Full wwPDB EM Validation Report ⓘ

Jan 26, 2023 – 05:19 am GMT

PDB ID	:	8BEF
EMDB ID	:	EMD-16000
Title	:	Cryo-EM structure of the Arabidopsis thaliana I+III2 supercomplex (CI membrane core)
Authors	:	Klusch, N.; Kuehlbrandt, W.
Deposited on	:	2022-10-21
Resolution	:	2.13 Å(reported)

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

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

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

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

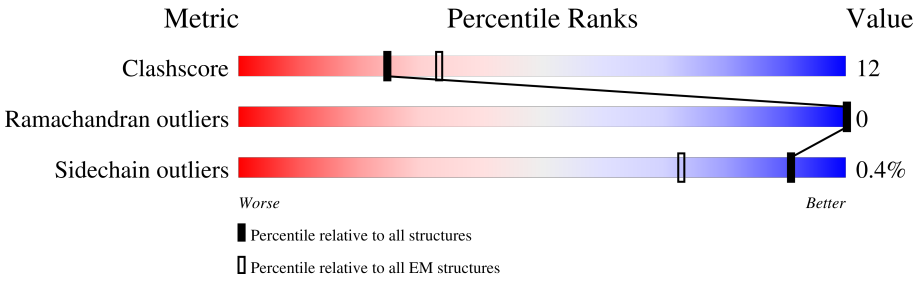
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.13 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	119	5% 60% 18% 21%
2	H	325	78% 22%
3	J	205	66% 19% 15%
4	K	100	73% 26%
5	L	669	9% 89%
6	M	495	40% 14% 46%
7	N	499	79% 19%
8	O	159	64% 14% 23%

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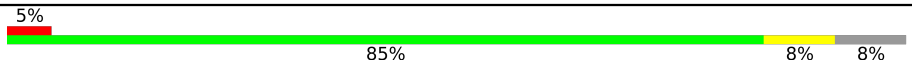
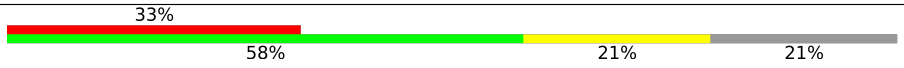
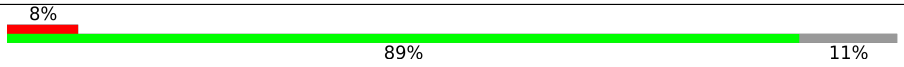
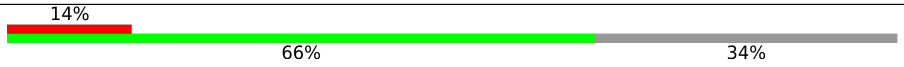
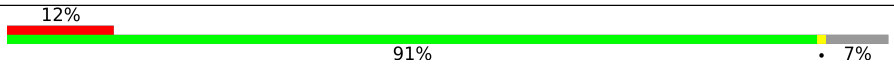
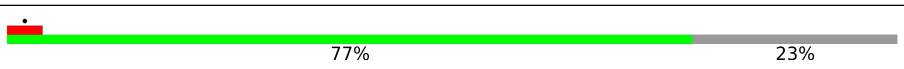
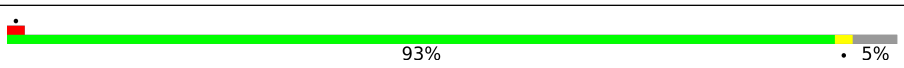
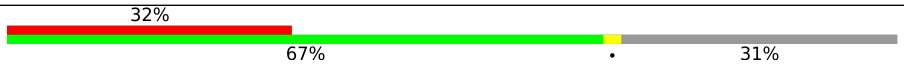
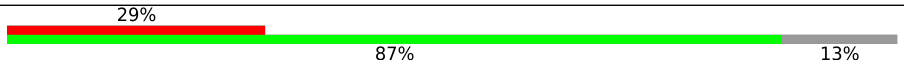
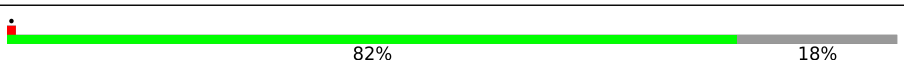
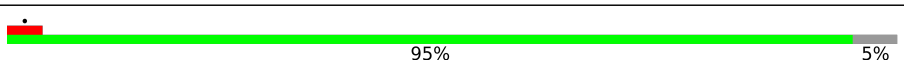
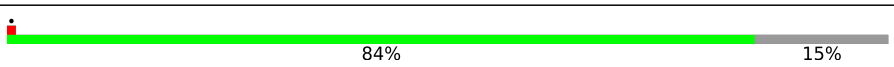
Mol	Chain	Length	Quality of chain
9	X	106	
10	Y	159	
11	Z	143	
12	a	65	
13	b	65	
14	d	81	
15	e	83	
16	f	106	
17	i	98	
18	u	63	
19	v	113	
20	x	256	
21	y	278	
22	z	275	

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 27758 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	94	802	565	110	123	4	0	0

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	324	2536	1719	386	416	15	0	0

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	174	1399	949	213	228	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	K	100	784	525	121	131	7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	SER	conflict	UNP Q04614

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L	76	623	416	97	107	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	91	PHE	SER	conflict	UNP B5TM94

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	269	Total	C	N	O	S	1	0
			2191	1498	328	352	13		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	146	PHE	PRO	variant	UNP P93313
M	326	LEU	PRO	variant	UNP P93313
M	383	PHE	SER	variant	UNP P93313

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	488	Total	C	N	O	S	2	0
			3839	2587	580	644	28		

- Molecule 8 is a protein called AT3G07480.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	123	Total	C	N	O	S	0	0
			963	603	170	186	4		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	X	98	Total	C	N	O	S	0	0
			776	486	134	144	12		

- Molecule 10 is a protein called Outer envelope pore protein 16-3, chloroplastic/mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Y	125	Total	C	N	O	S	0	0
			928	596	162	167	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Z	98	Total	C	N	O	S	0	0
			798	514	137	142	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	a	58	Total	C	N	O	S	0	0
			469	302	84	78	5		

- Molecule 13 is a protein called At2g46540/F11C10.23.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	b	43	Total	C	N	O	S	0	0
			315	206	51	55	3		

- Molecule 14 is a protein called Excitatory amino acid transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	75	Total	C	N	O	S	0	0
			592	382	106	99	5		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	64	Total	C	N	O	S	0	0
			546	338	102	99	7		

- Molecule 16 is a protein called At4g16450.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	101	Total	C	N	O	S	0	0
			765	491	126	143	5		

- Molecule 17 is a protein called P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	i	68	Total	C	N	O	S	0	0
			598	376	113	106	3		

- Molecule 18 is a protein called Uncharacterized protein At1g67785.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	u	55	Total	C	N	O	S	0	0
			463	298	84	78	3		

- Molecule 19 is a protein called Uncharacterized protein At2g27730, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	v	29	Total	C	N	O	0	0
			219	142	38	39		

- Molecule 20 is a protein called Gamma carbonic anhydrase-like 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	x	210	Total	C	N	O	S	0	0
			1629	1043	280	301	5		

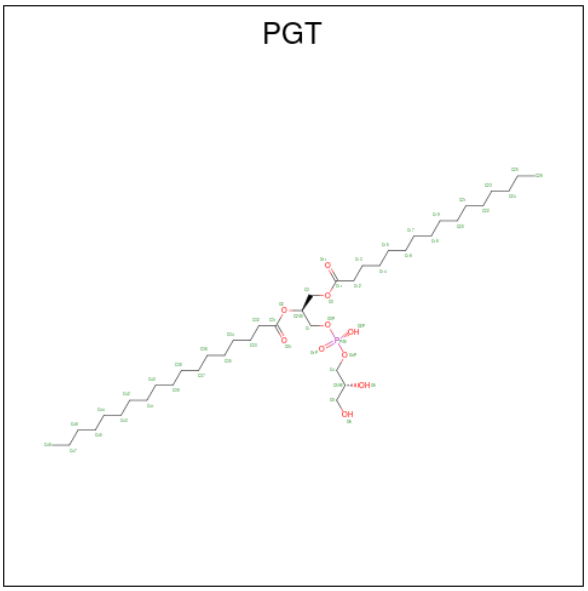
- Molecule 21 is a protein called Gamma carbonic anhydrase 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	y	265	Total	C	N	O	S	0	0
			2013	1258	359	388	8		

- Molecule 22 is a protein called Gamma carbonic anhydrase 1, mitochondrial.

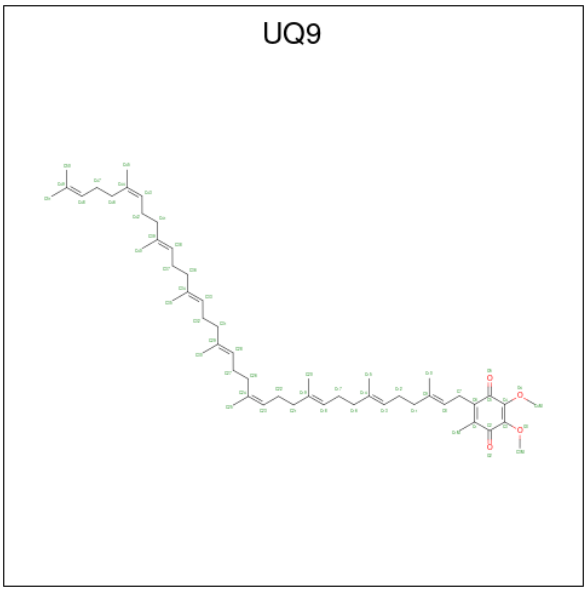
Mol	Chain	Residues	Atoms					AltConf	Trace
22	z	233	Total	C	N	O	S	0	0
			1772	1111	325	330	6		

- Molecule 23 is (1S)-2-{[{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: $C_{40}H_{79}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



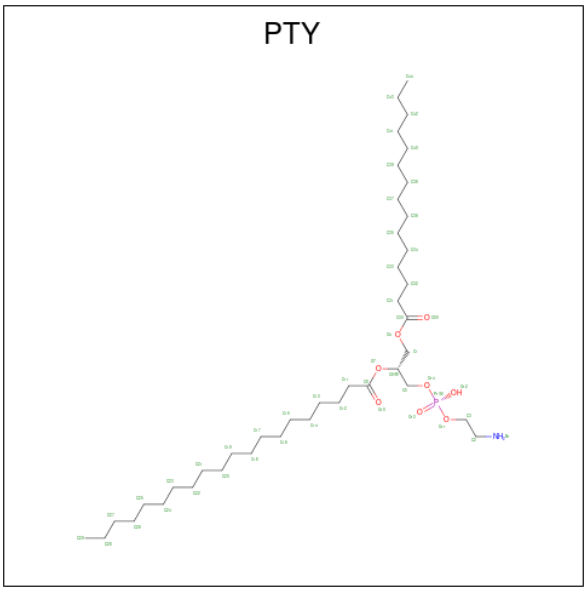
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total 51	C 40	O 10	P 1	0
23	L	1	Total 87	C 65	O 20	P 2	0
23	L	1	Total 87	C 65	O 20	P 2	0
23	M	1	Total 29	C 18	O 10	P 1	0
23	y	1	Total 41	C 30	O 10	P 1	0

- Molecule 24 is Ubiquinone-9 (three-letter code: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
24	H	1	Total	C	O	0
			35	31	4	

- Molecule 25 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
25	H	1	Total	C	N	O	P	0
			50	40	1	8	1	
25	L	1	Total	C	N	O	P	0
			31	21	1	8	1	

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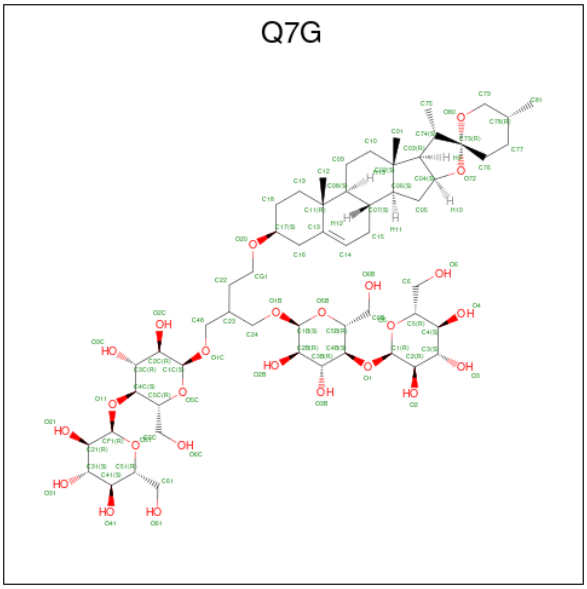
Mol	Chain	Residues	Atoms					AltConf
25	M	1	Total	C	N	O	P	0
			87	67	2	16	2	
25	M	1	Total	C	N	O	P	0
			87	67	2	16	2	
25	N	1	Total	C	N	O	P	0
			174	134	4	32	4	
25	N	1	Total	C	N	O	P	0
			174	134	4	32	4	
25	N	1	Total	C	N	O	P	0
			174	134	4	32	4	
25	N	1	Total	C	N	O	P	0
			174	134	4	32	4	
25	Y	1	Total	C	N	O	P	0
			50	40	1	8	1	
25	z	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 26 is 2-{[(4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranosyl)oxy]methyl}-4-{[(3beta,9beta,14beta,17beta,25R)-spirost-5-en-3-yl]oxy}butyl 4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranoside (three-letter code: Q7G) (formula: $C_{56}H_{92}O_{25}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
26	H	1	Total	C	O	0
			81	56	25	
26	K	1	Total	C	O	0
			81	56	25	

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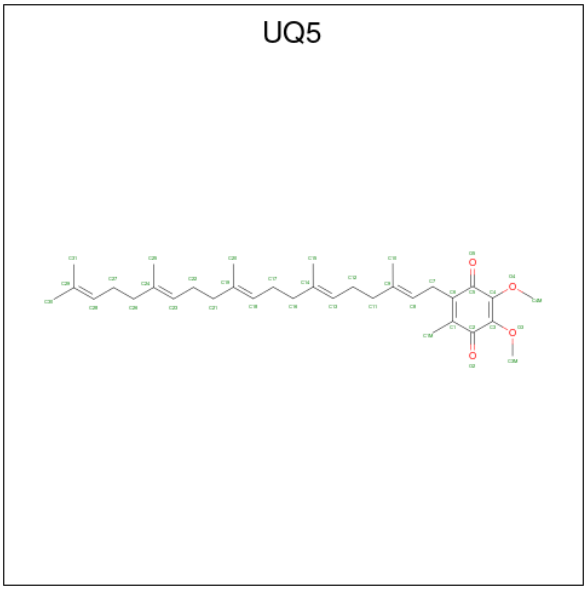
Mol	Chain	Residues	Atoms	AltConf
26	M	1	Total C O 39 34 5	0
26	a	1	Total C O 39 34 5	0

- Molecule 27 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

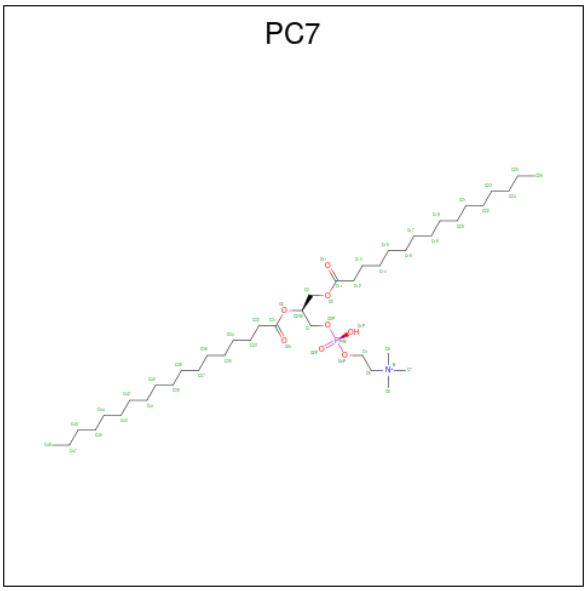
Mol	Chain	Residues	Atoms	AltConf
27	O	1	Total Fe 1 1	0

- Molecule 28 is 2,3-DIMETHOXY-5-METHYL-6-(3,11,15,19-TETRAMETHYL-EICOSA-2,6,10,14,18-PENTAENYL)-[1,4]BENZOQUINONE (three-letter code: UQ5) (formula: $C_{34}H_{50}O_4$) (labeled as "Ligand of Interest" by depositor).



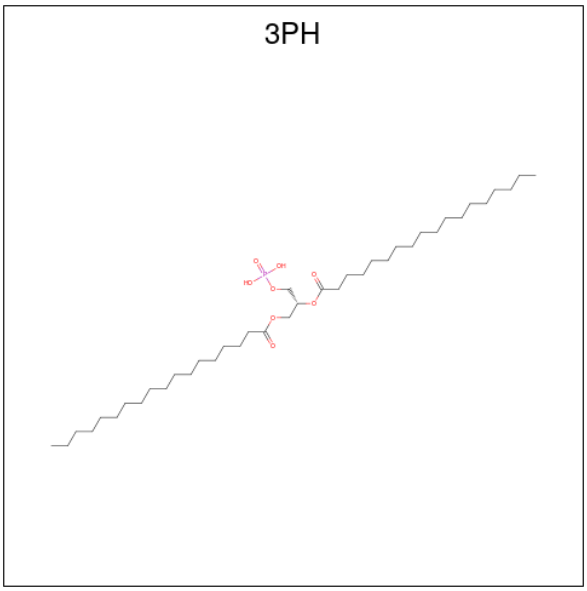
Mol	Chain	Residues	Atoms	AltConf
28	Y	1	Total C O 38 34 4	0

- Molecule 29 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PC7) (formula: $C_{42}H_{85}NO_8P$) (labeled as "Ligand of Interest" by depositor).



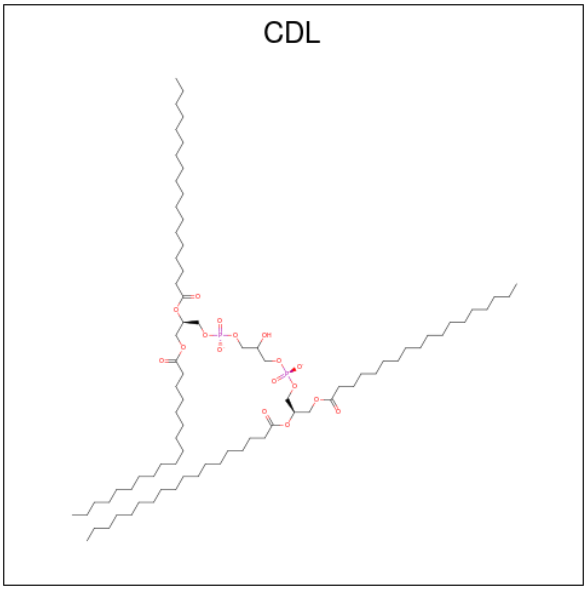
Mol	Chain	Residues	Atoms					AltConf
29	d	1	Total	C	N	O	P	0
			52	42	1	8	1	
29	f	1	Total	C	N	O	P	0
			48	38	1	8	1	
29	v	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 30 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
30	f	1	Total	C	O	P	0
			84	66	16	2	
30	f	1	Total	C	O	P	0
			84	66	16	2	

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

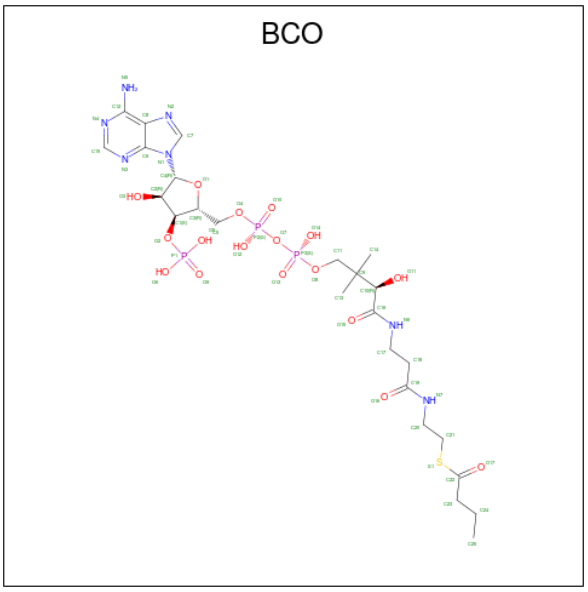


Mol	Chain	Residues	Atoms				AltConf
31	u	1	Total	C	O	P	0
			200	162	34	4	
31	u	1	Total	C	O	P	0
			200	162	34	4	

- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
32	y	1	Total	Zn	0
			1	1	

- Molecule 33 is Butyryl Coenzyme A (three-letter code: BCO) (formula: $C_{25}H_{42}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
33	y	1	Total	C	N	O	P	S	0
			53	25	7	17	3	1	

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		AltConf
34	A	20	Total	O	0
			20	20	
34	H	128	Total	O	0
			128	128	
34	J	63	Total	O	0
			63	63	
34	K	50	Total	O	0
			50	50	
34	L	11	Total	O	0
			11	11	
34	M	30	Total	O	0
			30	30	
34	N	200	Total	O	0
			200	200	
34	O	86	Total	O	0
			86	86	
34	X	19	Total	O	0
			19	19	
34	Y	4	Total	O	0
			4	4	
34	Z	47	Total	O	0
			47	47	

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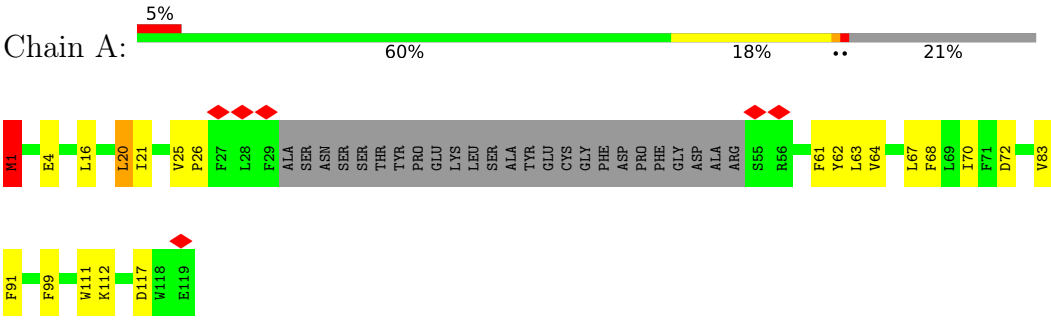
Mol	Chain	Residues	Atoms	AltConf
34	a	19	Total O 19 19	0
34	b	2	Total O 2 2	0
34	d	19	Total O 19 19	0
34	e	30	Total O 30 30	0
34	f	49	Total O 49 49	0
34	i	23	Total O 23 23	0
34	u	10	Total O 10 10	0
34	v	10	Total O 10 10	0
34	x	179	Total O 179 179	0
34	y	165	Total O 165 165	0
34	z	120	Total O 120 120	0

3 Residue-property plots (i)

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

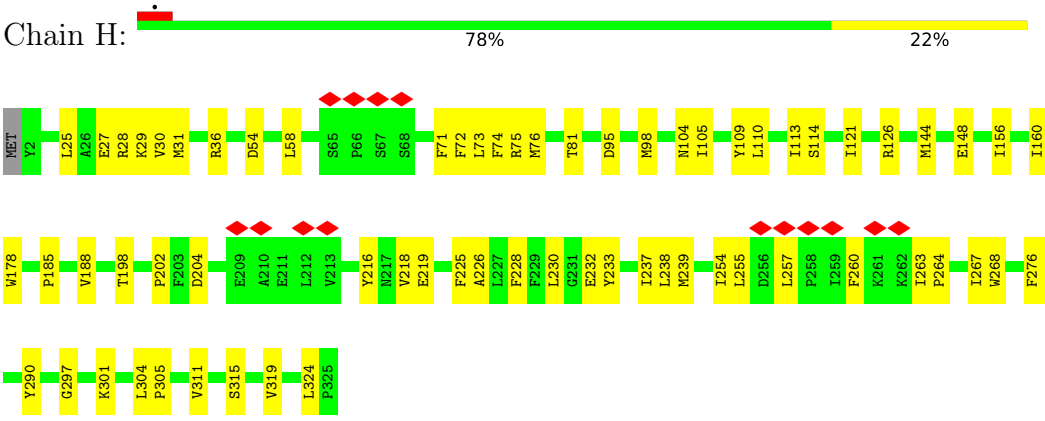
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:



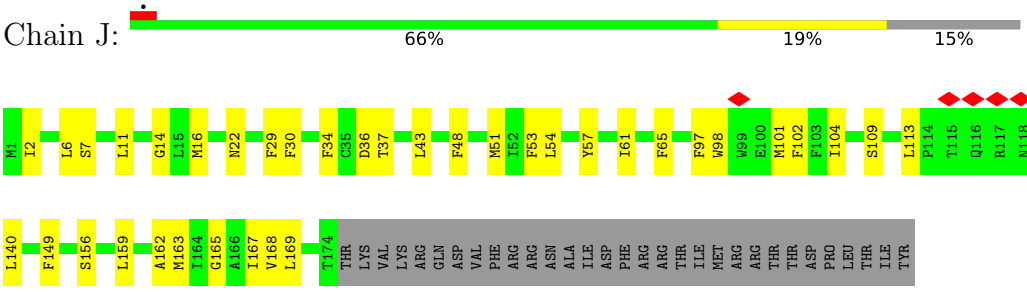
• Molecule 2: NADH-ubiquinone oxidoreductase chain 1

Chain H:



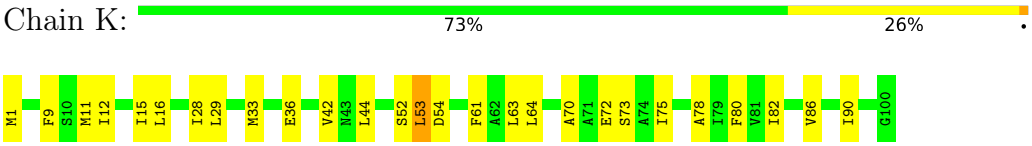
• Molecule 3: NADH-ubiquinone oxidoreductase chain 6

Chain J:



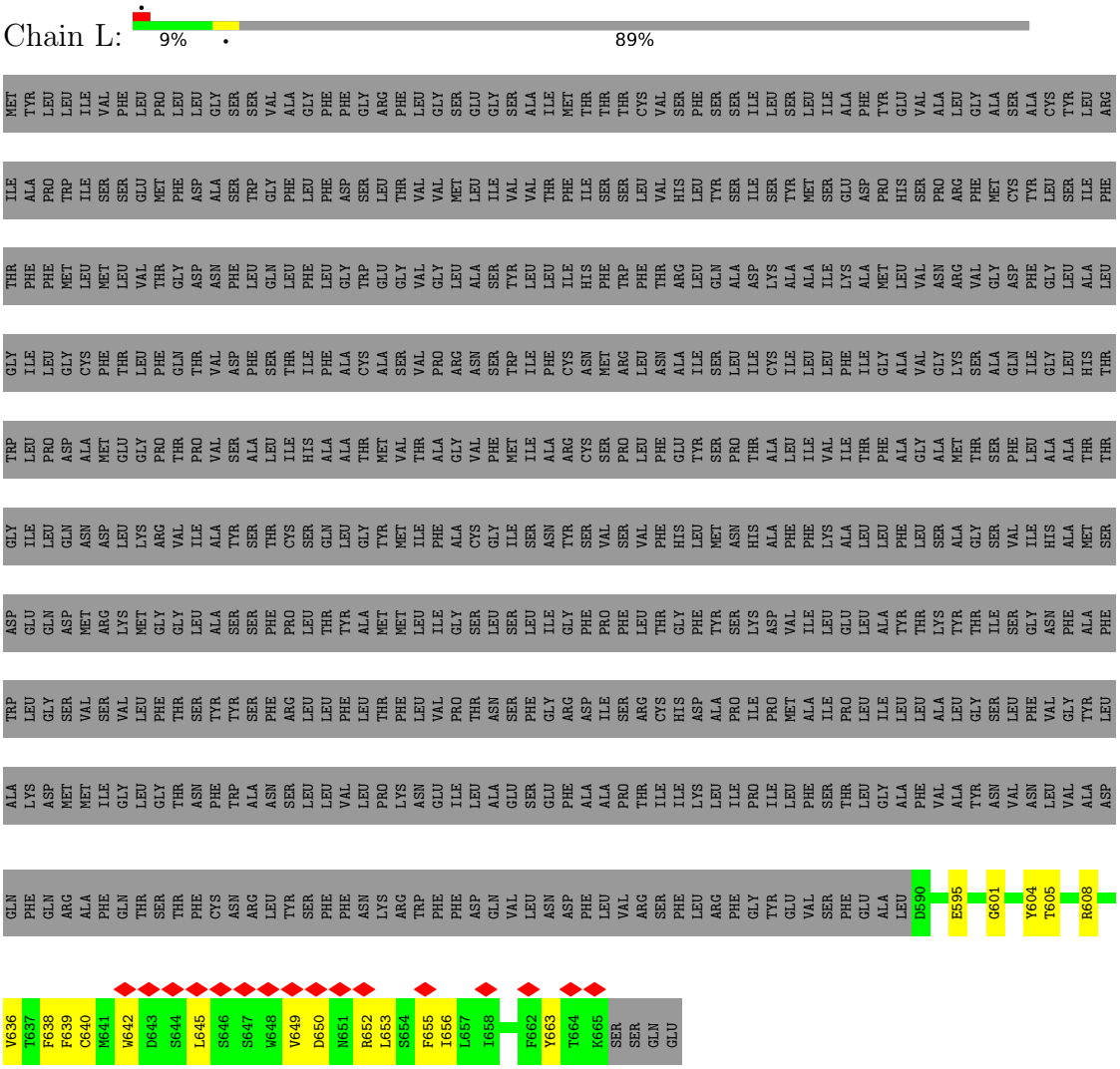
• Molecule 4: NADH-ubiquinone oxidoreductase chain 4L

Chain K:



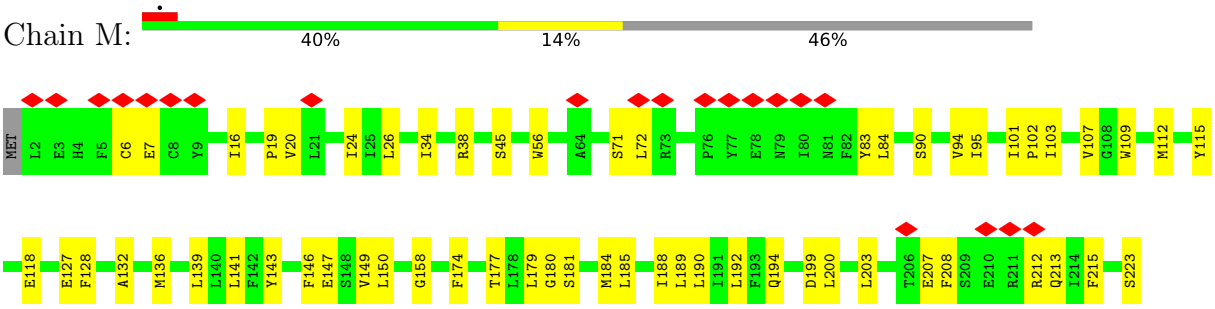
• Molecule 5: NADH-ubiquinone oxidoreductase chain 5

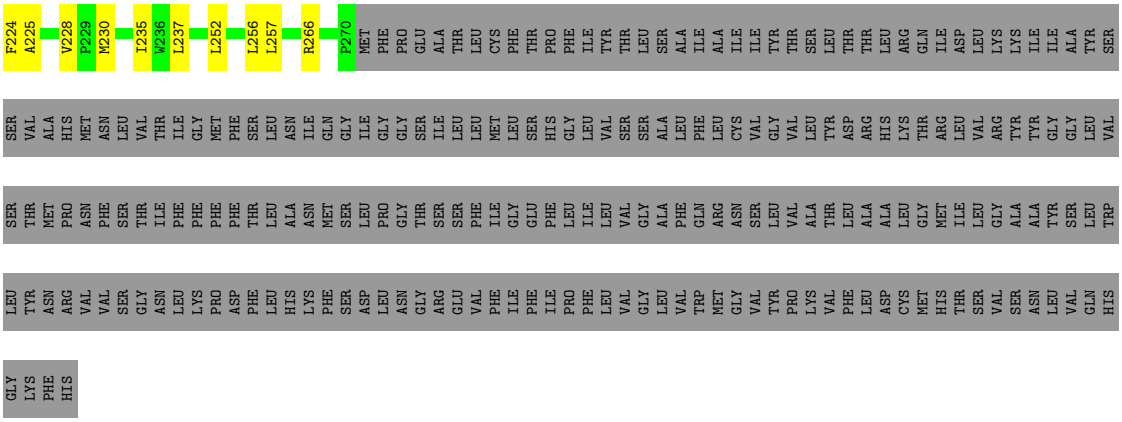
Chain L:



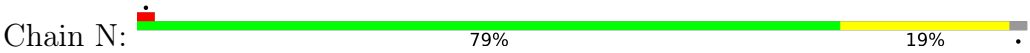
• Molecule 6: NADH-ubiquinone oxidoreductase chain 4

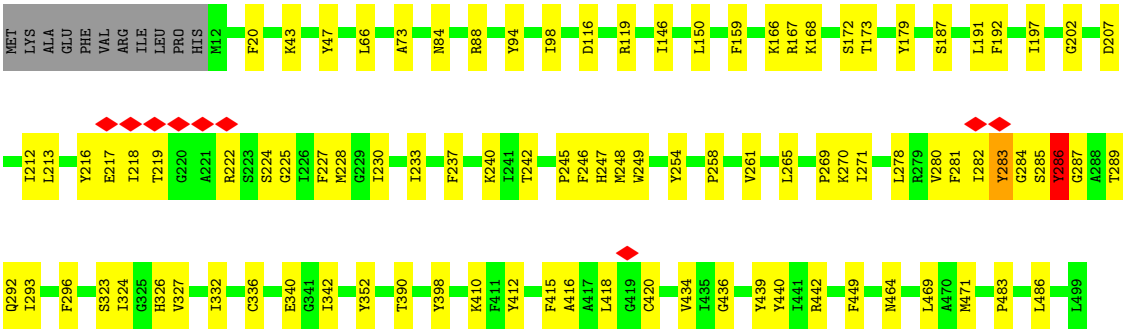
Chain M:



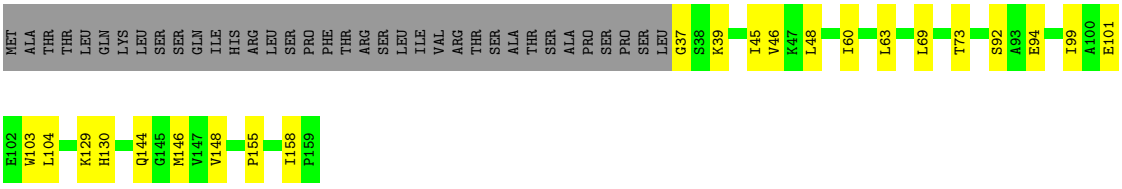


• Molecule 7: NADH-ubiquinone oxidoreductase chain 2

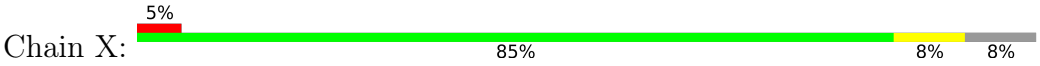


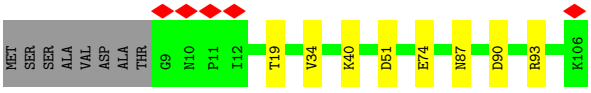


• Molecule 8: AT3G07480.1

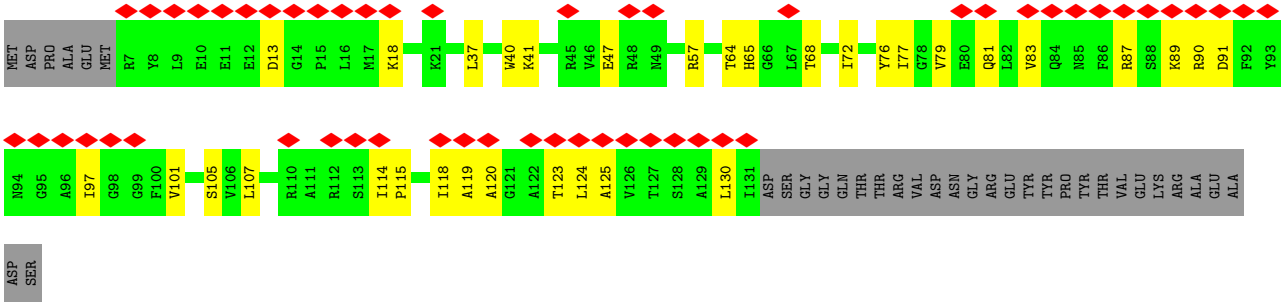


• Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B

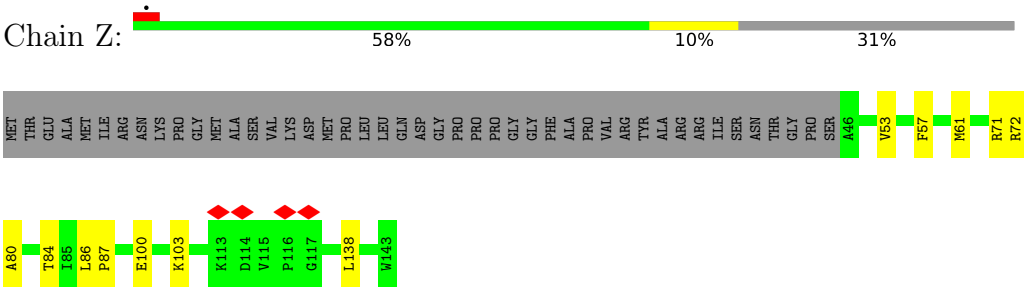




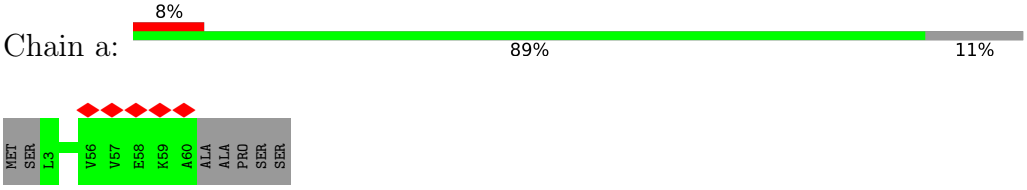
• Molecule 10: Outer envelope pore protein 16-3, chloroplastic/mitochondrial



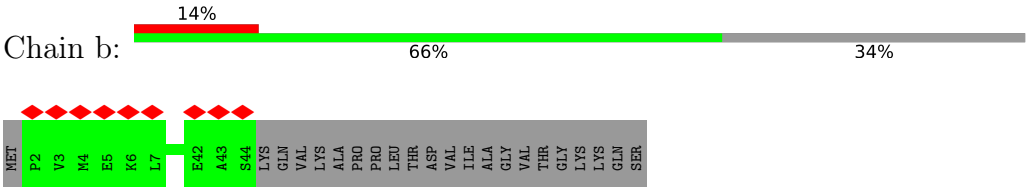
• Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A



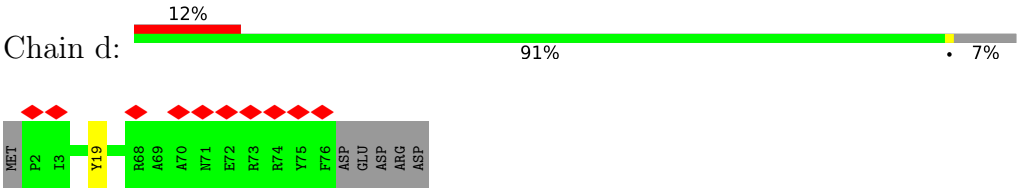
• Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



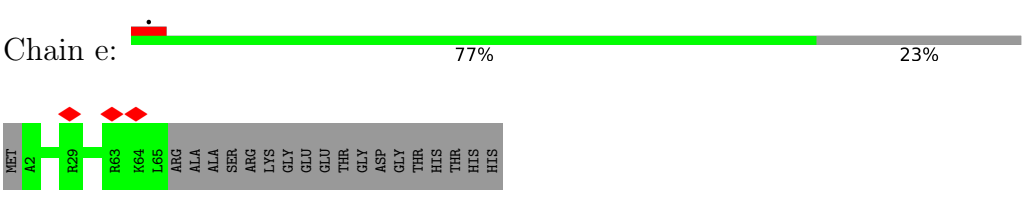
• Molecule 13: At2g46540/F11C10.23



• Molecule 14: Excitatory amino acid transporter

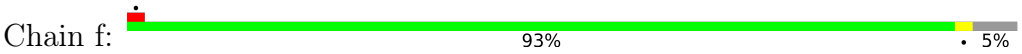


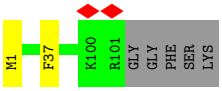
• Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-B



• Molecule 16: At4g16450

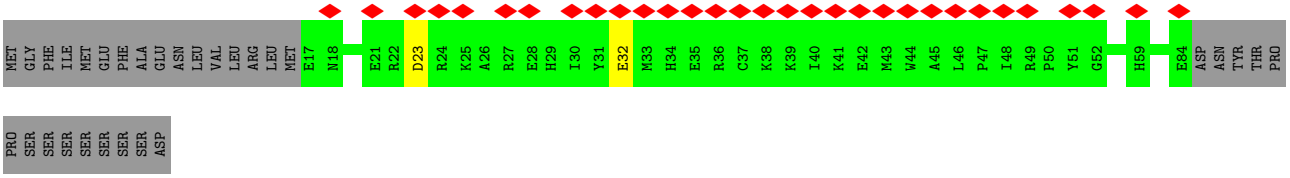
Chain f:





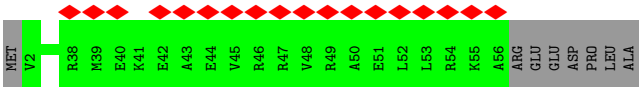
• Molecule 17: P1

Chain i:



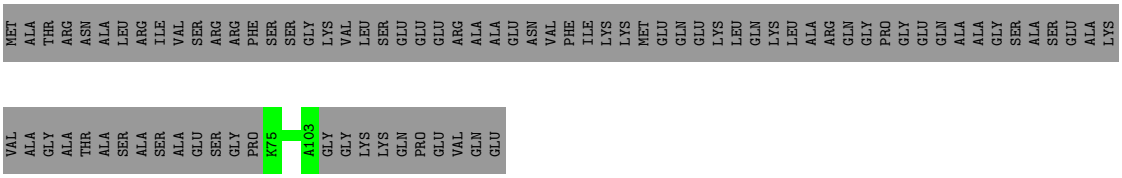
• Molecule 18: Uncharacterized protein At1g67785

Chain u:



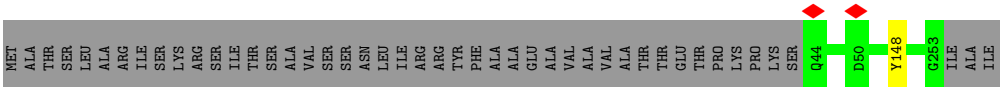
• Molecule 19: Uncharacterized protein At2g27730, mitochondrial

Chain v:



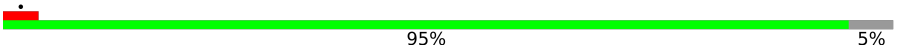
• Molecule 20: Gamma carbonic anhydrase-like 2, mitochondrial

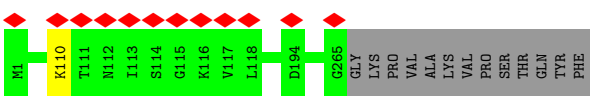
Chain x:



• Molecule 21: Gamma carbonic anhydrase 2, mitochondrial

Chain y:

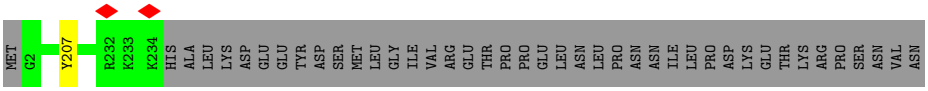




• Molecule 22: Gamma carbonic anhydrase 1, mitochondrial

Chain z:


84%
15%


MET
G2
Y207
R232
K233
K234
HIS
ALA
LEU
LYS
ASP
GLU
GLU
TYR
ASP
SER
MET
LEU
GLY
ILE
VAL
ARG
GLU
THR
PRO
PRO
GLU
LEU
ASN
LEU
PRO
ASN
ASN
ILE
LEU
PRO
ASP
LYS
GLU
THR
LYS
ARG
PRO
SER
ASN
VAL
ASN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	213993	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	215000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	5.559	Depositor
Minimum map value	-2.997	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.262	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	169.608, 156.429, 182.787	wwPDB
Map dimensions	319, 273, 296	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.573, 0.573, 0.573	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, 3PH, FME, PTY, FE, PC7, BCO, UQ5, PGT, Q7G, UQ9, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.30	0/820	0.50	1/1113 (0.1%)
2	H	0.28	0/2609	0.49	0/3553
3	J	0.43	0/1435	0.59	0/1957
4	K	0.70	1/785 (0.1%)	0.74	0/1062
5	L	0.46	1/641 (0.2%)	0.69	1/867 (0.1%)
6	M	0.31	0/2258	0.50	0/3070
7	N	0.47	0/3948	0.62	2/5360 (0.0%)
8	O	0.44	0/979	0.62	0/1326
9	X	0.28	0/790	0.51	0/1060
10	Y	0.41	1/944 (0.1%)	0.58	0/1277
11	Z	0.31	0/820	0.55	0/1108
12	a	0.28	0/481	0.54	0/646
13	b	0.26	0/320	0.54	0/434
14	d	0.44	0/605	0.58	0/815
15	e	0.50	0/559	0.65	0/745
16	f	0.27	0/771	0.48	0/1042
17	i	0.48	0/616	0.80	2/830 (0.2%)
18	u	0.25	0/472	0.45	0/632
19	v	0.25	0/222	0.42	0/300
20	x	0.51	0/1669	0.61	0/2279
21	y	0.41	0/2046	0.59	0/2772
22	z	0.44	0/1804	0.64	0/2441
All	All	0.41	3/25594 (0.0%)	0.58	6/34689 (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
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	650	ASP	C-O	5.71	1.34	1.23
4	K	53	LEU	C-O	-5.40	1.13	1.23
10	Y	125	ALA	C-O	-5.19	1.13	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	650	ASP	CB-CA-C	-9.75	90.89	110.40
17	i	32	GLU	C-N-CA	-7.91	101.92	121.70
7	N	286	TYR	CB-CA-C	5.63	121.66	110.40
1	A	20	LEU	CA-CB-CG	5.43	127.79	115.30
17	i	23	ASP	O-C-N	-5.32	114.18	122.70
7	N	287	GLY	N-CA-C	5.19	126.08	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	FME	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	802	0	817	20	0
2	H	2536	0	2641	73	0
3	J	1399	0	1472	37	0
4	K	784	0	843	33	0
5	L	623	0	617	24	0
6	M	2191	0	2282	54	0
7	N	3839	0	3943	99	0
8	O	963	0	975	14	0
9	X	776	0	775	8	0
10	Y	928	0	960	37	0
11	Z	798	0	780	14	0
12	a	469	0	472	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	b	315	0	338	0	0
14	d	592	0	610	0	0
15	e	546	0	510	0	0
16	f	765	0	766	0	0
17	i	598	0	567	0	0
18	u	463	0	471	0	0
19	v	219	0	227	0	0
20	x	1629	0	1636	0	0
21	y	2013	0	2024	0	0
22	z	1772	0	1771	0	0
23	A	51	0	78	3	0
23	L	87	0	120	3	0
23	M	29	0	28	4	0
23	y	41	0	52	0	0
24	H	35	0	43	4	0
25	H	50	0	79	6	0
25	L	31	0	35	0	0
25	M	87	0	126	3	0
25	N	174	0	252	13	0
25	Y	50	0	79	3	0
25	z	50	0	79	0	0
26	H	81	0	0	3	0
26	K	81	0	0	1	0
26	M	39	0	0	0	0
26	a	39	0	0	0	0
27	O	1	0	0	0	0
28	Y	38	0	50	9	0
29	d	52	0	84	0	0
29	f	48	0	73	0	0
29	v	52	0	84	0	0
30	f	84	0	120	0	0
31	u	200	0	312	0	0
32	y	1	0	0	0	0
33	y	53	0	40	0	0
34	A	20	0	0	3	0
34	H	128	0	0	35	0
34	J	63	0	0	13	0
34	K	50	0	0	16	0
34	L	11	0	0	3	0
34	M	30	0	0	4	0
34	N	200	0	0	28	0
34	O	86	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	X	19	0	0	1	0
34	Y	4	0	0	0	0
34	Z	47	0	0	1	0
34	a	19	0	0	0	0
34	b	2	0	0	0	0
34	d	19	0	0	0	0
34	e	30	0	0	0	0
34	f	49	0	0	0	0
34	i	23	0	0	0	0
34	u	10	0	0	0	0
34	v	10	0	0	0	0
34	x	179	0	0	0	0
34	y	165	0	0	0	0
34	z	120	0	0	0	0
All	All	27758	0	27231	387	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 12.

All (387) 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)
7:N:254:TYR:HA	34:N:647:HOH:O	1.38	1.19
2:H:232:GLU:HB3	34:H:501:HOH:O	1.44	1.16
7:N:412[B]:TYR:HE2	34:N:608:HOH:O	1.22	1.15
34:L:801:HOH:O	6:M:235:ILE:HD12	1.45	1.13
2:H:31:MET:SD	34:H:604:HOH:O	2.07	1.12
2:H:25:LEU:HD11	34:H:520:HOH:O	1.45	1.12
7:N:352:TYR:HD2	34:N:629:HOH:O	1.32	1.11
7:N:412[B]:TYR:CE2	34:N:608:HOH:O	1.94	1.10
3:J:167:ILE:HA	34:J:344:HOH:O	1.51	1.10
5:L:653:LEU:HD11	10:Y:77:ILE:HD11	1.43	1.01
34:J:356:HOH:O	4:K:75:ILE:HD13	1.59	0.99
2:H:232:GLU:OE2	34:H:501:HOH:O	1.79	0.99
5:L:653:LEU:HD11	10:Y:77:ILE:CD1	1.97	0.95
34:M:613:HOH:O	7:N:483:PRO:HD2	1.69	0.93
7:N:412[B]:TYR:CD2	34:N:799:HOH:O	2.20	0.93
9:X:90:ASP:OD1	11:Z:74:LEU:HD11	1.68	0.92
7:N:336:CYS:CB	7:N:420:CYS:SG	2.59	0.91
10:Y:90:ARG:O	10:Y:91:ASP:OD1	1.88	0.91
2:H:198:THR:HB	34:H:508:HOH:O	1.69	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:72:GLU:HG3	34:K:338:HOH:O	1.71	0.90
9:X:34:VAL:HB	34:X:202:HOH:O	1.71	0.89
7:N:167:ARG:HG3	7:N:168:LYS:HE3	1.55	0.89
2:H:202:PRO:HB2	34:H:515:HOH:O	1.75	0.87
2:H:284:ARG:HG2	34:H:604:HOH:O	1.76	0.86
3:J:61:ILE:HG12	34:K:337:HOH:O	1.77	0.84
2:H:104:ASN:ND2	34:H:503:HOH:O	2.10	0.83
7:N:336:CYS:HB3	7:N:420:CYS:SG	2.18	0.83
1:A:91:PHE:H	23:A:201:PGT:H5	1.44	0.81
4:K:54:ASP:HB2	34:K:342:HOH:O	1.81	0.80
7:N:412[B]:TYR:CE2	34:N:799:HOH:O	2.35	0.77
5:L:652:ARG:O	5:L:656:ILE:HG12	1.85	0.76
2:H:73:LEU:HA	2:H:76:MET:HG2	1.68	0.76
3:J:2:ILE:HG22	34:J:355:HOH:O	1.85	0.76
8:O:129:LYS:HE3	8:O:130:HIS:CE1	2.20	0.76
1:A:67:LEU:CD1	34:A:312:HOH:O	2.34	0.75
2:H:216:TYR:CD1	34:H:533:HOH:O	2.39	0.73
2:H:73:LEU:HD23	2:H:76:MET:SD	2.30	0.72
3:J:43:LEU:CD1	34:J:355:HOH:O	2.36	0.72
2:H:264:PRO:HD2	2:H:267:ILE:HD12	1.71	0.72
3:J:65:PHE:CE2	34:K:305:HOH:O	2.43	0.71
6:M:184:MET:HB2	6:M:223:SER:OG	1.89	0.70
6:M:174:PHE:CD1	34:M:626:HOH:O	2.43	0.70
34:K:345:HOH:O	8:O:155:PRO:HG3	1.91	0.70
2:H:204:ASP:OD1	34:H:502:HOH:O	2.09	0.69
5:L:653:LEU:CD1	10:Y:77:ILE:HD11	2.21	0.69
7:N:281:PHE:CG	7:N:290:LEU:HD21	2.28	0.69
11:Z:72:ARG:O	11:Z:76:GLU:HG2	1.94	0.68
2:H:230:LEU:HD11	24:H:401:UQ9:H11A	1.73	0.68
4:K:70:ALA:HA	34:K:337:HOH:O	1.93	0.67
2:H:290:TYR:CD2	34:H:515:HOH:O	2.46	0.67
11:Z:76:GLU:OE1	34:Z:201:HOH:O	2.13	0.67
7:N:116:ASP:OD2	34:N:601:HOH:O	2.13	0.67
2:H:31:MET:CE	34:H:604:HOH:O	2.40	0.66
7:N:119:ARG:NH2	34:N:607:HOH:O	2.28	0.66
2:H:114:SER:OG	2:H:148:GLU:OE1	2.12	0.66
4:K:64:LEU:HD13	7:N:150:LEU:HD11	1.78	0.66
1:A:16:LEU:O	1:A:20:LEU:HD22	1.97	0.64
7:N:436:GLY:HA2	7:N:439:TYR:CE2	2.32	0.64
6:M:252:LEU:HD23	6:M:256:LEU:HD12	1.80	0.64
9:X:90:ASP:OD2	11:Z:74:LEU:HD21	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:68:THR:O	10:Y:72:ILE:HD12	1.98	0.64
7:N:240:LYS:HD3	34:N:613:HOH:O	1.96	0.64
3:J:97:PHE:O	3:J:101:MET:HB3	1.98	0.63
6:M:208:PHE:O	6:M:213:GLN:NE2	2.30	0.63
7:N:248:MET:HG3	34:N:610:HOH:O	1.98	0.63
2:H:232:GLU:CB	34:H:501:HOH:O	2.21	0.62
2:H:279:LEU:HD21	25:H:402:PTY:H221	1.80	0.62
3:J:37:THR:HG23	4:K:44:LEU:HD21	1.81	0.62
7:N:84:ASN:HB3	34:N:734:HOH:O	2.00	0.62
2:H:72:PHE:CE2	2:H:76:MET:SD	2.93	0.62
3:J:43:LEU:HD11	34:J:355:HOH:O	1.96	0.62
5:L:653:LEU:HD11	10:Y:77:ILE:HD12	1.81	0.62
7:N:237:PHE:HD1	34:N:785:HOH:O	1.83	0.62
2:H:284:ARG:CG	34:H:604:HOH:O	2.41	0.61
7:N:43:LYS:HE2	7:N:47:TYR:OH	2.00	0.61
6:M:132:ALA:O	6:M:136:MET:HG2	2.01	0.61
7:N:187:SER:OG	34:N:602:HOH:O	2.14	0.61
2:H:324:LEU:O	11:Z:72:ARG:NH2	2.34	0.60
2:H:126:ARG:HH22	3:J:22:ASN:HD21	1.49	0.60
6:M:56:TRP:HB2	6:M:95:ILE:HD11	1.82	0.60
7:N:283:TYR:C	34:N:628:HOH:O	2.40	0.60
2:H:31:MET:SD	34:H:572:HOH:O	2.57	0.60
6:M:71:SER:OG	6:M:83:TYR:CE1	2.55	0.59
4:K:11:MET:CE	34:K:309:HOH:O	2.50	0.59
10:Y:101:VAL:O	10:Y:105:SER:OG	2.18	0.59
6:M:136:MET:HE3	6:M:141:LEU:HB3	1.83	0.59
7:N:410:LYS:NZ	34:N:617:HOH:O	2.36	0.59
3:J:43:LEU:HD12	34:J:355:HOH:O	1.99	0.59
6:M:150:LEU:HD11	6:M:177:THR:HG21	1.85	0.59
7:N:197:ILE:HD11	7:N:230:ILE:HD13	1.85	0.59
1:A:25:VAL:HG23	1:A:26:PRO:HD3	1.83	0.59
1:A:117:ASP:OD2	2:H:301:LYS:NZ	2.36	0.59
10:Y:47:GLU:OE1	10:Y:57:ARG:NH2	2.33	0.59
7:N:245:PRO:HB3	28:Y:202:UQ5:H23	1.85	0.58
34:L:801:HOH:O	6:M:235:ILE:CD1	2.20	0.58
8:O:99:ILE:HG12	8:O:148:VAL:HG22	1.85	0.58
25:H:402:PTY:H421	11:Z:53:VAL:HG12	1.86	0.57
2:H:58:LEU:HD13	2:H:226:ALA:HB2	1.86	0.57
3:J:104:ILE:HG13	7:N:224:SER:OG	2.04	0.57
25:N:503:PTY:HC21	34:N:748:HOH:O	2.02	0.57
3:J:104:ILE:HD11	7:N:225:GLY:HA2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:73:ALA:HB1	34:N:748:HOH:O	2.05	0.57
7:N:296:PHE:HB3	28:Y:202:UQ5:H311	1.86	0.57
7:N:340:GLU:CD	7:N:340:GLU:H	2.07	0.57
7:N:278:LEU:O	7:N:282:ILE:HB	2.05	0.56
25:N:501:PTY:H162	10:Y:130:LEU:CD1	2.35	0.56
25:N:501:PTY:C16	10:Y:130:LEU:HD12	2.35	0.56
2:H:238:LEU:HD23	34:H:619:HOH:O	2.05	0.56
4:K:28:ILE:HD11	4:K:90:ILE:HD11	1.86	0.56
2:H:233:TYR:CD1	34:H:501:HOH:O	2.53	0.56
6:M:143:TYR:CE1	6:M:185:LEU:HB2	2.41	0.56
10:Y:97:ILE:O	10:Y:101:VAL:HG12	2.06	0.56
6:M:103:ILE:O	6:M:107:VAL:HG23	2.06	0.56
2:H:74:PHE:CE2	34:H:591:HOH:O	2.53	0.56
4:K:11:MET:O	4:K:15:ILE:HG12	2.05	0.55
10:Y:79:VAL:HG11	10:Y:101:VAL:HG11	1.88	0.55
3:J:159:LEU:O	3:J:163:MET:HG3	2.07	0.55
6:M:101:ILE:HG13	6:M:127:GLU:HB2	1.87	0.55
2:H:297:GLY:O	2:H:301:LYS:HB2	2.06	0.55
6:M:71:SER:OG	6:M:83:TYR:CD1	2.56	0.55
3:J:109:SER:CB	34:J:307:HOH:O	2.55	0.55
7:N:227:PHE:CZ	7:N:289:THR:HG21	2.43	0.54
10:Y:107:LEU:HD12	10:Y:120:ALA:HB1	1.89	0.54
2:H:74:PHE:CD2	34:H:591:HOH:O	2.60	0.54
10:Y:115:PRO:HD3	25:Y:201:PTY:HC52	1.90	0.54
2:H:263:ILE:HD11	2:H:268:TRP:CZ2	2.42	0.54
5:L:595:GLU:OE2	34:L:801:HOH:O	2.18	0.54
6:M:112:MET:HA	6:M:115:TYR:HB2	1.89	0.54
2:H:290:TYR:HD2	34:H:531:HOH:O	1.91	0.54
4:K:11:MET:HE1	34:K:309:HOH:O	2.08	0.53
7:N:282:ILE:HD11	7:N:342:ILE:HD11	1.89	0.53
7:N:281:PHE:CD1	7:N:290:LEU:HD21	2.43	0.53
10:Y:87:ARG:HE	10:Y:89:LYS:HB2	1.72	0.53
2:H:218:VAL:HG13	2:H:219:GLU:OE2	2.08	0.53
6:M:199:ASP:O	6:M:203:LEU:HG	2.09	0.53
5:L:663:TYR:HB2	10:Y:107:LEU:HD13	1.90	0.53
7:N:270:LYS:CE	34:N:671:HOH:O	2.55	0.53
7:N:245:PRO:HB3	28:Y:202:UQ5:C23	2.39	0.52
7:N:265:LEU:HB3	34:N:772:HOH:O	2.07	0.52
1:A:67:LEU:HD12	34:A:312:HOH:O	2.01	0.52
1:A:99:PHE:CD1	3:J:156:SER:HB3	2.45	0.52
7:N:352:TYR:CD2	34:N:629:HOH:O	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:257:LEU:HD12	2:H:260:PHE:HE2	1.74	0.52
6:M:225:ALA:HA	6:M:230:MET:HG3	1.91	0.52
34:K:346:HOH:O	7:N:192:PHE:CD2	2.53	0.52
1:A:62:TYR:OH	4:K:78:ALA:HB2	2.10	0.52
7:N:88:ARG:NH2	7:N:207:ASP:OD1	2.43	0.52
3:J:162:ALA:HA	4:K:75:ILE:HD11	1.92	0.52
2:H:232:GLU:CG	34:H:501:HOH:O	2.51	0.51
4:K:82:ILE:HD12	7:N:173:THR:HG22	1.92	0.51
25:N:502:PTY:H312	25:N:502:PTY:H142	1.93	0.51
5:L:653:LEU:HD23	10:Y:76:TYR:HD2	1.74	0.51
7:N:216:TYR:O	7:N:219:THR:OG1	2.27	0.51
8:O:103:TRP:CE2	8:O:146:MET:HA	2.44	0.51
6:M:146:PHE:O	6:M:149:VAL:HG22	2.11	0.51
25:N:501:PTY:H161	10:Y:130:LEU:HD12	1.93	0.51
2:H:160:ILE:HD13	2:H:315:SER:HB3	1.93	0.51
5:L:601:GLY:O	5:L:605:THR:HG22	2.12	0.50
5:L:656:ILE:HG23	10:Y:124:LEU:HD22	1.93	0.50
7:N:261:VAL:O	7:N:265:LEU:HG	2.11	0.50
4:K:11:MET:HE1	7:N:192:PHE:CE2	2.46	0.50
34:K:346:HOH:O	7:N:192:PHE:CE2	2.65	0.50
7:N:247:HIS:N	34:N:610:HOH:O	2.30	0.50
6:M:136:MET:CE	6:M:141:LEU:HB3	2.40	0.50
11:Z:100:GLU:OE2	11:Z:100:GLU:HA	2.10	0.50
6:M:207:GLU:C	34:M:606:HOH:O	2.49	0.50
7:N:218:ILE:HG23	7:N:222:ARG:HD3	1.94	0.50
11:Z:103:LYS:NZ	11:Z:103:LYS:HB3	2.26	0.50
9:X:74:GLU:OE1	9:X:74:GLU:N	2.46	0.49
11:Z:80:ALA:O	11:Z:84:THR:HG23	2.12	0.49
7:N:207:ASP:OD2	34:N:604:HOH:O	2.17	0.49
4:K:33:MET:HA	4:K:36:GLU:OE2	2.13	0.49
4:K:61:PHE:CZ	7:N:191:LEU:HD11	2.47	0.49
2:H:185:PRO:HB3	25:H:402:PTY:H351	1.94	0.49
4:K:86:VAL:HA	34:K:302:HOH:O	2.13	0.49
2:H:81:THR:HG21	2:H:228:PHE:CD1	2.47	0.49
3:J:109:SER:HB3	34:J:307:HOH:O	2.13	0.49
8:O:129:LYS:HE3	8:O:130:HIS:HE1	1.72	0.49
4:K:9:PHE:O	4:K:12:ILE:HG22	2.12	0.49
7:N:324:ILE:O	7:N:327:VAL:HG22	2.13	0.49
10:Y:40:TRP:CZ3	28:Y:202:UQ5:H13	2.48	0.49
2:H:290:TYR:N	34:H:515:HOH:O	2.46	0.48
4:K:53:LEU:HD13	7:N:202:GLY:HA2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:73:SER:HB2	34:K:337:HOH:O	2.12	0.48
6:M:45:SER:HB2	6:M:102:PRO:HG3	1.94	0.48
6:M:136:MET:HE1	6:M:141:LEU:HD13	1.95	0.48
6:M:180:GLY:O	6:M:223:SER:OG	2.23	0.48
6:M:208:PHE:CD2	34:M:606:HOH:O	2.66	0.48
9:X:19:THR:HG21	9:X:87:ASN:HB3	1.94	0.48
7:N:390:THR:HG21	7:N:469:LEU:HG	1.95	0.48
2:H:110:LEU:HD11	2:H:167:LEU:HD11	1.95	0.48
6:M:189:LEU:HD22	7:N:415:PHE:HD2	1.77	0.48
7:N:323:SER:O	7:N:327:VAL:HG13	2.13	0.48
26:H:403:Q7G:O3B	26:H:403:Q7G:O2	2.31	0.48
25:M:503:PTY:HC32	7:N:442:ARG:HD2	1.96	0.48
7:N:285:SER:O	7:N:286:TYR:HD1	1.96	0.48
26:H:403:Q7G:C5B	34:H:523:HOH:O	2.61	0.48
3:J:14:GLY:HA3	4:K:16:LEU:HD13	1.95	0.48
3:J:57:TYR:OH	34:J:301:HOH:O	2.18	0.48
4:K:72:GLU:CG	34:K:338:HOH:O	2.44	0.47
5:L:640:CYS:SG	7:N:222:ARG:NH2	2.87	0.47
4:K:28:ILE:HD13	4:K:80:PHE:CE2	2.49	0.47
5:L:639:PHE:CD2	7:N:289:THR:HG23	2.49	0.47
5:L:645:LEU:O	5:L:649:VAL:HG22	2.14	0.47
7:N:284:GLY:N	34:N:628:HOH:O	2.47	0.47
7:N:289:THR:O	7:N:293:ILE:HG12	2.14	0.47
2:H:109:TYR:CZ	2:H:113:ILE:HD11	2.49	0.47
4:K:61:PHE:CG	7:N:146:ILE:HG12	2.49	0.47
5:L:638:PHE:HA	5:L:642:TRP:CE3	2.49	0.47
23:M:501:PGT:H11	7:N:418:LEU:HD11	1.96	0.47
2:H:54:ASP:HB3	24:H:401:UQ9:H7A	1.95	0.47
23:L:702:PGT:H172	23:L:702:PGT:H142	1.56	0.47
9:X:51:ASP:N	9:X:51:ASP:OD1	2.47	0.47
3:J:149:PHE:N	34:J:310:HOH:O	2.47	0.47
3:J:53:PHE:O	3:J:57:TYR:HB2	2.15	0.47
6:M:224:PHE:O	6:M:228:VAL:HG23	2.15	0.47
10:Y:13:ASP:HA	10:Y:18:LYS:HE2	1.96	0.47
2:H:95:ASP:HB3	2:H:98:MET:HG3	1.97	0.46
1:A:1:FME:O	34:A:301:HOH:O	2.20	0.46
7:N:282:ILE:CD1	7:N:342:ILE:HD11	2.45	0.46
1:A:89:ASP:HB3	23:A:201:PGT:H61	1.97	0.46
25:Y:201:PTY:H232	25:Y:201:PTY:H351	1.97	0.46
6:M:200:LEU:HD21	6:M:266:ARG:HD2	1.97	0.46
7:N:285:SER:HA	34:N:750:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:52:SER:HB2	11:Z:138:LEU:HD11	1.98	0.46
7:N:242:THR:HG22	7:N:249:TRP:CZ2	2.50	0.46
5:L:639:PHE:HZ	7:N:292:GLN:HB3	1.81	0.46
5:L:604:TYR:O	5:L:608:ARG:HG2	2.16	0.46
6:M:184:MET:CB	6:M:223:SER:OG	2.59	0.46
6:M:190:LEU:HD11	23:M:501:PGT:H12	1.98	0.46
2:H:36:ARG:HG2	2:H:36:ARG:HH11	1.79	0.45
7:N:280:VAL:HG12	7:N:281:PHE:CD1	2.51	0.45
6:M:118:GLU:H	6:M:118:GLU:CD	2.20	0.45
7:N:271:ILE:HG23	25:N:503:PTY:H431	1.97	0.45
3:J:11:LEU:HG	4:K:12:ILE:HG12	1.98	0.45
5:L:653:LEU:CD2	10:Y:76:TYR:HD2	2.29	0.45
7:N:94:TYR:OH	25:N:503:PTY:HC51	2.16	0.45
7:N:166:LYS:O	7:N:172:SER:HB3	2.17	0.45
10:Y:124:LEU:HD23	10:Y:124:LEU:HA	1.81	0.45
6:M:208:PHE:HB2	6:M:213:GLN:HG3	1.99	0.45
7:N:486:LEU:N	34:N:621:HOH:O	2.39	0.45
8:O:101:GLU:HA	8:O:104:LEU:HB2	1.99	0.45
3:J:48:PHE:CD1	3:J:137:LEU:HD13	2.51	0.45
6:M:147[A]:GLU:OE2	6:M:181:SER:HB2	2.16	0.45
2:H:254:ILE:O	2:H:255:LEU:HD23	2.16	0.45
3:J:51:MET:HA	3:J:51:MET:HE2	1.98	0.45
25:N:501:PTY:H352	28:Y:202:UQ5:H302	1.99	0.45
6:M:34:ILE:HD11	6:M:112:MET:HB3	1.98	0.45
10:Y:37:LEU:O	10:Y:41:LYS:HG3	2.17	0.44
6:M:194:GLN:HE21	6:M:194:GLN:HB3	1.68	0.44
2:H:188:VAL:HG22	25:H:402:PTY:H232	2.00	0.44
10:Y:119:ALA:O	10:Y:123:THR:OG1	2.32	0.44
2:H:169:GLU:OE2	11:Z:71:ARG:NH1	2.51	0.44
25:H:402:PTY:O12	34:H:504:HOH:O	2.21	0.44
5:L:655:PHE:HE1	25:N:501:PTY:H312	1.82	0.44
7:N:412[A]:TYR:CZ	7:N:416:ALA:HB2	2.52	0.44
8:O:94:GLU:N	34:O:318:HOH:O	2.50	0.44
2:H:27:GLU:HA	2:H:281:ILE:HD13	1.99	0.44
8:O:48:LEU:HB3	8:O:60:ILE:HG12	1.98	0.44
4:K:75:ILE:HB	34:K:324:HOH:O	2.17	0.44
7:N:292:GLN:O	7:N:296:PHE:HD1	2.01	0.44
10:Y:18:LYS:HB3	10:Y:77:ILE:HG21	1.99	0.44
3:J:140:LEU:HD21	4:K:63:LEU:HD22	1.98	0.44
6:M:72:LEU:HD11	6:M:84:LEU:HG	1.99	0.44
7:N:336:CYS:SG	7:N:416:ALA:HB1	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:90:SER:O	6:M:94:VAL:HG23	2.17	0.44
23:M:501:PGT:H322	23:M:501:PGT:H351	1.63	0.44
7:N:159:PHE:CE2	7:N:269:PRO:HG3	2.52	0.44
8:O:92:SER:HB2	8:O:94:GLU:OE2	2.18	0.44
1:A:68:PHE:O	1:A:72:ASP:HB2	2.18	0.43
2:H:202:PRO:HG2	34:H:531:HOH:O	2.18	0.43
5:L:636:VAL:HG13	7:N:228:MET:HE1	1.99	0.43
7:N:213:LEU:HB3	7:N:285:SER:O	2.18	0.43
7:N:464:ASN:HA	25:N:504:PTY:H332	1.99	0.43
8:O:37:GLY:C	8:O:39:LYS:H	2.22	0.43
10:Y:40:TRP:NE1	28:Y:202:UQ5:H102	2.33	0.43
6:M:179:LEU:HD13	7:N:434:VAL:HG21	2.00	0.43
6:M:194:GLN:OE1	6:M:212:ARG:HD2	2.18	0.43
7:N:240:LYS:HD2	7:N:240:LYS:HA	1.82	0.43
25:N:502:PTY:H201	25:N:502:PTY:H172	1.73	0.43
1:A:21:ILE:O	1:A:25:VAL:HG22	2.19	0.43
6:M:20:VAL:O	6:M:24:ILE:HD12	2.18	0.43
8:O:46:VAL:HA	8:O:144:GLN:NE2	2.32	0.43
4:K:54:ASP:CB	34:K:342:HOH:O	2.53	0.43
6:M:237:LEU:HD12	6:M:257:LEU:HD21	2.00	0.43
7:N:284:GLY:CA	34:N:628:HOH:O	2.65	0.43
8:O:48:LEU:HD12	8:O:48:LEU:HA	1.85	0.43
25:Y:201:PTY:H162	25:Y:201:PTY:H191	1.75	0.43
1:A:4:GLU:OE2	1:A:4:GLU:HA	2.17	0.43
1:A:111:TRP:CE2	2:H:301:LYS:HE3	2.53	0.43
2:H:36:ARG:HG2	2:H:36:ARG:NH1	2.34	0.43
26:H:403:Q7G:C3B	34:H:523:HOH:O	2.66	0.43
6:M:237:LEU:HD11	6:M:257:LEU:HD11	2.01	0.43
2:H:28:ARG:HH11	24:H:401:UQ9:H1M	1.84	0.43
2:H:304:LEU:HB3	2:H:305:PRO:HD3	2.00	0.43
2:H:311:VAL:HG13	34:H:592:HOH:O	2.18	0.43
4:K:28:ILE:HD12	4:K:29:LEU:N	2.34	0.43
6:M:139:LEU:HB3	6:M:188:ILE:HG12	2.01	0.43
7:N:270:LYS:HD3	34:N:671:HOH:O	2.19	0.43
2:H:160:ILE:HD12	34:H:592:HOH:O	2.17	0.43
25:H:402:PTY:H231	25:H:402:PTY:H262	1.60	0.43
7:N:326[B]:HIS:CE1	7:N:352:TYR:HB2	2.54	0.43
2:H:71:PHE:CZ	2:H:75:ARG:NH1	2.86	0.43
25:M:503:PTY:H212	25:M:503:PTY:H241	1.78	0.43
10:Y:47:GLU:CD	10:Y:57:ARG:HH22	2.18	0.43
2:H:156:ILE:HG22	34:H:592:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:16:MET:HB3	3:J:29:PHE:CD2	2.53	0.43
23:L:701:PGT:H321	23:L:701:PGT:H351	1.70	0.43
6:M:26:LEU:HD23	6:M:26:LEU:HA	1.88	0.43
9:X:90:ASP:OD1	9:X:93:ARG:NH2	2.52	0.43
23:A:201:PGT:H391	23:A:201:PGT:H361	1.54	0.43
5:L:652:ARG:H	5:L:652:ARG:HG2	1.53	0.43
5:L:656:ILE:HG23	10:Y:124:LEU:CD2	2.48	0.42
7:N:191:LEU:HD12	7:N:191:LEU:HA	1.87	0.42
6:M:20:VAL:HG12	6:M:24:ILE:HD11	2.00	0.42
7:N:398:TYR:HB3	7:N:440:TYR:CZ	2.55	0.42
2:H:81:THR:HG21	2:H:228:PHE:CE1	2.55	0.42
2:H:237:ILE:HA	2:H:277:LEU:HD21	2.02	0.42
3:J:165:GLY:HA2	3:J:168:VAL:HG22	2.00	0.42
1:A:112:LYS:HD2	1:A:112:LYS:HA	1.80	0.42
2:H:121:ILE:HD12	2:H:144:MET:SD	2.60	0.42
2:H:276:PHE:HB3	34:H:556:HOH:O	2.19	0.42
7:N:216:TYR:O	7:N:217:GLU:C	2.57	0.42
3:J:98:TRP:HA	3:J:102:PHE:CD1	2.55	0.42
25:M:503:PTY:H111	25:M:503:PTY:HC6	1.78	0.42
7:N:66:LEU:HD21	7:N:98:ILE:HG23	2.01	0.42
7:N:270:LYS:HE2	34:N:671:HOH:O	2.16	0.42
7:N:471:MET:HG2	25:N:504:PTY:H241	2.02	0.42
8:O:45:ILE:HD13	8:O:63:LEU:HD23	2.02	0.42
28:Y:202:UQ5:H23	28:Y:202:UQ5:H272	1.83	0.42
2:H:225:PHE:HZ	24:H:401:UQ9:H4M	1.83	0.42
3:J:113:LEU:O	34:J:302:HOH:O	2.21	0.42
10:Y:114:ILE:N	10:Y:115:PRO:HD2	2.35	0.42
11:Z:86:LEU:HB3	11:Z:87:PRO:HD3	2.02	0.42
2:H:105:ILE:HD12	2:H:105:ILE:HA	1.94	0.42
2:H:239:MET:CE	34:H:619:HOH:O	2.68	0.42
6:M:6:CYS:SG	6:M:7:GLU:N	2.93	0.42
7:N:197:ILE:HD12	7:N:233:ILE:HD12	2.01	0.42
25:N:504:PTY:H292	25:N:504:PTY:H262	1.87	0.42
9:X:40:LYS:HD2	9:X:40:LYS:HA	1.79	0.42
1:A:61:PHE:HA	1:A:64:VAL:HG12	2.02	0.41
3:J:167:ILE:HD13	34:J:344:HOH:O	2.19	0.41
4:K:61:PHE:CD1	7:N:146:ILE:HG23	2.55	0.41
2:H:178:TRP:CE3	34:H:622:HOH:O	2.71	0.41
2:H:284:ARG:CD	34:H:604:HOH:O	2.65	0.41
5:L:653:LEU:HD21	10:Y:77:ILE:HG13	2.02	0.41
6:M:38:ARG:HG2	6:M:112:MET:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:VAL:HG21	3:J:137:LEU:HG	2.01	0.41
4:K:42:VAL:HG11	7:N:191:LEU:HG	2.02	0.41
7:N:245:PRO:HD2	7:N:246:PHE:CE2	2.54	0.41
2:H:263:ILE:HA	2:H:264:PRO:HD3	1.94	0.41
3:J:7:SER:OG	4:K:9:PHE:HD2	2.02	0.41
23:L:702:PGT:H372	23:L:702:PGT:H401	1.79	0.41
28:Y:202:UQ5:H121	28:Y:202:UQ5:H101	1.75	0.41
11:Z:57:PHE:O	11:Z:61:MET:HG2	2.20	0.41
2:H:319:VAL:HG22	2:H:324:LEU:HD11	2.03	0.41
10:Y:64:THR:O	10:Y:68:THR:HG22	2.19	0.41
1:A:70:ILE:HG13	3:J:163:MET:HG2	2.01	0.41
2:H:29:LYS:HA	2:H:29:LYS:HD2	1.82	0.41
3:J:34:PHE:HE2	34:J:362:HOH:O	2.03	0.41
6:M:38:ARG:HD2	6:M:109:TRP:CD2	2.55	0.41
6:M:158:GLY:HA3	7:N:449:PHE:CE1	2.56	0.41
10:Y:83:VAL:O	10:Y:87:ARG:HB3	2.20	0.41
6:M:200:LEU:CD2	6:M:266:ARG:HD2	2.51	0.41
7:N:332:ILE:HD13	7:N:332:ILE:HA	1.78	0.41
5:L:638:PHE:HA	5:L:642:TRP:HE3	1.85	0.41
11:Z:75:LYS:HE2	11:Z:75:LYS:HB2	1.90	0.41
1:A:85:LEU:HD23	1:A:85:LEU:HA	1.93	0.41
7:N:212:ILE:HG22	7:N:213:LEU:HD23	2.02	0.41
8:O:69:LEU:O	8:O:73:THR:HG23	2.20	0.41
10:Y:65:HIS:HA	10:Y:68:THR:HG22	2.03	0.41
10:Y:114:ILE:HG22	10:Y:118:ILE:HD12	2.02	0.41
7:N:166:LYS:HG3	7:N:258:PRO:HG3	2.02	0.41
2:H:71:PHE:N	34:H:528:HOH:O	2.54	0.40
5:L:653:LEU:HD23	10:Y:76:TYR:CD2	2.55	0.40
6:M:192:LEU:HD23	7:N:415:PHE:HE2	1.86	0.40
1:A:63:LEU:HD23	1:A:63:LEU:HA	1.94	0.40
3:J:169:LEU:HD13	34:K:336:HOH:O	2.21	0.40
6:M:215:PHE:HE2	23:M:501:PGT:P	2.43	0.40
2:H:216:TYR:CG	34:H:533:HOH:O	2.70	0.40
3:J:54:LEU:HD13	26:K:201:Q7G:C79	2.52	0.40
7:N:245:PRO:HD3	28:Y:202:UQ5:H28	2.03	0.40
2:H:30:VAL:HB	2:H:281:ILE:HG21	2.03	0.40
3:J:6:LEU:HB3	3:J:36:ASP:OD1	2.20	0.40
6:M:16:ILE:O	6:M:19:PRO:HD2	2.21	0.40
6:M:38:ARG:HD2	6:M:109:TRP:CE2	2.57	0.40
10:Y:77:ILE:O	10:Y:81:GLN:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	90/119 (76%)	89 (99%)	1 (1%)	0	100	100
2	H	322/325 (99%)	316 (98%)	6 (2%)	0	100	100
3	J	172/205 (84%)	168 (98%)	4 (2%)	0	100	100
4	K	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
5	L	74/669 (11%)	68 (92%)	6 (8%)	0	100	100
6	M	268/495 (54%)	264 (98%)	4 (2%)	0	100	100
7	N	488/499 (98%)	472 (97%)	16 (3%)	0	100	100
8	O	121/159 (76%)	117 (97%)	4 (3%)	0	100	100
9	X	96/106 (91%)	95 (99%)	1 (1%)	0	100	100
10	Y	123/159 (77%)	116 (94%)	7 (6%)	0	100	100
11	Z	96/143 (67%)	96 (100%)	0	0	100	100
12	a	56/65 (86%)	55 (98%)	1 (2%)	0	100	100
13	b	41/65 (63%)	39 (95%)	2 (5%)	0	100	100
14	d	73/81 (90%)	71 (97%)	2 (3%)	0	100	100
15	e	62/83 (75%)	61 (98%)	1 (2%)	0	100	100
16	f	99/106 (93%)	98 (99%)	1 (1%)	0	100	100
17	i	66/98 (67%)	65 (98%)	1 (2%)	0	100	100
18	u	53/63 (84%)	53 (100%)	0	0	100	100
19	v	27/113 (24%)	27 (100%)	0	0	100	100
20	x	208/256 (81%)	206 (99%)	2 (1%)	0	100	100
21	y	263/278 (95%)	261 (99%)	2 (1%)	0	100	100
22	z	231/275 (84%)	228 (99%)	3 (1%)	0	100	100
All	All	3127/4462 (70%)	3061 (98%)	66 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	85/105 (81%)	85 (100%)	0	100	100
2	H	271/272 (100%)	271 (100%)	0	100	100
3	J	156/186 (84%)	155 (99%)	1 (1%)	86	89
4	K	85/85 (100%)	85 (100%)	0	100	100
5	L	67/568 (12%)	67 (100%)	0	100	100
6	M	240/434 (55%)	239 (100%)	1 (0%)	91	93
7	N	408/416 (98%)	404 (99%)	4 (1%)	76	79
8	O	108/141 (77%)	107 (99%)	1 (1%)	78	81
9	X	88/94 (94%)	88 (100%)	0	100	100
10	Y	92/120 (77%)	92 (100%)	0	100	100
11	Z	79/115 (69%)	79 (100%)	0	100	100
12	a	48/53 (91%)	48 (100%)	0	100	100
13	b	35/53 (66%)	35 (100%)	0	100	100
14	d	60/66 (91%)	59 (98%)	1 (2%)	60	63
15	e	59/73 (81%)	59 (100%)	0	100	100
16	f	80/83 (96%)	79 (99%)	1 (1%)	69	73
17	i	62/90 (69%)	62 (100%)	0	100	100
18	u	47/54 (87%)	47 (100%)	0	100	100
19	v	22/84 (26%)	22 (100%)	0	100	100
20	x	179/216 (83%)	178 (99%)	1 (1%)	86	89
21	y	221/232 (95%)	220 (100%)	1 (0%)	88	91
22	z	188/228 (82%)	187 (100%)	1 (0%)	88	91
All	All	2680/3768 (71%)	2668 (100%)	12 (0%)	91	93

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	30	PHE
6	M	128	PHE
7	N	20	PHE
7	N	179	TYR
7	N	283	TYR
7	N	286	TYR
8	O	158	ILE
14	d	19	TYR
16	f	37	PHE
20	x	148	TYR
21	y	110	LYS
22	z	207	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	FME	A	1	1	8,9,10	1.69	1 (12%)	7,9,11	1.60	1 (14%)
16	FME	f	1	16	8,9,10	1.69	1 (12%)	7,9,11	1.56	1 (14%)
4	FME	K	1	4	8,9,10	0.83	0	7,9,11	2.08	3 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	0/7/9/11	-
16	FME	f	1	16	-	5/7/9/11	-
4	FME	K	1	4	-	5/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	f	1	FME	O-C	4.12	1.36	1.19
1	A	1	FME	O-C	4.09	1.36	1.19

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	FME	O-C-CA	-3.68	115.14	124.78
4	K	1	FME	C-CA-N	3.60	116.22	109.73
16	f	1	FME	O-C-CA	-3.40	115.87	124.78
4	K	1	FME	O-C-CA	-2.97	116.99	124.78
4	K	1	FME	CG-CB-CA	-2.40	106.29	112.95

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	1	FME	O1-CN-N-CA
4	K	1	FME	N-CA-CB-CG
16	f	1	FME	O1-CN-N-CA
16	f	1	FME	C-CA-CB-CG
16	f	1	FME	O-C-CA-CB
16	f	1	FME	CA-CB-CG-SD
4	K	1	FME	CA-CB-CG-SD
16	f	1	FME	CB-CG-SD-CE
4	K	1	FME	C-CA-CB-CG
4	K	1	FME	CB-CG-SD-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 2 are monoatomic - leaving 29 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	$\#\|Z\| > 2$
23	PGT	L	701	-	35,35,50	1.24	3 (8%)	38,41,56	1.10	2 (5%)
31	CDL	u	101	-	99,99,99	0.89	7 (7%)	105,111,111	1.07	5 (4%)
33	BCO	y	302	-	47,55,55	3.80	21 (44%)	58,81,81	2.38	12 (20%)
23	PGT	M	501	-	28,28,50	1.35	3 (10%)	31,34,56	1.20	2 (6%)
23	PGT	L	702	-	50,50,50	1.08	3 (6%)	53,56,56	1.08	2 (3%)
31	CDL	u	102	-	99,99,99	0.87	8 (8%)	105,111,111	1.07	4 (3%)
26	Q7G	K	201	-	90,90,90	0.78	2 (2%)	136,138,138	1.33	19 (13%)
29	PC7	f	203	-	47,47,51	1.00	4 (8%)	53,55,59	1.07	2 (3%)
29	PC7	v	201	-	51,51,51	0.97	4 (7%)	57,59,59	1.13	3 (5%)
30	3PH	f	201	-	40,40,47	0.67	1 (2%)	44,45,52	0.73	2 (4%)
25	PTY	N	504	-	49,49,49	0.86	4 (8%)	52,54,54	1.10	2 (3%)
26	Q7G	H	403	-	90,90,90	0.70	3 (3%)	136,138,138	1.17	10 (7%)
26	Q7G	a	101	-	44,44,90	0.65	0	66,68,138	1.32	9 (13%)
25	PTY	N	501	-	39,39,49	0.97	4 (10%)	42,44,54	1.11	2 (4%)
28	UQ5	Y	202	-	38,38,38	0.48	0	46,49,49	0.97	4 (8%)
25	PTY	z	301	-	49,49,49	0.85	3 (6%)	52,54,54	1.17	3 (5%)
26	Q7G	M	504	-	44,44,90	0.75	1 (2%)	66,68,138	1.56	14 (21%)
24	UQ9	H	401	-	35,35,58	2.48	11 (31%)	42,45,73	2.16	13 (30%)
25	PTY	H	402	-	49,49,49	0.88	4 (8%)	52,54,54	1.03	2 (3%)
23	PGT	y	303	-	40,40,50	1.17	5 (12%)	43,46,56	1.11	2 (4%)
25	PTY	L	703	-	30,30,49	1.10	4 (13%)	33,35,54	1.16	2 (6%)
25	PTY	N	502	-	38,38,49	0.98	4 (10%)	41,43,54	1.15	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	PC7	d	101	-	51,51,51	0.42	0	57,59,59	0.52	0
25	PTY	Y	201	-	49,49,49	0.89	4 (8%)	52,54,54	1.05	2 (3%)
25	PTY	M	502	-	36,36,49	0.99	4 (11%)	39,41,54	1.12	2 (5%)
25	PTY	M	503	-	49,49,49	0.89	4 (8%)	52,54,54	1.20	3 (5%)
23	PGT	A	201	-	50,50,50	1.08	4 (8%)	53,56,56	1.08	3 (5%)
25	PTY	N	503	-	44,44,49	0.93	4 (9%)	47,49,54	1.05	2 (4%)
30	3PH	f	202	-	42,42,47	0.67	1 (2%)	46,47,52	0.64	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PGT	L	701	-	-	18/40/40/55	-
31	CDL	u	101	-	-	49/110/110/110	-
33	BCO	y	302	-	-	10/50/70/70	0/3/3/3
23	PGT	M	501	-	-	19/33/33/55	-
23	PGT	L	702	-	-	25/55/55/55	-
31	CDL	u	102	-	-	44/110/110/110	-
26	Q7G	K	201	-	-	6/32/200/200	0/10/10/10
29	PC7	f	203	-	-	22/51/51/55	-
29	PC7	v	201	-	-	25/55/55/55	-
30	3PH	f	201	-	-	14/42/42/49	-
25	PTY	N	504	-	-	15/53/53/53	-
26	Q7G	H	403	-	-	12/32/200/200	0/10/10/10
26	Q7G	a	101	-	-	4/12/100/200	0/6/6/10
25	PTY	N	501	-	-	22/43/43/53	-
28	UQ5	Y	202	-	-	12/33/57/57	0/1/1/1
25	PTY	z	301	-	-	27/53/53/53	-
26	Q7G	M	504	-	-	1/12/100/200	0/6/6/10
24	UQ9	H	401	-	-	9/30/54/81	0/1/1/1
25	PTY	H	402	-	-	19/53/53/53	-
23	PGT	y	303	-	-	28/45/45/55	-
25	PTY	L	703	-	-	18/34/34/53	-
25	PTY	N	502	-	-	19/42/42/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PC7	d	101	-	-	27/55/55/55	-
25	PTY	Y	201	-	-	19/53/53/53	-
25	PTY	M	502	-	-	18/40/40/53	-
25	PTY	M	503	-	-	25/53/53/53	-
23	PGT	A	201	-	-	26/55/55/55	-
25	PTY	N	503	-	-	22/48/48/53	-
30	3PH	f	202	-	-	18/44/44/49	-

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	y	302	BCO	C15-N4	-14.64	1.06	1.33
24	H	401	UQ9	C6-C1	9.79	1.53	1.35
33	y	302	BCO	C15-N3	-8.60	1.18	1.32
33	y	302	BCO	C8-C6	7.86	1.61	1.40
33	y	302	BCO	C19-N7	6.89	1.49	1.33
33	y	302	BCO	C16-N6	6.76	1.48	1.33
33	y	302	BCO	C6-N3	6.16	1.44	1.35
33	y	302	BCO	C12-N4	-5.45	1.13	1.37
33	y	302	BCO	O1-C4	4.41	1.47	1.41
24	H	401	UQ9	C4-C3	4.39	1.54	1.36
33	y	302	BCO	C8-N2	-4.20	1.24	1.39
24	H	401	UQ9	C7-C8	4.20	1.56	1.50
33	y	302	BCO	C22-S1	3.51	1.84	1.76
33	y	302	BCO	O15-C16	-3.31	1.16	1.23
30	f	202	3PH	P-O11	3.28	1.70	1.60
33	y	302	BCO	C24-C23	-3.25	1.34	1.51
30	f	201	3PH	P-O11	3.23	1.70	1.60
33	y	302	BCO	P1-O2	3.22	1.65	1.59
33	y	302	BCO	C12-N5	3.21	1.45	1.34
23	M	501	PGT	O3-C11	3.21	1.42	1.33
23	A	201	PGT	O3-C11	3.18	1.42	1.33
23	L	701	PGT	O3-C11	3.12	1.42	1.33
23	L	702	PGT	O3-C11	3.08	1.42	1.33
33	y	302	BCO	O16-C19	-3.08	1.17	1.23
23	L	702	PGT	O2-C31	3.03	1.42	1.34
23	L	701	PGT	O2-C31	3.02	1.42	1.34
23	M	501	PGT	O2-C31	3.02	1.42	1.34
33	y	302	BCO	C2-C4	-3.02	1.49	1.53
33	y	302	BCO	O11-C10	-2.90	1.37	1.42
23	y	303	PGT	O2-C31	2.89	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	K	201	Q7G	O1B-C1B	2.89	1.45	1.40
23	A	201	PGT	O2-C31	2.86	1.42	1.34
31	u	101	CDL	OA6-CA4	-2.82	1.39	1.46
23	y	303	PGT	O3-C11	2.79	1.41	1.33
31	u	102	CDL	OA6-CA4	-2.70	1.39	1.46
25	z	301	PTY	O7-C6	-2.59	1.40	1.46
25	Y	201	PTY	O7-C6	-2.58	1.40	1.46
26	H	403	Q7G	C11-C08	-2.57	1.51	1.56
25	z	301	PTY	O4-C1	-2.54	1.39	1.45
24	H	401	UQ9	C11-C9	2.53	1.56	1.51
31	u	101	CDL	OA8-CA7	2.53	1.40	1.33
31	u	101	CDL	OB8-CB7	2.53	1.40	1.33
25	H	402	PTY	O7-C6	-2.52	1.40	1.46
25	L	703	PTY	O7-C6	-2.51	1.40	1.46
33	y	302	BCO	C18-C19	2.51	1.56	1.51
25	N	503	PTY	O7-C6	-2.50	1.40	1.46
31	u	101	CDL	OB6-CB5	2.49	1.41	1.34
31	u	102	CDL	OB6-CB4	-2.49	1.40	1.46
25	N	502	PTY	O7-C6	-2.49	1.40	1.46
25	N	503	PTY	O4-C30	2.48	1.40	1.33
31	u	102	CDL	OB8-CB7	2.47	1.40	1.33
25	M	503	PTY	O7-C6	-2.47	1.40	1.46
29	f	203	PC7	O2-C2	-2.46	1.40	1.46
24	H	401	UQ9	C16-C14	2.46	1.56	1.51
29	v	201	PC7	O3-C11	2.46	1.40	1.33
25	Y	201	PTY	O4-C30	2.42	1.40	1.33
25	N	501	PTY	O4-C30	2.42	1.40	1.33
25	M	503	PTY	O4-C30	2.41	1.40	1.33
25	M	503	PTY	O7-C8	2.40	1.41	1.34
25	H	402	PTY	O4-C30	2.40	1.40	1.33
24	H	401	UQ9	C21-C19	2.39	1.56	1.51
25	M	502	PTY	O4-C30	2.39	1.40	1.33
33	y	302	BCO	P2-O4	2.39	1.69	1.59
25	N	502	PTY	O4-C30	2.38	1.40	1.33
26	M	504	Q7G	C11-C08	-2.38	1.52	1.56
29	v	201	PC7	O2-C2	-2.37	1.40	1.46
23	M	501	PGT	P-O3P	2.37	1.68	1.59
31	u	102	CDL	OA8-CA7	2.37	1.40	1.33
25	N	504	PTY	O4-C30	2.36	1.40	1.33
29	v	201	PC7	O3-C3	-2.35	1.39	1.45
25	N	501	PTY	O7-C8	2.35	1.40	1.34
29	f	203	PC7	O3-C3	-2.34	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	504	PTY	O7-C6	-2.34	1.40	1.46
24	H	401	UQ9	C26-C24	2.33	1.56	1.51
29	f	203	PC7	O3-C11	2.32	1.40	1.33
25	L	703	PTY	O4-C30	2.31	1.40	1.33
25	L	703	PTY	O4-C1	-2.29	1.39	1.45
31	u	101	CDL	OA8-CA6	-2.28	1.40	1.45
24	H	401	UQ9	C7-C6	2.27	1.55	1.51
23	L	701	PGT	P-O3P	2.26	1.68	1.59
24	H	401	UQ9	O4-C4M	-2.26	1.40	1.45
25	M	502	PTY	O7-C8	2.25	1.40	1.34
23	L	702	PGT	P-O3P	2.23	1.68	1.59
26	K	201	Q7G	O1C-C1C	2.21	1.44	1.40
29	f	203	PC7	O2-C31	2.21	1.40	1.34
23	y	303	PGT	P-O3P	2.20	1.68	1.59
33	y	302	BCO	O17-C22	-2.20	1.17	1.21
25	N	501	PTY	O7-C6	-2.20	1.41	1.46
25	N	503	PTY	O4-C1	-2.20	1.40	1.45
25	N	502	PTY	O4-C1	-2.19	1.40	1.45
25	N	504	PTY	O4-C1	-2.19	1.40	1.45
25	Y	201	PTY	O4-C1	-2.19	1.40	1.45
23	A	201	PGT	P-O3P	2.19	1.68	1.59
25	M	502	PTY	O7-C6	-2.18	1.41	1.46
31	u	102	CDL	OB6-CB5	2.17	1.40	1.34
25	M	502	PTY	O4-C1	-2.17	1.40	1.45
25	N	501	PTY	O4-C1	-2.15	1.40	1.45
25	Y	201	PTY	O7-C8	2.15	1.40	1.34
25	H	402	PTY	O4-C1	-2.14	1.40	1.45
25	L	703	PTY	O7-C8	2.14	1.40	1.34
25	H	402	PTY	O7-C8	2.12	1.40	1.34
25	N	502	PTY	O7-C8	2.11	1.40	1.34
23	A	201	PGT	O2-C2	-2.11	1.41	1.46
24	H	401	UQ9	O5-C5	-2.10	1.18	1.23
25	N	503	PTY	O7-C8	2.10	1.40	1.34
25	N	504	PTY	O7-C8	2.10	1.40	1.34
29	v	201	PC7	O2-C31	2.08	1.40	1.34
23	y	303	PGT	O3-C3	-2.08	1.40	1.45
26	H	403	Q7G	O1B-C1B	2.08	1.43	1.40
26	H	403	Q7G	O1C-C1C	2.08	1.43	1.40
31	u	101	CDL	OB8-CB6	-2.07	1.40	1.45
31	u	101	CDL	OB6-CB4	-2.07	1.41	1.46
24	H	401	UQ9	C6-C5	2.05	1.52	1.46
31	u	102	CDL	OA8-CA6	-2.05	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	z	301	PTY	O4-C30	2.04	1.39	1.33
31	u	102	CDL	OB8-CB6	-2.03	1.40	1.45
33	y	302	BCO	C2-C1	-2.03	1.48	1.52
23	y	303	PGT	O2-C2	-2.02	1.41	1.46
31	u	102	CDL	OA6-CA5	2.02	1.40	1.34
25	M	503	PTY	O4-C1	-2.00	1.40	1.45

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	y	302	BCO	C6-C8-N2	-13.77	95.05	109.40
24	H	401	UQ9	C7-C8-C9	-7.99	113.50	126.79
25	M	503	PTY	O7-C8-C11	5.05	122.39	111.50
33	y	302	BCO	C15-N4-C12	4.71	126.80	118.75
24	H	401	UQ9	C7-C6-C5	4.63	124.05	118.48
25	N	504	PTY	O7-C8-C11	4.49	121.17	111.50
26	M	504	Q7G	C12-C11-C08	-4.46	106.37	111.68
26	K	201	Q7G	C15-C07-C06	-4.37	104.58	110.91
29	v	201	PC7	O2-C31-C32	4.33	120.82	111.50
25	N	501	PTY	O7-C8-C11	4.12	120.39	111.50
23	M	501	PGT	O2-C31-C32	4.12	120.39	111.50
25	N	503	PTY	O7-C8-C11	4.12	120.38	111.50
23	L	701	PGT	O2-C31-C32	4.11	120.36	111.50
23	A	201	PGT	O2-C31-C32	4.07	120.28	111.50
25	M	502	PTY	O7-C8-C11	4.06	120.25	111.50
29	f	203	PC7	O2-C31-C32	4.06	120.25	111.50
26	K	201	Q7G	C76-C73-C74	-4.05	107.36	115.69
31	u	102	CDL	OB6-CB5-C51	4.03	120.19	111.50
23	L	702	PGT	O2-C31-C32	4.00	120.13	111.50
25	z	301	PTY	O7-C8-C11	3.97	120.06	111.50
33	y	302	BCO	C1-C2-C4	3.95	108.64	99.89
23	y	303	PGT	O2-C31-C32	3.91	119.94	111.50
33	y	302	BCO	C8-C12-N5	-3.88	114.46	120.35
25	N	502	PTY	O7-C8-C11	3.86	119.81	111.50
25	L	703	PTY	O7-C8-C11	3.84	119.78	111.50
26	K	201	Q7G	O80-C73-C76	-3.82	107.22	110.77
31	u	101	CDL	OA6-CA5-C11	3.72	119.52	111.50
25	Y	201	PTY	O7-C8-C11	3.67	119.42	111.50
25	H	402	PTY	O7-C8-C11	3.60	119.26	111.50
31	u	102	CDL	OA6-CA5-C11	3.55	119.14	111.50
26	K	201	Q7G	C16-C13-C14	-3.47	115.60	120.61
26	M	504	Q7G	C16-C13-C11	3.43	120.98	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	M	504	Q7G	C05-C06-C02	-3.40	99.38	103.91
24	H	401	UQ9	C1M-C1-C6	-3.39	118.87	124.40
33	y	302	BCO	C17-C18-C19	-3.36	106.77	112.36
31	u	101	CDL	OB6-CB5-C51	3.27	118.56	111.50
26	a	101	Q7G	C02-C06-C07	-3.20	109.65	114.38
24	H	401	UQ9	C27-C26-C24	-3.18	109.42	114.62
26	M	504	Q7G	C09-C10-C02	-3.16	107.36	112.78
26	H	403	Q7G	C3B-C4B-C5B	-3.11	103.79	110.93
26	H	403	Q7G	C09-C10-C02	-3.11	107.44	112.78
26	a	101	Q7G	C76-C73-C74	-3.11	109.29	115.69
31	u	101	CDL	OA8-CA7-C31	3.10	121.63	111.91
26	M	504	Q7G	C76-C73-C74	-3.09	109.33	115.69
24	H	401	UQ9	C22-C23-C24	-3.07	120.26	127.66
24	H	401	UQ9	C17-C18-C19	-3.04	120.34	127.66
24	H	401	UQ9	C12-C13-C14	-2.95	120.57	127.66
26	M	504	Q7G	C09-C08-C11	-2.94	109.21	113.08
24	H	401	UQ9	C8-C7-C6	2.88	119.80	112.05
26	M	504	Q7G	C15-C07-C08	-2.88	106.23	109.71
24	H	401	UQ9	C20-C19-C21	2.87	120.10	115.27
25	M	503	PTY	O4-C30-C31	2.86	120.87	111.91
29	v	201	PC7	O3-C11-C12	2.83	120.78	111.91
29	f	203	PC7	O3-C11-C12	2.79	120.65	111.91
26	K	201	Q7G	O1B-C1B-C2B	2.78	112.65	108.30
28	Y	202	UQ5	C7-C6-C5	2.78	121.83	118.48
26	M	504	Q7G	C02-C03-C74	-2.76	111.18	120.56
26	M	504	Q7G	C19-C11-C13	2.74	113.77	108.75
23	L	702	PGT	O3-C11-C12	2.73	120.49	111.91
26	H	403	Q7G	C76-C73-C74	-2.73	110.07	115.69
26	K	201	Q7G	C81-C78-C79	-2.71	106.41	111.18
26	H	403	Q7G	C02-C03-C74	-2.71	111.36	120.56
26	H	403	Q7G	C09-C08-C11	-2.70	109.52	113.08
26	M	504	Q7G	C02-C06-C07	-2.70	110.38	114.38
28	Y	202	UQ5	C8-C7-C6	2.69	119.30	112.05
25	N	502	PTY	O4-C30-C31	2.69	120.34	111.91
28	Y	202	UQ5	C6-C1-C2	2.68	121.30	119.18
31	u	102	CDL	OB8-CB7-C71	2.68	120.31	111.91
33	y	302	BCO	O8-C11-C9	-2.68	106.25	110.55
25	Y	201	PTY	O4-C30-C31	2.66	120.24	111.91
26	M	504	Q7G	C75-C74-C03	-2.65	108.61	114.50
25	H	402	PTY	O4-C30-C31	2.65	120.22	111.91
26	a	101	Q7G	C02-C03-C74	-2.65	111.56	120.56
24	H	401	UQ9	C25-C24-C26	2.64	119.72	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	M	501	PGT	O3-C11-C12	2.64	120.20	111.91
31	u	101	CDL	OB8-CB7-C71	2.62	120.13	111.91
26	H	403	Q7G	C12-C11-C08	-2.61	108.57	111.68
25	N	501	PTY	O4-C30-C31	2.60	120.08	111.91
26	K	201	Q7G	CG1-C22-C23	-2.59	110.61	113.88
23	y	303	PGT	O3-C11-C12	2.58	119.99	111.91
26	K	201	Q7G	C02-C03-C74	-2.56	111.84	120.56
25	L	703	PTY	O4-C30-C31	2.56	119.96	111.91
25	M	502	PTY	O4-C30-C31	2.56	119.95	111.91
33	y	302	BCO	C23-C22-S1	2.53	116.41	113.46
31	u	102	CDL	OA8-CA7-C31	2.53	119.85	111.91
24	H	401	UQ9	C15-C14-C16	2.53	119.52	115.27
33	y	302	BCO	P3-O7-P2	-2.53	124.16	132.83
26	a	101	Q7G	C12-C11-C08	-2.52	108.68	111.68
26	H	403	Q7G	C05-C06-C02	-2.50	100.58	103.91
29	v	201	PC7	C2-O2-C31	-2.48	111.69	117.79
26	a	101	Q7G	O80-C79-C78	-2.45	108.65	112.18
26	K	201	Q7G	C76-C77-C78	-2.45	106.65	111.81
23	A	201	PGT	O3-C11-C12	2.44	119.58	111.91
28	Y	202	UQ5	O5-C5-C4	-2.44	115.75	120.93
30	f	202	3PH	O13-P-O11	-2.44	100.25	106.73
23	L	701	PGT	O3-C11-C12	2.43	119.54	111.91
25	N	504	PTY	O4-C30-C31	2.43	119.53	111.91
26	K	201	Q7G	C61-C51-C41	-2.42	107.33	113.00
26	M	504	Q7G	CG1-C22-C23	-2.40	110.84	113.88
26	H	403	Q7G	CF1-O11-C4C	-2.39	112.06	117.96
26	a	101	Q7G	C08-C11-C13	2.38	113.38	109.65
33	y	302	BCO	C8-C12-N4	2.37	125.72	120.35
26	a	101	Q7G	CG1-C22-C23	-2.37	110.89	113.88
30	f	201	3PH	C3-C2-C1	2.36	117.37	111.79
26	M	504	Q7G	C16-C13-C14	-2.36	117.21	120.61
26	K	201	Q7G	C1C-O5C-C5C	2.33	118.26	113.69
26	a	101	Q7G	C75-C74-C73	-2.33	110.67	114.92
25	z	301	PTY	O4-C30-C31	2.33	119.21	111.91
26	H	403	Q7G	C75-C74-C73	-2.30	110.72	114.92
33	y	302	BCO	C25-C24-C23	2.27	122.36	112.67
33	y	302	BCO	O1-C3-C1	2.27	109.72	104.87
26	K	201	Q7G	C05-C06-C02	-2.26	100.90	103.91
26	K	201	Q7G	O80-C73-C74	2.24	115.24	107.38
24	H	401	UQ9	C6-C1-C2	2.24	120.95	119.18
26	M	504	Q7G	O80-C79-C78	-2.21	108.99	112.18
26	K	201	Q7G	C77-C76-C73	-2.21	108.12	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	201	3PH	O13-P-O11	-2.19	100.92	106.73
26	K	201	Q7G	O72-C73-C76	2.18	113.64	108.60
26	K	201	Q7G	C48-O1C-C1C	2.17	117.97	113.74
26	a	101	Q7G	C07-C15-C14	-2.16	109.63	112.73
33	y	302	BCO	C18-C17-N6	-2.16	107.54	111.90
24	H	401	UQ9	C10-C9-C8	-2.12	118.23	123.68
26	K	201	Q7G	C08-C07-C06	-2.10	106.27	109.09
26	K	201	Q7G	C03-C02-C06	-2.09	97.15	100.23
25	z	301	PTY	C6-O7-C8	-2.09	112.64	117.79
25	N	503	PTY	O4-C30-C31	2.09	118.47	111.91
30	f	202	3PH	O14-P-O13	2.08	115.57	107.64
26	K	201	Q7G	C19-C11-C08	2.04	111.57	108.73
26	H	403	Q7G	C08-C07-C06	-2.02	106.39	109.09
23	A	201	PGT	C2-O2-C31	-2.02	112.83	117.79
31	u	101	CDL	OA8-CA7-OA9	-2.01	118.52	123.59
25	M	503	PTY	O7-C8-O10	-2.00	118.86	123.70

There are no chirality outliers.

All (573) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	201	PGT	C32-C31-O2-C2
23	A	201	PGT	O4P-C4-C5-O5
23	L	702	PGT	C32-C31-O2-C2
23	L	702	PGT	C1-O3P-P-O4P
23	M	501	PGT	C1-O3P-P-O2P
23	M	501	PGT	C4-C5-C6-O6
23	M	501	PGT	O5-C5-C6-O6
23	y	303	PGT	O2-C2-C3-O3
24	H	401	UQ9	C12-C11-C9-C10
24	H	401	UQ9	C12-C11-C9-C8
24	H	401	UQ9	C1-C6-C7-C8
24	H	401	UQ9	C5-C6-C7-C8
25	H	402	PTY	C3-O11-P1-O12
25	L	703	PTY	C6-C5-O14-P1
25	M	502	PTY	N1-C2-C3-O11
25	M	502	PTY	O10-C8-O7-C6
25	M	502	PTY	C11-C8-O7-C6
25	M	502	PTY	C3-O11-P1-O12
25	M	502	PTY	C3-O11-P1-O13
25	M	503	PTY	N1-C2-C3-O11
25	M	503	PTY	C31-C30-O4-C1

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Mol	Chain	Res	Type	Atoms
25	M	503	PTY	O30-C30-O4-C1
25	M	503	PTY	O10-C8-O7-C6
25	M	503	PTY	C11-C8-O7-C6
25	M	503	PTY	C3-O11-P1-O12
25	M	503	PTY	C3-O11-P1-O14
25	M	503	PTY	C5-O14-P1-O11
25	M	503	PTY	C5-O14-P1-O12
25	M	503	PTY	C5-O14-P1-O13
25	N	501	PTY	N1-C2-C3-O11
25	N	501	PTY	C11-C8-O7-C6
25	N	502	PTY	N1-C2-C3-O11
25	N	502	PTY	C11-C8-O7-C6
25	N	503	PTY	C5-O14-P1-O13
25	N	504	PTY	N1-C2-C3-O11
25	Y	201	PTY	C11-C8-O7-C6
25	Y	201	PTY	C5-O14-P1-O12
25	Y	201	PTY	C5-O14-P1-O13
25	z	301	PTY	O10-C8-O7-C6
25	z	301	PTY	C11-C8-O7-C6
26	H	403	Q7G	CG1-C22-C23-C48
26	H	403	Q7G	C48-C23-C24-O1B
26	K	201	Q7G	C2B-C1B-O1B-C24
26	K	201	Q7G	O5B-C1B-O1B-C24
26	a	101	Q7G	C18-C17-O20-CG1
28	Y	202	UQ5	C1-C6-C7-C8
28	Y	202	UQ5	C5-C6-C7-C8
28	Y	202	UQ5	C9-C11-C12-C13
28	Y	202	UQ5	C24-C26-C27-C28
29	f	203	PC7	C32-C31-O2-C2
29	f	203	PC7	C1-O3P-P-O1P
29	f	203	PC7	C1-O3P-P-O2P
29	f	203	PC7	C1-O3P-P-O4P
29	f	203	PC7	C4-O4P-P-O1P
29	f	203	PC7	C4-O4P-P-O2P
30	f	201	3PH	C1-O11-P-O13
30	f	201	3PH	C1-O11-P-O12
30	f	202	3PH	C22-C21-O21-C2
31	u	101	CDL	O1-C1-CB2-OB2
31	u	101	CDL	OA9-CA7-OA8-CA6
31	u	101	CDL	C31-CA7-OA8-CA6
31	u	102	CDL	CB3-OB5-PB2-OB4
31	u	102	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
31	u	102	CDL	C51-CB5-OB6-CB4
33	y	302	BCO	C5-O4-P2-O12
33	y	302	BCO	C5-O4-P2-O10
33	y	302	BCO	C20-C21-S1-C22
25	M	502	PTY	O30-C30-O4-C1
23	A	201	PGT	O31-C31-O2-C2
23	L	702	PGT	O31-C31-O2-C2
25	N	501	PTY	O10-C8-O7-C6
25	N	502	PTY	O10-C8-O7-C6
25	N	503	PTY	O10-C8-O7-C6
25	Y	201	PTY	O10-C8-O7-C6
25	M	502	PTY	C31-C30-O4-C1
25	N	502	PTY	C31-C30-O4-C1
25	N	503	PTY	C11-C8-O7-C6
28	Y	202	UQ5	C12-C11-C9-C10
23	M	501	PGT	C12-C11-O3-C3
29	d	101	PC7	C12-C11-O3-C3
29	f	203	PC7	O31-C31-O2-C2
30	f	202	3PH	O22-C21-O21-C2
25	N	502	PTY	O30-C30-O4-C1
29	d	101	PC7	O11-C11-O3-C3
23	L	702	PGT	C14-C15-C16-C17
29	v	201	PC7	C2-C1-O3P-P
23	M	501	PGT	O11-C11-O3-C3
25	L	703	PTY	C31-C30-O4-C1
33	y	302	BCO	C3-C1-O2-P1
23	y	303	PGT	O4P-C4-C5-C6
25	L	703	PTY	O30-C30-O4-C1
29	v	201	PC7	C4-C5-N-C6
23	y	303	PGT	C12-C11-O3-C3
31	u	101	CDL	C71-CB7-OB8-CB6
23	y	303	PGT	C14-C15-C16-C17
25	H	402	PTY	C35-C36-C37-C38
23	L	702	PGT	O4P-C4-C5-O5
28	Y	202	UQ5	C12-C11-C9-C8
23	L	701	PGT	C32-C31-O2-C2
25	z	301	PTY	C38-C39-C40-C41
23	L	701	PGT	C11-C12-C13-C14
31	u	101	CDL	CB5-C51-C52-C53
25	z	301	PTY	C31-C32-C33-C34
29	d	101	PC7	C17-C18-C19-C20
23	y	303	PGT	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
31	u	101	CDL	C32-C33-C34-C35
23	A	201	PGT	O5-C5-C6-O6
23	L	702	PGT	C31-C32-C33-C34
23	M	501	PGT	C11-C12-C13-C14
25	M	503	PTY	C8-C11-C12-C13
31	u	101	CDL	CA5-C11-C12-C13
23	A	201	PGT	C17-C18-C19-C20
25	N	501	PTY	C33-C34-C35-C36
23	L	702	PGT	C5-C4-O4P-P
25	z	301	PTY	C8-C11-C12-C13
26	H	403	Q7G	C22-C23-C24-O1B
28	Y	202	UQ5	C19-C21-C22-C23
23	M	501	PGT	O4P-C4-C5-O5
23	y	303	PGT	O4P-C4-C5-O5
33	y	302	BCO	C2-C1-O2-P1
23	A	201	PGT	C36-C37-C38-C39
23	y	303	PGT	O11-C11-O3-C3
31	u	101	CDL	OB9-CB7-OB8-CB6
23	M	501	PGT	C32-C31-O2-C2
25	L	703	PTY	C11-C8-O7-C6
23	M	501	PGT	C1-O3P-P-O4P
23	y	303	PGT	C4-O4P-P-O3P
25	H	402	PTY	C3-O11-P1-O14
25	L	703	PTY	C3-O11-P1-O14
25	L	703	PTY	C5-O14-P1-O11
25	N	501	PTY	C3-O11-P1-O14
25	Y	201	PTY	C5-O14-P1-O11
25	z	301	PTY	C3-O11-P1-O14
29	f	203	PC7	C4-O4P-P-O3P
31	u	101	CDL	CB3-OB5-PB2-OB2
31	u	102	CDL	CB3-OB5-PB2-OB2
23	A	201	PGT	O4P-C4-C5-C6
23	L	702	PGT	O4P-C4-C5-C6
23	M	501	PGT	O4P-C4-C5-C6
31	u	101	CDL	CA2-C1-CB2-OB2
23	L	701	PGT	O31-C31-O2-C2
23	M	501	PGT	O31-C31-O2-C2
25	L	703	PTY	O10-C8-O7-C6
29	v	201	PC7	C4-C5-N-C8
25	N	504	PTY	C13-C14-C15-C16
29	v	201	PC7	C32-C31-O2-C2
23	y	303	PGT	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
25	M	502	PTY	C31-C32-C33-C34
25	N	502	PTY	C13-C14-C15-C16
25	N	504	PTY	C37-C38-C39-C40
29	d	101	PC7	C39-C40-C41-C42
29	d	101	PC7	C32-C33-C34-C35
30	f	202	3PH	C2C-C2D-C2E-C2F
23	A	201	PGT	C15-C16-C17-C18
23	A	201	PGT	C20-C21-C22-C23
23	L	702	PGT	C40-C41-C42-C43
25	N	502	PTY	C12-C13-C14-C15
23	y	303	PGT	C13-C14-C15-C16
25	Y	201	PTY	C33-C34-C35-C36
25	Y	201	PTY	C39-C40-C41-C42
25	z	301	PTY	C33-C34-C35-C36
31	u	101	CDL	C76-C77-C78-C79
31	u	102	CDL	C37-C38-C39-C40
29	d	101	PC7	C37-C38-C39-C40
29	v	201	PC7	C12-C13-C14-C15
31	u	101	CDL	C36-C37-C38-C39
23	A	201	PGT	C22-C23-C24-C25
25	Y	201	PTY	C37-C38-C39-C40
29	d	101	PC7	C43-C44-C45-C46
29	v	201	PC7	C18-C19-C20-C21
25	H	402	PTY	C17-C18-C19-C20
25	N	501	PTY	C11-C12-C13-C14
25	N	501	PTY	C37-C38-C39-C40
25	Y	201	PTY	C11-C12-C13-C14
23	A	201	PGT	C4-C5-C6-O6
23	L	701	PGT	C4-C5-C6-O6
23	L	702	PGT	C4-C5-C6-O6
26	H	403	Q7G	O5-C1-O1-C4B
26	K	201	Q7G	C22-CG1-O20-C17
25	H	402	PTY	C33-C34-C35-C36
29	v	201	PC7	C38-C39-C40-C41
23	A	201	PGT	C13-C14-C15-C16
23	y	303	PGT	C15-C16-C17-C18
29	v	201	PC7	C4-C5-N-C7
25	N	503	PTY	C37-C38-C39-C40
25	N	504	PTY	C36-C37-C38-C39
25	z	301	PTY	C32-C33-C34-C35
29	f	203	PC7	C33-C34-C35-C36
30	f	202	3PH	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
25	Y	201	PTY	N1-C2-C3-O11
31	u	101	CDL	CB7-C71-C72-C73
23	L	701	PGT	C14-C15-C16-C17
29	d	101	PC7	C18-C19-C20-C21
31	u	101	CDL	C61-C62-C63-C64
23	y	303	PGT	C38-C39-C40-C41
25	L	703	PTY	C13-C14-C15-C16
29	v	201	PC7	C13-C14-C15-C16
25	M	503	PTY	C15-C16-C17-C18
25	N	503	PTY	C16-C17-C18-C19
31	u	102	CDL	CA5-C11-C12-C13
25	H	402	PTY	C14-C15-C16-C17
26	H	403	Q7G	CG1-C22-C23-C24
26	M	504	Q7G	CG1-C22-C23-C48
23	A	201	PGT	C34-C35-C36-C37
23	y	303	PGT	C34-C35-C36-C37
29	d	101	PC7	C36-C37-C38-C39
31	u	101	CDL	C51-C52-C53-C54
26	H	403	Q7G	C2-C1-O1-C4B
25	Y	201	PTY	C23-C24-C25-C26
30	f	202	3PH	C38-C39-C3A-C3B
29	v	201	PC7	O31-C31-O2-C2
25	N	504	PTY	C11-C12-C13-C14
29	d	101	PC7	C15-C16-C17-C18
31	u	102	CDL	C11-CA5-OA6-CA4
25	H	402	PTY	C12-C13-C14-C15
25	H	402	PTY	C37-C38-C39-C40
25	Y	201	PTY	C31-C32-C33-C34
29	f	203	PC7	C16-C17-C18-C19
30	f	201	3PH	C23-C24-C25-C26
28	Y	202	UQ5	C23-C24-C26-C27
29	v	201	PC7	C33-C34-C35-C36
23	L	702	PGT	C36-C37-C38-C39
23	y	303	PGT	C36-C37-C38-C39
25	N	503	PTY	C15-C16-C17-C18
29	v	201	PC7	C32-C33-C34-C35
25	N	501	PTY	C39-C40-C41-C42
25	M	502	PTY	C11-C12-C13-C14
23	A	201	PGT	C12-C13-C14-C15
24	H	401	UQ9	C24-C26-C27-C28
25	N	503	PTY	C13-C14-C15-C16
25	N	501	PTY	O4-C1-C6-O7

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Mol	Chain	Res	Type	Atoms
31	u	102	CDL	C16-C17-C18-C19
25	N	504	PTY	C20-C21-C22-C23
28	Y	202	UQ5	C25-C24-C26-C27
31	u	102	CDL	CB5-C51-C52-C53
33	y	302	BCO	O1-C3-C5-O4
29	f	203	PC7	C18-C19-C20-C21
31	u	102	CDL	C51-C52-C53-C54
31	u	102	CDL	C53-C54-C55-C56
25	z	301	PTY	C34-C35-C36-C37
29	d	101	PC7	C33-C34-C35-C36
31	u	102	CDL	OA7-CA5-OA6-CA4
31	u	102	CDL	C77-C78-C79-C80
25	M	502	PTY	C3-O11-P1-O14
25	N	503	PTY	C5-O14-P1-O11
25	N	503	PTY	C6-C5-O14-P1
25	M	503	PTY	C11-C12-C13-C14
25	z	301	PTY	C36-C37-C38-C39
31	u	102	CDL	C12-C13-C14-C15
25	N	501	PTY	O14-C5-C6-C1
25	z	301	PTY	O14-C5-C6-C1
30	f	202	3PH	O11-C1-C2-C3
31	u	102	CDL	OB5-CB3-CB4-CB6
25	N	502	PTY	C14-C15-C16-C17
29	f	203	PC7	C39-C40-C41-C42
30	f	201	3PH	C37-C38-C39-C3A
25	z	301	PTY	C20-C21-C22-C23
23	y	303	PGT	C35-C36-C37-C38
31	u	102	CDL	C58-C59-C60-C61
29	v	201	PC7	C16-C17-C18-C19
31	u	101	CDL	C15-C16-C17-C18
25	N	503	PTY	C18-C19-C20-C21
25	N	503	PTY	C20-C21-C22-C23
25	N	501	PTY	O4-C1-C6-C5
25	Y	201	PTY	O4-C1-C6-C5
29	d	101	PC7	C1-C2-C3-O3
30	f	202	3PH	C23-C24-C25-C26
25	H	402	PTY	C15-C16-C17-C18
31	u	101	CDL	C44-C45-C46-C47
31	u	101	CDL	C11-C12-C13-C14
31	u	101	CDL	C33-C34-C35-C36
30	f	202	3PH	C35-C36-C37-C38
26	H	403	Q7G	O5C-C5C-C6C-O6C

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Mol	Chain	Res	Type	Atoms
30	f	201	3PH	C3F-C3G-C3H-C3I
25	M	502	PTY	C1-C6-O7-C8
25	N	501	PTY	C5-C6-O7-C8
25	N	503	PTY	C19-C20-C21-C22
25	N	501	PTY	C32-C33-C34-C35
29	f	203	PC7	C17-C18-C19-C20
31	u	102	CDL	C44-C45-C46-C47
29	v	201	PC7	C21-C22-C23-C24
26	H	403	Q7G	C2C-C1C-O1C-C48
25	M	503	PTY	C35-C36-C37-C38
29	f	203	PC7	C45-C46-C47-C48
25	M	502	PTY	O4-C1-C6-O7
25	M	503	PTY	C33-C34-C35-C36
23	A	201	PGT	C37-C38-C39-C40
31	u	102	CDL	C34-C35-C36-C37
31	u	102	CDL	C79-C80-C81-C82
25	N	501	PTY	C35-C36-C37-C38
30	f	202	3PH	C21-C22-C23-C24
23	L	701	PGT	C15-C16-C17-C18
26	H	403	Q7G	C3C-C4C-O11-CF1
31	u	101	CDL	C11-CA5-OA6-CA4
29	v	201	PC7	C45-C46-C47-C48
29	v	201	PC7	C40-C41-C42-C43
30	f	202	3PH	C32-C31-O31-C3
25	N	502	PTY	O14-C5-C6-C1
29	d	101	PC7	O3P-C1-C2-C3
25	N	503	PTY	C38-C39-C40-C41
29	f	203	PC7	C15-C16-C17-C18
31	u	102	CDL	C72-C71-CB7-OB8
29	v	201	PC7	C41-C42-C43-C44
30	f	202	3PH	C36-C37-C38-C39
25	H	402	PTY	C39-C40-C41-C42
25	M	503	PTY	C24-C25-C26-C27
23	y	303	PGT	C16-C17-C18-C19
23	L	701	PGT	C1-C2-C3-O3
23	M	501	PGT	C1-C2-C3-O3
23	y	303	PGT	C1-C2-C3-O3
25	N	503	PTY	O4-C1-C6-C5
25	z	301	PTY	O4-C1-C6-C5
31	u	101	CDL	CA3-CA4-CA6-OA8
31	u	102	CDL	CA3-CA4-CA6-OA8
25	N	504	PTY	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
29	d	101	PC7	C38-C39-C40-C41
31	u	101	CDL	C31-C32-C33-C34
23	A	201	PGT	C32-C33-C34-C35
25	L	703	PTY	C14-C15-C16-C17
25	N	503	PTY	C14-C15-C16-C17
28	Y	202	UQ5	C26-C27-C28-C29
23	L	702	PGT	C19-C20-C21-C22
29	f	203	PC7	C11-C12-C13-C14
23	y	303	PGT	O5-C5-C6-O6
26	H	403	Q7G	C5C-C4C-O11-CF1
25	N	502	PTY	O14-C5-C6-O7
29	d	101	PC7	O3P-C1-C2-O2
33	y	302	BCO	C1-C3-C5-O4
31	u	102	CDL	C36-C37-C38-C39
31	u	101	CDL	OA7-CA5-OA6-CA4
25	M	502	PTY	C8-C11-C12-C13
31	u	101	CDL	C12-C13-C14-C15
23	M	501	PGT	C2-C1-O3P-P
23	M	501	PGT	C5-C4-O4P-P
31	u	102	CDL	CB4-CB3-OB5-PB2
31	u	101	CDL	CA7-C31-C32-C33
31	u	102	CDL	C20-C21-C22-C23
25	z	301	PTY	C21-C22-C23-C24
25	H	402	PTY	C23-C24-C25-C26
25	N	503	PTY	C40-C41-C42-C43
25	L	703	PTY	O14-C5-C6-C1
23	A	201	PGT	C33-C34-C35-C36
25	M	503	PTY	C22-C23-C24-C25
29	d	101	PC7	C12-C13-C14-C15
30	f	201	3PH	C3A-C3B-C3C-C3D
25	N	504	PTY	C31-C32-C33-C34
31	u	101	CDL	C14-C15-C16-C17
31	u	101	CDL	CB6-CB4-OB6-CB5
23	L	701	PGT	C34-C35-C36-C37
30	f	202	3PH	C2D-C2E-C2F-C2G
23	L	702	PGT	C1-C2-C3-O3
25	L	703	PTY	O14-C5-C6-O7
29	f	203	PC7	O3P-C1-C2-O2
30	f	202	3PH	O32-C31-O31-C3
25	M	502	PTY	C12-C13-C14-C15
25	z	301	PTY	C40-C41-C42-C43
23	L	701	PGT	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
23	M	501	PGT	O2-C2-C3-O3
25	N	503	PTY	O4-C1-C6-O7
25	Y	201	PTY	O4-C1-C6-O7
25	z	301	PTY	O4-C1-C6-O7
29	v	201	PC7	O2-C2-C3-O3
31	u	101	CDL	OA6-CA4-CA6-OA8
31	u	101	CDL	OB6-CB4-CB6-OB8
31	u	102	CDL	OA6-CA4-CA6-OA8
33	y	302	BCO	C1-O2-P1-O6
31	u	102	CDL	C75-C76-C77-C78
25	M	502	PTY	C32-C33-C34-C35
23	L	702	PGT	C39-C40-C41-C42
25	H	402	PTY	C40-C41-C42-C43
25	Y	201	PTY	C38-C39-C40-C41
25	N	501	PTY	C5-O14-P1-O11
25	N	501	PTY	C6-C5-O14-P1
23	y	303	PGT	C4-O4P-P-O1P
25	H	402	PTY	C3-O11-P1-O13
25	L	703	PTY	C3-O11-P1-O13
25	L	703	PTY	C5-O14-P1-O12
25	M	503	PTY	C3-O11-P1-O13
25	N	501	PTY	C3-O11-P1-O13
25	N	502	PTY	C3-O11-P1-O13
25	z	301	PTY	C3-O11-P1-O12
25	z	301	PTY	C3-O11-P1-O13
31	u	101	CDL	CB2-OB2-PB2-OB3
31	u	101	CDL	CB3-OB5-PB2-OB3
31	u	101	CDL	CB3-OB5-PB2-OB4
31	u	102	CDL	CB3-OB5-PB2-OB3
23	y	303	PGT	C11-C12-C13-C14
26	H	403	Q7G	O5C-C1C-O1C-C48
23	A	201	PGT	C12-C11-O3-C3
29	v	201	PC7	C12-C11-O3-C3
29	f	203	PC7	O3P-C1-C2-C3
24	H	401	UQ9	C5-C4-O4-C4M
25	z	301	PTY	C25-C26-C27-C28
29	d	101	PC7	C13-C14-C15-C16
25	L	703	PTY	C2-C3-O11-P1
25	N	502	PTY	C2-C3-O11-P1
25	L	703	PTY	C8-C11-C12-C13
31	u	101	CDL	OB7-CB5-OB6-CB4
25	N	501	PTY	O14-C5-C6-O7

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Mol	Chain	Res	Type	Atoms
25	z	301	PTY	O14-C5-C6-O7
30	f	202	3PH	O11-C1-C2-O21
31	u	102	CDL	OB5-CB3-CB4-OB6
31	u	102	CDL	CB7-C71-C72-C73
31	u	102	CDL	C22-C23-C24-C25
25	N	502	PTY	C24-C25-C26-C27
29	d	101	PC7	C4-C5-N-C8
25	M	502	PTY	O4-C1-C6-C5
30	f	202	3PH	C39-C3A-C3B-C3C
23	M	501	PGT	C31-C32-C33-C34
23	A	201	PGT	C41-C42-C43-C44
29	f	203	PC7	C42-C43-C44-C45
23	A	201	PGT	C19-C20-C21-C22
29	d	101	PC7	C19-C20-C21-C22
30	f	201	3PH	C22-C23-C24-C25
31	u	101	CDL	C37-C38-C39-C40
25	Y	201	PTY	C25-C26-C27-C28
29	v	201	PC7	O11-C11-O3-C3
26	a	101	Q7G	CG1-C22-C23-C48
23	A	201	PGT	C21-C22-C23-C24
31	u	101	CDL	C41-C42-C43-C44
23	A	201	PGT	O11-C11-O3-C3
23	A	201	PGT	C42-C43-C44-C45
25	H	402	PTY	C6-C5-O14-P1
29	d	101	PC7	C4-C5-N-C7
31	u	102	CDL	C59-C60-C61-C62
23	M	501	PGT	C32-C33-C34-C35
31	u	101	CDL	C51-CB5-OB6-CB4
29	d	101	PC7	O2-C2-C3-O3
23	A	201	PGT	C1-O3P-P-O4P
23	L	701	PGT	C4-O4P-P-O3P
23	M	501	PGT	C4-O4P-P-O3P
23	y	303	PGT	C1-O3P-P-O4P
25	H	402	PTY	C5-O14-P1-O11
25	N	503	PTY	C3-O11-P1-O14
25	z	301	PTY	C5-O14-P1-O11
29	v	201	PC7	C4-O4P-P-O3P
25	H	402	PTY	C22-C23-C24-C25
23	A	201	PGT	C39-C40-C41-C42
31	u	102	CDL	C78-C79-C80-C81
25	N	502	PTY	C18-C19-C20-C21
31	u	102	CDL	C56-C57-C58-C59

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Mol	Chain	Res	Type	Atoms
25	Y	201	PTY	C13-C14-C15-C16
31	u	102	CDL	C42-C43-C44-C45
25	N	501	PTY	C31-C32-C33-C34
30	f	201	3PH	C2-C1-O11-P
31	u	102	CDL	C73-C74-C75-C76
31	u	102	CDL	C72-C73-C74-C75
29	f	203	PC7	C19-C20-C21-C22
25	N	504	PTY	C21-C22-C23-C24
23	L	702	PGT	C16-C17-C18-C19
28	Y	202	UQ5	C14-C16-C17-C18
29	d	101	PC7	C14-C15-C16-C17
23	L	702	PGT	C12-C11-O3-C3
23	L	702	PGT	C35-C36-C37-C38
23	L	702	PGT	C37-C38-C39-C40
25	N	503	PTY	C36-C37-C38-C39
31	u	102	CDL	C21-C22-C23-C24
30	f	202	3PH	C2B-C2C-C2D-C2E
23	L	701	PGT	O4P-C4-C5-O5
23	L	701	PGT	C32-C33-C34-C35
30	f	201	3PH	C1-C2-O21-C21
25	N	502	PTY	C17-C18-C19-C20
25	N	504	PTY	C41-C42-C43-C44
29	d	101	PC7	C4-C5-N-C6
31	u	101	CDL	CB2-OB2-PB2-OB5
29	f	203	PC7	C44-C45-C46-C47
26	a	101	Q7G	CG1-C22-C23-C24
25	M	503	PTY	C30-C31-C32-C33
25	M	502	PTY	O14-C5-C6-O7
31	u	101	CDL	OA5-CA3-CA4-OA6
25	L	703	PTY	C12-C11-C8-O7
30	f	202	3PH	C24-C25-C26-C27
26	K	201	Q7G	C3C-C4C-O11-CF1
25	z	301	PTY	C26-C27-C28-C29
30	f	201	3PH	C24-C25-C26-C27
25	N	504	PTY	C24-C25-C26-C27
23	L	702	PGT	O2-C2-C3-O3
25	L	703	PTY	O4-C1-C6-O7
29	v	201	PC7	C17-C18-C19-C20
31	u	101	CDL	C81-C82-C83-C84
26	K	201	Q7G	C5C-C4C-O11-CF1
23	y	303	PGT	C37-C38-C39-C40
23	L	702	PGT	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
29	v	201	PC7	C1-C2-C3-O3
31	u	102	CDL	CB3-CB4-CB6-OB8
31	u	102	CDL	C72-C71-CB7-OB9
31	u	101	CDL	C62-C63-C64-C65
23	y	303	PGT	O3P-C1-C2-O2
31	u	101	CDL	C21-C22-C23-C24
31	u	101	CDL	OA5-CA3-CA4-CA6
31	u	102	CDL	C24-C25-C26-C27
23	L	701	PGT	O5-C5-C6-O6
29	v	201	PC7	O3-C11-C12-C13
30	f	201	3PH	O31-C31-C32-C33
30	f	201	3PH	C1-O11-P-O14
24	H	401	UQ9	C15-C14-C16-C17
29	d	101	PC7	C4-O4P-P-O3P
25	H	402	PTY	C21-C22-C23-C24
25	N	504	PTY	C33-C34-C35-C36
26	a	101	Q7G	C23-C48-O1C-C1C
25	M	503	PTY	C31-C32-C33-C34
29	d	101	PC7	C23-C24-C25-C26
30	f	201	3PH	O22-C21-O21-C2
30	f	202	3PH	C31-C32-C33-C34
23	L	701	PGT	O2-C31-C32-C33
25	N	504	PTY	O4-C30-C31-C32
31	u	101	CDL	CB3-CB4-CB6-OB8
23	y	303	PGT	O3-C11-C12-C13
25	N	501	PTY	O4-C30-C31-C32
24	H	401	UQ9	C13-C14-C16-C17
31	u	101	CDL	C40-C41-C42-C43
25	Y	201	PTY	C12-C13-C14-C15
23	y	303	PGT	O3P-C1-C2-C3
31	u	102	CDL	C43-C44-C45-C46
25	M	503	PTY	O4-C1-C6-O7
33	y	302	BCO	C1-O2-P1-O5
33	y	302	BCO	C5-O4-P2-O7
29	d	101	PC7	C45-C46-C47-C48
25	M	503	PTY	C36-C37-C38-C39
25	M	503	PTY	C34-C35-C36-C37
25	N	503	PTY	C21-C22-C23-C24
24	H	401	UQ9	C3-C4-O4-C4M
26	K	201	Q7G	C23-C22-CG1-O20
23	y	303	PGT	O11-C11-C12-C13
23	L	701	PGT	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
23	L	702	PGT	C15-C16-C17-C18
23	y	303	PGT	C4-C5-C6-O6
25	Y	201	PTY	C32-C33-C34-C35
26	H	403	Q7G	C22-CG1-O20-C17
30	f	201	3PH	O32-C31-C32-C33
25	N	503	PTY	C32-C33-C34-C35
23	L	702	PGT	O2-C31-C32-C33
23	L	702	PGT	C13-C14-C15-C16
25	N	504	PTY	O30-C30-C31-C32
31	u	101	CDL	C17-C18-C19-C20
25	N	501	PTY	O30-C30-C31-C32
25	H	402	PTY	C41-C42-C43-C44
25	N	504	PTY	C35-C36-C37-C38
25	z	301	PTY	C15-C16-C17-C18
31	u	102	CDL	C52-C53-C54-C55
23	L	701	PGT	C4-O4P-P-O1P
23	M	501	PGT	C4-O4P-P-O1P
25	z	301	PTY	C5-O14-P1-O13
28	Y	202	UQ5	C6-C7-C8-C9
29	d	101	PC7	C4-O4P-P-O2P
31	u	101	CDL	CA3-OA5-PA1-OA3
25	L	703	PTY	C15-C16-C17-C18
25	z	301	PTY	N1-C2-C3-O11
31	u	101	CDL	C54-C55-C56-C57
25	H	402	PTY	C2-C3-O11-P1
25	M	503	PTY	C2-C3-O11-P1
25	N	503	PTY	C2-C3-O11-P1
23	L	701	PGT	C31-C32-C33-C34
23	L	702	PGT	O5-C5-C6-O6
25	N	502	PTY	C21-C22-C23-C24
25	N	501	PTY	C12-C11-C8-O7
25	N	502	PTY	O4-C30-C31-C32
23	L	701	PGT	O3-C11-C12-C13
31	u	101	CDL	C43-C44-C45-C46
29	v	201	PC7	C11-C12-C13-C14
25	N	502	PTY	C6-C5-O14-P1
23	L	702	PGT	O31-C31-C32-C33
25	z	301	PTY	O4-C30-C31-C32
31	u	102	CDL	C32-C31-CA7-OA8
25	M	502	PTY	C34-C35-C36-C37
23	y	303	PGT	C31-C32-C33-C34
31	u	101	CDL	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
25	M	503	PTY	C12-C11-C8-O7
29	f	203	PC7	O3-C11-C12-C13
25	z	301	PTY	O30-C30-C31-C32
31	u	102	CDL	C32-C31-CA7-OA9
25	N	502	PTY	O30-C30-C31-C32
23	A	201	PGT	O3-C11-C12-C13

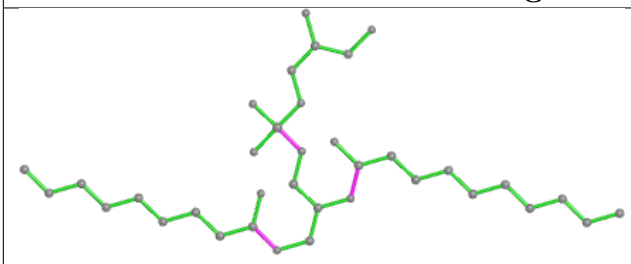
There are no ring outliers.

15 monomers are involved in 51 short contacts:

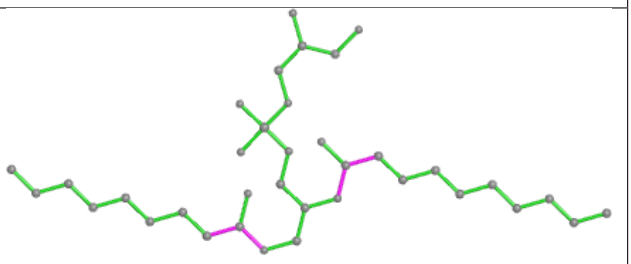
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	L	701	PGT	1	0
23	M	501	PGT	4	0
23	L	702	PGT	2	0
26	K	201	Q7G	1	0
25	N	504	PTY	3	0
26	H	403	Q7G	3	0
25	N	501	PTY	5	0
28	Y	202	UQ5	9	0
24	H	401	UQ9	4	0
25	H	402	PTY	6	0
25	N	502	PTY	2	0
25	Y	201	PTY	3	0
25	M	503	PTY	3	0
23	A	201	PGT	3	0
25	N	503	PTY	3	0

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.

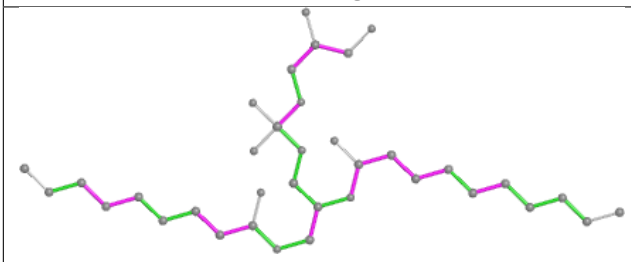
Ligand PGT L 701



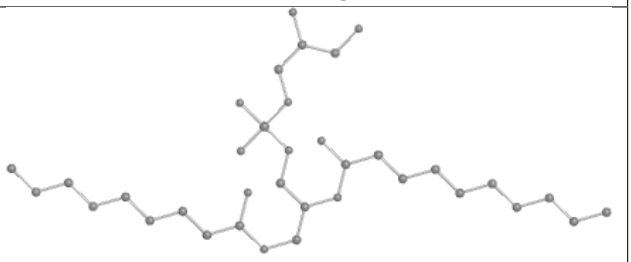
Bond lengths



Bond angles

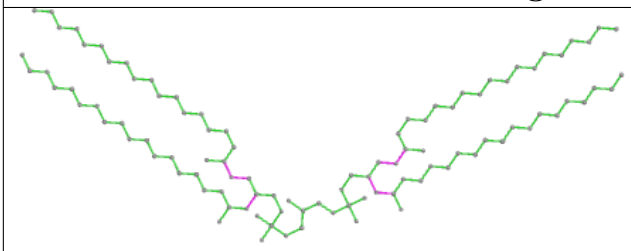


Torsions

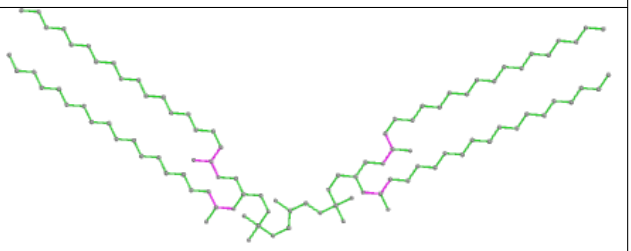


Rings

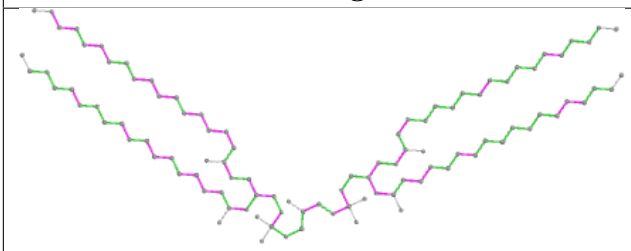
Ligand CDL u 101



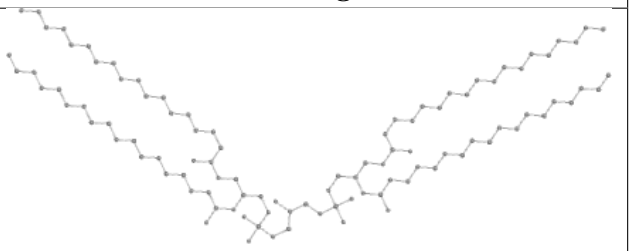
Bond lengths



Bond angles

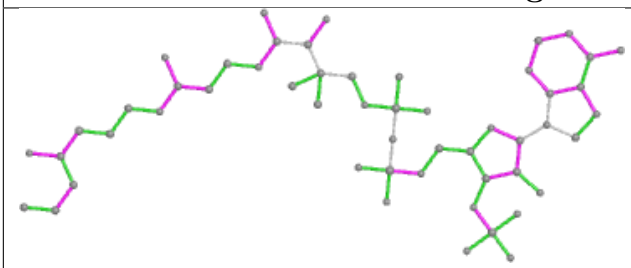


Torsions

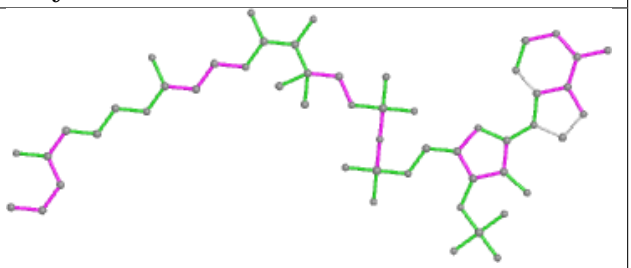


Rings

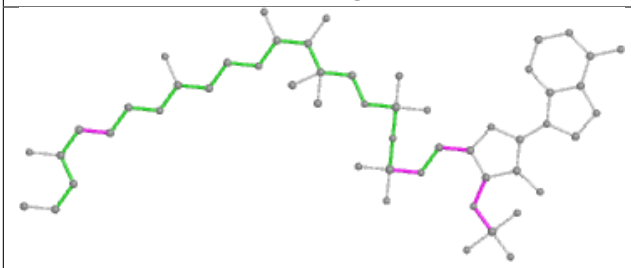
Ligand BCO y 302



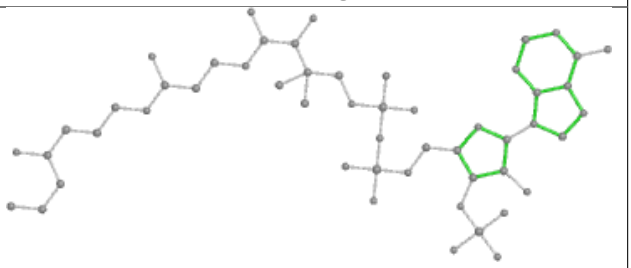
Bond lengths



Bond angles

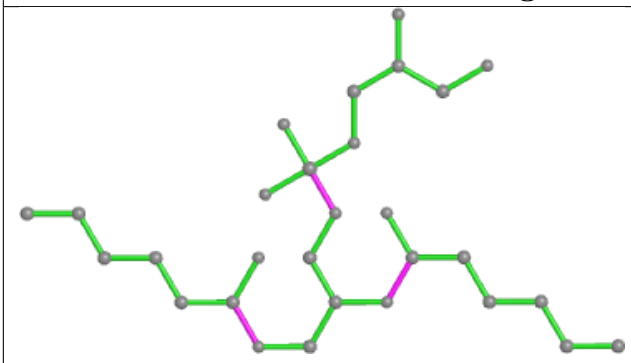


Torsions

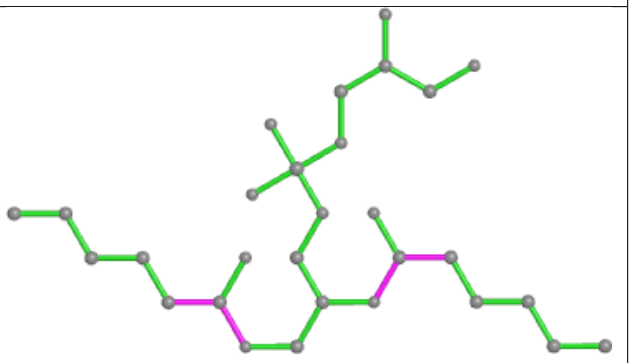


Rings

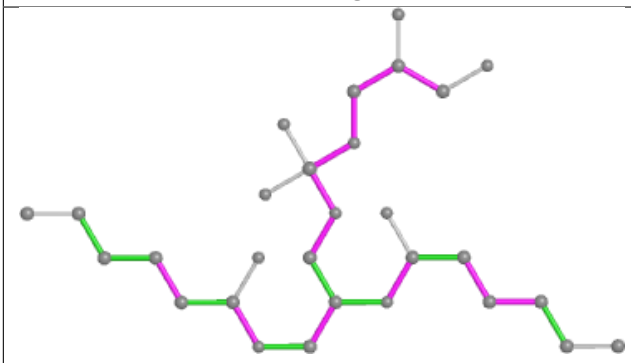
Ligand PGT M 501



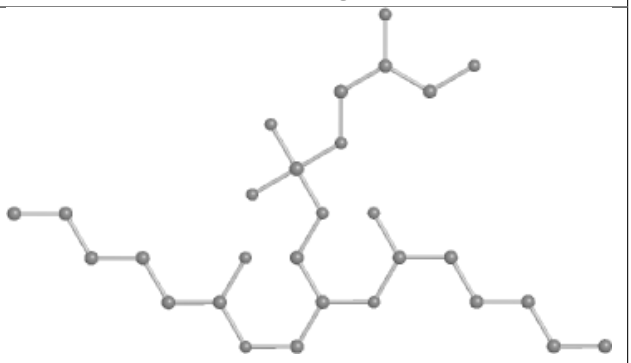
Bond lengths



Bond angles

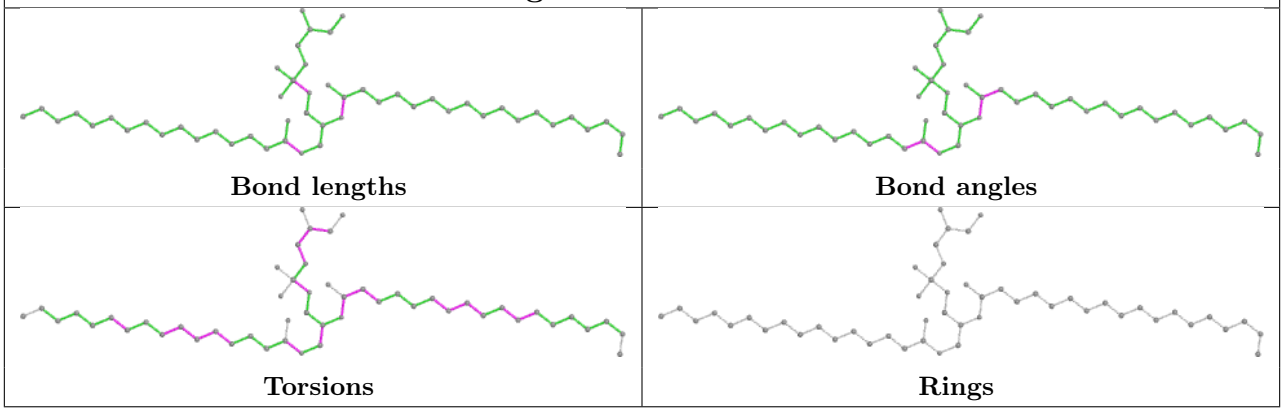


Torsions

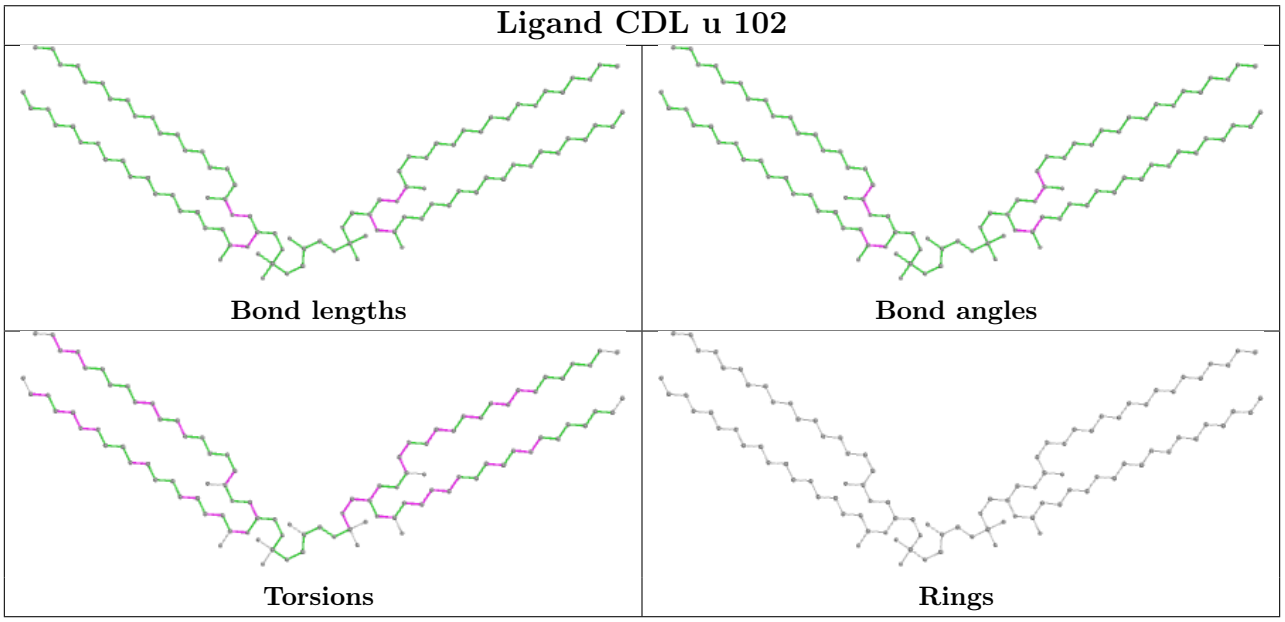


Rings

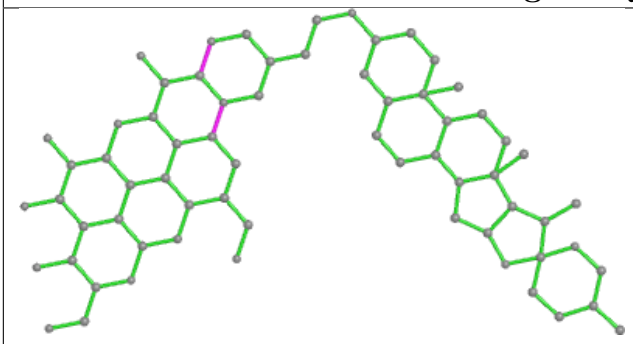
Ligand PGT L 702



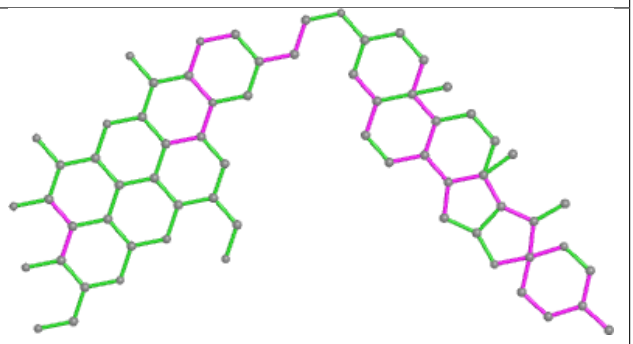
Ligand CDL u 102



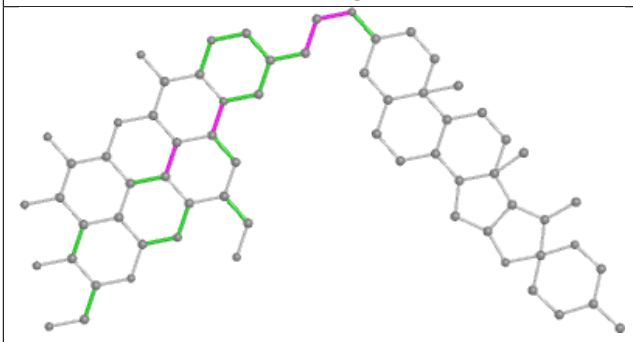
Ligand Q7G K 201



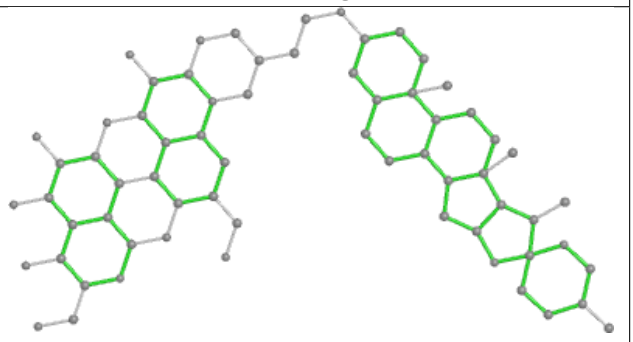
Bond lengths



Bond angles

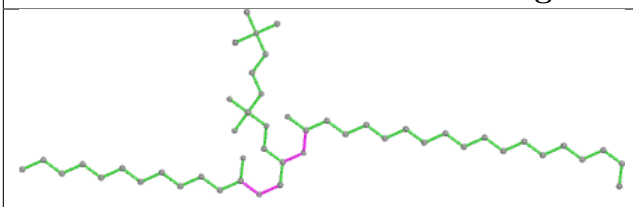


Torsions

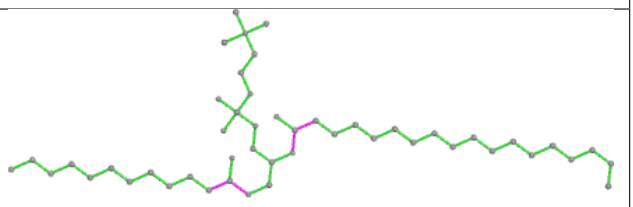


Rings

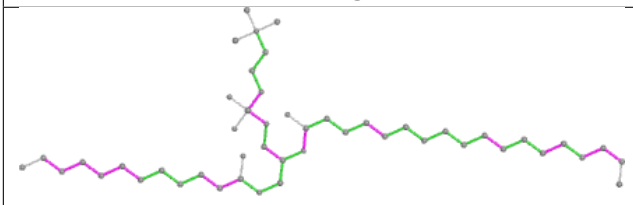
Ligand PC7 f 203



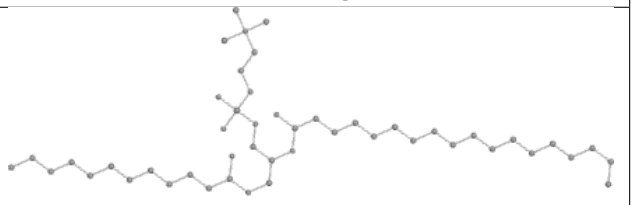
Bond lengths



Bond angles

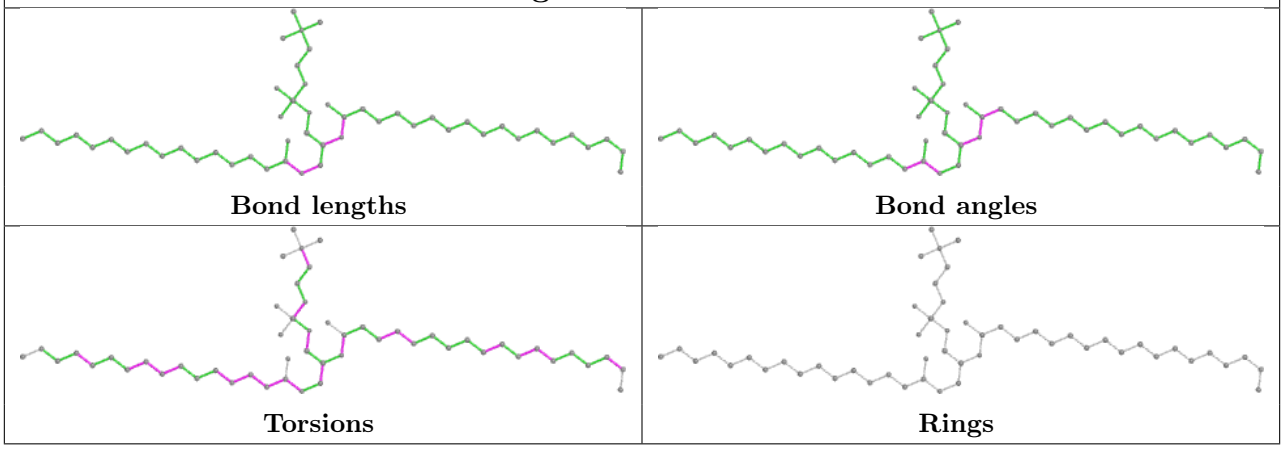


Torsions

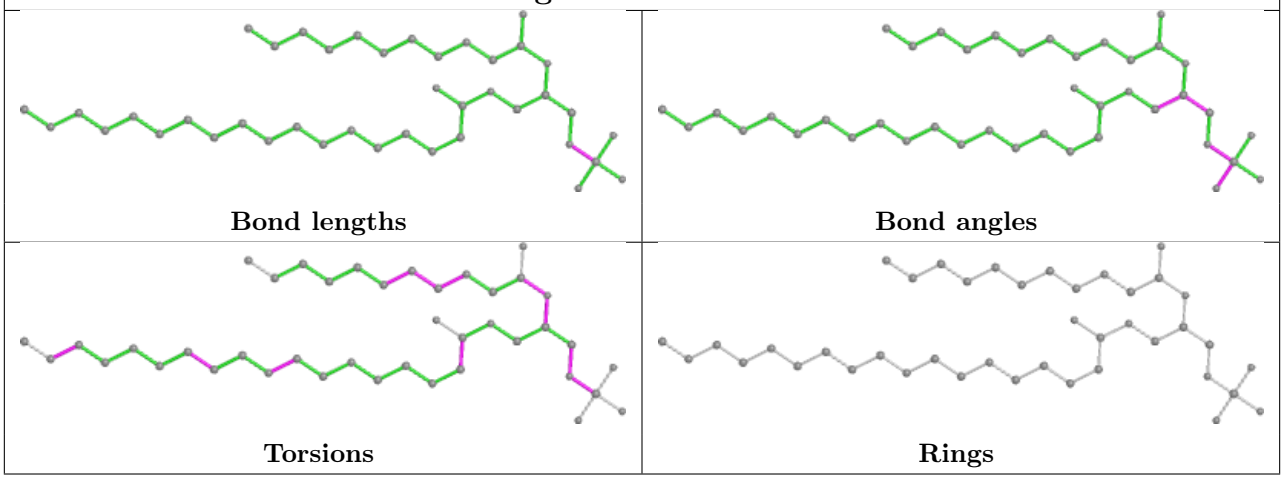


Rings

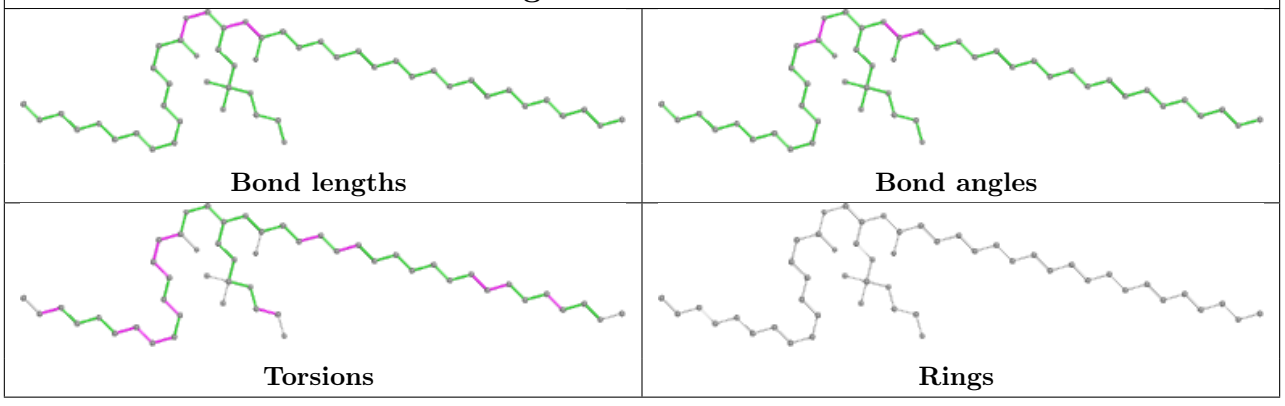
Ligand PC7 v 201



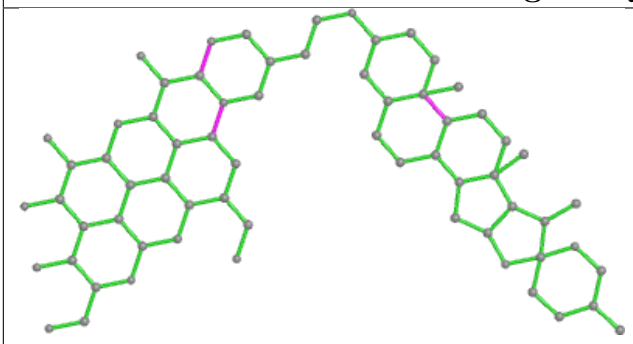
Ligand 3PH f 201



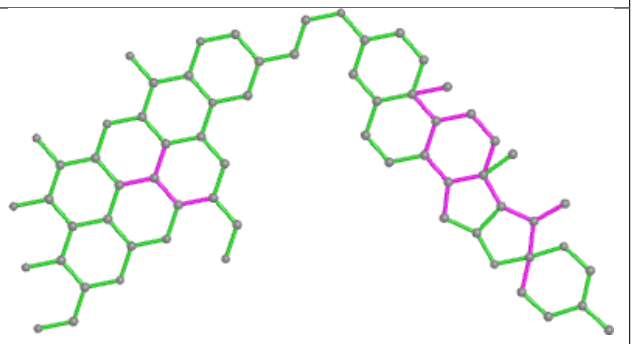
Ligand PTY N 504



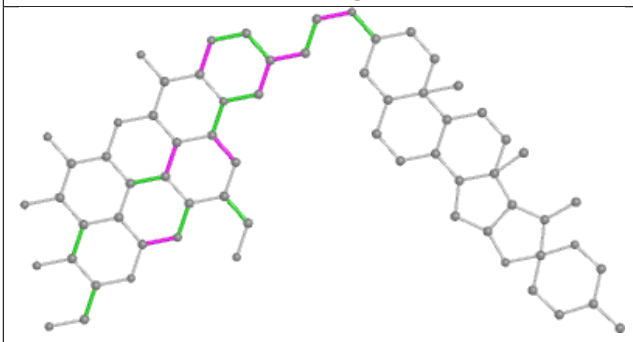
Ligand Q7G H 403



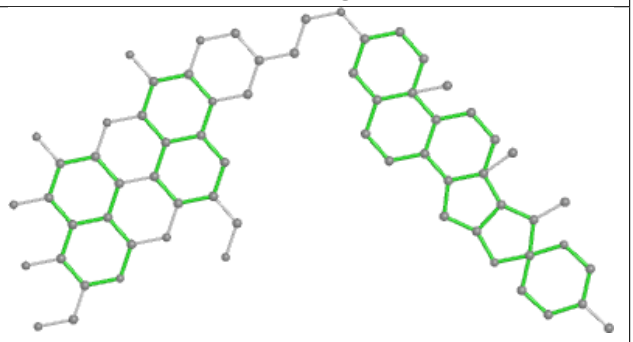
Bond lengths



Bond angles

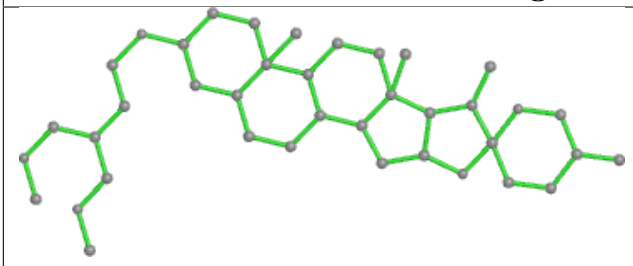


Torsions

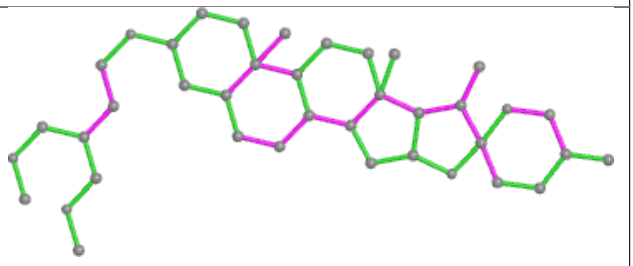


Rings

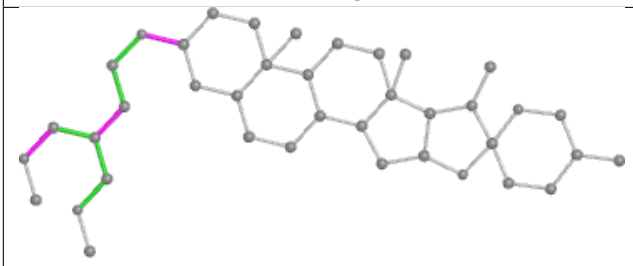
Ligand Q7G a 101



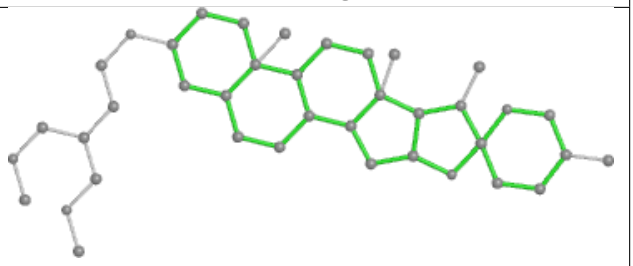
Bond lengths



Bond angles

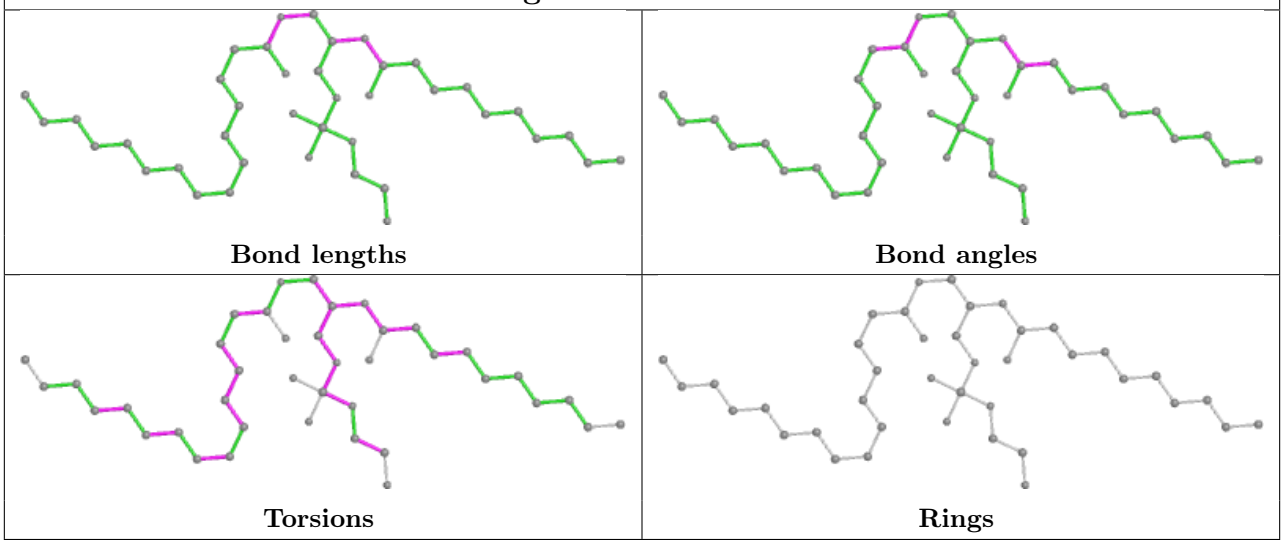


Torsions

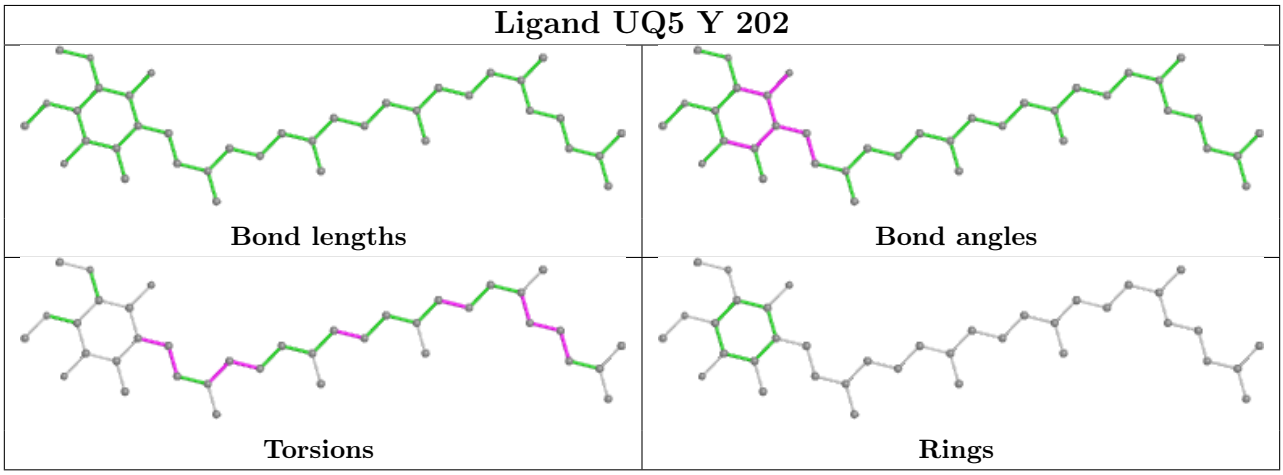


Rings

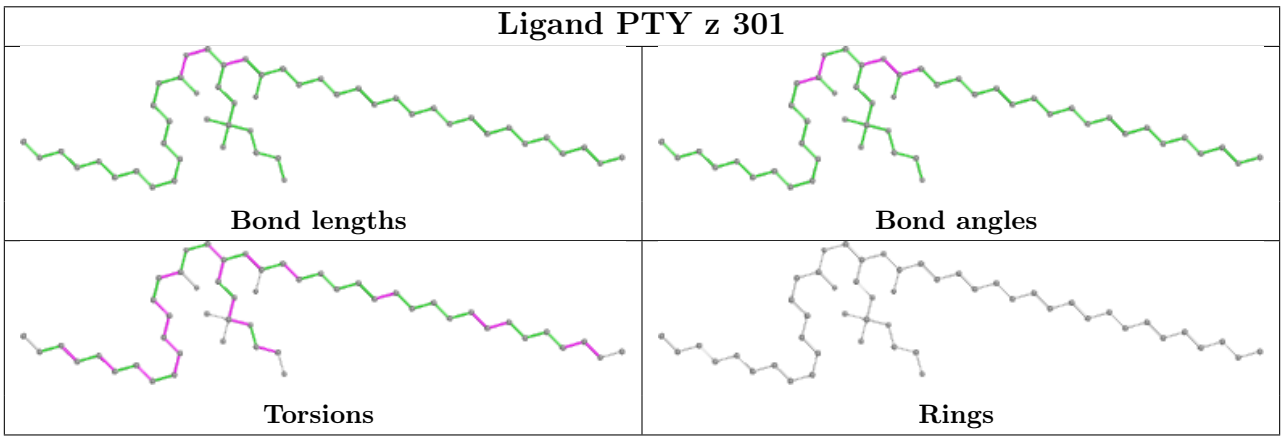
Ligand PTY N 501



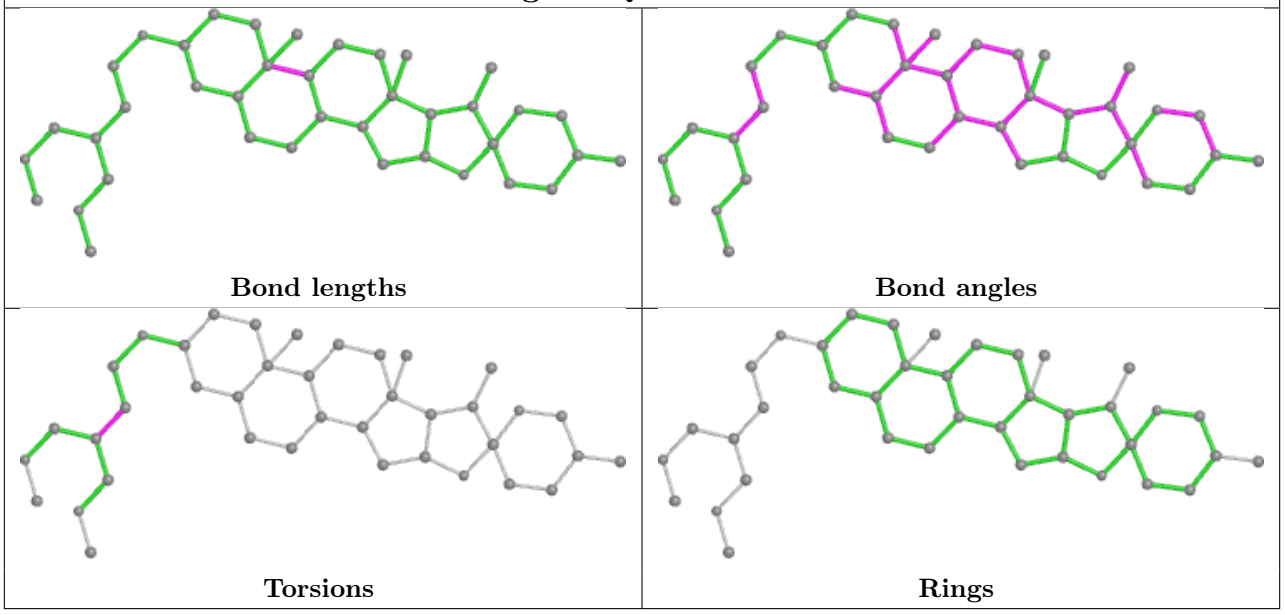
Ligand UQ5 Y 202



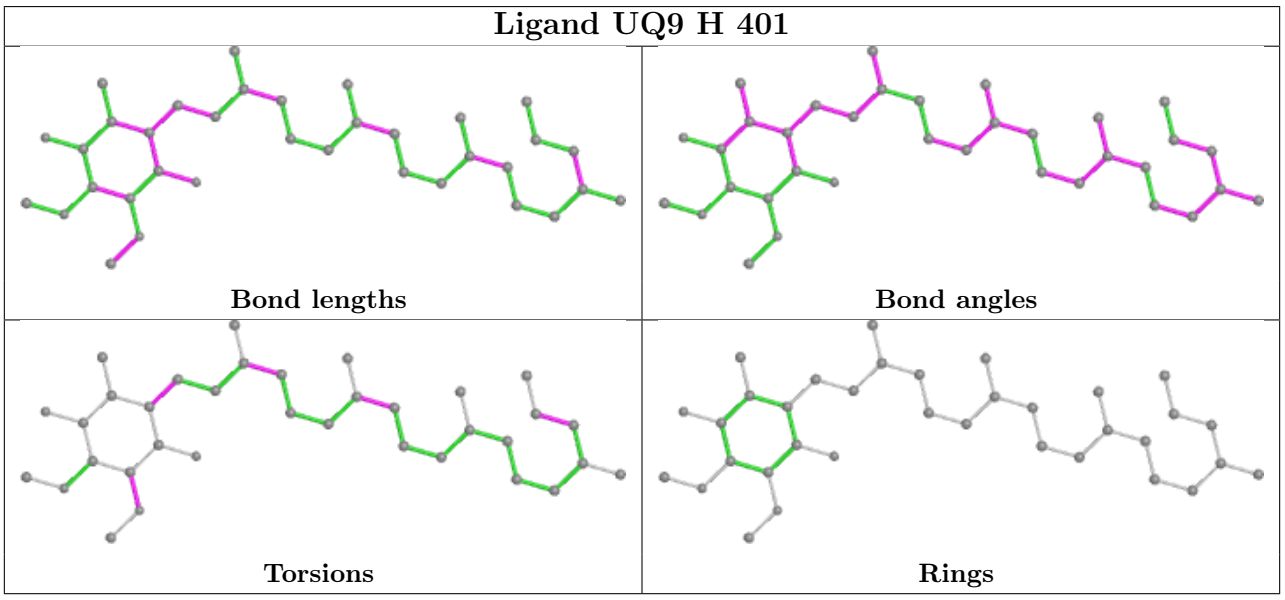
Ligand PTY z 301



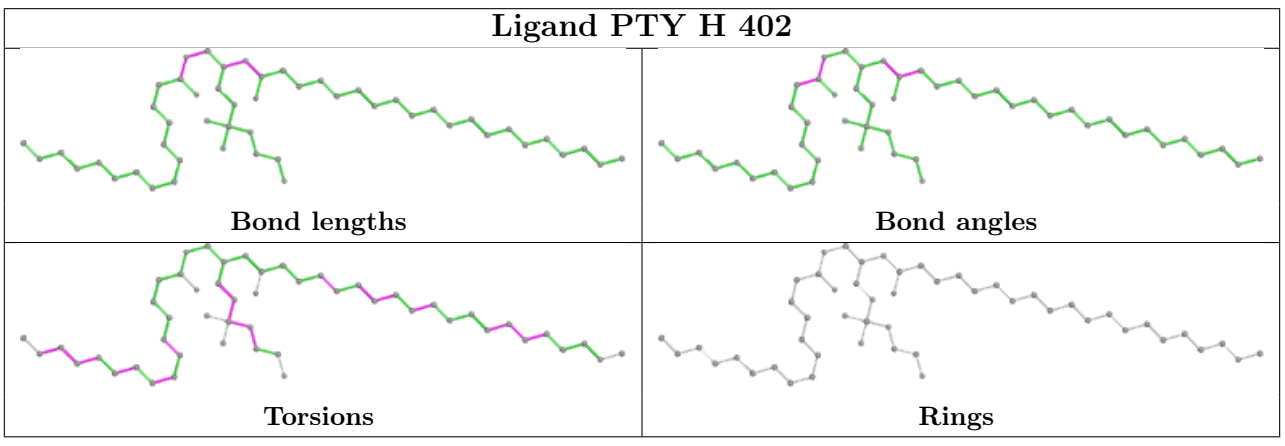
Ligand Q7G M 504



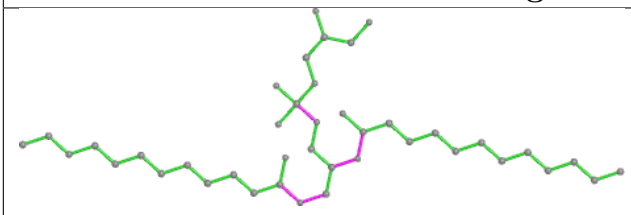
Ligand UQ9 H 401



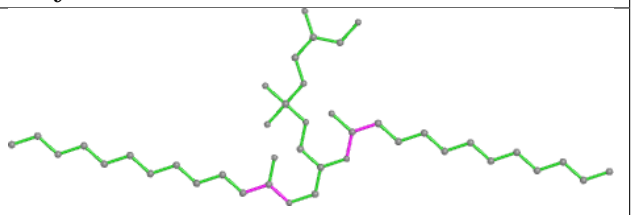
Ligand PTY H 402



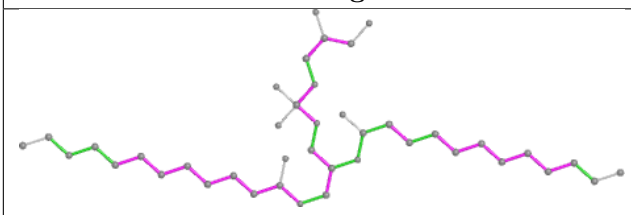
Ligand PGT y 303



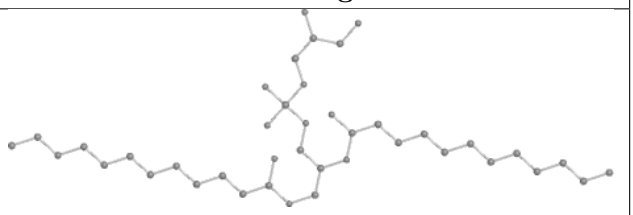
Bond lengths



Bond angles

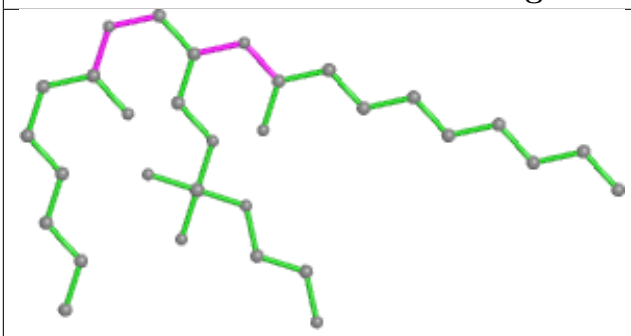


Torsions

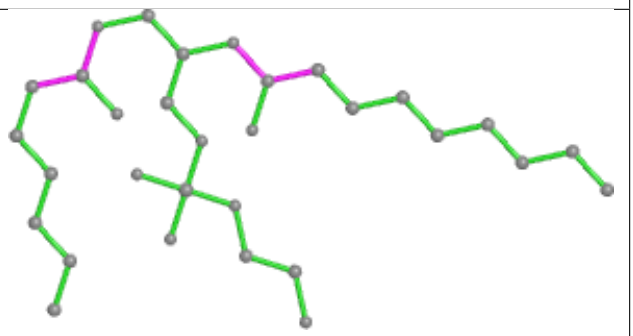


Rings

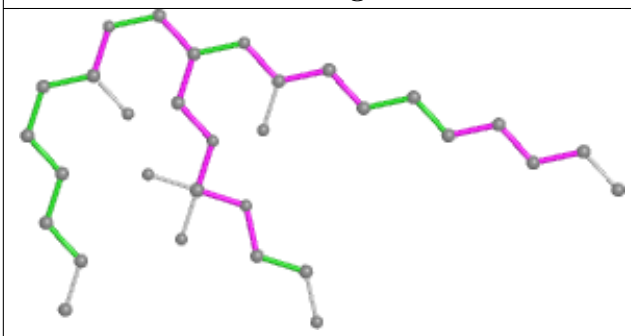
Ligand PTY L 703



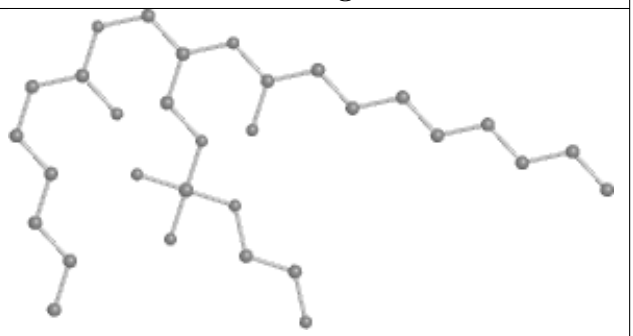
Bond lengths



Bond angles

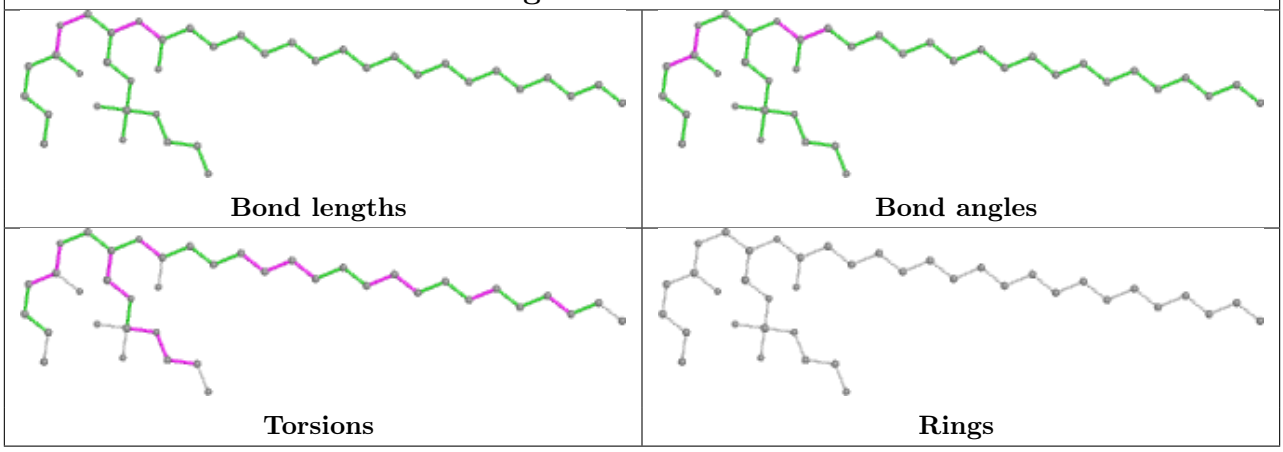


Torsions

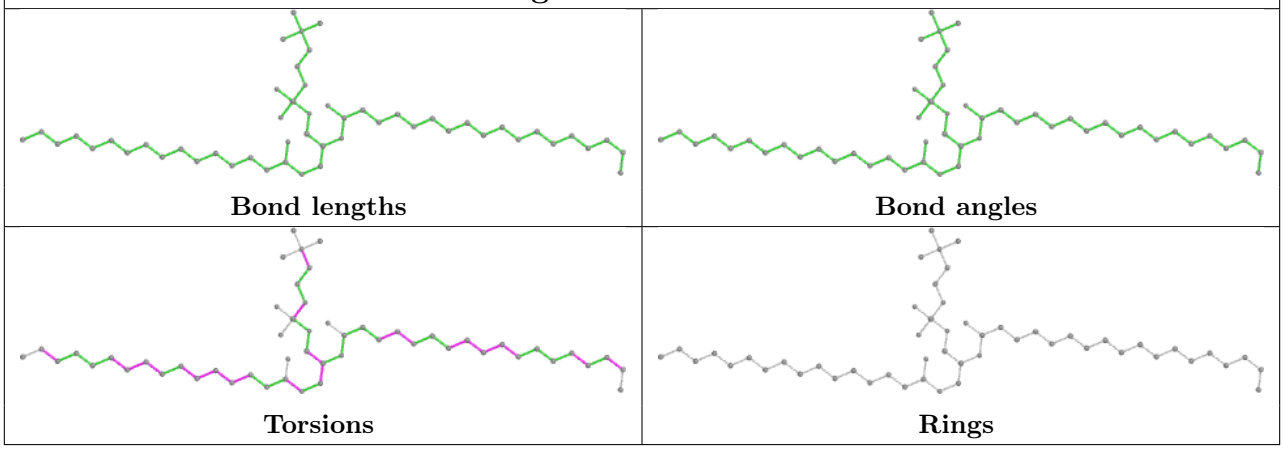


Rings

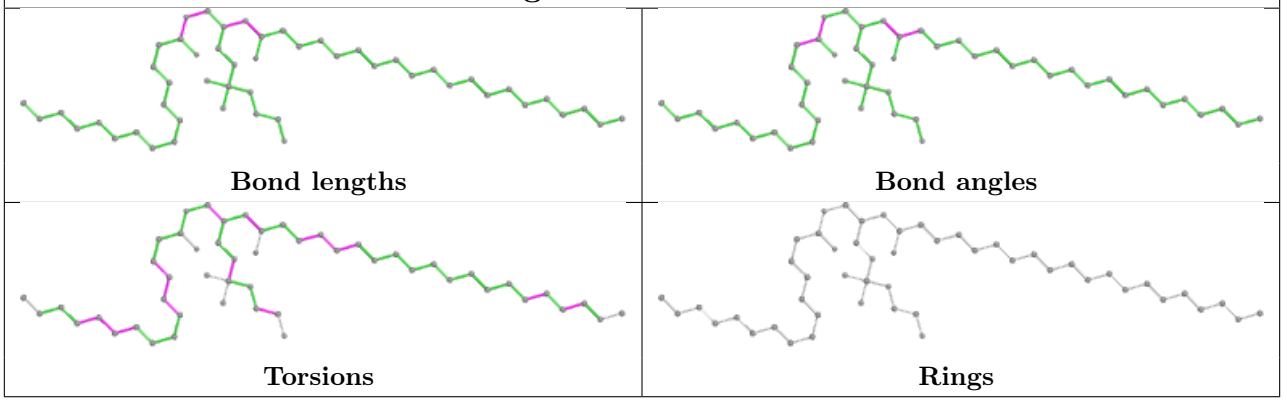
Ligand PTY N 502



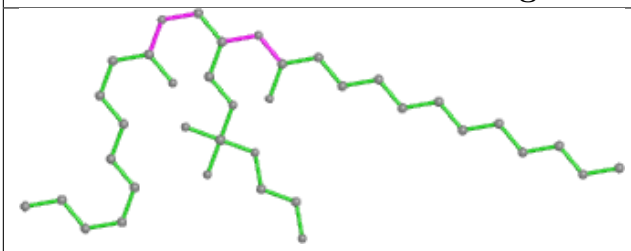
Ligand PC7 d 101



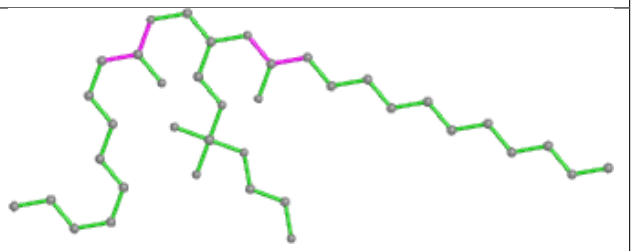
Ligand PTY Y 201



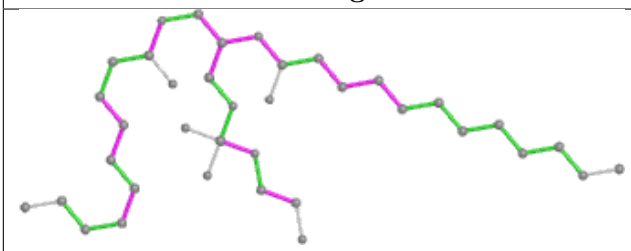
Ligand PTY M 502



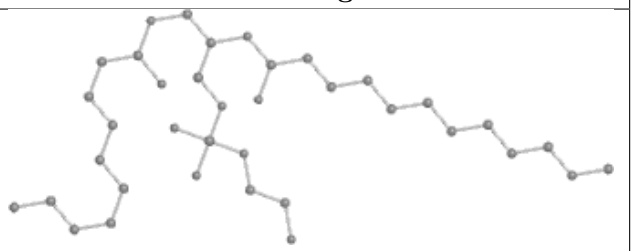
Bond lengths



Bond angles

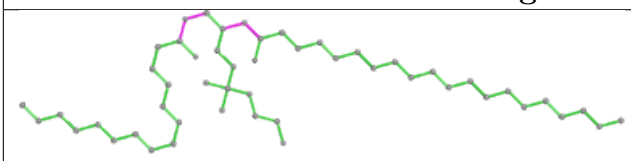


Torsions

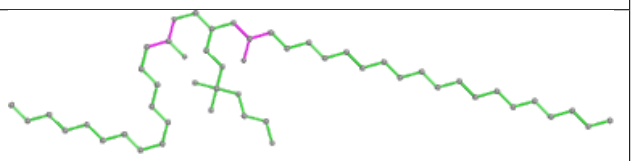


Rings

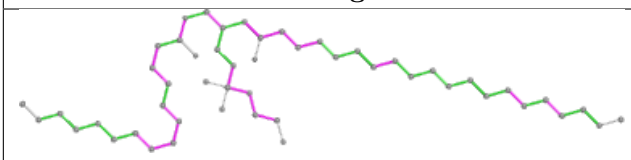
Ligand PTY M 503



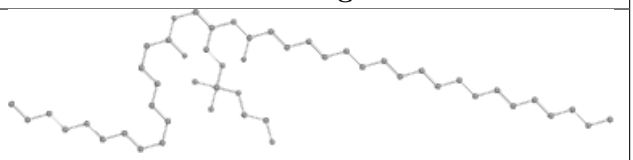
Bond lengths



Bond angles

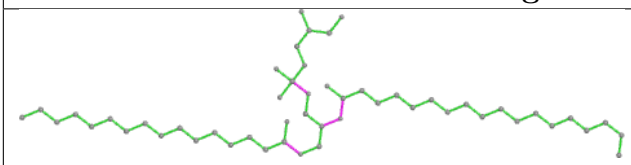


Torsions

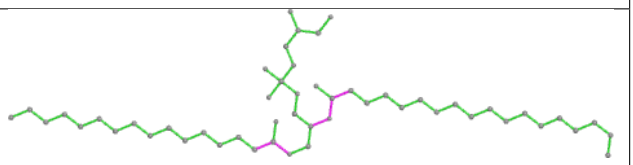


Rings

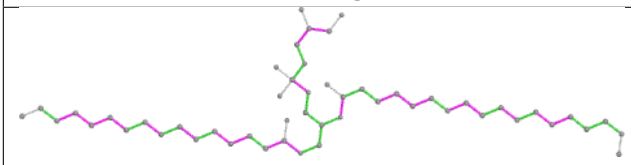
Ligand PGT A 201



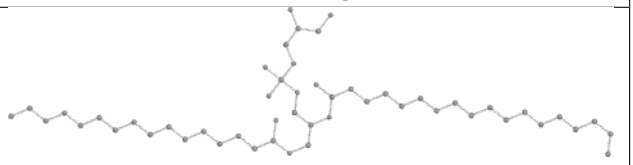
Bond lengths



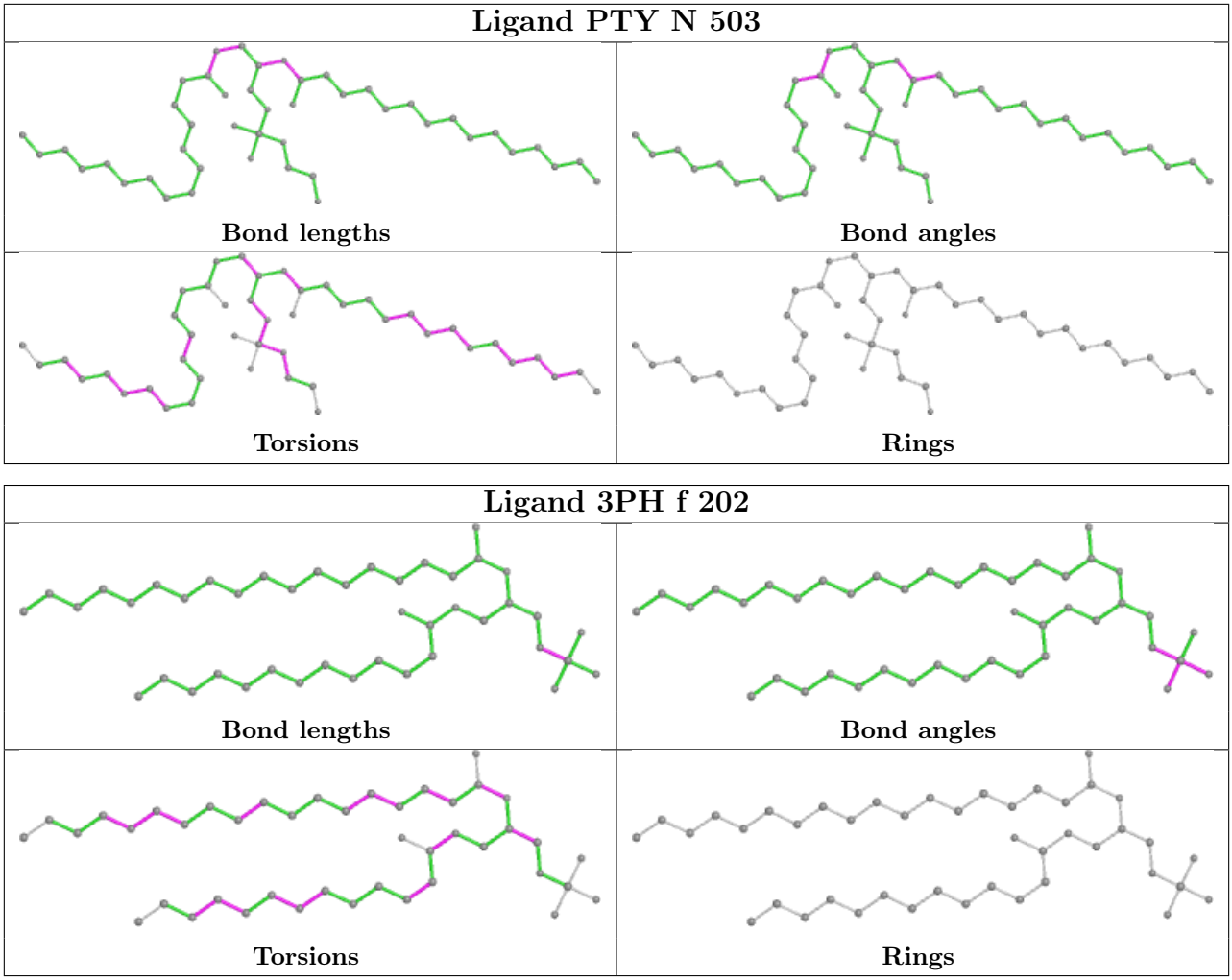
Bond angles



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.

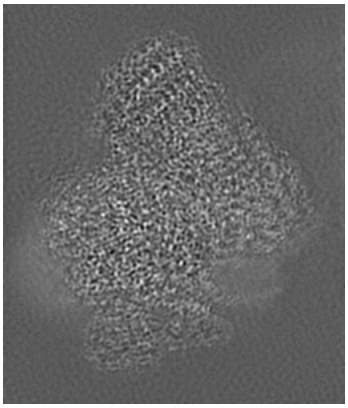
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16000. These allow visual inspection of the internal detail of the map and identification of artifacts.

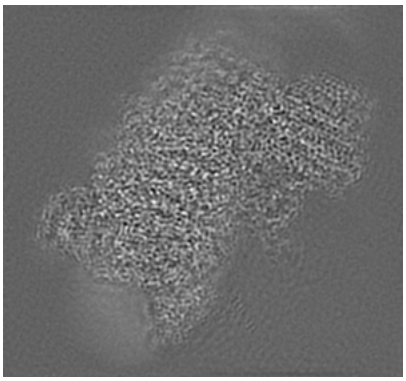
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

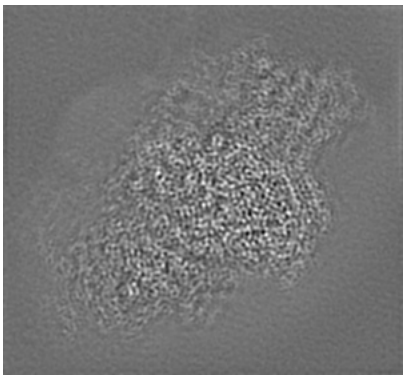
6.1.1 Primary map



X

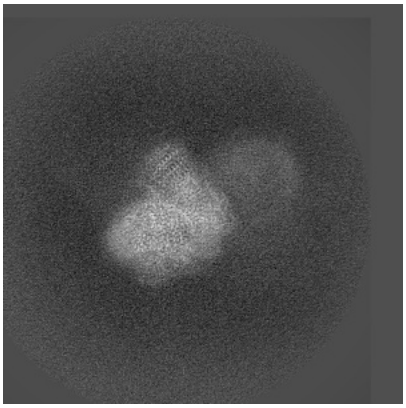


Y

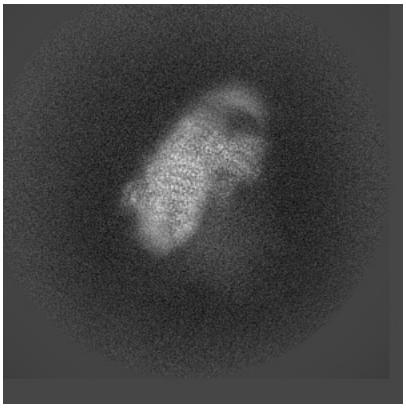


Z

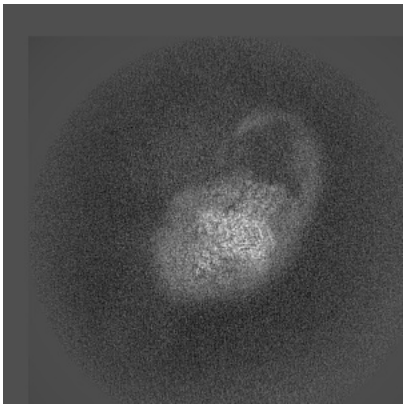
6.1.2 Raw map



X



Y

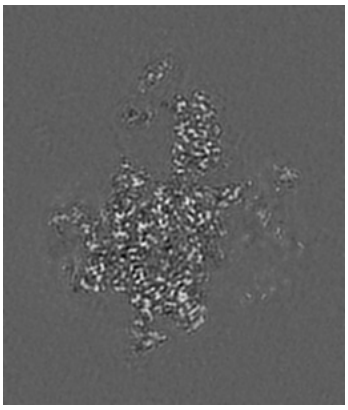


Z

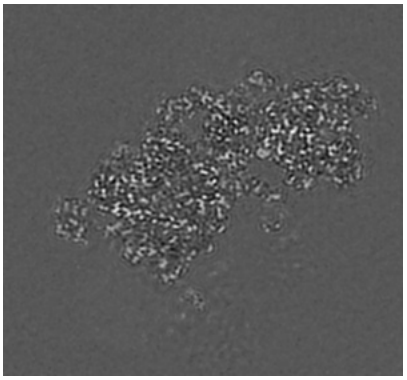
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

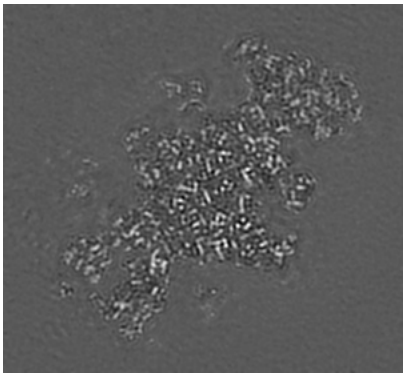
6.2.1 Primary map



X Index: 148

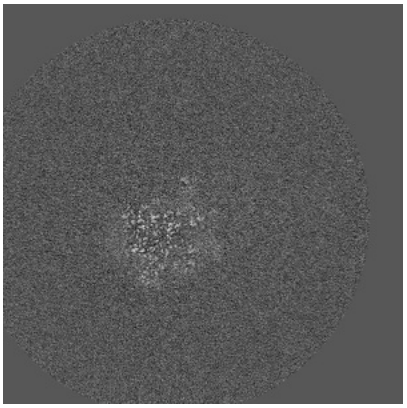


Y Index: 136

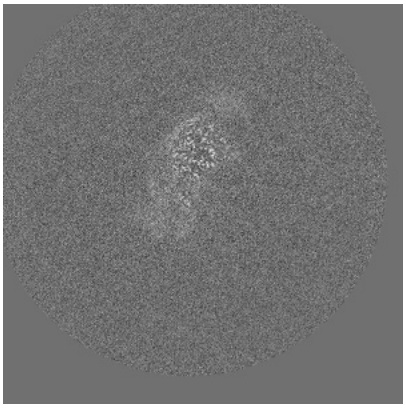


Z Index: 159

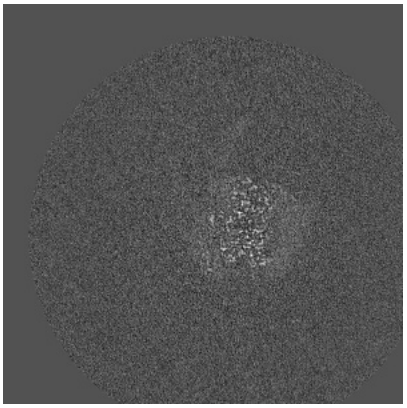
6.2.2 Raw map



X Index: 375



Y Index: 375

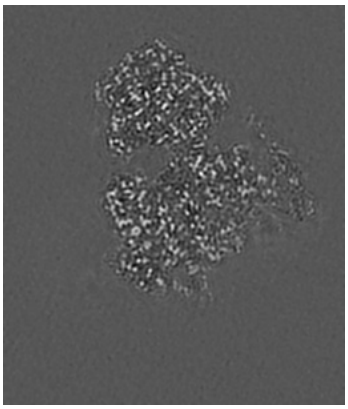


Z Index: 375

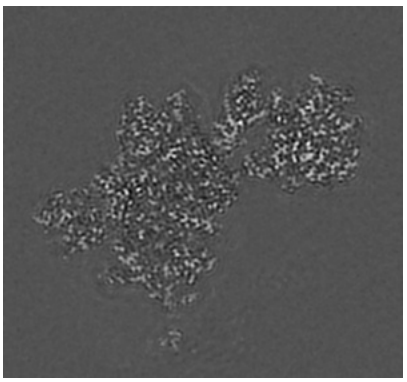
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

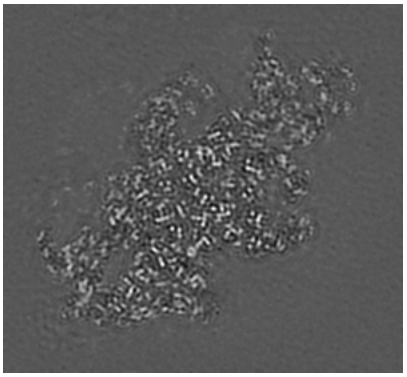
6.3.1 Primary map



X Index: 182

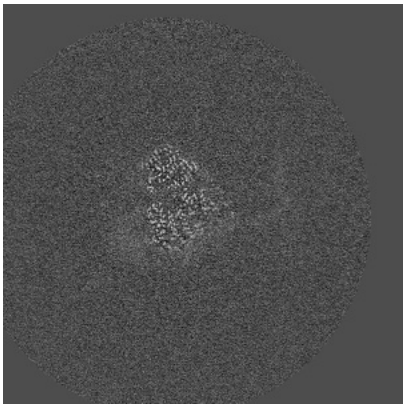


Y Index: 107

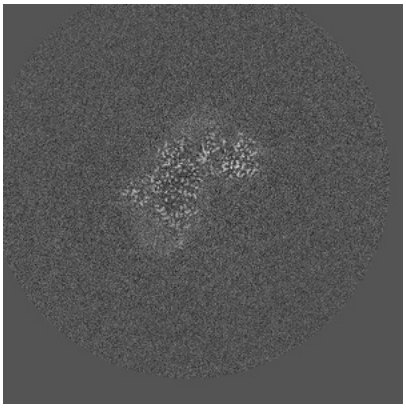


Z Index: 143

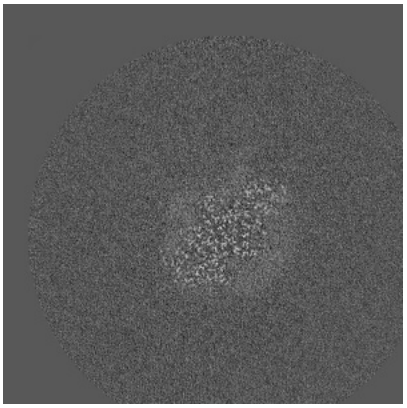
6.3.2 Raw map



X Index: 451



Y Index: 293



Z Index: 340

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

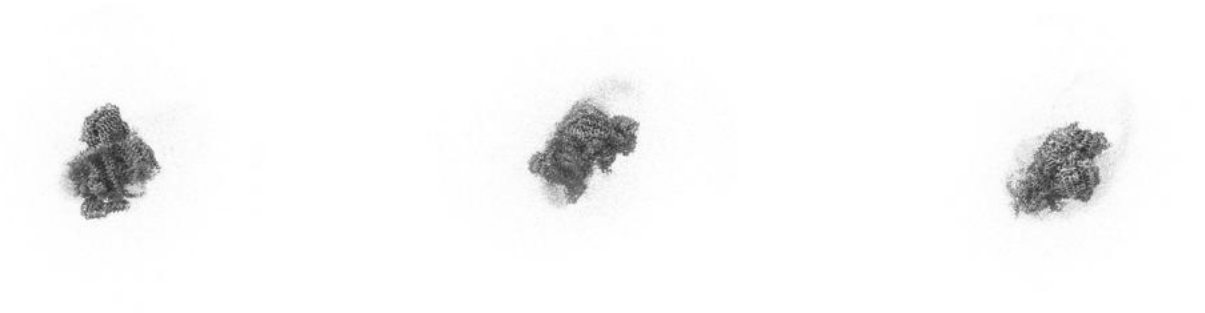
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

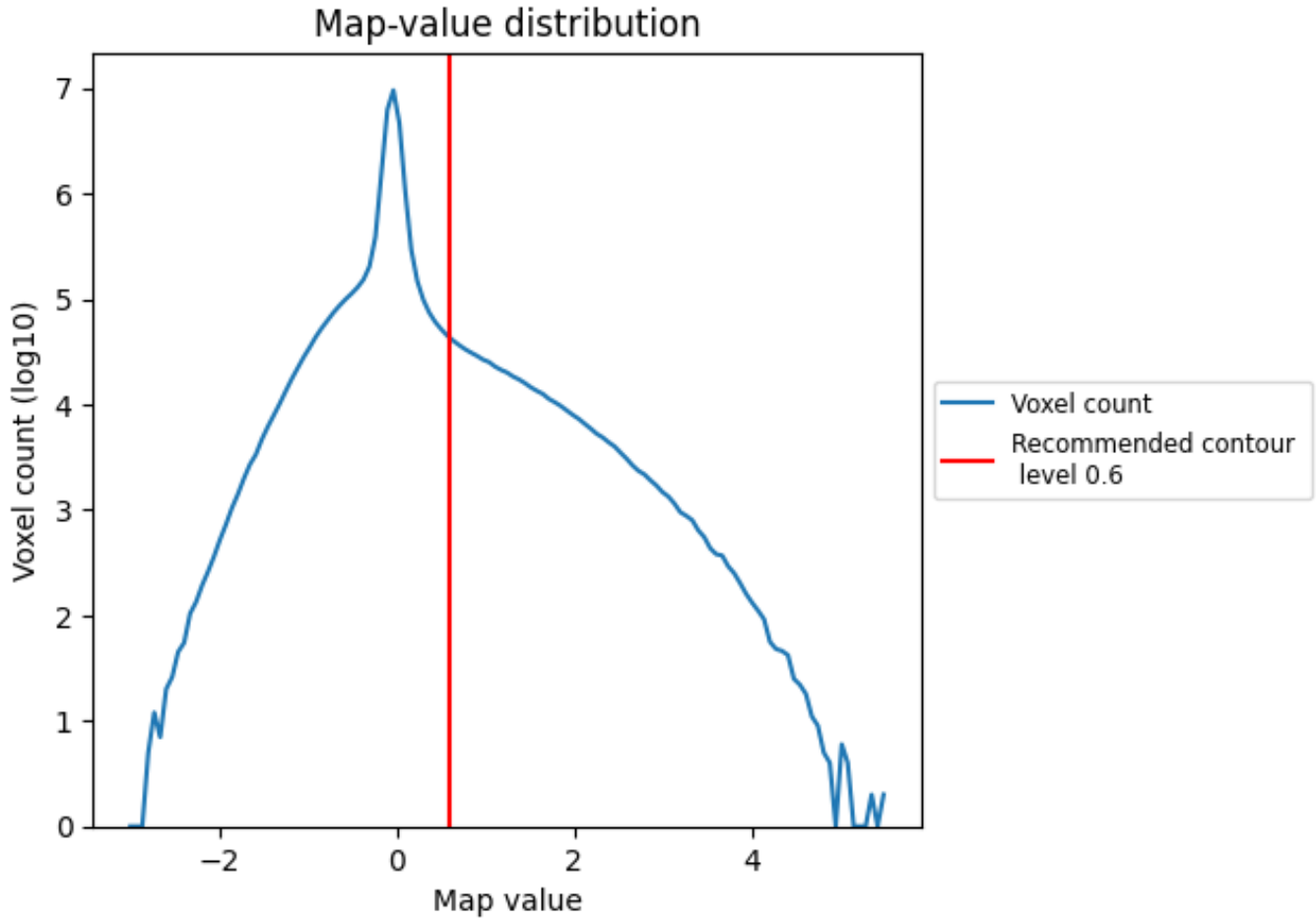
6.5 Mask visualisation (i)

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

7 Map analysis

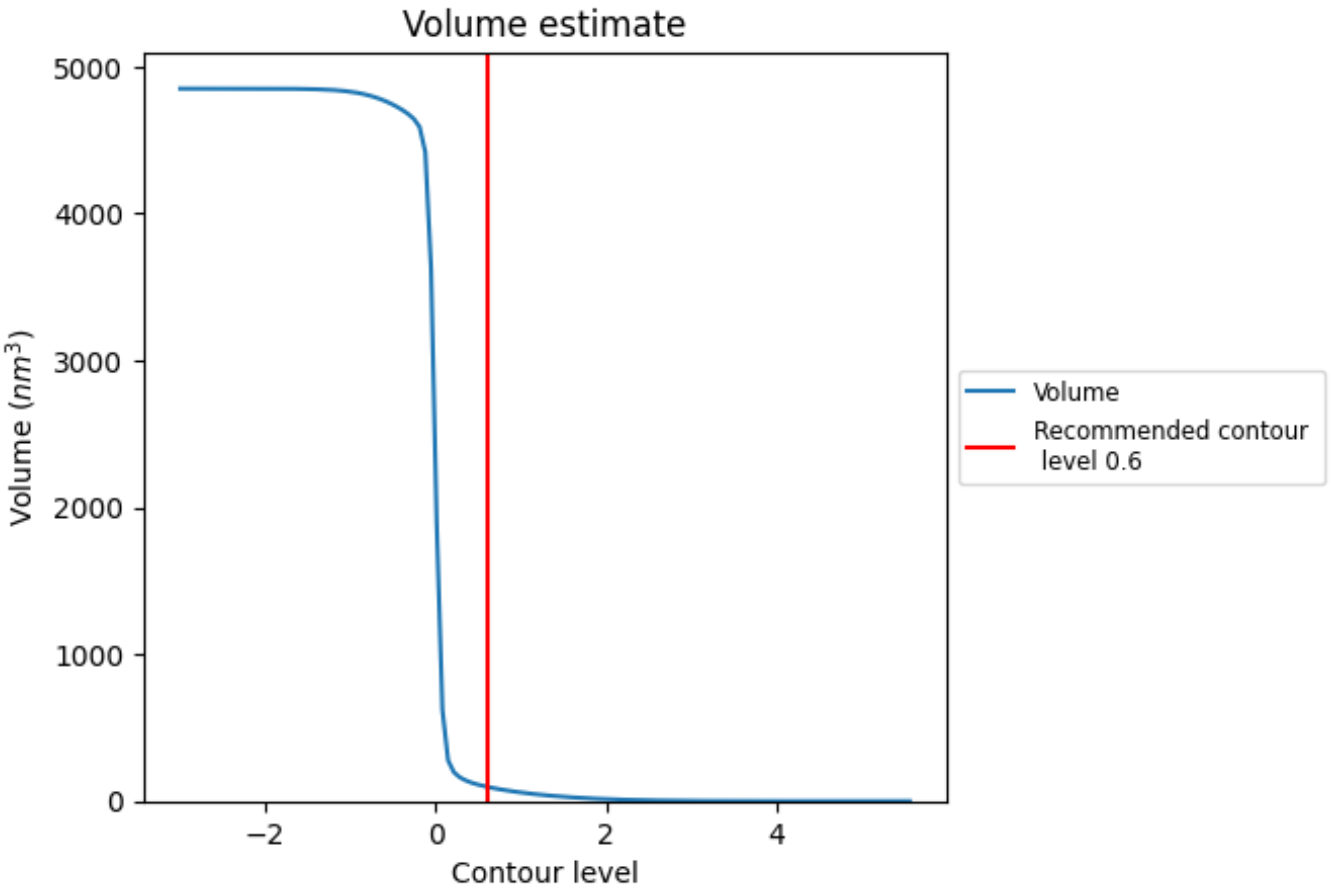
This section contains the results of statistical analysis of the map.

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 (i)



The volume at the recommended contour level is 98 nm^3; this corresponds to an approximate mass of 88 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.

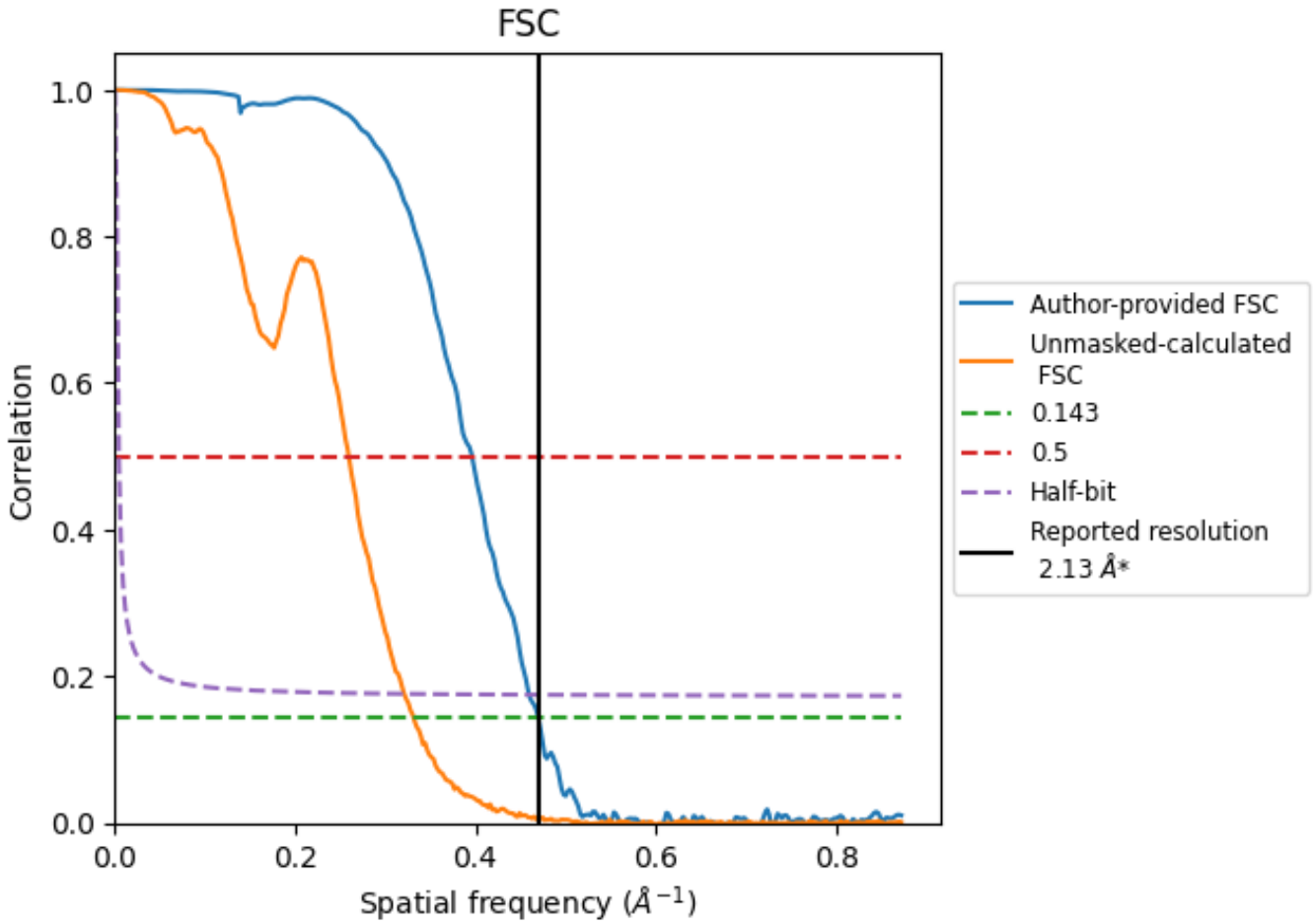
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.469 Å^{-1}

8.2 Resolution estimates (i)

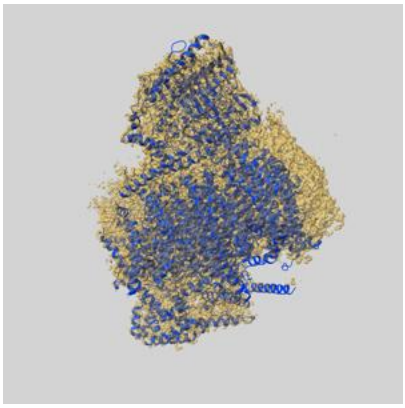
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.13	-	-
Author-provided FSC curve	2.13	2.52	2.17
Unmasked-calculated*	3.02	3.85	3.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.02 differs from the reported value 2.13 by more than 10 %

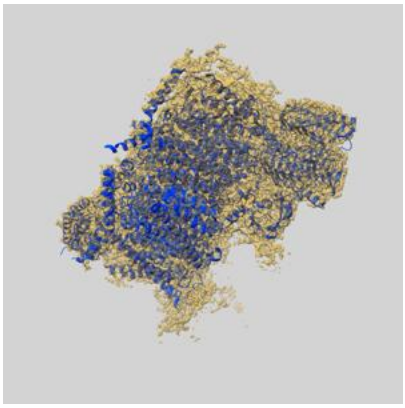
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16000 and PDB model 8BEF. Per-residue inclusion information can be found in section 3 on page 16.

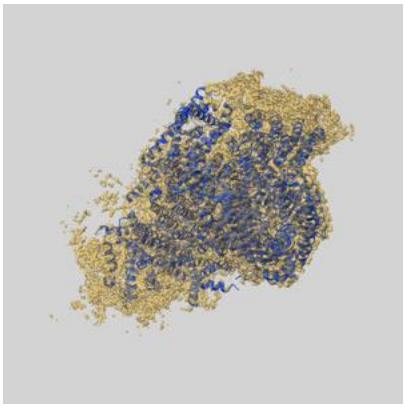
9.1 Map-model overlay



X



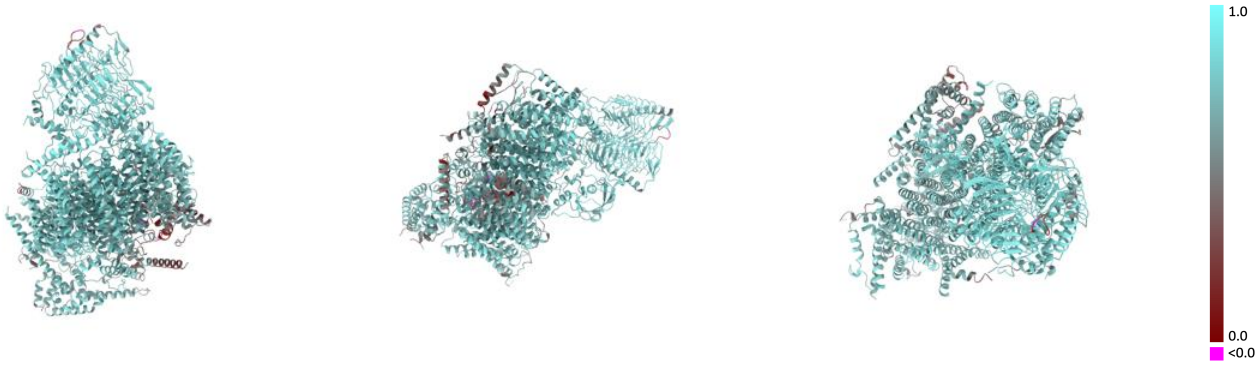
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 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.

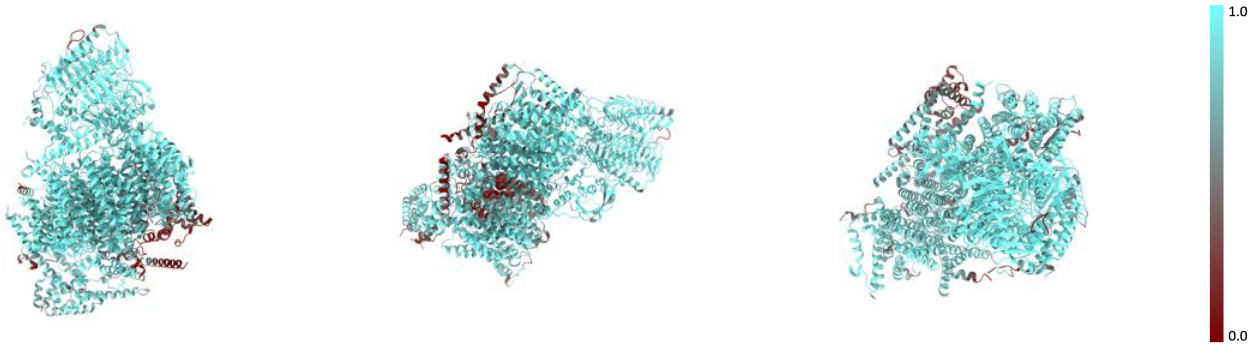
9.2 Q-score mapped to coordinate model



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.

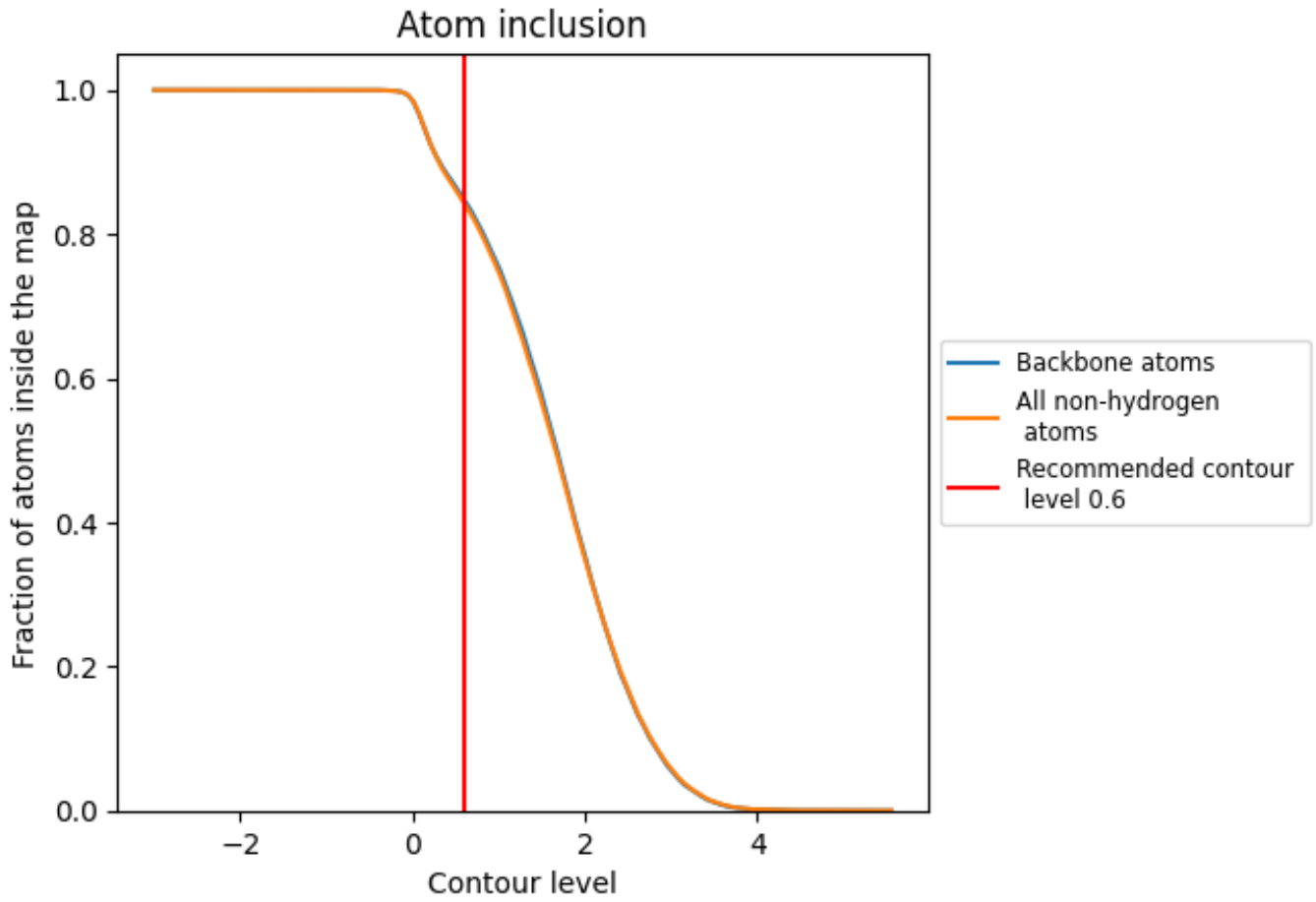
9.3 Atom inclusion mapped to coordinate model



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 (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 84% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8431	0.7290
A	0.9048	0.7590
H	0.8922	0.7620
J	0.8895	0.7460
K	0.9041	0.7630
L	0.6212	0.6430
M	0.7999	0.6770
N	0.9350	0.7760
O	0.9215	0.7670
X	0.8063	0.7000
Y	0.4588	0.5610
Z	0.8773	0.7350
a	0.8249	0.7060
b	0.7106	0.6600
d	0.7933	0.7010
e	0.8691	0.7200
f	0.8842	0.7540
i	0.5017	0.5450
u	0.5092	0.5820
v	0.8872	0.7440
x	0.9598	0.8020
y	0.9103	0.7600
z	0.9060	0.7460