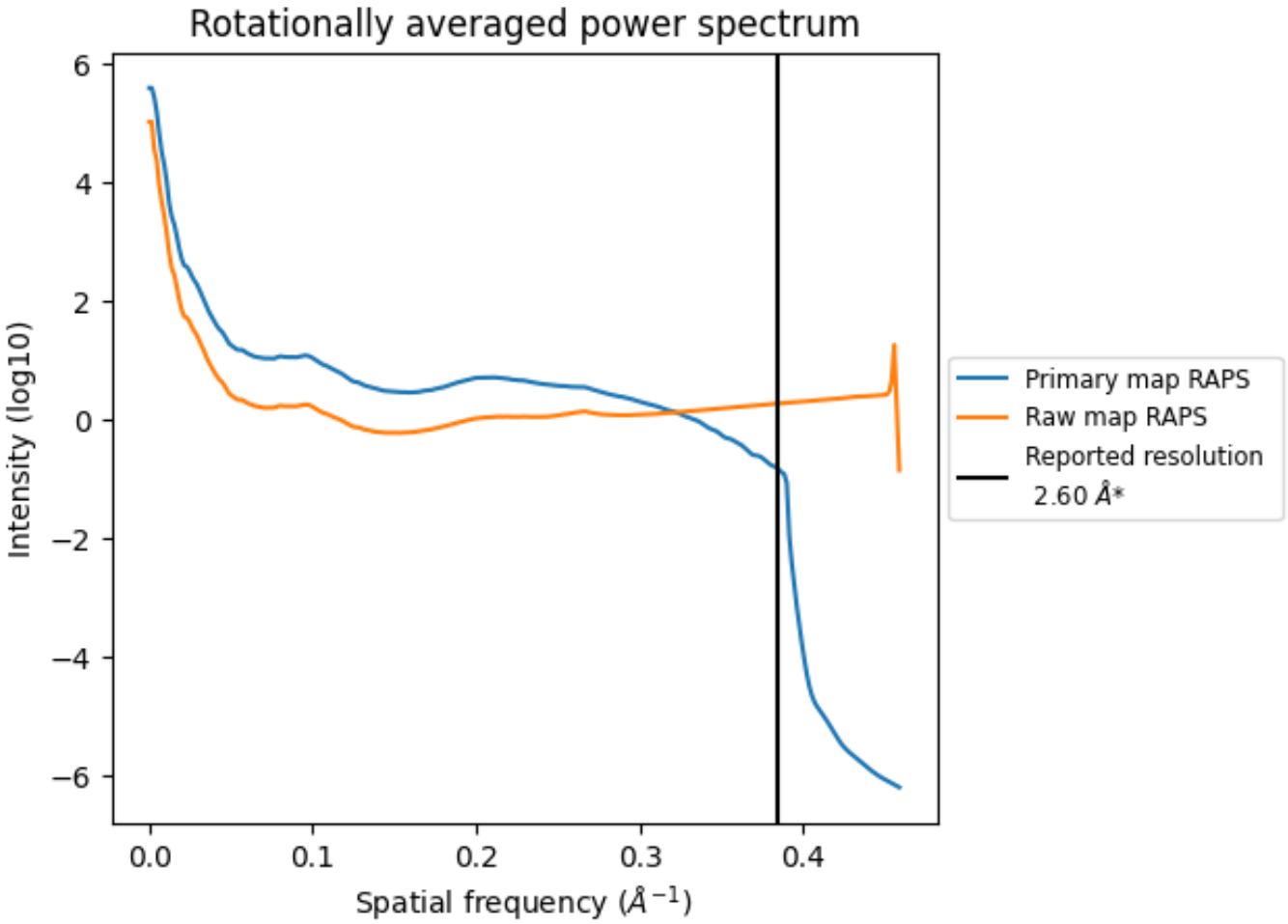
7.2 Volume estimate



The volume at the recommended contour level is 472 nm^3; this corresponds to an approximate mass of 426 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)

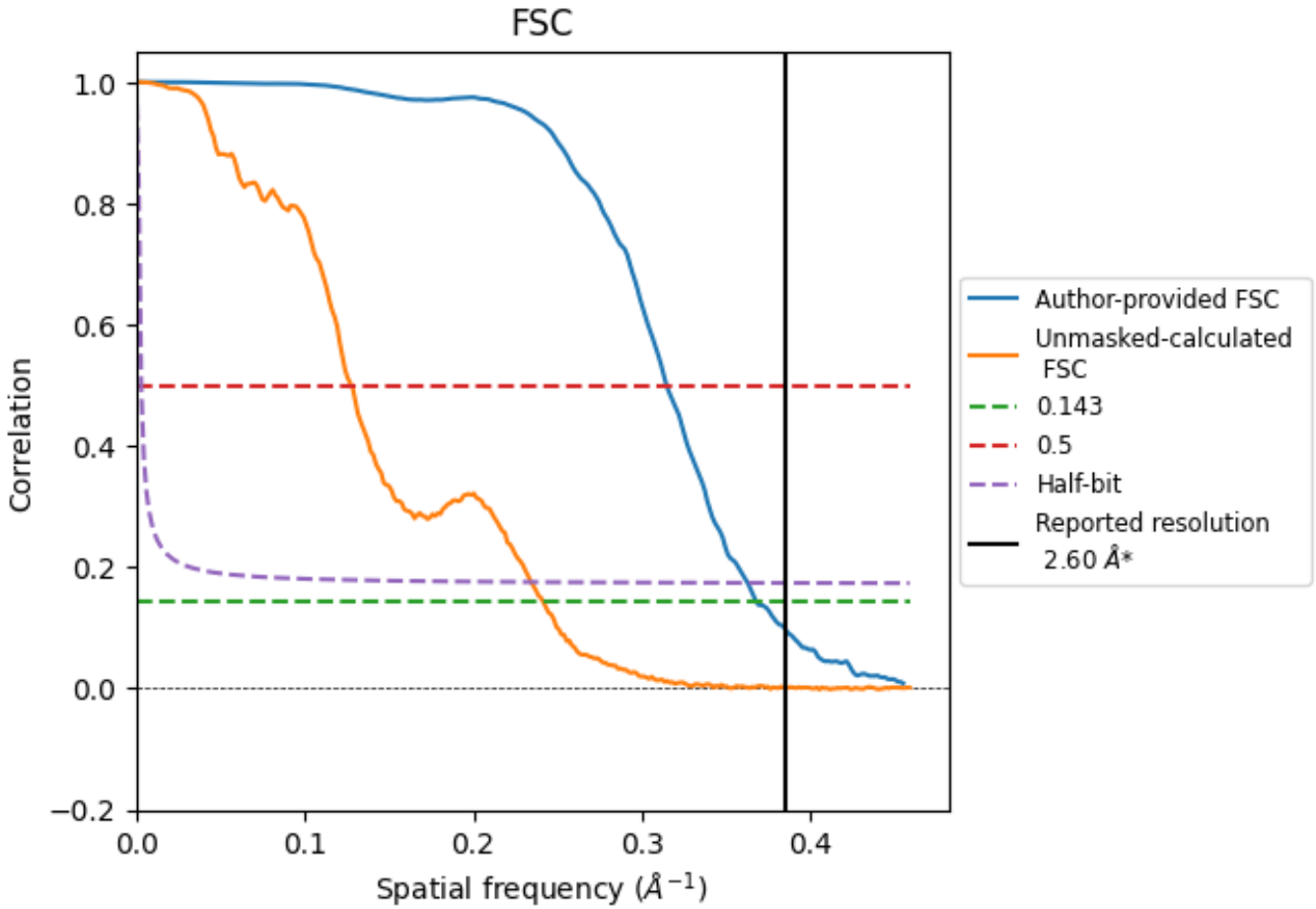


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

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 0.385 Å^{-1}

8.2 Resolution estimates (i)

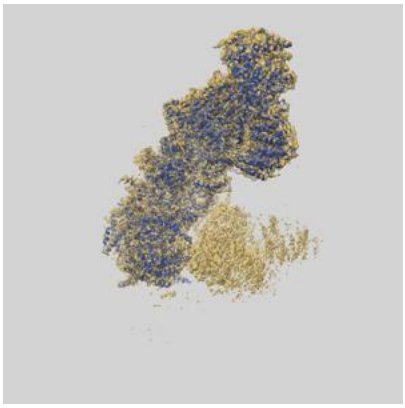
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.72	3.18	2.76
Unmasked-calculated*	4.14	7.83	4.27

*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 4.14 differs from the reported value 2.6 by more than 10 %

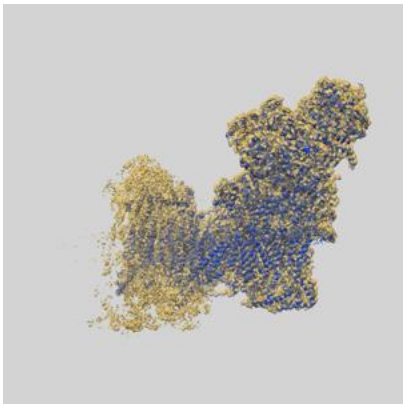
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-65580 and PDB model 9W2U. Per-residue inclusion information can be found in section 3 on page 22.

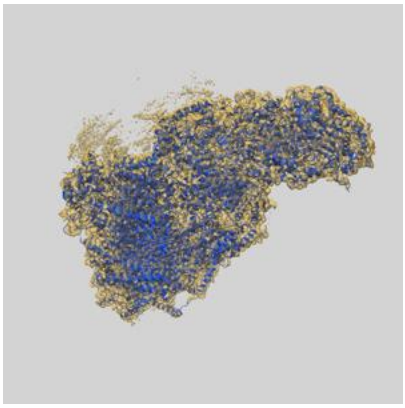
9.1 Map-model overlay



X



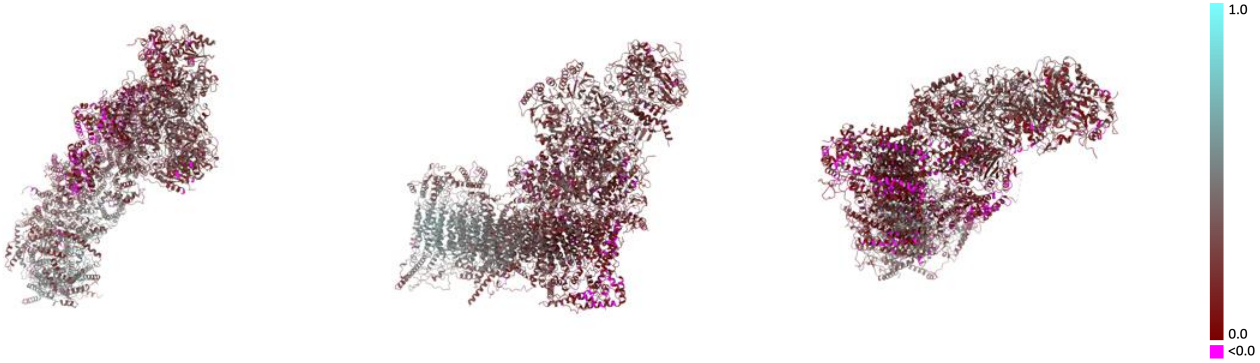
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

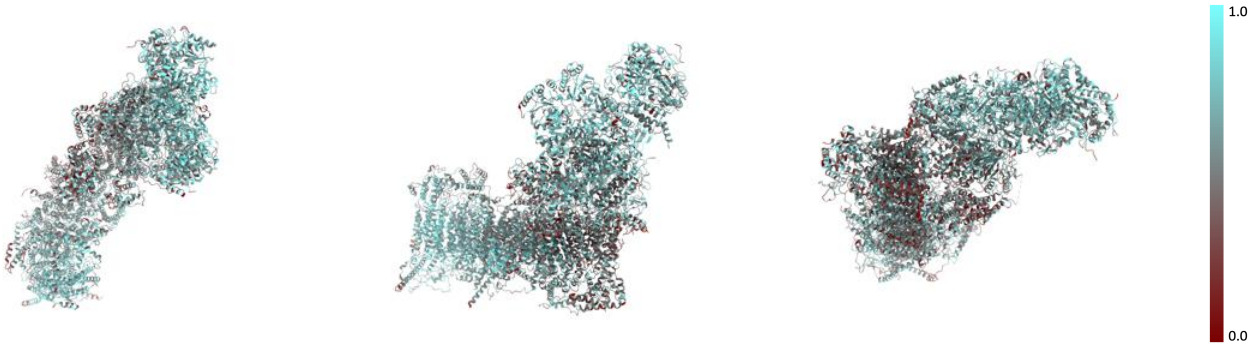
9.2 Q-score mapped to coordinate model



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.

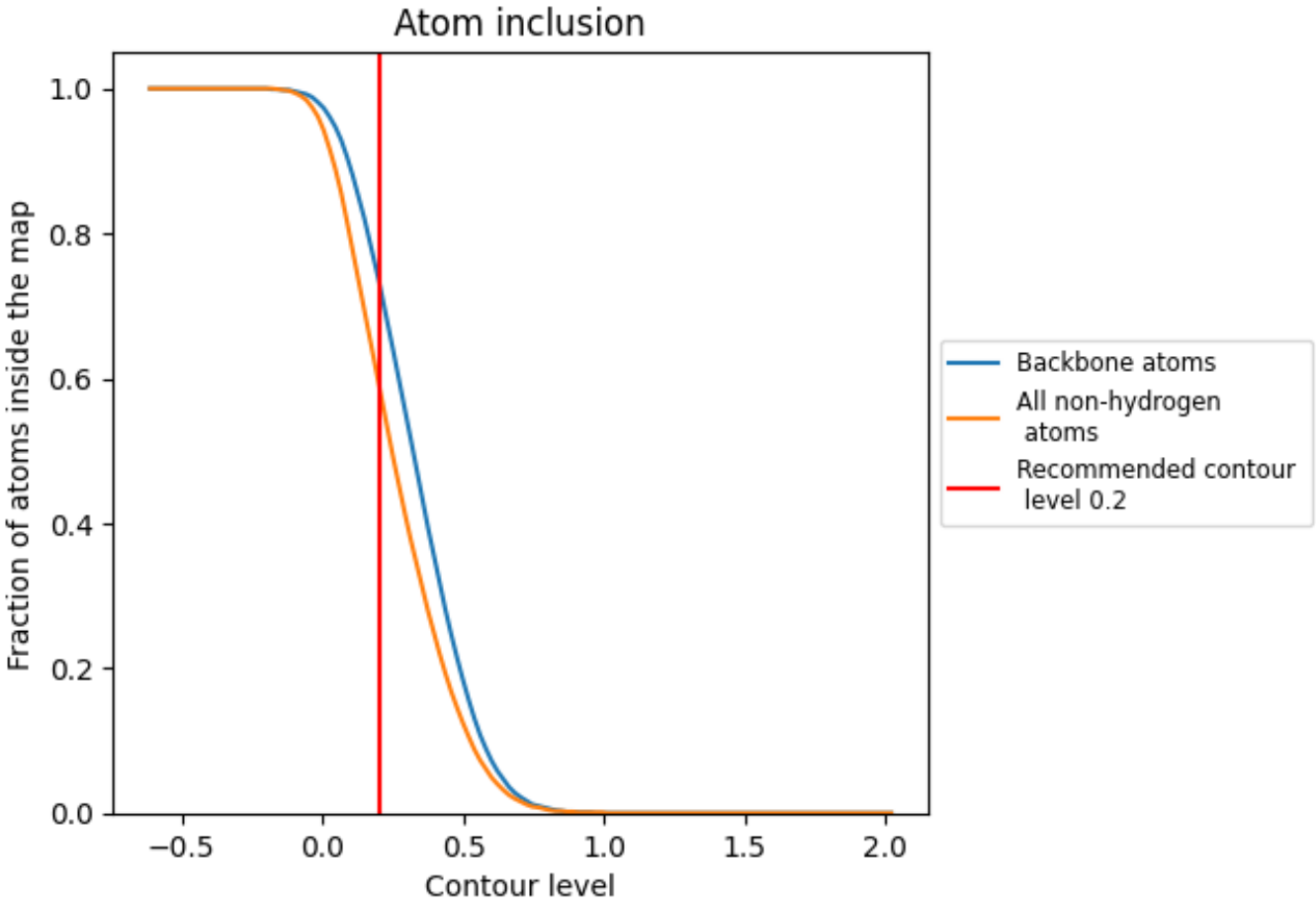
9.3 Atom inclusion mapped to coordinate model



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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5920	0.2670
A	0.4440	0.1710
B	0.6120	0.2540
C	0.5590	0.2030
D	0.5700	0.2150
E	0.6730	0.2690
F	0.6160	0.2130
G	0.6580	0.2860
H	0.4920	0.1790
I	0.6250	0.2360
J	0.5320	0.2400
K	0.5400	0.2520
L	0.7670	0.4830
M	0.6640	0.3410
N	0.5760	0.2420
O	0.4330	0.1360
P	0.5390	0.2640
Q	0.6080	0.2820
R	0.6580	0.3150
S	0.5830	0.2620
T	0.4370	0.2570
U	0.6160	0.3150
V	0.4340	0.1260
W	0.5720	0.2720
X	0.4950	0.1220
Z	0.4810	0.1170
a	0.5050	0.1400
b	0.4070	0.1180
c	0.4120	0.0950
d	0.4470	0.1550
e	0.5550	0.1840
f	0.4660	0.1840
g	0.5520	0.2220
h	0.5700	0.2400
j	0.6340	0.4210



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Continued from previous page...

Chain	Atom inclusion	Q-score
k	0.5970	0.3920
l	0.7240	0.4150
m	0.6520	0.3910
n	0.6620	0.3400
o	0.6980	0.3670
p	0.6520	0.2870
q	0.6110	0.2510
s	0.6390	0.2590
t	0.6160	0.4050
u	0.5440	0.3040
v	0.4910	0.1550