Full wwPDB EM Validation Report ⓘ

Dec 7, 2022 – 02:31 PM JST

PDB ID	:	7V2R
EMDB ID	:	EMD-31647
Title	:	Active state complex I from Q1-NADH dataset
Authors	:	Gu, J.K.; Yang, M.J.
Deposited on	:	2021-08-09
Resolution	:	2.60 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:

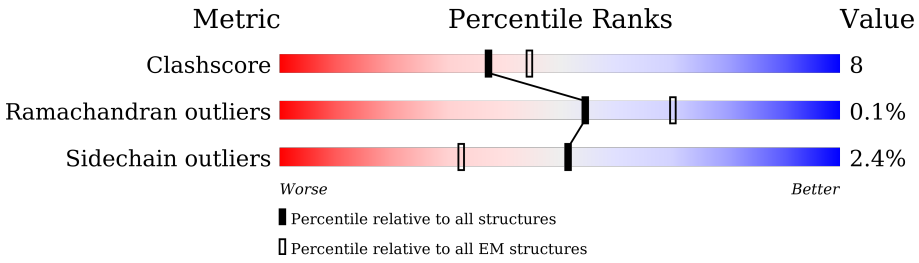
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.60 Å.

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



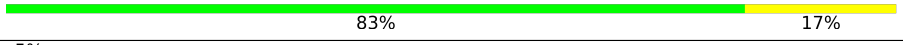
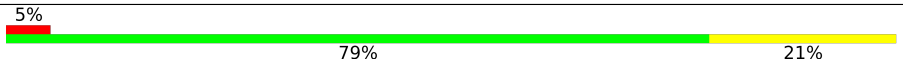
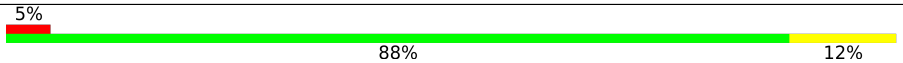
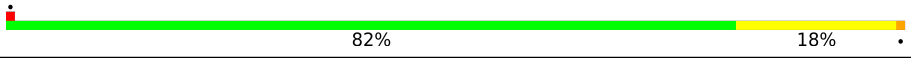
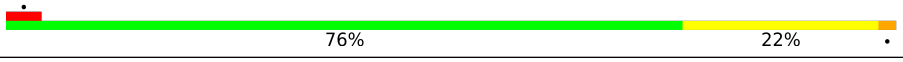
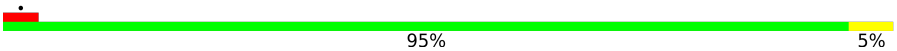
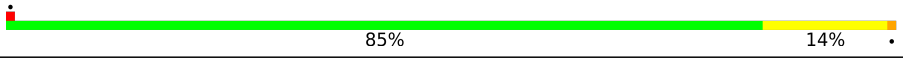
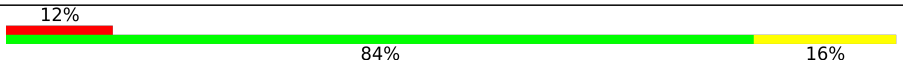
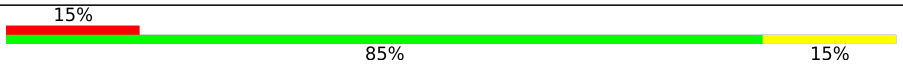
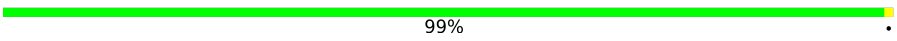
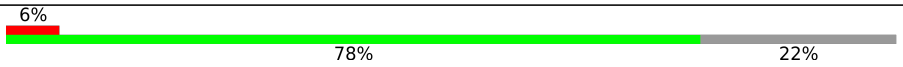
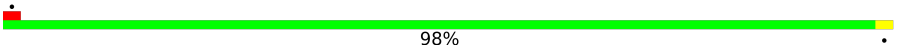
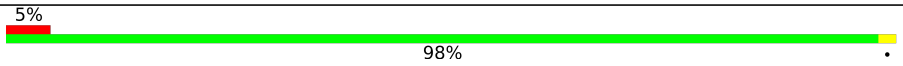
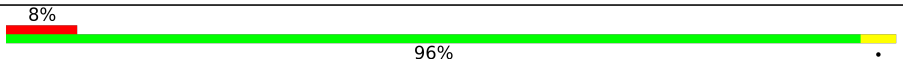
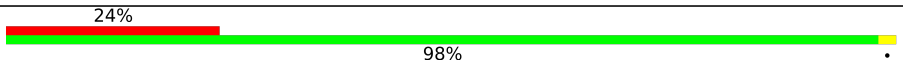
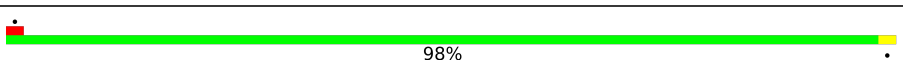
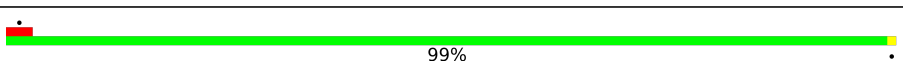
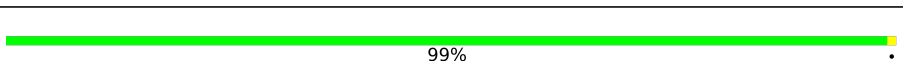
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	433	78% 21%
2	B	176	90% 9%
3	C	156	88% 12%
4	E	115	83% 16%
5	F	86	6% 70% 27%
6	G	88	15% 75% 22%
6	X	88	5% 82% 17%
7	H	112	88% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	I	112	
9	J	342	
10	K	43	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	67	
23	Z	80	
24	a	138	
25	b	126	
26	c	156	
27	d	175	
28	e	104	
29	f	49	
30	g	122	
31	h	105	
32	i	347	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	j	115	99%
34	k	98	96%
35	l	606	97%
36	m	175	14% 97%
37	n	56	16% 100%
38	o	128	98%
39	p	178	97%
40	r	459	98%
41	s	318	98%
42	u	171	94% 6%
43	v	125	15% 94% 5%
44	w	320	98%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	A	501	-	-	X	-
45	SF4	M	802	-	-	X	-
54	FES	O	301	-	-	X	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 68260 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	433	3330	2103	593	614	20	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	176	1412	887	243	269	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	156	1248	794	227	213	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	115	971	619	179	168	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	86	687	432	129	124	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			693	447	102	139	5		
6	X	88	Total	C	N	O	S	0	0
			703	453	104	141	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	97	Total	C	N	O	S	0	0
			780	491	147	139	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	342	Total	C	N	O	S	0	0
			2751	1783	481	478	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	43	Total	C	N	O	S	0	0
			366	228	68	69	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	125	Total	C	N	O	S	0	0
			1016	642	181	190	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	690	Total	C	N	O	S	0	0
			5296	3320	923	1014	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	144	Total	C	N	O	S	0	0
			1204	770	218	212	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	217	Total	C	N	O	S	0	0
			1671	1065	281	315	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1738	1124	298	314	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	430	Total	C	N	O	S	0	0
			3459	2212	594	629	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			566	364	103	94	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	142	Total	C	N	O	S	0	0
			1167	752	200	206	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	67	Total	C	N	O	S	0	0
			584	385	95	103	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	80	Total	C	N	O	S	0	0
			641	418	108	114	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	98	Total	C	N	O	S	0	0
			819	537	144	137	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	156	Total	C	N	O	S	0	0
			1315	853	213	241	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	175	Total	C	N	O	S	0	0
			1461	916	265	272	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	104	Total	C	N	O	S	0	0
			867	553	142	168	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	49	Total	C	N	O	0	0
			378	246	65	67		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	122	Total	C	N	O	S	0	0
			1005	653	174	172	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	347	Total	C	N	O	S	0	0
			2710	1782	420	462	46		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	115	Total	C	N	O	S	0	0
			914	615	134	158	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	98	Total	C	N	O	S	0	0
			748	493	113	128	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	606	Total	C	N	O	S	0	0
			4816	3193	746	826	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	175	Total	C	N	O	S	0	0
			1292	863	188	228	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

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

4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	o	128	Total	C	N	O	0	0
			1062	691	182	189		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	459	Total	C	N	O	S	0	0
			3631	2412	572	609	38		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	318	Total	C	N	O	S	0	0
			2508	1678	385	424	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			1028	642	195	182	9		

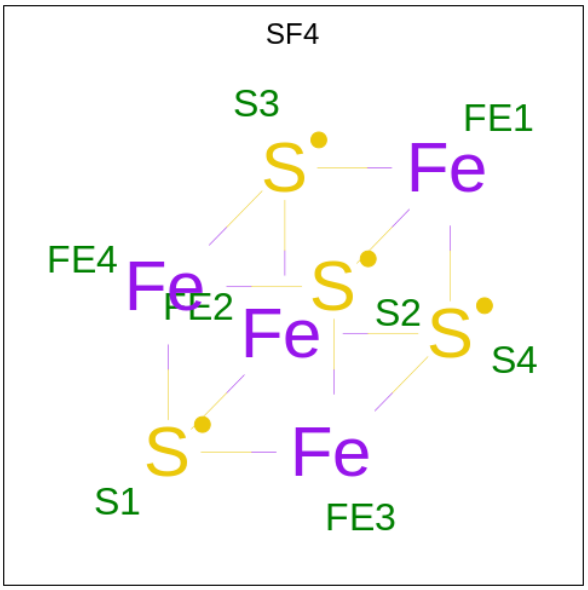
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	1	MYR	-	acetylation	UNP F1SCH1

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

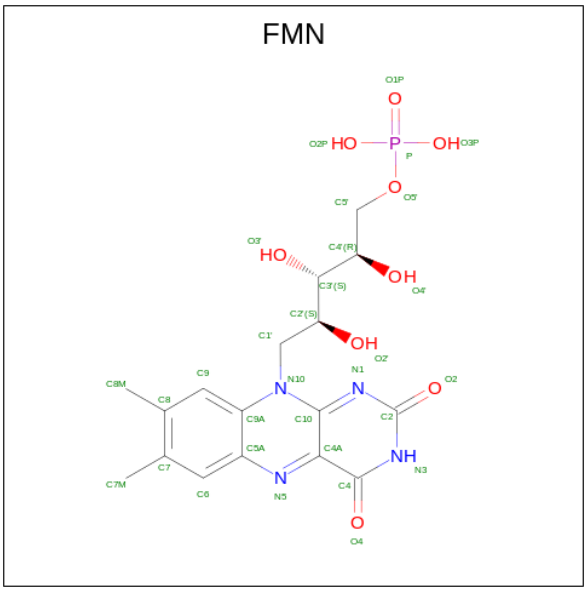
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2582	1643	438	491	10		

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



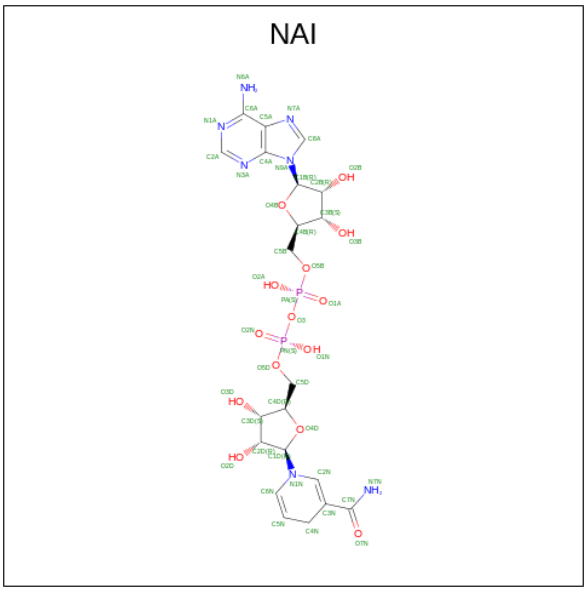
Mol	Chain	Residues	Atoms				AltConf
45	A	1	Total	Fe	S		0
			8	4	4		
45	B	1	Total	Fe	S		0
			16	8	8		
45	B	1	Total	Fe	S		0
			16	8	8		
45	C	1	Total	Fe	S		0
			8	4	4		
45	M	1	Total	Fe	S		0
			16	8	8		
45	M	1	Total	Fe	S		0
			16	8	8		

- Molecule 46 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



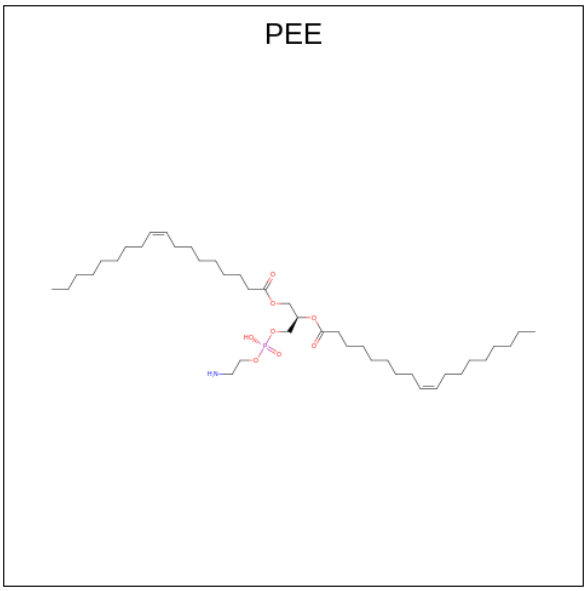
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



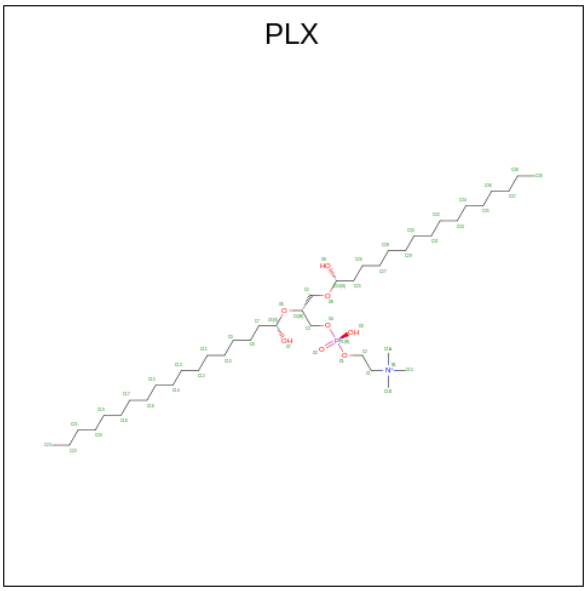
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 48 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



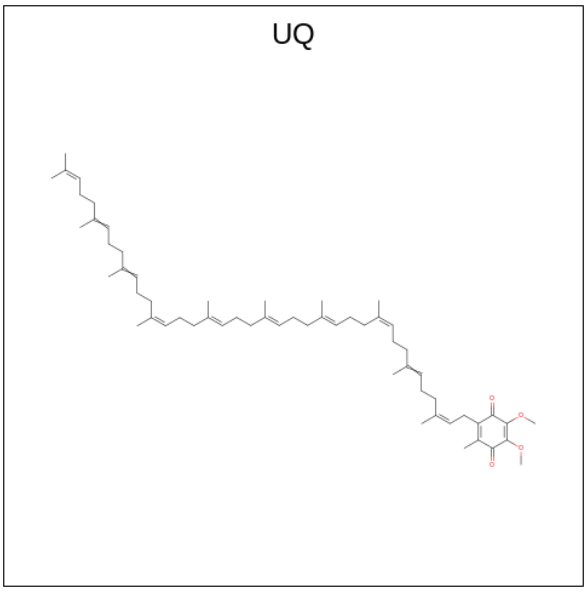
Mol	Chain	Residues	Atoms					AltConf
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	Q	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	V	1	Total	C	N	O	P	0
			91	71	2	16	2	
48	V	1	Total	C	N	O	P	0
			91	71	2	16	2	
48	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	j	1	Total	C	N	O	P	0
			92	72	2	16	2	
48	j	1	Total	C	N	O	P	0
			92	72	2	16	2	
48	l	1	Total	C	N	O	P	0
			97	77	2	16	2	
48	l	1	Total	C	N	O	P	0
			97	77	2	16	2	
48	s	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 49 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (three-letter code: PLX) (formula: $C_{42}H_{89}NO_8P$) (labeled as "Ligand of Interest" by depositor).



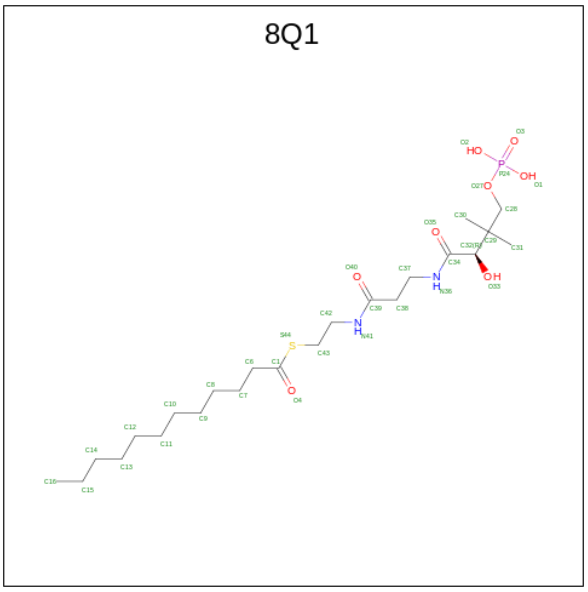
Mol	Chain	Residues	Atoms					AltConf
49	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	J	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	e	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 50 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
50	C	1	Total	C	O	0
			38	34	4	
50	J	1	Total	C	O	0
			33	29	4	

- Molecule 51 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



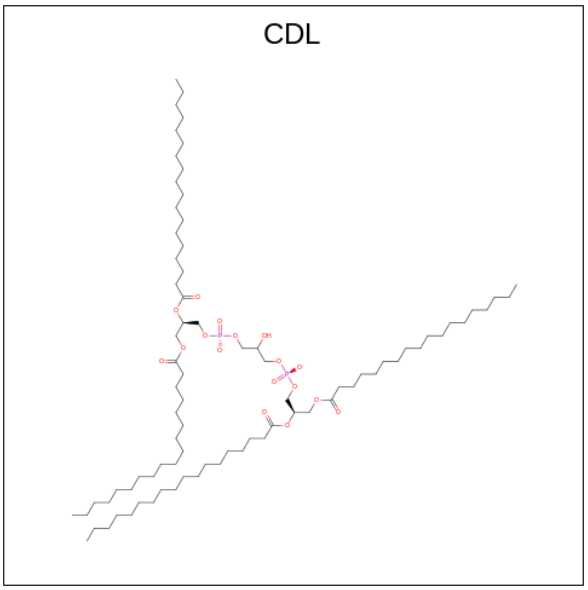
Mol	Chain	Residues	Atoms					AltConf
51	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

Continued on next page...

Continued from previous page...

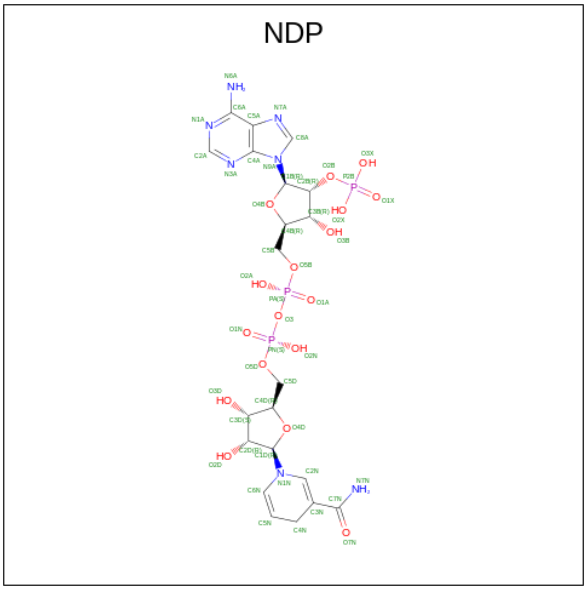
Mol	Chain	Residues	Atoms						AltConf
51	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 52 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



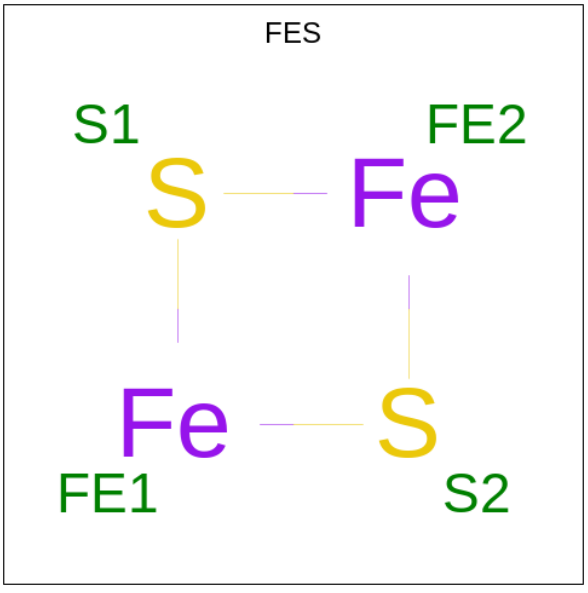
Mol	Chain	Residues	Atoms				AltConf
52	I	1	Total	C	O	P	0
			51	32	17	2	
52	J	1	Total	C	O	P	0
			89	70	17	2	
52	V	1	Total	C	O	P	0
			194	156	34	4	
52	V	1	Total	C	O	P	0
			194	156	34	4	
52	a	1	Total	C	O	P	0
			100	81	17	2	
52	k	1	Total	C	O	P	0
			94	75	17	2	
52	l	1	Total	C	O	P	0
			199	161	34	4	
52	l	1	Total	C	O	P	0
			199	161	34	4	
52	r	1	Total	C	O	P	0
			100	81	17	2	
52	u	1	Total	C	O	P	0
			55	36	17	2	

- Molecule 53 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

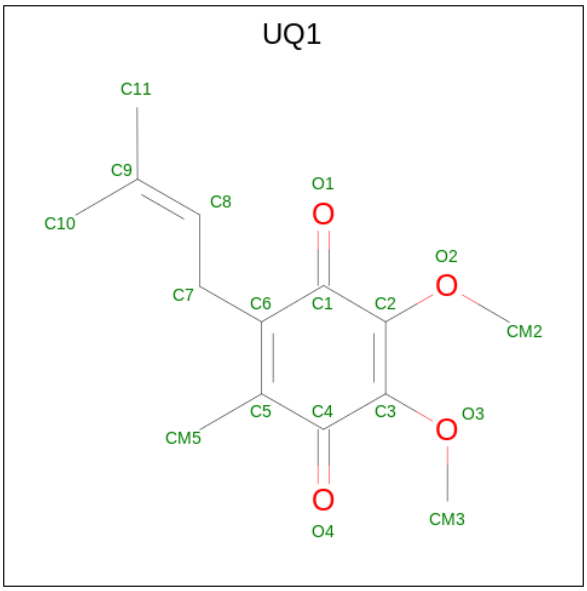


Mol	Chain	Residues	Atoms	AltConf
54	M	1	Total Fe S 4 2 2	0
54	O	1	Total Fe S 4 2 2	0

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 56 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$) (labeled as "Ligand of Interest" by depositor).

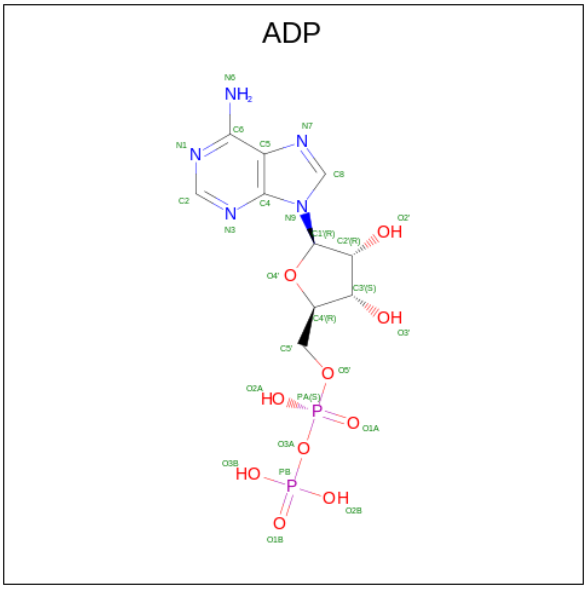


Mol	Chain	Residues	Atoms	AltConf
56	Q	1	Total C O 36 28 8	0
56	Q	1	Total C O 36 28 8	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 58 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



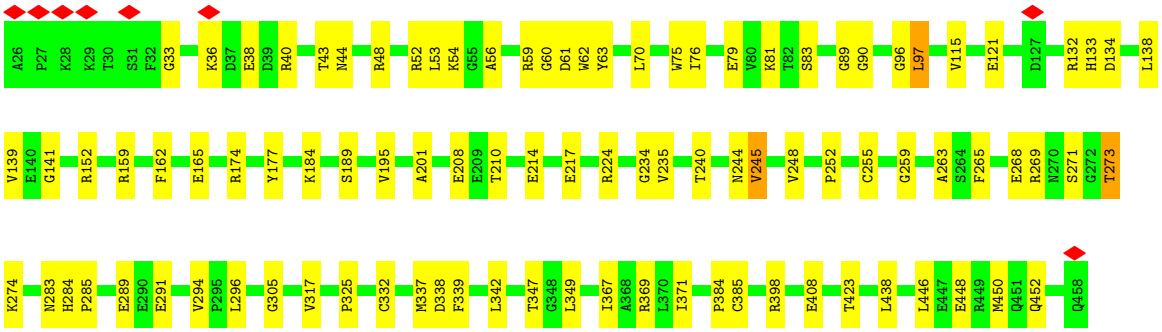
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	w	1	27	10	5	10	2	0

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.

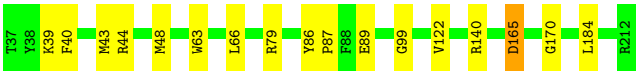
• Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain A:



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

Chain B:



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

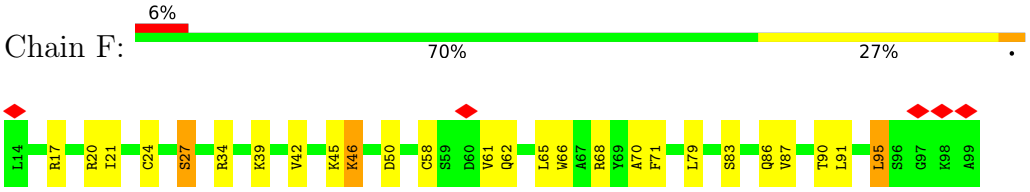
Chain C:

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

Chain E:

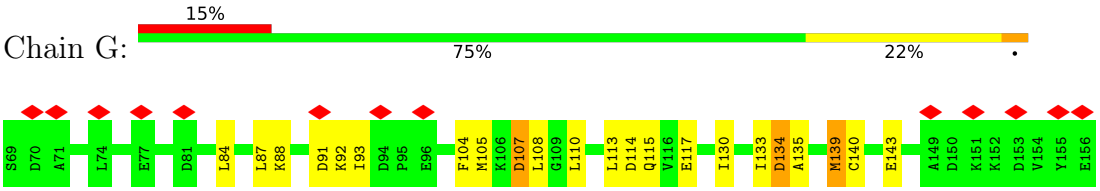
• Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain F:



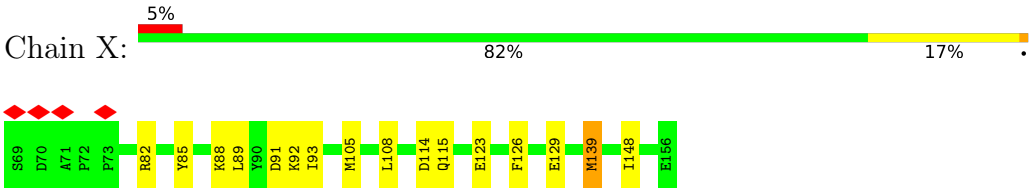
• Molecule 6: Acyl carrier protein, mitochondrial

Chain G:



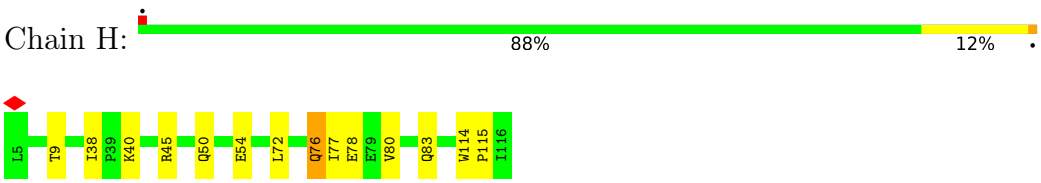
• Molecule 6: Acyl carrier protein, mitochondrial

Chain X:



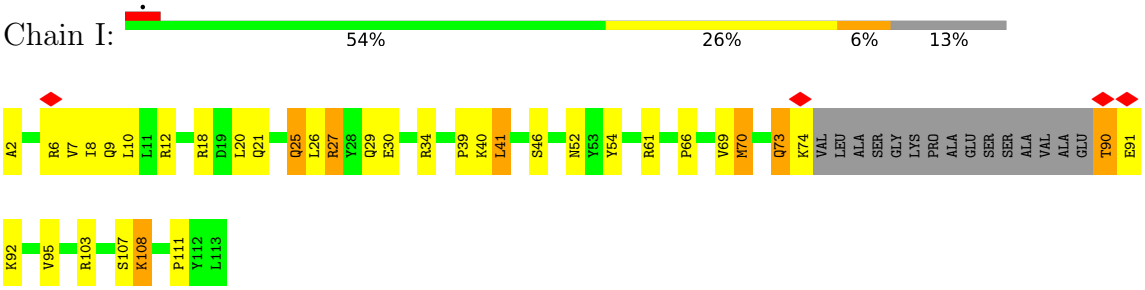
• Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain H:



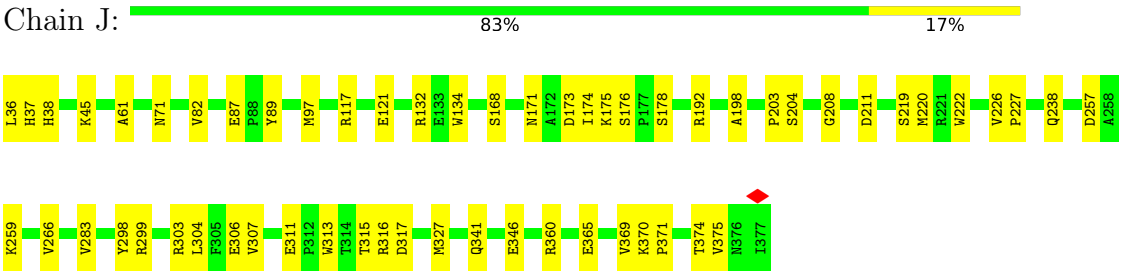
• Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain I:



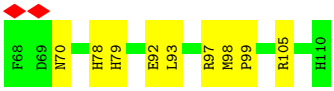
• Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain J:



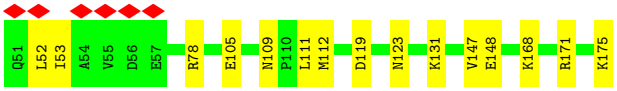
• Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain K:



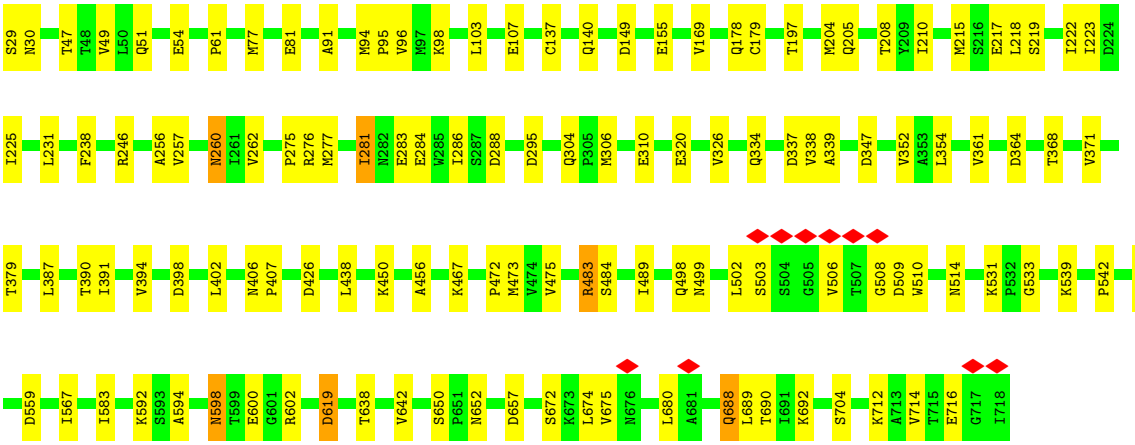
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain L:



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

Chain M:

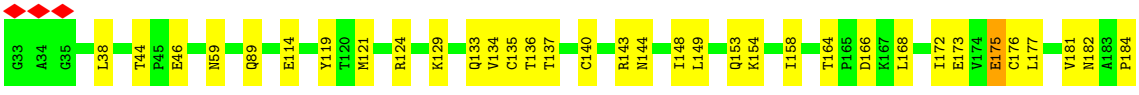


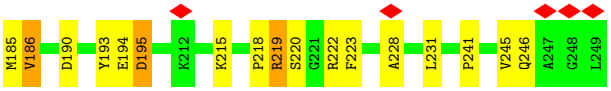
• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain N:

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

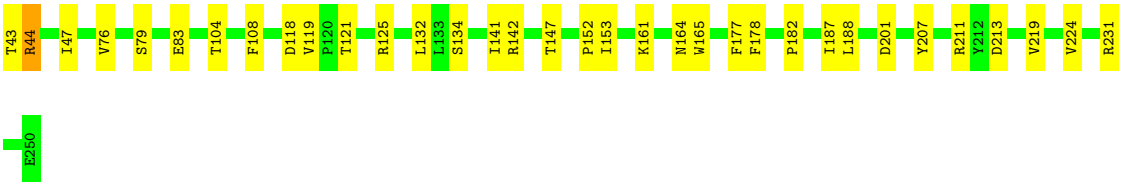
Chain O:





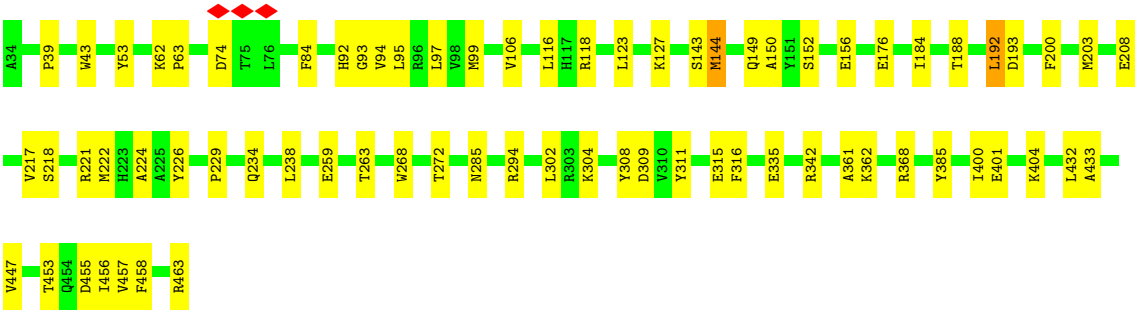
• Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain P:



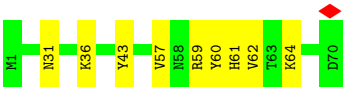
• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain Q:



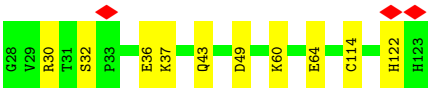
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S:



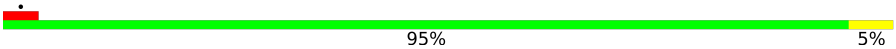
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

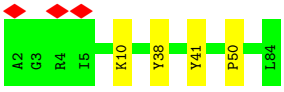
Chain T:



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

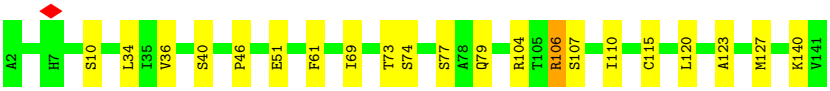
Chain U:





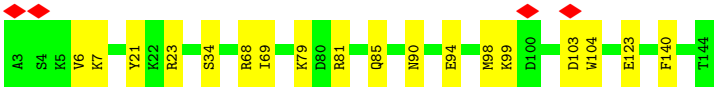
• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:



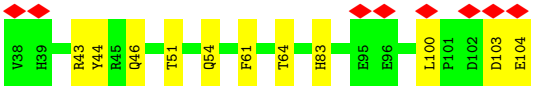
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:



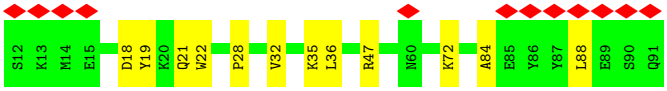
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y:



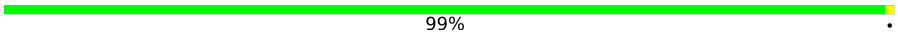
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z:



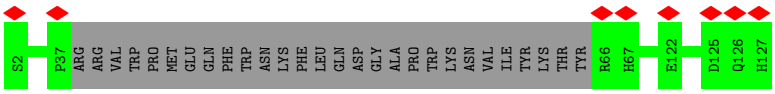
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:



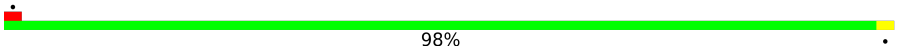
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

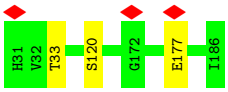
Chain b:



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

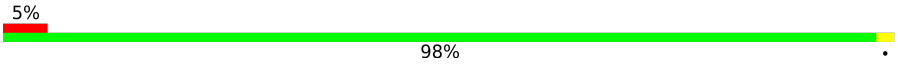
Chain c:

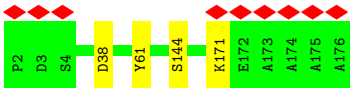




• Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

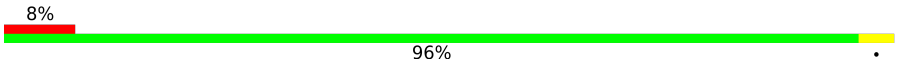
Chain d:

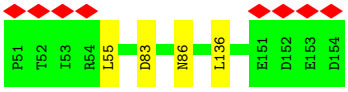




• Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

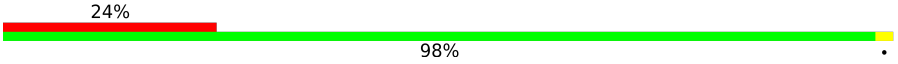
Chain e:

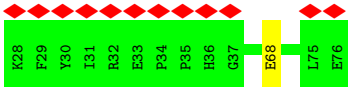




• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

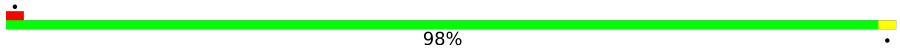
Chain f:

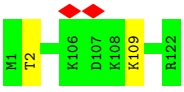




• Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

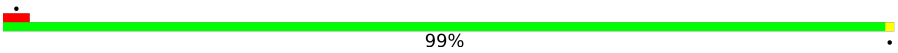
Chain g:

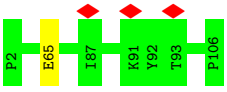




• Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

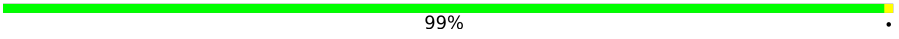
Chain h:





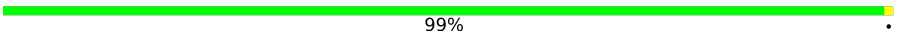
• Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain i:



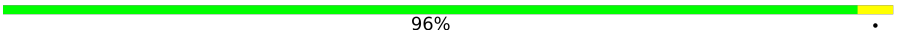
• Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j:



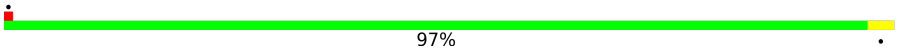
• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain k:



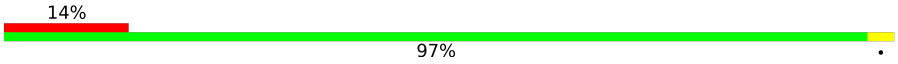
• Molecule 35: NADH-ubiquinone oxidoreductase chain 5

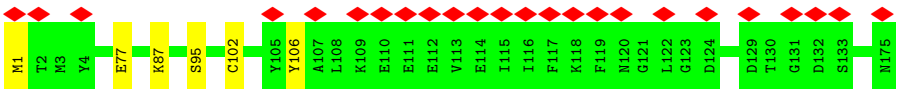
Chain l:



• Molecule 36: NADH-ubiquinone oxidoreductase chain 6

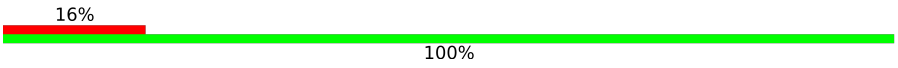
Chain m:

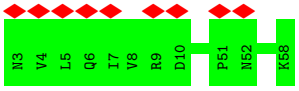




• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

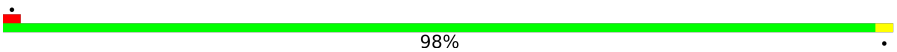
Chain n:

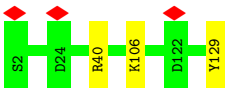




• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

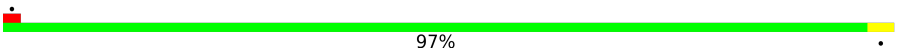
Chain o:

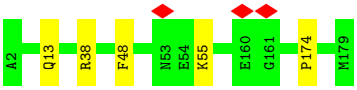




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

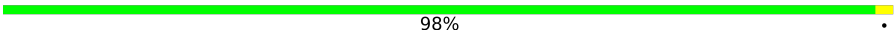
Chain p:





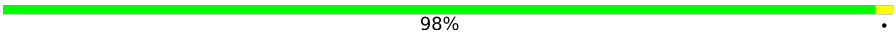
• Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r:



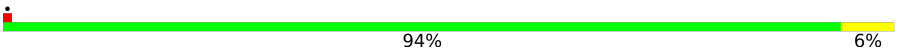
• Molecule 41: NADH-ubiquinone oxidoreductase chain 1

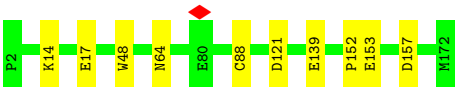
Chain s:



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

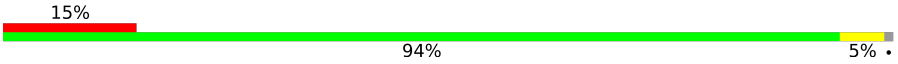
Chain u:

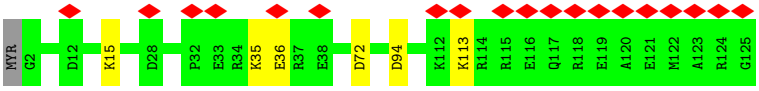




• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

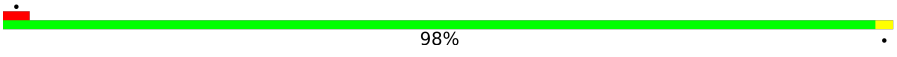
Chain v:

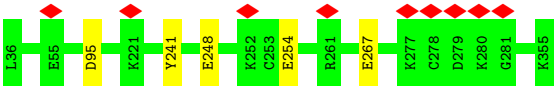




• Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain w:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	302353	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)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.268	Depositor
Minimum map value	-0.140	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	333.7616, 333.7616, 333.7616	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEE, SF4, NDP, UQ1, 8Q1, 2MR, ADP, FES, ZN, PLX, UQ, CDL, NAI, MG, FMN

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	0.27	0/3406	0.50	0/4603
2	B	0.29	0/1443	0.52	0/1952
3	C	0.29	0/1279	0.54	0/1730
4	E	0.27	0/995	0.52	0/1340
5	F	0.25	0/698	0.56	0/940
6	G	0.25	0/705	0.47	0/956
6	X	0.26	0/715	0.42	0/967
7	H	0.25	0/929	0.45	0/1258
8	I	0.28	0/798	0.63	0/1079
9	J	0.27	0/2828	0.48	0/3834
10	K	0.26	0/377	0.54	0/509
11	L	0.26	0/1039	0.50	0/1403
12	M	0.27	0/5384	0.53	0/7295
13	N	0.27	0/1245	0.51	0/1694
14	O	0.26	0/1711	0.49	0/2328
15	P	0.30	0/1789	0.55	0/2436
16	Q	0.35	2/3538 (0.1%)	0.54	0/4796
17	S	0.26	0/581	0.46	0/781
18	T	0.28	0/755	0.54	0/1018
19	U	0.26	0/664	0.46	0/912
20	V	0.26	0/1042	0.47	0/1411
21	W	0.28	0/1198	0.54	0/1617
22	Y	0.25	0/610	0.47	0/836
23	Z	0.26	0/660	0.47	0/892
24	a	0.28	0/1184	0.50	0/1603
25	b	0.27	0/844	0.51	0/1149
26	c	0.28	0/1371	0.48	0/1875
27	d	0.27	0/1494	0.52	0/2015
28	e	0.26	0/891	0.50	1/1210 (0.1%)
29	f	0.26	0/386	0.46	0/523
30	g	0.29	0/1036	0.49	0/1401
31	h	0.25	0/889	0.51	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	i	0.27	0/2773	0.49	1/3768 (0.0%)
33	j	0.26	0/938	0.42	0/1281
34	k	0.28	0/759	0.47	0/1029
35	l	0.27	0/4947	0.46	0/6728
36	m	0.29	0/1325	0.48	0/1800
37	n	0.24	0/491	0.48	0/663
38	o	0.28	0/1092	0.52	0/1481
39	p	0.26	0/1590	0.49	0/2155
40	r	0.27	0/3723	0.47	0/5078
41	s	0.28	0/2581	0.51	0/3529
42	u	0.26	0/1436	0.49	0/1938
43	v	0.25	0/1052	0.50	0/1411
44	w	0.26	0/2642	0.48	0/3580
All	All	0.27	2/67833 (0.0%)	0.50	2/91994 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	92	HIS	C-N	8.14	1.47	1.33
16	Q	193	ASP	C-N	5.40	1.46	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	e	55	LEU	CA-CB-CG	5.16	127.18	115.30
32	i	109	SER	C-N-CD	-5.09	109.40	120.60

There are no chirality outliers.

There are no planarity outliers.

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	3330	0	3292	80	0
2	B	1412	0	1363	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1248	0	1254	16	0
4	E	971	0	975	18	0
5	F	687	0	700	18	0
6	G	693	0	671	26	0
6	X	703	0	693	16	0
7	H	910	0	950	8	0
8	I	780	0	808	28	0
9	J	2751	0	2773	42	0
10	K	366	0	338	9	0
11	L	1016	0	1016	13	0
12	M	5296	0	5327	93	0
13	N	1204	0	1162	12	0
14	O	1671	0	1675	52	0
15	P	1738	0	1693	26	0
16	Q	3459	0	3395	50	0
17	S	566	0	561	5	0
18	T	741	0	702	9	0
19	U	643	0	642	3	0
20	V	1021	0	1025	13	0
21	W	1167	0	1155	13	0
22	Y	584	0	529	6	0
23	Z	641	0	620	7	0
24	a	1151	0	1164	0	0
25	b	819	0	835	0	0
26	c	1315	0	1208	0	0
27	d	1461	0	1429	0	0
28	e	867	0	817	0	0
29	f	378	0	356	0	0
30	g	1005	0	999	0	0
31	h	867	0	873	0	0
32	i	2710	0	2874	0	0
33	j	914	0	951	0	0
34	k	748	0	799	0	0
35	l	4816	0	4955	0	0
36	m	1292	0	1261	0	0
37	n	479	0	486	0	0
38	o	1062	0	1072	0	0
39	p	1534	0	1470	0	0
40	r	3631	0	3839	0	0
41	s	2508	0	2607	0	0
42	u	1398	0	1374	0	0
43	v	1028	0	982	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	w	2582	0	2531	0	0
45	A	8	0	0	2	0
45	B	16	0	0	0	0
45	C	8	0	0	1	0
45	M	16	0	0	3	0
46	A	31	0	19	3	0
47	A	44	0	27	4	0
48	C	47	0	71	5	0
48	Q	47	0	71	11	0
48	V	91	0	136	8	0
48	W	41	0	59	6	0
48	j	92	0	141	0	0
48	l	97	0	151	0	0
48	s	51	0	82	0	0
49	C	52	0	88	7	0
49	J	52	0	88	2	0
49	a	52	0	88	0	0
49	e	52	0	88	0	0
49	g	52	0	88	0	0
49	j	52	0	88	0	0
49	r	52	0	88	0	0
50	C	38	0	47	5	0
50	J	33	0	39	13	0
51	G	35	0	0	4	0
51	X	35	0	0	0	0
52	I	51	0	46	2	0
52	J	89	0	125	6	0
52	V	194	0	294	8	0
52	a	100	0	156	0	0
52	k	94	0	141	0	0
52	l	199	0	307	0	0
52	r	100	0	156	0	0
52	u	55	0	54	0	0
53	J	48	0	26	1	0
54	M	4	0	0	0	0
54	O	4	0	0	3	0
55	M	1	0	0	0	0
56	Q	36	0	36	7	0
57	T	1	0	0	0	0
58	w	27	0	11	0	0
All	All	68260	0	69012	548	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 8.

All (548) 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)
4:E:68:MET:CE	51:G:201:8Q1:C30	2.09	1.30
4:E:68:MET:HE3	51:G:201:8Q1:C30	1.65	1.24
48:Q:503:PEE:H42	48:Q:503:PEE:H34	1.26	1.16
16:Q:208:GLU:OE2	16:Q:221:ARG:NH2	1.83	1.11
1:A:285:PRO:HG3	14:O:143:ARG:NH1	1.67	1.10
6:X:139:MET:HE3	6:X:139:MET:HA	1.33	1.10
6:G:133:ILE:O	6:G:134:ASP:HB2	1.46	1.09
14:O:135:CYS:SG	14:O:175:GLU:O	2.11	1.07
14:O:134:VAL:HG12	14:O:186:VAL:HG22	1.37	1.03
14:O:140:CYS:SG	54:O:301:FES:FE1	1.49	1.03
4:E:68:MET:HE1	51:G:201:8Q1:C30	1.83	1.02
8:I:40:LYS:HB3	21:W:7:LYS:H	1.22	1.00
14:O:134:VAL:HG12	14:O:186:VAL:CG2	1.93	0.99
4:E:64:ARG:NH2	6:G:114:ASP:OD1	1.95	0.99
1:A:48:ARG:NH1	10:K:70:ASN:O	1.97	0.97
12:M:391:ILE:N	12:M:600:GLU:OE2	1.98	0.96
21:W:140:PHE:O	48:W:201:PEE:H11	1.65	0.95
48:Q:503:PEE:H37	48:Q:503:PEE:C37	1.96	0.95
12:M:179:CYS:SG	45:M:802:SF4:FE1	1.61	0.93
48:Q:503:PEE:H37	48:Q:503:PEE:H60	1.50	0.91
16:Q:156:GLU:OE2	16:Q:229:PRO:O	1.90	0.89
6:G:133:ILE:O	6:G:134:ASP:CB	2.19	0.88
12:M:483:ARG:NH1	12:M:489:ILE:HD11	1.89	0.87
9:J:313:TRP:CG	50:J:402:UQ:H8	2.12	0.85
6:G:139:MET:HA	6:G:139:MET:HE3	1.59	0.83
12:M:295:ASP:OD1	12:M:704:SER:OG	1.95	0.83
12:M:179:CYS:HG	45:M:802:SF4:FE1	0.96	0.82
9:J:313:TRP:CD1	50:J:402:UQ:H8	2.14	0.82
6:G:130:ILE:CG2	6:G:135:ALA:HB2	2.09	0.81
48:Q:503:PEE:H34	48:Q:503:PEE:C25	2.09	0.81
9:J:304:LEU:HD11	49:J:403:PLX:H312	1.63	0.80
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.16	0.79
15:P:125:ARG:NH2	15:P:201:ASP:OD1	2.16	0.78
11:L:109:ASN:ND2	11:L:111:LEU:O	2.17	0.77
6:X:139:MET:HA	6:X:139:MET:CE	2.14	0.77
48:W:201:PEE:H42	48:W:201:PEE:H33	1.64	0.77
14:O:136:THR:HG21	14:O:173:GLU:OE1	1.86	0.76
3:C:73:ALA:HB1	56:Q:501:UQ1:H112	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:PRO:CG	14:O:143:ARG:NH1	2.48	0.76
9:J:306:GLU:HG2	9:J:315:THR:HG22	1.68	0.76
48:Q:503:PEE:H37	48:Q:503:PEE:H61	1.67	0.75
9:J:220:MET:CE	9:J:227:PRO:HD2	2.17	0.75
6:G:105:MET:HE3	6:G:139:MET:SD	2.27	0.75
2:B:48:MET:O	19:U:10:LYS:NZ	2.20	0.74
12:M:338:VAL:HG21	12:M:361:VAL:HG11	1.70	0.74
15:P:231:ARG:HG3	15:P:231:ARG:HH11	1.54	0.73
6:X:85:TYR:HH	23:Z:22:TRP:HE1	0.75	0.73
12:M:483:ARG:HH11	12:M:489:ILE:HD11	1.52	0.72
22:Y:43:ARG:O	22:Y:46:GLN:NE2	2.22	0.72
14:O:177:LEU:HD12	14:O:185:MET:SD	2.30	0.71
14:O:140:CYS:HG	54:O:301:FES:FE1	0.42	0.71
6:G:139:MET:HA	6:G:139:MET:CE	2.21	0.71
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.73	0.71
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.72	0.71
12:M:179:CYS:SG	45:M:802:SF4:S4	2.89	0.71
48:Q:503:PEE:H28	48:Q:503:PEE:H36	1.72	0.71
12:M:256:ALA:O	12:M:598:ASN:ND2	2.24	0.70
16:Q:62:LYS:HE2	16:Q:63:PRO:HD2	1.73	0.70
48:W:201:PEE:H33	48:W:201:PEE:C25	2.21	0.70
5:F:20:ARG:HB2	5:F:66:TRP:HB2	1.73	0.70
50:J:402:UQ:C24	50:J:402:UQ:H201	2.22	0.70
8:I:92:LYS:HA	8:I:92:LYS:HE2	1.74	0.69
8:I:46:SER:O	8:I:52:ASN:ND2	2.24	0.69
50:J:402:UQ:H103	50:J:402:UQ:O1	1.93	0.69
12:M:337:ASP:O	12:M:542:PRO:HB2	1.93	0.69
2:B:44:ARG:HH11	2:B:44:ARG:HG2	1.59	0.68
6:G:130:ILE:HG22	6:G:135:ALA:HB2	1.74	0.68
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.27	0.68
9:J:37:HIS:CE1	18:T:49:ASP:HA	2.28	0.68
16:Q:156:GLU:CG	16:Q:229:PRO:O	2.42	0.68
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.75	0.67
48:W:201:PEE:H42	48:W:201:PEE:C21	2.24	0.67
1:A:285:PRO:HG3	14:O:143:ARG:HH11	1.56	0.67
9:J:192:ARG:NH1	9:J:198:ALA:O	2.28	0.67
1:A:337:MET:HE2	1:A:342:LEU:HD11	1.75	0.66
10:K:78:HIS:CE1	10:K:79:HIS:CE1	2.83	0.66
9:J:304:LEU:O	9:J:307:VAL:HG22	1.94	0.66
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.77	0.66
8:I:40:LYS:HB3	21:W:7:LYS:N	2.05	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Q:503:PEE:H60	48:Q:503:PEE:C23	2.24	0.66
16:Q:259:GLU:OE2	21:W:23:ARG:NH1	2.26	0.65
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.77	0.65
5:F:71:PHE:HE1	12:M:334:GLN:NE2	1.94	0.65
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.78	0.65
52:V:201:CDL:H731	52:V:201:CDL:H601	1.79	0.65
14:O:215:LYS:O	14:O:219:ARG:NH2	2.31	0.64
1:A:89:GLY:O	47:A:503:NAI:H2N	1.97	0.64
1:A:385:CYS:HB3	45:A:501:SF4:S2	2.37	0.63
5:F:71:PHE:CE1	12:M:334:GLN:NE2	2.66	0.63
1:A:56:ALA:HB1	1:A:61:ASP:HB2	1.81	0.63
12:M:178:GLN:HG2	12:M:204:MET:HE3	1.81	0.63
14:O:166:ASP:HB3	14:O:168:LEU:HD22	1.79	0.63
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.27	0.63
16:Q:192:LEU:HD21	56:Q:502:UQ1:HM22	1.81	0.62
1:A:285:PRO:HG3	14:O:143:ARG:HH12	1.63	0.62
7:H:83:GLN:HG3	15:P:104:THR:HG22	1.80	0.62
3:C:92:VAL:HG11	50:C:304:UQ:H103	1.81	0.62
4:E:64:ARG:NH1	6:G:117:GLU:OE1	2.32	0.62
4:E:96:VAL:HG12	4:E:96:VAL:O	2.00	0.62
15:P:211:ARG:NH2	15:P:213:ASP:OD2	2.33	0.62
6:X:139:MET:HE3	6:X:139:MET:CA	2.17	0.62
12:M:275:PRO:HG3	12:M:286:ILE:HG12	1.81	0.62
11:L:123:ASN:OD1	12:M:246:ARG:NH2	2.33	0.61
14:O:181:VAL:CG1	14:O:222:ARG:HH22	2.14	0.61
12:M:47:THR:O	12:M:96:VAL:HG22	2.01	0.61
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.83	0.60
1:A:159:ARG:NH2	14:O:176:CYS:O	2.34	0.60
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.33	0.60
1:A:285:PRO:CG	14:O:143:ARG:HH12	2.15	0.60
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.84	0.60
12:M:506:VAL:HG12	12:M:508:GLY:H	1.66	0.60
23:Z:84:ALA:O	23:Z:88:LEU:HB2	2.01	0.60
1:A:268:GLU:OE1	1:A:269:ARG:NH1	2.35	0.60
52:V:203:CDL:H622	52:V:203:CDL:H762	1.83	0.60
1:A:48:ARG:NH2	14:O:231:LEU:HD11	2.17	0.60
1:A:195:VAL:O	10:K:97:ARG:NH1	2.33	0.60
9:J:283:VAL:HG22	9:J:369:VAL:HG21	1.83	0.60
14:O:38:LEU:O	14:O:124:ARG:NH2	2.35	0.59
48:Q:503:PEE:H36	48:Q:503:PEE:C18	2.31	0.59
12:M:472:PRO:O	12:M:510:TRP:NE1	2.29	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:483:ARG:HH11	12:M:489:ILE:CD1	2.15	0.59
14:O:182:ASN:HD22	14:O:194:GLU:CD	2.05	0.59
14:O:59:ASN:ND2	14:O:89:GLN:OE1	2.32	0.59
5:F:24:CYS:N	5:F:58:CYS:SG	2.75	0.59
13:N:8:ARG:O	13:N:12:GLN:HG2	2.03	0.59
14:O:44:THR:HG22	14:O:46:GLU:H	1.68	0.59
48:Q:503:PEE:H42	48:Q:503:PEE:C21	2.10	0.59
9:J:313:TRP:CD2	50:J:402:UQ:C8	2.85	0.59
12:M:456:ALA:O	12:M:499:ASN:ND2	2.35	0.59
4:E:71:ALA:HB1	51:G:201:8Q1:O33	2.01	0.59
1:A:214:GLU:OE1	11:L:175:LYS:NZ	2.32	0.59
6:G:139:MET:HE3	6:G:139:MET:CA	2.32	0.59
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.37	0.59
20:V:61:PHE:HD2	20:V:104:ARG:HH21	1.51	0.59
5:F:68:ARG:NH2	12:M:364:ASP:OD1	2.36	0.58
12:M:368:THR:O	12:M:533:GLY:O	2.21	0.58
12:M:674:LEU:HD12	12:M:675:VAL:HG23	1.85	0.58
15:P:231:ARG:HG3	15:P:231:ARG:NH1	2.14	0.58
16:Q:226:TYR:OH	16:Q:234:GLN:O	2.14	0.58
1:A:52:ARG:O	1:A:54:LYS:N	2.37	0.58
12:M:498:GLN:O	12:M:498:GLN:NE2	2.35	0.58
8:I:8:ILE:HG13	52:I:201:CDL:OA4	2.03	0.58
11:L:78:ARG:NH1	11:L:148:GLU:OE2	2.36	0.58
3:C:54:VAL:HG21	48:C:302:PEE:H55	1.84	0.58
20:V:110:ILE:HD11	48:V:204:PEE:H8	1.85	0.58
21:W:90:ASN:ND2	21:W:123:GLU:O	2.37	0.58
5:F:71:PHE:HE1	12:M:334:GLN:HE21	1.51	0.58
9:J:313:TRP:CD2	50:J:402:UQ:H8	2.38	0.58
14:O:134:VAL:HG21	14:O:149:LEU:HD13	1.84	0.58
10:K:78:HIS:HE1	10:K:79:HIS:CE1	2.21	0.58
16:Q:144:MET:HG2	16:Q:222:MET:O	2.03	0.57
16:Q:152:SER:HB3	16:Q:229:PRO:HA	1.86	0.57
9:J:173:ASP:HB3	9:J:176:SER:HB2	1.87	0.57
14:O:148:ILE:HG13	14:O:184:PRO:HG2	1.87	0.57
50:C:304:UQ:HM31	56:Q:502:UQ1:HM31	1.86	0.57
6:G:104:PHE:HD1	6:G:108:LEU:HD12	1.70	0.57
12:M:257:VAL:C	12:M:598:ASN:HD21	2.08	0.57
1:A:56:ALA:HB1	1:A:61:ASP:CB	2.35	0.57
1:A:60:GLY:HA2	14:O:241:PRO:HA	1.87	0.56
8:I:7:VAL:HA	8:I:10:LEU:HD12	1.87	0.56
1:A:56:ALA:O	1:A:61:ASP:HB2	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:PRO:O	1:A:347:THR:OG1	2.19	0.56
50:J:402:UQ:O1	50:J:402:UQ:HM23	2.04	0.56
11:L:112:MET:SD	13:N:126:PRO:HB2	2.46	0.56
12:M:509:ASP:N	12:M:509:ASP:OD1	2.39	0.56
16:Q:304:LYS:NZ	16:Q:316:PHE:O	2.35	0.56
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.38	0.56
52:J:404:CDL:H561	48:W:201:PEE:H45	1.88	0.56
18:T:43:GLN:NE2	18:T:60:LYS:NZ	2.54	0.56
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.38	0.56
5:F:65:LEU:HB2	5:F:79:LEU:HD11	1.87	0.56
1:A:265:PHE:HB3	1:A:291:GLU:HG3	1.88	0.55
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.87	0.55
12:M:371:VAL:HG22	12:M:533:GLY:HA2	1.87	0.55
6:G:105:MET:CE	6:G:139:MET:CE	2.84	0.55
12:M:337:ASP:O	12:M:542:PRO:CB	2.54	0.55
3:C:188:LYS:HG2	3:C:191:ARG:HH11	1.71	0.55
12:M:390:THR:HB	12:M:600:GLU:OE2	2.06	0.55
48:C:302:PEE:H31	49:C:303:PLX:H392	1.88	0.55
7:H:9:THR:O	7:H:76:GLN:NE2	2.39	0.55
14:O:135:CYS:SG	14:O:176:CYS:HA	2.47	0.55
16:Q:156:GLU:HG3	16:Q:229:PRO:O	2.06	0.55
9:J:219:SER:HB2	50:J:402:UQ:HM52	1.88	0.55
14:O:148:ILE:HG13	14:O:184:PRO:CG	2.37	0.55
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.87	0.55
14:O:129:LYS:H	14:O:168:LEU:HA	1.72	0.55
15:P:201:ASP:OD1	15:P:201:ASP:N	2.40	0.55
48:C:302:PEE:O5	48:C:302:PEE:H52	2.07	0.55
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.88	0.54
6:G:92:LYS:HE2	6:G:114:ASP:OD2	2.07	0.54
14:O:164:THR:HG22	14:O:166:ASP:H	1.71	0.54
9:J:299:ARG:HG3	9:J:316:ARG:HG2	1.88	0.54
1:A:285:PRO:O	14:O:222:ARG:NH2	2.40	0.54
9:J:204:SER:OG	9:J:238:GLN:O	2.25	0.54
16:Q:404:LYS:HE2	16:Q:457:VAL:HG23	1.89	0.54
1:A:210:THR:HB	1:A:224:ARG:HG2	1.90	0.54
1:A:217:GLU:CD	11:L:171:ARG:HH22	2.12	0.54
9:J:178:SER:OG	9:J:317:ASP:OD1	2.23	0.54
5:F:61:VAL:HG23	5:F:62:GLN:H	1.73	0.54
9:J:117:ARG:O	9:J:121:GLU:HG3	2.08	0.54
9:J:313:TRP:CG	50:J:402:UQ:C8	2.89	0.54
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:217:GLU:HG2	12:M:218:LEU:HG	1.90	0.53
6:G:93:ILE:HD11	6:G:110:LEU:HD11	1.88	0.53
14:O:140:CYS:SG	54:O:301:FES:S2	3.06	0.53
12:M:51:GLN:HA	12:M:54:GLU:HG2	1.89	0.53
52:V:203:CDL:H742	52:V:203:CDL:H601	1.90	0.53
6:X:126:PHE:CE2	6:X:148:ILE:HD13	2.44	0.53
6:G:115:GLN:HG3	6:G:139:MET:HE1	1.89	0.53
8:I:12:ARG:HB3	8:I:20:LEU:HD12	1.90	0.53
9:J:168:SER:O	9:J:203:PRO:HD2	2.09	0.53
14:O:177:LEU:HD12	14:O:185:MET:CE	2.38	0.53
15:P:43:THR:HA	15:P:47:ILE:HD12	1.89	0.53
21:W:103:ASP:OD1	21:W:103:ASP:N	2.40	0.53
16:Q:156:GLU:CD	16:Q:229:PRO:O	2.47	0.53
12:M:390:THR:HA	12:M:600:GLU:HG2	1.91	0.53
1:A:263:ALA:HA	1:A:271:SER:HB3	1.91	0.52
1:A:448:GLU:O	1:A:452:GLN:HG2	2.10	0.52
20:V:106:ARG:HA	20:V:106:ARG:NE	2.24	0.52
4:E:120:SER:O	4:E:124:VAL:HG22	2.08	0.52
1:A:369:ARG:NH2	14:O:136:THR:OG1	2.41	0.52
3:C:126:GLU:HG2	9:J:89:TYR:OH	2.09	0.52
1:A:235:VAL:H	1:A:240:THR:HG21	1.74	0.52
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.45	0.52
12:M:98:LYS:HD3	12:M:98:LYS:C	2.30	0.52
15:P:44:ARG:HB2	15:P:44:ARG:CZ	2.39	0.52
1:A:296:LEU:HD22	1:A:332:CYS:HB3	1.91	0.52
4:E:48:HIS:NE2	9:J:365:GLU:OE1	2.37	0.52
5:F:86:GLN:O	5:F:90:THR:HG22	2.11	0.52
16:Q:53:TYR:OH	48:Q:503:PEE:O2P	2.12	0.52
46:A:502:FMN:N5	47:A:503:NAI:H4N	2.25	0.51
9:J:222:TRP:HZ3	52:J:404:CDL:HA4	1.74	0.51
1:A:217:GLU:OE1	11:L:171:ARG:NH2	2.43	0.51
6:G:107:ASP:OD1	6:G:107:ASP:N	2.44	0.51
20:V:110:ILE:HD11	48:V:204:PEE:C3	2.41	0.51
1:A:83:SER:HB2	1:A:259:GLY:HA2	1.92	0.51
1:A:115:VAL:HG22	1:A:248:VAL:HG21	1.93	0.51
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.38	0.51
20:V:46:PRO:HB2	20:V:51:GLU:HG2	1.93	0.51
22:Y:100:LEU:HD13	22:Y:104:GLU:HB2	1.92	0.51
5:F:42:VAL:O	5:F:46:LYS:HG2	2.10	0.51
8:I:54:TYR:CZ	16:Q:362:LYS:HD2	2.46	0.51
12:M:306:MET:HB2	12:M:583:ILE:HB	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:161:LYS:HG2	16:Q:285:ASN:HD22	1.76	0.51
6:X:91:ASP:OD1	23:Z:47:ARG:NH2	2.31	0.51
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.46	0.51
6:G:130:ILE:HG21	6:G:135:ALA:HB2	1.92	0.51
12:M:379:THR:O	12:M:379:THR:HG22	2.10	0.50
6:G:105:MET:HE3	6:G:139:MET:CE	2.41	0.50
9:J:220:MET:HE2	9:J:227:PRO:HD2	1.92	0.50
3:C:80:ALA:HA	3:C:86:MET:HG2	1.94	0.50
23:Z:32:VAL:O	23:Z:36:LEU:HG	2.12	0.50
1:A:234:GLY:HA3	1:A:240:THR:HG22	1.93	0.50
1:A:56:ALA:C	1:A:61:ASP:HB2	2.31	0.50
1:A:367:ILE:HG13	1:A:438:LEU:HD13	1.94	0.50
13:N:7:LEU:O	13:N:11:LEU:HG	2.11	0.50
1:A:214:GLU:OE2	1:A:224:ARG:NH2	2.40	0.50
16:Q:218:SER:OG	16:Q:224:ALA:HB1	2.12	0.50
9:J:87:GLU:HG3	9:J:89:TYR:H	1.77	0.50
7:H:38:ILE:O	7:H:45:ARG:NH1	2.36	0.50
16:Q:218:SER:CB	16:Q:224:ALA:HB1	2.42	0.50
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.47	0.49
52:J:404:CDL:HB61	52:J:404:CDL:H322	1.94	0.49
6:G:105:MET:HE2	6:G:139:MET:CE	2.42	0.49
6:X:89:LEU:HD21	23:Z:19:TYR:HB2	1.93	0.49
8:I:66:PRO:HB3	15:P:79:SER:HA	1.94	0.49
8:I:69:VAL:O	15:P:76:VAL:HB	2.11	0.49
1:A:134:ASP:N	1:A:134:ASP:OD1	2.45	0.49
6:G:84:LEU:O	6:G:88:LYS:HG2	2.13	0.49
12:M:531:LYS:HB2	12:M:531:LYS:NZ	2.27	0.49
1:A:255:CYS:O	14:O:246:GLN:OE1	2.30	0.49
1:A:283:ASN:ND2	1:A:305:GLY:O	2.46	0.49
15:P:147:THR:HB	15:P:153:ILE:HD11	1.94	0.49
8:I:26:LEU:HD13	13:N:55:PHE:CD2	2.48	0.49
9:J:238:GLN:HG2	9:J:266:VAL:HB	1.94	0.49
50:J:402:UQ:H201	50:J:402:UQ:C23	2.43	0.48
20:V:69:ILE:O	20:V:73:THR:HG23	2.12	0.48
12:M:29:SER:OG	12:M:30:ASN:N	2.45	0.48
14:O:175:GLU:OE1	14:O:175:GLU:HA	2.11	0.48
1:A:44:ASN:ND2	1:A:133:HIS:O	2.47	0.48
1:A:273:THR:OG1	1:A:274:LYS:N	2.47	0.48
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.53	0.48
4:E:101:THR:OG1	15:P:219:VAL:O	2.21	0.48
3:C:59:ARG:NH1	49:C:303:PLX:O2	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:94:VAL:HG21	16:Q:116:LEU:HB2	1.95	0.48
9:J:174:ILE:HG23	9:J:175:LYS:HG2	1.95	0.48
18:T:64:GLU:OE2	18:T:64:GLU:HA	2.14	0.48
3:C:52:ASP:HB3	49:C:303:PLX:H251	1.96	0.48
5:F:91:LEU:O	5:F:95:LEU:HD12	2.12	0.48
12:M:619:ASP:OD1	12:M:619:ASP:N	2.46	0.48
20:V:40:SER:HA	52:V:201:CDL:HB61	1.95	0.48
48:V:204:PEE:O2P	48:V:204:PEE:H7	2.14	0.48
22:Y:103:ASP:OD1	22:Y:103:ASP:N	2.47	0.48
12:M:638:THR:O	12:M:642:VAL:HG23	2.13	0.48
2:B:44:ARG:HG2	2:B:44:ARG:NH1	2.22	0.48
8:I:2:ALA:HB3	8:I:21:GLN:HE22	1.78	0.48
12:M:222:ILE:HD12	12:M:231:LEU:HD13	1.96	0.47
12:M:347:ASP:HB3	12:M:594:ALA:HB1	1.96	0.47
12:M:391:ILE:HG13	12:M:600:GLU:CD	2.34	0.47
6:G:93:ILE:HD13	6:G:108:LEU:HD13	1.95	0.47
15:P:165:TRP:CD2	16:Q:433:ALA:HB2	2.48	0.47
17:S:43:TYR:CZ	21:W:68:ARG:HG3	2.49	0.47
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.70	0.47
49:C:303:PLX:H102	49:C:303:PLX:H261	1.97	0.47
12:M:169:VAL:HG22	12:M:223:ILE:HD11	1.95	0.47
12:M:262:VAL:HG23	12:M:276:ARG:HB2	1.96	0.47
12:M:483:ARG:HH12	12:M:489:ILE:HD11	1.78	0.47
12:M:690:THR:CG2	12:M:692:LYS:HG2	2.45	0.47
8:I:30:GLU:CD	8:I:30:GLU:H	2.17	0.47
23:Z:28:PRO:O	23:Z:32:VAL:HG23	2.15	0.47
1:A:36:LYS:HG3	1:A:38:GLU:HG2	1.96	0.47
1:A:40:ARG:NH2	1:A:289:GLU:O	2.43	0.47
48:C:302:PEE:H31	49:C:303:PLX:C39	2.45	0.47
12:M:347:ASP:OD1	12:M:347:ASP:N	2.39	0.47
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.97	0.47
1:A:90:GLY:HA3	47:A:503:NAI:H1D	1.97	0.47
12:M:394:VAL:HA	12:M:473:MET:HE1	1.97	0.47
12:M:406:ASN:ND2	12:M:688:GLN:O	2.47	0.47
6:X:123:GLU:HG2	6:X:129:GLU:HA	1.97	0.47
4:E:23:ARG:NH2	11:L:52:LEU:O	2.48	0.47
8:I:40:LYS:CG	21:W:6:VAL:HA	2.44	0.47
18:T:43:GLN:HE21	18:T:60:LYS:HZ1	1.61	0.47
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.29	0.46
9:J:71:ASN:HA	9:J:97:MET:HG2	1.97	0.46
16:Q:176:GLU:OE2	16:Q:311:TYR:OH	2.24	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:294:ARG:NH2	16:Q:401:GLU:OE2	2.48	0.46
16:Q:432:LEU:HB2	16:Q:456:ILE:HD13	1.97	0.46
18:T:37:LYS:HB2	18:T:37:LYS:HE3	1.54	0.46
3:C:63:TRP:HH2	50:C:304:UQ:H153	1.80	0.46
12:M:260:ASN:HD22	12:M:260:ASN:N	2.12	0.46
15:P:161:LYS:HG2	16:Q:285:ASN:ND2	2.30	0.46
4:E:16:SER:HA	11:L:52:LEU:HD13	1.97	0.46
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.51	0.46
1:A:62:TRP:HZ2	1:A:139:VAL:HG12	1.81	0.46
1:A:81:LYS:HG2	1:A:96:GLY:HA3	1.96	0.46
12:M:257:VAL:O	12:M:598:ASN:ND2	2.48	0.46
13:N:129:THR:HA	18:T:43:GLN:HG2	1.98	0.46
1:A:63:TYR:CE2	14:O:245:VAL:HG21	2.50	0.46
3:C:188:LYS:HG2	3:C:191:ARG:NH1	2.31	0.46
50:C:304:UQ:H262	50:C:304:UQ:H221	1.41	0.46
48:V:204:PEE:H7	48:V:204:PEE:P	2.56	0.46
21:W:98:MET:HE2	21:W:104:TRP:CD2	2.51	0.46
1:A:338:ASP:OD1	1:A:338:ASP:N	2.49	0.46
4:E:101:THR:O	4:E:105:ARG:HG3	2.15	0.46
9:J:134:TRP:CZ2	9:J:311:GLU:HG2	2.50	0.46
12:M:407:PRO:HD2	12:M:438:LEU:HD21	1.98	0.46
15:P:164:ASN:ND2	15:P:182:PRO:HG2	2.31	0.46
20:V:140:LYS:HB3	20:V:140:LYS:HE2	1.54	0.46
22:Y:51:THR:O	22:Y:54:GLN:HG2	2.15	0.46
1:A:33:GLY:HA2	1:A:294:VAL:HB	1.98	0.46
18:T:32:SER:OG	18:T:36:GLU:O	2.29	0.46
5:F:45:LYS:HA	5:F:45:LYS:HD2	1.73	0.45
7:H:76:GLN:O	7:H:78:GLU:N	2.49	0.45
14:O:153:GLN:HG2	14:O:158:ILE:O	2.15	0.45
1:A:62:TRP:CZ2	1:A:139:VAL:HG12	2.51	0.45
14:O:148:ILE:CG1	14:O:184:PRO:CG	2.94	0.45
3:C:73:ALA:HB1	56:Q:501:UQ1:C11	2.43	0.45
8:I:40:LYS:HG2	21:W:6:VAL:HA	1.98	0.45
52:J:404:CDL:H381	52:J:404:CDL:H742	1.98	0.45
1:A:63:TYR:HE2	14:O:245:VAL:HG21	1.81	0.45
5:F:61:VAL:O	5:F:62:GLN:HG2	2.15	0.45
12:M:208:THR:OG1	12:M:210:ILE:O	2.34	0.45
5:F:65:LEU:HD11	5:F:91:LEU:HD13	1.98	0.45
5:F:83:SER:O	5:F:87:VAL:HG13	2.17	0.45
8:I:90:THR:OG1	8:I:91:GLU:N	2.49	0.45
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:193:TYR:HD1	14:O:219:ARG:HH21	1.63	0.45
17:S:59:ARG:HD2	17:S:61:HIS:NE2	2.31	0.45
1:A:177:TYR:CD2	10:K:93:LEU:HD22	2.51	0.45
14:O:195:ASP:OD2	14:O:220:SER:OG	2.28	0.45
16:Q:188:THR:HB	16:Q:200:PHE:HA	1.98	0.45
1:A:75:TRP:O	1:A:79:GLU:HG2	2.17	0.45
3:C:83:ARG:HH22	8:I:27:ARG:NH2	2.15	0.45
11:L:168:LYS:N	11:L:168:LYS:HD2	2.31	0.45
6:X:105:MET:HE3	6:X:139:MET:HE1	1.98	0.45
12:M:197:THR:O	14:O:114:GLU:HG2	2.17	0.45
12:M:197:THR:HA	12:M:205:GLN:O	2.17	0.45
6:X:88:LYS:HB2	6:X:88:LYS:HE3	1.59	0.45
4:E:25:MET:O	4:E:29:LYS:HG3	2.17	0.44
12:M:650:SER:OG	12:M:652:ASN:OD1	2.35	0.44
1:A:43:THR:OG1	1:A:59:ARG:HD2	2.17	0.44
12:M:391:ILE:HG13	12:M:600:GLU:OE2	2.17	0.44
16:Q:218:SER:OG	16:Q:224:ALA:CB	2.64	0.44
17:S:31:ASN:ND2	17:S:36:LYS:HB2	2.31	0.44
20:V:110:ILE:CG1	48:V:204:PEE:H8	2.47	0.44
2:B:39:LYS:HD2	16:Q:335:GLU:HG2	1.99	0.44
3:C:59:ARG:HH12	49:C:303:PLX:P1	2.40	0.44
4:E:19:PRO:HB3	11:L:53:ILE:HG21	1.99	0.44
7:H:72:LEU:HD13	7:H:80:VAL:HG11	1.99	0.44
12:M:402:LEU:HD23	12:M:475:VAL:HB	1.98	0.44
12:M:688:GLN:H	12:M:688:GLN:HG2	1.60	0.44
16:Q:268:TRP:O	16:Q:272:THR:OG1	2.30	0.44
20:V:34:LEU:HD23	20:V:34:LEU:HA	1.82	0.44
6:G:139:MET:CE	6:G:139:MET:CA	2.93	0.44
12:M:483:ARG:H	12:M:483:ARG:HG2	1.57	0.44
20:V:123:ALA:O	20:V:127:MET:HG3	2.17	0.44
48:V:202:PEE:O2P	48:V:202:PEE:H12	2.17	0.44
2:B:99:GLY:HA3	2:B:170:GLY:O	2.17	0.44
6:G:113:LEU:HD23	6:G:113:LEU:HA	1.75	0.44
8:I:39:PRO:HB2	8:I:41:LEU:HD13	1.99	0.44
11:L:131:LYS:HD2	11:L:147:VAL:HG11	1.99	0.44
52:V:201:CDL:H341	52:V:201:CDL:H371	1.81	0.44
22:Y:61:PHE:HA	22:Y:64:THR:HG22	1.98	0.44
1:A:76:ILE:HG23	1:A:255:CYS:SG	2.58	0.44
13:N:85:GLU:HG2	13:N:86:TRP:H	1.83	0.44
3:C:107:GLY:HA2	45:C:301:SF4:S1	2.58	0.44
9:J:220:MET:HE2	9:J:226:VAL:HG13	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:284:GLU:HG2	12:M:284:GLU:O	2.17	0.44
7:H:40:LYS:HE2	7:H:40:LYS:HB2	1.90	0.43
8:I:103:ARG:HH11	8:I:103:ARG:HB3	1.82	0.43
2:B:184:LEU:HD23	11:L:112:MET:HG3	2.00	0.43
15:P:119:VAL:HG12	15:P:121:THR:HG22	2.00	0.43
1:A:115:VAL:HG11	1:A:138:LEU:HD11	2.00	0.43
9:J:222:TRP:CZ3	52:J:404:CDL:HA4	2.52	0.43
50:J:402:UQ:HM51	50:J:402:UQ:H72	1.69	0.43
17:S:64:LYS:HE2	17:S:64:LYS:HA	2.00	0.43
18:T:43:GLN:HE21	18:T:60:LYS:NZ	2.14	0.43
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.99	0.43
9:J:220:MET:HE3	9:J:227:PRO:HD2	1.96	0.43
6:X:139:MET:CE	6:X:139:MET:CA	2.86	0.43
4:E:35:LEU:HD21	4:E:86:GLY:HA3	2.00	0.43
9:J:303:ARG:HB2	9:J:316:ARG:HD2	2.01	0.43
12:M:94:MET:HA	12:M:95:PRO:HD3	1.91	0.43
15:P:161:LYS:HD3	15:P:161:LYS:HA	1.77	0.43
6:X:126:PHE:CE2	6:X:148:ILE:CD1	3.01	0.43
10:K:105:ARG:NH2	12:M:426:ASP:OD1	2.51	0.43
1:A:446:LEU:O	1:A:450:MET:HG3	2.19	0.43
8:I:27:ARG:HB2	8:I:30:GLU:OE2	2.17	0.43
13:N:8:ARG:HA	13:N:11:LEU:HD12	2.01	0.43
14:O:134:VAL:O	14:O:134:VAL:HG23	2.18	0.43
16:Q:184:ILE:HG23	16:Q:203:MET:HB3	1.99	0.43
8:I:108:LYS:HD3	8:I:108:LYS:HA	1.83	0.43
12:M:339:ALA:HB3	12:M:542:PRO:HG3	2.00	0.43
12:M:484:SER:OG	12:M:680:LEU:HD11	2.19	0.43
14:O:218:PRO:HD2	14:O:223:PHE:HA	2.00	0.43
16:Q:342:ARG:HD2	21:W:21:TYR:CZ	2.53	0.43
18:T:43:GLN:NE2	18:T:60:LYS:HZ1	2.16	0.43
21:W:7:LYS:HA	21:W:7:LYS:HD3	1.83	0.43
2:B:79:ARG:HH11	8:I:25:GLN:NE2	2.16	0.43
15:P:152:PRO:HB3	15:P:177:PHE:HD2	1.84	0.43
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	2.01	0.43
48:W:201:PEE:H20	48:W:201:PEE:H14	1.55	0.43
13:N:68:MET:CG	13:N:69:ASN:H	2.32	0.43
1:A:201:ALA:HB1	14:O:121:MET:HB2	2.00	0.42
12:M:712:LYS:O	12:M:716:GLU:HG2	2.19	0.42
16:Q:99:MET:HB3	16:Q:99:MET:HE2	1.83	0.42
1:A:56:ALA:O	1:A:61:ASP:N	2.47	0.42
1:A:152:ARG:NH2	10:K:99:PRO:O	2.47	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:107:SER:HB3	8:I:111:PRO:HA	2.00	0.42
12:M:178:GLN:HG2	12:M:204:MET:CE	2.49	0.42
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.49	0.42
12:M:531:LYS:HB2	12:M:531:LYS:HZ3	1.82	0.42
6:G:140:CYS:SG	6:G:143:GLU:HG3	2.59	0.42
13:N:132:LYS:NZ	13:N:136:GLU:OE1	2.51	0.42
15:P:132:LEU:HB2	15:P:141:ILE:HG22	2.01	0.42
5:F:27:SER:O	5:F:34:ARG:NH2	2.44	0.42
8:I:6:ARG:HA	8:I:9:GLN:HG3	2.02	0.42
9:J:132:ARG:NH1	53:J:401:NDP:O3X	2.51	0.42
12:M:689:LEU:HD12	12:M:689:LEU:HA	1.85	0.42
20:V:36:VAL:HG22	52:V:201:CDL:H741	2.02	0.42
2:B:40:PHE:HB3	2:B:43:MET:HB2	2.02	0.42
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.84	0.42
49:J:403:PLX:H251	49:J:403:PLX:H282	1.69	0.42
14:O:154:LYS:HB3	14:O:154:LYS:HE3	1.78	0.42
17:S:57:VAL:HG21	17:S:62:VAL:HG21	2.02	0.42
1:A:339:PHE:CE1	1:A:349:LEU:HD23	2.55	0.42
49:C:303:PLX:H21	49:C:303:PLX:H1C3	1.86	0.42
9:J:36:LEU:N	12:M:304:GLN:HE22	2.17	0.42
12:M:219:SER:OG	12:M:288:ASP:OD2	2.36	0.42
12:M:277:MET:HG2	12:M:283:GLU:O	2.19	0.42
56:Q:502:UQ1:H113	56:Q:502:UQ1:H72	1.83	0.42
19:U:50:PRO:HB2	21:W:69:ILE:HD11	2.01	0.42
1:A:97:LEU:HD23	1:A:97:LEU:HA	1.92	0.42
3:C:190:LEU:HD22	48:C:302:PEE:H14	2.02	0.42
12:M:81:GLU:OE2	12:M:103:LEU:HD12	2.20	0.42
14:O:133:GLN:HG2	14:O:172:ILE:HD11	2.01	0.42
16:Q:208:GLU:CD	16:Q:221:ARG:HH22	2.21	0.42
56:Q:501:UQ1:HM22	56:Q:502:UQ1:H103	2.00	0.42
52:V:203:CDL:H812	52:V:203:CDL:H781	1.88	0.42
1:A:138:LEU:HD13	1:A:245:VAL:HG23	2.02	0.42
9:J:61:ALA:HB3	9:J:82:VAL:HG13	2.02	0.42
9:J:313:TRP:CE2	50:J:402:UQ:H8	2.55	0.42
12:M:219:SER:O	12:M:222:ILE:HG12	2.19	0.42
16:Q:123:LEU:O	16:Q:127:LYS:HG2	2.19	0.42
16:Q:404:LYS:HG2	16:Q:455:ASP:OD2	2.20	0.42
48:Q:503:PEE:H14	48:Q:503:PEE:H1	1.92	0.42
19:U:38:TYR:HD1	19:U:41:TYR:HD2	1.68	0.42
6:X:93:ILE:HG23	6:X:108:LEU:HD11	2.01	0.42
9:J:208:GLY:H	9:J:211:ASP:HB3	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:215:MET:HG2	12:M:714:VAL:HG12	2.02	0.41
12:M:326:VAL:HG13	12:M:567:ILE:HD13	2.02	0.41
12:M:354:LEU:HD22	12:M:548:LEU:HD22	2.01	0.41
16:Q:238:LEU:HD23	16:Q:238:LEU:HA	1.85	0.41
16:Q:315:GLU:HA	16:Q:315:GLU:OE1	2.19	0.41
13:N:53:LYS:HD3	13:N:53:LYS:HA	1.75	0.41
1:A:60:GLY:CA	14:O:241:PRO:HA	2.50	0.41
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.55	0.41
4:E:127:ASP:OD2	9:J:45:LYS:HD3	2.21	0.41
8:I:73:GLN:OE1	8:I:74:LYS:N	2.53	0.41
9:J:375:VAL:HG23	9:J:375:VAL:O	2.21	0.41
12:M:602:ARG:HD3	12:M:657:ASP:OD1	2.20	0.41
52:V:203:CDL:H792	52:V:203:CDL:H761	1.65	0.41
10:K:98:MET:HE2	10:K:98:MET:HB3	1.90	0.41
12:M:49:VAL:HB	12:M:91:ALA:HA	2.01	0.41
20:V:107:SER:HB3	20:V:110:ILE:HB	2.02	0.41
6:X:82:ARG:HD2	22:Y:44:TYR:CE1	2.55	0.41
1:A:201:ALA:O	14:O:119:TYR:HB3	2.20	0.41
50:J:402:UQ:C13	50:J:402:UQ:H101	2.50	0.41
48:V:202:PEE:H68	48:V:202:PEE:H62	1.66	0.41
6:X:115:GLN:HG3	6:X:139:MET:HE1	2.03	0.41
3:C:184:ILE:O	3:C:187:GLU:HG2	2.21	0.41
50:C:304:UQ:H152	50:C:304:UQ:H121	1.82	0.41
8:I:8:ILE:HD11	52:I:201:CDL:H111	2.02	0.41
14:O:148:ILE:HG12	14:O:184:PRO:HG3	2.01	0.41
14:O:181:VAL:CG1	14:O:222:ARG:NH2	2.81	0.41
16:Q:259:GLU:HG3	16:Q:263:THR:OG1	2.20	0.41
48:V:202:PEE:H71	48:V:202:PEE:H33	2.03	0.41
15:P:207:TYR:C	15:P:224:VAL:HG23	2.41	0.41
16:Q:74:ASP:OD1	16:Q:74:ASP:N	2.48	0.41
1:A:70:LEU:HD21	1:A:189:SER:HA	2.03	0.41
1:A:367:ILE:O	1:A:371:ILE:HG12	2.20	0.41
9:J:171:ASN:HA	9:J:327:MET:SD	2.61	0.41
12:M:61:PRO:HB2	12:M:77:MET:HG3	2.03	0.41
15:P:108:PHE:CD2	15:P:134:SER:HB2	2.56	0.41
16:Q:404:LYS:HE3	16:Q:455:ASP:O	2.20	0.41
6:G:104:PHE:CD1	6:G:108:LEU:HD12	2.52	0.41
7:H:50:GLN:O	7:H:54:GLU:HG3	2.20	0.41
15:P:118:ASP:OD1	15:P:125:ARG:HG2	2.21	0.41
5:F:17:ARG:HH21	5:F:70:ALA:HB2	1.86	0.40
14:O:185:MET:SD	14:O:185:MET:O	2.79	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:87:LEU:HD23	6:G:87:LEU:HA	2.11	0.40
12:M:502:LEU:HD12	12:M:502:LEU:HA	1.90	0.40
15:P:153:ILE:O	15:P:178:PHE:HA	2.20	0.40
1:A:141:GLY:HA2	1:A:252:PRO:HD3	2.04	0.40
1:A:284:HIS:ND1	14:O:228:ALA:HB3	2.37	0.40
8:I:34:ARG:HA	8:I:34:ARG:HD2	1.89	0.40
52:J:404:CDL:H162	52:J:404:CDL:H191	1.92	0.40
12:M:592:LYS:HG3	12:M:594:ALA:HB2	2.03	0.40
16:Q:150:ALA:HB2	16:Q:400:ILE:HG12	2.03	0.40
1:A:296:LEU:HD11	1:A:317:VAL:HG11	2.03	0.40
5:F:21:ILE:HG12	5:F:65:LEU:HD12	2.04	0.40
23:Z:18:ASP:O	23:Z:21:GLN:HG2	2.21	0.40
8:I:70:MET:SD	8:I:70:MET:O	2.79	0.40
9:J:259:LYS:HD3	9:J:259:LYS:HA	1.87	0.40
12:M:379:THR:O	12:M:379:THR:CG2	2.70	0.40
12:M:467:LYS:HE2	12:M:503:SER:HB3	2.02	0.40
16:Q:93:GLY:HA2	56:Q:501:UQ1:H71	2.04	0.40
6:X:92:LYS:NZ	6:X:114:ASP:OD2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	431/433 (100%)	416 (96%)	14 (3%)	1 (0%)	47 71
2	B	174/176 (99%)	168 (97%)	6 (3%)	0	100 100
3	C	154/156 (99%)	151 (98%)	3 (2%)	0	100 100
4	E	113/115 (98%)	109 (96%)	3 (3%)	1 (1%)	17 35
5	F	84/86 (98%)	79 (94%)	5 (6%)	0	100 100
6	G	86/88 (98%)	81 (94%)	4 (5%)	1 (1%)	13 27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	X	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
7	H	110/112 (98%)	102 (93%)	7 (6%)	1 (1%)	17	35
8	I	93/112 (83%)	84 (90%)	7 (8%)	2 (2%)	6	12
9	J	340/342 (99%)	327 (96%)	12 (4%)	1 (0%)	41	64
10	K	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	668 (97%)	19 (3%)	1 (0%)	51	75
13	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
14	O	215/217 (99%)	203 (94%)	11 (5%)	1 (0%)	29	52
15	P	206/208 (99%)	199 (97%)	7 (3%)	0	100	100
16	Q	427/430 (99%)	418 (98%)	9 (2%)	0	100	100
17	S	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
18	T	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
19	U	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
20	V	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
21	W	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
22	Y	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
23	Z	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
24	a	136/138 (99%)	132 (97%)	4 (3%)	0	100	100
25	b	94/126 (75%)	86 (92%)	8 (8%)	0	100	100
26	c	154/156 (99%)	145 (94%)	9 (6%)	0	100	100
27	d	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
28	e	102/104 (98%)	97 (95%)	5 (5%)	0	100	100
29	f	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
30	g	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
31	h	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
32	i	345/347 (99%)	329 (95%)	16 (5%)	0	100	100
33	j	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
34	k	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
35	l	604/606 (100%)	581 (96%)	23 (4%)	0	100	100
36	m	173/175 (99%)	161 (93%)	12 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
37	n	54/56 (96%)	54 (100%)	0	0	100 100
38	o	126/128 (98%)	125 (99%)	1 (1%)	0	100 100
39	p	176/178 (99%)	165 (94%)	10 (6%)	1 (1%)	25 47
40	r	457/459 (100%)	451 (99%)	6 (1%)	0	100 100
41	s	316/318 (99%)	304 (96%)	11 (4%)	1 (0%)	41 64
42	u	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	25 47
43	v	122/125 (98%)	114 (93%)	8 (7%)	0	100 100
44	w	318/320 (99%)	304 (96%)	14 (4%)	0	100 100
All	All	8175/8314 (98%)	7866 (96%)	297 (4%)	12 (0%)	54 75

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	LEU
6	G	134	ASP
7	H	77	ILE
8	I	29	GLN
14	O	175	GLU
9	J	38	HIS
12	M	281	ILE
8	I	41	LEU
41	s	208	VAL
42	u	152	PRO
39	p	174	PRO
4	E	96	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	346/346 (100%)	342 (99%)	4 (1%)	71 87
2	B	151/151 (100%)	150 (99%)	1 (1%)	84 94

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	132/132 (100%)	130 (98%)	2 (2%)	65 83
4	E	107/107 (100%)	106 (99%)	1 (1%)	78 91
5	F	75/76 (99%)	70 (93%)	5 (7%)	16 33
6	G	76/81 (94%)	73 (96%)	3 (4%)	32 58
6	X	79/81 (98%)	78 (99%)	1 (1%)	69 86
7	H	99/99 (100%)	98 (99%)	1 (1%)	76 90
8	I	87/97 (90%)	78 (90%)	9 (10%)	7 13
9	J	296/296 (100%)	290 (98%)	6 (2%)	55 78
10	K	42/42 (100%)	41 (98%)	1 (2%)	49 74
11	L	113/113 (100%)	111 (98%)	2 (2%)	59 80
12	M	580/580 (100%)	566 (98%)	14 (2%)	49 74
13	N	130/130 (100%)	128 (98%)	2 (2%)	65 83
14	O	183/183 (100%)	177 (97%)	6 (3%)	38 64
15	P	190/190 (100%)	189 (100%)	1 (0%)	88 96
16	Q	370/370 (100%)	363 (98%)	7 (2%)	57 79
17	S	57/58 (98%)	56 (98%)	1 (2%)	59 80
18	T	79/79 (100%)	76 (96%)	3 (4%)	33 59
19	U	69/69 (100%)	69 (100%)	0	100 100
20	V	101/101 (100%)	94 (93%)	7 (7%)	15 31
21	W	122/123 (99%)	116 (95%)	6 (5%)	25 48
22	Y	62/62 (100%)	61 (98%)	1 (2%)	62 82
23	Z	62/62 (100%)	60 (97%)	2 (3%)	39 65
24	a	121/121 (100%)	120 (99%)	1 (1%)	81 92
25	b	90/119 (76%)	90 (100%)	0	100 100
26	c	141/141 (100%)	138 (98%)	3 (2%)	53 77
27	d	155/155 (100%)	151 (97%)	4 (3%)	46 72
28	e	96/96 (100%)	93 (97%)	3 (3%)	40 66
29	f	36/45 (80%)	35 (97%)	1 (3%)	43 69
30	g	108/109 (99%)	106 (98%)	2 (2%)	57 79
31	h	93/93 (100%)	92 (99%)	1 (1%)	73 88
32	i	311/311 (100%)	308 (99%)	3 (1%)	76 90

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
33	j	100/100 (100%)	99 (99%)	1 (1%)	76 90
34	k	85/85 (100%)	81 (95%)	4 (5%)	26 50
35	l	540/540 (100%)	523 (97%)	17 (3%)	40 66
36	m	129/141 (92%)	123 (95%)	6 (5%)	26 50
37	n	53/53 (100%)	53 (100%)	0	100 100
38	o	113/113 (100%)	110 (97%)	3 (3%)	44 71
39	p	159/159 (100%)	155 (98%)	4 (2%)	47 73
40	r	410/410 (100%)	403 (98%)	7 (2%)	60 81
41	s	275/275 (100%)	270 (98%)	5 (2%)	59 80
42	u	153/153 (100%)	144 (94%)	9 (6%)	19 39
43	v	104/111 (94%)	98 (94%)	6 (6%)	20 40
44	w	281/283 (99%)	276 (98%)	5 (2%)	59 80
All	All	7161/7241 (99%)	6990 (98%)	171 (2%)	51 74

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	LEU
1	A	184	LYS
1	A	245	VAL
1	A	273	THR
2	B	165	ASP
3	C	142	TYR
3	C	195	ARG
4	E	31	ARG
5	F	27	SER
5	F	39	LYS
5	F	46	LYS
5	F	50	ASP
5	F	95	LEU
6	G	91	ASP
6	G	107	ASP
6	G	139	MET
7	H	76	GLN
8	I	18	ARG
8	I	25	GLN
8	I	27	ARG
8	I	61	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	I	70	MET
8	I	73	GLN
8	I	90	THR
8	I	95	VAL
8	I	108	LYS
9	J	257	ASP
9	J	298	TYR
9	J	341	GLN
9	J	360	ARG
9	J	370	LYS
9	J	374	THR
10	K	92	GLU
11	L	105	GLU
11	L	119	ASP
12	M	107	GLU
12	M	260	ASN
12	M	281	ILE
12	M	310	GLU
12	M	352	VAL
12	M	398	ASP
12	M	450	LYS
12	M	483	ARG
12	M	539	LYS
12	M	559	ASP
12	M	598	ASN
12	M	619	ASP
12	M	672	SER
12	M	688	GLN
13	N	21	ARG
13	N	144	TYR
14	O	137	THR
14	O	144	ASN
14	O	186	VAL
14	O	190	ASP
14	O	195	ASP
14	O	219	ARG
15	P	44	ARG
16	Q	143	SER
16	Q	144	MET
16	Q	192	LEU
16	Q	217	VAL
16	Q	308	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	Q	453	THR
16	Q	463	ARG
17	S	60	TYR
18	T	30	ARG
18	T	114	CYS
18	T	122	HIS
20	V	10	SER
20	V	74	SER
20	V	77	SER
20	V	79	GLN
20	V	106	ARG
20	V	115	CYS
20	V	120	LEU
21	W	34	SER
21	W	79	LYS
21	W	81	ARG
21	W	85	GLN
21	W	94	GLU
21	W	99	LYS
6	X	139	MET
22	Y	83	HIS
23	Z	35	LYS
23	Z	72	LYS
24	a	114	LYS
26	c	33	THR
26	c	120	SER
26	c	177	GLU
27	d	38	ASP
27	d	61	TYR
27	d	144	SER
27	d	171	LYS
28	e	83	ASP
28	e	86	ASN
28	e	136	LEU
29	f	68	GLU
30	g	2	THR
30	g	109	LYS
31	h	65	GLU
32	i	111	PHE
32	i	299	SER
32	i	336	VAL
33	j	87	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	k	24	SER
34	k	37	MET
34	k	53	PHE
34	k	59	MET
35	l	23	ASN
35	l	70	THR
35	l	72	GLN
35	l	73	THR
35	l	140	LEU
35	l	185	SER
35	l	190	LEU
35	l	197	ASP
35	l	252	MET
35	l	271	LYS
35	l	308	SER
35	l	314	MET
35	l	340	PHE
35	l	349	SER
35	l	496	MET
35	l	498	PHE
35	l	554	ASP
36	m	1	MET
36	m	77	GLU
36	m	87	LYS
36	m	95	SER
36	m	102	CYS
36	m	106	TYR
38	o	40	ARG
38	o	106	LYS
38	o	129	TYR
39	p	13	GLN
39	p	38	ARG
39	p	48	PHE
39	p	55	LYS
40	r	1	MET
40	r	116	ILE
40	r	122	PHE
40	r	183	SER
40	r	243	MET
40	r	336	ARG
40	r	375	LEU
41	s	40	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	s	54	LYS
41	s	145	THR
41	s	202	GLU
41	s	296	LEU
42	u	14	LYS
42	u	17	GLU
42	u	48	TRP
42	u	64	ASN
42	u	88	CYS
42	u	121	ASP
42	u	139	GLU
42	u	153	GLU
42	u	157	ASP
43	v	15	LYS
43	v	35	LYS
43	v	36	GLU
43	v	72	ASP
43	v	94	ASP
43	v	113	LYS
44	w	95	ASP
44	w	241	TYR
44	w	248	GLU
44	w	254	GLU
44	w	267	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	204	ASN
4	E	70	ASN
7	H	76	GLN
10	K	78	HIS
10	K	79	HIS
12	M	39	GLN
12	M	300	GLN
12	M	334	GLN
12	M	598	ASN
14	O	182	ASN
16	Q	285	ASN
17	S	68	ASN
18	T	43	GLN
21	W	61	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	i	150	ASN
35	l	2	ASN
35	l	59	GLN
35	l	605	HIS
38	o	75	ASN
38	o	79	ASN
39	p	12	HIS
40	r	180	HIS
40	r	304	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
16	2MR	Q	118	16	10,12,13	2.00	1 (10%)	5,13,15	5.97	3 (60%)

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
16	2MR	Q	118	16	-	3/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.65	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Q	118	2MR	NE-CZ-NH2	12.07	130.55	119.48
16	Q	118	2MR	CD-NE-CZ	3.90	130.72	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.60	131.82	123.86

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	Q	118	2MR	NE-CD-CG-CB
16	Q	118	2MR	CA-CB-CG-CD
16	Q	118	2MR	CG-CD-NE-CZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 47 ligands modelled in this entry, 2 are monoatomic - leaving 45 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	$\#\|Z\| > 2$
51	8Q1	X	201	-	31,34,34	2.11	6 (19%)	40,43,43	1.70	9 (22%)
52	CDL	l	701	-	98,98,99	1.10	8 (8%)	104,110,111	0.87	4 (3%)
58	ADP	w	401	-	24,29,29	3.12	6 (25%)	29,45,45	1.38	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
49	PLX	J	403	-	51,51,51	1.14	2 (3%)	55,59,59	0.61	1 (1%)
50	UQ	C	304	-	38,38,63	3.53	10 (26%)	46,49,79	2.84	16 (34%)
52	CDL	V	203	-	99,99,99	1.08	8 (8%)	105,111,111	0.89	4 (3%)
52	CDL	I	201	-	50,50,99	1.28	4 (8%)	56,62,111	1.36	7 (12%)
52	CDL	k	101	-	93,93,99	1.11	7 (7%)	99,105,111	0.84	4 (4%)
51	8Q1	G	201	-	31,34,34	2.08	6 (19%)	40,43,43	1.83	11 (27%)
54	FES	O	301	14	0,4,4	-	-	-		
48	PEE	W	201	-	40,40,50	1.14	5 (12%)	43,45,55	1.03	2 (4%)
48	PEE	j	202	-	40,40,50	1.16	4 (10%)	43,45,55	1.04	2 (4%)
49	PLX	g	201	-	51,51,51	1.13	3 (5%)	55,59,59	0.63	1 (1%)
48	PEE	V	204	-	39,39,50	1.31	6 (15%)	41,44,55	1.07	2 (4%)
45	SF4	A	501	1	0,12,12	-	-	-		
45	SF4	M	802	12	0,12,12	-	-	-		
45	SF4	B	301	2	0,12,12	-	-	-		
45	SF4	C	301	3	0,12,12	-	-	-		
48	PEE	s	401	-	50,50,50	1.15	5 (10%)	53,55,55	1.01	2 (3%)
49	PLX	a	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.59	1 (1%)
52	CDL	V	201	-	93,93,99	1.11	8 (8%)	99,105,111	0.84	4 (4%)
45	SF4	B	302	2	0,12,12	-	-	-		
47	NAI	A	503	-	42,48,48	4.92	18 (42%)	47,73,73	1.36	7 (14%)
48	PEE	C	302	-	46,46,50	1.21	6 (13%)	49,51,55	0.99	2 (4%)
52	CDL	l	702	-	99,99,99	0.92	4 (4%)	105,111,111	1.15	8 (7%)
49	PLX	e	201	-	51,51,51	1.14	4 (7%)	55,59,59	0.53	1 (1%)
52	CDL	a	201	-	99,99,99	1.09	8 (8%)	105,111,111	0.88	4 (3%)
49	PLX	j	203	-	51,51,51	1.14	4 (7%)	55,59,59	0.64	1 (1%)
56	UQ1	Q	501	-	18,18,18	2.34	6 (33%)	22,25,25	1.86	6 (27%)
52	CDL	r	502	-	99,99,99	1.08	8 (8%)	105,111,111	0.87	4 (3%)
48	PEE	j	201	-	50,50,50	1.14	6 (12%)	53,55,55	0.97	2 (3%)
46	FMN	A	502	-	33,33,33	1.10	2 (6%)	48,50,50	1.27	9 (18%)
56	UQ1	Q	502	-	18,18,18	2.32	6 (33%)	22,25,25	1.68	4 (18%)
49	PLX	r	501	-	51,51,51	1.14	5 (9%)	55,59,59	0.64	1 (1%)
45	SF4	M	801	12	0,12,12	-	-	-		
48	PEE	V	202	-	50,50,50	1.16	6 (12%)	53,55,55	0.94	2 (3%)
50	UQ	J	402	-	33,33,63	3.43	8 (24%)	40,43,79	2.82	13 (32%)
52	CDL	u	201	-	54,54,99	1.22	4 (7%)	60,66,111	1.25	5 (8%)
48	PEE	l	704	-	45,45,50	1.22	6 (13%)	48,50,55	0.98	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
52	CDL	J	404	-	88,88,99	1.13	8 (9%)	94,100,111	0.91	4 (4%)
48	PEE	Q	503	-	46,46,50	1.19	6 (13%)	49,51,55	1.03	2 (4%)
49	PLX	C	303	-	51,51,51	1.13	3 (5%)	55,59,59	0.60	1 (1%)
53	NDP	J	401	-	45,52,52	2.20	4 (8%)	53,80,80	1.71	10 (18%)
54	FES	M	803	12	0,4,4	-	-	-		
48	PEE	l	703	-	50,50,50	1.15	5 (10%)	53,55,55	0.95	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	8Q1	X	201	-	-	16/41/41/41	-
52	CDL	l	701	-	-	66/109/109/110	-
58	ADP	w	401	-	-	6/12/32/32	0/3/3/3
49	PLX	J	403	-	-	34/55/55/55	-
50	UQ	C	304	-	-	11/33/57/87	0/1/1/1
52	CDL	V	203	-	-	55/110/110/110	-
52	CDL	I	201	-	-	25/61/61/110	-
52	CDL	k	101	-	-	53/104/104/110	-
51	8Q1	G	201	-	-	11/41/41/41	-
54	FES	O	301	14	-	-	0/1/1/1
48	PEE	W	201	-	-	20/44/44/54	-
48	PEE	j	202	-	-	17/44/44/54	-
49	PLX	g	201	-	-	25/55/55/55	-
48	PEE	V	204	-	-	20/43/43/54	-
45	SF4	A	501	1	-	-	0/6/5/5
45	SF4	M	802	12	-	-	0/6/5/5
45	SF4	B	301	2	-	-	0/6/5/5
48	PEE	s	401	-	-	20/54/54/54	-
45	SF4	C	301	3	-	-	0/6/5/5
49	PLX	a	202	-	-	30/55/55/55	-
52	CDL	V	201	-	-	61/104/104/110	-
47	NAI	A	503	-	-	4/25/72/72	0/5/5/5
45	SF4	B	302	2	-	-	0/6/5/5
48	PEE	C	302	-	-	25/50/50/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	CDL	l	702	-	-	43/110/110/110	-
49	PLX	e	201	-	-	36/55/55/55	-
52	CDL	a	201	-	-	57/110/110/110	-
49	PLX	j	203	-	-	24/55/55/55	-
56	UQ1	Q	501	-	-	3/9/33/33	0/1/1/1
52	CDL	r	502	-	-	54/110/110/110	-
48	PEE	j	201	-	-	24/54/54/54	-
46	FMN	A	502	-	-	11/18/18/18	0/3/3/3
56	UQ1	Q	502	-	-	2/9/33/33	0/1/1/1
49	PLX	r	501	-	-	31/55/55/55	-
45	SF4	M	801	12	-	-	0/6/5/5
48	PEE	V	202	-	-	29/54/54/54	-
50	UQ	J	402	-	-	14/27/51/87	0/1/1/1
52	CDL	u	201	-	-	26/65/65/110	-
48	PEE	l	704	-	-	22/49/49/54	-
52	CDL	J	404	-	-	48/99/99/110	-
48	PEE	Q	503	-	-	22/50/50/54	-
49	PLX	C	303	-	-	24/55/55/55	-
53	NDP	J	401	-	-	6/30/77/77	0/5/5/5
54	FES	M	803	12	-	-	0/1/1/1
48	PEE	l	703	-	-	24/54/54/54	-

All (219) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	O4B-C1B	16.00	1.63	1.41
47	A	503	NAI	C2B-C1B	-15.47	1.30	1.53
53	J	401	NDP	P2B-O2B	12.27	1.82	1.59
47	A	503	NAI	C3D-C4D	-10.43	1.26	1.53
50	C	304	UQ	C18-C19	9.63	1.56	1.33
50	J	402	UQ	C18-C19	9.56	1.55	1.33
50	C	304	UQ	C13-C14	9.17	1.55	1.33
50	J	402	UQ	C13-C14	9.10	1.54	1.33
50	C	304	UQ	C23-C24	9.09	1.54	1.33
50	C	304	UQ	C8-C9	9.04	1.54	1.33
50	J	402	UQ	C8-C9	8.95	1.54	1.33
58	w	401	ADP	C3'-C4'	-8.95	1.30	1.53
47	A	503	NAI	O4B-C4B	-8.38	1.26	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	J	402	UQ	C23-C24	7.81	1.54	1.32
58	w	401	ADP	O4'-C4'	7.69	1.62	1.45
51	X	201	8Q1	P24-O27	7.69	1.85	1.60
50	C	304	UQ	C28-C29	7.65	1.54	1.32
47	A	503	NAI	C2D-C1D	-7.58	1.29	1.53
51	G	201	8Q1	P24-O27	7.51	1.84	1.60
56	Q	501	UQ1	C8-C9	7.24	1.53	1.32
56	Q	502	UQ1	C8-C9	7.15	1.52	1.32
58	w	401	ADP	O4'-C1'	-6.87	1.31	1.41
47	A	503	NAI	O4D-C4D	6.77	1.60	1.45
47	A	503	NAI	C2D-C3D	5.90	1.69	1.53
47	A	503	NAI	C7N-N7N	5.70	1.48	1.33
47	A	503	NAI	O4D-C1D	5.29	1.54	1.42
47	A	503	NAI	C4N-C3N	-5.07	1.40	1.49
47	A	503	NAI	O2B-C2B	4.57	1.53	1.43
52	I	201	CDL	OB8-CB7	4.32	1.46	1.33
52	u	201	CDL	OA8-CA7	4.32	1.46	1.33
52	I	201	CDL	OA8-CA7	4.27	1.45	1.33
52	l	702	CDL	OA8-CA7	4.26	1.45	1.33
52	l	702	CDL	OB8-CB7	4.21	1.45	1.33
52	l	702	CDL	OA6-CA5	4.14	1.46	1.34
52	I	201	CDL	OA6-CA5	4.11	1.45	1.34
52	u	201	CDL	OB6-CB5	4.08	1.45	1.34
52	l	702	CDL	OB6-CB5	4.07	1.45	1.34
52	u	201	CDL	OB8-CB7	4.04	1.45	1.33
52	u	201	CDL	OA6-CA5	3.99	1.45	1.34
51	X	201	8Q1	C1-S44	3.98	1.85	1.76
47	A	503	NAI	C6N-C5N	3.94	1.40	1.33
52	I	201	CDL	OB6-CB5	3.94	1.45	1.34
51	G	201	8Q1	C1-S44	3.93	1.85	1.76
58	w	401	ADP	C6-N6	3.86	1.48	1.34
51	G	201	8Q1	C6-C1	3.81	1.54	1.50
53	J	401	NDP	PN-O5D	3.77	1.74	1.59
48	C	302	PEE	C18-C19	3.76	1.53	1.31
48	l	703	PEE	C18-C19	3.74	1.53	1.31
48	V	204	PEE	C18-C19	3.74	1.53	1.31
48	l	704	PEE	C18-C19	3.74	1.53	1.31
48	j	202	PEE	C18-C19	3.72	1.53	1.31
48	s	401	PEE	C18-C19	3.72	1.53	1.31
46	A	502	FMN	C4A-N5	3.71	1.38	1.30
48	V	202	PEE	C18-C19	3.70	1.53	1.31
48	j	201	PEE	C18-C19	3.70	1.53	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	W	201	PEE	C18-C19	3.69	1.53	1.31
48	Q	503	PEE	C18-C19	3.67	1.53	1.31
48	V	204	PEE	C39-C38	3.66	1.53	1.31
48	C	302	PEE	C39-C38	3.64	1.52	1.31
48	V	202	PEE	C39-C38	3.63	1.52	1.31
48	l	704	PEE	C39-C38	3.63	1.52	1.31
48	s	401	PEE	C39-C38	3.62	1.52	1.31
48	Q	503	PEE	C39-C38	3.62	1.52	1.31
48	l	703	PEE	C39-C38	3.62	1.52	1.31
48	j	201	PEE	C39-C38	3.61	1.52	1.31
47	A	503	NAI	C6A-N6A	3.51	1.46	1.34
51	X	201	8Q1	C34-N36	3.49	1.41	1.33
52	V	203	CDL	OA8-CA7	3.46	1.43	1.33
47	A	503	NAI	C7N-C3N	3.43	1.56	1.48
52	l	701	CDL	OA8-CA7	3.43	1.43	1.33
52	a	201	CDL	OA8-CA7	3.43	1.43	1.33
52	V	201	CDL	OA8-CA7	3.42	1.43	1.33
52	r	502	CDL	OA8-CA7	3.40	1.43	1.33
51	G	201	8Q1	O27-C28	-3.39	1.32	1.43
52	k	101	CDL	OA8-CA7	3.38	1.43	1.33
51	X	201	8Q1	C6-C1	3.36	1.54	1.50
52	J	404	CDL	OA8-CA7	3.34	1.43	1.33
47	A	503	NAI	C4N-C5N	-3.33	1.40	1.48
52	k	101	CDL	OA6-CA5	3.27	1.43	1.34
51	X	201	8Q1	O27-C28	-3.26	1.33	1.43
58	w	401	ADP	O2'-C2'	-3.25	1.35	1.43
51	G	201	8Q1	C34-N36	3.20	1.40	1.33
58	w	401	ADP	O3'-C3'	3.14	1.50	1.43
53	J	401	NDP	O2B-C2B	-3.14	1.32	1.44
52	a	201	CDL	OB6-CB5	3.10	1.43	1.34
52	r	502	CDL	OB6-CB5	3.08	1.43	1.34
52	V	201	CDL	OA6-CA5	3.06	1.43	1.34
51	X	201	8Q1	C39-N41	3.06	1.40	1.33
52	a	201	CDL	OB8-CB7	3.05	1.42	1.33
52	J	404	CDL	OB6-CB5	3.05	1.42	1.34
52	l	701	CDL	OB8-CB7	3.03	1.42	1.33
52	l	701	CDL	OB6-CB5	3.01	1.42	1.34
52	V	201	CDL	OB8-CB7	2.99	1.42	1.33
52	J	404	CDL	OA6-CA5	2.99	1.42	1.34
52	k	101	CDL	OB6-CB5	2.97	1.42	1.34
52	r	502	CDL	OA6-CA5	2.96	1.42	1.34
52	V	201	CDL	OB6-CB5	2.96	1.42	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	V	203	CDL	OB6-CB5	2.95	1.42	1.34
52	k	101	CDL	OB8-CB7	2.95	1.41	1.33
52	r	502	CDL	OB8-CB7	2.94	1.41	1.33
52	V	203	CDL	OB8-CB7	2.91	1.41	1.33
52	l	701	CDL	OA6-CA5	2.91	1.42	1.34
52	V	203	CDL	OA6-CA5	2.90	1.42	1.34
52	a	201	CDL	OA6-CA5	2.89	1.42	1.34
52	J	404	CDL	OB8-CB7	2.86	1.41	1.33
49	C	303	PLX	O6-C4	-2.73	1.41	1.44
48	s	401	PEE	O2-C2	-2.73	1.39	1.46
51	G	201	8Q1	C39-N41	2.70	1.39	1.33
49	g	201	PLX	O6-C4	-2.68	1.41	1.44
49	a	202	PLX	O6-C4	-2.66	1.41	1.44
49	e	201	PLX	O6-C4	-2.65	1.41	1.44
50	C	304	UQ	C6-C1	2.64	1.54	1.46
48	C	302	PEE	O2-C2	-2.61	1.40	1.46
50	J	402	UQ	C6-C1	2.60	1.53	1.46
49	j	203	PLX	O6-C4	-2.58	1.41	1.44
48	j	202	PEE	O3-C30	2.57	1.40	1.33
48	V	204	PEE	O3-C30	2.53	1.40	1.33
48	Q	503	PEE	O2-C2	-2.51	1.40	1.46
49	J	403	PLX	O6-C4	-2.50	1.41	1.44
48	l	704	PEE	O3-C30	2.49	1.40	1.33
47	A	503	NAI	O3B-C3B	-2.49	1.37	1.43
48	l	703	PEE	O2-C2	-2.48	1.40	1.46
52	a	201	CDL	OA6-CA4	-2.46	1.40	1.46
48	j	201	PEE	O3-C30	2.46	1.40	1.33
50	C	304	UQ	C7-C8	2.46	1.54	1.50
56	Q	501	UQ1	C6-C1	2.46	1.53	1.46
48	W	201	PEE	O2-C2	-2.43	1.40	1.46
52	V	203	CDL	OA6-CA4	-2.42	1.40	1.46
52	l	701	CDL	OA6-CA4	-2.41	1.40	1.46
46	A	502	FMN	C10-N1	2.41	1.38	1.33
48	j	202	PEE	O2-C2	-2.40	1.40	1.46
49	a	202	PLX	C7-C6	2.40	1.55	1.50
52	J	404	CDL	OA6-CA4	-2.39	1.40	1.46
48	l	704	PEE	O2-C2	-2.39	1.40	1.46
56	Q	501	UQ1	O2-CM2	-2.39	1.39	1.45
49	j	203	PLX	C7-C6	2.38	1.55	1.50
48	l	703	PEE	O3-C30	2.36	1.40	1.33
52	r	502	CDL	OA6-CA4	-2.35	1.40	1.46
56	Q	501	UQ1	O1-C1	-2.34	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	J	402	UQ	C7-C8	2.34	1.54	1.50
48	V	204	PEE	O2-C2	-2.34	1.40	1.46
48	V	202	PEE	O3-C30	2.34	1.40	1.33
56	Q	502	UQ1	C6-C1	2.33	1.53	1.46
49	e	201	PLX	C7-C6	2.33	1.55	1.50
56	Q	502	UQ1	O4-C4	-2.33	1.18	1.23
48	W	201	PEE	O3-C30	2.32	1.40	1.33
48	V	202	PEE	O2-C2	-2.32	1.40	1.46
49	r	501	PLX	C7-C6	2.31	1.55	1.50
47	A	503	NAI	PN-O5D	2.31	1.68	1.59
48	j	201	PEE	O2-C2	-2.29	1.40	1.46
49	J	403	PLX	C7-C6	2.29	1.55	1.50
49	r	501	PLX	O6-C4	-2.29	1.41	1.44
48	l	704	PEE	O2-C10	2.29	1.40	1.34
48	C	302	PEE	O3-C30	2.28	1.40	1.33
48	j	202	PEE	O2-C10	2.28	1.40	1.34
48	Q	503	PEE	O3-C30	2.28	1.40	1.33
48	s	401	PEE	O3-C30	2.28	1.40	1.33
49	g	201	PLX	C7-C6	2.27	1.55	1.50
52	k	101	CDL	OB6-CB4	-2.27	1.40	1.46
56	Q	502	UQ1	O1-C1	-2.27	1.18	1.23
48	C	302	PEE	O3-C3	-2.26	1.40	1.45
52	V	203	CDL	PB2-OB2	2.26	1.68	1.59
48	V	202	PEE	O2-C10	2.25	1.40	1.34
52	l	701	CDL	OB6-CB4	-2.25	1.41	1.46
48	V	204	PEE	O2-C10	2.25	1.40	1.34
48	Q	503	PEE	O2-C10	2.24	1.40	1.34
52	V	203	CDL	OB6-CB4	-2.23	1.41	1.46
52	V	201	CDL	OB6-CB4	-2.23	1.41	1.46
49	C	303	PLX	C7-C6	2.23	1.55	1.50
52	V	201	CDL	PB2-OB2	2.22	1.68	1.59
48	j	201	PEE	O2-C10	2.22	1.40	1.34
52	a	201	CDL	PB2-OB5	2.22	1.68	1.59
56	Q	501	UQ1	O4-C4	-2.22	1.18	1.23
56	Q	502	UQ1	O3-CM3	-2.22	1.40	1.45
48	V	202	PEE	O3-C3	-2.21	1.40	1.45
52	V	201	CDL	PB2-OB5	2.21	1.68	1.59
48	W	201	PEE	O3-C3	-2.21	1.40	1.45
50	C	304	UQ	O4-C4	-2.20	1.18	1.23
48	Q	503	PEE	O3-C3	-2.20	1.40	1.45
48	W	201	PEE	O2-C10	2.19	1.40	1.34
52	r	502	CDL	PB2-OB2	2.18	1.68	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	J	404	CDL	PB2-OB2	2.18	1.68	1.59
52	J	404	CDL	OB6-CB4	-2.18	1.41	1.46
48	s	401	PEE	O3-C3	-2.17	1.40	1.45
52	r	502	CDL	OB6-CB4	-2.17	1.41	1.46
52	l	701	CDL	PB2-OB5	2.16	1.68	1.59
50	J	402	UQ	O1-C1	-2.16	1.18	1.23
56	Q	502	UQ1	O2-CM2	-2.15	1.40	1.45
52	l	701	CDL	PB2-OB2	2.15	1.68	1.59
49	j	203	PLX	P1-O4	2.15	1.68	1.59
49	a	202	PLX	P1-O4	2.15	1.68	1.59
52	V	203	CDL	PB2-OB5	2.14	1.68	1.59
48	C	302	PEE	O2-C10	2.14	1.40	1.34
49	r	501	PLX	P1-O4	2.14	1.68	1.59
52	a	201	CDL	PB2-OB2	2.14	1.67	1.59
52	r	502	CDL	PB2-OB5	2.12	1.67	1.59
52	V	201	CDL	OA6-CA4	-2.12	1.41	1.46
49	g	201	PLX	P1-O4	2.11	1.67	1.59
49	r	501	PLX	P1-O1	2.11	1.67	1.59
50	J	402	UQ	O4-C4	-2.11	1.18	1.23
52	J	404	CDL	PB2-OB5	2.10	1.67	1.59
47	A	503	NAI	C5B-C4B	2.10	1.58	1.51
52	k	101	CDL	PB2-OB5	2.10	1.67	1.59
52	a	201	CDL	OB6-CB4	-2.09	1.41	1.46
53	J	401	NDP	O5D-C5D	-2.08	1.36	1.44
49	e	201	PLX	P1-O4	2.07	1.67	1.59
48	l	703	PEE	O3-C3	-2.07	1.40	1.45
49	j	203	PLX	P1-O1	2.05	1.67	1.59
49	r	501	PLX	C25-C24	2.04	1.55	1.50
56	Q	501	UQ1	O3-CM3	-2.04	1.40	1.45
52	k	101	CDL	PB2-OB2	2.04	1.67	1.59
49	C	303	PLX	P1-O4	2.04	1.67	1.59
49	a	202	PLX	P1-O1	2.03	1.67	1.59
50	C	304	UQ	O1-C1	-2.03	1.19	1.23
48	j	201	PEE	O3-C3	-2.02	1.40	1.45
50	C	304	UQ	O3-CM3	-2.02	1.40	1.45
49	e	201	PLX	P1-O1	2.01	1.67	1.59
48	l	704	PEE	O3-C3	-2.01	1.40	1.45
48	V	204	PEE	O3-C3	-2.01	1.40	1.45

All (164) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	J	402	UQ	C7-C8-C9	-8.63	112.43	126.79
50	C	304	UQ	C7-C8-C9	-8.16	113.20	126.79
53	J	401	NDP	PN-O3-PA	-6.86	109.30	132.83
50	J	402	UQ	C12-C13-C14	-6.05	113.10	127.66
50	C	304	UQ	C17-C18-C19	-5.95	113.34	127.66
50	J	402	UQ	C17-C18-C19	-5.89	113.47	127.66
50	C	304	UQ	C12-C13-C14	-5.89	113.48	127.66
50	C	304	UQ	C22-C23-C24	-5.69	113.96	127.66
51	G	201	8Q1	C6-C1-S44	5.49	119.85	113.46
56	Q	501	UQ1	C7-C6-C1	4.94	124.42	118.48
52	l	702	CDL	OA6-CA5-C11	4.83	121.92	111.50
56	Q	502	UQ1	C7-C8-C9	-4.76	112.33	127.26
52	l	702	CDL	OB6-CB5-C51	4.66	121.55	111.50
58	w	401	ADP	N3-C2-N1	-4.52	121.61	128.68
50	J	402	UQ	C20-C19-C18	-4.41	112.36	123.68
47	A	503	NAI	N3A-C2A-N1A	-4.39	121.82	128.68
48	j	202	PEE	O2-C10-C11	4.37	120.92	111.50
50	C	304	UQ	C10-C9-C8	-4.33	112.57	123.68
50	J	402	UQ	C22-C23-C24	-4.32	112.99	127.75
50	C	304	UQ	C25-C24-C23	-4.29	112.66	123.68
52	a	201	CDL	OB6-CB5-C51	4.26	120.69	111.50
51	X	201	8Q1	C43-S44-C1	4.24	115.08	101.87
50	C	304	UQ	C27-C28-C29	-4.24	113.25	127.75
52	I	201	CDL	OB6-CB5-C51	4.18	120.50	111.50
48	V	204	PEE	O2-C10-C11	4.15	120.45	111.50
48	V	202	PEE	O2-C10-C11	4.15	120.44	111.50
50	J	402	UQ	C21-C19-C18	-4.14	112.73	121.12
48	j	201	PEE	O2-C10-C11	4.14	120.42	111.50
50	J	402	UQ	C16-C14-C13	-4.14	112.74	121.12
50	J	402	UQ	C15-C14-C13	-4.13	113.09	123.68
52	r	502	CDL	OA6-CA5-C11	4.11	120.37	111.50
48	l	704	PEE	O2-C10-C11	4.11	120.35	111.50
50	C	304	UQ	C21-C19-C18	-4.09	112.83	121.12
51	X	201	8Q1	C6-C1-S44	4.08	118.20	113.46
52	l	701	CDL	OA6-CA5-C11	4.03	120.19	111.50
52	J	404	CDL	OB6-CB5-C51	4.03	120.18	111.50
52	I	201	CDL	OA6-CA5-C11	4.02	120.17	111.50
50	C	304	UQ	C16-C14-C13	-4.02	112.99	121.12
52	V	203	CDL	OA6-CA5-C11	4.01	120.14	111.50
50	C	304	UQ	C11-C9-C8	-3.99	113.05	121.12
48	W	201	PEE	O2-C10-C11	3.97	120.07	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	u	201	CDL	OB6-CB5-C51	3.97	120.06	111.50
50	J	402	UQ	C10-C9-C8	-3.96	113.52	123.68
50	C	304	UQ	C20-C19-C18	-3.95	113.54	123.68
52	V	203	CDL	OB6-CB5-C51	3.94	120.00	111.50
48	Q	503	PEE	O2-C10-C11	3.94	119.98	111.50
48	s	401	PEE	O2-C10-C11	3.93	119.96	111.50
52	J	404	CDL	OA6-CA5-C11	3.92	119.95	111.50
52	r	502	CDL	OB6-CB5-C51	3.91	119.93	111.50
52	a	201	CDL	OA6-CA5-C11	3.90	119.91	111.50
50	J	402	UQ	C11-C9-C8	-3.89	113.24	121.12
48	l	703	PEE	O2-C10-C11	3.88	119.86	111.50
48	C	302	PEE	O2-C10-C11	3.87	119.85	111.50
52	V	201	CDL	OA6-CA5-C11	3.82	119.74	111.50
50	C	304	UQ	C15-C14-C13	-3.82	113.88	123.68
52	k	101	CDL	OB6-CB5-C51	3.79	119.68	111.50
51	G	201	8Q1	C43-S44-C1	3.76	113.57	101.87
52	u	201	CDL	OA6-CA5-C11	3.73	119.53	111.50
52	V	201	CDL	OB6-CB5-C51	3.72	119.53	111.50
52	l	701	CDL	OB6-CB5-C51	3.70	119.47	111.50
50	C	304	UQ	C26-C24-C23	-3.66	113.71	121.12
56	Q	501	UQ1	C7-C8-C9	-3.51	116.26	127.26
51	G	201	8Q1	O35-C34-N36	-3.44	115.61	122.99
50	J	402	UQ	C25-C24-C23	-3.40	112.82	122.65
50	C	304	UQ	C30-C29-C28	-3.38	112.87	122.65
50	J	402	UQ	C26-C24-C23	-3.34	112.99	122.65
52	k	101	CDL	OA6-CA5-C11	3.33	118.69	111.50
46	A	502	FMN	C4-N3-C2	-3.29	119.56	125.64
47	A	503	NAI	C4D-O4D-C1D	-3.29	102.22	109.47
50	C	304	UQ	C31-C29-C28	-3.28	113.16	122.65
47	A	503	NAI	C3D-C2D-C1D	3.23	107.56	101.43
52	u	201	CDL	OB8-CB7-C71	3.20	121.96	111.91
56	Q	502	UQ1	C10-C9-C8	-3.20	113.41	122.65
48	s	401	PEE	O3-C30-C31	3.16	121.84	111.91
53	J	401	NDP	O2B-P2B-O1X	-3.14	97.27	109.39
51	X	201	8Q1	O35-C34-N36	-3.14	116.26	122.99
52	u	201	CDL	OA8-CA7-C31	3.13	119.59	111.38
56	Q	501	UQ1	C10-C9-C8	-3.13	113.61	122.65
56	Q	502	UQ1	C11-C9-C8	-3.11	113.65	122.65
53	J	401	NDP	PA-O5B-C5B	-3.05	103.81	121.68
52	l	702	CDL	CB4-OB6-CB5	-3.04	110.30	117.79
52	a	201	CDL	OB8-CB7-C71	2.91	121.04	111.91
52	l	702	CDL	OA8-CA7-C31	2.90	120.99	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	Q	503	PEE	O3-C30-C31	2.88	120.94	111.91
52	I	201	CDL	CA6-CA4-CA3	-2.86	105.03	111.79
53	J	401	NDP	PN-O5D-C5D	-2.79	105.30	121.68
58	w	401	ADP	PA-O3A-PB	-2.78	123.27	132.83
52	I	201	CDL	OA8-CA7-C31	2.78	120.64	111.91
51	G	201	8Q1	C32-C34-N36	2.78	122.11	116.58
51	X	201	8Q1	C37-C38-C39	2.78	116.98	112.36
51	X	201	8Q1	O2-P24-O27	-2.78	99.35	106.73
46	A	502	FMN	C4A-C4-N3	2.77	120.22	113.19
51	G	201	8Q1	O40-C39-N41	-2.77	117.79	123.01
52	V	203	CDL	OB8-CB7-C71	2.77	120.59	111.91
52	k	101	CDL	OA8-CA7-C31	2.76	120.58	111.91
52	I	201	CDL	CB4-OB6-CB5	-2.76	111.00	117.79
51	G	201	8Q1	C37-C38-C39	2.73	116.91	112.36
52	l	702	CDL	OB8-CB7-C71	2.71	120.42	111.91
52	I	201	CDL	OB8-CB7-C71	2.71	120.42	111.91
51	G	201	8Q1	O2-P24-O27	-2.70	99.54	106.73
50	J	402	UQ	CM5-C5-C6	-2.70	120.00	124.40
51	G	201	8Q1	O4-C1-S44	-2.69	119.12	122.61
48	C	302	PEE	O3-C30-C31	2.68	120.32	111.91
47	A	503	NAI	C4A-C5A-N7A	-2.68	106.61	109.40
52	V	201	CDL	OB8-CB7-C71	2.67	120.30	111.91
48	W	201	PEE	O3-C30-C31	2.67	120.28	111.91
48	V	204	PEE	O3-C30-C31	2.67	120.27	111.91
52	l	701	CDL	OA8-CA7-C31	2.65	120.22	111.91
53	J	401	NDP	O4B-C4B-C3B	2.64	110.35	105.11
48	l	703	PEE	O3-C30-C31	2.63	120.17	111.91
48	j	201	PEE	O3-C30-C31	2.63	120.17	111.91
48	j	202	PEE	O3-C30-C31	2.63	120.15	111.91
52	l	701	CDL	OB8-CB7-C71	2.62	120.14	111.91
52	V	203	CDL	OA8-CA7-C31	2.60	120.08	111.91
52	J	404	CDL	OA8-CA7-C31	2.60	120.07	111.91
47	A	503	NAI	C3B-C2B-C1B	2.59	104.88	100.98
52	r	502	CDL	OA8-CA7-C31	2.59	120.02	111.91
52	k	101	CDL	OB8-CB7-C71	2.57	119.97	111.91
46	A	502	FMN	O4-C4-C4A	-2.56	119.81	126.60
53	J	401	NDP	O3X-P2B-O2X	2.53	117.32	107.64
51	G	201	8Q1	O4-C1-C6	-2.51	121.03	123.99
52	V	201	CDL	OA8-CA7-C31	2.50	119.75	111.91
49	r	501	PLX	C1A-N1-C1	2.49	120.12	109.92
51	X	201	8Q1	O40-C39-N41	-2.49	118.31	123.01
49	g	201	PLX	C1A-N1-C1	2.49	120.09	109.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	A	502	FMN	C4A-C10-N1	-2.49	118.96	124.73
52	a	201	CDL	OA8-CA7-C31	2.47	119.65	111.91
52	u	201	CDL	OB8-CB7-OB9	-2.46	117.39	123.59
56	Q	501	UQ1	C11-C9-C8	-2.45	115.58	122.65
52	r	502	CDL	OB8-CB7-C71	2.44	119.57	111.91
51	X	201	8Q1	C32-C34-N36	2.44	121.44	116.58
48	V	202	PEE	O3-C30-C31	2.43	119.54	111.91
51	X	201	8Q1	O27-P24-O3	-2.42	99.69	106.47
48	l	704	PEE	O3-C30-C31	2.41	119.49	111.91
53	J	401	NDP	O5D-PN-O1N	-2.41	99.67	109.07
53	J	401	NDP	C2A-N1A-C6A	-2.39	114.67	118.75
56	Q	501	UQ1	C6-C5-C4	2.37	121.06	119.18
49	j	203	PLX	C1A-N1-C1	2.37	119.61	109.92
53	J	401	NDP	O2N-PN-O1N	2.36	123.92	112.24
46	A	502	FMN	C4A-C10-N10	2.32	119.88	116.48
53	J	401	NDP	C5B-C4B-C3B	-2.31	106.52	115.18
52	J	404	CDL	OB8-CB7-C71	2.30	119.14	111.91
46	A	502	FMN	C5A-C9A-N10	2.30	120.33	117.95
51	G	201	8Q1	O1-P24-O2	2.28	116.35	107.64
51	X	201	8Q1	O1-P24-O2	2.28	116.34	107.64
56	Q	502	UQ1	CM5-C5-C6	-2.27	120.69	124.40
49	a	202	PLX	C1A-N1-C1	2.27	119.21	109.92
49	J	403	PLX	C1A-N1-C1	2.26	119.14	109.92
50	C	304	UQ	CM5-C5-C6	-2.24	120.75	124.40
49	C	303	PLX	C1A-N1-C1	2.23	119.02	109.92
46	A	502	FMN	C9A-C5A-N5	-2.23	120.01	122.43
47	A	503	NAI	PN-O3-PA	-2.21	125.25	132.83
52	l	702	CDL	OA6-CA5-OA7	-2.20	118.39	123.70
52	l	702	CDL	OB6-CB5-OB7	-2.18	118.43	123.70
56	Q	501	UQ1	CM5-C5-C6	-2.18	120.85	124.40
51	G	201	8Q1	C38-C39-N41	2.15	120.03	116.42
52	l	702	CDL	CA4-OA6-CA5	-2.12	112.58	117.79
49	e	201	PLX	C1A-N1-C1	2.11	118.55	109.92
46	A	502	FMN	C10-C4A-N5	-2.11	120.39	124.86
58	w	401	ADP	C4-C5-N7	-2.10	107.21	109.40
47	A	503	NAI	C2D-C3D-C4D	2.07	106.67	102.64
52	I	201	CDL	OB6-CB5-OB7	-2.04	118.76	123.70
46	A	502	FMN	C4-C4A-C10	2.03	120.20	116.79
58	w	401	ADP	O4'-C1'-C2'	-2.00	104.00	106.93

There are no chirality outliers.

All (999) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C1'-C2'-C3'-O3'
46	A	502	FMN	C1'-C2'-C3'-C4'
46	A	502	FMN	C3'-C4'-C5'-O5'
46	A	502	FMN	O4'-C4'-C5'-O5'
46	A	502	FMN	C5'-O5'-P-O1P
46	A	502	FMN	C5'-O5'-P-O2P
47	A	503	NAI	PN-O3-PA-O5B
48	C	302	PEE	O4P-C4-C5-N
48	Q	503	PEE	C11-C10-O2-C2
48	Q	503	PEE	O4-C10-O2-C2
48	Q	503	PEE	C4-O4P-P-O1P
48	V	202	PEE	C5-C4-O4P-P
48	V	204	PEE	O4P-C4-C5-N
48	W	201	PEE	C4-O4P-P-O3P
48	W	201	PEE	C4-O4P-P-O2P
48	W	201	PEE	C4-O4P-P-O1P
48	j	201	PEE	O4P-C4-C5-N
48	j	202	PEE	C11-C10-O2-C2
48	j	202	PEE	O4P-C4-C5-N
48	l	703	PEE	C11-C10-O2-C2
48	l	703	PEE	C4-O4P-P-O1P
48	l	704	PEE	C1-O3P-P-O2P
48	l	704	PEE	C1-O3P-P-O1P
48	l	704	PEE	O4P-C4-C5-N
49	C	303	PLX	O6-C6-C7-C8
49	J	403	PLX	O7-C6-O6-C4
49	J	403	PLX	C3-C4-O6-C6
49	J	403	PLX	C2-O1-P1-O2
49	J	403	PLX	N1-C1-C2-O1
49	J	403	PLX	O8-C24-C25-C26
49	a	202	PLX	O7-C6-O6-C4
49	a	202	PLX	C2-O1-P1-O2
49	a	202	PLX	N1-C1-C2-O1
49	a	202	PLX	O9-C24-O8-C5
49	a	202	PLX	O9-C24-C25-C26
49	e	201	PLX	C3-O4-P1-O2
49	e	201	PLX	C2-O1-P1-O4
49	e	201	PLX	O9-C24-O8-C5
49	g	201	PLX	C3-O4-P1-O2
49	g	201	PLX	C2-O1-P1-O4
49	g	201	PLX	C2-O1-P1-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	g	201	PLX	C2-O1-P1-O3
49	j	203	PLX	O7-C6-C7-C8
49	j	203	PLX	O9-C24-O8-C5
49	r	501	PLX	C5-C4-O6-C6
49	r	501	PLX	O9-C24-C25-C26
50	C	304	UQ	C7-C8-C9-C10
50	C	304	UQ	C7-C8-C9-C11
50	C	304	UQ	C12-C13-C14-C16
50	C	304	UQ	C22-C23-C24-C25
50	J	402	UQ	C1-C6-C7-C8
50	J	402	UQ	C5-C6-C7-C8
50	J	402	UQ	C7-C8-C9-C10
50	J	402	UQ	C12-C11-C9-C8
50	J	402	UQ	C12-C13-C14-C15
50	J	402	UQ	C12-C13-C14-C16
50	J	402	UQ	C17-C18-C19-C21
50	J	402	UQ	C20-C19-C21-C22
51	G	201	8Q1	C28-C29-C32-C34
51	G	201	8Q1	C28-C29-C32-O33
51	G	201	8Q1	C30-C29-C32-C34
51	G	201	8Q1	C30-C29-C32-O33
51	G	201	8Q1	C31-C29-C32-C34
51	G	201	8Q1	C31-C29-C32-O33
51	X	201	8Q1	C1-C6-C7-C8
51	X	201	8Q1	C28-O27-P24-O3
51	X	201	8Q1	C28-O27-P24-O2
51	X	201	8Q1	C28-O27-P24-O1
52	I	201	CDL	O1-C1-CA2-OA2
52	I	201	CDL	CB2-C1-CA2-OA2
52	I	201	CDL	CA2-OA2-PA1-OA3
52	I	201	CDL	CA2-OA2-PA1-OA4
52	I	201	CDL	CA2-OA2-PA1-OA5
52	I	201	CDL	CA3-OA5-PA1-OA4
52	I	201	CDL	CB2-OB2-PB2-OB4
52	I	201	CDL	CB3-OB5-PB2-OB2
52	J	404	CDL	CA2-OA2-PA1-OA3
52	J	404	CDL	OA5-CA3-CA4-OA6
52	J	404	CDL	OA9-CA7-OA8-CA6
52	J	404	CDL	C31-CA7-OA8-CA6
52	V	201	CDL	CA2-C1-CB2-OB2
52	V	201	CDL	CB2-OB2-PB2-OB3
52	V	201	CDL	CB2-OB2-PB2-OB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	V	201	CDL	CB3-OB5-PB2-OB4
52	V	203	CDL	CA3-OA5-PA1-OA2
52	V	203	CDL	CA3-OA5-PA1-OA3
52	V	203	CDL	CA3-OA5-PA1-OA4
52	V	203	CDL	CB2-OB2-PB2-OB3
52	V	203	CDL	OB5-CB3-CB4-OB6
52	a	201	CDL	CB2-C1-CA2-OA2
52	a	201	CDL	CA2-OA2-PA1-OA3
52	a	201	CDL	CB2-OB2-PB2-OB3
52	a	201	CDL	CB3-OB5-PB2-OB4
52	a	201	CDL	OB7-CB5-OB6-CB4
52	a	201	CDL	C51-CB5-OB6-CB4
52	k	101	CDL	CA2-OA2-PA1-OA3
52	k	101	CDL	CA3-OA5-PA1-OA2
52	k	101	CDL	CA3-OA5-PA1-OA3
52	k	101	CDL	CA3-OA5-PA1-OA4
52	k	101	CDL	CB2-OB2-PB2-OB3
52	l	701	CDL	CA2-C1-CB2-OB2
52	l	701	CDL	CA2-OA2-PA1-OA4
52	l	701	CDL	C31-CA7-OA8-CA6
52	l	701	CDL	CB2-OB2-PB2-OB3
52	l	701	CDL	CB2-OB2-PB2-OB4
52	l	701	CDL	CB3-OB5-PB2-OB3
52	l	701	CDL	OB5-CB3-CB4-OB6
52	l	702	CDL	CA2-OA2-PA1-OA4
52	l	702	CDL	CA3-OA5-PA1-OA2
52	l	702	CDL	CA3-OA5-PA1-OA3
52	l	702	CDL	CA3-OA5-PA1-OA4
52	l	702	CDL	CB2-OB2-PB2-OB3
52	l	702	CDL	CB2-OB2-PB2-OB4
52	l	702	CDL	CB2-OB2-PB2-OB5
52	r	502	CDL	CB3-OB5-PB2-OB3
52	r	502	CDL	C51-CB5-OB6-CB4
52	u	201	CDL	CA2-OA2-PA1-OA4
52	u	201	CDL	CA3-OA5-PA1-OA2
52	u	201	CDL	CA3-OA5-PA1-OA3
52	u	201	CDL	CA3-OA5-PA1-OA4
52	u	201	CDL	CB2-OB2-PB2-OB5
52	u	201	CDL	CB3-OB5-PB2-OB2
52	u	201	CDL	CB3-OB5-PB2-OB3
52	u	201	CDL	CB3-OB5-PB2-OB4
53	J	401	NDP	C5B-O5B-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	J	401	NDP	O4D-C4D-C5D-O5D
56	Q	501	UQ1	C1-C6-C7-C8
56	Q	501	UQ1	C5-C6-C7-C8
56	Q	501	UQ1	C7-C8-C9-C10
58	w	401	ADP	C5'-O5'-PA-O2A
58	w	401	ADP	C5'-O5'-PA-O3A
48	Q	503	PEE	O5-C30-O3-C3
48	V	204	PEE	O5-C30-O3-C3
52	l	701	CDL	OA9-CA7-OA8-CA6
48	Q	503	PEE	C31-C30-O3-C3
48	j	201	PEE	O5-C30-O3-C3
48	l	703	PEE	O4-C10-O2-C2
52	r	502	CDL	OB7-CB5-OB6-CB4
48	V	204	PEE	C31-C30-O3-C3
48	j	201	PEE	C31-C30-O3-C3
50	J	402	UQ	C12-C11-C9-C10
50	C	304	UQ	C18-C19-C21-C22
48	l	704	PEE	C2-C3-O3-C30
48	V	204	PEE	C17-C18-C19-C20
48	j	201	PEE	C17-C18-C19-C20
48	s	401	PEE	C17-C18-C19-C20
52	V	201	CDL	C11-C12-C13-C14
48	j	202	PEE	O4-C10-O2-C2
50	C	304	UQ	C17-C18-C19-C21
52	V	201	CDL	C62-C63-C64-C65
52	I	201	CDL	O1-C1-CB2-OB2
52	V	201	CDL	O1-C1-CB2-OB2
52	a	201	CDL	O1-C1-CA2-OA2
52	a	201	CDL	O1-C1-CB2-OB2
52	l	702	CDL	O1-C1-CA2-OA2
52	r	502	CDL	O1-C1-CA2-OA2
52	l	701	CDL	C71-CB7-OB8-CB6
52	V	201	CDL	C11-CA5-OA6-CA4
52	l	702	CDL	C11-CA5-OA6-CA4
49	r	501	PLX	C9-C10-C11-C12
52	l	701	CDL	OB9-CB7-OB8-CB6
48	l	704	PEE	C34-C35-C36-C37
49	j	203	PLX	C13-C14-C15-C16
49	r	501	PLX	C11-C12-C13-C14
58	w	401	ADP	O4'-C4'-C5'-O5'
58	w	401	ADP	C3'-C4'-C5'-O5'
49	r	501	PLX	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
50	J	402	UQ	C22-C23-C24-C26
50	J	402	UQ	C15-C14-C16-C17
52	k	101	CDL	C36-C37-C38-C39
52	l	702	CDL	C31-C32-C33-C34
52	l	702	CDL	C33-C34-C35-C36
50	C	304	UQ	C27-C28-C29-C31
56	Q	502	UQ1	C7-C8-C9-C11
52	V	201	CDL	CB2-C1-CA2-OA2
52	a	201	CDL	CA2-C1-CB2-OB2
52	r	502	CDL	CB2-C1-CA2-OA2
52	V	201	CDL	OA7-CA5-OA6-CA4
48	j	201	PEE	C40-C41-C42-C43
49	g	201	PLX	C2-C1-N1-C1A
48	W	201	PEE	C31-C30-O3-C3
52	I	201	CDL	C31-CA7-OA8-CA6
52	V	201	CDL	C31-CA7-OA8-CA6
52	V	203	CDL	C31-CA7-OA8-CA6
52	l	702	CDL	C71-CB7-OB8-CB6
52	l	701	CDL	CB7-C71-C72-C73
48	l	703	PEE	C33-C34-C35-C36
49	J	403	PLX	C25-C26-C27-C28
52	k	101	CDL	O1-C1-CB2-OB2
52	u	201	CDL	O1-C1-CA2-OA2
52	J	404	CDL	CB7-C71-C72-C73
52	a	201	CDL	C34-C35-C36-C37
48	W	201	PEE	O5-C30-O3-C3
52	V	203	CDL	OA9-CA7-OA8-CA6
50	J	402	UQ	C18-C19-C21-C22
52	V	203	CDL	C51-CB5-OB6-CB4
52	l	701	CDL	C58-C59-C60-C61
48	V	202	PEE	C10-C11-C12-C13
52	r	502	CDL	CB7-C71-C72-C73
52	k	101	CDL	CA7-C31-C32-C33
52	l	701	CDL	CB5-C51-C52-C53
52	r	502	CDL	CB5-C51-C52-C53
52	J	404	CDL	CA7-C31-C32-C33
52	V	201	CDL	CB7-C71-C72-C73
52	l	702	CDL	CA5-C11-C12-C13
52	r	502	CDL	CA7-C31-C32-C33
53	J	401	NDP	C3D-C4D-C5D-O5D
48	l	704	PEE	C21-C22-C23-C24
52	l	701	CDL	C18-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	l	702	CDL	OA7-CA5-OA6-CA4
48	V	204	PEE	C10-C11-C12-C13
52	V	203	CDL	CA5-C11-C12-C13
48	W	201	PEE	C11-C12-C13-C14
52	l	702	CDL	C35-C36-C37-C38
49	J	403	PLX	C34-C35-C36-C37
52	V	201	CDL	OA9-CA7-OA8-CA6
52	l	702	CDL	OB9-CB7-OB8-CB6
50	C	304	UQ	C14-C16-C17-C18
52	V	201	CDL	O1-C1-CA2-OA2
52	V	203	CDL	O1-C1-CB2-OB2
52	l	702	CDL	O1-C1-CB2-OB2
52	I	201	CDL	OA9-CA7-OA8-CA6
48	s	401	PEE	C11-C12-C13-C14
52	I	201	CDL	C11-CA5-OA6-CA4
48	l	703	PEE	C4-O4P-P-O3P
48	l	704	PEE	C1-O3P-P-O4P
49	a	202	PLX	C2-O1-P1-O4
49	g	201	PLX	C3-O4-P1-O1
49	r	501	PLX	C3-O4-P1-O1
52	I	201	CDL	CA3-OA5-PA1-OA2
52	I	201	CDL	CB2-OB2-PB2-OB5
52	V	201	CDL	CB2-OB2-PB2-OB5
52	V	201	CDL	CB3-OB5-PB2-OB2
52	V	203	CDL	CB3-OB5-PB2-OB2
52	a	201	CDL	CB2-OB2-PB2-OB5
52	l	701	CDL	CA2-OA2-PA1-OA5
52	l	701	CDL	CB2-OB2-PB2-OB5
52	l	702	CDL	CA2-OA2-PA1-OA5
52	r	502	CDL	CA3-OA5-PA1-OA2
52	r	502	CDL	CB2-OB2-PB2-OB5
52	u	201	CDL	CA2-OA2-PA1-OA5
52	J	404	CDL	C33-C34-C35-C36
52	l	701	CDL	C81-C82-C83-C84
52	V	203	CDL	CA2-C1-CB2-OB2
52	I	201	CDL	OA7-CA5-OA6-CA4
52	V	203	CDL	OB7-CB5-OB6-CB4
49	g	201	PLX	C2-C1-N1-C1B
48	j	202	PEE	C31-C30-O3-C3
52	k	101	CDL	C71-CB7-OB8-CB6
52	u	201	CDL	CB5-C51-C52-C53
49	C	303	PLX	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	l	702	CDL	C41-C42-C43-C44
48	C	302	PEE	C11-C12-C13-C14
52	V	201	CDL	C73-C74-C75-C76
52	l	701	CDL	C75-C76-C77-C78
48	l	704	PEE	C11-C10-O2-C2
48	W	201	PEE	C12-C13-C14-C15
48	l	703	PEE	C21-C22-C23-C24
48	s	401	PEE	C34-C35-C36-C37
49	J	403	PLX	C31-C32-C33-C34
49	a	202	PLX	C9-C10-C11-C12
49	a	202	PLX	C31-C32-C33-C34
49	g	201	PLX	C27-C28-C29-C30
49	j	203	PLX	C12-C13-C14-C15
49	r	501	PLX	C11-C10-C9-C8
52	J	404	CDL	C51-C52-C53-C54
52	J	404	CDL	C52-C53-C54-C55
52	V	203	CDL	C75-C76-C77-C78
52	k	101	CDL	C20-C21-C22-C23
52	k	101	CDL	C81-C82-C83-C84
48	s	401	PEE	C31-C30-O3-C3
49	C	303	PLX	C14-C15-C16-C17
49	e	201	PLX	C13-C14-C15-C16
49	j	203	PLX	C14-C15-C16-C17
51	G	201	8Q1	C11-C12-C13-C14
51	X	201	8Q1	C12-C13-C14-C15
52	V	203	CDL	C12-C13-C14-C15
52	V	203	CDL	C34-C35-C36-C37
52	l	701	CDL	C71-C72-C73-C74
52	l	701	CDL	C74-C75-C76-C77
48	l	704	PEE	O4-C10-O2-C2
48	j	202	PEE	C12-C13-C14-C15
49	C	303	PLX	C11-C12-C13-C14
49	g	201	PLX	C11-C10-C9-C8
49	j	203	PLX	C33-C34-C35-C36
52	J	404	CDL	C71-C72-C73-C74
52	k	101	CDL	C32-C33-C34-C35
52	l	701	CDL	C14-C15-C16-C17
52	l	701	CDL	C31-C32-C33-C34
48	l	704	PEE	C37-C38-C39-C40
48	C	302	PEE	C34-C35-C36-C37
49	e	201	PLX	C25-C26-C27-C28
49	e	201	PLX	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	j	203	PLX	C30-C31-C32-C33
52	J	404	CDL	C32-C33-C34-C35
52	V	201	CDL	C55-C56-C57-C58
52	k	101	CDL	C15-C16-C17-C18
52	k	101	CDL	C75-C76-C77-C78
52	l	701	CDL	C36-C37-C38-C39
52	l	701	CDL	O1-C1-CB2-OB2
49	C	303	PLX	C28-C29-C30-C31
52	V	203	CDL	C76-C77-C78-C79
52	a	201	CDL	C11-C12-C13-C14
52	a	201	CDL	C62-C63-C64-C65
52	k	101	CDL	C21-C22-C23-C24
52	r	502	CDL	C14-C15-C16-C17
52	J	404	CDL	CB5-C51-C52-C53
49	C	303	PLX	C10-C11-C12-C13
49	j	203	PLX	C7-C8-C9-C10
51	X	201	8Q1	C10-C11-C12-C13
52	l	701	CDL	C62-C63-C64-C65
52	r	502	CDL	C43-C44-C45-C46
48	j	202	PEE	O5-C30-O3-C3
48	V	202	PEE	C11-C12-C13-C14
48	V	202	PEE	C40-C41-C42-C43
49	a	202	PLX	C7-C8-C9-C10
49	e	201	PLX	C14-C15-C16-C17
49	g	201	PLX	C10-C11-C12-C13
49	g	201	PLX	C28-C29-C30-C31
49	r	501	PLX	C27-C28-C29-C30
52	V	201	CDL	C75-C76-C77-C78
52	V	203	CDL	C17-C18-C19-C20
52	V	203	CDL	C40-C41-C42-C43
52	a	201	CDL	C21-C22-C23-C24
52	l	701	CDL	C11-C12-C13-C14
52	l	701	CDL	C51-C52-C53-C54
48	l	704	PEE	C20-C21-C22-C23
49	C	303	PLX	C33-C34-C35-C36
49	r	501	PLX	C18-C19-C20-C21
49	r	501	PLX	C28-C29-C30-C31
52	V	201	CDL	C37-C38-C39-C40
52	r	502	CDL	C75-C76-C77-C78
48	j	201	PEE	C34-C35-C36-C37
52	a	201	CDL	C22-C23-C24-C25
52	l	701	CDL	C56-C57-C58-C59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	V	202	PEE	C33-C34-C35-C36
48	V	204	PEE	C31-C32-C33-C34
49	J	403	PLX	C10-C11-C12-C13
49	r	501	PLX	C33-C34-C35-C36
52	V	203	CDL	C32-C33-C34-C35
52	a	201	CDL	C71-C72-C73-C74
52	l	702	CDL	C11-C12-C13-C14
48	W	201	PEE	C19-C20-C21-C22
52	a	201	CDL	CA5-C11-C12-C13
48	V	202	PEE	C21-C22-C23-C24
48	j	202	PEE	C23-C24-C25-C26
49	J	403	PLX	C33-C34-C35-C36
49	g	201	PLX	C14-C15-C16-C17
49	g	201	PLX	C25-C26-C27-C28
49	g	201	PLX	C32-C33-C34-C35
49	j	203	PLX	C10-C11-C12-C13
52	J	404	CDL	C73-C74-C75-C76
52	V	201	CDL	C31-C32-C33-C34
52	V	203	CDL	C59-C60-C61-C62
52	k	101	CDL	C16-C17-C18-C19
52	k	101	CDL	C33-C34-C35-C36
52	k	101	CDL	C37-C38-C39-C40
52	k	101	CDL	C71-C72-C73-C74
52	l	701	CDL	C37-C38-C39-C40
52	r	502	CDL	C60-C61-C62-C63
49	g	201	PLX	C2-C1-N1-C1C
49	J	403	PLX	C27-C28-C29-C30
49	a	202	PLX	C12-C13-C14-C15
52	V	201	CDL	C56-C57-C58-C59
52	u	201	CDL	C73-C74-C75-C76
48	V	202	PEE	C31-C32-C33-C34
49	a	202	PLX	C13-C14-C15-C16
52	a	201	CDL	C51-C52-C53-C54
52	k	101	CDL	C78-C79-C80-C81
48	V	202	PEE	C13-C14-C15-C16
52	J	404	CDL	C35-C36-C37-C38
48	C	302	PEE	C31-C30-O3-C3
52	J	404	CDL	C59-C60-C61-C62
52	a	201	CDL	C54-C55-C56-C57
49	a	202	PLX	C14-C15-C16-C17
52	r	502	CDL	C34-C35-C36-C37
52	r	502	CDL	C57-C58-C59-C60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	J	403	PLX	C14-C15-C16-C17
52	J	404	CDL	C14-C15-C16-C17
52	J	404	CDL	C75-C76-C77-C78
52	V	203	CDL	C42-C43-C44-C45
52	l	701	CDL	C35-C36-C37-C38
52	r	502	CDL	C41-C42-C43-C44
48	s	401	PEE	C37-C38-C39-C40
48	V	202	PEE	C20-C21-C22-C23
49	e	201	PLX	C10-C11-C12-C13
49	g	201	PLX	C30-C31-C32-C33
52	l	701	CDL	C52-C53-C54-C55
52	l	702	CDL	CB5-C51-C52-C53
52	k	101	CDL	OB9-CB7-OB8-CB6
52	I	201	CDL	C51-CB5-OB6-CB4
52	J	404	CDL	C51-CB5-OB6-CB4
49	a	202	PLX	C27-C28-C29-C30
51	X	201	8Q1	C11-C12-C13-C14
49	C	303	PLX	O7-C6-C7-C8
49	J	403	PLX	O9-C24-C25-C26
49	e	201	PLX	O9-C24-C25-C26
49	r	501	PLX	O7-C6-C7-C8
52	k	101	CDL	C53-C54-C55-C56
48	l	704	PEE	C15-C16-C17-C18
49	J	403	PLX	C7-C8-C9-C10
52	a	201	CDL	C60-C61-C62-C63
52	r	502	CDL	C32-C33-C34-C35
49	e	201	PLX	C28-C29-C30-C31
49	e	201	PLX	C33-C34-C35-C36
52	V	203	CDL	C37-C38-C39-C40
52	l	701	CDL	C82-C83-C84-C85
52	J	404	CDL	OB7-CB5-OB6-CB4
50	C	304	UQ	C27-C28-C29-C30
48	W	201	PEE	C24-C25-C26-C27
49	e	201	PLX	C12-C13-C14-C15
52	J	404	CDL	C37-C38-C39-C40
52	J	404	CDL	C82-C83-C84-C85
52	l	701	CDL	C40-C41-C42-C43
49	J	403	PLX	C26-C27-C28-C29
49	a	202	PLX	C25-C26-C27-C28
52	V	201	CDL	C40-C41-C42-C43
52	k	101	CDL	C34-C35-C36-C37
52	r	502	CDL	C54-C55-C56-C57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	r	502	CDL	C62-C63-C64-C65
52	u	201	CDL	CB7-C71-C72-C73
49	J	403	PLX	C18-C19-C20-C21
52	V	201	CDL	C51-C52-C53-C54
52	V	201	CDL	C14-C15-C16-C17
48	s	401	PEE	O5-C30-O3-C3
48	l	704	PEE	C30-C31-C32-C33
49	r	501	PLX	C30-C31-C32-C33
48	j	202	PEE	C13-C14-C15-C16
49	C	303	PLX	C11-C10-C9-C8
49	a	202	PLX	C11-C12-C13-C14
49	j	203	PLX	C11-C12-C13-C14
52	V	201	CDL	C71-C72-C73-C74
48	V	202	PEE	C17-C18-C19-C20
48	C	302	PEE	O5-C30-O3-C3
48	l	703	PEE	C44-C45-C46-C47
48	l	703	PEE	C15-C16-C17-C18
50	J	402	UQ	C3-C2-O2-CM2
48	C	302	PEE	O4-C10-O2-C2
48	s	401	PEE	O4-C10-O2-C2
52	I	201	CDL	OB7-CB5-OB6-CB4
52	V	201	CDL	CB5-C51-C52-C53
48	j	201	PEE	C41-C42-C43-C44
52	V	203	CDL	C74-C75-C76-C77
49	e	201	PLX	C11-C10-C9-C8
52	l	702	CDL	C72-C73-C74-C75
49	r	501	PLX	C13-C14-C15-C16
52	r	502	CDL	C71-C72-C73-C74
48	l	704	PEE	C13-C14-C15-C16
52	V	203	CDL	C54-C55-C56-C57
52	k	101	CDL	C40-C41-C42-C43
48	s	401	PEE	C13-C14-C15-C16
51	G	201	8Q1	C9-C10-C11-C12
52	a	201	CDL	C33-C34-C35-C36
52	k	101	CDL	C52-C53-C54-C55
52	l	701	CDL	CA7-C31-C32-C33
48	C	302	PEE	C11-C10-O2-C2
48	s	401	PEE	C11-C10-O2-C2
52	J	404	CDL	C11-CA5-OA6-CA4
52	l	701	CDL	C11-CA5-OA6-CA4
52	l	702	CDL	C51-CB5-OB6-CB4
52	l	701	CDL	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	r	502	CDL	C83-C84-C85-C86
48	j	201	PEE	C14-C15-C16-C17
49	r	501	PLX	C14-C15-C16-C17
49	e	201	PLX	C27-C28-C29-C30
52	l	701	CDL	C34-C35-C36-C37
52	r	502	CDL	C76-C77-C78-C79
52	J	404	CDL	OB6-CB4-CB6-OB8
52	V	203	CDL	OB6-CB4-CB6-OB8
48	j	201	PEE	C22-C23-C24-C25
49	g	201	PLX	C33-C34-C35-C36
52	V	203	CDL	C14-C15-C16-C17
49	a	202	PLX	C15-C16-C17-C18
48	j	201	PEE	C19-C20-C21-C22
48	s	401	PEE	C35-C36-C37-C38
48	j	202	PEE	C11-C12-C13-C14
51	X	201	8Q1	C7-C8-C9-C10
52	a	201	CDL	C35-C36-C37-C38
48	V	202	PEE	C14-C15-C16-C17
52	V	201	CDL	C32-C33-C34-C35
52	V	201	CDL	C52-C53-C54-C55
52	k	101	CDL	C42-C43-C44-C45
52	J	404	CDL	OA7-CA5-OA6-CA4
52	l	702	CDL	OB7-CB5-OB6-CB4
48	Q	503	PEE	C34-C35-C36-C37
48	j	201	PEE	C21-C22-C23-C24
48	V	202	PEE	C36-C37-C38-C39
48	V	202	PEE	C38-C39-C40-C41
48	j	201	PEE	C38-C39-C40-C41
46	A	502	FMN	O2'-C2'-C3'-C4'
48	Q	503	PEE	C4-O4P-P-O3P
48	V	202	PEE	C1-O3P-P-O4P
49	J	403	PLX	C2-O1-P1-O4
52	a	201	CDL	CA2-OA2-PA1-OA5
52	a	201	CDL	CB3-OB5-PB2-OB2
52	k	101	CDL	CB2-OB2-PB2-OB5
52	r	502	CDL	CB3-OB5-PB2-OB2
49	g	201	PLX	C9-C10-C11-C12
52	l	701	CDL	C59-C60-C61-C62
52	V	201	CDL	C1-CB2-OB2-PB2
52	l	701	CDL	OB5-CB3-CB4-CB6
48	s	401	PEE	C23-C24-C25-C26
49	C	303	PLX	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	r	502	CDL	C12-C13-C14-C15
52	r	502	CDL	C37-C38-C39-C40
48	C	302	PEE	C10-C11-C12-C13
48	l	703	PEE	C11-C12-C13-C14
52	V	203	CDL	C60-C61-C62-C63
49	j	203	PLX	C31-C32-C33-C34
52	u	201	CDL	C52-C53-C54-C55
48	C	302	PEE	C19-C20-C21-C22
48	C	302	PEE	C35-C36-C37-C38
48	Q	503	PEE	C35-C36-C37-C38
48	W	201	PEE	C15-C16-C17-C18
49	C	303	PLX	C31-C32-C33-C34
52	a	201	CDL	C52-C53-C54-C55
52	k	101	CDL	C58-C59-C60-C61
52	r	502	CDL	C84-C85-C86-C87
49	C	303	PLX	C7-C8-C9-C10
49	e	201	PLX	C11-C12-C13-C14
49	g	201	PLX	C13-C14-C15-C16
52	J	404	CDL	C11-C12-C13-C14
52	l	702	CDL	C51-C52-C53-C54
49	J	403	PLX	C13-C14-C15-C16
52	J	404	CDL	CB3-CB4-CB6-OB8
52	V	203	CDL	C16-C17-C18-C19
52	k	101	CDL	CB3-CB4-CB6-OB8
52	l	702	CDL	CA3-CA4-CA6-OA8
48	l	703	PEE	C2-C3-O3-C30
52	J	404	CDL	C17-C18-C19-C20
49	J	403	PLX	C30-C31-C32-C33
49	r	501	PLX	C31-C32-C33-C34
51	X	201	8Q1	C13-C14-C15-C16
49	a	202	PLX	O6-C6-C7-C8
49	r	501	PLX	O6-C6-C7-C8
52	a	201	CDL	C23-C24-C25-C26
48	C	302	PEE	C15-C16-C17-C18
52	V	201	CDL	C59-C60-C61-C62
52	k	101	CDL	C43-C44-C45-C46
52	V	201	CDL	C19-C20-C21-C22
52	l	701	CDL	C78-C79-C80-C81
52	a	201	CDL	C82-C83-C84-C85
52	r	502	CDL	C64-C65-C66-C67
52	a	201	CDL	C71-CB7-OB8-CB6
49	J	403	PLX	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	a	201	CDL	C37-C38-C39-C40
52	I	201	CDL	CA6-CA4-OA6-CA5
52	V	201	CDL	CA6-CA4-OA6-CA5
52	l	701	CDL	C73-C74-C75-C76
52	J	404	CDL	C55-C56-C57-C58
52	r	502	CDL	C11-C12-C13-C14
52	r	502	CDL	C52-C53-C54-C55
48	j	201	PEE	C36-C37-C38-C39
52	k	101	CDL	C12-C13-C14-C15
52	l	702	CDL	C14-C15-C16-C17
52	a	201	CDL	OA5-CA3-CA4-OA6
52	k	101	CDL	OA5-CA3-CA4-OA6
52	k	101	CDL	CA5-C11-C12-C13
48	W	201	PEE	C20-C21-C22-C23
52	u	201	CDL	C72-C73-C74-C75
52	V	201	CDL	C74-C75-C76-C77
48	j	201	PEE	C44-C45-C46-C47
48	l	703	PEE	O2-C2-C3-O3
49	C	303	PLX	O6-C4-C5-O8
49	a	202	PLX	O6-C4-C5-O8
52	k	101	CDL	OB6-CB4-CB6-OB8
52	l	701	CDL	OA7-CA5-OA6-CA4
48	C	302	PEE	C13-C14-C15-C16
48	V	202	PEE	C24-C25-C26-C27
52	J	404	CDL	C54-C55-C56-C57
52	a	201	CDL	C17-C18-C19-C20
48	s	401	PEE	C38-C39-C40-C41
49	e	201	PLX	C7-C8-C9-C10
52	V	201	CDL	C44-C45-C46-C47
52	V	203	CDL	C31-C32-C33-C34
48	C	302	PEE	C42-C43-C44-C45
52	k	101	CDL	C11-C12-C13-C14
49	J	403	PLX	C12-C13-C14-C15
52	a	201	CDL	C44-C45-C46-C47
52	l	701	CDL	C63-C64-C65-C66
52	V	203	CDL	C39-C40-C41-C42
47	A	503	NAI	C3D-C4D-C5D-O5D
49	g	201	PLX	C12-C13-C14-C15
49	r	501	PLX	C12-C13-C14-C15
52	l	702	CDL	C39-C40-C41-C42
49	a	202	PLX	C34-C35-C36-C37
49	g	201	PLX	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	r	501	PLX	C16-C17-C18-C19
52	V	203	CDL	C84-C85-C86-C87
49	g	201	PLX	C17-C18-C19-C20
52	a	201	CDL	C42-C43-C44-C45
48	Q	503	PEE	C30-C31-C32-C33
52	a	201	CDL	C32-C33-C34-C35
52	r	502	CDL	C33-C34-C35-C36
52	a	201	CDL	OB9-CB7-OB8-CB6
48	l	704	PEE	C11-C12-C13-C14
52	a	201	CDL	C53-C54-C55-C56
52	l	701	CDL	C21-C22-C23-C24
48	C	302	PEE	C1-C2-C3-O3
48	l	704	PEE	C1-C2-C3-O3
49	J	403	PLX	C3-C4-C5-O8
49	a	202	PLX	C3-C4-C5-O8
49	e	201	PLX	C3-C4-C5-O8
49	j	203	PLX	C3-C4-C5-O8
49	r	501	PLX	C3-C4-C5-O8
52	V	201	CDL	CA3-CA4-CA6-OA8
52	V	203	CDL	CB3-CB4-CB6-OB8
52	r	502	CDL	CA3-CA4-CA6-OA8
51	X	201	8Q1	C11-C10-C9-C8
52	u	201	CDL	C74-C75-C76-C77
48	s	401	PEE	C4-O4P-P-O3P
49	e	201	PLX	C5-C4-O6-C6
49	e	201	PLX	C3-O4-P1-O1
52	l	701	CDL	CB3-OB5-PB2-OB2
52	r	502	CDL	C63-C64-C65-C66
52	V	201	CDL	OB5-CB3-CB4-OB6
52	k	101	CDL	C84-C85-C86-C87
48	C	302	PEE	O2-C2-C3-O3
48	V	204	PEE	O2-C2-C3-O3
48	W	201	PEE	O2-C2-C3-O3
52	V	201	CDL	OA6-CA4-CA6-OA8
52	l	701	CDL	OA6-CA4-CA6-OA8
52	l	701	CDL	OB6-CB4-CB6-OB8
52	l	702	CDL	OA6-CA4-CA6-OA8
52	r	502	CDL	OA6-CA4-CA6-OA8
48	j	202	PEE	C24-C25-C26-C27
48	C	302	PEE	C12-C13-C14-C15
49	r	501	PLX	C25-C26-C27-C28
52	V	203	CDL	C64-C65-C66-C67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	V	203	CDL	CB2-C1-CA2-OA2
52	l	702	CDL	CB2-C1-CA2-OA2
48	C	302	PEE	C41-C42-C43-C44
52	V	201	CDL	C72-C73-C74-C75
52	r	502	CDL	C17-C18-C19-C20
52	r	502	CDL	C59-C60-C61-C62
52	V	203	CDL	C1-CB2-OB2-PB2
51	G	201	8Q1	C11-C10-C9-C8
52	V	201	CDL	C54-C55-C56-C57
52	J	404	CDL	C12-C13-C14-C15
52	r	502	CDL	C44-C45-C46-C47
48	V	204	PEE	C36-C37-C38-C39
48	j	201	PEE	C13-C14-C15-C16
52	r	502	CDL	C21-C22-C23-C24
48	V	204	PEE	C11-C10-O2-C2
52	J	404	CDL	C36-C37-C38-C39
52	r	502	CDL	C74-C75-C76-C77
48	V	204	PEE	C18-C19-C20-C21
48	j	202	PEE	C34-C35-C36-C37
49	e	201	PLX	O8-C24-C25-C26
49	r	501	PLX	O8-C24-C25-C26
49	J	403	PLX	O4-C3-C4-C5
52	V	201	CDL	OB5-CB3-CB4-CB6
52	V	203	CDL	OB5-CB3-CB4-CB6
52	a	201	CDL	OA5-CA3-CA4-CA6
48	l	703	PEE	C24-C25-C26-C27
48	Q	503	PEE	C24-C25-C26-C27
52	k	101	CDL	C73-C74-C75-C76
52	l	702	CDL	C61-C62-C63-C64
52	V	201	CDL	C33-C34-C35-C36
49	C	303	PLX	C27-C28-C29-C30
49	J	403	PLX	C11-C10-C9-C8
52	l	701	CDL	C55-C56-C57-C58
52	V	201	CDL	C34-C35-C36-C37
48	l	703	PEE	C13-C14-C15-C16
52	r	502	CDL	C35-C36-C37-C38
52	k	101	CDL	C39-C40-C41-C42
52	a	201	CDL	C81-C82-C83-C84
48	W	201	PEE	C1-C2-C3-O3
48	l	703	PEE	C1-C2-C3-O3
52	l	701	CDL	CB3-CB4-CB6-OB8
52	V	201	CDL	OA5-CA3-CA4-OA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	u	201	CDL	OB5-CB3-CB4-OB6
48	j	201	PEE	C32-C33-C34-C35
52	V	201	CDL	C53-C54-C55-C56
52	l	702	CDL	CA2-C1-CB2-OB2
48	V	204	PEE	O4-C10-O2-C2
52	V	203	CDL	C24-C25-C26-C27
52	J	404	CDL	C34-C35-C36-C37
52	l	701	CDL	C54-C55-C56-C57
52	r	502	CDL	C77-C78-C79-C80
49	J	403	PLX	O6-C4-C5-O8
49	j	203	PLX	O6-C4-C5-O8
49	r	501	PLX	O6-C4-C5-O8
49	j	203	PLX	C36-C37-C38-C39
52	a	201	CDL	C64-C65-C66-C67
52	k	101	CDL	C54-C55-C56-C57
49	e	201	PLX	C9-C10-C11-C12
52	V	201	CDL	C22-C23-C24-C25
52	l	702	CDL	C40-C41-C42-C43
49	e	201	PLX	C24-C25-C26-C27
49	e	201	PLX	C18-C19-C20-C21
53	J	401	NDP	O4B-C4B-C5B-O5B
49	j	203	PLX	C9-C10-C11-C12
52	V	201	CDL	C64-C65-C66-C67
49	a	202	PLX	C29-C30-C31-C32
48	V	204	PEE	C33-C34-C35-C36
48	C	302	PEE	C4-O4P-P-O3P
48	Q	503	PEE	C1-O3P-P-O4P
48	V	204	PEE	C4-O4P-P-O3P
48	j	201	PEE	C4-O4P-P-O3P
49	r	501	PLX	C2-O1-P1-O4
53	J	401	NDP	O4D-C1D-N1N-C6N
52	a	201	CDL	C14-C15-C16-C17
52	u	201	CDL	C71-C72-C73-C74
48	V	204	PEE	C2-C1-O3P-P
52	r	502	CDL	C1-CB2-OB2-PB2
49	a	202	PLX	C16-C17-C18-C19
52	V	203	CDL	C33-C34-C35-C36
48	C	302	PEE	C4-O4P-P-O2P
48	C	302	PEE	C4-O4P-P-O1P
48	Q	503	PEE	C1-O3P-P-O1P
48	Q	503	PEE	C4-O4P-P-O2P
48	V	202	PEE	C1-O3P-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	l	703	PEE	C4-O4P-P-O2P
49	C	303	PLX	C2-O1-P1-O3
49	J	403	PLX	C2-O1-P1-O3
49	g	201	PLX	C3-O4-P1-O3
49	r	501	PLX	C3-O4-P1-O2
49	r	501	PLX	C3-O4-P1-O3
49	r	501	PLX	C2-O1-P1-O3
52	I	201	CDL	CB3-OB5-PB2-OB4
52	J	404	CDL	CB2-OB2-PB2-OB4
52	V	201	CDL	CB3-OB5-PB2-OB3
52	V	203	CDL	CB3-OB5-PB2-OB4
52	a	201	CDL	CB2-OB2-PB2-OB4
52	a	201	CDL	CB3-OB5-PB2-OB3
52	k	101	CDL	CB2-OB2-PB2-OB4
52	l	701	CDL	CA2-OA2-PA1-OA3
52	l	701	CDL	CB3-OB5-PB2-OB4
52	r	502	CDL	CA3-OA5-PA1-OA3
52	r	502	CDL	CB2-OB2-PB2-OB3
52	r	502	CDL	CB2-OB2-PB2-OB4
52	r	502	CDL	CB3-OB5-PB2-OB4
52	u	201	CDL	CA2-OA2-PA1-OA3
52	u	201	CDL	CB2-OB2-PB2-OB4
58	w	401	ADP	C5'-O5'-PA-O1A
48	Q	503	PEE	O3P-C1-C2-C3
52	J	404	CDL	OA5-CA3-CA4-CA6
52	V	201	CDL	OA5-CA3-CA4-CA6
52	k	101	CDL	OA5-CA3-CA4-CA6
52	u	201	CDL	OB5-CB3-CB4-CB6
51	G	201	8Q1	C13-C14-C15-C16
48	l	704	PEE	C5-C4-O4P-P
49	C	303	PLX	C25-C24-O8-C5
49	J	403	PLX	C1-C2-O1-P1
49	J	403	PLX	C25-C24-O8-C5
49	e	201	PLX	C32-C33-C34-C35
52	k	101	CDL	C23-C24-C25-C26
46	A	502	FMN	O2'-C2'-C3'-O3'
52	a	201	CDL	CB5-C51-C52-C53
52	J	404	CDL	CA2-C1-CB2-OB2
52	k	101	CDL	CA2-C1-CB2-OB2
52	V	201	CDL	OB7-CB5-OB6-CB4
49	e	201	PLX	C16-C17-C18-C19
52	l	702	CDL	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	J	403	PLX	O4-C3-C4-O6
52	k	101	CDL	C14-C15-C16-C17
52	r	502	CDL	C72-C71-CB7-OB8
52	V	201	CDL	C51-CB5-OB6-CB4
52	a	201	CDL	C11-CA5-OA6-CA4
52	l	701	CDL	C51-CB5-OB6-CB4
52	V	203	CDL	O1-C1-CA2-OA2
52	r	502	CDL	C15-C16-C17-C18
49	j	203	PLX	C34-C35-C36-C37
49	C	303	PLX	C3-C4-C5-O8
49	C	303	PLX	N1-C1-C2-O1
49	e	201	PLX	C26-C27-C28-C29
51	X	201	8Q1	O27-C28-C29-C32
49	e	201	PLX	O6-C4-C5-O8
52	J	404	CDL	C31-C32-C33-C34
52	V	203	CDL	C55-C56-C57-C58
52	l	701	CDL	C24-C25-C26-C27
48	Q	503	PEE	C18-C19-C20-C21
48	C	302	PEE	C20-C21-C22-C23
48	j	202	PEE	C21-C22-C23-C24
48	s	401	PEE	C24-C25-C26-C27
49	C	303	PLX	C16-C17-C18-C19
52	V	203	CDL	C83-C84-C85-C86
49	a	202	PLX	O8-C24-C25-C26
49	j	203	PLX	O6-C6-C7-C8
52	V	201	CDL	C12-C13-C14-C15
52	l	702	CDL	C38-C39-C40-C41
48	l	703	PEE	C40-C41-C42-C43
48	V	202	PEE	C34-C35-C36-C37
48	W	201	PEE	C10-C11-C12-C13
48	V	204	PEE	C30-C31-C32-C33
52	I	201	CDL	CA2-C1-CB2-OB2
52	u	201	CDL	CB2-C1-CA2-OA2
49	r	501	PLX	C19-C20-C21-C22
48	W	201	PEE	O4-C10-O2-C2
52	l	701	CDL	OB7-CB5-OB6-CB4
52	V	203	CDL	C77-C78-C79-C80
48	Q	503	PEE	C16-C17-C18-C19
48	l	704	PEE	C2-C1-O3P-P
52	a	201	CDL	OA7-CA5-OA6-CA4
52	I	201	CDL	C51-C52-C53-C54
52	V	201	CDL	C36-C37-C38-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	W	201	PEE	C11-C10-O2-C2
48	l	704	PEE	O2-C2-C3-O3
52	k	101	CDL	C44-C45-C46-C47
48	V	202	PEE	C4-O4P-P-O3P
48	V	204	PEE	C1-O3P-P-O4P
48	j	201	PEE	C1-O3P-P-O4P
48	l	704	PEE	C4-O4P-P-O3P
49	C	303	PLX	C3-O4-P1-O1
49	a	202	PLX	C3-O4-P1-O1
52	J	404	CDL	CB3-OB5-PB2-OB2
52	V	201	CDL	CA2-OA2-PA1-OA5
52	V	203	CDL	CA2-OA2-PA1-OA5
52	V	203	CDL	CB2-OB2-PB2-OB5
52	k	101	CDL	CA2-OA2-PA1-OA5
48	j	201	PEE	C23-C24-C25-C26
47	A	503	NAI	O4D-C1D-N1N-C2N
52	l	702	CDL	C12-C13-C14-C15
51	X	201	8Q1	C6-C7-C8-C9
52	l	702	CDL	CB7-C71-C72-C73
49	a	202	PLX	C35-C36-C37-C38
52	k	101	CDL	CA4-CA3-OA5-PA1
48	V	202	PEE	O4-C10-O2-C2
52	a	201	CDL	C18-C19-C20-C21
52	r	502	CDL	C13-C14-C15-C16
52	V	203	CDL	CA7-C31-C32-C33
49	e	201	PLX	C17-C18-C19-C20
48	Q	503	PEE	C12-C13-C14-C15
49	C	303	PLX	C9-C10-C11-C12
49	C	303	PLX	C26-C27-C28-C29
48	Q	503	PEE	C14-C15-C16-C17
52	a	201	CDL	OB5-CB3-CB4-OB6
52	l	702	CDL	OA5-CA3-CA4-OA6
52	V	201	CDL	C43-C44-C45-C46
48	j	201	PEE	C33-C34-C35-C36
52	V	203	CDL	C53-C54-C55-C56
52	J	404	CDL	C84-C85-C86-C87
49	g	201	PLX	C6-C7-C8-C9
48	j	202	PEE	O2-C2-C3-O3
52	J	404	CDL	C56-C57-C58-C59
47	A	503	NAI	C2D-C1D-N1N-C2N
49	J	403	PLX	C36-C37-C38-C39
52	J	404	CDL	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	j	203	PLX	C28-C29-C30-C31
48	l	703	PEE	C1-C2-O2-C10
52	k	101	CDL	CA6-CA4-OA6-CA5
49	J	403	PLX	C28-C29-C30-C31
52	k	101	CDL	C76-C77-C78-C79
49	J	403	PLX	C19-C20-C21-C22
49	j	203	PLX	C25-C26-C27-C28
52	l	702	CDL	C53-C54-C55-C56
52	J	404	CDL	C72-C71-CB7-OB8
49	r	501	PLX	C4-C3-O4-P1
52	V	201	CDL	CA4-CA3-OA5-PA1
52	l	701	CDL	CB4-CB3-OB5-PB2
48	j	201	PEE	C11-C12-C13-C14
52	a	201	CDL	C61-C62-C63-C64
52	l	701	CDL	OA5-CA3-CA4-OA6
50	C	304	UQ	C6-C7-C8-C9
56	Q	502	UQ1	C6-C7-C8-C9
52	u	201	CDL	C55-C56-C57-C58
52	a	201	CDL	C56-C57-C58-C59
48	j	202	PEE	C32-C33-C34-C35
49	g	201	PLX	C15-C16-C17-C18
49	e	201	PLX	C15-C16-C17-C18
49	e	201	PLX	C31-C32-C33-C34
51	X	201	8Q1	C42-C43-S44-C1
52	k	101	CDL	OA6-CA4-CA6-OA8
52	u	201	CDL	OB6-CB4-CB6-OB8
52	a	201	CDL	C84-C85-C86-C87
48	W	201	PEE	C22-C23-C24-C25
48	j	201	PEE	C43-C44-C45-C46
52	l	702	CDL	C22-C23-C24-C25
48	j	201	PEE	C37-C38-C39-C40
48	Q	503	PEE	C11-C12-C13-C14
48	l	704	PEE	C38-C39-C40-C41
52	l	701	CDL	C12-C11-CA5-OA6
48	C	302	PEE	C44-C45-C46-C47
52	V	201	CDL	C32-C31-CA7-OA8
49	j	203	PLX	C24-C25-C26-C27
48	j	202	PEE	C18-C19-C20-C21
48	Q	503	PEE	O3P-C1-C2-O2
48	s	401	PEE	O3P-C1-C2-O2
49	e	201	PLX	C36-C37-C38-C39
52	V	201	CDL	CA7-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	V	203	CDL	C18-C19-C20-C21
52	r	502	CDL	OB5-CB3-CB4-CB6
51	X	201	8Q1	O33-C32-C34-O35
49	C	303	PLX	C15-C16-C17-C18
52	V	203	CDL	C13-C14-C15-C16
52	I	201	CDL	OB6-CB4-CB6-OB8
48	V	202	PEE	O2-C10-C11-C12
46	A	502	FMN	C5'-O5'-P-O3P
51	X	201	8Q1	O33-C32-C34-N36
49	r	501	PLX	C36-C37-C38-C39
51	X	201	8Q1	O27-C28-C29-C31
52	k	101	CDL	CB5-C51-C52-C53
52	J	404	CDL	OB9-CB7-OB8-CB6
48	V	202	PEE	C16-C17-C18-C19
48	l	703	PEE	C3-C2-O2-C10
48	l	703	PEE	C10-C11-C12-C13
49	a	202	PLX	C30-C31-C32-C33
52	l	701	CDL	C39-C40-C41-C42
48	V	204	PEE	C16-C17-C18-C19
48	W	201	PEE	C18-C19-C20-C21
48	j	201	PEE	C16-C17-C18-C19
48	s	401	PEE	C18-C19-C20-C21
48	V	204	PEE	C1-C2-C3-O3
49	j	203	PLX	C7-C6-O6-C4
52	l	701	CDL	CA3-CA4-CA6-OA8
52	I	201	CDL	OA5-CA3-CA4-OA6
52	r	502	CDL	OB5-CB3-CB4-OB6
48	W	201	PEE	C17-C18-C19-C20
52	a	201	CDL	C38-C39-C40-C41
52	u	201	CDL	C51-C52-C53-C54
52	J	404	CDL	C74-C75-C76-C77
49	J	403	PLX	C24-C25-C26-C27
50	J	402	UQ	C22-C23-C24-C25
48	C	302	PEE	C18-C19-C20-C21
48	C	302	PEE	C36-C37-C38-C39
48	l	703	PEE	C18-C19-C20-C21
48	l	703	PEE	C16-C17-C18-C19
52	a	201	CDL	OB5-CB3-CB4-CB6
52	l	702	CDL	OA5-CA3-CA4-CA6
48	V	202	PEE	C22-C23-C24-C25
52	V	203	CDL	C71-C72-C73-C74
52	a	201	CDL	C41-C42-C43-C44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	a	201	CDL	C12-C11-CA5-OA6
49	j	203	PLX	C29-C30-C31-C32
49	j	203	PLX	C32-C33-C34-C35
48	V	204	PEE	C38-C39-C40-C41
52	V	203	CDL	C52-C51-CB5-OB6
49	C	303	PLX	O9-C24-C25-C26
53	J	401	NDP	C2B-O2B-P2B-O2X
48	V	202	PEE	C11-C10-O2-C2
48	Q	503	PEE	C2-C1-O3P-P
48	Q	503	PEE	C38-C39-C40-C41
48	l	703	PEE	C36-C37-C38-C39
52	I	201	CDL	C72-C71-CB7-OB8
52	J	404	CDL	O1-C1-CB2-OB2
58	w	401	ADP	PB-O3A-PA-O2A
48	V	202	PEE	C41-C42-C43-C44
48	C	302	PEE	C37-C38-C39-C40
52	V	203	CDL	C19-C20-C21-C22
52	l	702	CDL	C18-C19-C20-C21
48	s	401	PEE	O2-C10-C11-C12
52	k	101	CDL	C41-C42-C43-C44
48	W	201	PEE	C16-C17-C18-C19
52	J	404	CDL	C71-CB7-OB8-CB6
49	a	202	PLX	C10-C11-C12-C13
52	a	201	CDL	C12-C13-C14-C15
52	r	502	CDL	C53-C54-C55-C56
48	j	202	PEE	C1-C2-C3-O3
48	l	703	PEE	C14-C15-C16-C17
52	l	701	CDL	C84-C85-C86-C87
48	V	204	PEE	C32-C33-C34-C35
52	l	702	CDL	C13-C14-C15-C16
52	u	201	CDL	O1-C1-CB2-OB2
52	V	203	CDL	C52-C51-CB5-OB7
52	J	404	CDL	C19-C20-C21-C22
52	V	203	CDL	C82-C83-C84-C85
48	V	202	PEE	C30-C31-C32-C33
48	V	202	PEE	O4-C10-C11-C12
48	V	202	PEE	C1-O3P-P-O2P
48	l	704	PEE	C4-O4P-P-O1P
48	s	401	PEE	C1-O3P-P-O1P
49	J	403	PLX	C2-C1-N1-C1A
49	e	201	PLX	C2-C1-N1-C1C
49	e	201	PLX	C2-C1-N1-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	e	201	PLX	C2-C1-N1-C1A
52	J	404	CDL	CB3-OB5-PB2-OB3
52	V	201	CDL	CA2-OA2-PA1-OA3
52	V	201	CDL	CA3-OA5-PA1-OA3
52	l	701	CDL	CA3-OA5-PA1-OA3
52	r	502	CDL	CA5-C11-C12-C13
49	e	201	PLX	C30-C31-C32-C33
49	a	202	PLX	O4-C3-C4-C5
48	V	202	PEE	C12-C13-C14-C15
48	j	202	PEE	O3-C30-C31-C32
52	V	201	CDL	C21-C22-C23-C24
48	s	401	PEE	C20-C21-C22-C23
49	a	202	PLX	C25-C24-O8-C5
49	j	203	PLX	C25-C24-O8-C5
52	J	404	CDL	CA6-CA4-OA6-CA5
52	I	201	CDL	C72-C71-CB7-OB9
49	a	202	PLX	C19-C20-C21-C22
52	l	701	CDL	C72-C71-CB7-OB8
48	V	202	PEE	C15-C16-C17-C18
52	k	101	CDL	C12-C11-CA5-OA6
51	G	201	8Q1	C6-C7-C8-C9
50	C	304	UQ	C25-C24-C26-C27
49	e	201	PLX	O4-C3-C4-O6
52	l	701	CDL	C52-C51-CB5-OB6
52	a	201	CDL	C32-C31-CA7-OA8
48	s	401	PEE	C41-C42-C43-C44
49	r	501	PLX	C6-C7-C8-C9
52	l	701	CDL	C33-C34-C35-C36
52	a	201	CDL	C12-C11-CA5-OA7
52	l	701	CDL	C72-C71-CB7-OB9
52	r	502	CDL	C23-C24-C25-C26
48	l	703	PEE	C38-C39-C40-C41

There are no ring outliers.

23 monomers are involved in 96 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	J	403	PLX	2	0
50	C	304	UQ	5	0
52	V	203	CDL	4	0
52	I	201	CDL	2	0
51	G	201	8Q1	4	0

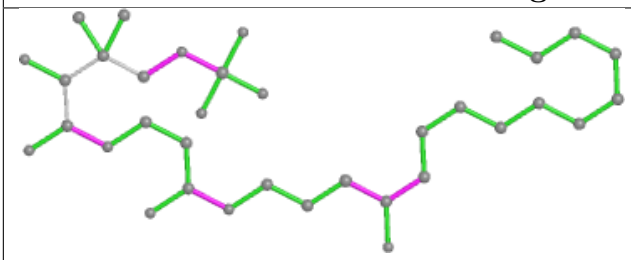
Continued on next page...

Continued from previous page...

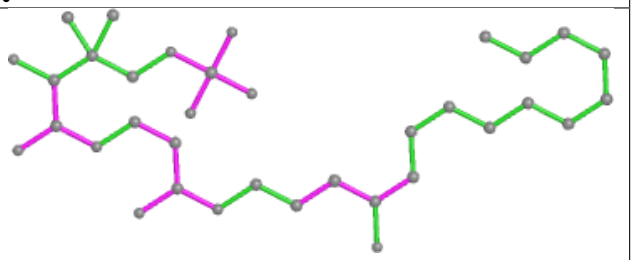
Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	O	301	FES	3	0
48	W	201	PEE	6	0
48	V	204	PEE	5	0
45	A	501	SF4	2	0
45	M	802	SF4	3	0
45	C	301	SF4	1	0
52	V	201	CDL	4	0
47	A	503	NAI	4	0
48	C	302	PEE	5	0
56	Q	501	UQ1	4	0
46	A	502	FMN	3	0
56	Q	502	UQ1	4	0
48	V	202	PEE	3	0
50	J	402	UQ	13	0
52	J	404	CDL	6	0
48	Q	503	PEE	11	0
49	C	303	PLX	7	0
53	J	401	NDP	1	0

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

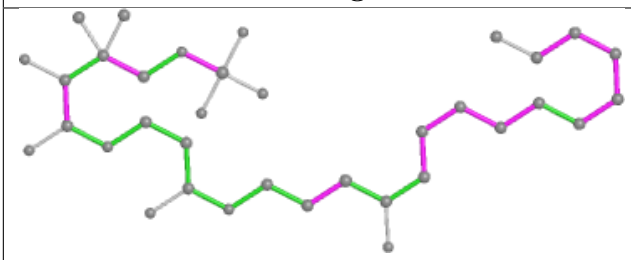
Ligand 8Q1 X 201



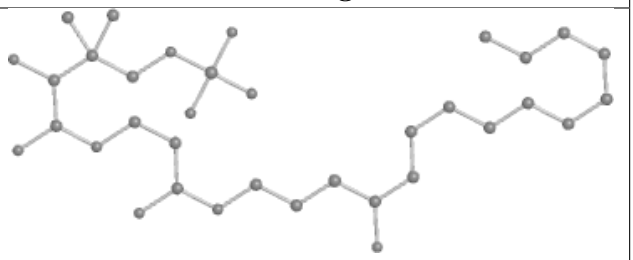
Bond lengths



Bond angles

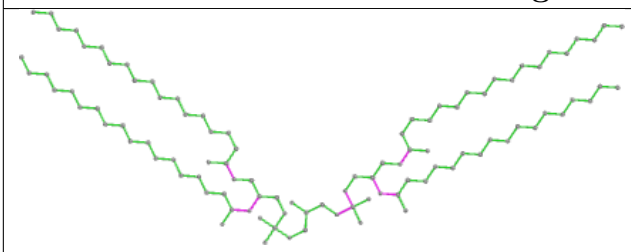


Torsions

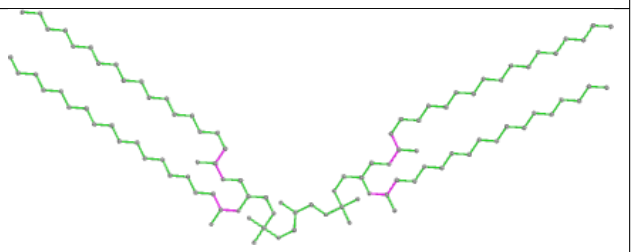


Rings

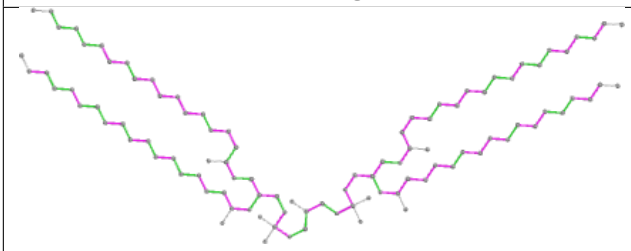
Ligand CDL l 701



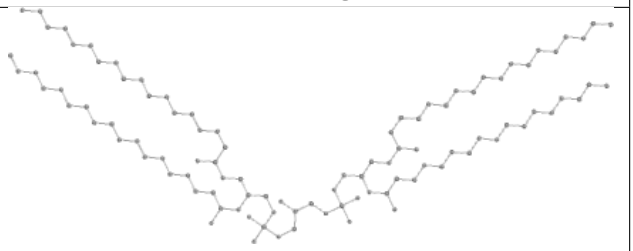
Bond lengths



Bond angles

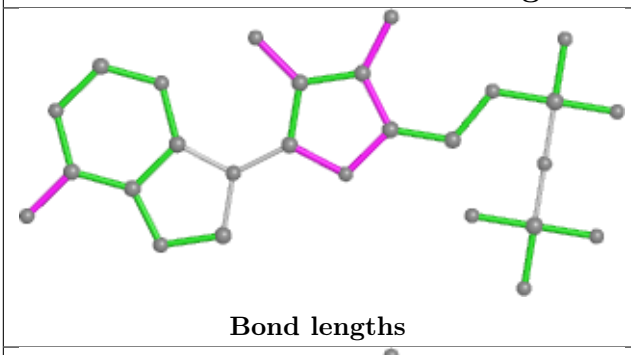


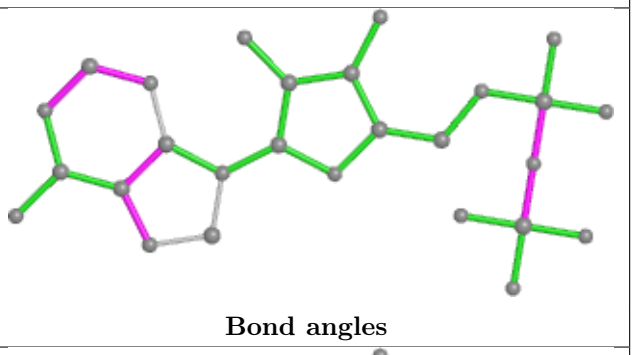
Torsions

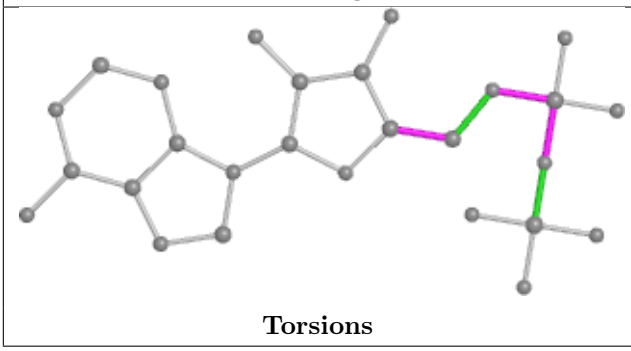


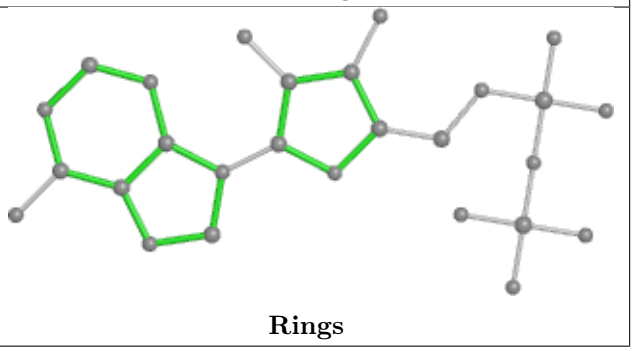
Rings

Ligand ADP w 401

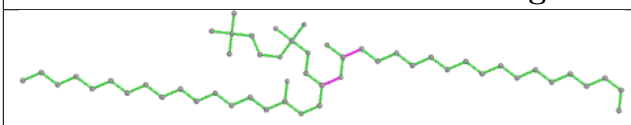

Bond lengths

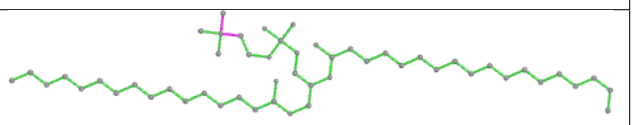

Bond angles

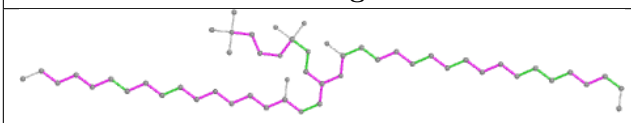

Torsions

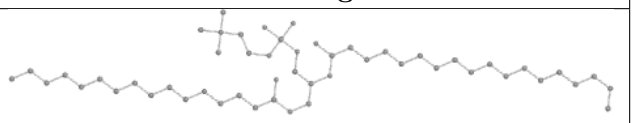

Rings

Ligand PLX J 403

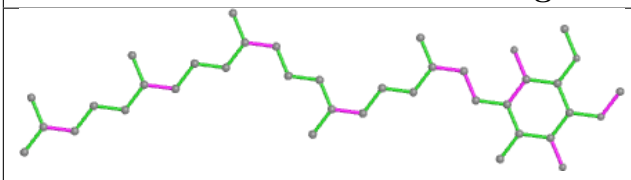

Bond lengths

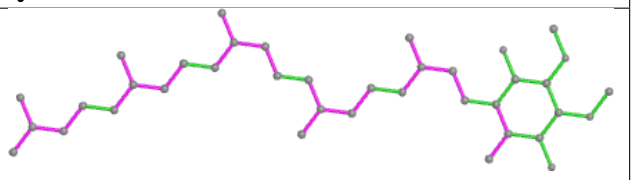

Bond angles

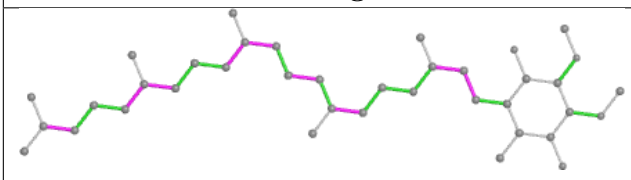

Torsions

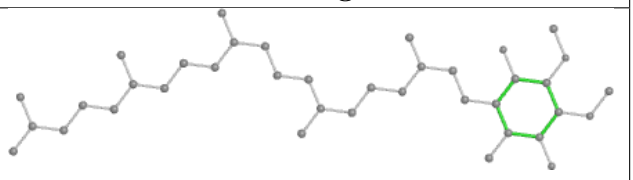

Rings

Ligand UQ C 304

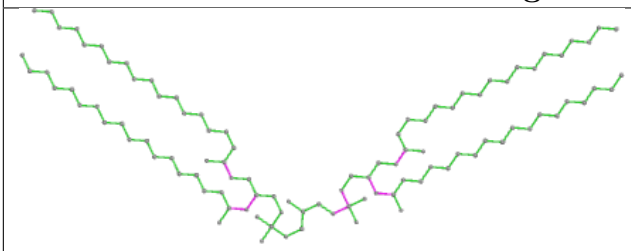

Bond lengths


Bond angles

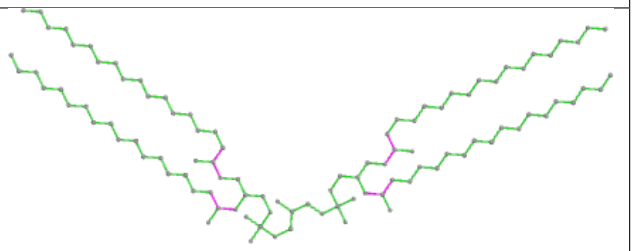

Torsions


Rings

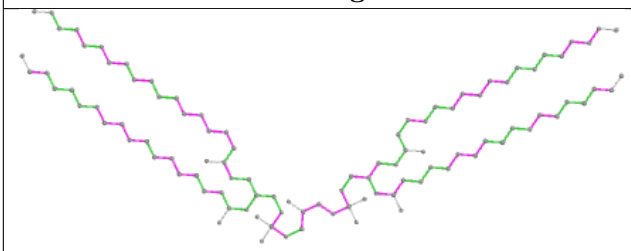
Ligand CDL V 203



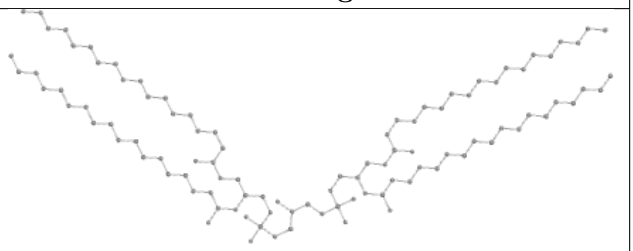
Bond lengths



Bond angles

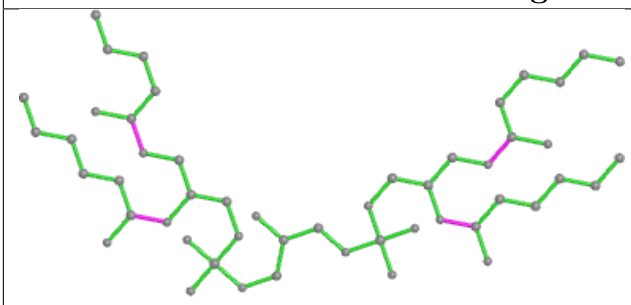


Torsions

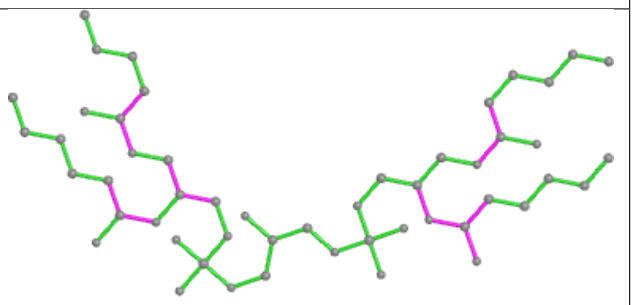


Rings

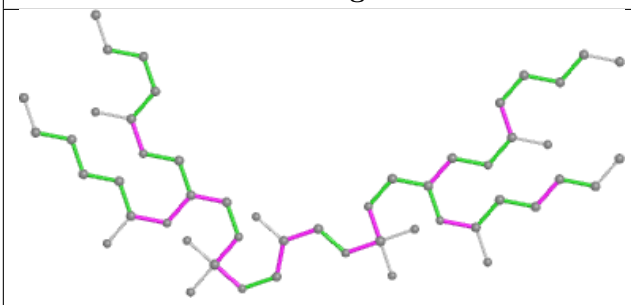
Ligand CDL I 201



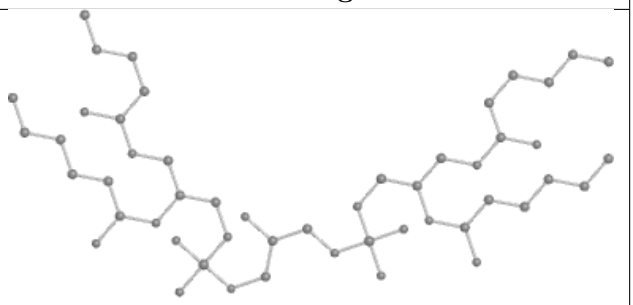
Bond lengths



Bond angles

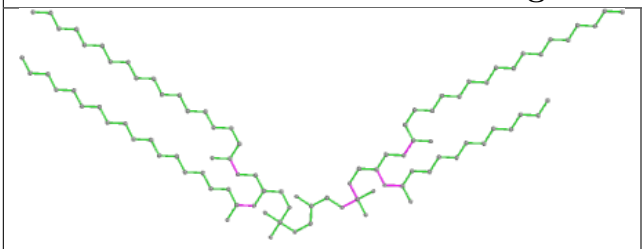


Torsions

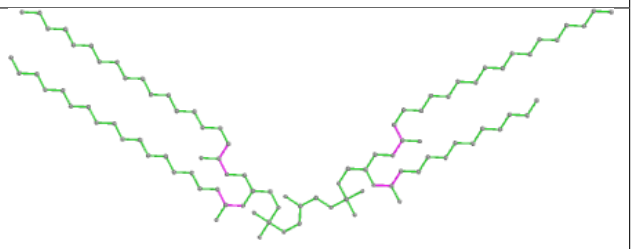


Rings

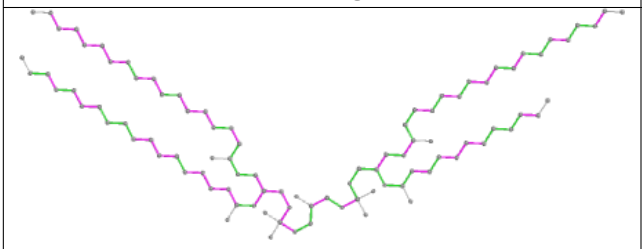
Ligand CDL k 101



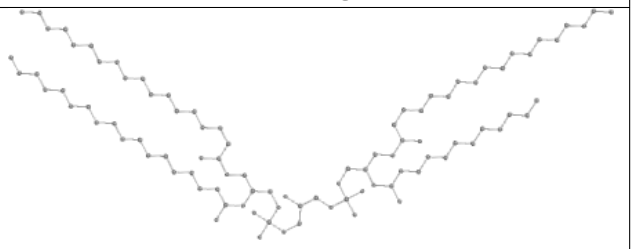
Bond lengths



Bond angles

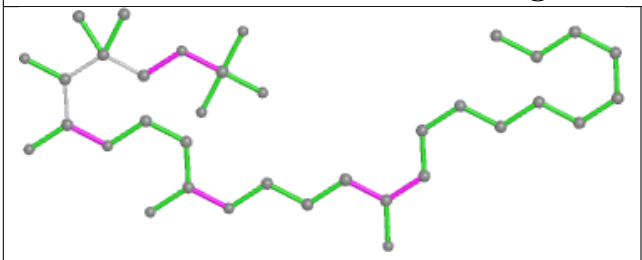


Torsions

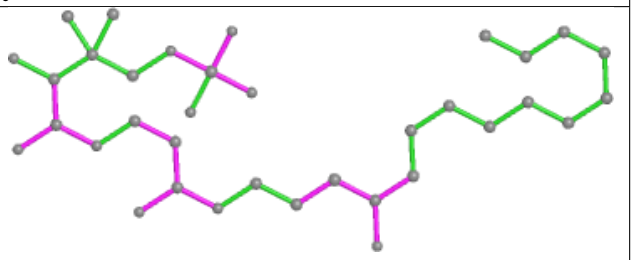


Rings

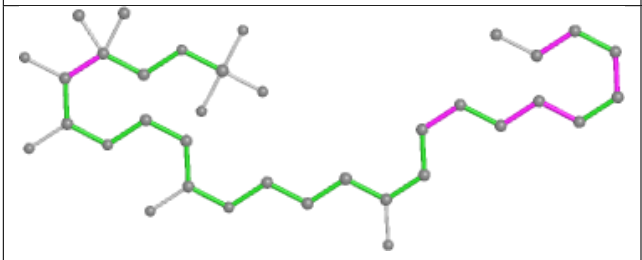
Ligand 8Q1 G 201



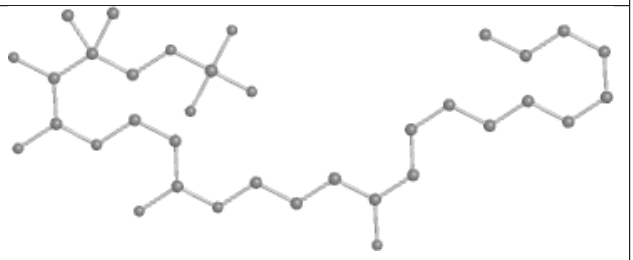
Bond lengths



Bond angles

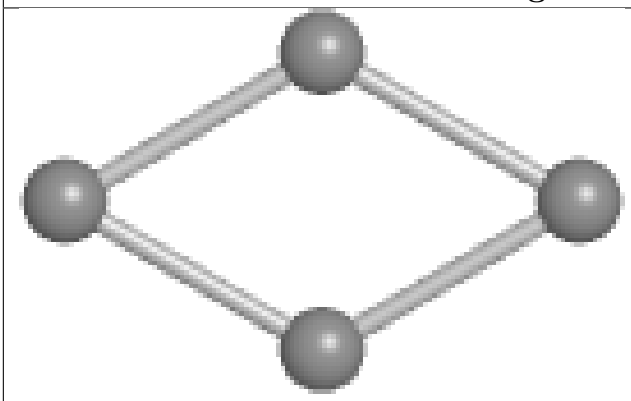


Torsions

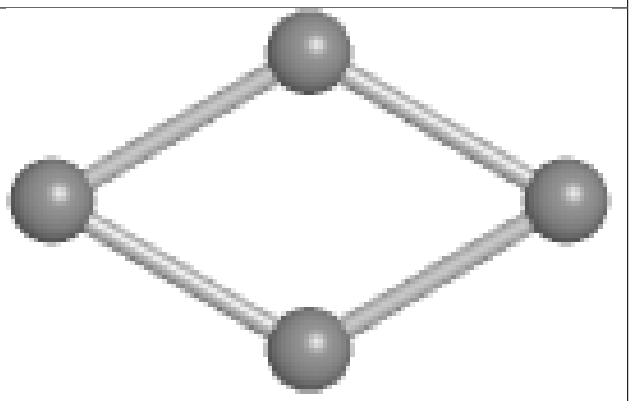


Rings

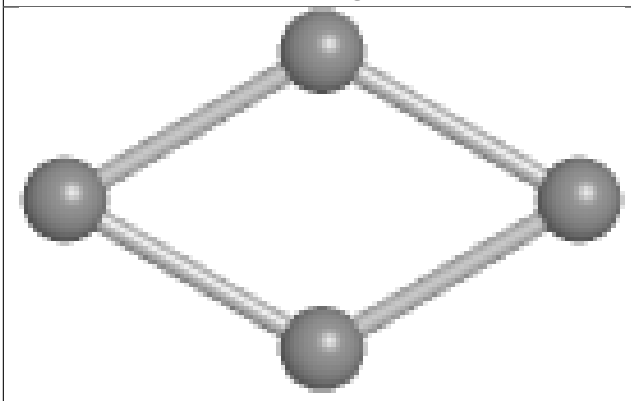
Ligand FES O 301



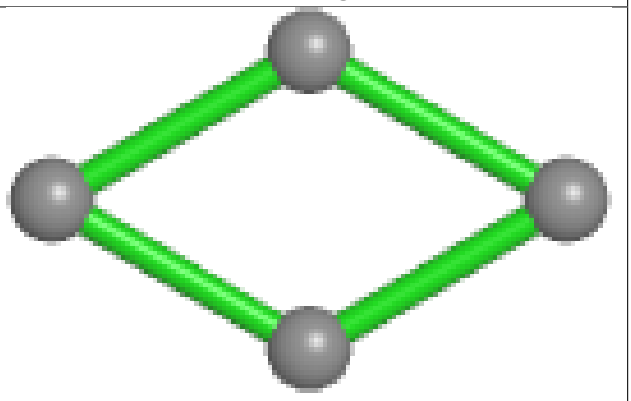
Bond lengths



Bond angles



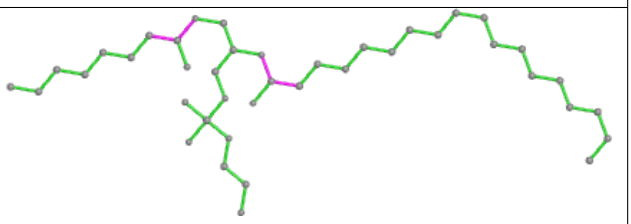
Torsions



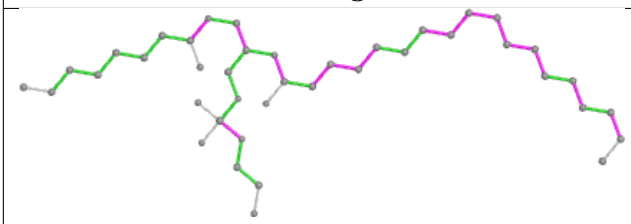
Rings

Ligand PEE W 201

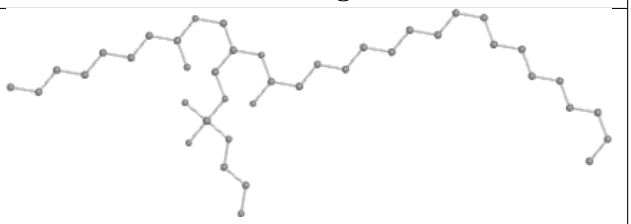
Bond lengths



Bond angles

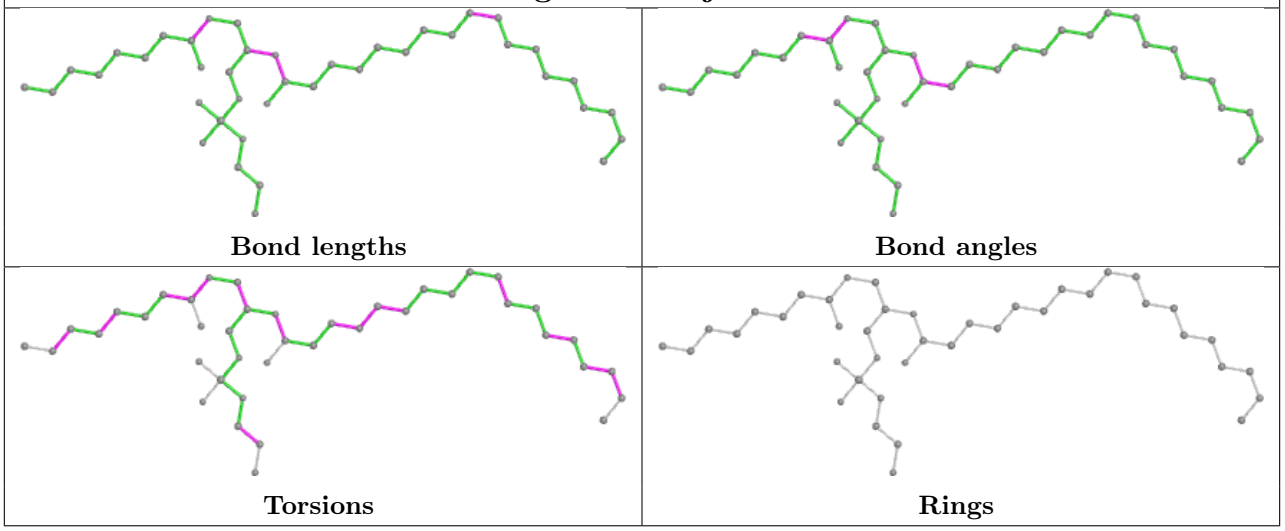


Torsions

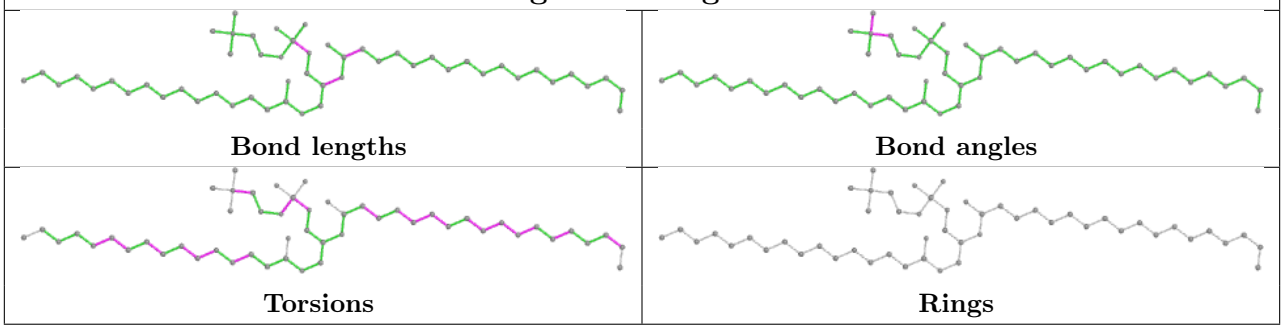


Rings

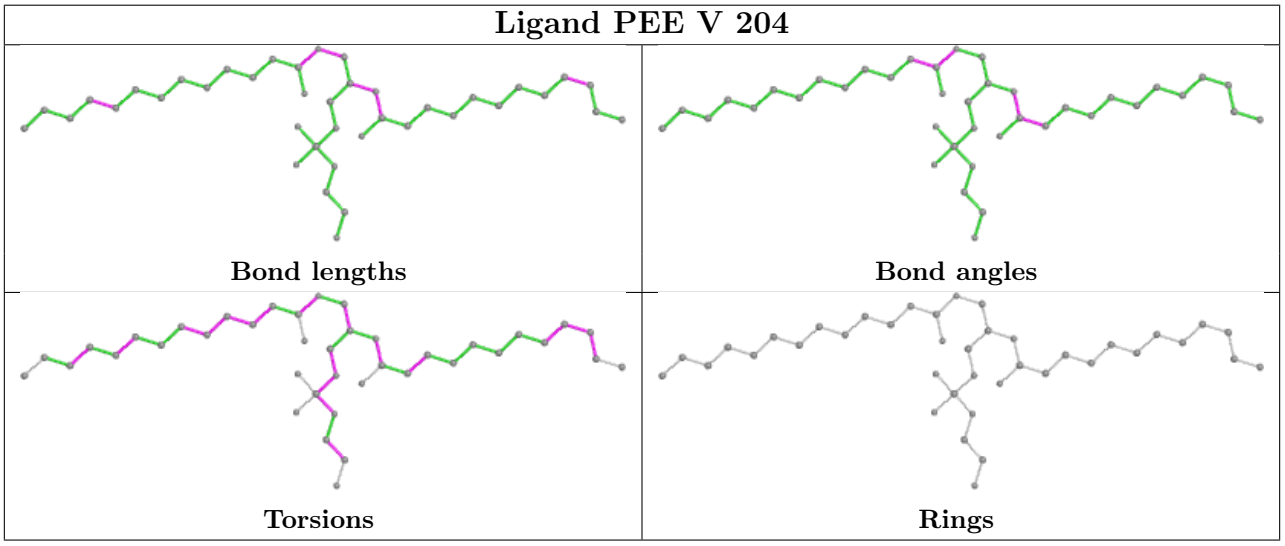
Ligand PEE j 202



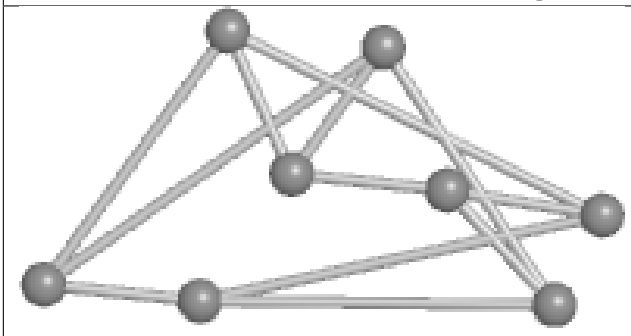
Ligand PLX g 201



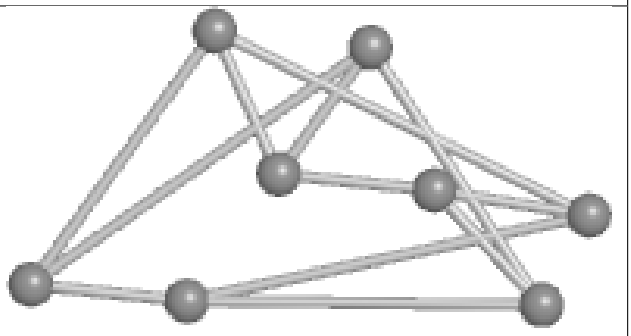
Ligand PEE V 204



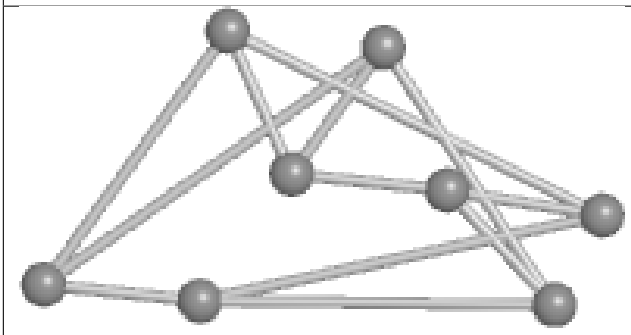
Ligand SF4 A 501



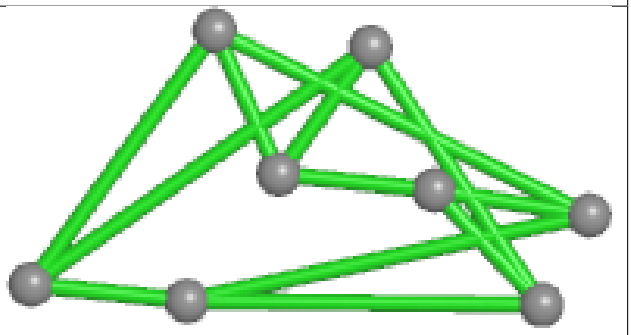
Bond lengths



Bond angles

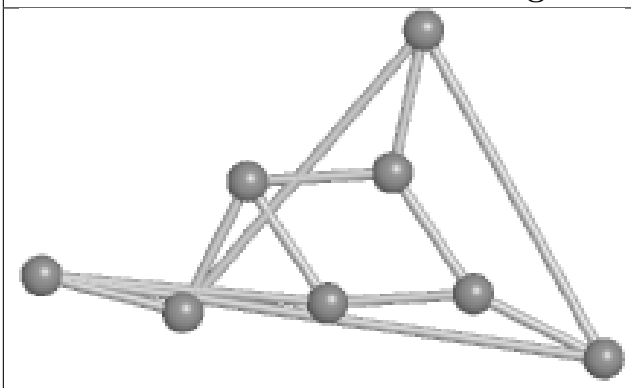


Torsions

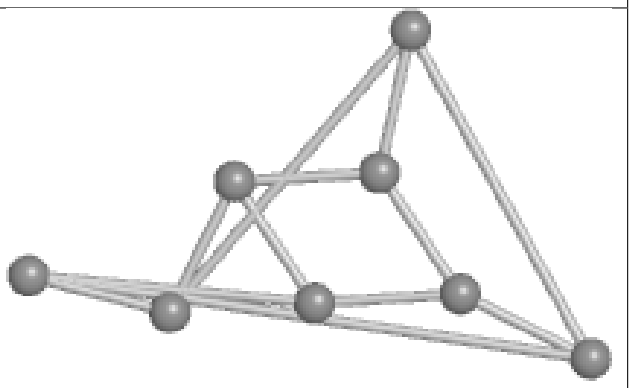


Rings

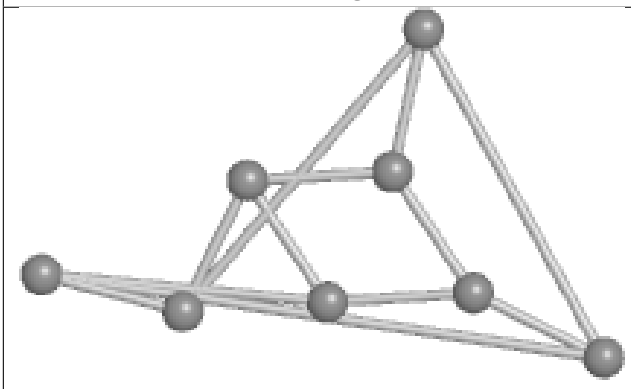
Ligand SF4 M 802



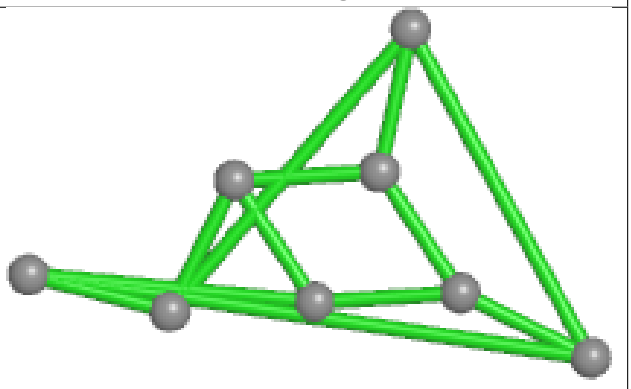
Bond lengths



Bond angles

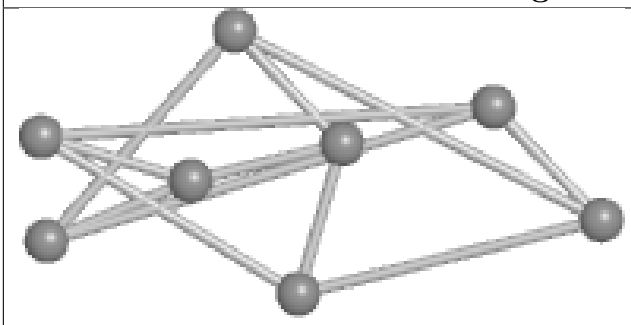


Torsions

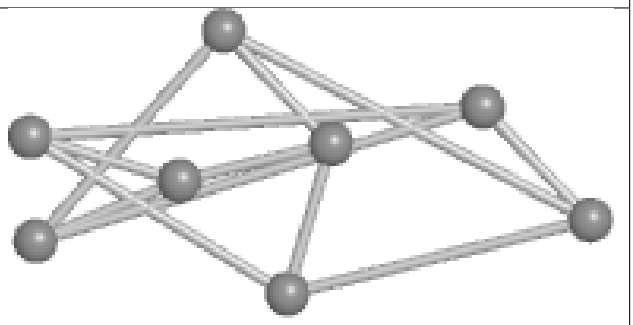


Rings

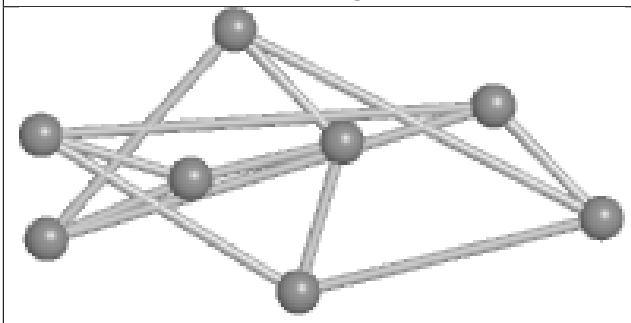
Ligand SF4 B 301



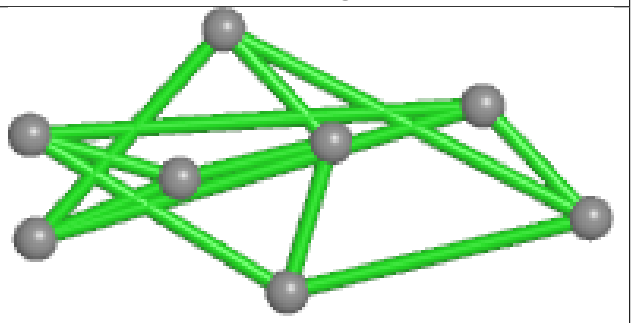
Bond lengths



Bond angles

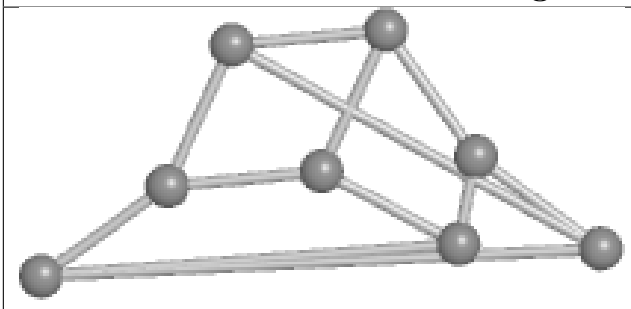


Torsions

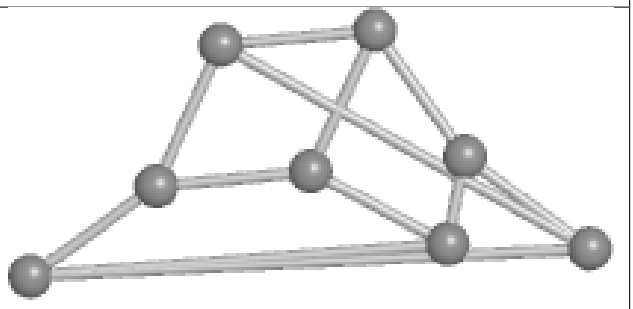


Rings

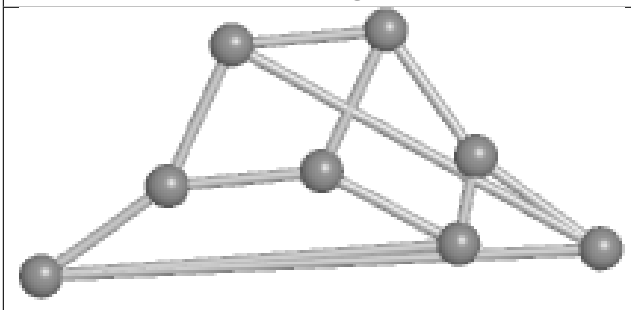
Ligand SF4 C 301



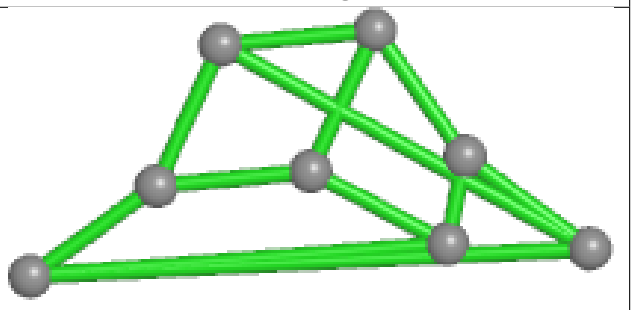
Bond lengths



Bond angles

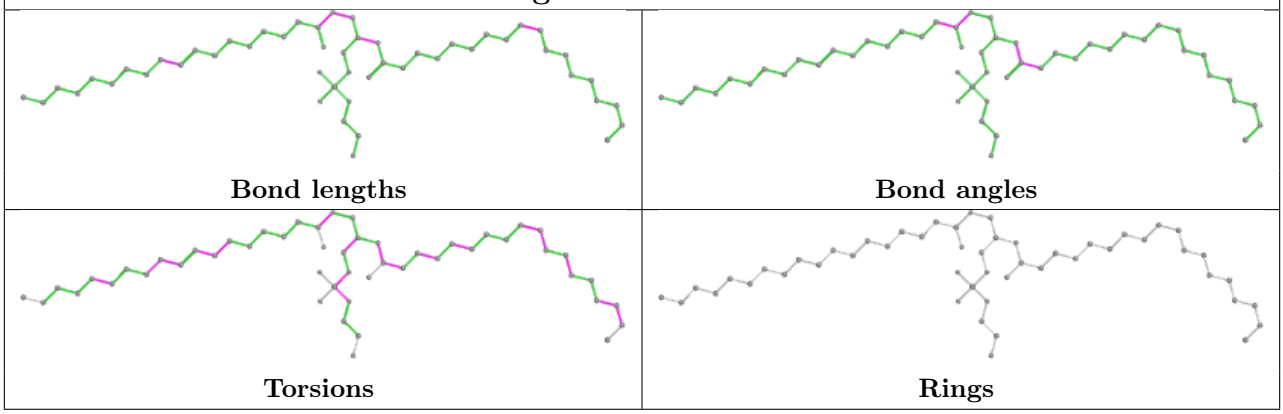


Torsions

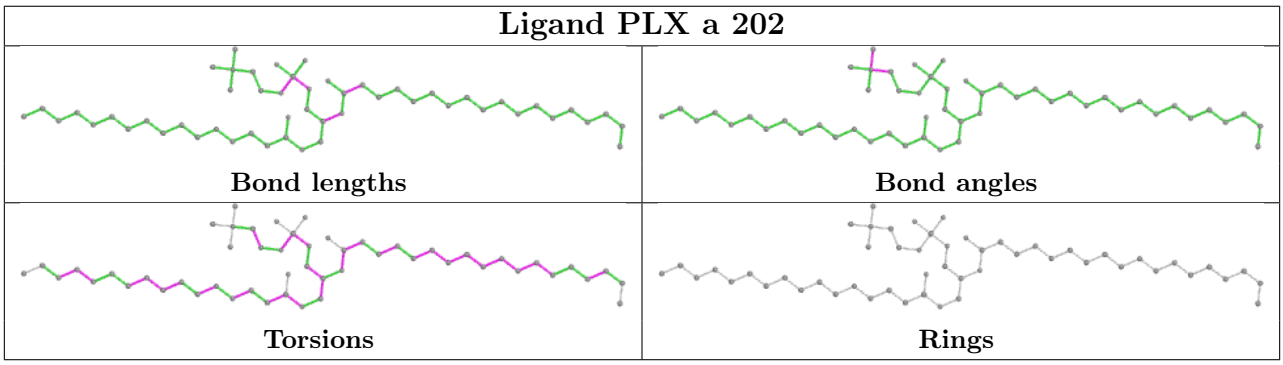


Rings

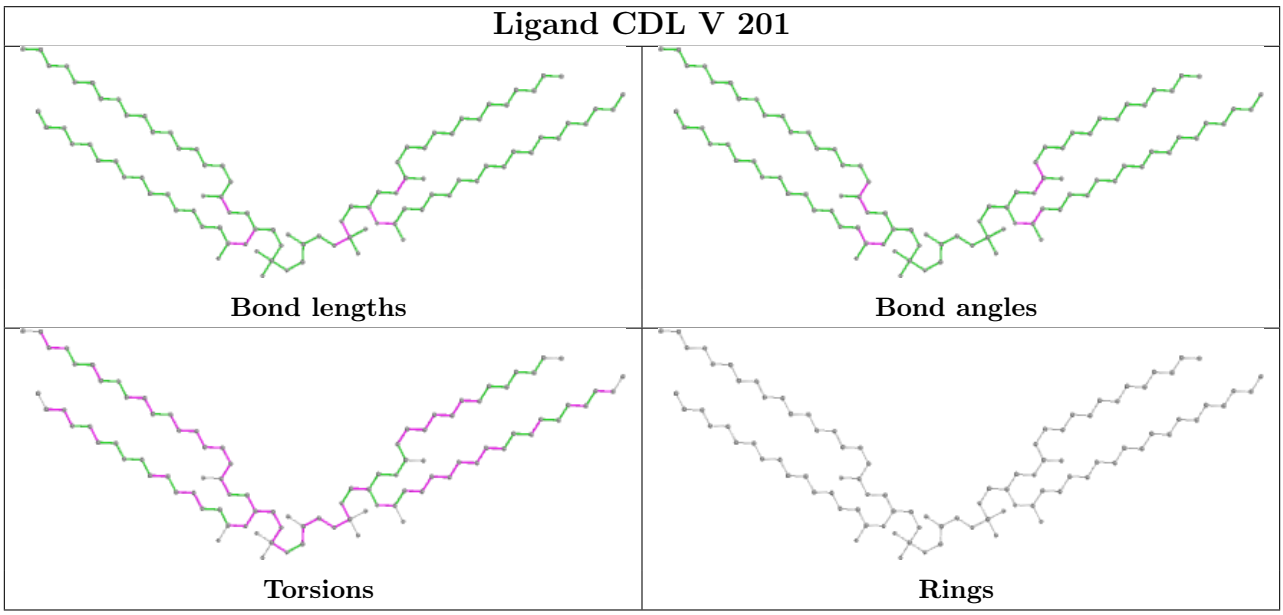
Ligand PEE s 401



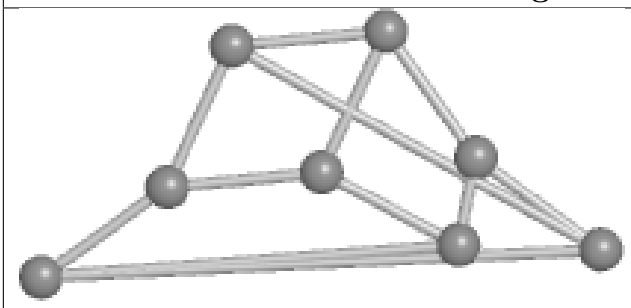
Ligand PLX a 202



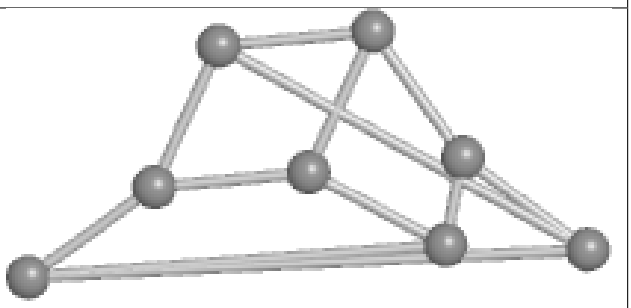
Ligand CDL V 201



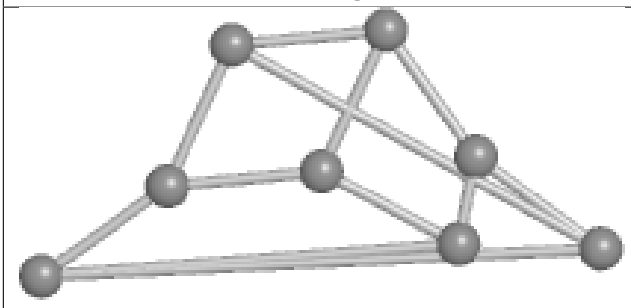
Ligand SF4 B 302



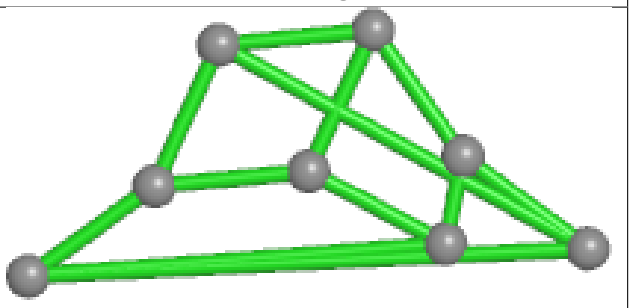
Bond lengths



Bond angles

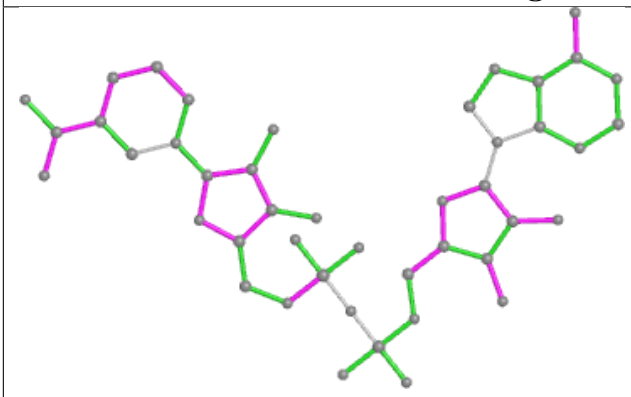


Torsions

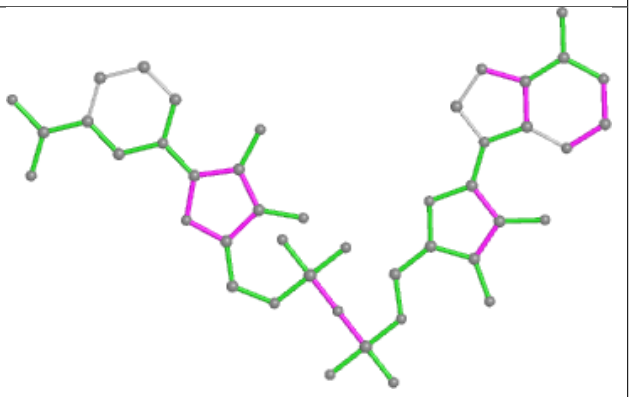


Rings

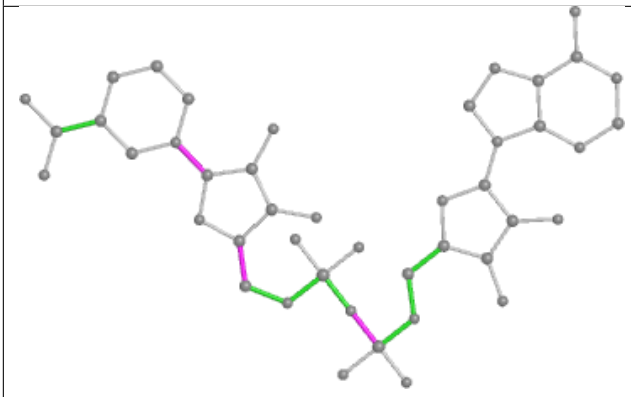
Ligand NAI A 503



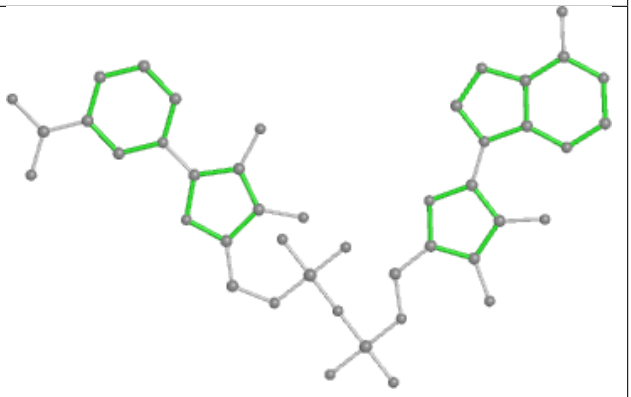
Bond lengths



Bond angles

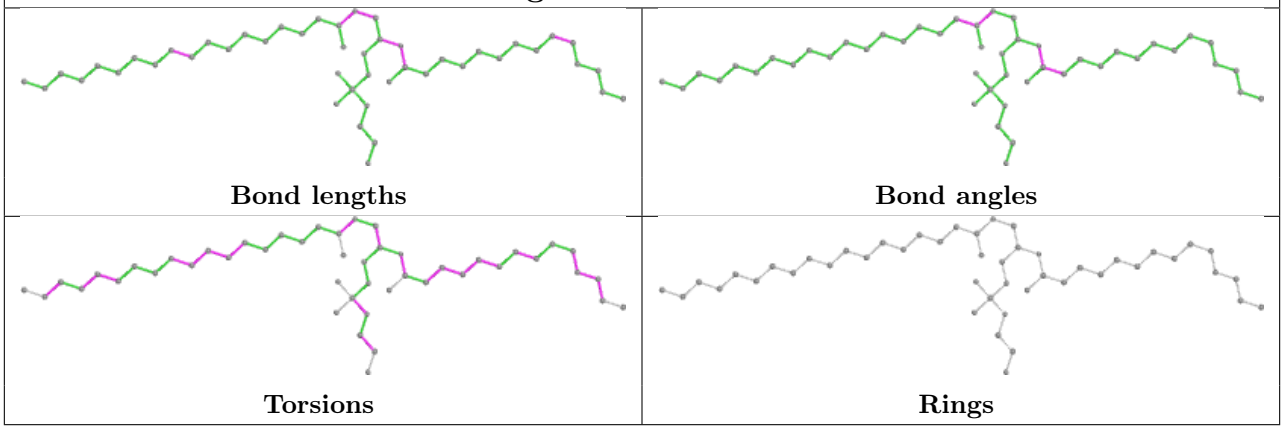


Torsions

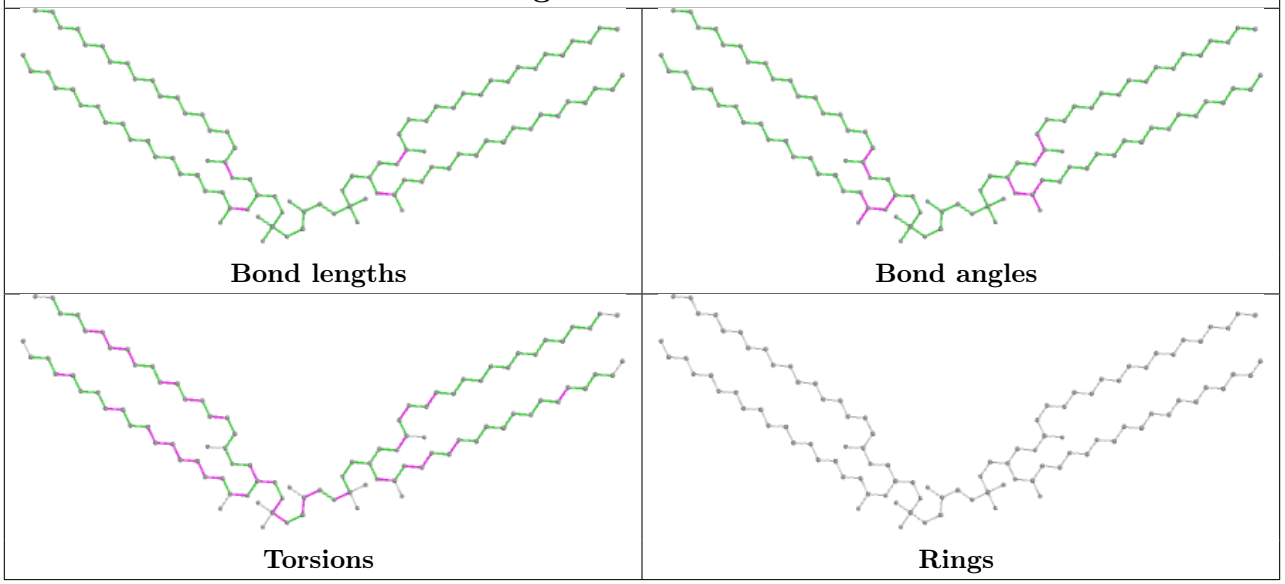


Rings

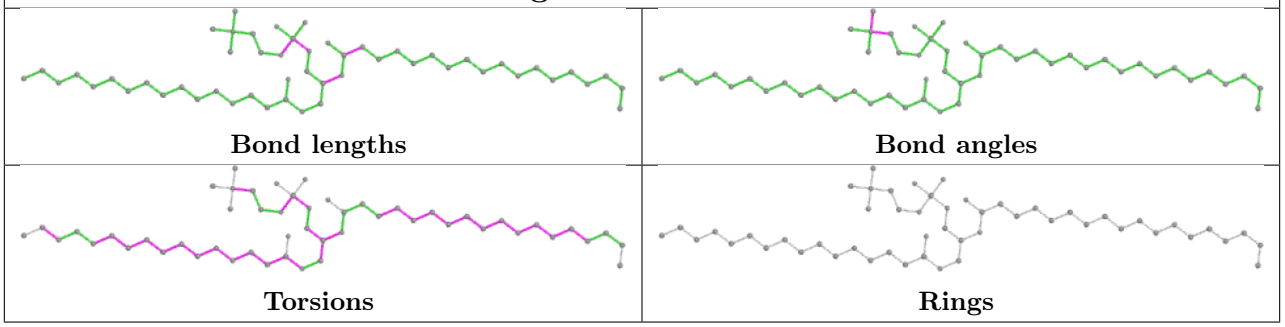
Ligand PEE C 302



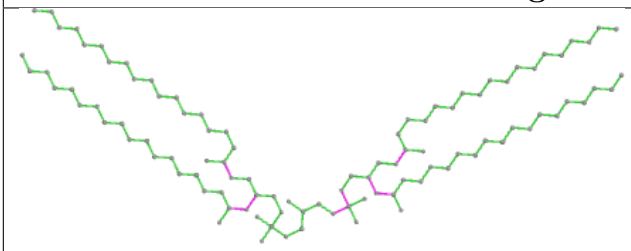
Ligand CDL l 702



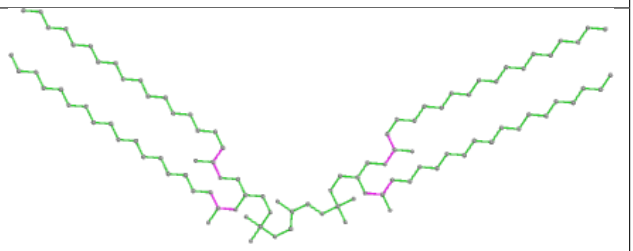
Ligand PLX e 201



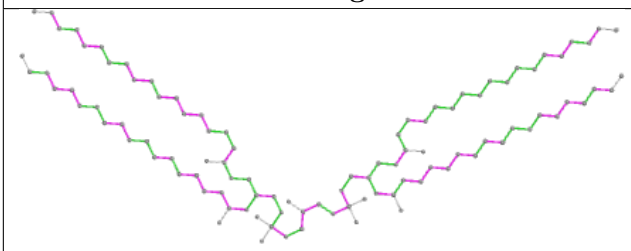
Ligand CDL a 201



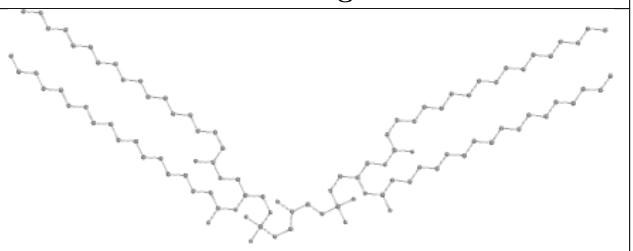
Bond lengths



Bond angles

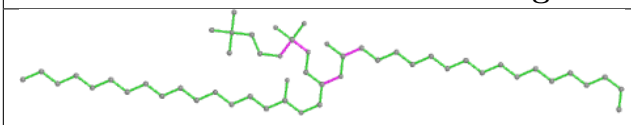


Torsions

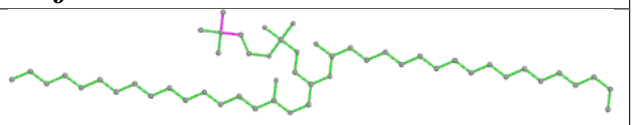


Rings

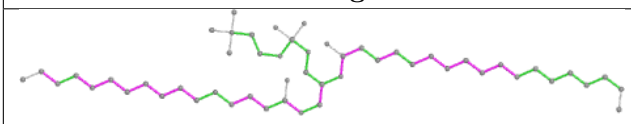
Ligand PLX j 203



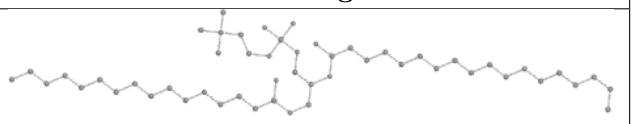
Bond lengths



Bond angles

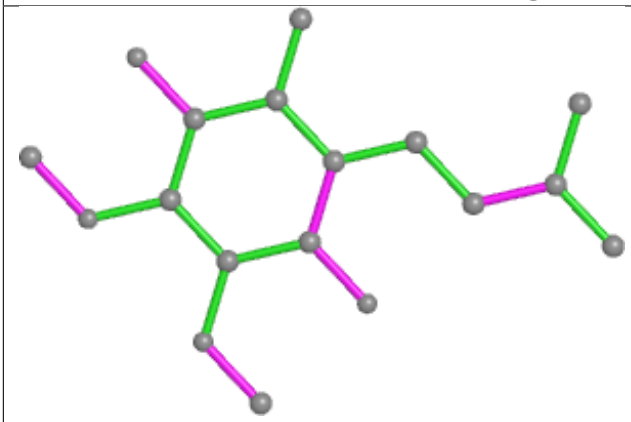


Torsions

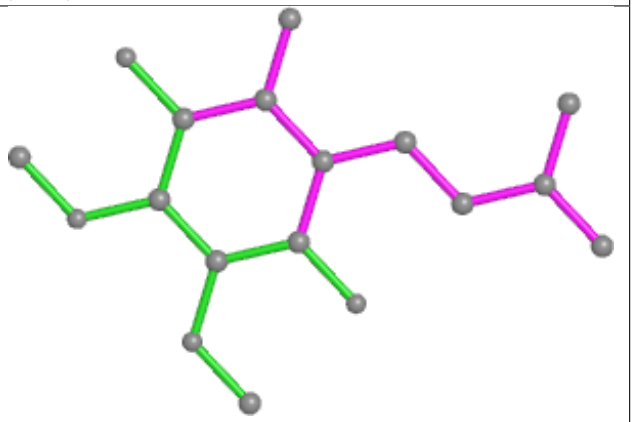


Rings

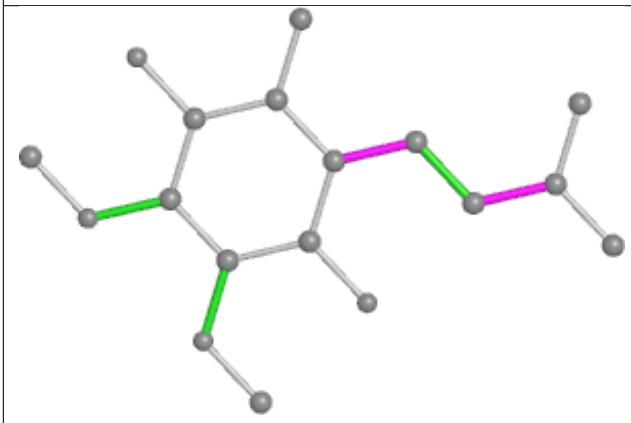
Ligand UQ1 Q 501



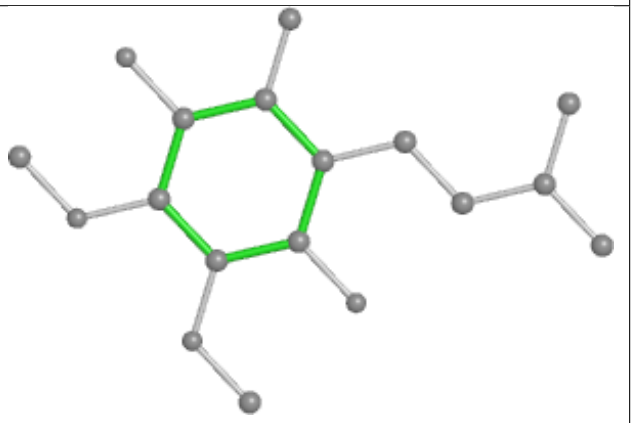
Bond lengths



Bond angles

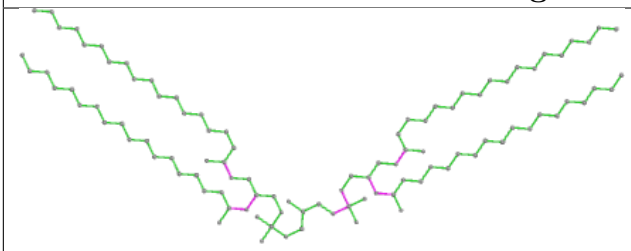


Torsions

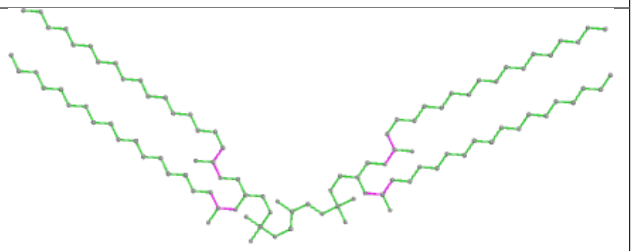


Rings

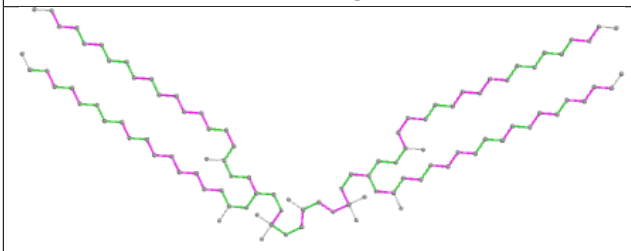
Ligand CDL r 502



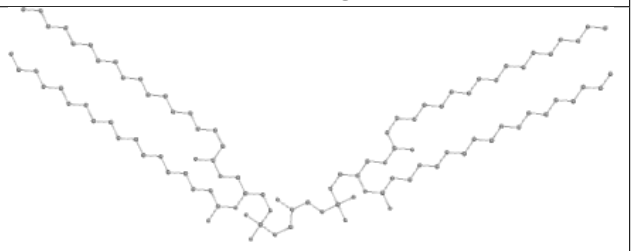
Bond lengths



Bond angles

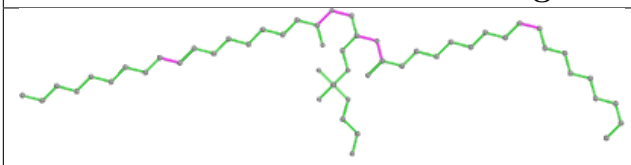


Torsions

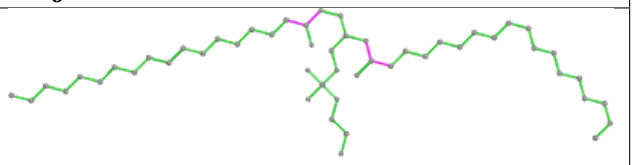


Rings

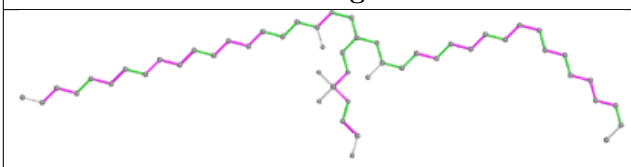
Ligand PEE j 201



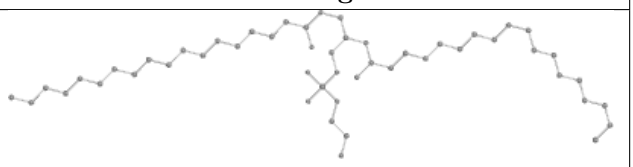
Bond lengths



Bond angles

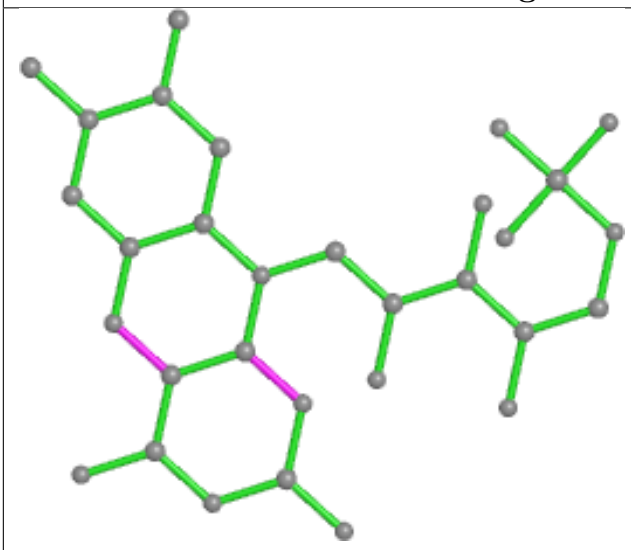


Torsions

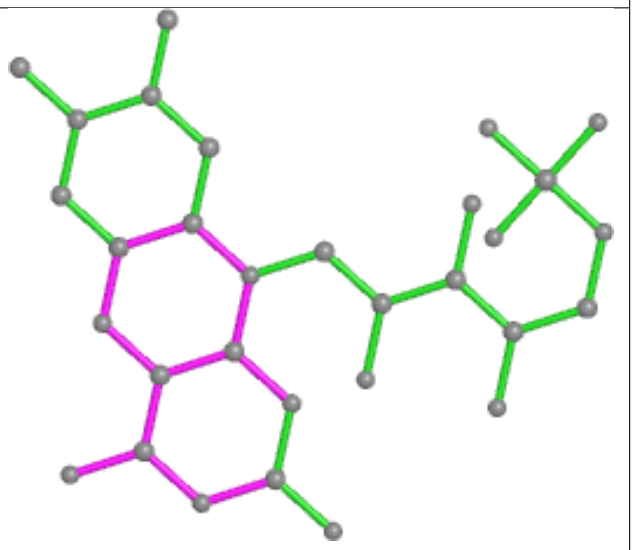


Rings

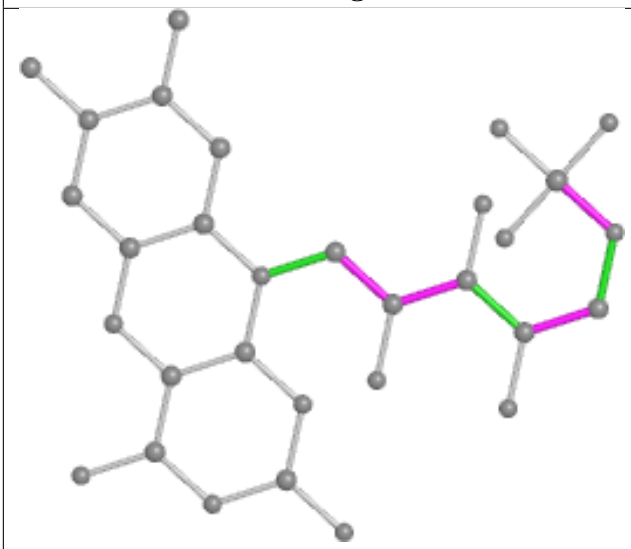
Ligand FMN A 502



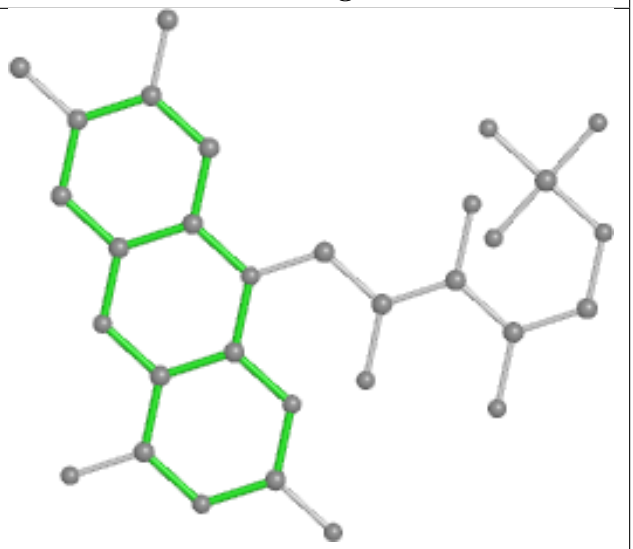
Bond lengths



Bond angles

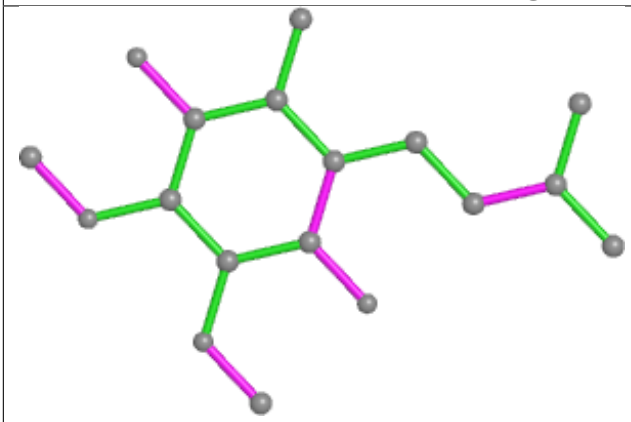


Torsions

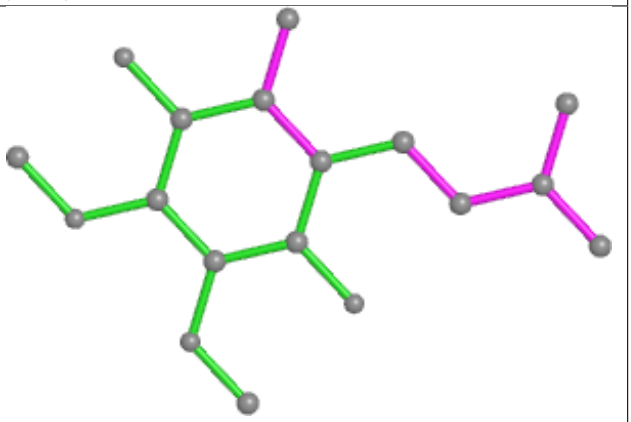


Rings

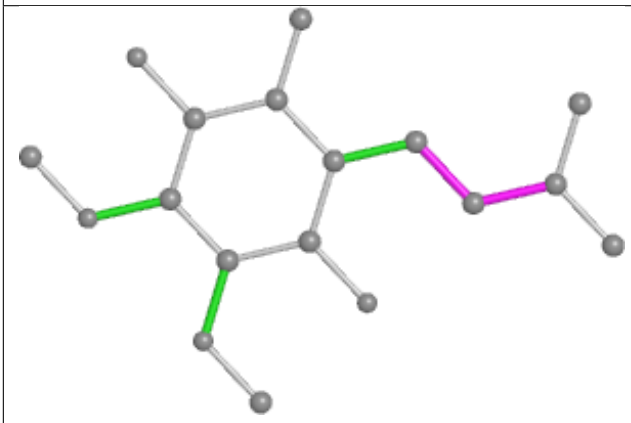
Ligand UQ1 Q 502



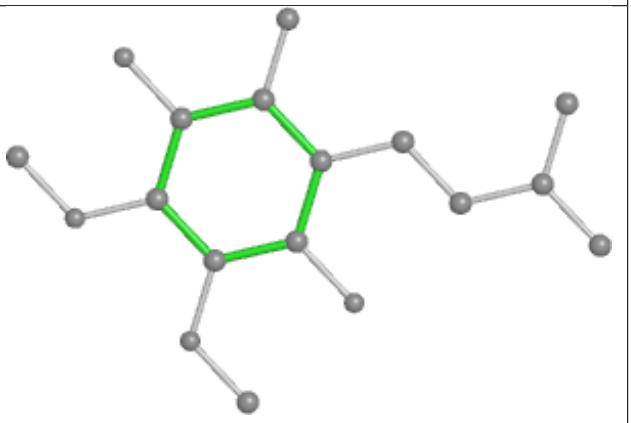
Bond lengths



Bond angles

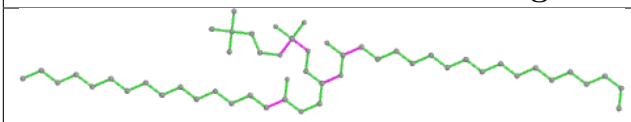


Torsions

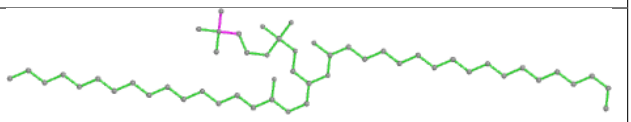


Rings

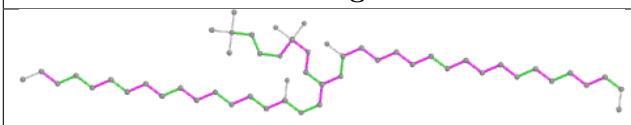
Ligand PLX r 501



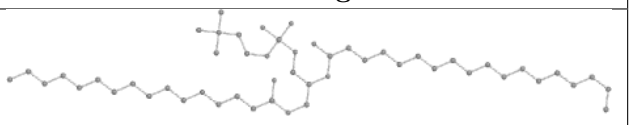
Bond lengths



Bond angles

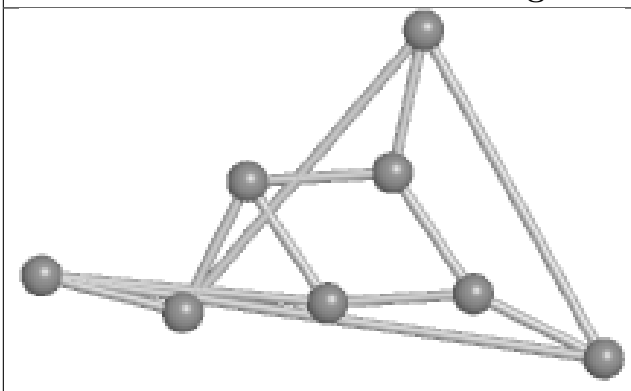


Torsions

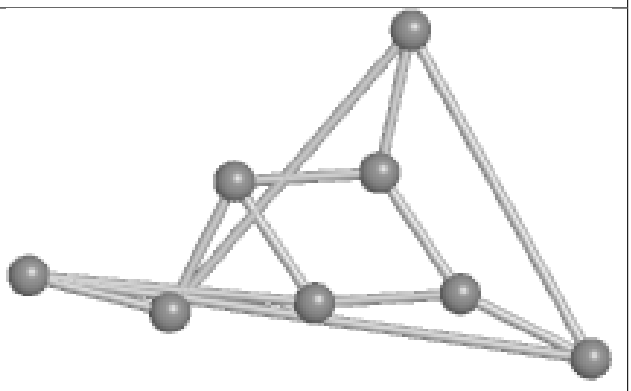


Rings

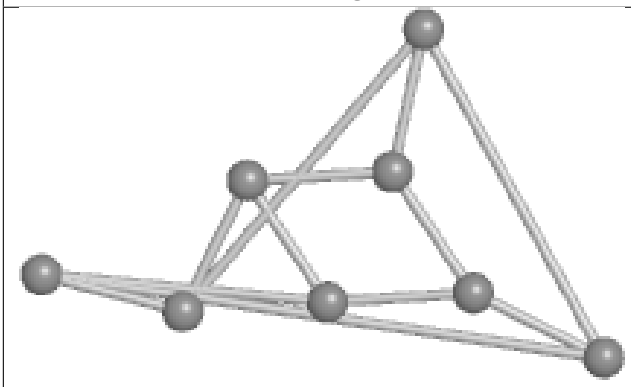
Ligand SF4 M 801



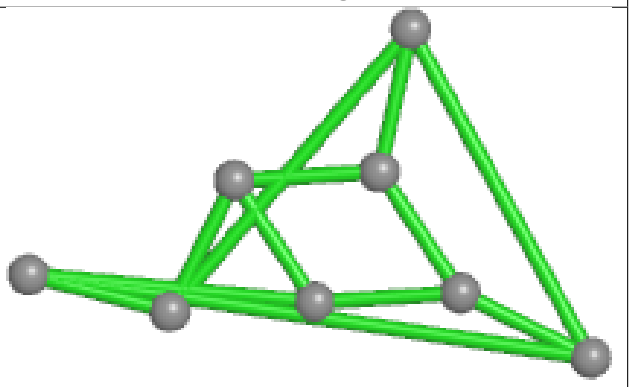
Bond lengths



Bond angles

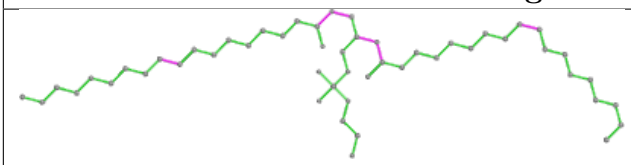


Torsions

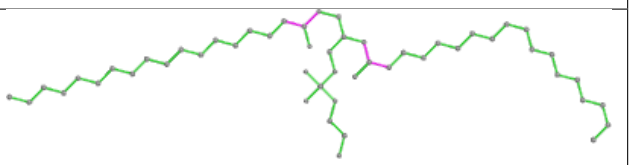


Rings

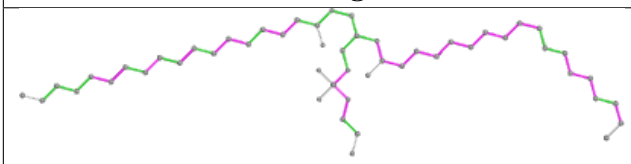
Ligand PEE V 202



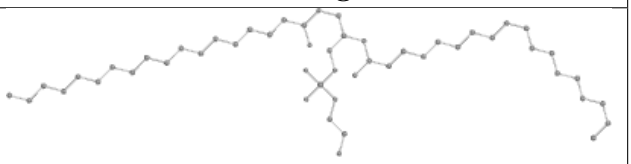
Bond lengths



Bond angles

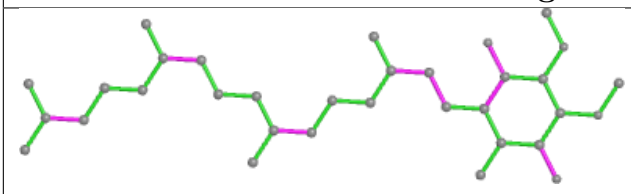


Torsions

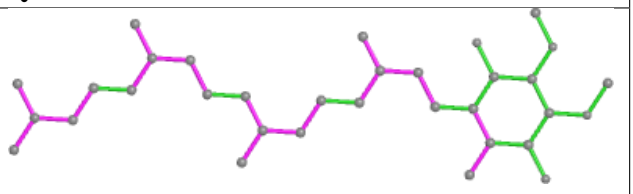


Rings

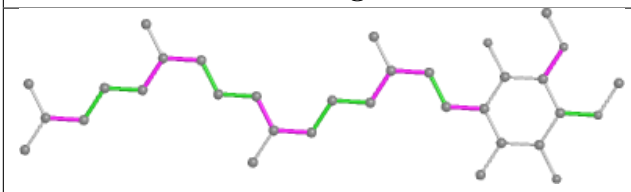
Ligand UQ J 402



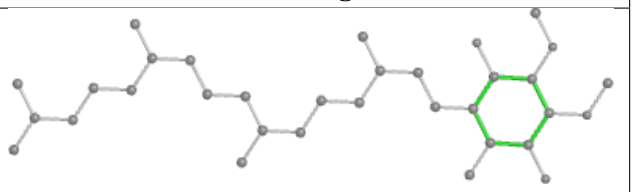
Bond lengths



Bond angles

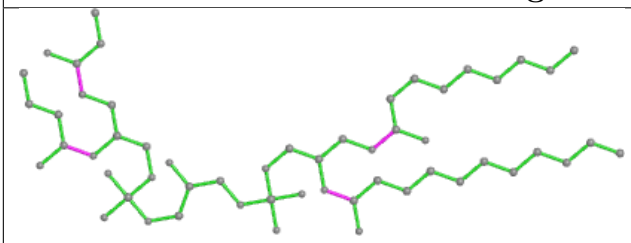


Torsions

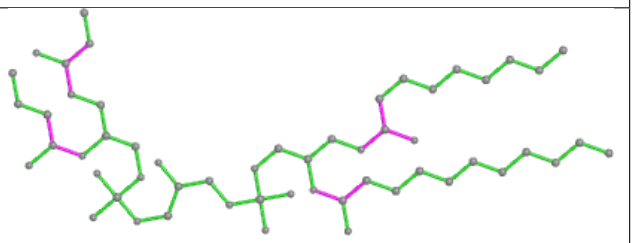


Rings

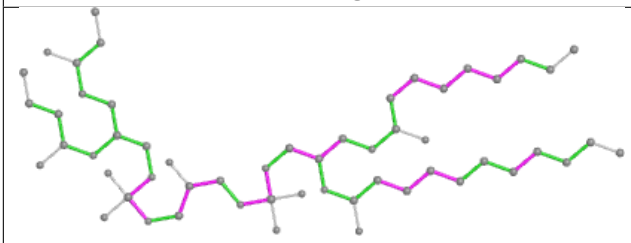
Ligand CDL u 201



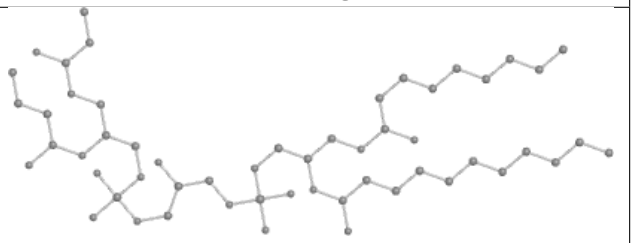
Bond lengths



Bond angles

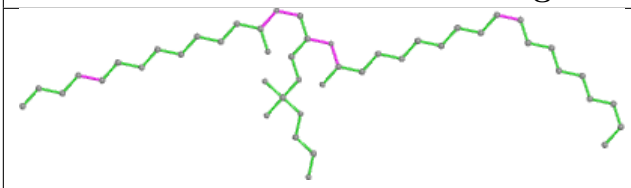


Torsions

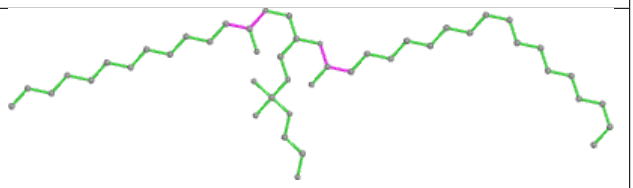


Rings

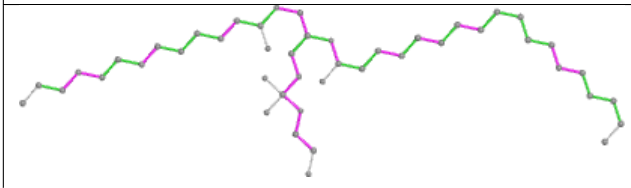
Ligand PEE l 704



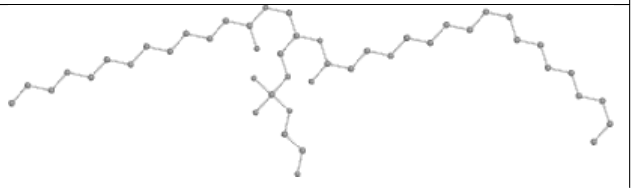
Bond lengths



Bond angles

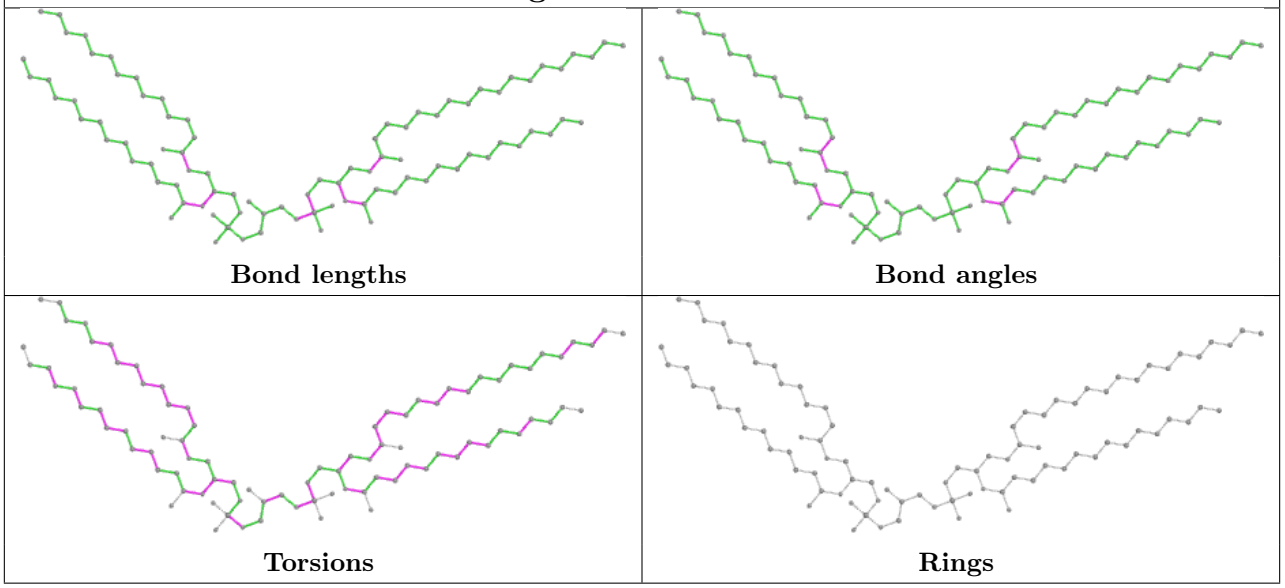


Torsions

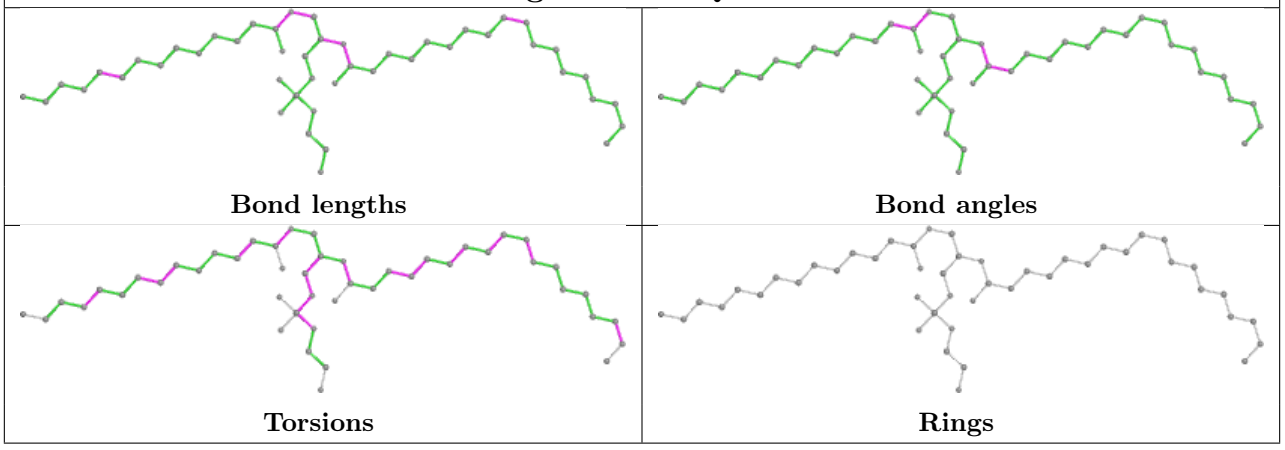


Rings

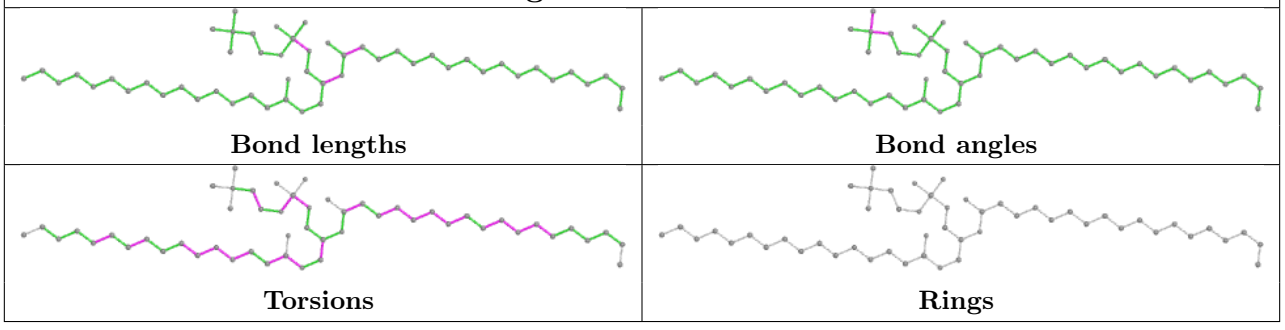
Ligand CDL J 404



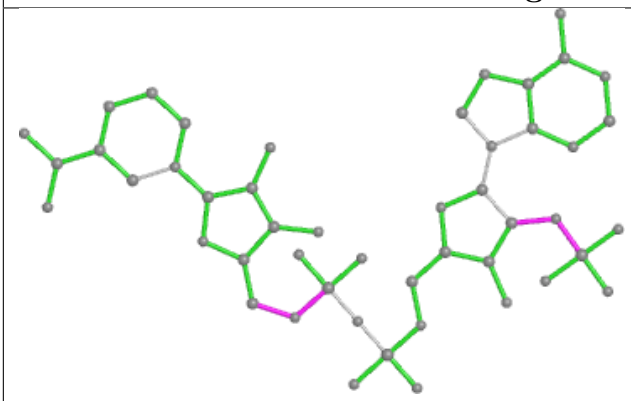
Ligand PEE Q 503



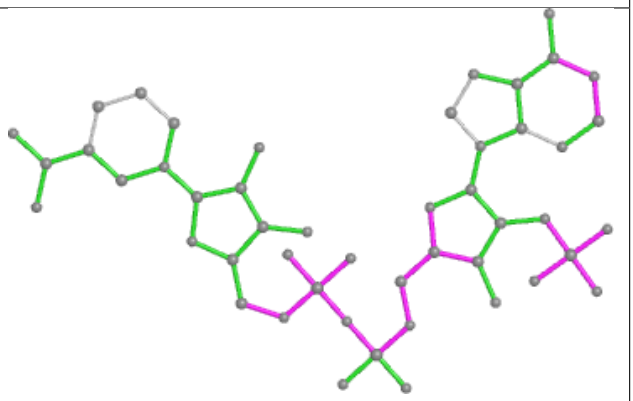
Ligand PLX C 303



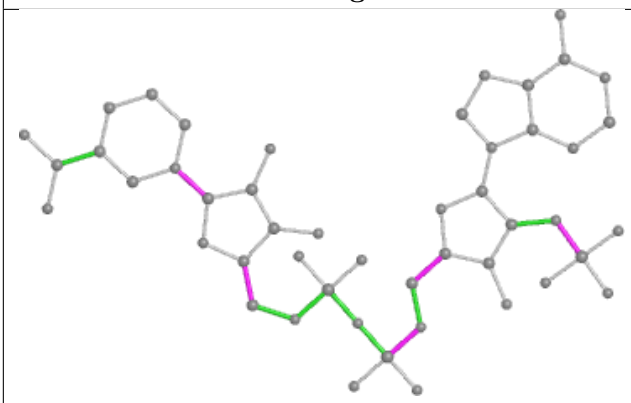
Ligand NDP J 401



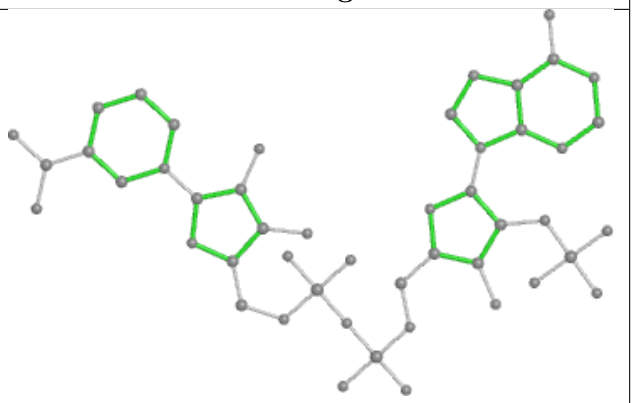
Bond lengths



Bond angles

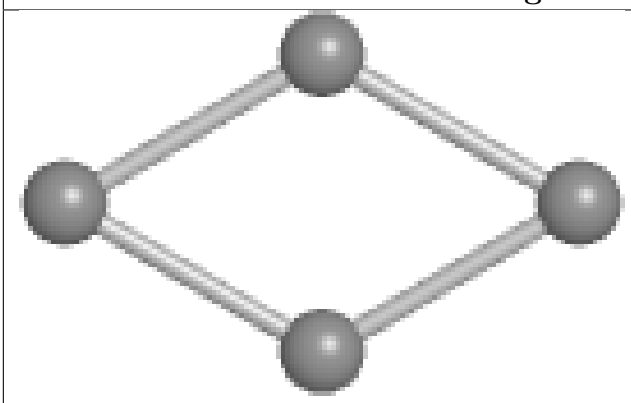


Torsions

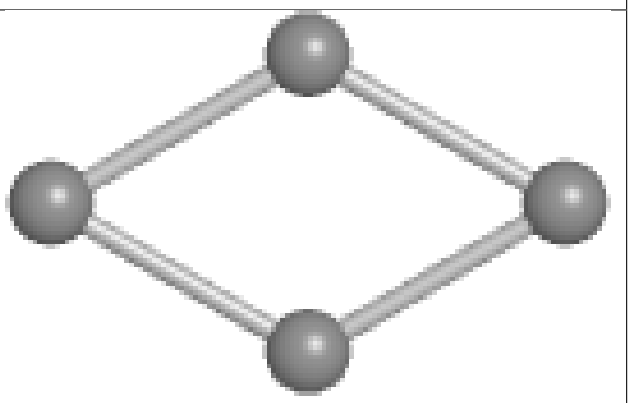


Rings

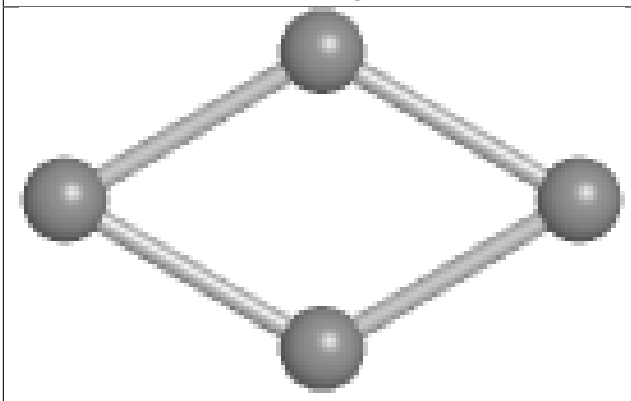
Ligand FES M 803



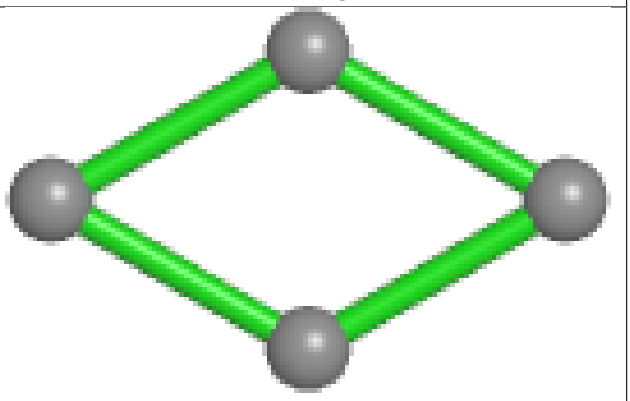
Bond lengths



Bond angles

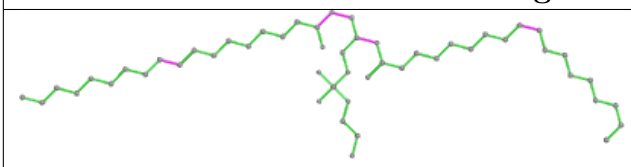


Torsions

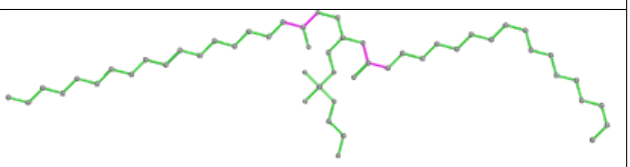


Rings

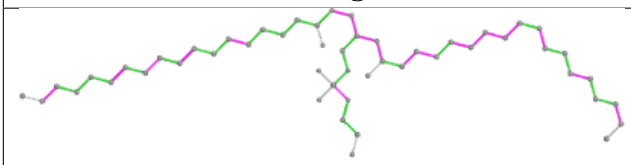
Ligand PEE l 703



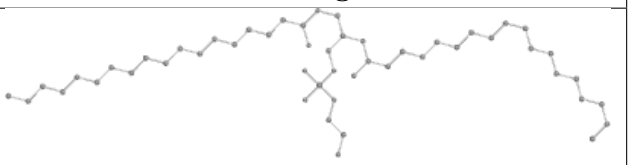
Bond lengths



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.

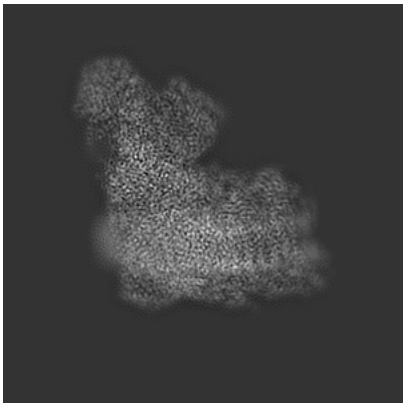
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31647. These allow visual inspection of the internal detail of the map and identification of artifacts.

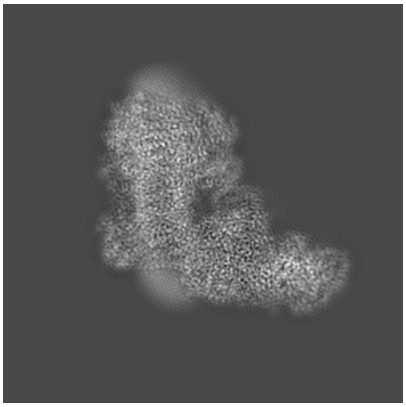
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

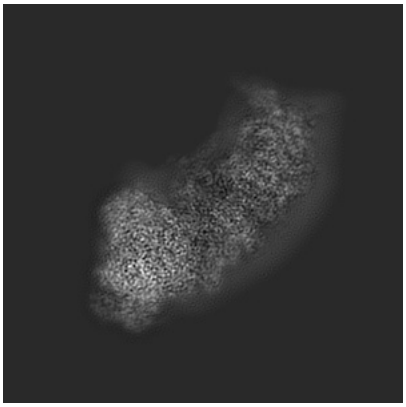
6.1.1 Primary map



X



Y

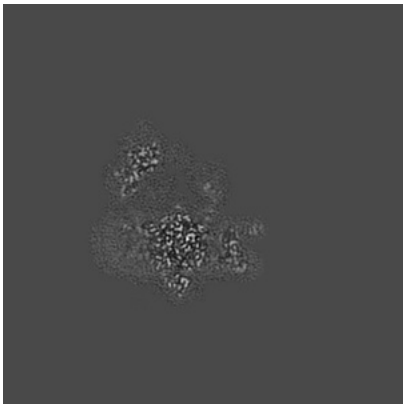


Z

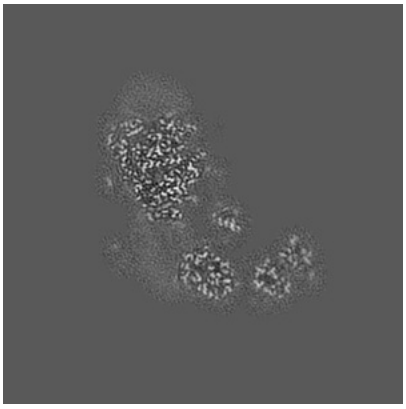
The images above show the map projected in three orthogonal directions.

6.2 Central slices

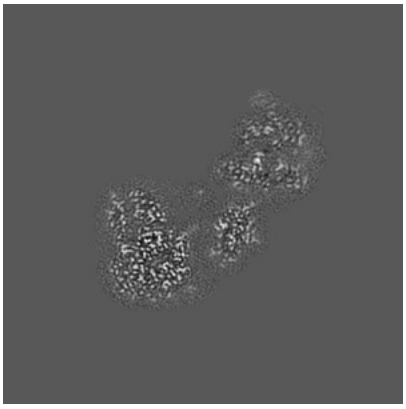
6.2.1 Primary map



X Index: 152



Y Index: 152



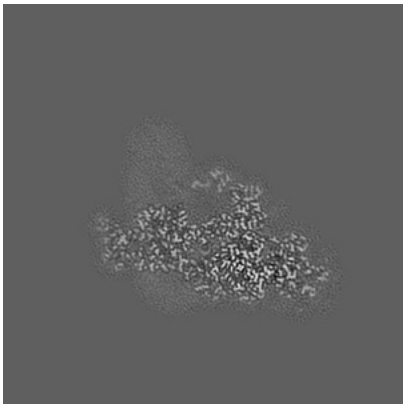
Z Index: 152

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: 105



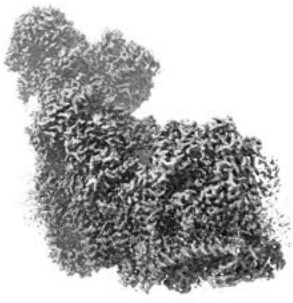
Y Index: 106

Z Index: 130

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

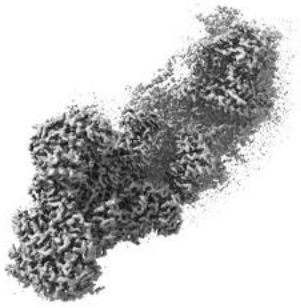
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

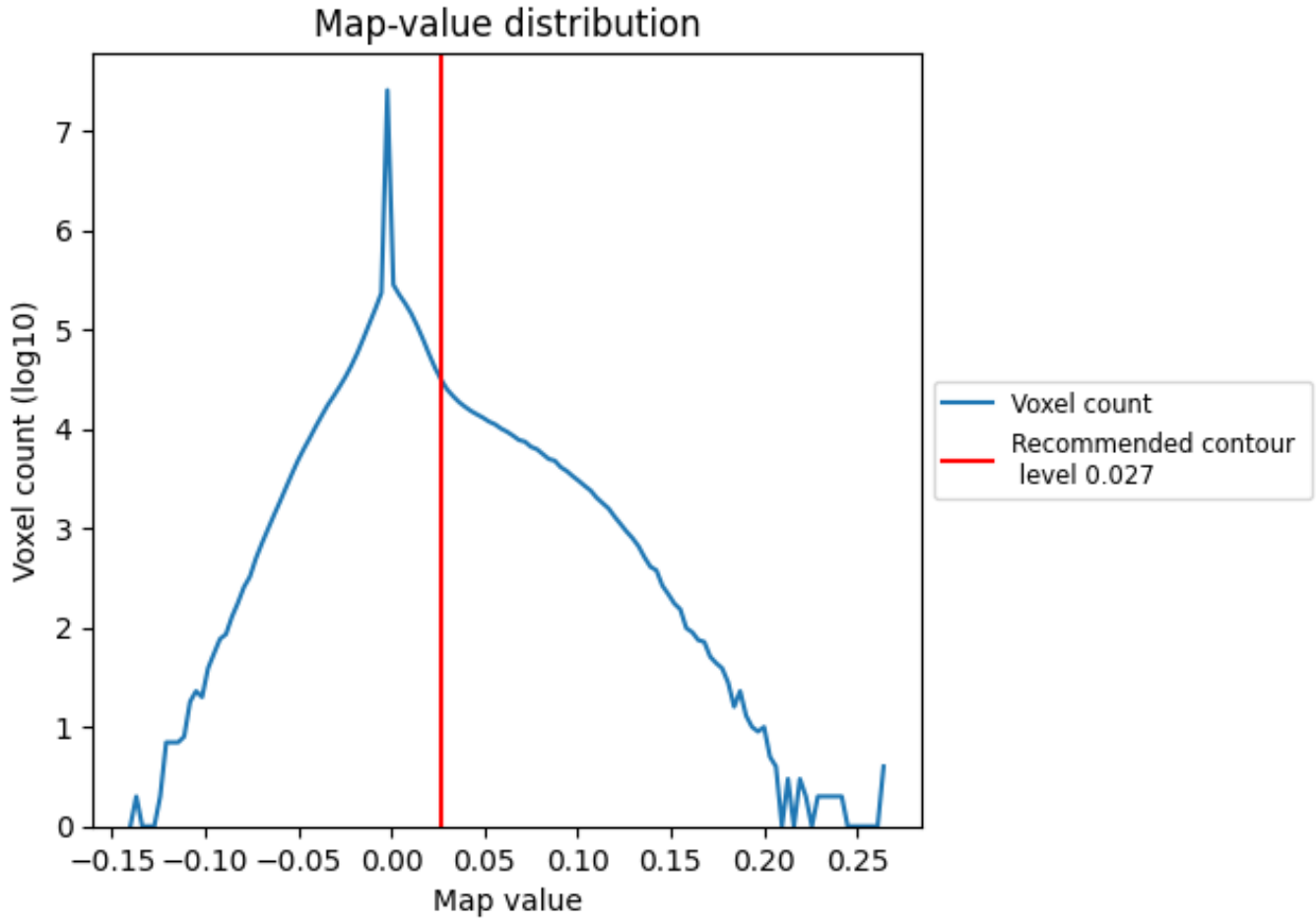
6.5 Mask visualisation (i)

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

7 Map analysis

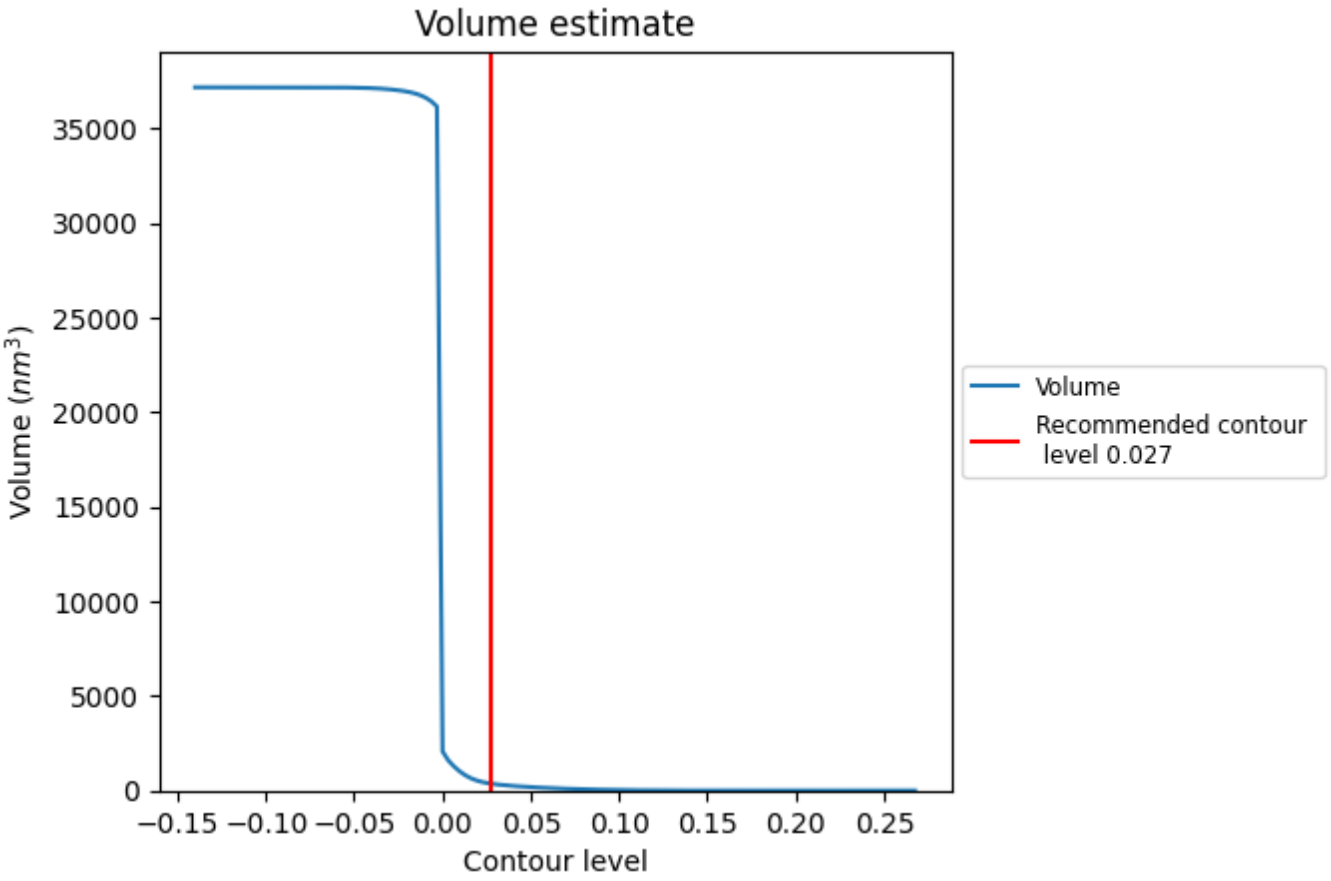
This section contains the results of statistical analysis of the map.

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.

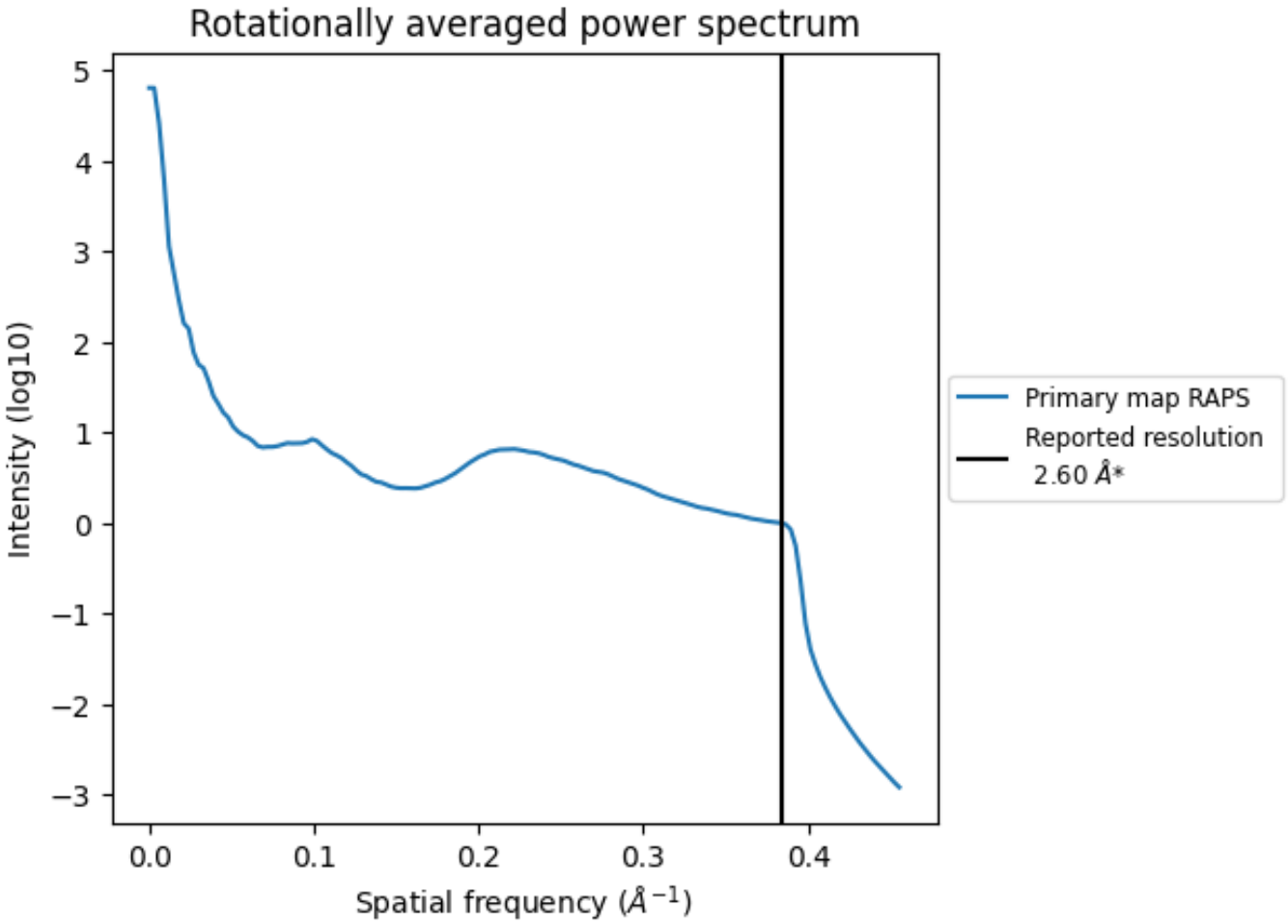
7.2 Volume estimate



The volume at the recommended contour level is 373 nm^3; this corresponds to an approximate mass of 337 kDa.

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

7.3 Rotationally averaged power spectrum (i)



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

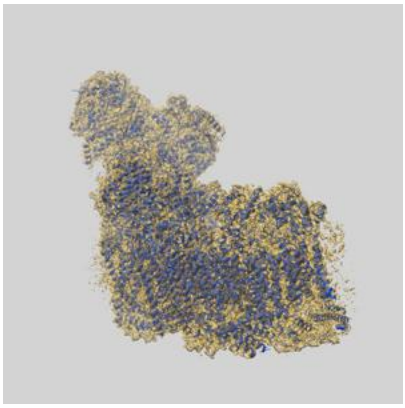
8 Fourier-Shell correlation (i)

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

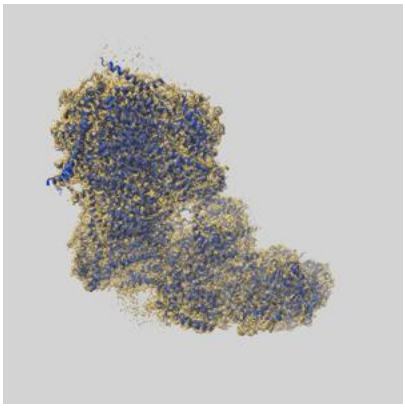
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31647 and PDB model 7V2R. Per-residue inclusion information can be found in section 3 on page 21.

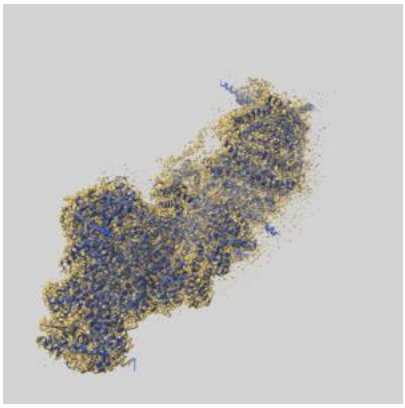
9.1 Map-model overlay



X



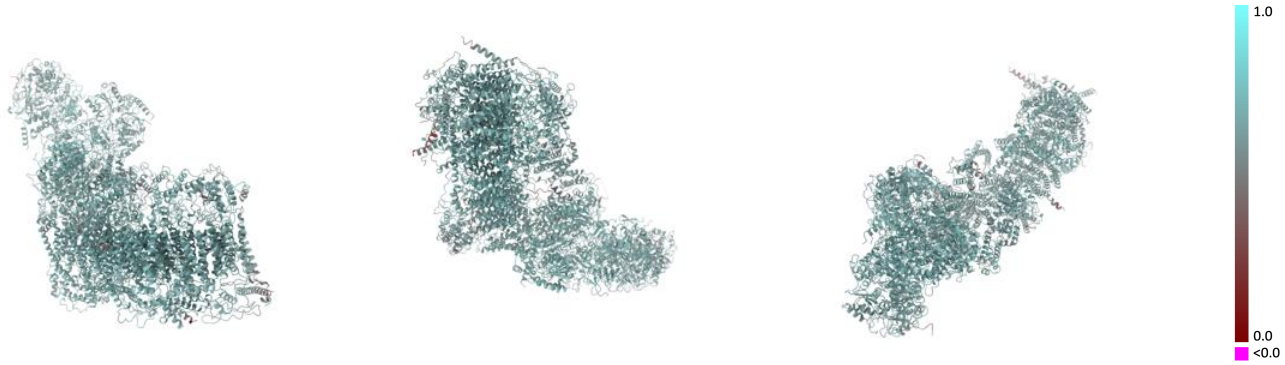
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.027 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.

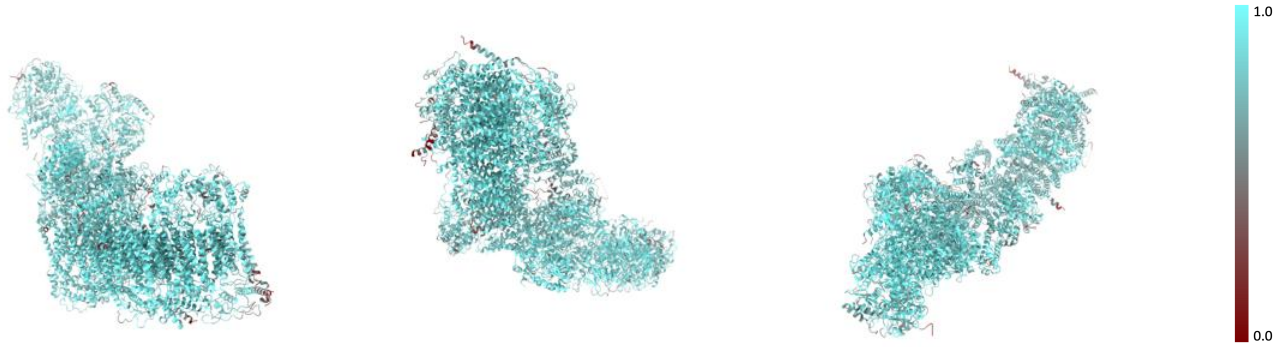
9.2 Q-score mapped to coordinate model



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.

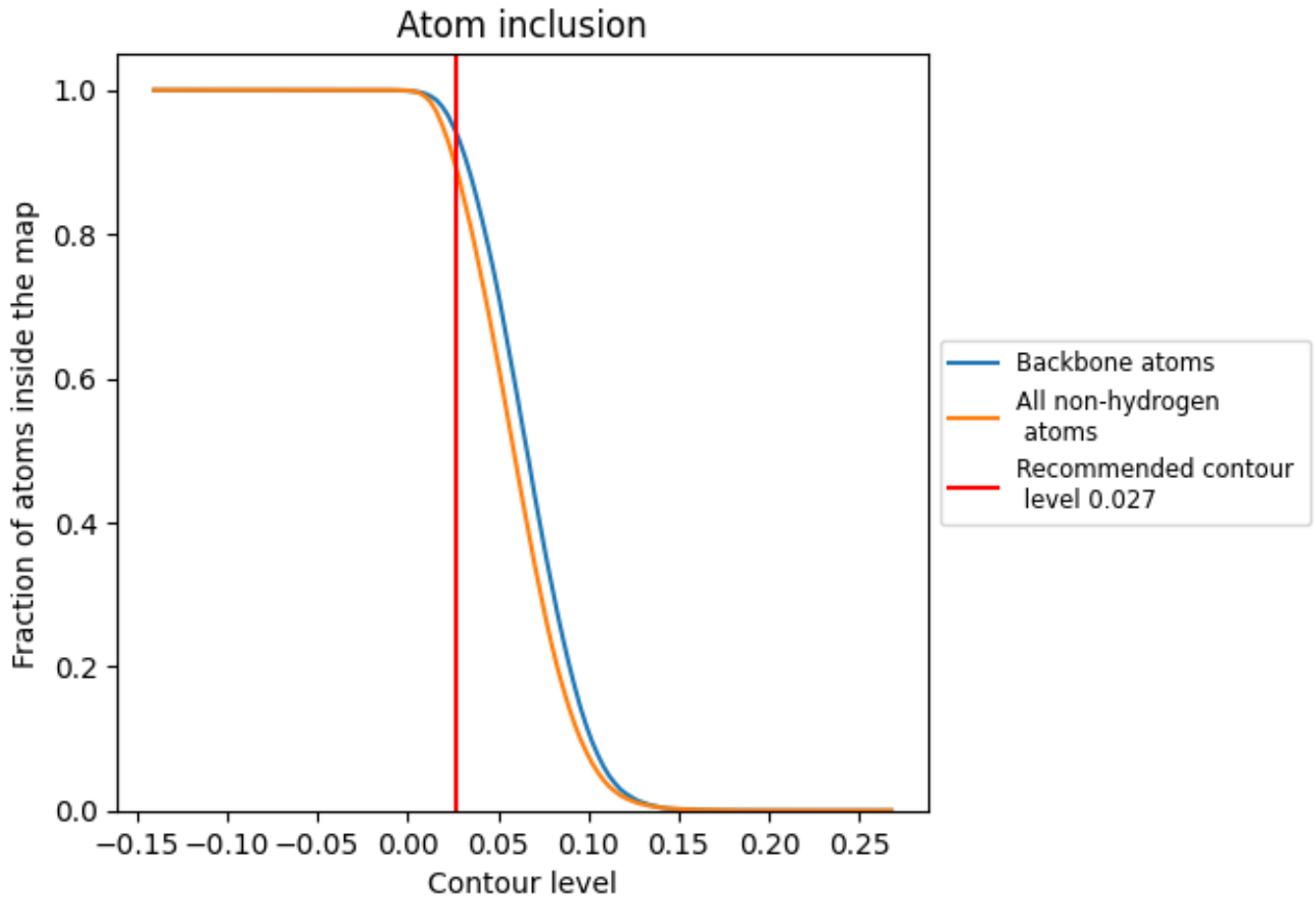
9.3 Atom inclusion mapped to coordinate model



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 (0.027).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 89% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8911	0.6460
A	0.8620	0.6190
B	0.9712	0.6880
C	0.9428	0.6830
E	0.9108	0.6600
F	0.7769	0.5920
G	0.6814	0.5480
H	0.8816	0.6310
I	0.8674	0.6370
J	0.8921	0.6530
K	0.8028	0.6010
L	0.9074	0.6690
M	0.9181	0.6510
N	0.9150	0.6660
O	0.8267	0.6090
P	0.9698	0.6870
Q	0.9598	0.6830
S	0.9366	0.6600
T	0.9169	0.6600
U	0.8792	0.6390
V	0.8072	0.6320
W	0.8865	0.6290
X	0.7855	0.6030
Y	0.7364	0.5760
Z	0.6736	0.5620
a	0.8819	0.6560
b	0.8086	0.6090
c	0.8694	0.6370
d	0.8537	0.6290
e	0.8140	0.6180
f	0.7378	0.5740
g	0.9113	0.6560
h	0.8688	0.6360
i	0.9747	0.6830
j	0.9047	0.6700

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	0.9342	0.6740
l	0.9002	0.6500
m	0.8487	0.6280
n	0.7759	0.5930
o	0.8814	0.6450
p	0.8714	0.6330
r	0.9638	0.6740
s	0.9750	0.6800
u	0.8747	0.6300
v	0.7231	0.5700
w	0.8609	0.6290