Full wwPDB EM Validation Report ⓘ

May 6, 2025 – 04:11 AM EDT

PDB ID	:	8ESZ / pdb_00008esz
EMDB ID	:	EMD-28582
Title	:	Structure of mitochondrial complex I from Drosophila melanogaster, Helix-locked state
Authors	:	Padavannil, A.; Letts, J.A.
Deposited on	:	2022-10-15
Resolution	:	3.40 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:

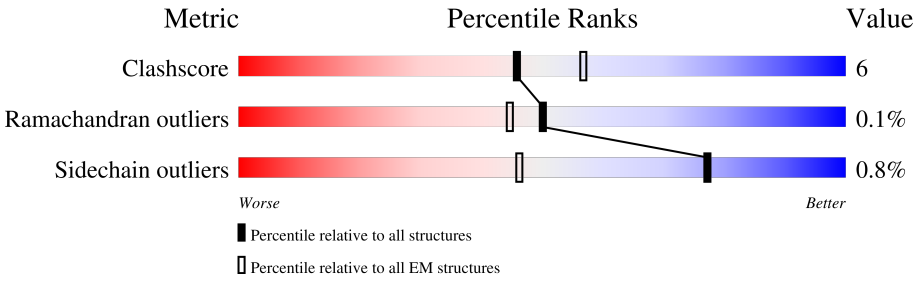
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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.



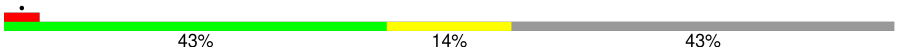
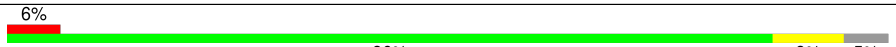
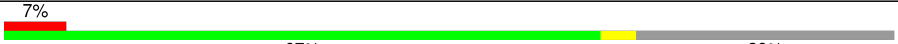
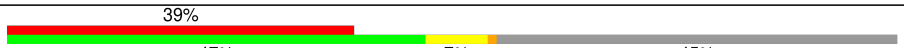
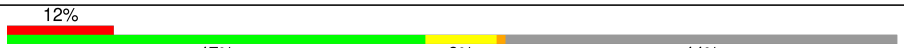
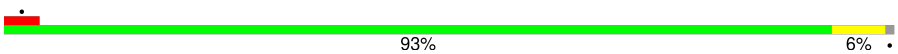
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	AN	142	12% 80% 15%
2	S6	126	63% 7% 29%
3	S1	731	8% 80% 13% 7%
4	S3	265	64% 14% 23%
5	V2	242	14% 78% 10% 12%
6	S7	221	61% 21% 18%
7	S8	217	72% 14% 14%
8	1	315	79% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	4	446	
10	5	577	
11	A8	175	
12	A1	123	
13	AO	154	
14	S5	101	
15	AM	170	
16	BL	159	
17	B6	167	
18	B4	113	
19	B7	117	
20	B5	186	
21	B9	144	
22	BM	150	
23	B8	175	
24	B3	110	
25	AB	152	
25	AC	152	
26	C2	116	
27	B1	56	
28	S4	183	
29	A9	416	
30	B2	94	
31	S2	468	
32	V3	37	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	V1	474	6% 78% 14% 8%
34	2	341	80% 19%
35	A7	103	9% 76% 12% 12%
36	A3	77	6% 74% 12% 14%
37	4L	96	82% 18%
38	6	174	78% 22%
39	3	117	83% 17%
40	A5	124	9% 85% 9% 6%
41	AL	407	76% 14% 10%
42	A6	124	6% 82% 10% 7%

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
46	SF4	S7	301	-	-	X	-

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 67757 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] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AN	136	1145	747	191	202	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	S6	89	716	453	130	129	4	0	0

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	S1	683	5181	3246	919	987	29	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	S3	205	1699	1086	298	310	5	0	0

- Molecule 5 is a protein called NADH dehydrogenase (Ubiquinone) 24 kDa subunit, isoform A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	V2	214	1680	1062	285	321	12	0	0

- Molecule 6 is a protein called LD31474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S7	182	Total	C	N	O	S	0	0
			1435	920	251	250	14		

- Molecule 7 is a protein called NADH dehydrogenase (ubiquinone) 23 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S8	186	Total	C	N	O	S	0	0
			1485	935	251	287	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1	315	Total	C	N	O	S	0	0
			2571	1764	367	418	22		

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	4	446	Total	C	N	O	S	0	0
			3606	2450	533	581	42		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	5	577	Total	C	N	O	S	0	0
			4606	3092	680	774	60		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A8	174	Total	C	N	O	S	0	0
			1384	867	240	267	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A1	70	Total	C	N	O	S	0	0
			581	375	97	103	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AO	146	Total	C	N	O	S	0	0
			1202	787	203	210	2		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S5	100	Total	C	N	O	S	0	0
			828	523	145	149	11		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AM	168	Total	C	N	O	S	0	0
			1281	832	212	230	7		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BL	151	Total	C	N	O	S	0	0
			1266	794	232	230	10		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	B6	161	Total	C	N	O	S	0	0
			1302	829	242	226	5		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B4	107	Total	C	N	O	S	0	0
			884	566	162	155	1		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	B7	117	Total	C	N	O	S	0	0
			972	617	170	175	10		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B5	143	Total	C	N	O	S	0	0
			1221	787	209	222	3		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B9	134	Total	C	N	O	S	0	0
			1148	732	217	196	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BM	106	Total	C	N	O	S	0	0
			871	560	140	170	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B8	144	Total	C	N	O	S	0	0
			1201	783	191	223	4		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B3	81	Total	C	N	O	S	0	0
			646	421	113	111	1		

- Molecule 25 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AC	85	Total	C	N	O	S	0	0
			680	438	103	137	2		
25	AB	84	Total	C	N	O	S	0	0
			670	433	102	133	2		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	C2	115	Total	C	N	O	S	0	0
			908	590	159	158	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B1	55	Total	C	N	O	S	0	0
			430	278	76	74	2		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S4	151	Total	C	N	O	S	0	0
			1214	756	227	227	4		

- Molecule 29 is a protein called NADH dehydrogenase (Ubiquinone) 39 kDa subunit, isoform A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A9	377	Total	C	N	O	S	0	0
			3030	1931	546	543	10		

- Molecule 30 is a protein called GEO11417p1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B2	60	Total	C	N	O	S	0	0
			495	323	88	83	1		

- Molecule 31 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	S2	429	Total	C	N	O	S	0	0
			3427	2197	578	629	23		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	V3	27	Total	C	N	O	0	0
			135	81	27	27		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochon-

drial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	V1	438	Total	C	N	O	S	0	0
			3361	2121	599	615	26		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	2	341	Total	C	N	O	S	0	0
			2797	1893	411	459	34		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	A7	91	Total	C	N	O	S	0	0
			736	463	138	134	1		

- Molecule 36 is a protein called RH45008p.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	A3	66	Total	C	N	O	S	0	0
			519	327	95	96	1		

- Molecule 37 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	4L	96	Total	C	N	O	S	0	0
			794	540	113	128	13		

- Molecule 38 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	6	174	Total	C	N	O	S	0	0
			1404	949	202	236	17		

- Molecule 39 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	3	117	Total	C	N	O	S	0	0
			956	652	141	156	7		

- Molecule 40 is a protein called NADH dehydrogenase (Ubiquinone) 13 kDa B subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A5	117	Total	C	N	O	S	0	0
			914	584	161	165	4		

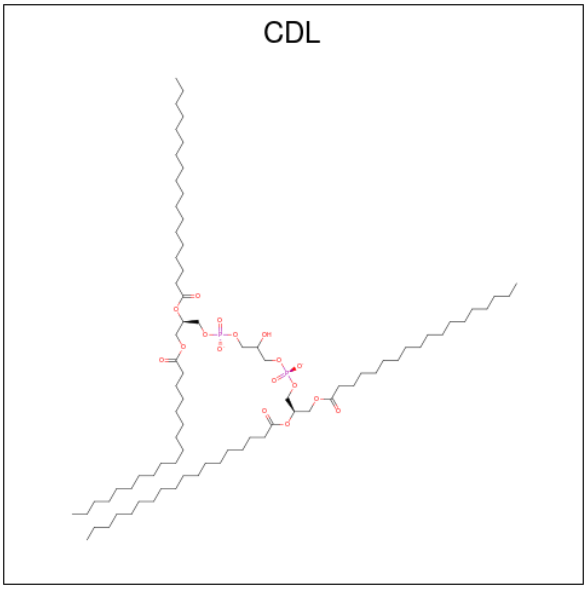
- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AL	368	Total	C	N	O	S	0	0
			3008	1927	504	561	16		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	A6	115	Total	C	N	O	S	0	0
			977	624	174	173	6		

- Molecule 43 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



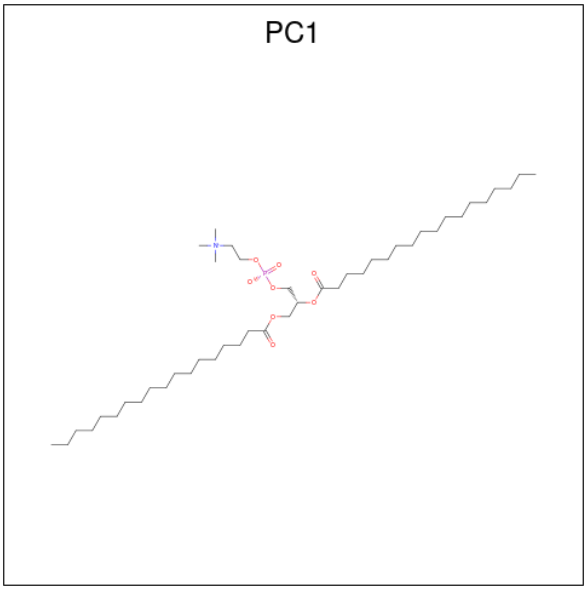
Mol	Chain	Residues	Atoms				AltConf
43	AN	1	Total	C	O	P	0
			67	48	17	2	
43	AM	1	Total	C	O	P	0
			76	57	17	2	
43	B6	1	Total	C	O	P	0
			47	28	17	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
43	B5	1	Total	C	O	P	0
			76	57	17	2	
43	B5	1	Total	C	O	P	0
			66	47	17	2	
43	2	1	Total	C	O	P	0
			45	27	16	2	
43	6	1	Total	C	O	P	0
			86	67	17	2	
43	3	1	Total	C	O	P	0
			54	35	17	2	

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



Mol	Chain	Residues	Atoms					AltConf
44	AN	1	Total	C	N	O	P	0
			44	34	1	8	1	
44	S7	1	Total	C	N	O	P	0
			46	36	1	8	1	
44	1	1	Total	C	N	O	P	0
			54	44	1	8	1	
44	4	1	Total	C	N	O	P	0
			39	29	1	8	1	
44	4	1	Total	C	N	O	P	0
			39	29	1	8	1	
44	5	1	Total	C	N	O	P	0
			34	24	1	8	1	

Continued on next page...

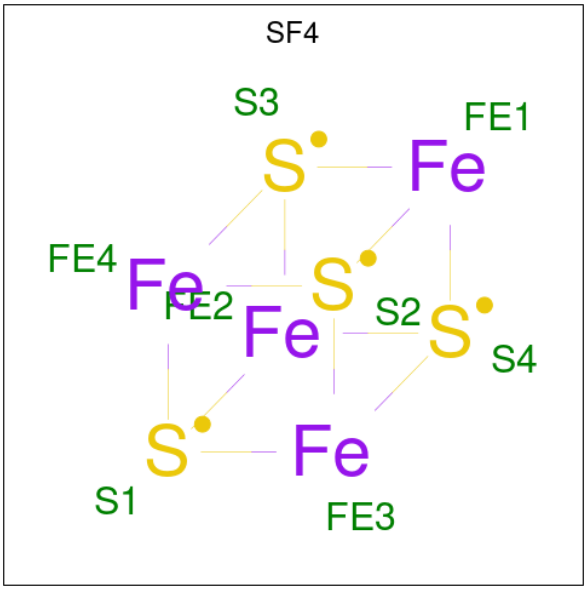
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
44	AM	1	Total	C	N	O	P	0
			37	27	1	8	1	
44	AM	1	Total	C	N	O	P	0
			44	34	1	8	1	
44	AM	1	Total	C	N	O	P	0
			32	22	1	8	1	
44	B6	1	Total	C	N	O	P	0
			37	27	1	8	1	
44	A9	1	Total	C	N	O	P	0
			44	34	1	8	1	
44	2	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 45 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
45	S6	1	Total	Zn	0
			1	1	

- Molecule 46 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



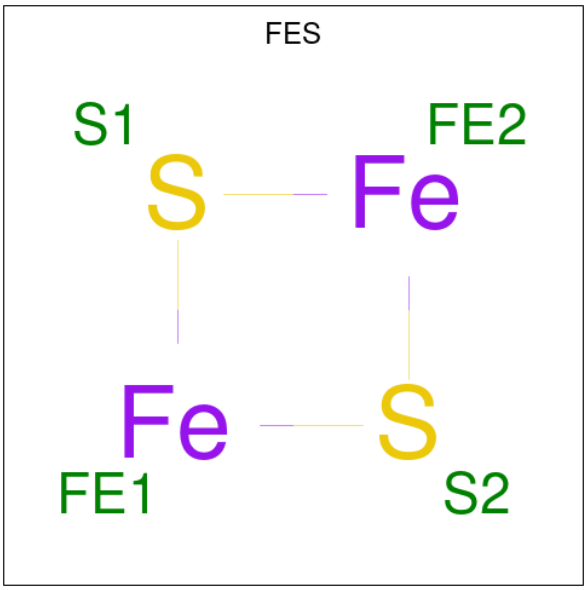
Mol	Chain	Residues	Atoms			AltConf
46	S1	1	Total	Fe	S	0
			8	4	4	
46	S1	1	Total	Fe	S	0
			8	4	4	

Continued on next page...

Continued from previous page...

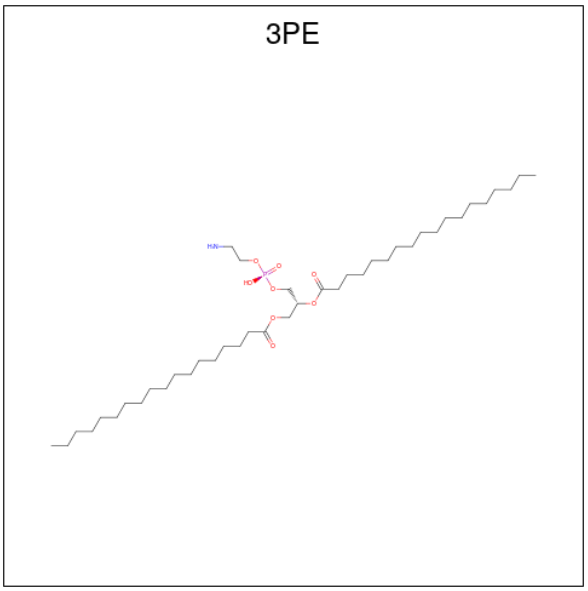
Mol	Chain	Residues	Atoms	AltConf
46	S7	1	Total Fe S 8 4 4	0
46	S8	1	Total Fe S 8 4 4	0
46	S8	1	Total Fe S 8 4 4	0
46	V1	1	Total Fe S 8 4 4	0

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	AltConf
47	S1	1	Total Fe S 4 2 2	0
47	V2	1	Total Fe S 4 2 2	0

- Molecule 48 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



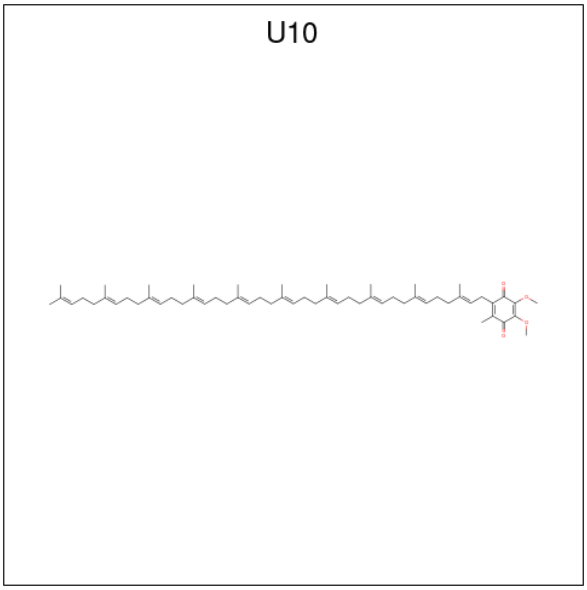
Mol	Chain	Residues	Atoms	AltConf
48	S7	1	Total C N O P 33 23 1 8 1	0
48	S7	1	Total C N O P 33 23 1 8 1	0
48	1	1	Total C N O P 51 41 1 8 1	0
48	4	1	Total C N O P 32 22 1 8 1	0
48	4	1	Total C N O P 45 35 1 8 1	0
48	4	1	Total C N O P 36 26 1 8 1	0
48	4	1	Total C N O P 39 29 1 8 1	0
48	5	1	Total C O P 32 23 8 1	0
48	5	1	Total C N O P 51 41 1 8 1	0
48	5	1	Total C N O P 33 23 1 8 1	0
48	5	1	Total C N O P 30 20 1 8 1	0
48	5	1	Total C N O P 33 23 1 8 1	0
48	5	1	Total C N O P 51 41 1 8 1	0
48	5	1	Total C N O P 45 35 1 8 1	0

Continued on next page...

Continued from previous page...

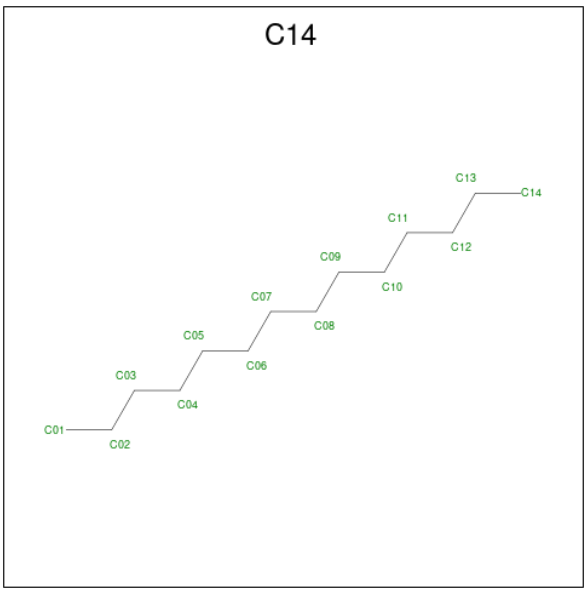
Mol	Chain	Residues	Atoms	AltConf
48	AM	1	Total C N O P 41 31 1 8 1	0
48	AM	1	Total C N O P 31 21 1 8 1	0
48	B6	1	Total C O P 48 39 8 1	0
48	B4	1	Total C N O P 47 37 1 8 1	0
48	C2	1	Total C N O P 45 35 1 8 1	0
48	B1	1	Total C N O P 37 27 1 8 1	0
48	2	1	Total C N O P 30 20 1 8 1	0
48	6	1	Total C N O P 35 25 1 8 1	0
48	3	1	Total C N O P 51 41 1 8 1	0
48	3	1	Total C N O P 41 31 1 8 1	0

- Molecule 49 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



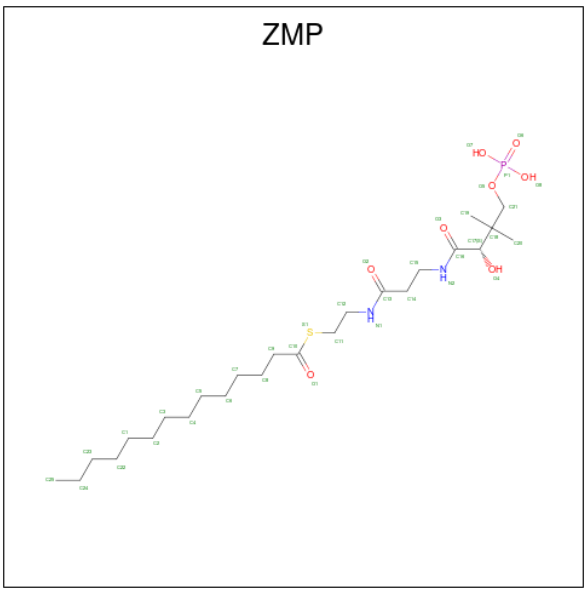
Mol	Chain	Residues	Atoms	AltConf
49	1	1	Total C O 63 59 4	0

- Molecule 50 is TETRADECANE (CCD ID: C14) (formula: $C_{14}H_{30}$).



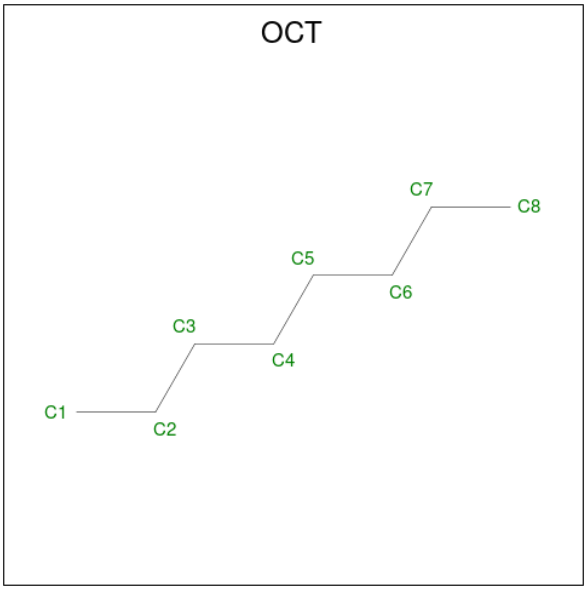
Mol	Chain	Residues	Atoms	AltConf
50	AO	1	Total C 14 14	0
50	B5	1	Total C 14 14	0
50	C2	1	Total C 14 14	0

- Molecule 51 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



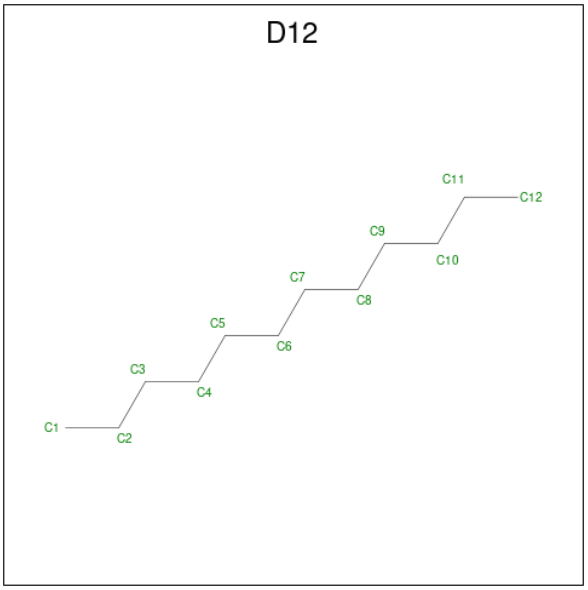
Mol	Chain	Residues	Atoms						AltConf
51	AC	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	
51	AB	1	Total	C	N	O	P	S	0
			32	21	2	7	1	1	

- Molecule 52 is N-OCTANE (CCD ID: OCT) (formula: C_8H_{18}).



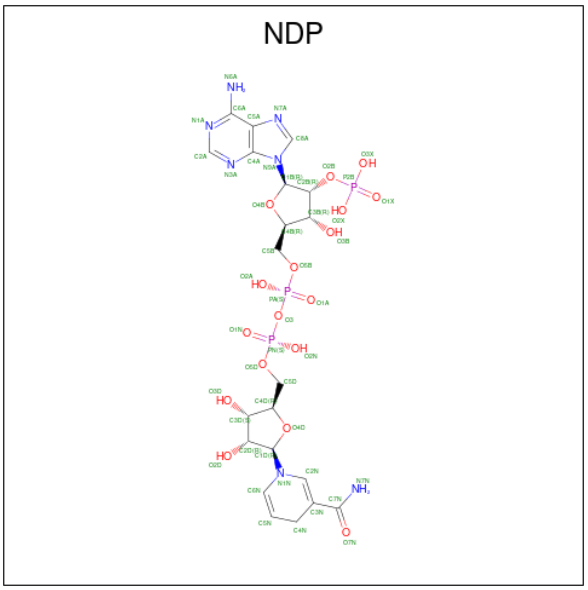
Mol	Chain	Residues	Atoms		AltConf
52	B1	1	Total	C	0
			8	8	

- Molecule 53 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$).



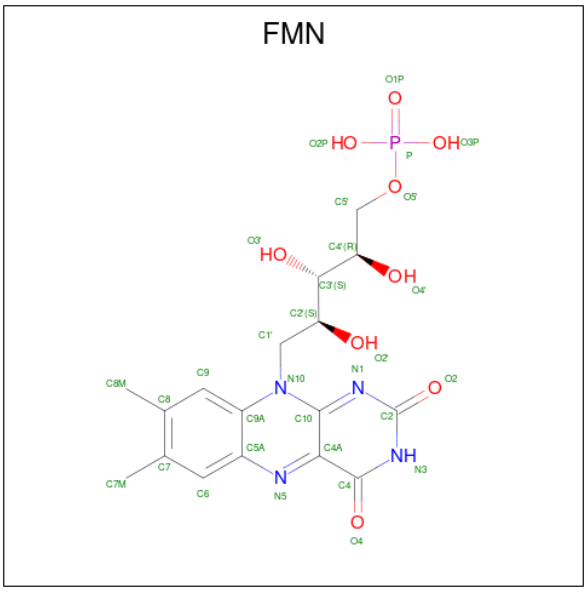
Mol	Chain	Residues	Atoms	AltConf
53	B1	1	Total C 12 12	0
53	A9	1	Total C 12 12	0
53	A9	1	Total C 12 12	0
53	A3	1	Total C 12 12	0

- Molecule 54 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



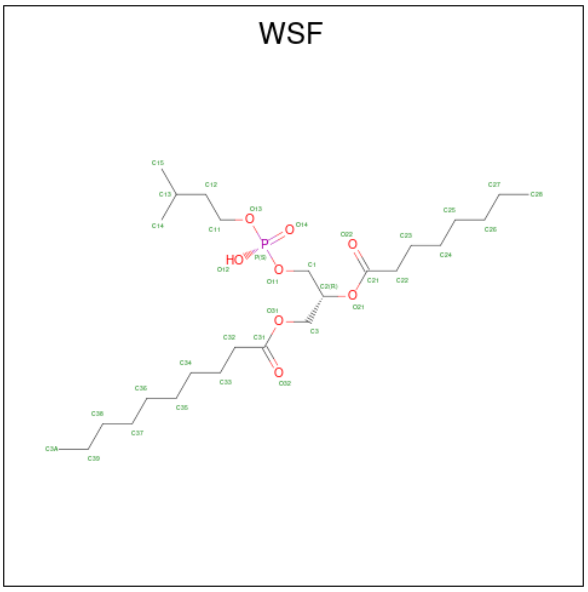
Mol	Chain	Residues	Atoms	AltConf
54	A9	1	Total C N O P 48 21 7 17 3	0

- Molecule 55 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



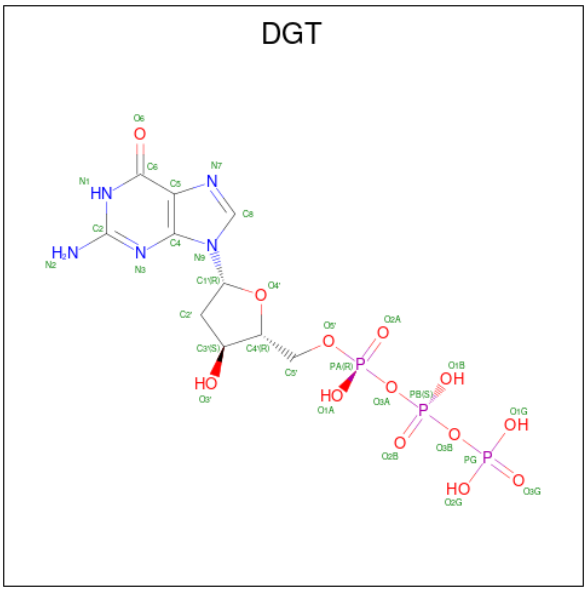
Mol	Chain	Residues	Atoms					AltConf
55	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 56 is (2R)-3-{[(S)-hydroxy(3-methylbutoxy)phosphoryl]oxy}-2-(octanoyloxy)propyl decanoate (CCD ID: WSF) (formula: $C_{26}H_{51}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
56	6	1	Total	C	O	P	0
			35	26	8	1	

- Molecule 57 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



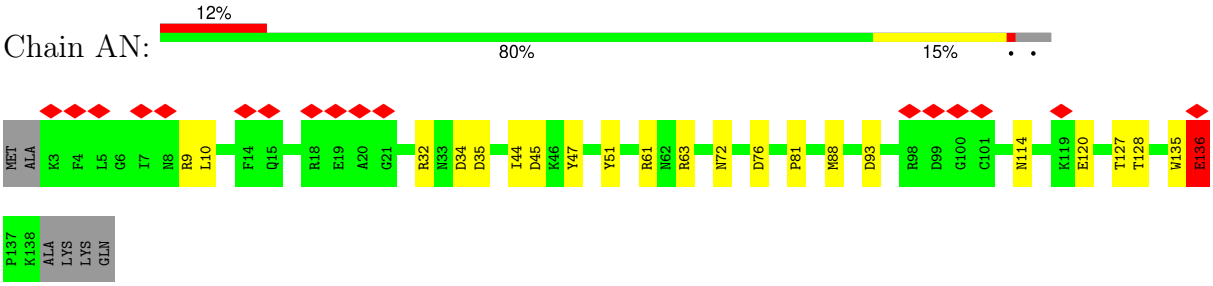
Mol	Chain	Residues	Atoms					AltConf
57	AL	1	Total	C	N	O	P	0
			31	10	5	13	3	

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.

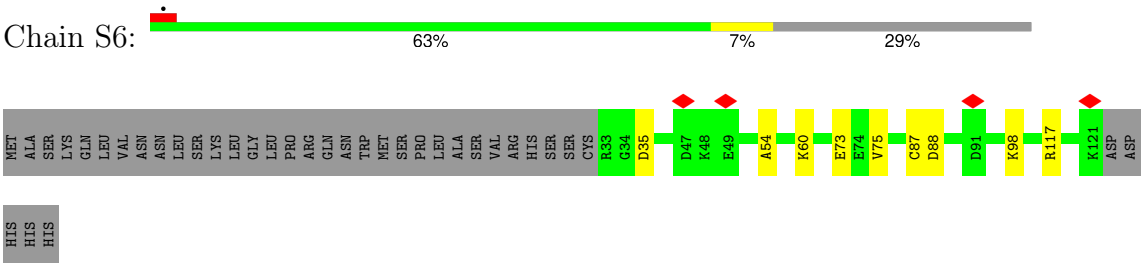
• Molecule 1: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain AN:



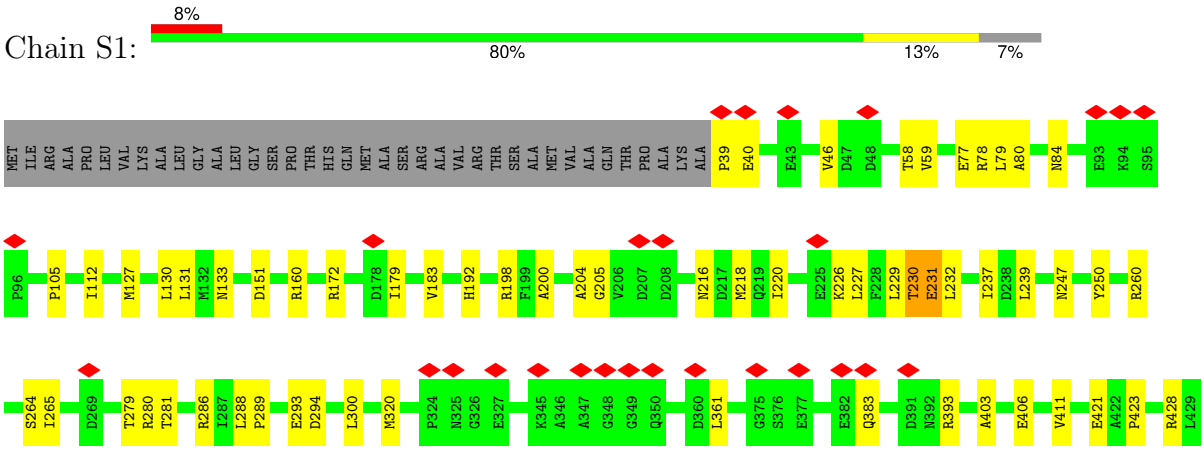
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

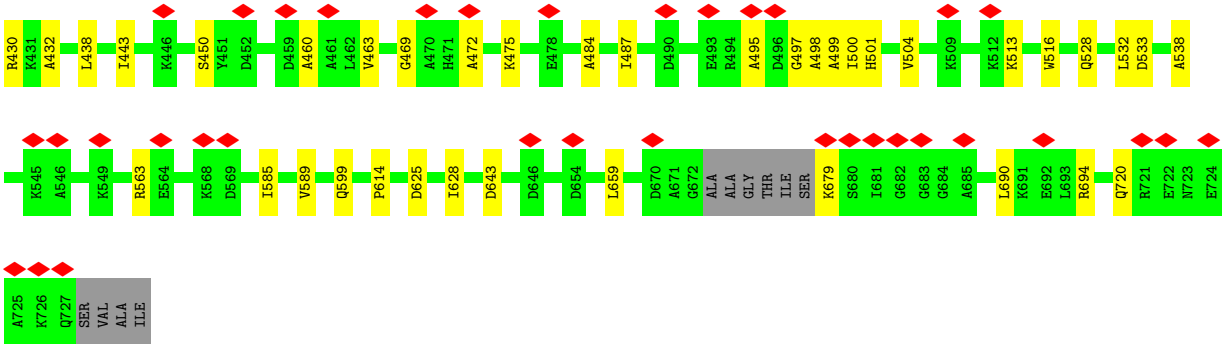
Chain S6:



• Molecule 3: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

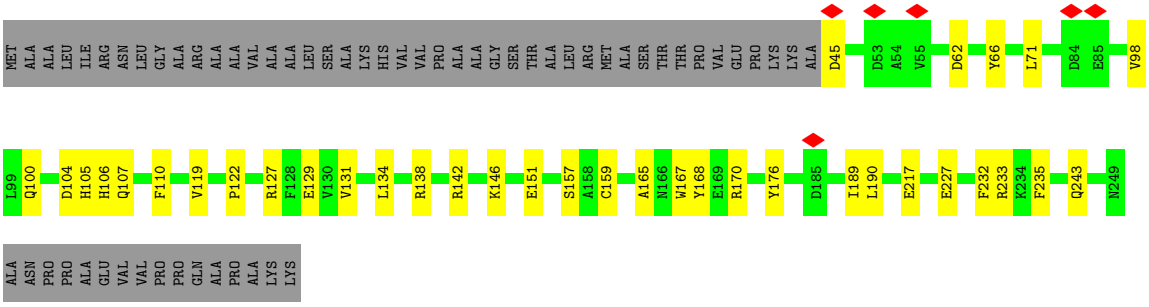
Chain S1:





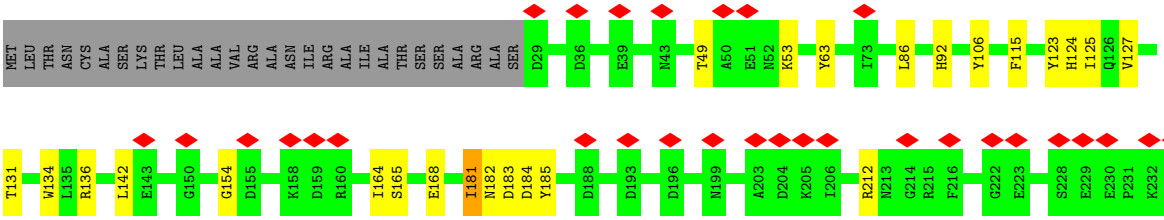
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain S3:



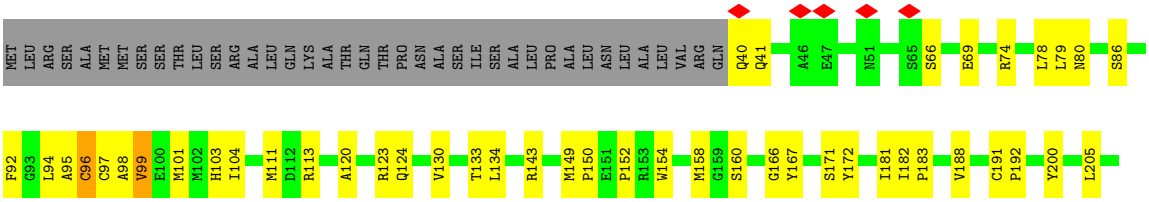
• Molecule 5: NADH dehydrogenase (Ubiquinone) 24 kDa subunit, isoform A

Chain V2:



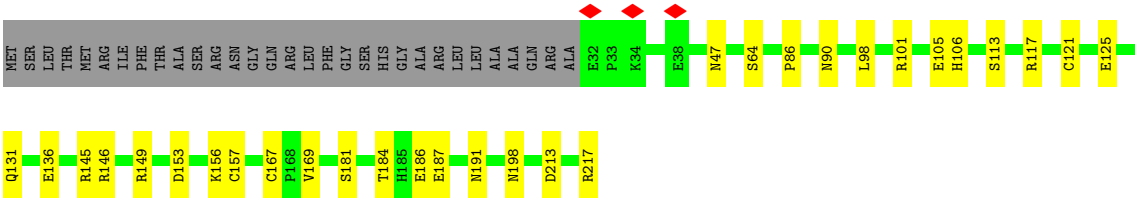
• Molecule 6: LD31474p

Chain S7:



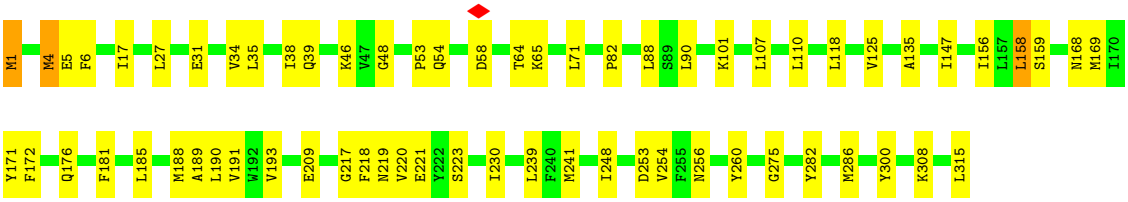
• Molecule 7: NADH dehydrogenase (ubiquinone) 23 kDa subunit

Chain S8:



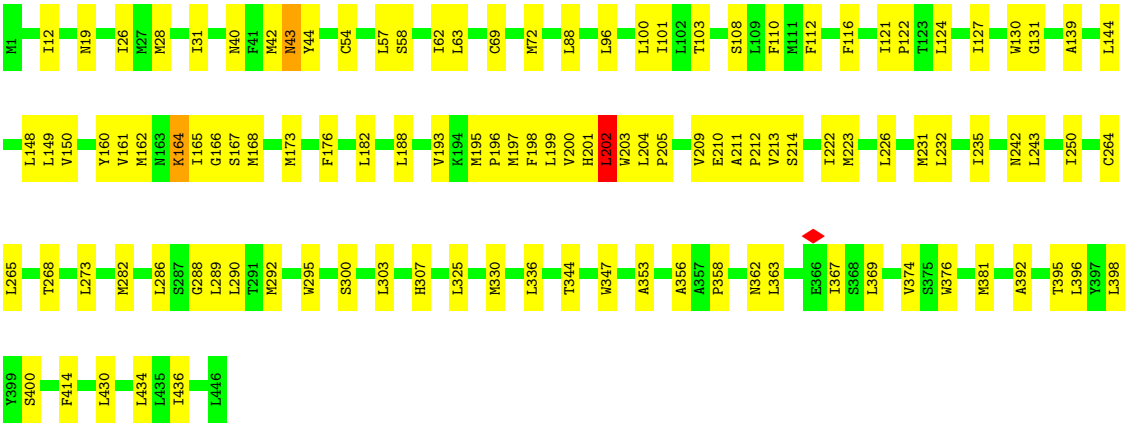
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain 1:



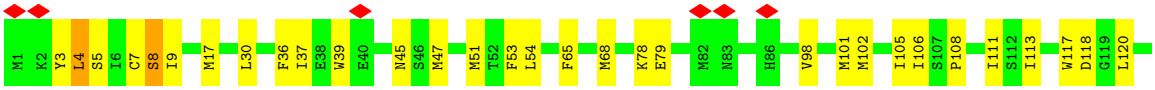
• Molecule 9: NADH-ubiquinone oxidoreductase chain 4

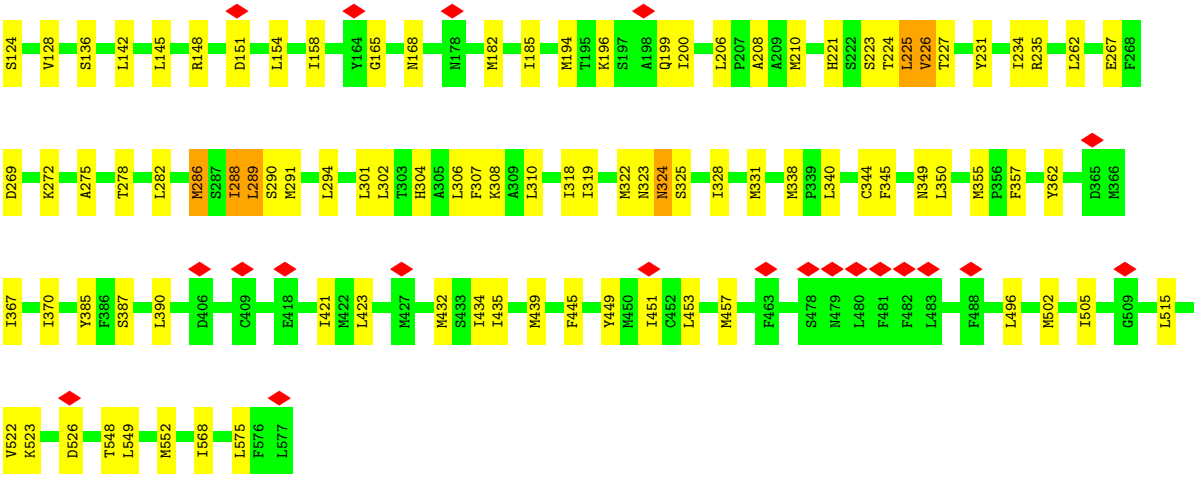
Chain 4:



• Molecule 10: NADH-ubiquinone oxidoreductase chain 5

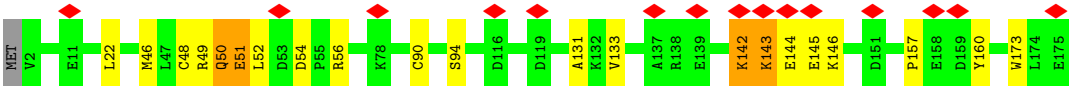
Chain 5:





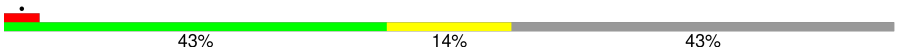
• Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

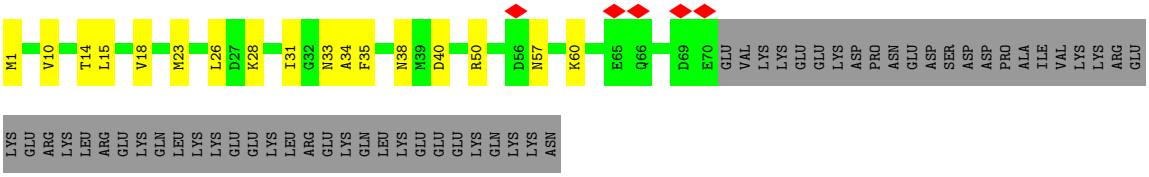
Chain A8:



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

Chain A1:



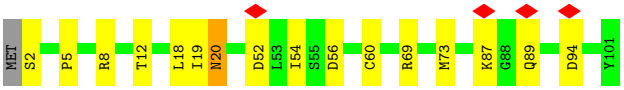


• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain AO:

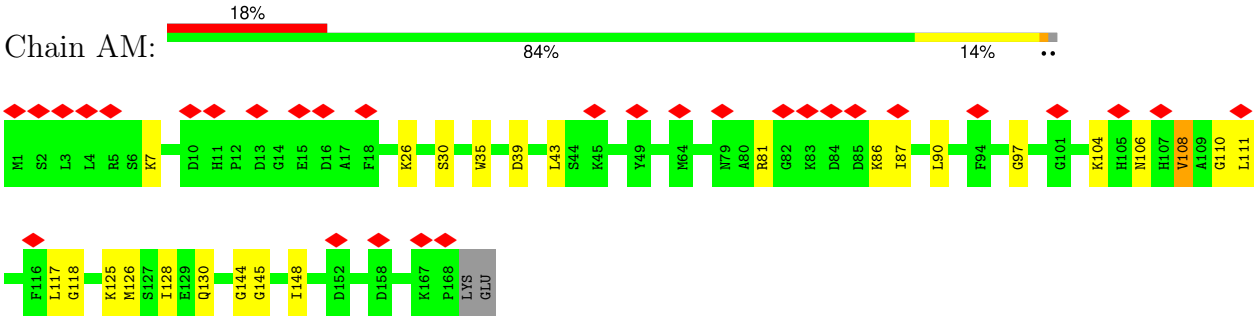
• Molecule 14: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain S5:



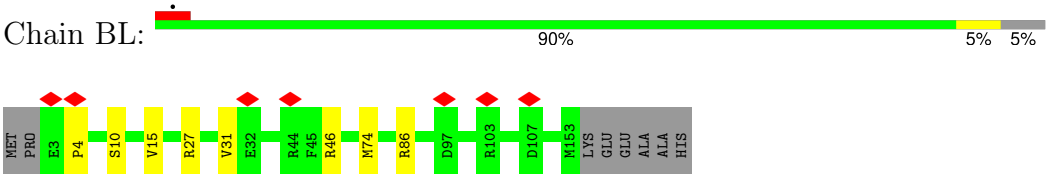
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain AM:



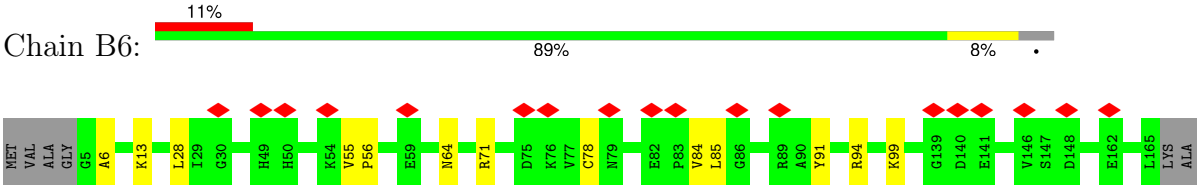
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain BL:



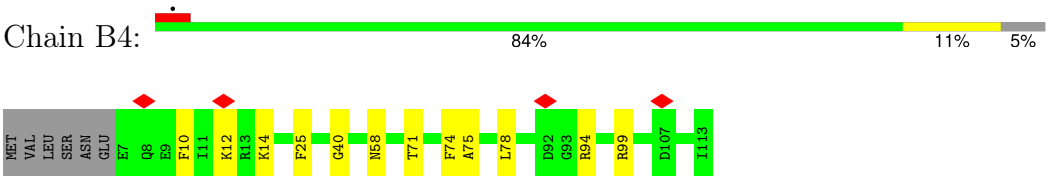
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain B6:



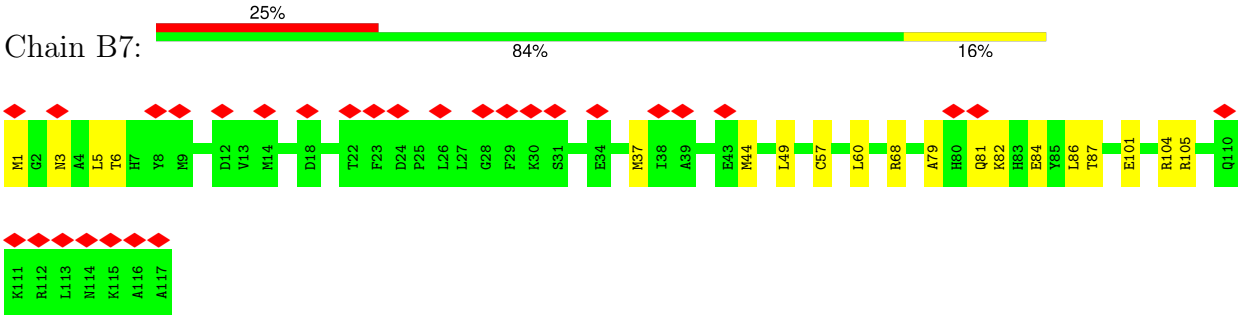
• Molecule 18: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain B4:



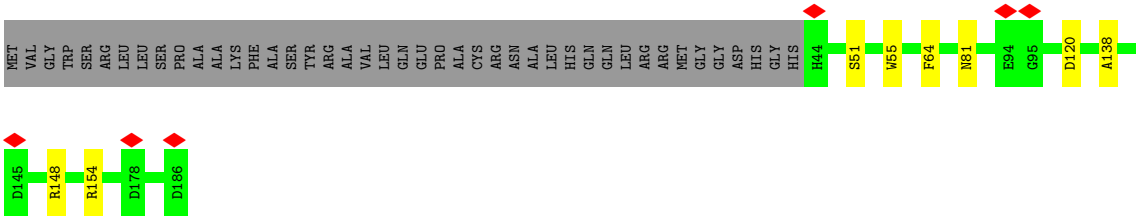
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain B7:



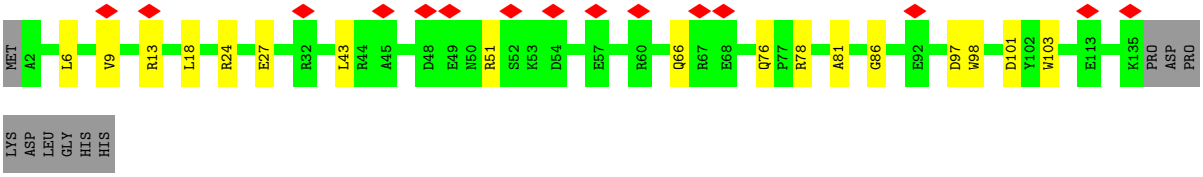
• Molecule 20: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain B5:



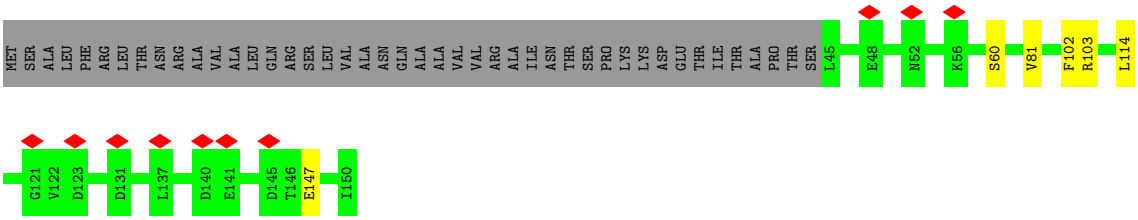
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain B9:



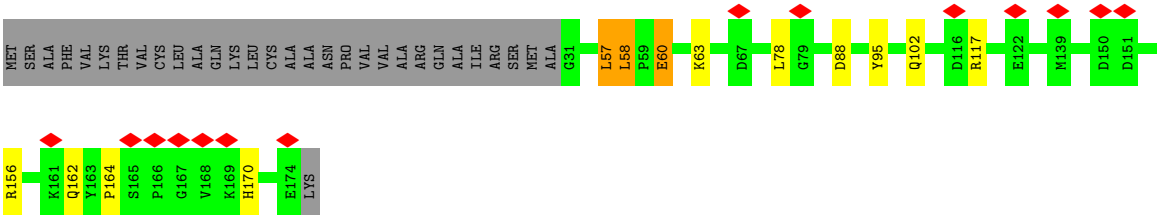
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain BM:



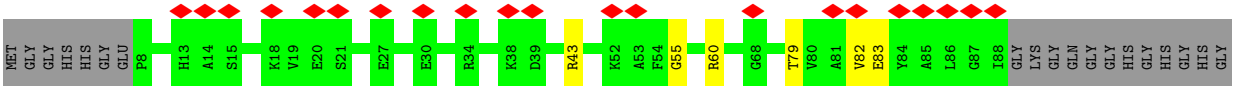
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain B8:



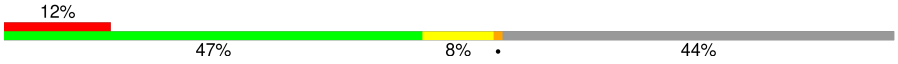
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

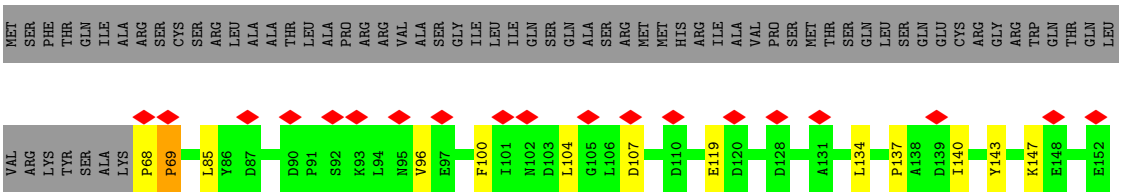
Chain B3:



• Molecule 25: Acyl carrier protein, mitochondrial

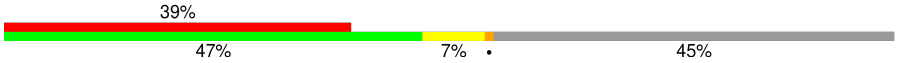
Chain AC:

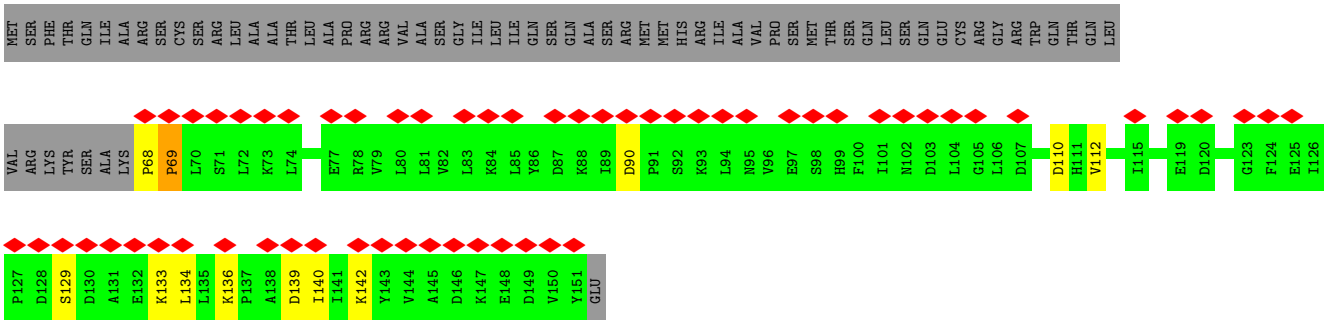




• Molecule 25: Acyl carrier protein, mitochondrial

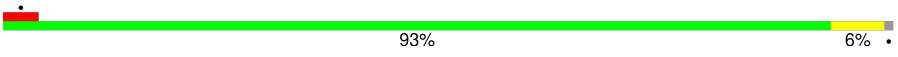
Chain AB:

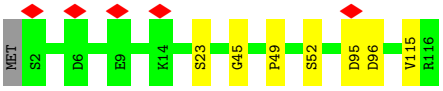




• Molecule 26: NADH dehydrogenase [ubiquinone] 1 subunit C2

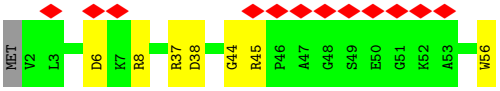
Chain C2:





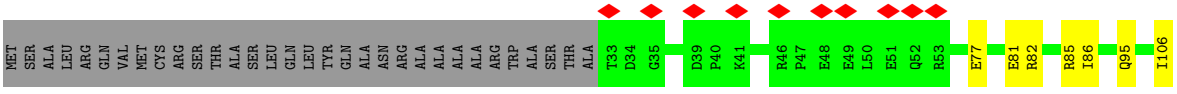
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

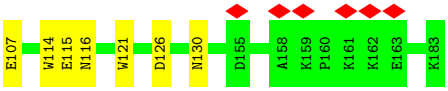
Chain B1:



• Molecule 28: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

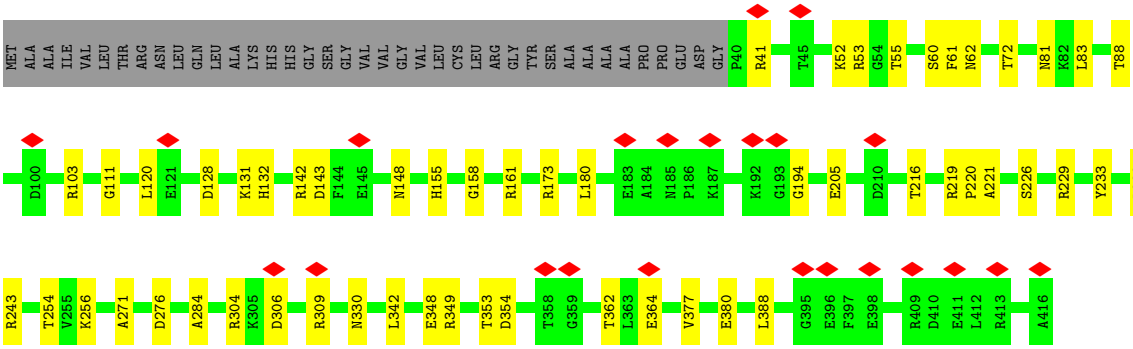
Chain S4:





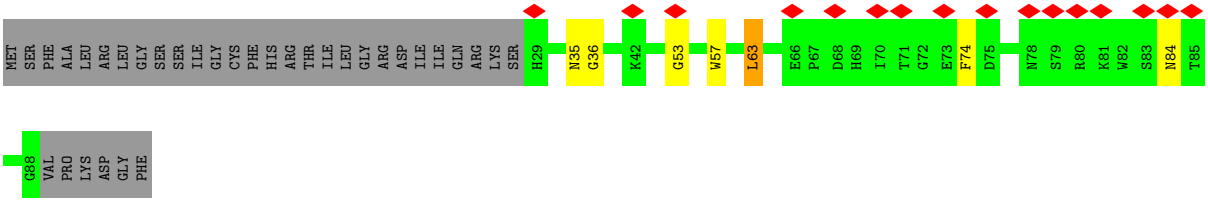
• Molecule 29: NADH dehydrogenase (Ubiquinone) 39 kDa subunit, isoform A

Chain A9:



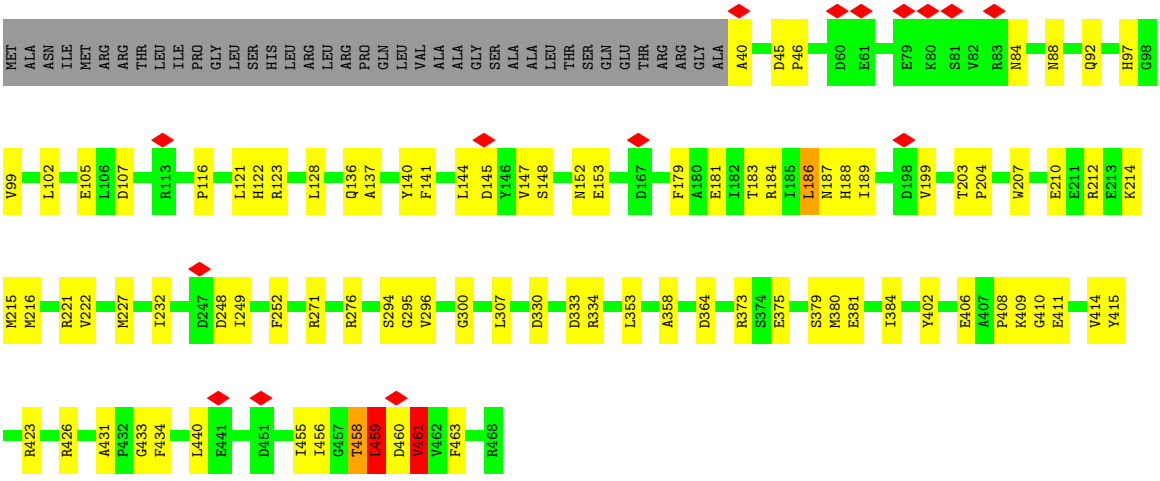
• Molecule 30: GEO11417p1

Chain B2:



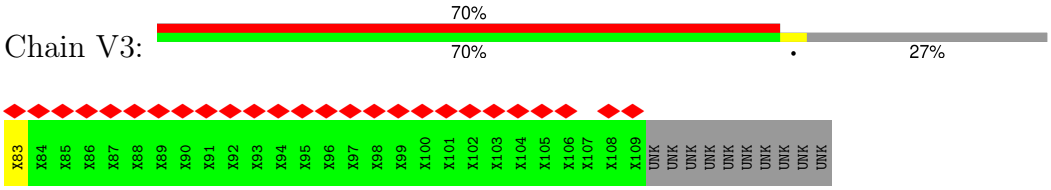
• Molecule 31: Complex I-49kD

Chain S2:



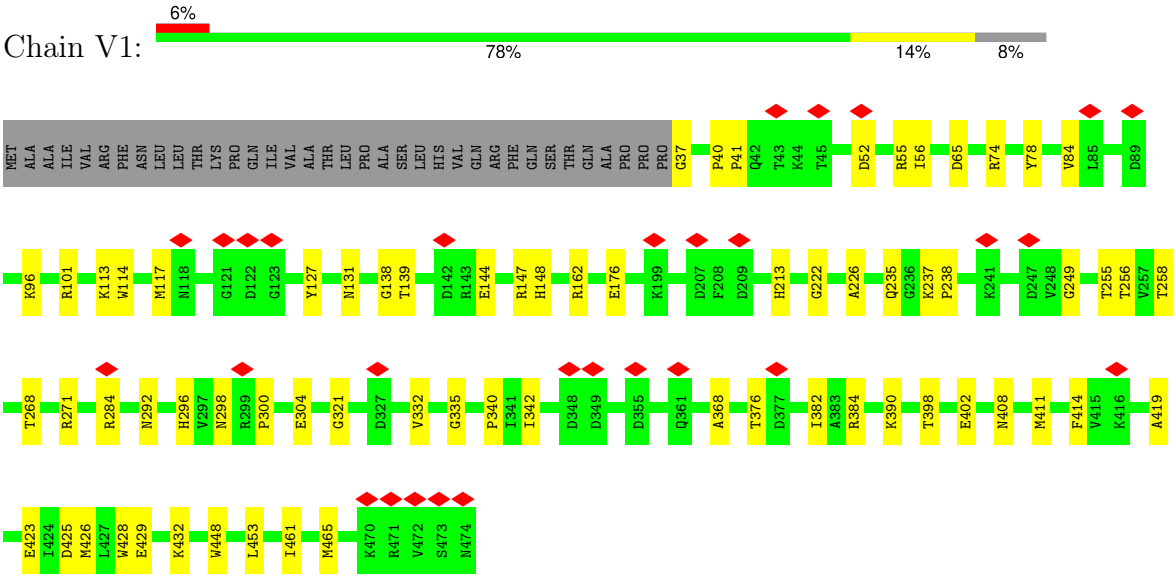
• Molecule 32: NADH dehydrogenase [ubiquinone] flavoprotein 3

Chain V3:



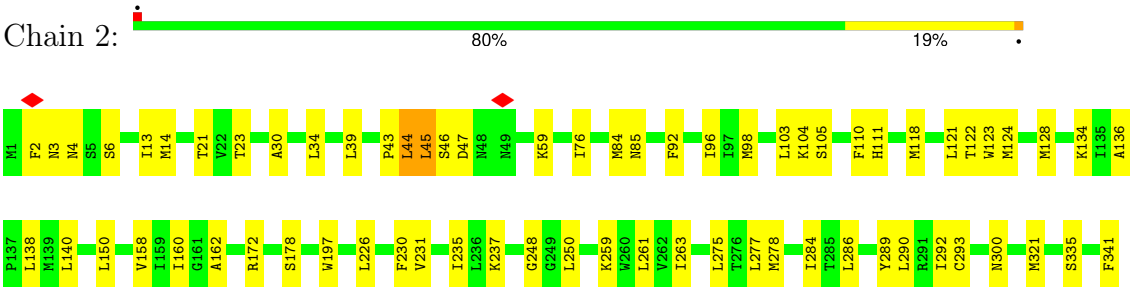
• Molecule 33: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain V1:



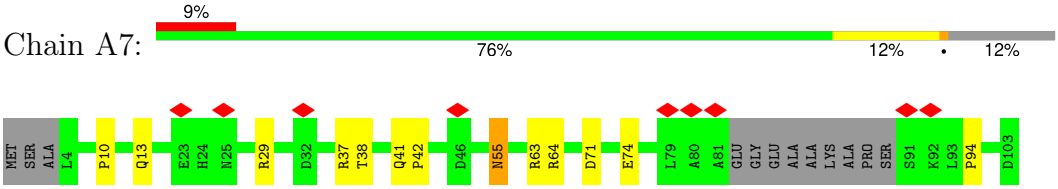
• Molecule 34: NADH-ubiquinone oxidoreductase chain 2

Chain 2:



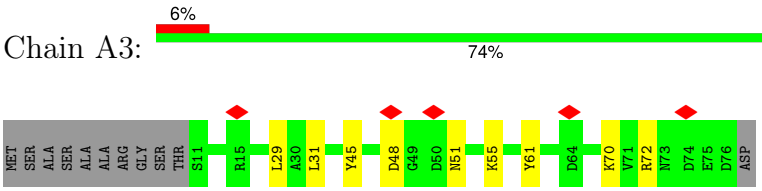
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain A7:



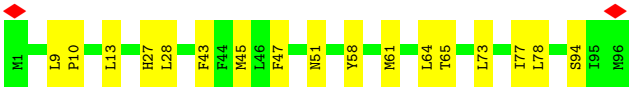
• Molecule 36: RH45008p

Chain A3:



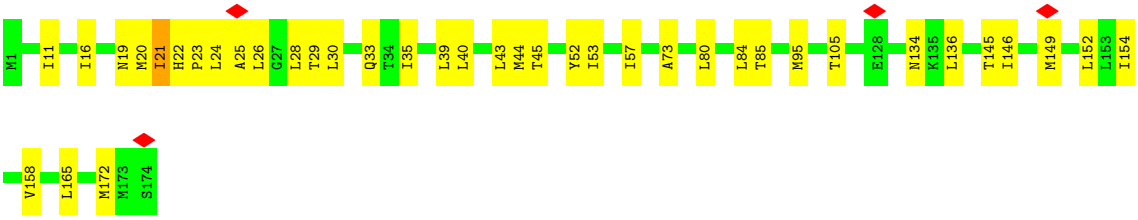
• Molecule 37: NADH-ubiquinone oxidoreductase chain 4L

Chain 4L:



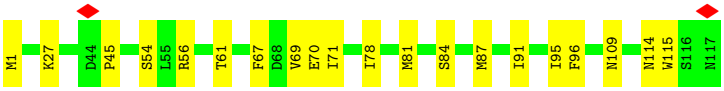
• Molecule 38: NADH-ubiquinone oxidoreductase chain 6

Chain 6:



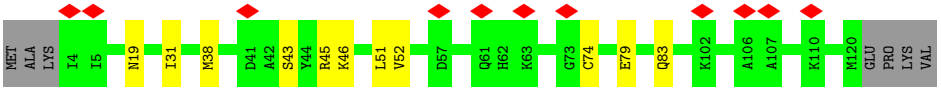
• Molecule 39: NADH-ubiquinone oxidoreductase chain 3

Chain 3:



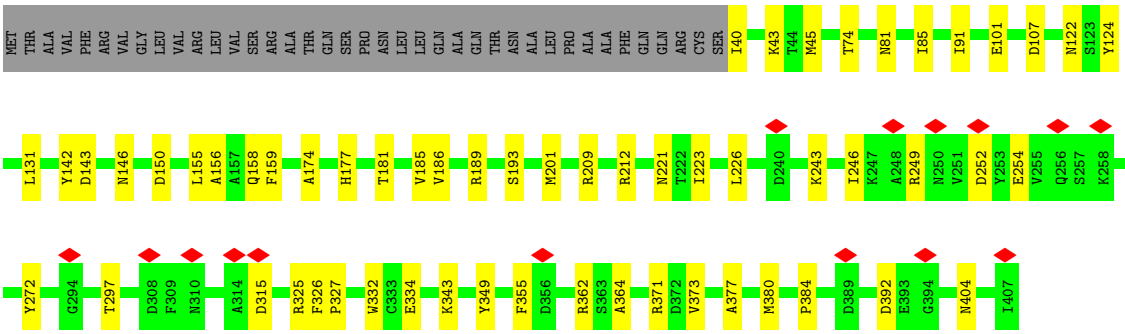
• Molecule 40: NADH dehydrogenase (Ubiquinone) 13 kDa B subunit

Chain A5:



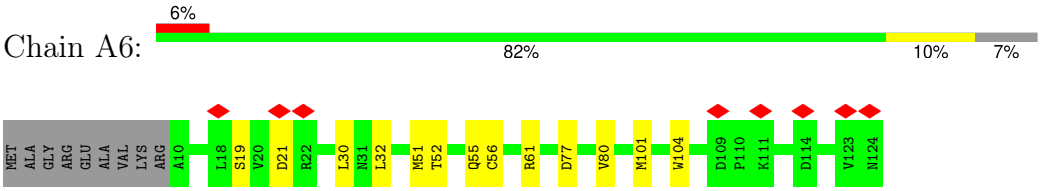
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain AL:



• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain A6:


6%
82%
10%
7%
MET
ALA
GLY
ARG
GLU
ALA
VAL
LYS
ARG
A10
L18
S19
V20
D21
R22
L30
N31
L32
M51
T52
Q55
C56
R61
D77
V80
M101
W104
D109
P110
K111
D114
V123
N124

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	293389	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.876	Depositor
Minimum map value	-1.949	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	450.56, 450.56, 450.56	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, NDP, OCT, SF4, U10, DGT, FMN, ZMP, C14, FES, D12, ZN, CDL, WSF, 3PE

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	AN	0.26	0/1185	0.54	0/1605
2	S6	0.13	0/733	0.33	0/987
3	S1	0.21	0/5264	0.52	1/7133 (0.0%)
4	S3	0.21	0/1745	0.49	0/2370
5	V2	0.24	0/1719	0.56	0/2328
6	S7	0.34	0/1473	0.66	1/1997 (0.1%)
7	S8	0.22	0/1518	0.50	0/2050
8	1	0.32	0/2651	0.62	0/3593
9	4	0.35	1/3711 (0.0%)	0.69	1/5029 (0.0%)
10	5	0.38	0/4726	0.71	1/6396 (0.0%)
11	A8	0.32	0/1417	0.57	0/1911
12	A1	0.24	0/594	0.57	0/801
13	AO	0.24	0/1240	0.47	0/1682
14	S5	0.22	0/846	0.54	0/1128
15	AM	0.27	0/1318	0.53	0/1790
16	BL	0.25	0/1299	0.57	0/1754
17	B6	0.21	0/1338	0.52	0/1808
18	B4	0.23	0/905	0.50	0/1210
19	B7	0.27	0/995	0.58	0/1336
20	B5	0.19	0/1255	0.44	0/1694
21	B9	0.21	0/1181	0.43	0/1593
22	BM	0.19	0/896	0.44	0/1222
23	B8	0.28	0/1250	0.53	0/1701
24	B3	0.17	0/665	0.41	0/903
25	AB	0.23	0/680	0.62	2/919 (0.2%)
25	AC	0.24	0/690	0.67	2/931 (0.2%)
26	C2	0.24	0/936	0.46	0/1271
27	B1	0.19	0/441	0.47	0/590
28	S4	0.24	0/1245	0.54	0/1687
29	A9	0.20	0/3105	0.49	2/4200 (0.0%)
30	B2	0.20	0/519	0.47	0/713
31	S2	0.29	0/3512	0.63	5/4761 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	V1	0.24	0/3438	0.54	0/4643
34	2	0.26	0/2876	0.60	3/3890 (0.1%)
35	A7	0.18	0/752	0.45	0/1018
36	A3	0.18	0/528	0.43	0/714
37	4L	0.26	0/815	0.57	0/1095
38	6	0.34	0/1431	0.69	0/1933
39	3	0.33	0/979	0.69	2/1325 (0.2%)
40	A5	0.20	0/933	0.48	0/1265
41	AL	0.20	0/3083	0.46	0/4168
42	A6	0.25	0/997	0.56	0/1340
All	All	0.27	1/66884 (0.0%)	0.57	20/90484 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	S7	0	1
16	BL	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	4	12	ILE	C-N	5.66	1.39	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	2	44	LEU	N-CA-C	-7.79	98.96	110.48
25	AC	69	PRO	N-CA-CB	7.42	111.04	103.25
25	AB	69	PRO	N-CA-CB	7.24	110.85	103.25
25	AC	68	PRO	N-CA-CB	6.75	110.42	103.00
25	AB	68	PRO	N-CA-CB	6.74	110.42	103.00
31	S2	459	LEU	N-CA-C	-6.47	100.70	110.28
9	4	40	ASN	N-CA-C	-6.38	104.72	114.16
3	S1	231	GLU	N-CA-C	-5.92	106.40	113.21
6	S7	95	ALA	N-CA-C	5.89	115.79	108.19
39	3	45	PRO	CA-C-N	5.70	132.42	121.54
39	3	45	PRO	C-N-CA	5.70	132.42	121.54
34	2	2	PHE	CA-C-N	5.67	133.31	123.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	2	2	PHE	C-N-CA	5.67	133.31	123.91
29	A9	226	SER	CA-C-N	5.46	130.10	122.08
29	A9	226	SER	C-N-CA	5.46	130.10	122.08
31	S2	461	VAL	CA-C-N	-5.40	113.60	121.71
31	S2	461	VAL	C-N-CA	-5.40	113.60	121.71
31	S2	459	LEU	CA-C-N	-5.36	115.33	122.72
31	S2	459	LEU	C-N-CA	-5.36	115.33	122.72
10	5	385	TYR	CB-CA-C	5.12	119.29	110.79

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	BL	86	ARG	Sidechain
6	S7	191	CYS	Peptide

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	AN	1145	0	1102	20	0
2	S6	716	0	700	7	0
3	S1	5181	0	5227	62	0
4	S3	1699	0	1648	26	0
5	V2	1680	0	1657	15	0
6	S7	1435	0	1448	42	0
7	S8	1485	0	1422	24	0
8	1	2571	0	2628	52	0
9	4	3606	0	3740	82	0
10	5	4606	0	4742	90	0
11	A8	1384	0	1324	13	0
12	A1	581	0	582	12	0
13	AO	1202	0	1211	12	0
14	S5	828	0	807	12	0
15	AM	1281	0	1267	19	0
16	BL	1266	0	1205	5	0
17	B6	1302	0	1295	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	B4	884	0	879	12	0
19	B7	972	0	959	13	0
20	B5	1221	0	1186	8	0
21	B9	1148	0	1113	12	0
22	BM	871	0	822	6	0
23	B8	1201	0	1107	12	0
24	B3	646	0	641	4	0
25	AB	670	0	669	7	0
25	AC	680	0	675	8	0
26	C2	908	0	896	7	0
27	B1	430	0	436	5	0
28	S4	1214	0	1186	10	0
29	A9	3030	0	3032	38	0
30	B2	495	0	457	5	0
31	S2	3427	0	3399	74	0
32	V3	135	0	30	1	0
33	V1	3361	0	3339	41	0
34	2	2797	0	2879	49	0
35	A7	736	0	737	10	0
36	A3	519	0	517	7	0
37	4L	794	0	818	16	0
38	6	1404	0	1517	34	0
39	3	956	0	1030	18	0
40	A5	914	0	944	8	0
41	AL	3008	0	2945	39	0
42	A6	977	0	997	8	0
43	2	45	0	34	1	0
43	3	54	0	52	0	0
43	6	86	0	122	4	0
43	AM	76	0	96	5	0
43	AN	67	0	78	3	0
43	B5	142	0	172	7	0
43	B6	47	0	38	2	0
44	1	54	0	88	2	0
44	2	45	0	67	1	0
44	4	78	0	104	4	0
44	5	34	0	41	3	0
44	A9	44	0	62	3	0
44	AM	113	0	151	5	0
44	AN	44	0	62	2	0
44	B6	37	0	48	1	0
44	S7	46	0	69	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	S6	1	0	0	0	0
46	S1	16	0	0	0	0
46	S7	8	0	0	7	0
46	S8	16	0	0	0	0
46	V1	8	0	0	0	0
47	S1	4	0	0	0	0
47	V2	4	0	0	0	0
48	1	51	0	82	1	0
48	2	30	0	34	2	0
48	3	92	0	141	3	0
48	4	152	0	203	3	0
48	5	275	0	377	9	0
48	6	35	0	43	2	0
48	AM	72	0	95	3	0
48	B1	37	0	48	0	0
48	B4	47	0	71	0	0
48	B6	48	0	75	2	0
48	C2	45	0	67	1	0
48	S7	66	0	80	3	0
49	1	63	0	87	3	0
50	AO	14	0	30	0	0
50	B5	14	0	30	0	0
50	C2	14	0	30	0	0
51	AB	32	0	36	0	0
51	AC	34	0	40	1	0
52	B1	8	0	18	0	0
53	A3	12	0	26	0	0
53	A9	24	0	52	0	0
53	B1	12	0	26	0	0
54	A9	48	0	26	0	0
55	V1	31	0	19	2	0
56	6	35	0	0	8	0
57	AL	31	0	12	5	0
All	All	67757	0	68247	819	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 6.

All (819) 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)
6:S7:97:CYS:SG	46:S7:301:SF4:FE1	1.46	1.06
31:S2:186:LEU:HD12	31:S2:212:ARG:HG3	1.42	1.02
38:6:20:MET:HE3	38:6:25:ALA:HB1	1.43	0.97
56:6:201:WSF:C13	56:6:201:WSF:C15	2.43	0.96
56:6:201:WSF:C15	56:6:201:WSF:C14	2.44	0.96
56:6:201:WSF:C13	56:6:201:WSF:C14	2.43	0.96
56:6:201:WSF:C13	56:6:201:WSF:C12	2.46	0.93
56:6:201:WSF:C15	56:6:201:WSF:C12	2.47	0.92
56:6:201:WSF:C14	56:6:201:WSF:C12	2.48	0.90
10:5:262:LEU:HD12	10:5:390:LEU:HD21	1.51	0.89
31:S2:186:LEU:CD1	31:S2:212:ARG:HG3	2.06	0.86
31:S2:186:LEU:HD13	31:S2:215:MET:SD	2.16	0.85
9:4:396:LEU:O	9:4:400:SER:HB2	1.83	0.79
6:S7:97:CYS:HG	46:S7:301:SF4:FE1	1.02	0.77
9:4:198:PHE:O	9:4:201:HIS:ND1	2.20	0.74
6:S7:96:CYS:SG	46:S7:301:SF4:FE4	1.78	0.73
8:1:189:ALA:O	8:1:193:VAL:HG23	1.88	0.73
31:S2:187:ASN:HD21	31:S2:409:LYS:HE2	1.53	0.73
10:5:234:ILE:HG13	10:5:289:LEU:HD11	1.70	0.72
3:S1:497:GLY:O	3:S1:500:ILE:HB	1.90	0.71
9:4:162:MET:HB2	9:4:168:MET:HE3	1.71	0.71
38:6:22:HIS:HE1	38:6:24:LEU:HD12	1.56	0.70
5:V2:131:THR:HA	5:V2:134:TRP:HB3	1.75	0.69
9:4:130:TRP:O	9:4:212:PRO:HB3	1.91	0.69
7:S8:106:HIS:HE1	7:S8:157:CYS:SG	2.07	0.68
3:S1:498:ALA:O	3:S1:501:HIS:HB3	1.95	0.66
38:6:16:ILE:O	38:6:20:MET:HG2	1.96	0.66
4:S3:165:ALA:HA	4:S3:168:TYR:HB2	1.78	0.66
38:6:20:MET:HE1	43:6:203:CDL:OA8	1.96	0.65
33:V1:335:GLY:HA2	33:V1:368:ALA:H	1.61	0.65
34:2:44:LEU:O	34:2:45:LEU:HB3	1.96	0.65
8:1:282:TYR:CE2	39:3:115:TRP:HH2	2.16	0.64
6:S7:99:VAL:HG13	31:S2:212:ARG:HH12	1.63	0.64
10:5:234:ILE:HA	10:5:289:LEU:HD21	1.79	0.63
12:A1:31:ILE:HG22	12:A1:33:ASN:H	1.63	0.63
10:5:120:LEU:HG	10:5:225:LEU:HD12	1.80	0.63
6:S7:133:THR:HG21	31:S2:123:ARG:HG2	1.80	0.62
9:4:188:LEU:HD11	9:4:235:ILE:HD11	1.79	0.62
44:4:501:PC1:H152	22:BM:103:ARG:HH12	1.64	0.62
10:5:101:MET:HE3	10:5:105:ILE:HD11	1.82	0.62
10:5:345:PHE:O	10:5:349:ASN:HB2	1.98	0.61
37:4L:51:ASN:HD22	38:6:44:MET:HB2	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:A7:10:PRO:HA	35:A7:13:GLN:HB2	1.83	0.61
4:S3:167:TRP:O	4:S3:170:ARG:HB2	2.00	0.61
10:5:568:ILE:HD12	34:2:96:ILE:HG23	1.83	0.60
3:S1:205:GLY:HA3	3:S1:450:SER:HB2	1.83	0.60
9:4:108:SER:HB3	9:4:168:MET:HB2	1.83	0.60
33:V1:226:ALA:HB2	33:V1:238:PRO:HG3	1.82	0.60
10:5:120:LEU:HG	10:5:225:LEU:CD1	2.32	0.60
10:5:304:HIS:HA	10:5:307:PHE:CE2	2.36	0.60
15:AM:106:ASN:HD21	15:AM:108:VAL:HG12	1.65	0.60
6:S7:98:ALA:HA	6:S7:101:MET:HE3	1.84	0.59
31:S2:409:LYS:HG2	31:S2:460:ASP:HB3	1.83	0.59
6:S7:103:HIS:NE2	31:S2:216:MET:SD	2.75	0.59
9:4:162:MET:CB	9:4:168:MET:HE3	2.32	0.59
38:6:85:THR:HG22	43:6:203:CDL:H132	1.85	0.59
4:S3:176:TYR:HH	31:S2:426:ARG:HE	1.50	0.59
5:V2:63:TYR:HH	33:V1:213:HIS:HD1	1.49	0.59
18:B4:10:PHE:CD1	23:B8:60:GLU:HG3	2.38	0.59
8:1:1:MET:HE1	8:1:5:GLU:CB	2.33	0.59
44:4:505:PC1:H133	34:2:335:SER:HB2	1.83	0.59
31:S2:431:ALA:HB3	31:S2:434:PHE:HB2	1.85	0.59
41:AL:201:MET:HE2	57:AL:501:DGT:HN2	1.67	0.59
5:V2:136:ARG:HH12	33:V1:300:PRO:HG3	1.68	0.58
38:6:22:HIS:CE1	38:6:24:LEU:HD12	2.36	0.58
9:4:96:LEU:HD22	9:4:122:PRO:HB2	1.85	0.58
6:S7:66:SER:HB2	6:S7:69:GLU:HB2	1.85	0.58
4:S3:232:PHE:O	28:S4:130:ASN:ND2	2.32	0.58
34:2:263:ILE:HG12	34:2:275:LEU:HD11	1.86	0.58
10:5:234:ILE:HG23	10:5:294:LEU:HB2	1.84	0.58
19:B7:44:MET:HG3	19:B7:49:LEU:HD12	1.85	0.58
44:A9:501:PC1:H32	38:6:80:LEU:HD12	1.85	0.58
34:2:231:VAL:HG21	34:2:237:LYS:HB2	1.85	0.58
1:AN:10:LEU:HD11	43:AN:201:CDL:H522	1.86	0.58
6:S7:78:LEU:HB2	48:S7:303:3PE:H242	1.86	0.57
8:1:209:GLU:HA	8:1:217:GLY:HA3	1.86	0.57
9:4:292:MET:HB2	26:C2:115:VAL:HG11	1.85	0.57
10:5:288:ILE:HG12	10:5:367:ILE:HG23	1.86	0.57
29:A9:377:VAL:HA	29:A9:380:GLU:HB2	1.87	0.57
36:A3:51:ASN:ND2	36:A3:70:LYS:O	2.38	0.57
9:4:358:PRO:HG3	10:5:118:ASP:HB2	1.86	0.57
44:4:505:PC1:H112	26:C2:23:SER:HA	1.85	0.57
10:5:221:HIS:HB3	10:5:278:THR:HG21	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:AL:91:ILE:HD12	57:AL:501:DGT:H2'A	1.85	0.57
43:B5:201:CDL:HA32	43:B5:201:CDL:H542	1.85	0.57
10:5:350:LEU:HD12	10:5:355:MET:HB2	1.87	0.57
34:2:162:ALA:HB1	34:2:284:ILE:HB	1.87	0.57
35:A7:63:ARG:HH21	35:A7:64:ARG:HH21	1.52	0.57
48:1:403:3PE:H3F2	38:6:28:LEU:HD21	1.87	0.56
9:4:161:VAL:HG13	9:4:165:ILE:HD12	1.86	0.56
9:4:273:LEU:HD22	9:4:398:LEU:HD12	1.87	0.56
11:A8:142:LYS:HE2	11:A8:144:GLU:HA	1.87	0.56
3:S1:280:ARG:HG2	3:S1:281:THR:HG23	1.86	0.56
21:B9:98:TRP:O	21:B9:101:ASP:HB2	2.05	0.56
25:AB:134:LEU:HD23	25:AB:140:ILE:HD13	1.86	0.56
28:S4:114:TRP:HB2	29:A9:53:ARG:HD2	1.87	0.56
6:S7:124:GLN:NE2	8:1:219:ASN:O	2.38	0.56
42:A6:52:THR:HB	42:A6:55:GLN:HG3	1.88	0.56
31:S2:148:SER:O	31:S2:152:ASN:ND2	2.38	0.56
1:AN:93:ASP:H	35:A7:38:THR:HG23	1.70	0.56
10:5:262:LEU:CD1	10:5:390:LEU:HD21	2.31	0.56
14:S5:20:ASN:HD22	14:S5:20:ASN:C	2.13	0.56
15:AM:7:LYS:HE3	43:AM:204:CDL:HA21	1.87	0.56
34:2:158:VAL:HG11	34:2:278:MET:HG2	1.88	0.56
7:S8:64:SER:O	31:S2:271:ARG:NH2	2.39	0.56
37:4L:43:PHE:O	37:4L:47:PHE:HB2	2.05	0.56
9:4:162:MET:HB2	9:4:168:MET:CE	2.36	0.55
8:1:147:ILE:HD13	39:3:61:THR:HG22	1.88	0.55
3:S1:231:GLU:HG3	3:S1:423:PRO:HB3	1.88	0.55
8:1:168:ASN:ND2	12:A1:40:ASP:OD2	2.39	0.55
9:4:242:ASN:ND2	9:4:292:MET:SD	2.77	0.55
10:5:194:MET:HG3	10:5:199:GLN:HB2	1.88	0.55
9:4:131:GLY:O	31:S2:40:ALA:N	2.39	0.55
1:AN:34:ASP:OD2	6:S7:113:ARG:NH2	2.40	0.55
1:AN:35:ASP:OD2	1:AN:61:ARG:NH2	2.39	0.55
10:5:223:SER:HA	10:5:227:THR:HG21	1.89	0.55
1:AN:135:TRP:O	1:AN:136:GLU:HB2	2.05	0.55
3:S1:472:ALA:HA	3:S1:475:LYS:HD2	1.89	0.55
9:4:26:ILE:HG23	22:BM:81:VAL:HG11	1.87	0.55
10:5:221:HIS:HA	10:5:226:VAL:CG1	2.37	0.55
13:AO:98:GLU:OE2	14:S5:69:ARG:NH2	2.39	0.55
18:B4:12:LYS:HZ1	21:B9:6:LEU:HD21	1.72	0.55
1:AN:9:ARG:HB3	43:AN:201:CDL:HA22	1.88	0.55
13:AO:89:ARG:HD2	13:AO:93:ARG:HH21	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S1:411:VAL:HG22	3:S1:438:LEU:HD21	1.90	0.54
33:V1:139:THR:HA	33:V1:292:ASN:HD21	1.72	0.54
9:4:162:MET:O	9:4:166:GLY:N	2.38	0.54
31:S2:99:VAL:HG11	31:S2:121:LEU:HD13	1.88	0.54
34:2:263:ILE:HG23	34:2:275:LEU:HD21	1.89	0.54
41:AL:201:MET:CE	57:AL:501:DGT:HN2	2.20	0.54
8:1:88:LEU:HD13	8:1:118:LEU:HB3	1.88	0.54
33:V1:419:ALA:HB1	33:V1:423:GLU:HG3	1.88	0.54
7:S8:101:ARG:NH1	31:S2:222:VAL:O	2.40	0.54
9:4:165:ILE:HD13	9:4:173:MET:HG2	1.89	0.54
9:4:196:PRO:HG3	9:4:204:LEU:HD22	1.88	0.54
9:4:325:LEU:HD11	9:4:336:LEU:HD21	1.90	0.54
29:A9:60:SER:OG	29:A9:61:PHE:N	2.41	0.54
1:AN:9:ARG:NH1	43:AN:201:CDL:O1	2.40	0.54
9:4:198:PHE:O	9:4:201:HIS:CE1	2.60	0.54
10:5:36:PHE:CD1	10:5:108:PRO:HG2	2.43	0.54
10:5:357:PHE:HE2	30:B2:63:LEU:HD13	1.72	0.54
8:1:169:MET:O	8:1:172:PHE:HB2	2.08	0.54
3:S1:160:ARG:NH2	31:S2:364:ASP:O	2.41	0.54
28:S4:77:GLU:O	28:S4:81:GLU:HB2	2.07	0.54
3:S1:151:ASP:OD2	28:S4:95:GLN:NE2	2.41	0.54
6:S7:113:ARG:NH2	7:S8:90:ASN:OD1	2.40	0.54
9:4:72:MET:HG3	9:4:214:SER:HA	1.89	0.54
9:4:295:TRP:HE1	10:5:45:ASN:HB2	1.73	0.54
9:4:374:VAL:HG13	9:4:381:MET:HE2	1.89	0.54
3:S1:183:VAL:HG12	3:S1:237:ILE:HD11	1.90	0.53
9:4:264:CYS:HB3	9:4:273:LEU:HG	1.90	0.53
29:A9:143:ASP:OD1	29:A9:349:ARG:NH1	2.42	0.53
8:1:158:LEU:HD23	39:3:78:ILE:HD11	1.88	0.53
11:A8:46:MET:HE3	11:A8:50:GLN:HE22	1.73	0.53
8:1:1:MET:HE1	8:1:5:GLU:HB2	1.90	0.53
31:S2:204:PRO:HA	31:S2:207:TRP:HB2	1.90	0.53
33:V1:131:ASN:ND2	33:V1:222:GLY:O	2.41	0.53
7:S8:98:LEU:O	35:A7:37:ARG:NH2	2.41	0.53
7:S8:121:CYS:HA	7:S8:145:ARG:HH21	1.72	0.53
42:A6:32:LEU:HD11	42:A6:80:VAL:HA	1.90	0.53
9:4:62:ILE:HG23	9:4:101:ILE:HG12	1.90	0.53
14:S5:5:PRO:HB2	14:S5:8:ARG:HB3	1.90	0.53
29:A9:72:THR:O	29:A9:103:ARG:NH2	2.40	0.53
31:S2:455:ILE:O	31:S2:459:LEU:HG	2.08	0.53
34:2:121:LEU:O	34:2:172:ARG:NH1	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S1:443:ILE:HD13	3:S1:463:VAL:HG22	1.89	0.53
5:V2:127:VAL:HG21	5:V2:142:LEU:HD13	1.90	0.53
6:S7:74:ARG:HB3	48:S7:303:3PE:H251	1.90	0.53
31:S2:199:VAL:HG13	31:S2:276:ARG:HG2	1.91	0.53
37:4L:64:LEU:HD22	38:6:57:ILE:HG21	1.91	0.53
7:S8:213:ASP:OD2	7:S8:217:ARG:NH2	2.41	0.53
8:1:27:LEU:HD22	8:1:239:LEU:HG	1.90	0.53
10:5:267:GLU:OE1	21:B9:76:GLN:NE2	2.42	0.53
3:S1:411:VAL:HG12	3:S1:484:ALA:HB3	1.91	0.53
8:1:188:MET:HA	8:1:191:VAL:HB	1.89	0.53
10:5:221:HIS:HA	10:5:226:VAL:HG11	1.90	0.53
19:B7:105:ARG:NH1	30:B2:84:ASN:OD1	2.42	0.53
31:S2:184:ARG:NH2	31:S2:406:GLU:O	2.42	0.53
3:S1:532:LEU:HD21	3:S1:538:ALA:HB2	1.90	0.53
10:5:515:LEU:HD13	23:B8:117:ARG:HD3	1.91	0.53
31:S2:188:HIS:CE1	31:S2:408:PRO:HB3	2.43	0.53
34:2:178:SER:OG	34:2:289:TYR:OH	2.27	0.53
6:S7:134:LEU:HD21	6:S7:181:ILE:HD12	1.91	0.53
9:4:121:ILE:HD11	34:2:250:LEU:HB3	1.91	0.53
16:BL:46:ARG:NH1	27:B1:44:GLY:O	2.41	0.53
21:B9:97:ASP:N	21:B9:97:ASP:OD1	2.41	0.53
31:S2:141:PHE:HA	31:S2:144:LEU:HD23	1.91	0.53
41:AL:85:ILE:O	41:AL:186:VAL:HA	2.08	0.53
3:S1:289:PRO:HG3	3:S1:300:LEU:HB2	1.92	0.52
33:V1:37:GLY:HA2	33:V1:96:LYS:HB3	1.91	0.52
3:S1:77:GLU:OE2	3:S1:78:ARG:NH2	2.42	0.52
5:V2:92:HIS:NE2	5:V2:106:TYR:OH	2.43	0.52
13:AO:152:LEU:O	39:3:1:MET:N	2.42	0.52
21:B9:24:ARG:NH2	25:AC:119:GLU:OE1	2.41	0.52
25:AC:100:PHE:HA	25:AC:104:LEU:HD12	1.89	0.52
38:6:30:LEU:HA	38:6:33:GLN:HB2	1.92	0.52
38:6:20:MET:HE2	38:6:29:THR:OG1	2.08	0.52
2:S6:87:CYS:O	2:S6:98:LYS:HA	2.10	0.52
8:1:315:LEU:HD13	13:AO:62:LYS:HD3	1.92	0.52
15:AM:144:GLY:HA3	15:AM:148:ILE:HD12	1.90	0.52
3:S1:495:ALA:O	3:S1:498:ALA:HB3	2.09	0.52
8:1:39:GLN:HG3	31:S2:203:THR:HG23	1.92	0.52
14:S5:94:ASP:OD1	14:S5:94:ASP:N	2.43	0.52
15:AM:81:ARG:HH12	15:AM:87:ILE:HD11	1.75	0.52
17:B6:71:ARG:HD2	17:B6:94:ARG:HH22	1.75	0.52
31:S2:145:ASP:OD2	31:S2:148:SER:OG	2.22	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:6:203:CDL:H222	43:6:203:CDL:H341	1.90	0.52
1:AN:72:ASN:HD22	44:AN:202:PC1:H111	1.75	0.52
4:S3:131:VAL:HG22	4:S3:146:LYS:HG2	1.92	0.52
4:S3:189:ILE:HG23	4:S3:190:LEU:HG	1.90	0.52
9:4:127:ILE:CD1	9:4:211:ALA:HB2	2.40	0.51
14:S5:18:LEU:HG	14:S5:19:ILE:HG12	1.93	0.51
15:AM:126:MET:O	15:AM:130:GLN:HB2	2.09	0.51
29:A9:233:TYR:OH	29:A9:239:ARG:NH1	2.44	0.51
8:1:176:GLN:NE2	8:1:248:ILE:O	2.41	0.51
12:A1:33:ASN:ND2	12:A1:35:PHE:O	2.43	0.51
31:S2:179:PHE:O	31:S2:183:THR:OG1	2.28	0.51
3:S1:230:THR:C	3:S1:232:LEU:H	2.18	0.51
3:S1:293:GLU:O	3:S1:428:ARG:NH2	2.43	0.51
9:4:112:PHE:O	9:4:116:PHE:HB3	2.09	0.51
10:5:54:LEU:HD13	10:5:108:PRO:HG3	1.92	0.51
10:5:124:SER:HB2	10:5:225:LEU:HD13	1.92	0.51
11:A8:90:CYS:O	11:A8:94:SER:HB2	2.09	0.51
31:S2:295:GLY:HA3	31:S2:410:GLY:HA2	1.92	0.51
4:S3:100:GLN:NE2	4:S3:104:ASP:OD2	2.43	0.51
4:S3:233:ARG:HH21	7:S8:131:GLN:HB3	1.76	0.51
8:1:125:VAL:HG11	44:A9:501:PC1:H392	1.93	0.51
29:A9:120:LEU:O	29:A9:161:ARG:NH1	2.43	0.51
42:A6:61:ARG:NH2	25:AB:110:ASP:OD1	2.43	0.51
3:S1:599:GLN:HB2	3:S1:614:PRO:HD3	1.91	0.51
8:1:31:GLU:O	8:1:35:LEU:HB3	2.09	0.51
10:5:128:VAL:O	10:5:136:SER:OG	2.29	0.51
11:A8:49:ARG:HH22	13:AO:84:ASP:HB3	1.75	0.51
4:S3:138:ARG:NH1	40:A5:74:CYS:O	2.43	0.51
4:S3:217:GLU:OE1	29:A9:81:ASN:ND2	2.43	0.51
6:S7:80:ASN:ND2	6:S7:212:MET:O	2.44	0.51
10:5:310:LEU:HD21	10:5:344:CYS:HB3	1.93	0.51
20:B5:81:ASN:ND2	43:B5:202:CDL:OA3	2.44	0.51
29:A9:330:ASN:HD22	29:A9:342:LEU:HB3	1.76	0.51
31:S2:334:ARG:HH21	31:S2:458:THR:HG21	1.75	0.51
33:V1:138:GLY:O	33:V1:292:ASN:ND2	2.44	0.51
3:S1:131:LEU:HD13	31:S2:381:GLU:HG2	1.93	0.51
3:S1:205:GLY:HA2	3:S1:430:ARG:HH21	1.76	0.51
9:4:201:HIS:O	9:4:203:TRP:N	2.44	0.51
21:B9:9:VAL:HG23	21:B9:13:ARG:HD3	1.93	0.51
9:4:88:LEU:HD22	34:2:235:ILE:HG23	1.93	0.51
15:AM:30:SER:HB3	43:AM:204:CDL:H312	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A9:304:ARG:O	29:A9:309:ARG:NH2	2.44	0.51
31:S2:187:ASN:ND2	31:S2:409:LYS:HE2	2.24	0.51
33:V1:55:ARG:NH1	33:V1:304:GLU:O	2.44	0.51
33:V1:101:ARG:NH1	33:V1:284:ARG:O	2.44	0.51
9:4:197:MET:HB3	9:4:200:VAL:HG22	1.93	0.51
3:S1:460:ALA:O	3:S1:463:VAL:HB	2.11	0.50
10:5:323:ASN:O	10:5:325:SER:N	2.43	0.50
18:B4:99:ARG:NH2	22:BM:147:GLU:OE2	2.44	0.50
25:AB:136:LYS:HG3	25:AB:139:ASP:H	1.74	0.50
3:S1:286:ARG:HH12	3:S1:288:LEU:HD22	1.76	0.50
6:S7:104:ILE:HG13	6:S7:111:MET:HE2	1.91	0.50
1:AN:128:THR:HG23	7:S8:149:ARG:HB2	1.92	0.50
31:S2:107:ASP:O	39:3:56:ARG:NH1	2.45	0.50
33:V1:114:TRP:HE1	33:V1:258:THR:HG21	1.76	0.50
20:B5:154:ARG:NH1	26:C2:96:ASP:OD2	2.45	0.50
34:2:231:VAL:O	41:AL:371:ARG:NH1	2.45	0.50
36:A3:48:ASP:O	36:A3:72:ARG:NH2	2.45	0.50
9:4:165:ILE:HG12	9:4:176:PHE:CD1	2.47	0.50
12:A1:28:LYS:HE3	12:A1:34:ALA:HB2	1.92	0.50
3:S1:383:GLN:HB3	3:S1:528:GLN:HE21	1.77	0.50
7:S8:105:GLU:OE2	7:S8:198:ASN:ND2	2.45	0.50
14:S5:56:ASP:O	14:S5:60:CYS:HB2	2.12	0.50
27:B1:37:ARG:NH1	27:B1:56:TRP:OXT	2.42	0.50
31:S2:210:GLU:OE2	31:S2:214:LYS:NZ	2.45	0.50
37:4L:61:MET:HE2	38:6:53:ILE:HG13	1.94	0.50
4:S3:122:PRO:HA	4:S3:127:ARG:HG3	1.92	0.50
5:V2:168:GLU:OE1	33:V1:384:ARG:NH2	2.44	0.50
9:4:69:CYS:HA	9:4:72:MET:HE3	1.94	0.50
10:5:575:LEU:HD13	34:2:92:PHE:HB2	1.93	0.50
19:B7:79:ALA:O	19:B7:82:LYS:HB3	2.12	0.50
34:2:39:LEU:HA	37:4L:73:LEU:HD11	1.93	0.50
2:S6:75:VAL:HG21	7:S8:113:SER:HB2	1.94	0.49
29:A9:362:THR:HG23	29:A9:364:GLU:H	1.77	0.49
41:AL:315:ASP:O	41:AL:325:ARG:NH1	2.45	0.49
1:AN:34:ASP:OD2	8:1:46:LYS:NZ	2.41	0.49
3:S1:469:GLY:O	3:S1:475:LYS:NZ	2.45	0.49
10:5:223:SER:HA	10:5:227:THR:CG2	2.42	0.49
17:B6:78:CYS:HB2	17:B6:94:ARG:HG3	1.94	0.49
33:V1:78:TYR:O	33:V1:271:ARG:NH1	2.45	0.49
40:A5:31:ILE:HG21	40:A5:52:VAL:HG21	1.93	0.49
3:S1:643:ASP:OD1	3:S1:643:ASP:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S7:172:TYR:OH	31:S2:122:HIS:NE2	2.39	0.49
8:1:253:ASP:OD2	8:1:256:ASN:ND2	2.43	0.49
29:A9:243:ARG:HE	44:A9:501:PC1:H142	1.77	0.49
37:4L:28:LEU:HD22	37:4L:78:LEU:HD13	1.94	0.49
40:A5:38:MET:O	40:A5:45:ARG:NH1	2.46	0.49
11:A8:133:VAL:HG12	36:A3:61:TYR:HB2	1.95	0.49
16:BL:4:PRO:HB3	16:BL:10:SER:HB2	1.94	0.49
33:V1:425:ASP:O	33:V1:428:TRP:HB3	2.12	0.49
33:V1:298:ASN:ND2	33:V1:321:GLY:O	2.45	0.49
38:6:19:ASN:HD22	38:6:84:LEU:HD13	1.78	0.49
48:6:202:3PE:N	41:AL:334:GLU:OE2	2.44	0.49
41:AL:189:ARG:NH1	41:AL:272:TYR:OH	2.45	0.49
41:AL:209:ARG:HH12	41:AL:212:ARG:HH21	1.59	0.49
6:S7:192:PRO:HB3	31:S2:227:MET:HE2	1.94	0.49
7:S8:153:ASP:HB3	7:S8:156:LYS:HB2	1.94	0.49
10:5:124:SER:HB2	10:5:225:LEU:CD1	2.43	0.49
10:5:231:TYR:OH	10:5:235:ARG:NH2	2.45	0.49
31:S2:88:ASN:HA	31:S2:102:LEU:O	2.13	0.49
5:V2:125:ILE:HG12	5:V2:181:ILE:HD13	1.94	0.49
40:A5:19:ASN:HD22	41:AL:45:MET:HA	1.77	0.49
41:AL:91:ILE:HG23	57:AL:501:DGT:H3'	1.95	0.49
3:S1:127:MET:HA	3:S1:130:LEU:HB2	1.95	0.49
3:S1:421:GLU:HG2	3:S1:690:LEU:HD12	1.93	0.49
6:S7:219:TYR:O	29:A9:148:ASN:ND2	2.44	0.49
38:6:23:PRO:HA	38:6:26:LEU:HD12	1.95	0.49
9:4:19:ASN:O	27:B1:8:ARG:NH1	2.46	0.49
9:4:414:PHE:HB3	18:B4:40:GLY:HA3	1.95	0.49
10:5:206:LEU:HD22	10:5:221:HIS:CD2	2.48	0.49
29:A9:83:LEU:HD22	29:A9:88:THR:HG21	1.94	0.49
34:2:30:ALA:HB1	34:2:140:LEU:HD21	1.95	0.49
38:6:152:LEU:HD13	39:3:70:GLU:HG2	1.94	0.49
8:1:181:PHE:HB3	8:1:185:LEU:HD12	1.94	0.49
9:4:376:TRP:O	18:B4:94:ARG:NH2	2.45	0.49
17:B6:28:LEU:HD11	25:AC:147:LYS:HB2	1.94	0.49
3:S1:320:MET:HB2	3:S1:589:VAL:HB	1.94	0.48
8:1:275:GLY:O	31:S2:203:THR:OG1	2.27	0.48
9:4:57:LEU:HD11	9:4:232:LEU:HD13	1.94	0.48
10:5:227:THR:HB	10:5:301:LEU:HD11	1.95	0.48
23:B8:88:ASP:OD1	23:B8:88:ASP:N	2.46	0.48
38:6:52:TYR:OH	56:6:201:WSF:O12	2.27	0.48
21:B9:18:LEU:HD13	21:B9:66:GLN:HG3	1.93	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:4:353:ALA:O	9:4:362:ASN:ND2	2.46	0.48
14:S5:52:ASP:OD1	14:S5:52:ASP:N	2.46	0.48
41:AL:221:ASN:ND2	41:AL:349:TYR:O	2.46	0.48
1:AN:76:ASP:OD1	1:AN:76:ASP:N	2.45	0.48
43:AM:204:CDL:H132	48:2:401:3PE:H252	1.95	0.48
48:B6:201:3PE:H342	48:B6:201:3PE:H262	1.95	0.48
30:B2:53:GLY:O	30:B2:57:TRP:HB3	2.14	0.48
34:2:43:PRO:HG3	38:6:158:VAL:HG22	1.95	0.48
41:AL:177:HIS:O	41:AL:181:THR:OG1	2.31	0.48
1:AN:114:ASN:ND2	7:S8:181:SER:O	2.46	0.48
9:4:392:ALA:HA	9:4:395:THR:HG22	1.95	0.48
25:AB:90:ASP:OD1	25:AB:90:ASP:N	2.46	0.48
3:S1:133:ASN:ND2	33:V1:402:GLU:OE1	2.43	0.48
4:S3:157:SER:OG	4:S3:159:CYS:SG	2.72	0.48
7:S8:47:ASN:ND2	31:S2:333:ASP:OD1	2.46	0.48
8:1:48:GLY:HA3	8:1:53:PRO:HD2	1.95	0.48
8:1:190:LEU:HD22	44:1:401:PC1:H3B2	1.95	0.48
9:4:100:LEU:HD13	9:4:222:ILE:HD12	1.94	0.48
9:4:162:MET:CA	9:4:168:MET:HE3	2.43	0.48
9:4:303:LEU:O	9:4:307:HIS:HB3	2.14	0.48
9:4:367:ILE:HD11	10:5:158:ILE:HD13	1.95	0.48
18:B4:25:PHE:HB2	23:B8:102:GLN:HG3	1.95	0.48
31:S2:249:ILE:HG22	31:S2:353:LEU:HD11	1.95	0.48
39:3:91:ILE:O	39:3:95:ILE:HB	2.14	0.48
8:1:168:ASN:HB3	8:1:171:TYR:HD2	1.79	0.48
31:S2:221:ARG:NH1	31:S2:248:ASP:OD2	2.46	0.48
34:2:248:GLY:HA3	34:2:286:LEU:HD13	1.94	0.48
42:A6:56:CYS:HA	42:A6:104:TRP:HZ2	1.79	0.48
3:S1:204:ALA:HB1	3:S1:230:THR:HG21	1.95	0.48
10:5:113:ILE:O	10:5:117:TRP:HB2	2.14	0.48
48:B6:201:3PE:H271	48:B6:201:3PE:H391	1.96	0.48
7:S8:145:ARG:O	7:S8:146:ARG:NH1	2.41	0.48
9:4:243:LEU:HD21	26:C2:115:VAL:HG12	1.95	0.48
10:5:523:LYS:NZ	18:B4:58:ASN:OD1	2.44	0.48
15:AM:97:GLY:O	15:AM:110:GLY:HA2	2.13	0.48
31:S2:189:ILE:HD12	31:S2:215:MET:HE1	1.95	0.48
34:2:3:ASN:HB2	41:AL:334:GLU:HG3	1.95	0.48
41:AL:74:THR:HB	41:AL:332:TRP:HB3	1.96	0.48
2:S6:88:ASP:N	2:S6:88:ASP:OD1	2.47	0.47
17:B6:84:VAL:HG12	17:B6:85:LEU:HD12	1.96	0.47
19:B7:81:GLN:O	19:B7:84:GLU:HB3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S1:200:ALA:HA	3:S1:204:ALA:HB3	1.95	0.47
3:S1:625:ASP:HA	3:S1:628:ILE:HD12	1.95	0.47
6:S7:99:VAL:HG21	31:S2:147:VAL:HG12	1.96	0.47
8:1:17:ILE:HG23	8:1:90:LEU:HD13	1.95	0.47
9:4:250:ILE:HD11	9:4:290:LEU:HB2	1.95	0.47
9:4:288:GLY:HA3	9:4:369:LEU:HD22	1.95	0.47
11:A8:157:PRO:HG2	11:A8:160:TYR:HB2	1.96	0.47
43:B5:201:CDL:H122	43:B5:201:CDL:H552	1.96	0.47
41:AL:122:ASN:HD22	41:AL:380:MET:HG3	1.78	0.47
41:AL:142:TYR:OH	41:AL:150:ASP:O	2.31	0.47
10:5:108:PRO:HB2	10:5:168:ASN:HD22	1.80	0.47
14:S5:12:THR:HB	34:2:23:THR:HB	1.94	0.47
21:B9:27:GLU:O	21:B9:78:ARG:NH2	2.47	0.47
38:6:134:ASN:OD1	39:3:84:SER:OG	2.32	0.47
41:AL:193:SER:O	41:AL:193:SER:OG	2.29	0.47
1:AN:76:ASP:HB2	6:S7:200:TYR:HE1	1.79	0.47
6:S7:40:GLN:NE2	6:S7:41:GLN:O	2.46	0.47
7:S8:186:GLU:OE2	29:A9:111:GLY:N	2.47	0.47
8:1:31:GLU:O	8:1:35:LEU:CB	2.61	0.47
9:4:195:MET:HE3	9:4:286:LEU:HD22	1.95	0.47
10:5:102:MET:O	10:5:106:ILE:HG12	2.14	0.47
19:B7:37:MET:HE1	23:B8:164:PRO:HG3	1.96	0.47
29:A9:52:LYS:HG3	29:A9:62:ASN:HA	1.96	0.47
41:AL:124:TYR:OH	41:AL:392:ASP:OD2	2.33	0.47
3:S1:179:ILE:O	3:S1:227:LEU:HA	2.15	0.47
4:S3:233:ARG:NH1	7:S8:125:GLU:OE2	2.47	0.47
9:4:392:ALA:HB3	10:5:148:ARG:HG2	1.96	0.47
10:5:200:ILE:HD13	10:5:502:MET:HE1	1.96	0.47
13:AO:133:LYS:NZ	38:6:105:THR:O	2.48	0.47
34:2:230:PHE:HE1	41:AL:362:ARG:HH22	1.62	0.47
36:A3:31:LEU:HD12	48:3:202:3PE:H2I1	1.95	0.47
37:4L:10:PRO:HB2	37:4L:45:MET:HG3	1.96	0.47
9:4:436:ILE:HD11	44:B6:202:PC1:H2D2	1.96	0.47
25:AC:134:LEU:HD13	25:AC:140:ILE:HD13	1.97	0.47
42:A6:19:SER:OG	42:A6:77:ASP:OD2	2.30	0.47
4:S3:106:HIS:HB2	40:A5:51:LEU:HD13	1.96	0.47
6:S7:123:ARG:HB3	8:1:223:SER:HB3	1.97	0.47
10:5:288:ILE:HD13	10:5:288:ILE:HA	1.64	0.47
44:AM:205:PC1:H321	44:AM:205:PC1:H262	1.97	0.47
26:C2:95:ASP:OD1	26:C2:95:ASP:N	2.44	0.47
37:4L:64:LEU:HD13	38:6:57:ILE:HG13	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S1:80:ALA:O	3:S1:198:ARG:NH1	2.46	0.47
3:S1:361:LEU:HD21	3:S1:659:LEU:HD13	1.97	0.47
15:AM:26:LYS:HG3	43:AM:204:CDL:H322	1.96	0.47
9:4:160:TYR:O	9:4:164:LYS:HG2	2.15	0.47
9:4:265:LEU:O	23:B8:117:ARG:NH1	2.47	0.47
9:4:356:ALA:HB1	9:4:363:LEU:HD13	1.97	0.47
10:5:36:PHE:CE1	10:5:108:PRO:HG2	2.50	0.47
10:5:286:MET:HE2	10:5:286:MET:HB2	1.60	0.47
19:B7:3:ASN:O	19:B7:6:THR:OG1	2.30	0.47
55:V1:501:FMN:H1'2	55:V1:501:FMN:H4'	1.74	0.47
25:AB:129:SER:O	25:AB:133:LYS:HB2	2.14	0.47
4:S3:71:LEU:HD13	4:S3:98:VAL:HG22	1.95	0.47
31:S2:294:SER:HB3	31:S2:411:GLU:H	1.80	0.47
3:S1:59:VAL:HG13	3:S1:112:ILE:HD13	1.95	0.46
4:S3:110:PHE:HB3	4:S3:134:LEU:HB3	1.97	0.46
4:S3:235:PHE:O	31:S2:423:ARG:NH2	2.48	0.46
20:B5:148:ARG:NH2	34:2:341:PHE:OXT	2.48	0.46
1:AN:32:ARG:HG3	44:AN:202:PC1:H142	1.97	0.46
21:B9:81:ALA:HA	21:B9:86:GLY:HA3	1.97	0.46
33:V1:113:LYS:NZ	55:V1:501:FMN:O3P	2.48	0.46
3:S1:192:HIS:NE2	3:S1:218:MET:O	2.47	0.46
4:S3:127:ARG:NH1	4:S3:151:GLU:OE2	2.41	0.46
9:4:182:LEU:HD13	44:AM:205:PC1:H332	1.97	0.46
10:5:328:ILE:HA	10:5:331:MET:HE3	1.98	0.46
41:AL:131:LEU:HD13	41:AL:373:VAL:HG12	1.98	0.46
2:S6:54:ALA:HB2	29:A9:132:HIS:HB2	1.97	0.46
4:S3:45:ASP:OD1	4:S3:45:ASP:N	2.48	0.46
8:1:58:ASP:HB3	49:1:402:U10:H372	1.98	0.46
8:1:64:THR:O	39:3:27:LYS:N	2.49	0.46
10:5:182:MET:HA	10:5:185:ILE:HD12	1.98	0.46
29:A9:205:GLU:OE2	29:A9:219:ARG:NH2	2.48	0.46
31:S2:375:GLU:O	31:S2:379:SER:OG	2.31	0.46
33:V1:461:ILE:HG22	33:V1:465:MET:HE2	1.96	0.46
13:AO:77:PRO:HA	13:AO:80:VAL:HG12	1.96	0.46
16:BL:74:MET:HE1	22:BM:102:PHE:HB2	1.98	0.46
42:A6:30:LEU:HD22	25:AB:112:VAL:HG21	1.97	0.46
1:AN:88:MET:HE3	1:AN:88:MET:HB3	1.80	0.46
10:5:3:TYR:HD2	17:B6:91:TYR:CZ	2.34	0.46
10:5:47:MET:HG2	10:5:165:GLY:HA2	1.97	0.46
27:B1:38:ASP:OD2	27:B1:45:ARG:NH2	2.49	0.46
37:4L:58:TYR:HB2	38:6:136:LEU:HG	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S1:513:LYS:HB2	3:S1:516:TRP:HB3	1.97	0.46
8:1:82:PRO:HB3	8:1:230:ILE:HG13	1.98	0.46
8:1:308:LYS:HE3	39:3:81:MET:HE1	1.97	0.46
9:4:195:MET:HG3	9:4:282:MET:HE2	1.97	0.46
18:B4:74:PHE:HD1	18:B4:78:LEU:HD22	1.81	0.46
19:B7:57:CYS:HB2	19:B7:60:LEU:HD13	1.97	0.46
21:B9:43:LEU:HD11	51:AC:201:ZMP:H4A	1.96	0.46
41:AL:43:LYS:NZ	41:AL:107:ASP:OD1	2.44	0.46
41:AL:249:ARG:NH2	41:AL:254:GLU:OE1	2.49	0.46
9:4:201:HIS:O	9:4:202:LEU:C	2.58	0.46
11:A8:131:ALA:HB2	36:A3:55:LYS:HD2	1.98	0.46
15:AM:108:VAL:HA	15:AM:111:LEU:HD12	1.98	0.46
31:S2:440:LEU:HD13	31:S2:459:LEU:HD11	1.97	0.46
39:3:109:ASN:ND2	48:3:203:3PE:O32	2.48	0.46
6:S7:92:PHE:CE2	6:S7:94:LEU:HD11	2.51	0.46
6:S7:166:GLY:HA2	7:S8:156:LYS:HA	1.98	0.46
28:S4:86:ILE:HG13	28:S4:106:ILE:HG12	1.97	0.46
33:V1:84:VAL:HA	33:V1:162:ARG:HG2	1.98	0.46
37:4L:51:ASN:ND2	38:6:45:THR:OG1	2.43	0.46
38:6:35:ILE:O	38:6:39:LEU:HG	2.16	0.46
38:6:165:LEU:HD11	39:3:114:ASN:O	2.15	0.46
3:S1:563:ARG:NH1	3:S1:585:ILE:O	2.49	0.46
5:V2:123:TYR:HA	5:V2:182:ASN:HD21	1.81	0.46
9:4:430:LEU:O	9:4:434:LEU:HB2	2.16	0.46
10:5:262:LEU:HD23	10:5:496:LEU:HD22	1.98	0.46
10:5:322:MET:HE3	10:5:322:MET:HB3	1.75	0.46
3:S1:130:LEU:HG	33:V1:398:THR:HG21	1.98	0.45
6:S7:96:CYS:SG	46:S7:301:SF4:S3	3.05	0.45
9:4:112:PHE:O	9:4:116:PHE:CB	2.64	0.45
10:5:65:PHE:HE2	10:5:306:LEU:HD11	1.80	0.45
11:A8:22:LEU:O	12:A1:50:ARG:NH1	2.48	0.45
41:AL:101:GLU:HB3	41:AL:297:THR:HG21	1.97	0.45
3:S1:231:GLU:CD	3:S1:231:GLU:H	2.25	0.45
18:B4:71:THR:O	18:B4:75:ALA:CB	2.64	0.45
23:B8:57:LEU:HD11	23:B8:78:LEU:HD11	1.98	0.45
31:S2:181:GLU:OE1	31:S2:184:ARG:NH1	2.48	0.45
1:AN:127:THR:OG1	7:S8:191:ASN:OD1	2.34	0.45
9:4:344:THR:HB	43:B5:201:CDL:HB61	1.98	0.45
24:B3:79:THR:HA	24:B3:82:VAL:HG12	1.99	0.45
56:6:201:WSF:C14	56:6:201:WSF:C11	2.94	0.45
5:V2:123:TYR:HA	5:V2:182:ASN:ND2	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S7:160:SER:N	46:S7:301:SF4:S4	2.89	0.45
10:5:17:MET:HG3	48:5:607:3PE:H2H2	1.98	0.45
10:5:439:MET:HB3	48:5:604:3PE:H232	1.98	0.45
30:B2:35:ASN:OD1	30:B2:36:GLY:N	2.47	0.45
3:S1:172:ARG:NH1	3:S1:216:ASN:OD1	2.49	0.45
4:S3:119:VAL:HB	4:S3:129:GLU:HG2	1.98	0.45
48:5:601:3PE:H282	16:BL:15:VAL:HG11	1.97	0.45
44:5:606:PC1:H2	43:B5:201:CDL:H132	1.99	0.45
15:AM:86:LYS:HG3	15:AM:125:LYS:HB3	1.97	0.45
44:AM:205:PC1:H341	44:AM:205:PC1:H281	1.99	0.45
29:A9:180:LEU:HD22	29:A9:221:ALA:HB2	1.99	0.45
34:2:124:MET:HE3	43:2:403:CDL:HB31	1.98	0.45
4:S3:66:TYR:OH	4:S3:105:HIS:NE2	2.38	0.45
6:S7:97:CYS:SG	46:S7:301:SF4:S3	3.09	0.45
8:1:34:VAL:O	8:1:38:ILE:N	2.49	0.45
29:A9:41:ARG:NH2	29:A9:276:ASP:OD1	2.49	0.45
33:V1:235:GLN:HB2	33:V1:237:LYS:HG2	1.98	0.45
34:2:226:LEU:HD13	34:2:292:ILE:HG23	1.99	0.45
41:AL:143:ASP:OD1	41:AL:146:ASN:ND2	2.50	0.45
4:S3:243:GLN:OE1	35:A7:63:ARG:NH2	2.50	0.45
6:S7:130:VAL:HG21	6:S7:182:ILE:HD11	1.98	0.45
9:4:162:MET:HA	9:4:168:MET:HE3	1.99	0.45
34:2:98:MET:HE2	34:2:150:LEU:HD13	1.99	0.45
5:V2:86:LEU:HD22	5:V2:115:PHE:HB3	1.98	0.45
44:1:401:PC1:H2	31:S2:271:ARG:HD3	1.98	0.45
24:B3:43:ARG:HG2	25:AC:85:LEU:HD22	1.97	0.45
31:S2:380:MET:HE3	31:S2:384:ILE:HG13	1.99	0.45
34:2:45:LEU:O	34:2:45:LEU:HG	2.16	0.45
34:2:111:HIS:CE1	34:2:160:ILE:HG21	2.52	0.45
4:S3:142:ARG:NH1	31:S2:411:GLU:OE2	2.47	0.45
31:S2:186:LEU:CD1	31:S2:215:MET:SD	3.00	0.45
34:2:290:LEU:HA	34:2:293:CYS:HB2	1.98	0.45
41:AL:243:LYS:O	41:AL:246:ILE:HB	2.17	0.45
42:A6:51:MET:HE2	42:A6:101:MET:HE1	1.99	0.45
3:S1:260:ARG:HB2	3:S1:279:THR:O	2.17	0.44
7:S8:167:CYS:O	31:S2:373:ARG:NH2	2.51	0.44
8:1:220:VAL:HG13	8:1:221:GLU:HG2	1.99	0.44
10:5:275:ALA:O	10:5:278:THR:OG1	2.31	0.44
37:4L:65:THR:HA	39:3:69:VAL:HG21	1.99	0.44
3:S1:46:VAL:HG22	3:S1:112:ILE:HD12	1.99	0.44
19:B7:86:LEU:HB3	30:B2:74:PHE:HZ	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A9:194:GLY:HA3	29:A9:348:GLU:HG3	1.99	0.44
38:6:149:MET:HE2	39:3:96:PHE:HD1	1.82	0.44
41:AL:40:ILE:HG23	41:AL:81:ASN:HA	2.00	0.44
3:S1:79:LEU:HD11	3:S1:239:LEU:HD13	1.99	0.44
9:4:44:TYR:OH	20:B5:120:ASP:OD1	2.35	0.44
9:4:139:ALA:HB2	9:4:210:GLU:HG3	1.99	0.44
10:5:451:ILE:HG23	10:5:453:LEU:HD23	1.98	0.44
10:5:502:MET:HA	10:5:505:ILE:HB	1.99	0.44
17:B6:64:ASN:HD22	20:B5:64:PHE:HB2	1.82	0.44
24:B3:55:GLY:O	24:B3:60:ARG:NH1	2.50	0.44
32:V3:83:UNK:H2	33:V1:147:ARG:HD2	1.81	0.44
33:V1:144:GLU:O	33:V1:148:HIS:HB2	2.16	0.44
38:6:21:ILE:H	38:6:21:ILE:HG12	1.33	0.44
3:S1:406:GLU:HA	3:S1:432:ALA:HB2	1.99	0.44
10:5:445:PHE:O	19:B7:68:ARG:NH2	2.51	0.44
28:S4:115:GLU:O	29:A9:53:ARG:NE	2.50	0.44
10:5:549:LEU:HD21	34:2:160:ILE:HG23	1.99	0.44
16:BL:27:ARG:HA	16:BL:31:VAL:HB	2.00	0.44
17:B6:99:LYS:NZ	43:B6:203:CDL:OB4	2.48	0.44
19:B7:84:GLU:O	19:B7:87:THR:OG1	2.31	0.44
28:S4:85:ARG:NH1	28:S4:107:GLU:OE2	2.43	0.44
37:4L:27:HIS:CE1	38:6:73:ALA:HB2	2.52	0.44
1:AN:63:ARG:NH2	1:AN:93:ASP:OD1	2.50	0.44
3:S1:487:ILE:HD11	3:S1:504:VAL:HG11	1.98	0.44
6:S7:143:ARG:HA	6:S7:143:ARG:HD2	1.85	0.44
6:S7:171:SER:HB3	31:S2:128:LEU:HD11	2.00	0.44
10:5:37:ILE:HG12	10:5:53:PHE:HB2	1.99	0.44
10:5:54:LEU:N	10:5:106:ILE:O	2.51	0.44
10:5:522:VAL:HA	10:5:526:ASP:HB2	2.00	0.44
44:5:606:PC1:H241	43:B5:201:CDL:H171	1.98	0.44
20:B5:55:TRP:HZ2	43:B5:201:CDL:HA61	1.82	0.44
29:A9:120:LEU:HD13	29:A9:158:GLY:HA3	1.98	0.44
29:A9:254:THR:HA	29:A9:353:THR:HG22	2.00	0.44
1:AN:120:GLU:HA	2:S6:60:LYS:HG3	1.98	0.44
2:S6:35:ASP:OD1	2:S6:35:ASP:N	2.51	0.44
8:1:300:TYR:HD1	36:A3:29:LEU:HD13	1.82	0.44
9:4:100:LEU:HA	9:4:103:THR:HG22	1.99	0.44
10:5:323:ASN:O	10:5:324:ASN:C	2.61	0.44
34:2:21:THR:HG21	34:2:136:ALA:HB1	2.00	0.44
41:AL:155:LEU:O	41:AL:158:GLN:HB3	2.18	0.44
3:S1:247:ASN:HB3	3:S1:250:TYR:HB3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S7:183:PRO:HG3	29:A9:103:ARG:HA	2.00	0.44
10:5:302:LEU:O	10:5:306:LEU:HG	2.18	0.44
10:5:457:MET:SD	23:B8:156:ARG:NH1	2.91	0.44
10:5:548:THR:HG21	48:5:608:3PE:H122	1.99	0.44
29:A9:229:ARG:O	29:A9:233:TYR:HB2	2.18	0.44
33:V1:117:MET:SD	33:V1:256:THR:OG1	2.71	0.44
33:V1:249:GLY:HA3	33:V1:255:THR:HG22	2.00	0.44
41:AL:252:ASP:OD1	41:AL:252:ASP:N	2.47	0.44
29:A9:53:ARG:O	29:A9:60:SER:OG	2.34	0.44
48:2:401:3PE:H251	48:2:401:3PE:H321	2.00	0.44
3:S1:264:SER:OG	3:S1:265:ILE:N	2.50	0.43
48:5:605:3PE:H252	48:AM:202:3PE:H321	1.99	0.43
33:V1:296:HIS:NE2	33:V1:376:THR:OG1	2.51	0.43
9:4:42:MET:O	9:4:43:ASN:C	2.61	0.43
10:5:390:LEU:HD12	48:5:602:3PE:H271	2.00	0.43
31:S2:107:ASP:OD2	39:3:54:SER:OG	2.34	0.43
34:2:300:ASN:HB3	41:AL:364:ALA:HB1	1.99	0.43
38:6:145:THR:O	38:6:149:MET:HG3	2.17	0.43
3:S1:192:HIS:HD2	3:S1:220:ILE:HG12	1.84	0.43
4:S3:62:ASP:HB3	35:A7:94:PRO:HB3	1.98	0.43
49:1:402:U10:H8	49:1:402:U10:H122	1.68	0.43
11:A8:51:GLU:H	11:A8:51:GLU:HG3	1.41	0.43
15:AM:35:TRP:O	15:AM:39:ASP:HB2	2.18	0.43
25:AC:96:VAL:HA	25:AC:137:PRO:HB2	1.99	0.43
31:S2:45:ASP:OD1	31:S2:45:ASP:N	2.44	0.43
31:S2:99:VAL:HG21	31:S2:121:LEU:HD22	1.99	0.43
1:AN:47:TYR:HE2	1:AN:81:PRO:HB3	1.83	0.43
7:S8:86:PRO:HD2	12:A1:1:MET:HG2	1.99	0.43
8:1:107:LEU:HB3	8:1:110:LEU:HD12	1.99	0.43
13:AO:14:LEU:HD11	31:S2:358:ALA:HB2	2.01	0.43
15:AM:104:LYS:HA	15:AM:104:LYS:HD2	1.82	0.43
31:S2:46:PRO:HB3	41:AL:355:PHE:HB3	1.99	0.43
34:2:76:ILE:HG21	37:4L:45:MET:HB3	2.00	0.43
7:S8:184:THR:HB	7:S8:187:GLU:HG3	2.01	0.43
8:1:135:ALA:HA	8:1:218:PHE:HA	2.01	0.43
9:4:344:THR:HA	9:4:347:TRP:HB2	2.01	0.43
31:S2:307:LEU:HB2	31:S2:406:GLU:HB2	2.00	0.43
34:2:14:MET:HE1	34:2:128:MET:HB3	1.99	0.43
3:S1:383:GLN:O	3:S1:528:GLN:NE2	2.52	0.43
8:1:5:GLU:O	8:1:6:PHE:C	2.61	0.43
48:5:607:3PE:H351	48:5:607:3PE:H322	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:C2:201:3PE:H231	48:C2:201:3PE:H262	1.89	0.43
29:A9:229:ARG:O	29:A9:233:TYR:CB	2.66	0.43
31:S2:153:GLU:HB3	31:S2:232:ILE:HB	2.00	0.43
31:S2:402:TYR:HD2	31:S2:415:TYR:HB2	1.84	0.43
33:V1:340:PRO:HG3	33:V1:448:TRP:HB3	2.01	0.43
7:S8:117:ARG:NH1	7:S8:169:VAL:O	2.51	0.43
34:2:13:ILE:HG21	38:6:154:ILE:HG21	2.01	0.43
25:AB:142:LYS:HA	25:AB:142:LYS:HD3	1.82	0.43
1:AN:45:ASP:HB3	1:AN:51:TYR:HE2	1.83	0.43
3:S1:694:ARG:NH2	3:S1:720:GLN:OE1	2.51	0.43
10:5:4:LEU:HB3	10:5:9:ILE:HD11	2.01	0.43
18:B4:71:THR:O	18:B4:75:ALA:HB3	2.19	0.43
33:V1:429:GLU:HA	33:V1:432:LYS:HB2	2.00	0.43
6:S7:79:LEU:HD11	8:1:64:THR:HG21	2.01	0.43
10:5:340:LEU:HD23	10:5:423:LEU:HD23	2.01	0.43
10:5:370:ILE:HD11	10:5:449:TYR:HB3	2.01	0.43
15:AM:90:LEU:HD12	15:AM:118:GLY:HA3	1.99	0.43
23:B8:162:GLN:OE1	23:B8:170:HIS:ND1	2.51	0.43
31:S2:215:MET:HE2	31:S2:252:PHE:HZ	1.83	0.43
33:V1:52:ASP:HA	33:V1:55:ARG:HG3	2.00	0.43
3:S1:218:MET:HE3	3:S1:220:ILE:HD11	2.01	0.43
5:V2:212:ARG:HA	5:V2:212:ARG:HD2	1.93	0.43
10:5:226:VAL:HB	10:5:282:LEU:HD11	1.99	0.43
44:5:606:PC1:H221	43:B6:203:CDL:HA62	2.01	0.43
26:C2:49:PRO:HB2	26:C2:52:SER:HB3	2.01	0.43
29:A9:128:ASP:HA	29:A9:131:LYS:HD2	2.00	0.43
31:S2:97:HIS:HB2	31:S2:463:PHE:HE2	1.84	0.43
34:2:118:MET:HA	34:2:121:LEU:HD13	2.00	0.43
6:S7:149:MET:HA	6:S7:150:PRO:HD3	1.89	0.42
10:5:148:ARG:HD2	10:5:151:ASP:HB2	1.99	0.42
10:5:154:LEU:HD23	10:5:154:LEU:HA	1.92	0.42
12:A1:57:ASN:HB3	12:A1:60:LYS:HB2	2.01	0.42
17:B6:13:LYS:HD2	17:B6:13:LYS:HA	1.81	0.42
31:S2:433:GLY:HA3	31:S2:461:VAL:HG12	2.00	0.42
33:V1:127:TYR:O	33:V1:255:THR:HA	2.19	0.42
34:2:4:ASN:ND2	34:2:6:SER:OG	2.51	0.42
4:S3:227:GLU:OE2	29:A9:55:THR:OG1	2.29	0.42
5:V2:49:THR:O	5:V2:53:LYS:N	2.48	0.42
5:V2:185:TYR:OH	33:V1:176:GLU:HB3	2.19	0.42
8:1:101:LYS:HZ3	13:AO:154:SER:HB2	1.83	0.42
10:5:210:MET:SD	10:5:221:HIS:HE1	2.42	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:5:434:ILE:HG22	10:5:435:ILE:HG23	2.02	0.42
13:AO:68:MET:HE2	13:AO:68:MET:HB2	1.88	0.42
15:AM:35:TRP:HB2	48:AM:202:3PE:H2B1	2.00	0.42
27:B1:6:ASP:OD1	27:B1:6:ASP:N	2.49	0.42
33:V1:56:ILE:HG12	33:V1:268:THR:HG21	2.00	0.42
34:2:34:LEU:HD22	34:2:104:LYS:HE2	2.01	0.42
2:S6:73:GLU:HA	2:S6:117:ARG:HH12	1.85	0.42
6:S7:120:ALA:O	31:S2:92:GLN:NE2	2.48	0.42
49:1:402:U10:H372	49:1:402:U10:H351	1.85	0.42
12:A1:15:LEU:O	12:A1:18:VAL:HB	2.18	0.42
14:S5:2:SER:HA	34:2:85:ASN:HB2	2.02	0.42
33:V1:423:GLU:O	33:V1:426:MET:HB3	2.20	0.42
10:5:7:CYS:CB	10:5:78:LYS:HB3	2.50	0.42
11:A8:143:LYS:HB2	11:A8:143:LYS:HE2	1.49	0.42
18:B4:10:PHE:HD1	23:B8:58:LEU:HD12	1.84	0.42
6:S7:97:CYS:SG	46:S7:301:SF4:S2	3.18	0.42
12:A1:23:MET:HA	12:A1:26:LEU:HB2	2.01	0.42
22:BM:114:LEU:HD12	22:BM:114:LEU:HA	1.93	0.42
26:C2:45:GLY:HA3	34:2:321:MET:SD	2.60	0.42
33:V1:65:ASP:O	33:V1:74:ARG:NH1	2.45	0.42
6:S7:124:GLN:HE22	8:1:219:ASN:HB3	1.84	0.42
6:S7:158:MET:HA	6:S7:188:VAL:HB	2.00	0.42
8:1:71:LEU:HG	29:A9:388:LEU:HD13	2.02	0.42
13:AO:98:GLU:HG3	14:S5:73:MET:HE3	2.01	0.42
13:AO:140:ASP:OD1	13:AO:140:ASP:N	2.52	0.42
14:S5:54:ILE:HG12	34:2:84:MET:HE1	2.02	0.42
31:S2:373:ARG:HA	31:S2:373:ARG:HD2	1.90	0.42
33:V1:292:ASN:OD1	33:V1:292:ASN:N	2.53	0.42
3:S1:39:PRO:HB2	3:S1:40:GLU:H	1.66	0.42
10:5:5:SER:OG	10:5:8:SER:HB3	2.19	0.42
10:5:552:MET:HG3	15:AM:43:LEU:HD23	2.02	0.42
29:A9:142:ARG:H	29:A9:155:HIS:CE1	2.37	0.42
29:A9:306:ASP:OD1	29:A9:306:ASP:N	2.41	0.42
31:S2:330:ASP:OD1	31:S2:330:ASP:N	2.44	0.42
34:2:122:THR:OG1	34:2:123:TRP:N	2.53	0.42
40:A5:43:SER:HA	40:A5:46:LYS:HD3	2.00	0.42
3:S1:563:ARG:HD2	3:S1:563:ARG:HA	1.87	0.42
9:4:268:THR:O	9:4:330:MET:N	2.52	0.42
31:S2:84:ASN:HB2	31:S2:105:GLU:HG2	2.02	0.42
34:2:138:LEU:HD13	34:2:197:TRP:HE1	1.84	0.42
37:4L:9:LEU:HG	37:4L:13:LEU:HD11	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V2:154:GLY:N	5:V2:164:ILE:O	2.50	0.42
6:S7:86:SER:HB3	8:1:54:GLN:HE22	1.85	0.42
8:1:254:VAL:O	8:1:260:TYR:OH	2.36	0.42
28:S4:116:ASN:OD1	28:S4:116:ASN:N	2.53	0.42
29:A9:173:ARG:NH2	29:A9:216:THR:OG1	2.52	0.42
31:S2:116:PRO:HG3	31:S2:440:LEU:HD23	2.00	0.42
39:3:67:PHE:O	39:3:71:ILE:HG12	2.20	0.42
3:S1:230:THR:C	3:S1:232:LEU:N	2.78	0.42
48:S7:302:3PE:H321	48:S7:302:3PE:H252	2.01	0.42
8:1:1:MET:HE3	8:1:1:MET:HB3	1.70	0.42
9:4:149:LEU:HD13	48:4:502:3PE:H352	2.02	0.42
9:4:205:PRO:O	9:4:209:VAL:HG22	2.20	0.42
48:5:608:3PE:H3A2	34:2:277:LEU:HD21	2.02	0.42
24:B3:79:THR:O	24:B3:83:GLU:HB2	2.20	0.42
37:4L:77:ILE:HD13	37:4L:77:ILE:HA	1.95	0.42
8:1:241:MET:HE3	8:1:241:MET:HB3	1.96	0.41
11:A8:54:ASP:OD1	11:A8:56:ARG:HB2	2.20	0.41
29:A9:216:THR:HG21	29:A9:271:ALA:HB1	2.02	0.41
41:AL:156:ALA:O	41:AL:159:PHE:HB3	2.19	0.41
6:S7:167:TYR:OH	31:S2:136:GLN:O	2.38	0.41
9:4:164:LYS:HA	9:4:164:LYS:HD2	1.84	0.41
9:4:167:SER:HB3	20:B5:138:ALA:HB2	2.02	0.41
10:5:68:MET:HE1	10:5:432:MET:HG2	2.01	0.41
10:5:318:ILE:HA	10:5:338:MET:HE1	2.01	0.41
31:S2:137:ALA:HA	31:S2:140:TYR:HD2	1.84	0.41
44:2:402:PC1:H262	44:2:402:PC1:H372	2.02	0.41
38:6:20:MET:HE1	43:6:203:CDL:CA7	2.49	0.41
48:6:202:3PE:H341	48:3:203:3PE:H3F2	2.01	0.41
41:AL:343:LYS:HD3	41:AL:404:ASN:HB3	2.02	0.41
3:S1:406:GLU:OE1	3:S1:428:ARG:NH1	2.54	0.41
9:4:28:MET:HA	9:4:31:ILE:HD12	2.02	0.41
20:B5:51:SER:HB2	21:B9:103:TRP:HA	2.02	0.41
29:A9:142:ARG:HD3	29:A9:142:ARG:HA	1.84	0.41
41:AL:174:ALA:HB1	41:AL:185:VAL:HG21	2.02	0.41
9:4:110:PHE:HD2	11:A8:173:TRP:HZ3	1.68	0.41
9:4:124:LEU:HD22	9:4:144:LEU:HD13	2.02	0.41
17:B6:55:VAL:HA	17:B6:56:PRO:HD3	1.93	0.41
28:S4:82:ARG:NH1	28:S4:126:ASP:OD1	2.53	0.41
29:A9:220:PRO:HA	29:A9:284:ALA:HB3	2.02	0.41
34:2:105:SER:O	34:2:134:LYS:NZ	2.49	0.41
41:AL:124:TYR:OH	41:AL:384:PRO:O	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AM:125:LYS:HA	15:AM:128:ILE:HG22	2.02	0.41
19:B7:101:GLU:OE2	19:B7:104:ARG:NH2	2.53	0.41
35:A7:55:ASN:HD22	35:A7:55:ASN:C	2.27	0.41
9:4:231:MET:HE3	9:4:289:LEU:HD13	2.00	0.41
48:4:504:3PE:H2A2	44:AM:205:PC1:H2E1	2.01	0.41
48:AM:203:3PE:H272	38:6:146:ILE:HG21	2.01	0.41
23:B8:58:LEU:HD22	23:B8:58:LEU:HA	1.79	0.41
3:S1:294:ASP:HA	3:S1:403:ALA:HB2	2.01	0.41
9:4:63:LEU:HG	44:4:501:PC1:H3B2	2.02	0.41
9:4:148:LEU:HD11	34:2:250:LEU:HD21	2.03	0.41
12:A1:10:VAL:O	12:A1:14:THR:N	2.51	0.41
18:B4:14:LYS:HE3	18:B4:14:LYS:HB3	1.92	0.41
31:S2:128:LEU:HB3	31:S2:140:TYR:OH	2.21	0.41
33:V1:332:VAL:HG23	33:V1:342:ILE:HB	2.03	0.41
34:2:59:LYS:NZ	37:4L:94:SER:O	2.47	0.41
38:6:172:MET:HE3	38:6:172:MET:HB3	1.81	0.41
41:AL:131:LEU:HD11	41:AL:377:ALA:HB2	2.03	0.41
42:A6:21:ASP:OD1	42:A6:21:ASP:N	2.53	0.41
6:S7:152:PRO:HD2	8:1:65:LYS:HG3	2.03	0.41
8:1:101:LYS:HG3	12:A1:38:ASN:HA	2.02	0.41
9:4:54:CYS:HB2	9:4:58:SER:HB3	2.02	0.41
9:4:150:VAL:HG21	9:4:193:VAL:HB	2.03	0.41
9:4:223:MET:HE2	9:4:223:MET:HB3	1.91	0.41
10:5:79:GLU:HB2	10:5:421:ILE:HB	2.02	0.41
12:A1:23:MET:HE3	12:A1:23:MET:HB3	1.88	0.41
23:B8:95:TYR:HE1	23:B8:102:GLN:HA	1.86	0.41
28:S4:116:ASN:OD1	28:S4:121:TRP:N	2.54	0.41
35:A7:41:GLN:HA	35:A7:42:PRO:HD3	1.88	0.41
3:S1:58:THR:HA	3:S1:105:PRO:HA	2.02	0.41
8:1:185:LEU:O	8:1:189:ALA:N	2.51	0.41
9:4:116:PHE:HD1	9:4:226:LEU:HD13	1.86	0.41
10:5:39:TRP:HB3	10:5:51:MET:HB3	2.03	0.41
10:5:98:VAL:HG13	10:5:102:MET:HE3	2.03	0.41
10:5:142:LEU:HD23	10:5:208:ALA:HB2	2.01	0.41
10:5:319:ILE:HG23	10:5:324:ASN:O	2.21	0.41
17:B6:28:LEU:HD12	25:AC:143:TYR:CZ	2.56	0.41
19:B7:44:MET:HE3	19:B7:44:MET:HB2	1.86	0.41
29:A9:256:LYS:HA	29:A9:354:ASP:HB2	2.02	0.41
31:S2:186:LEU:HD12	31:S2:186:LEU:HA	1.90	0.41
31:S2:214:LYS:HD3	35:A7:29:ARG:HD3	2.01	0.41
31:S2:296:VAL:O	31:S2:300:GLY:N	2.48	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:S2:402:TYR:HA	31:S2:414:VAL:O	2.21	0.41
33:V1:40:PRO:HA	33:V1:41:PRO:HD3	1.97	0.41
34:2:103:LEU:HD13	34:2:110:PHE:HB3	2.02	0.41
35:A7:71:ASP:HB3	35:A7:74:GLU:HB2	2.02	0.41
38:6:11:ILE:HG21	38:6:95:MET:HE1	2.03	0.41
41:AL:159:PHE:HE2	57:AL:501:DGT:N2	2.19	0.41
41:AL:223:ILE:HD12	41:AL:226:LEU:HD12	2.03	0.41
41:AL:326:PHE:HA	41:AL:327:PRO:HD3	1.93	0.41
6:S7:154:TRP:HB3	6:S7:205:LEU:HD11	2.03	0.41
7:S8:136:GLU:HB2	7:S8:149:ARG:HB3	2.03	0.41
10:5:145:LEU:HD12	48:5:603:3PE:H221	2.02	0.41
14:S5:87:LYS:HE3	14:S5:89:GLN:HB3	2.03	0.41
33:V1:390:LYS:HD3	33:V1:408:ASN:HD22	1.85	0.41
34:2:261:LEU:HD23	34:2:261:LEU:HA	1.94	0.41
48:4:504:3PE:H252	15:AM:126:MET:HE1	2.03	0.40
19:B7:1:MET:HA	19:B7:5:LEU:HD22	2.03	0.40
3:S1:499:ALA:HB1	3:S1:679:LYS:HA	2.02	0.40
9:4:197:MET:HE3	9:4:199:LEU:HB2	2.03	0.40
10:5:196:LYS:HA	10:5:196:LYS:HD3	1.97	0.40
10:5:224:THR:OG1	10:5:225:LEU:N	2.54	0.40
15:AM:117:LEU:HD22	43:AM:204:CDL:H781	2.03	0.40
15:AM:145:GLY:H	44:AM:206:PC1:H111	1.86	0.40
36:A3:45:TYR:HE2	39:3:87:MET:HB2	1.86	0.40
3:S1:393:ARG:NH1	3:S1:533:ASP:OD2	2.54	0.40
21:B9:51:ARG:NH2	25:AC:107:ASP:OD2	2.55	0.40
34:2:259:LYS:HB3	34:2:259:LYS:HE2	1.84	0.40
4:S3:107:GLN:HE22	40:A5:51:LEU:HD21	1.87	0.40
5:V2:124:HIS:NE2	5:V2:165:SER:OG	2.42	0.40
8:1:4:MET:O	8:1:5:GLU:C	2.64	0.40
10:5:357:PHE:HA	10:5:362:TYR:CE1	2.57	0.40
11:A8:48:CYS:O	11:A8:52:LEU:HB2	2.20	0.40
17:B6:6:ALA:HB1	22:BM:60:SER:HB3	2.04	0.40
33:V1:411:MET:HA	33:V1:414:PHE:HB2	2.04	0.40
8:1:156:ILE:HG23	8:1:188:MET:SD	2.61	0.40
8:1:286:MET:SD	39:3:115:TRP:NE1	2.94	0.40
9:4:300:SER:HA	9:4:369:LEU:HD11	2.03	0.40
10:5:269:ASP:HB3	10:5:272:LYS:HB2	2.03	0.40
33:V1:382:ILE:HG13	33:V1:453:LEU:HD13	2.03	0.40
40:A5:79:GLU:OE1	40:A5:83:GLN:NE2	2.54	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	AN	134/142 (94%)	130 (97%)	3 (2%)	1 (1%)	19	47
2	S6	87/126 (69%)	87 (100%)	0	0	100	100
3	S1	679/731 (93%)	660 (97%)	19 (3%)	0	100	100
4	S3	203/265 (77%)	196 (97%)	7 (3%)	0	100	100
5	V2	212/242 (88%)	208 (98%)	4 (2%)	0	100	100
6	S7	180/221 (81%)	168 (93%)	12 (7%)	0	100	100
7	S8	184/217 (85%)	179 (97%)	5 (3%)	0	100	100
8	1	313/315 (99%)	300 (96%)	13 (4%)	0	100	100
9	4	444/446 (100%)	421 (95%)	21 (5%)	2 (0%)	25	54
10	5	575/577 (100%)	552 (96%)	22 (4%)	1 (0%)	44	72
11	A8	172/175 (98%)	164 (95%)	8 (5%)	0	100	100
12	A1	68/123 (55%)	68 (100%)	0	0	100	100
13	AO	144/154 (94%)	140 (97%)	4 (3%)	0	100	100
14	S5	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
15	AM	166/170 (98%)	161 (97%)	5 (3%)	0	100	100
16	BL	149/159 (94%)	148 (99%)	1 (1%)	0	100	100
17	B6	159/167 (95%)	155 (98%)	4 (2%)	0	100	100
18	B4	105/113 (93%)	101 (96%)	4 (4%)	0	100	100
19	B7	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
20	B5	141/186 (76%)	139 (99%)	2 (1%)	0	100	100
21	B9	132/144 (92%)	131 (99%)	1 (1%)	0	100	100
22	BM	104/150 (69%)	100 (96%)	4 (4%)	0	100	100
23	B8	142/175 (81%)	134 (94%)	8 (6%)	0	100	100
24	B3	79/110 (72%)	75 (95%)	4 (5%)	0	100	100
25	AB	82/152 (54%)	78 (95%)	3 (4%)	1 (1%)	11	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
25	AC	83/152 (55%)	79 (95%)	3 (4%)	1 (1%)	11 35
26	C2	113/116 (97%)	109 (96%)	4 (4%)	0	100 100
27	B1	53/56 (95%)	51 (96%)	2 (4%)	0	100 100
28	S4	149/183 (81%)	145 (97%)	4 (3%)	0	100 100
29	A9	375/416 (90%)	366 (98%)	9 (2%)	0	100 100
30	B2	58/94 (62%)	57 (98%)	1 (2%)	0	100 100
31	S2	427/468 (91%)	418 (98%)	8 (2%)	1 (0%)	44 72
33	V1	436/474 (92%)	421 (97%)	15 (3%)	0	100 100
34	2	339/341 (99%)	330 (97%)	9 (3%)	0	100 100
35	A7	87/103 (84%)	85 (98%)	2 (2%)	0	100 100
36	A3	64/77 (83%)	64 (100%)	0	0	100 100
37	4L	94/96 (98%)	93 (99%)	1 (1%)	0	100 100
38	6	172/174 (99%)	172 (100%)	0	0	100 100
39	3	115/117 (98%)	111 (96%)	4 (4%)	0	100 100
40	A5	115/124 (93%)	114 (99%)	1 (1%)	0	100 100
41	AL	366/407 (90%)	354 (97%)	12 (3%)	0	100 100
42	A6	113/124 (91%)	107 (95%)	6 (5%)	0	100 100
All	All	8026/9000 (89%)	7779 (97%)	240 (3%)	7 (0%)	50 78

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	4	43	ASN
9	4	202	LEU
10	5	324	ASN
25	AB	69	PRO
25	AC	69	PRO
31	S2	461	VAL
1	AN	136	GLU

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	AN	118/122 (97%)	116 (98%)	2 (2%)	56	74
2	S6	77/111 (69%)	77 (100%)	0	100	100
3	S1	549/582 (94%)	545 (99%)	4 (1%)	81	88
4	S3	184/225 (82%)	184 (100%)	0	100	100
5	V2	185/205 (90%)	182 (98%)	3 (2%)	58	75
6	S7	152/184 (83%)	150 (99%)	2 (1%)	65	78
7	S8	159/182 (87%)	159 (100%)	0	100	100
8	1	282/282 (100%)	278 (99%)	4 (1%)	62	77
9	4	403/404 (100%)	400 (99%)	3 (1%)	81	88
10	5	518/518 (100%)	505 (98%)	13 (2%)	42	65
11	A8	150/151 (99%)	144 (96%)	6 (4%)	27	52
12	A1	63/115 (55%)	63 (100%)	0	100	100
13	AO	128/134 (96%)	128 (100%)	0	100	100
14	S5	88/89 (99%)	87 (99%)	1 (1%)	70	81
15	AM	129/131 (98%)	128 (99%)	1 (1%)	79	87
16	BL	135/141 (96%)	135 (100%)	0	100	100
17	B6	133/136 (98%)	133 (100%)	0	100	100
18	B4	88/94 (94%)	88 (100%)	0	100	100
19	B7	104/104 (100%)	104 (100%)	0	100	100
20	B5	129/162 (80%)	129 (100%)	0	100	100
21	B9	116/126 (92%)	116 (100%)	0	100	100
22	BM	95/131 (72%)	95 (100%)	0	100	100
23	B8	121/145 (83%)	117 (97%)	4 (3%)	33	58
24	B3	66/84 (79%)	66 (100%)	0	100	100
25	AB	76/136 (56%)	76 (100%)	0	100	100
25	AC	77/136 (57%)	77 (100%)	0	100	100
26	C2	93/94 (99%)	93 (100%)	0	100	100
27	B1	42/43 (98%)	42 (100%)	0	100	100
28	S4	131/154 (85%)	131 (100%)	0	100	100
29	A9	319/346 (92%)	319 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	B2	51/80 (64%)	50 (98%)	1 (2%)	50 70
31	S2	368/398 (92%)	363 (99%)	5 (1%)	62 77
33	V1	350/381 (92%)	350 (100%)	0	100 100
34	2	317/317 (100%)	314 (99%)	3 (1%)	75 86
35	A7	79/86 (92%)	78 (99%)	1 (1%)	65 78
36	A3	52/59 (88%)	52 (100%)	0	100 100
37	4L	91/91 (100%)	91 (100%)	0	100 100
38	6	167/167 (100%)	164 (98%)	3 (2%)	54 73
39	3	110/110 (100%)	110 (100%)	0	100 100
40	A5	96/102 (94%)	96 (100%)	0	100 100
41	AL	324/356 (91%)	324 (100%)	0	100 100
42	A6	108/114 (95%)	108 (100%)	0	100 100
All	All	7023/7728 (91%)	6967 (99%)	56 (1%)	77 87

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AN	44	ILE
1	AN	136	GLU
3	S1	84	ASN
3	S1	226	LYS
3	S1	229	LEU
3	S1	230	THR
5	V2	181	ILE
5	V2	183	ASP
5	V2	184	ASP
6	S7	96	CYS
6	S7	99	VAL
8	1	1	MET
8	1	4	MET
8	1	158	LEU
8	1	159	SER
9	4	164	LYS
9	4	202	LEU
9	4	213	VAL
10	5	4	LEU
10	5	8	SER
10	5	30	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	5	111	ILE
10	5	225	LEU
10	5	226	VAL
10	5	286	MET
10	5	288	ILE
10	5	289	LEU
10	5	290	SER
10	5	291	MET
10	5	308	LYS
10	5	387	SER
11	A8	50	GLN
11	A8	51	GLU
11	A8	142	LYS
11	A8	143	LYS
11	A8	145	GLU
11	A8	146	LYS
14	S5	20	ASN
15	AM	108	VAL
23	B8	57	LEU
23	B8	58	LEU
23	B8	60	GLU
23	B8	63	LYS
30	B2	63	LEU
31	S2	186	LEU
31	S2	456	ILE
31	S2	458	THR
31	S2	459	LEU
31	S2	461	VAL
34	2	45	LEU
34	2	46	SER
34	2	47	ASP
35	A7	55	ASN
38	6	21	ILE
38	6	40	LEU
38	6	43	LEU

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

Mol	Chain	Res	Type
1	AN	33	ASN
3	S1	52	GLN
3	S1	436	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	S1	517	ASN
3	S1	528	GLN
3	S1	541	GLN
3	S1	555	ASN
4	S3	140	ASN
5	V2	43	ASN
5	V2	175	ASN
5	V2	199	ASN
9	4	87	ASN
9	4	138	GLN
9	4	239	GLN
10	5	31	ASN
10	5	168	ASN
10	5	304	HIS
10	5	321	ASN
10	5	324	ASN
11	A8	18	GLN
11	A8	50	GLN
12	A1	62	ASN
13	AO	90	GLN
14	S5	22	GLN
14	S5	64	GLN
14	S5	89	GLN
15	AM	25	ASN
16	BL	17	ASN
16	BL	43	GLN
16	BL	67	GLN
17	B6	79	ASN
19	B7	83	HIS
20	B5	88	GLN
20	B5	123	ASN
20	B5	135	ASN
20	B5	139	GLN
21	B9	50	ASN
22	BM	52	ASN
23	B8	128	ASN
28	S4	92	ASN
28	S4	132	ASN
29	A9	116	HIS
29	A9	249	HIS
29	A9	257	GLN
29	A9	266	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	A9	330	ASN
31	S2	84	ASN
31	S2	152	ASN
31	S2	270	ASN
31	S2	290	ASN
31	S2	311	GLN
34	2	85	ASN
34	2	86	ASN
34	2	145	ASN
34	2	271	GLN
34	2	304	ASN
34	2	316	ASN
34	2	318	ASN
35	A7	55	ASN
37	4L	24	ASN
37	4L	51	ASN
38	6	19	ASN
38	6	79	ASN
38	6	113	ASN
38	6	138	ASN
40	A5	19	ASN
40	A5	22	HIS
40	A5	83	GLN
40	A5	111	GLN
40	A5	118	GLN
41	AL	160	GLN
41	AL	176	GLN
41	AL	245	GLN
41	AL	274	GLN
41	AL	275	GLN
41	AL	404	ASN
42	A6	13	GLN
42	A6	99	HIS
42	A6	108	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 68 ligands modelled in this entry, 1 is monoatomic - leaving 67 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	$\#\|Z\| > 2$
43	CDL	B6	203	-	46,46,99	0.41	0	52,58,111	0.39	0
43	CDL	6	203	-	85,85,99	0.32	0	91,97,111	0.29	0
55	FMN	V1	501	-	33,33,33	0.31	0	48,50,50	0.43	0
48	3PE	5	603	-	32,32,50	0.40	0	35,37,55	0.69	1 (2%)
56	WSF	6	201	-	34,34,34	4.99	3 (8%)	37,40,40	2.85	4 (10%)
44	PC1	AM	201	-	36,36,53	0.34	0	42,44,61	0.36	0
43	CDL	B5	202	-	65,65,99	0.36	0	71,77,111	0.31	0
47	FES	V2	301	5	0,4,4	-	-	-		
44	PC1	AN	202	-	43,43,53	0.33	0	49,51,61	0.30	0
44	PC1	5	606	-	33,33,53	0.38	0	39,41,61	0.39	0
52	OCT	B1	101	-	7,7,7	0.12	0	6,6,6	0.05	0
44	PC1	2	402	-	44,44,53	0.31	0	50,52,61	0.32	0
48	3PE	B4	201	-	46,46,50	0.31	0	49,51,55	0.28	0
48	3PE	B6	201	-	47,47,50	0.38	0	50,52,55	0.39	1 (2%)
48	3PE	4	503	-	44,44,50	0.31	0	47,49,55	0.27	0
44	PC1	A9	501	-	43,43,53	0.31	0	49,51,61	0.30	0
48	3PE	5	608	-	44,44,50	0.34	0	47,49,55	0.59	1 (2%)
44	PC1	1	401	-	53,53,53	0.33	0	59,61,61	0.55	1 (1%)
48	3PE	4	502	-	31,31,50	0.37	0	34,36,55	0.33	0
48	3PE	5	605	-	32,32,50	0.37	0	35,37,55	0.32	0
43	CDL	B5	201	-	75,75,99	0.34	0	81,87,111	0.31	0
44	PC1	AM	206	-	31,31,53	0.39	0	37,39,61	0.41	0
48	3PE	5	602	-	50,50,50	0.31	0	53,55,55	0.32	0
51	ZMP	AC	201	-	28,33,36	0.81	1 (3%)	32,40,45	3.27	6 (18%)
50	C14	AO	201	-	13,13,13	0.11	0	12,12,12	0.07	0
50	C14	B5	203	-	13,13,13	0.11	0	12,12,12	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
53	D12	B1	102	-	11,11,11	0.10	0	10,10,10	0.06	0
48	3PE	S7	303	-	32,32,50	0.37	0	35,37,55	0.34	0
43	CDL	AM	204	-	75,75,99	0.36	0	81,87,111	0.49	1 (1%)
48	3PE	B1	103	-	36,36,50	0.37	0	39,41,55	0.64	1 (2%)
44	PC1	B6	202	-	36,36,53	0.36	0	42,44,61	0.64	1 (2%)
48	3PE	5	607	-	50,50,50	0.29	0	53,55,55	0.30	0
44	PC1	S7	304	-	45,45,53	0.33	0	51,53,61	0.33	0
48	3PE	5	601	-	31,31,50	0.38	0	34,36,55	0.34	0
46	SF4	V1	502	33	0,12,12	-	-	-		
48	3PE	4	504	-	35,35,50	0.35	0	38,40,55	0.34	0
48	3PE	4	506	-	38,38,50	0.36	0	41,43,55	0.63	1 (2%)
48	3PE	AM	202	-	40,40,50	0.33	0	43,45,55	0.35	0
54	NDP	A9	502	-	47,52,52	0.54	0	61,80,80	0.54	1 (1%)
44	PC1	AM	205	-	43,43,53	0.32	0	49,51,61	0.44	0
46	SF4	S8	302	7	0,12,12	-	-	-		
48	3PE	1	403	-	50,50,50	0.30	0	53,55,55	0.31	0
44	PC1	4	505	-	38,38,53	0.33	0	44,46,61	0.34	0
48	3PE	5	604	-	29,29,50	0.39	0	32,34,55	0.35	0
46	SF4	S1	801	3	0,12,12	-	-	-		
48	3PE	AM	203	-	30,30,50	0.38	0	33,35,55	0.35	0
47	FES	S1	803	3	0,4,4	-	-	-		
43	CDL	AN	201	-	66,66,99	0.36	0	72,78,111	0.38	0
48	3PE	C2	201	-	44,44,50	0.32	0	47,49,55	0.35	0
48	3PE	6	202	-	34,34,50	0.37	0	37,39,55	0.34	0
50	C14	C2	202	-	13,13,13	0.10	0	12,12,12	0.07	0
53	D12	A3	101	-	11,11,11	0.11	0	10,10,10	0.06	0
57	DGT	AL	501	-	29,33,33	0.96	3 (10%)	37,52,52	0.70	1 (2%)
48	3PE	3	202	-	50,50,50	0.30	0	53,55,55	0.37	0
46	SF4	S1	802	3	0,12,12	-	-	-		
53	D12	A9	503	-	11,11,11	0.11	0	10,10,10	0.05	0
43	CDL	2	403	-	43,43,99	0.60	1 (2%)	47,54,111	0.63	1 (2%)
49	U10	1	402	-	63,63,63	2.26	25 (39%)	78,79,79	1.48	19 (24%)
46	SF4	S8	301	7	0,12,12	-	-	-		
48	3PE	S7	302	-	32,32,50	0.37	0	35,37,55	0.31	0
48	3PE	2	401	-	29,29,50	0.38	0	32,34,55	0.36	0
46	SF4	S7	301	6	0,12,12	-	-	-		
53	D12	A9	504	-	11,11,11	0.11	0	10,10,10	0.07	0
44	PC1	4	501	-	38,38,53	0.35	0	44,46,61	0.37	0
51	ZMP	AB	201	-	26,31,36	0.77	1 (3%)	30,38,45	3.45	6 (20%)
48	3PE	3	203	-	40,40,50	0.36	0	43,45,55	0.60	1 (2%)
43	CDL	3	201	-	53,53,99	0.40	0	59,65,111	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	CDL	B6	203	-	-	21/56/56/110	-
43	CDL	6	203	-	-	16/96/96/110	-
55	FMN	V1	501	-	-	10/18/18/18	0/3/3/3
48	3PE	5	603	-	-	9/36/36/54	-
56	WSF	6	201	-	-	5/38/38/38	-
44	PC1	AM	201	-	-	5/40/40/57	-
43	CDL	B5	202	-	-	16/76/76/110	-
47	FES	V2	301	5	-	-	0/1/1/1
44	PC1	AN	202	-	-	6/47/47/57	-
44	PC1	5	606	-	-	9/37/37/57	-
52	OCT	B1	101	-	-	0/5/5/5	-
46	SF4	S8	302	7	-	-	0/6/5/5
44	PC1	2	402	-	-	6/48/48/57	-
48	3PE	B4	201	-	-	9/50/50/54	-
48	3PE	B6	201	-	-	6/49/49/54	-
48	3PE	4	503	-	-	5/48/48/54	-
44	PC1	A9	501	-	-	6/47/47/57	-
48	3PE	5	608	-	-	11/48/48/54	-
44	PC1	1	401	-	-	13/57/57/57	-
48	3PE	4	502	-	-	8/35/35/54	-
48	3PE	5	605	-	-	7/36/36/54	-
43	CDL	B5	201	-	-	18/86/86/110	-
44	PC1	AM	206	-	-	14/35/35/57	-
48	3PE	5	602	-	-	5/54/54/54	-
51	ZMP	AC	201	-	-	13/38/40/43	-
50	C14	AO	201	-	-	0/11/11/11	-
50	C14	B5	203	-	-	0/11/11/11	-
53	D12	B1	102	-	-	0/9/9/9	-
48	3PE	S7	303	-	-	6/36/36/54	-
43	CDL	AM	204	-	-	23/86/86/110	-
48	3PE	B1	103	-	-	7/40/40/54	-
44	PC1	B6	202	-	-	10/40/40/57	-
48	3PE	5	607	-	-	12/54/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	PC1	S7	304	-	-	14/49/49/57	-
48	3PE	5	601	-	-	8/35/35/54	-
48	3PE	4	504	-	-	12/39/39/54	-
48	3PE	AM	202	-	-	6/44/44/54	-
48	3PE	4	506	-	-	11/42/42/54	-
54	NDP	A9	502	-	-	2/30/77/77	0/5/5/5
46	SF4	V1	502	33	-	-	0/6/5/5
44	PC1	AM	205	-	-	9/47/47/57	-
48	3PE	1	403	-	-	9/54/54/54	-
48	3PE	5	604	-	-	8/33/33/54	-
44	PC1	4	505	-	-	6/42/42/57	-
48	3PE	AM	203	-	-	6/34/34/54	-
48	3PE	C2	201	-	-	8/48/48/54	-
48	3PE	6	202	-	-	11/38/38/54	-
46	SF4	S1	801	3	-	-	0/6/5/5
43	CDL	AN	201	-	-	28/77/77/110	-
50	C14	C2	202	-	-	1/11/11/11	-
53	D12	A3	101	-	-	0/9/9/9	-
57	DGT	AL	501	-	-	3/18/34/34	0/3/3/3
47	FES	S1	803	3	-	-	0/1/1/1
48	3PE	3	202	-	-	12/54/54/54	-
46	SF4	S1	802	3	-	-	0/6/5/5
53	D12	A9	503	-	-	0/9/9/9	-
43	CDL	2	403	-	-	20/53/53/110	-
49	U10	1	402	-	-	19/63/87/87	0/1/1/1
48	3PE	S7	302	-	-	6/36/36/54	-
46	SF4	S8	301	7	-	-	0/6/5/5
48	3PE	2	401	-	-	8/33/33/54	-
46	SF4	S7	301	6	-	-	0/6/5/5
53	D12	A9	504	-	-	0/9/9/9	-
44	PC1	4	501	-	-	17/42/42/57	-
51	ZMP	AB	201	-	-	5/36/38/43	-
48	3PE	3	203	-	-	12/44/44/54	-
43	CDL	3	201	-	-	17/64/64/110	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	6	201	WSF	C14-C13	17.63	2.43	1.51
56	6	201	WSF	C15-C13	17.59	2.43	1.51
56	6	201	WSF	C12-C13	14.87	2.46	1.51
49	1	402	U10	C6-C1	10.61	1.54	1.35
49	1	402	U10	C4-C3	4.81	1.53	1.36
49	1	402	U10	C7-C8	2.97	1.55	1.50
49	1	402	U10	C26-C24	2.83	1.57	1.51
49	1	402	U10	C41-C39	2.81	1.57	1.51
49	1	402	U10	C21-C19	2.76	1.57	1.51
57	AL	501	DGT	C5-C6	-2.69	1.42	1.47
49	1	402	U10	C31-C29	2.65	1.56	1.51
49	1	402	U10	O5-C5	-2.62	1.17	1.23
49	1	402	U10	C7-C6	2.61	1.56	1.51
51	AC	201	ZMP	C9-C10	2.58	1.53	1.50
49	1	402	U10	C11-C9	2.52	1.56	1.51
49	1	402	U10	C36-C34	2.49	1.56	1.51
49	1	402	U10	C46-C44	2.45	1.56	1.51
43	2	403	CDL	OA6-CA5	-2.43	1.34	1.43
49	1	402	U10	O2-C2	-2.37	1.18	1.23
49	1	402	U10	C6-C5	2.37	1.53	1.46
49	1	402	U10	C51-C49	2.36	1.56	1.51
49	1	402	U10	C22-C23	2.32	1.57	1.50
51	AB	201	ZMP	C9-C10	2.31	1.53	1.50
49	1	402	U10	C27-C28	2.29	1.57	1.50
49	1	402	U10	C16-C14	2.26	1.56	1.51
49	1	402	U10	C42-C43	2.24	1.57	1.50
49	1	402	U10	O3-C3M	-2.22	1.40	1.45
49	1	402	U10	C17-C18	2.19	1.57	1.50
49	1	402	U10	C12-C13	2.14	1.56	1.50
49	1	402	U10	C32-C33	2.13	1.56	1.50
57	AL	501	DGT	C8-N7	-2.09	1.31	1.34
57	AL	501	DGT	C5-C4	-2.07	1.38	1.43
49	1	402	U10	C37-C38	2.02	1.56	1.50
49	1	402	U10	O4-C4M	-2.01	1.40	1.45

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	6	201	WSF	C15-C13-C14	-11.30	60.13	110.53
51	AB	201	ZMP	C19-C18-C17	-10.47	90.92	108.77
51	AC	201	ZMP	C20-C18-C17	-9.61	92.38	108.77
51	AC	201	ZMP	C19-C18-C17	-9.44	92.67	108.77
51	AB	201	ZMP	C20-C18-C17	-9.25	92.99	108.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	6	201	WSF	C15-C13-C12	-8.59	60.69	111.55
56	6	201	WSF	C14-C13-C12	-8.54	60.95	111.55
51	AB	201	ZMP	C19-C18-C21	7.50	120.60	108.22
51	AC	201	ZMP	C19-C18-C21	7.17	120.06	108.22
51	AB	201	ZMP	C20-C18-C19	6.71	122.58	109.20
51	AC	201	ZMP	C20-C18-C21	6.70	119.28	108.22
51	AC	201	ZMP	C20-C18-C19	5.74	120.65	109.20
51	AB	201	ZMP	C20-C18-C21	5.06	116.58	108.22
56	6	201	WSF	C11-C12-C13	4.69	150.06	116.18
49	1	402	U10	C27-C28-C29	-2.99	120.77	127.62
49	1	402	U10	C37-C38-C39	-2.96	120.86	127.62
49	1	402	U10	C32-C33-C34	-2.83	121.14	127.62
49	1	402	U10	C12-C13-C14	-2.77	121.29	127.62
43	AM	204	CDL	CB4-OB6-CB5	2.74	124.35	117.80
49	1	402	U10	C47-C48-C49	-2.67	121.51	127.62
49	1	402	U10	C42-C43-C44	-2.64	121.58	127.62
49	1	402	U10	C25-C24-C26	2.64	119.81	115.23
49	1	402	U10	C35-C34-C36	2.64	119.81	115.23
48	5	603	3PE	C2-O21-C21	2.64	124.11	117.80
49	1	402	U10	C20-C19-C21	2.62	119.78	115.23
43	2	403	CDL	CB4-OB6-CB5	2.59	124.00	117.80
51	AB	201	ZMP	O1-C10-C9	-2.59	120.99	123.98
48	B1	103	3PE	C2-O21-C21	2.58	123.98	117.80
44	B6	202	PC1	C2-O21-C21	2.57	123.96	117.80
48	3	203	3PE	C2-O21-C21	2.54	123.87	117.80
49	1	402	U10	C10-C9-C11	2.53	119.61	115.23
48	4	506	3PE	C2-O21-C21	2.52	123.82	117.80
49	1	402	U10	C30-C29-C31	2.51	119.58	115.23
51	AC	201	ZMP	O1-C10-C9	-2.49	121.10	123.98
49	1	402	U10	C50-C49-C51	2.48	119.53	115.23
49	1	402	U10	C17-C18-C19	-2.47	121.96	127.62
44	1	401	PC1	C2-O21-C21	2.46	123.69	117.80
48	5	608	3PE	C2-O21-C21	2.42	123.59	117.80
49	1	402	U10	C15-C14-C16	2.42	119.43	115.23
49	1	402	U10	C40-C39-C41	2.40	119.40	115.23
49	1	402	U10	C22-C23-C24	-2.36	122.22	127.62
49	1	402	U10	C45-C44-C46	2.31	119.24	115.23
54	A9	502	NDP	C5A-C6A-N6A	2.28	123.78	120.31
48	B6	201	3PE	O12-P-O14	2.12	119.09	110.83
49	1	402	U10	C7-C8-C9	-2.11	123.20	126.83
49	1	402	U10	C56-C54-C55	2.09	119.40	114.59
57	AL	501	DGT	O6-C6-C5	2.01	128.31	124.32

There are no chirality outliers.

All (534) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	AN	201	CDL	CA2-OA2-PA1-OA3
43	AN	201	CDL	CA2-OA2-PA1-OA4
43	AN	201	CDL	CA2-OA2-PA1-OA5
43	AN	201	CDL	CA3-OA5-PA1-OA2
43	AN	201	CDL	OA5-CA3-CA4-OA6
43	AN	201	CDL	CB2-OB2-PB2-OB4
43	AN	201	CDL	CB2-OB2-PB2-OB5
43	AN	201	CDL	CB3-OB5-PB2-OB3
43	AN	201	CDL	CB3-OB5-PB2-OB4
43	AM	204	CDL	CB2-OB2-PB2-OB3
43	AM	204	CDL	CB2-OB2-PB2-OB4
43	AM	204	CDL	CB2-OB2-PB2-OB5
43	AM	204	CDL	CB3-OB5-PB2-OB2
43	AM	204	CDL	CB3-OB5-PB2-OB3
43	AM	204	CDL	CB3-OB5-PB2-OB4
43	B6	203	CDL	CA2-OA2-PA1-OA4
43	B6	203	CDL	CA2-OA2-PA1-OA5
43	B6	203	CDL	CA3-OA5-PA1-OA2
43	B6	203	CDL	CA3-OA5-PA1-OA3
43	B6	203	CDL	CB2-OB2-PB2-OB5
43	B6	203	CDL	CB3-OB5-PB2-OB2
43	B6	203	CDL	CB3-OB5-PB2-OB3
43	B6	203	CDL	CB3-OB5-PB2-OB4
43	B5	201	CDL	CA2-OA2-PA1-OA5
43	B5	201	CDL	CA3-OA5-PA1-OA2
43	B5	201	CDL	CA3-OA5-PA1-OA3
43	B5	201	CDL	CA3-OA5-PA1-OA4
43	B5	202	CDL	CA3-OA5-PA1-OA2
43	B5	202	CDL	CA3-OA5-PA1-OA3
43	B5	202	CDL	CB3-OB5-PB2-OB2
43	B5	202	CDL	CB3-OB5-PB2-OB4
43	2	403	CDL	CA2-OA2-PA1-OA3
43	2	403	CDL	CA3-OA5-PA1-OA2
43	2	403	CDL	CA3-OA5-PA1-OA3
43	2	403	CDL	CA3-OA5-PA1-OA4
43	2	403	CDL	CB3-OB5-PB2-OB2
43	2	403	CDL	CB3-OB5-PB2-OB4
43	6	203	CDL	CB3-OB5-PB2-OB2
43	6	203	CDL	CB3-OB5-PB2-OB3
43	6	203	CDL	CB3-OB5-PB2-OB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
43	3	201	CDL	CA2-OA2-PA1-OA4
43	3	201	CDL	CA3-OA5-PA1-OA2
43	3	201	CDL	CA3-OA5-PA1-OA4
43	3	201	CDL	CB2-OB2-PB2-OB3
43	3	201	CDL	CB2-OB2-PB2-OB4
43	3	201	CDL	CB2-OB2-PB2-OB5
44	AN	202	PC1	C1-O11-P-O13
44	S7	304	PC1	C11-O13-P-O12
44	S7	304	PC1	C11-O13-P-O11
44	1	401	PC1	C11-O13-P-O12
44	1	401	PC1	C11-O13-P-O14
44	1	401	PC1	C11-O13-P-O11
44	4	501	PC1	C11-O13-P-O12
44	4	501	PC1	C11-O13-P-O14
44	4	501	PC1	C11-O13-P-O11
44	4	501	PC1	C1-O11-P-O12
44	4	501	PC1	C1-O11-P-O13
44	4	505	PC1	O13-C11-C12-N
44	5	606	PC1	C11-O13-P-O14
44	5	606	PC1	C11-O13-P-O11
44	5	606	PC1	C1-O11-P-O12
44	5	606	PC1	C1-O11-P-O14
44	AM	201	PC1	C1-O11-P-O12
44	AM	205	PC1	C11-O13-P-O12
44	AM	205	PC1	C11-O13-P-O14
44	AM	205	PC1	C11-O13-P-O11
44	AM	205	PC1	O21-C2-C3-O31
44	AM	206	PC1	C11-O13-P-O11
44	AM	206	PC1	O13-C11-C12-N
44	B6	202	PC1	C11-O13-P-O12
44	B6	202	PC1	C11-O13-P-O11
44	B6	202	PC1	C1-O11-P-O14
44	B6	202	PC1	C1-O11-P-O13
44	A9	501	PC1	C11-O13-P-O12
44	A9	501	PC1	C11-O13-P-O11
44	2	402	PC1	C11-O13-P-O12
44	2	402	PC1	C11-O13-P-O14
44	2	402	PC1	C11-O13-P-O11
44	2	402	PC1	O13-C11-C12-N
48	S7	302	3PE	C11-O13-P-O11
48	S7	302	3PE	C11-O13-P-O12
48	S7	302	3PE	O21-C2-C3-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	S7	303	3PE	C1-O11-P-O13
48	1	403	3PE	C1-O11-P-O12
48	1	403	3PE	C1-O11-P-O13
48	1	403	3PE	C11-O13-P-O12
48	1	403	3PE	O13-C11-C12-N
48	4	502	3PE	C1-O11-P-O12
48	4	502	3PE	C1-O11-P-O13
48	4	502	3PE	C1-O11-P-O14
48	4	502	3PE	C11-O13-P-O11
48	4	502	3PE	C11-O13-P-O14
48	4	502	3PE	O13-C11-C12-N
48	4	503	3PE	C1-O11-P-O12
48	4	503	3PE	C1-O11-P-O13
48	4	504	3PE	C1-O11-P-O12
48	4	504	3PE	C1-O11-P-O13
48	4	504	3PE	C1-O11-P-O14
48	4	504	3PE	C11-O13-P-O11
48	4	504	3PE	C11-O13-P-O12
48	4	504	3PE	O13-C11-C12-N
48	4	506	3PE	C1-O11-P-O13
48	4	506	3PE	C1-O11-P-O14
48	4	506	3PE	C11-O13-P-O12
48	4	506	3PE	O13-C11-C12-N
48	5	601	3PE	C1-O11-P-O13
48	5	601	3PE	C11-O13-P-O11
48	5	602	3PE	C11-O13-P-O11
48	5	603	3PE	C1-O11-P-O13
48	5	603	3PE	C1-O11-P-O14
48	5	603	3PE	C11-O13-P-O11
48	5	603	3PE	C11-O13-P-O12
48	5	603	3PE	O13-C11-C12-N
48	5	604	3PE	C1-O11-P-O12
48	5	604	3PE	C1-O11-P-O13
48	5	604	3PE	C1-O11-P-O14
48	5	604	3PE	O13-C11-C12-N
48	5	605	3PE	C1-O11-P-O13
48	5	605	3PE	C11-O13-P-O11
48	5	605	3PE	C11-O13-P-O12
48	5	605	3PE	O13-C11-C12-N
48	5	607	3PE	C1-O11-P-O13
48	5	607	3PE	C1-O11-P-O14
48	5	607	3PE	C11-O13-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	5	607	3PE	C11-O13-P-O12
48	5	607	3PE	C11-O13-P-O14
48	5	608	3PE	C1-O11-P-O12
48	5	608	3PE	C1-O11-P-O13
48	5	608	3PE	C1-O11-P-O14
48	5	608	3PE	C11-O13-P-O11
48	5	608	3PE	C11-O13-P-O12
48	5	608	3PE	C11-O13-P-O14
48	AM	202	3PE	C1-O11-P-O12
48	AM	202	3PE	C1-O11-P-O13
48	AM	202	3PE	C11-O13-P-O12
48	AM	203	3PE	C1-O11-P-O12
48	AM	203	3PE	C1-O11-P-O13
48	B6	201	3PE	C1-O11-P-O12
48	B6	201	3PE	C1-O11-P-O13
48	B6	201	3PE	C1-O11-P-O14
48	B4	201	3PE	C1-O11-P-O12
48	B4	201	3PE	C1-O11-P-O14
48	B4	201	3PE	C11-O13-P-O11
48	B4	201	3PE	C11-O13-P-O12
48	C2	201	3PE	C1-O11-P-O13
48	B1	103	3PE	C1-O11-P-O13
48	B1	103	3PE	C1-O11-P-O14
48	B1	103	3PE	C11-O13-P-O14
48	B1	103	3PE	O13-C11-C12-N
48	2	401	3PE	C1-O11-P-O13
48	2	401	3PE	C1-O11-P-O14
48	2	401	3PE	C11-O13-P-O11
48	6	202	3PE	C1-O11-P-O13
48	6	202	3PE	C11-O13-P-O11
48	6	202	3PE	C11-O13-P-O14
48	3	202	3PE	C11-O13-P-O12
48	3	203	3PE	C1-O11-P-O12
48	3	203	3PE	C1-O11-P-O13
48	3	203	3PE	C1-O11-P-O14
48	3	203	3PE	C11-O13-P-O11
49	1	402	U10	C40-C39-C41-C42
51	AC	201	ZMP	C19-C18-C21-O5
51	AC	201	ZMP	C17-C18-C21-O5
51	AC	201	ZMP	C12-C11-S1-C10
51	AB	201	ZMP	C19-C18-C21-O5
55	V1	501	FMN	N10-C1'-C2'-O2'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
55	V1	501	FMN	N10-C1'-C2'-C3'
55	V1	501	FMN	C5'-O5'-P-O1P
55	V1	501	FMN	C5'-O5'-P-O2P
55	V1	501	FMN	C5'-O5'-P-O3P
56	6	201	WSF	O13-C11-C12-C13
49	1	402	U10	C38-C39-C41-C42
51	AC	201	ZMP	C14-C13-N1-C12
43	AN	201	CDL	O1-C1-CB2-OB2
49	1	402	U10	C14-C16-C17-C18
49	1	402	U10	C29-C31-C32-C33
49	1	402	U10	C34-C36-C37-C38
49	1	402	U10	C39-C41-C42-C43
49	1	402	U10	C49-C51-C52-C53
51	AC	201	ZMP	O2-C13-N1-C12
43	AN	201	CDL	CA2-C1-CB2-OB2
44	4	501	PC1	C31-C32-C33-C34
44	AM	206	PC1	O21-C2-C3-O31
57	AL	501	DGT	O4'-C4'-C5'-O5'
49	1	402	U10	C44-C46-C47-C48
44	1	401	PC1	C11-C12-N-C14
44	5	606	PC1	C11-C12-N-C15
48	4	502	3PE	C31-C32-C33-C34
43	AM	204	CDL	CB7-C71-C72-C73
48	4	504	3PE	C31-C32-C33-C34
44	S7	304	PC1	C11-C12-N-C15
44	1	401	PC1	C11-C12-N-C13
44	5	606	PC1	C11-C12-N-C14
44	AM	206	PC1	C11-C12-N-C14
57	AL	501	DGT	C3'-C4'-C5'-O5'
49	1	402	U10	C15-C14-C16-C17
49	1	402	U10	C35-C34-C36-C37
43	B5	202	CDL	O1-C1-CA2-OA2
44	S7	304	PC1	C11-C12-N-C14
48	5	605	3PE	C22-C23-C24-C25
43	6	203	CDL	C20-C21-C22-C23
44	1	401	PC1	C24-C25-C26-C27
48	4	504	3PE	C29-C2A-C2B-C2C
56	6	201	WSF	C11-C12-C13-C14
48	5	601	3PE	C27-C28-C29-C2A
43	AN	201	CDL	C53-C54-C55-C56
44	AM	205	PC1	C2B-C2C-C2D-C2E
43	B5	202	CDL	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
43	B5	202	CDL	CB2-C1-CA2-OA2
49	1	402	U10	C19-C21-C22-C23
44	AM	206	PC1	C23-C24-C25-C26
55	V1	501	FMN	O3'-C3'-C4'-O4'
48	3	202	3PE	C21-C22-C23-C24
43	AM	204	CDL	C31-C32-C33-C34
43	B5	201	CDL	C73-C74-C75-C76
48	C2	201	3PE	C37-C38-C39-C3A
44	S7	304	PC1	C11-C12-N-C13
44	1	401	PC1	C11-C12-N-C15
43	B5	201	CDL	CA7-C31-C32-C33
55	V1	501	FMN	C2'-C3'-C4'-O4'
43	AM	204	CDL	C76-C77-C78-C79
43	AM	204	CDL	C78-C79-C80-C81
51	AC	201	ZMP	C6-C7-C8-C9
48	C2	201	3PE	C28-C29-C2A-C2B
49	1	402	U10	C13-C14-C16-C17
49	1	402	U10	C33-C34-C36-C37
43	3	201	CDL	C51-C52-C53-C54
51	AC	201	ZMP	C4-C5-C6-C7
51	AB	201	ZMP	C4-C5-C6-C7
44	5	606	PC1	C11-C12-N-C13
44	AM	206	PC1	C11-C12-N-C13
43	B5	201	CDL	C55-C56-C57-C58
44	4	501	PC1	O11-C1-C2-O21
43	3	201	CDL	C14-C15-C16-C17
44	AN	202	PC1	O21-C2-C3-O31
43	3	201	CDL	C16-C17-C18-C19
48	4	506	3PE	C2-C1-O11-P
48	6	202	3PE	C2-C1-O11-P
44	AM	206	PC1	C24-C25-C26-C27
44	1	401	PC1	C37-C38-C39-C3A
44	AM	206	PC1	C11-C12-N-C15
51	AC	201	ZMP	O3-C16-C17-O4
43	AM	204	CDL	OB5-CB3-CB4-CB6
43	B5	201	CDL	OA5-CA3-CA4-CA6
43	B6	203	CDL	CB5-C51-C52-C53
48	B6	201	3PE	C31-C32-C33-C34
48	5	608	3PE	C34-C35-C36-C37
49	1	402	U10	C43-C44-C46-C47
43	B6	203	CDL	CA3-CA4-CA6-OA8
48	S7	302	3PE	C1-C2-C3-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
55	V1	501	FMN	C2'-C3'-C4'-C5'
49	1	402	U10	C45-C44-C46-C47
48	3	202	3PE	C2B-C2C-C2D-C2E
48	3	203	3PE	O11-C1-C2-O21
48	4	504	3PE	O21-C2-C3-O31
48	5	603	3PE	O21-C2-C3-O31
44	AM	205	PC1	C28-C29-C2A-C2B
44	4	501	PC1	C11-C12-N-C13
43	B5	201	CDL	C53-C54-C55-C56
48	B4	201	3PE	C37-C38-C39-C3A
43	AM	204	CDL	CB4-CB3-OB5-PB2
43	B5	202	CDL	CA4-CA3-OA5-PA1
43	AM	204	CDL	OA5-CA3-CA4-CA6
43	B6	203	CDL	OA5-CA3-CA4-CA6
44	4	501	PC1	O11-C1-C2-C3
48	6	202	3PE	O11-C1-C2-C3
43	B5	202	CDL	CA7-C31-C32-C33
49	1	402	U10	C50-C49-C51-C52
48	4	506	3PE	C2B-C2C-C2D-C2E
55	V1	501	FMN	O3'-C3'-C4'-C5'
43	AN	201	CDL	CA3-CA4-CA6-OA8
44	AN	202	PC1	C1-C2-C3-O31
44	AM	205	PC1	C1-C2-C3-O31
44	AM	206	PC1	C1-C2-C3-O31
48	3	202	3PE	C1-C2-C3-O31
44	4	505	PC1	C33-C34-C35-C36
49	1	402	U10	C48-C49-C51-C52
44	4	501	PC1	C11-C12-N-C15
48	6	202	3PE	O11-C1-C2-O21
43	B6	203	CDL	CA4-CA3-OA5-PA1
43	3	201	CDL	C1-CB2-OB2-PB2
48	3	203	3PE	C2-C1-O11-P
51	AC	201	ZMP	C5-C6-C7-C8
43	AM	204	CDL	OB6-CB4-CB6-OB8
43	B6	203	CDL	OA6-CA4-CA6-OA8
48	3	203	3PE	O21-C2-C3-O31
44	1	401	PC1	C3B-C3C-C3D-C3E
48	1	403	3PE	C26-C27-C28-C29
57	AL	501	DGT	PB-O3A-PA-O5'
54	A9	502	NDP	O4D-C1D-N1N-C6N
43	B5	201	CDL	C54-C55-C56-C57
51	AC	201	ZMP	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
43	AN	201	CDL	OA5-CA3-CA4-CA6
43	2	403	CDL	OB5-CB3-CB4-CB6
44	4	505	PC1	O11-C1-C2-C3
48	AM	203	3PE	O11-C1-C2-C3
48	C2	201	3PE	C26-C27-C28-C29
44	4	501	PC1	C11-C12-N-C14
48	5	602	3PE	C23-C24-C25-C26
43	B6	203	CDL	OA5-CA3-CA4-OA6
43	B5	202	CDL	OB5-CB3-CB4-OB6
43	6	203	CDL	OB5-CB3-CB4-OB6
43	3	201	CDL	OB5-CB3-CB4-OB6
44	4	505	PC1	O11-C1-C2-O21
48	5	608	3PE	O11-C1-C2-O21
49	1	402	U10	C9-C11-C12-C13
48	3	203	3PE	C21-C22-C23-C24
50	C2	202	C14	C04-C05-C06-C07
43	AM	204	CDL	C51-C52-C53-C54
44	4	501	PC1	C12-C11-O13-P
48	5	602	3PE	C12-C11-O13-P
48	2	401	3PE	C12-C11-O13-P
48	3	202	3PE	O21-C2-C3-O31
56	6	201	WSF	C2-C1-O11-P
44	AM	201	PC1	O13-C11-C12-N
44	AM	205	PC1	O13-C11-C12-N
44	B6	202	PC1	O13-C11-C12-N
44	A9	501	PC1	O13-C11-C12-N
44	1	401	PC1	C29-C2A-C2B-C2C
43	B5	202	CDL	OB5-CB3-CB4-CB6
43	3	201	CDL	OB5-CB3-CB4-CB6
51	AC	201	ZMP	C20-C18-C21-O5
44	AM	206	PC1	C31-C32-C33-C34
48	S7	303	3PE	C2-C1-O11-P
43	AM	204	CDL	OA5-CA3-CA4-OA6
43	AM	204	CDL	OB5-CB3-CB4-OB6
43	B5	201	CDL	OA5-CA3-CA4-OA6
48	AM	203	3PE	O11-C1-C2-O21
43	6	203	CDL	C75-C76-C77-C78
43	AN	201	CDL	OA6-CA4-CA6-OA8
48	5	607	3PE	O21-C2-C3-O31
48	5	607	3PE	C1-C2-C3-O31
48	3	203	3PE	C1-C2-C3-O31
51	AC	201	ZMP	C11-C12-N1-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	5	607	3PE	C39-C3A-C3B-C3C
48	AM	202	3PE	C24-C25-C26-C27
43	AN	201	CDL	CA3-OA5-PA1-OA3
43	AN	201	CDL	CB2-OB2-PB2-OB3
43	AN	201	CDL	CB3-OB5-PB2-OB2
43	AM	204	CDL	CA2-OA2-PA1-OA3
43	B6	203	CDL	CA3-OA5-PA1-OA4
43	B6	203	CDL	CB2-OB2-PB2-OB3
43	B5	201	CDL	CA2-OA2-PA1-OA3
43	B5	201	CDL	CB3-OB5-PB2-OB2
43	B5	202	CDL	CA3-OA5-PA1-OA4
43	2	403	CDL	CA2-OA2-PA1-OA4
43	2	403	CDL	CA2-OA2-PA1-OA5
43	2	403	CDL	CB2-OB2-PB2-OB3
43	2	403	CDL	CB2-OB2-PB2-OB4
43	2	403	CDL	CB2-OB2-PB2-OB5
43	6	203	CDL	CA2-OA2-PA1-OA3
43	6	203	CDL	CA2-OA2-PA1-OA4
43	6	203	CDL	CA2-OA2-PA1-OA5
43	3	201	CDL	CA2-OA2-PA1-OA3
43	3	201	CDL	CA2-OA2-PA1-OA5
44	AN	202	PC1	C1-O11-P-O14
44	S7	304	PC1	C1-O11-P-O12
44	S7	304	PC1	C1-O11-P-O14
44	S7	304	PC1	C1-O11-P-O13
44	4	501	PC1	C1-O11-P-O14
44	5	606	PC1	C1-O11-P-O13
44	AM	201	PC1	C11-O13-P-O14
44	AM	201	PC1	C1-O11-P-O14
44	AM	201	PC1	C1-O11-P-O13
44	B6	202	PC1	C1-O11-P-O12
48	S7	302	3PE	O13-C11-C12-N
48	S7	303	3PE	C1-O11-P-O12
48	S7	303	3PE	C1-O11-P-O14
48	1	403	3PE	C11-O13-P-O11
48	1	403	3PE	C11-O13-P-O14
48	4	502	3PE	C11-O13-P-O12
48	4	503	3PE	O13-C11-C12-N
48	4	506	3PE	C11-O13-P-O11
48	4	506	3PE	C11-O13-P-O14
48	5	601	3PE	C1-O11-P-O14
48	5	601	3PE	C11-O13-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	5	602	3PE	C11-O13-P-O14
48	5	603	3PE	C1-O11-P-O12
48	5	607	3PE	C1-O11-P-O12
48	B4	201	3PE	C1-O11-P-O13
48	B4	201	3PE	O13-C11-C12-N
48	C2	201	3PE	C1-O11-P-O14
48	C2	201	3PE	C11-O13-P-O14
48	B1	103	3PE	C1-O11-P-O12
48	2	401	3PE	C1-O11-P-O12
48	2	401	3PE	C11-O13-P-O14
48	6	202	3PE	C1-O11-P-O14
48	6	202	3PE	C11-O13-P-O12
48	3	202	3PE	C11-O13-P-O11
48	3	202	3PE	C11-O13-P-O14
48	3	203	3PE	C11-O13-P-O14
48	3	203	3PE	O13-C11-C12-N
43	AM	204	CDL	C71-C72-C73-C74
48	3	202	3PE	C37-C38-C39-C3A
43	AN	201	CDL	C1-CB2-OB2-PB2
43	B6	203	CDL	C1-CB2-OB2-PB2
43	2	403	CDL	C1-CA2-OA2-PA1
44	1	401	PC1	C2-C1-O11-P
55	V1	501	FMN	C4'-C5'-O5'-P
48	5	602	3PE	C24-C25-C26-C27
56	6	201	WSF	C31-C32-C33-C34
43	B5	202	CDL	C73-C74-C75-C76
48	AM	202	3PE	C23-C24-C25-C26
43	AM	204	CDL	CB5-C51-C52-C53
43	6	203	CDL	CB5-C51-C52-C53
43	AN	201	CDL	OB5-CB3-CB4-CB6
43	AN	201	CDL	OB5-CB3-CB4-OB6
43	AN	201	CDL	CB4-CB3-OB5-PB2
44	B6	202	PC1	C2-C1-O11-P
43	AN	201	CDL	C13-C14-C15-C16
48	3	202	3PE	C29-C2A-C2B-C2C
48	4	504	3PE	C1-C2-C3-O31
44	5	606	PC1	O31-C31-C32-C33
54	A9	502	NDP	C2B-O2B-P2B-O3X
43	B5	201	CDL	C1-CA2-OA2-PA1
44	AM	206	PC1	O11-C1-C2-O21
48	5	603	3PE	O11-C1-C2-O21
48	5	605	3PE	O21-C2-C3-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	2	401	3PE	C2-C1-O11-P
43	AN	201	CDL	C15-C16-C17-C18
43	B6	203	CDL	CB3-CB4-CB6-OB8
48	5	601	3PE	C1-C2-C3-O31
51	AC	201	ZMP	N2-C16-C17-O4
48	S7	303	3PE	O21-C21-C22-C23
44	S7	304	PC1	C3A-C3B-C3C-C3D
48	4	506	3PE	O11-C1-C2-O21
43	B5	202	CDL	C1-CA2-OA2-PA1
44	AN	202	PC1	C2-C1-O11-P
48	5	601	3PE	O21-C2-C3-O31
48	C2	201	3PE	C29-C2A-C2B-C2C
44	2	402	PC1	C27-C28-C29-C2A
48	5	605	3PE	C1-C2-C3-O31
48	5	608	3PE	C1-C2-C3-O31
48	5	608	3PE	O21-C21-C22-C23
56	6	201	WSF	O31-C31-C32-C33
44	S7	304	PC1	C39-C3A-C3B-C3C
43	B5	201	CDL	C72-C71-CB7-OB8
48	4	504	3PE	C2-C1-O11-P
44	A9	501	PC1	O31-C31-C32-C33
43	2	403	CDL	CB6-CB4-OB6-CB5
48	5	608	3PE	C1-C2-O21-C21
48	3	203	3PE	C3-C2-O21-C21
43	B5	201	CDL	CA4-CA3-OA5-PA1
43	3	201	CDL	CA4-CA3-OA5-PA1
48	S7	303	3PE	O11-C1-C2-O21
44	2	402	PC1	C2E-C2F-C2G-C2H
48	2	401	3PE	C22-C23-C24-C25
44	4	505	PC1	C36-C37-C38-C39
48	AM	202	3PE	C21-C22-C23-C24
44	4	501	PC1	O31-C31-C32-C33
48	5	601	3PE	C32-C33-C34-C35
43	AM	204	CDL	C13-C14-C15-C16
48	4	506	3PE	C26-C27-C28-C29
43	B6	203	CDL	C52-C51-CB5-OB6
48	6	202	3PE	O21-C21-C22-C23
48	B4	201	3PE	C39-C3A-C3B-C3C
51	AB	201	ZMP	C6-C7-C8-C9
48	3	202	3PE	C33-C34-C35-C36
43	6	203	CDL	C12-C11-CA5-OA6
48	B6	201	3PE	O31-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	C2	201	3PE	C36-C37-C38-C39
48	5	607	3PE	O21-C21-C22-C23
48	6	202	3PE	O31-C31-C32-C33
48	3	202	3PE	C2C-C2D-C2E-C2F
43	2	403	CDL	C72-C71-CB7-OB8
48	AM	203	3PE	O21-C21-C22-C23
51	AB	201	ZMP	O3-C16-C17-C18
43	B5	201	CDL	CB5-C51-C52-C53
44	S7	304	PC1	C3B-C3C-C3D-C3E
43	3	201	CDL	C15-C16-C17-C18
44	4	501	PC1	O21-C21-C22-C23
44	A9	501	PC1	O21-C21-C22-C23
44	AM	206	PC1	C32-C33-C34-C35
43	B5	202	CDL	CA5-C11-C12-C13
44	AM	206	PC1	O21-C21-C22-C23
48	B1	103	3PE	O31-C31-C32-C33
43	2	403	CDL	C52-C51-CB5-OB6
43	6	203	CDL	C32-C31-CA7-OA8
48	5	604	3PE	O21-C21-C22-C23
48	4	506	3PE	C35-C36-C37-C38
44	S7	304	PC1	C23-C24-C25-C26
48	5	604	3PE	O31-C31-C32-C33
43	AN	201	CDL	C14-C15-C16-C17
44	1	401	PC1	C1-C2-O21-C21
44	B6	202	PC1	C3-C2-O21-C21
48	5	603	3PE	C3-C2-O21-C21
43	2	403	CDL	C32-C31-CA7-OA8
44	S7	304	PC1	O31-C31-C32-C33
43	B6	203	CDL	C72-C71-CB7-OB8
43	AN	201	CDL	C52-C51-CB5-OB6
43	AN	201	CDL	CA5-C11-C12-C13
43	3	201	CDL	CB4-CB3-OB5-PB2
48	3	202	3PE	C2-C1-O11-P
49	1	402	U10	C30-C29-C31-C32
44	B6	202	PC1	O21-C21-C22-C23
48	5	607	3PE	O22-C21-C22-C23
43	AN	201	CDL	C51-C52-C53-C54
48	S7	302	3PE	C26-C27-C28-C29
43	B5	201	CDL	C12-C13-C14-C15
43	2	403	CDL	C72-C71-CB7-OB9
44	A9	501	PC1	O22-C21-C22-C23
43	B5	202	CDL	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	B4	201	3PE	C21-C22-C23-C24
44	4	501	PC1	O32-C31-C32-C33
48	B6	201	3PE	O32-C31-C32-C33
48	6	202	3PE	O22-C21-C22-C23
43	AM	204	CDL	C74-C75-C76-C77
48	5	607	3PE	C36-C37-C38-C39
43	6	203	CDL	C12-C11-CA5-OA7
48	5	604	3PE	O22-C21-C22-C23
44	AN	202	PC1	O21-C21-C22-C23
51	AB	201	ZMP	N2-C16-C17-O4
43	B6	203	CDL	C52-C51-CB5-OB7
43	2	403	CDL	C32-C31-CA7-OA9
48	1	403	3PE	O31-C31-C32-C33
48	1	403	3PE	O21-C21-C22-C23
43	6	203	CDL	C32-C31-CA7-OA9
48	5	604	3PE	O32-C31-C32-C33
44	1	401	PC1	C2C-C2D-C2E-C2F
43	6	203	CDL	C54-C55-C56-C57
43	6	203	CDL	OB5-CB3-CB4-CB6
44	AM	206	PC1	O22-C21-C22-C23
48	AM	203	3PE	O22-C21-C22-C23
43	2	403	CDL	C52-C51-CB5-OB7
44	4	501	PC1	O22-C21-C22-C23
48	4	503	3PE	C31-C32-C33-C34
43	AM	204	CDL	C32-C31-CA7-OA8
44	4	505	PC1	O21-C21-C22-C23
48	4	503	3PE	O21-C21-C22-C23
48	4	504	3PE	O21-C21-C22-C23
44	S7	304	PC1	O32-C31-C32-C33
44	B6	202	PC1	O22-C21-C22-C23
48	B1	103	3PE	O32-C31-C32-C33
44	AM	205	PC1	C23-C24-C25-C26

There are no ring outliers.

43 monomers are involved in 91 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	B6	203	CDL	2	0
43	6	203	CDL	4	0
55	V1	501	FMN	2	0
48	5	603	3PE	1	0
56	6	201	WSF	8	0

Continued on next page...

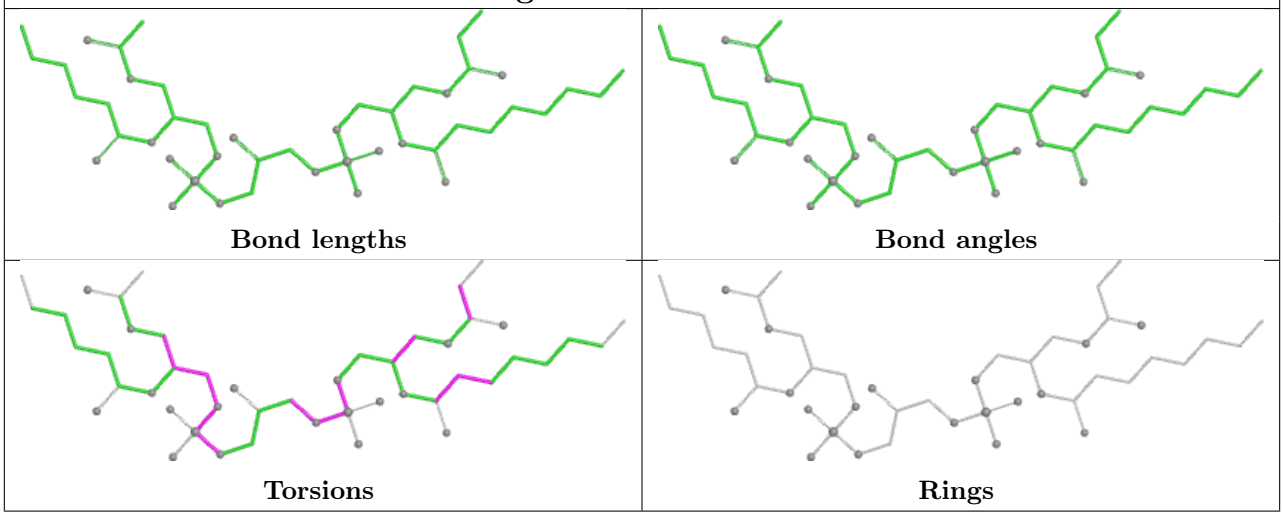
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	B5	202	CDL	1	0
44	AN	202	PC1	2	0
44	5	606	PC1	3	0
44	2	402	PC1	1	0
48	B6	201	3PE	2	0
44	A9	501	PC1	3	0
48	5	608	3PE	2	0
44	1	401	PC1	2	0
48	4	502	3PE	1	0
48	5	605	3PE	1	0
43	B5	201	CDL	6	0
44	AM	206	PC1	1	0
48	5	602	3PE	1	0
51	AC	201	ZMP	1	0
48	S7	303	3PE	2	0
43	AM	204	CDL	5	0
44	B6	202	PC1	1	0
48	5	607	3PE	2	0
48	5	601	3PE	1	0
48	4	504	3PE	2	0
48	AM	202	3PE	2	0
44	AM	205	PC1	4	0
48	1	403	3PE	1	0
44	4	505	PC1	2	0
48	5	604	3PE	1	0
48	AM	203	3PE	1	0
43	AN	201	CDL	3	0
48	C2	201	3PE	1	0
48	6	202	3PE	2	0
57	AL	501	DGT	5	0
48	3	202	3PE	1	0
43	2	403	CDL	1	0
49	1	402	U10	3	0
48	S7	302	3PE	1	0
48	2	401	3PE	2	0
46	S7	301	SF4	7	0
44	4	501	PC1	2	0
48	3	203	3PE	2	0

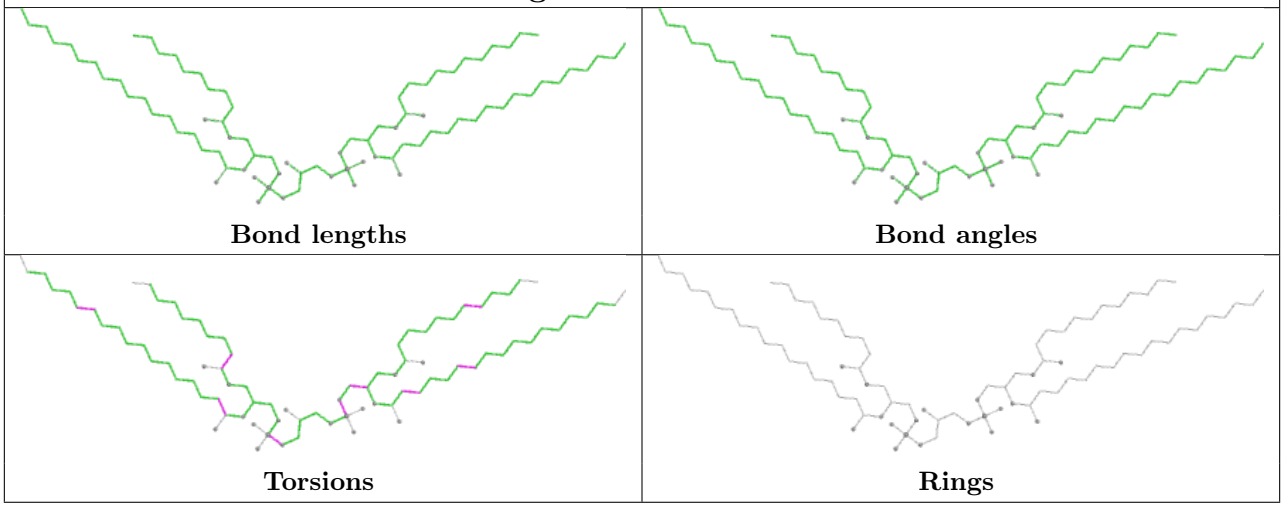
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

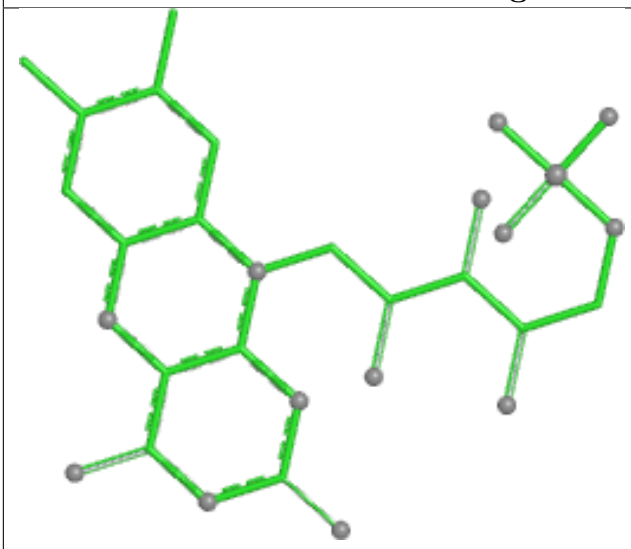
Ligand CDL B6 203



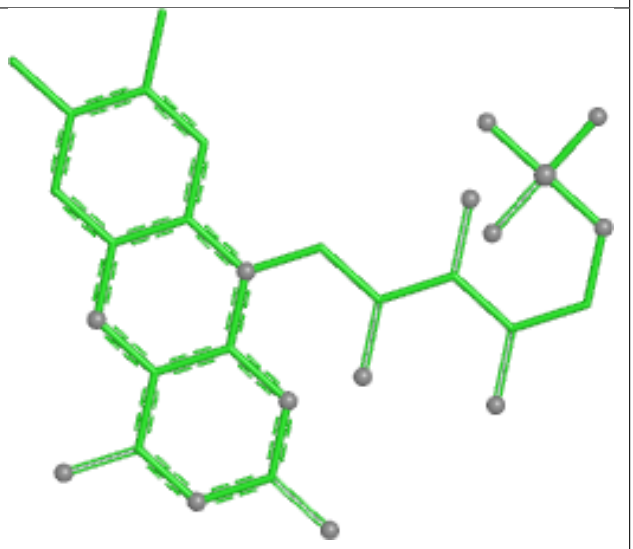
Ligand CDL 6 203



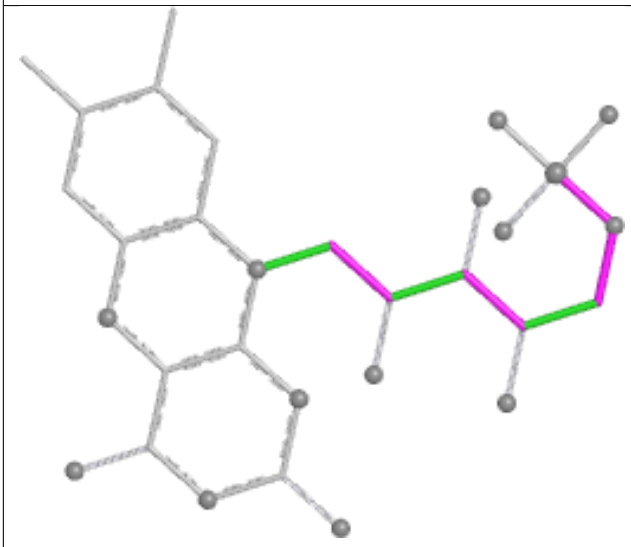
Ligand FMN V1 501



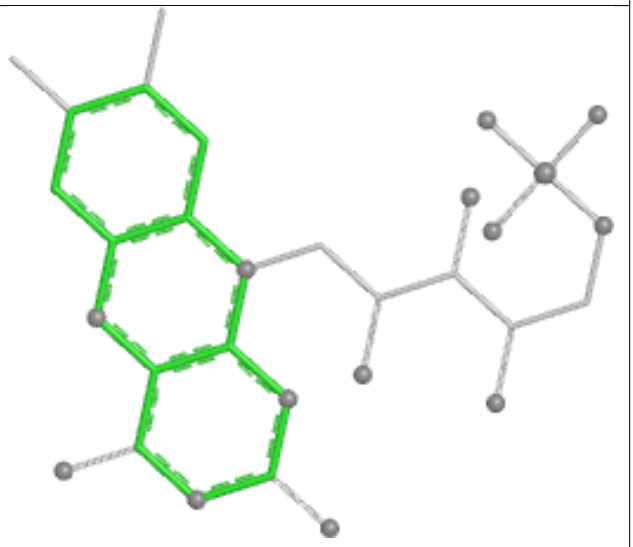
Bond lengths



Bond angles

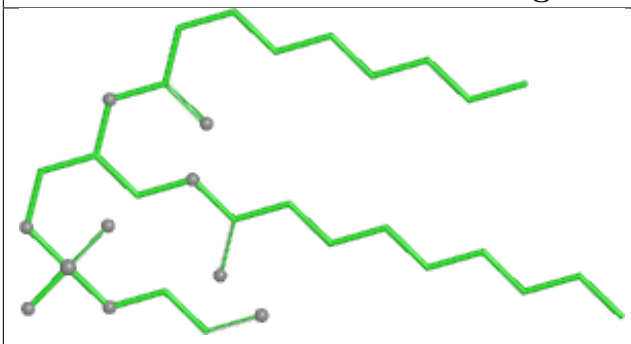


Torsions

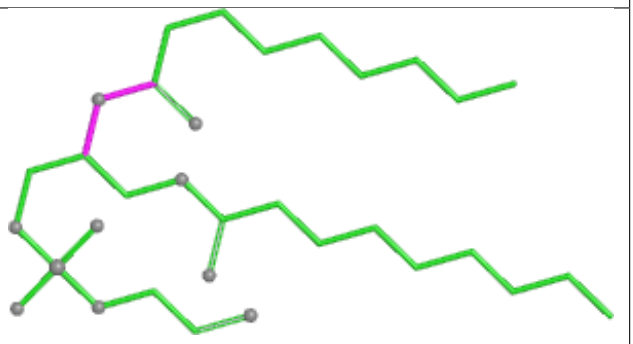


Rings

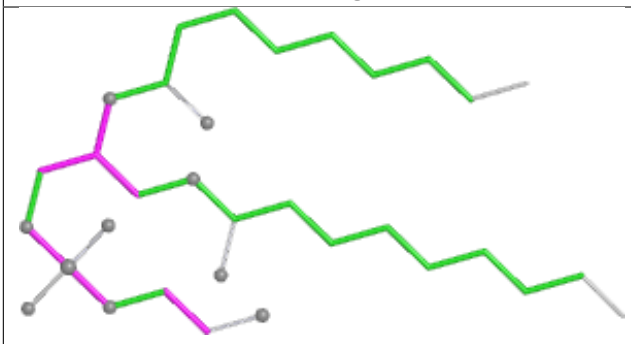
Ligand 3PE 5 603



Bond lengths



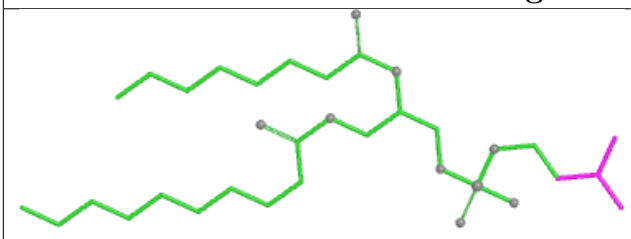
Bond angles



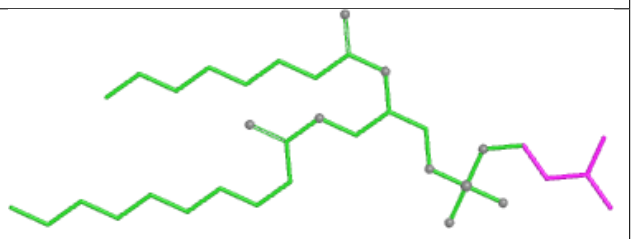
Torsions

Rings

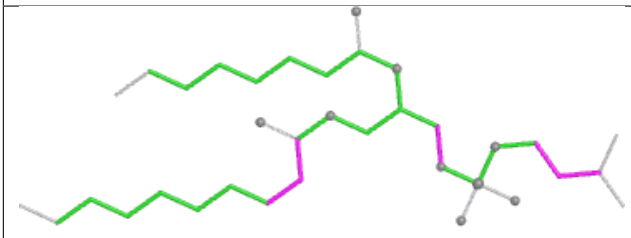
Ligand WSF 6 201



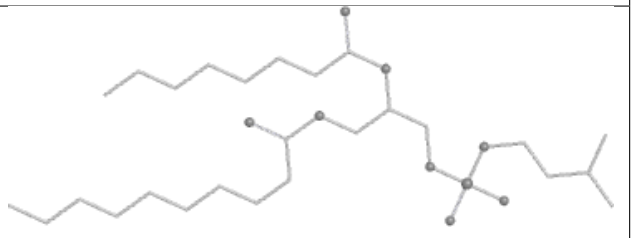
Bond lengths



Bond angles

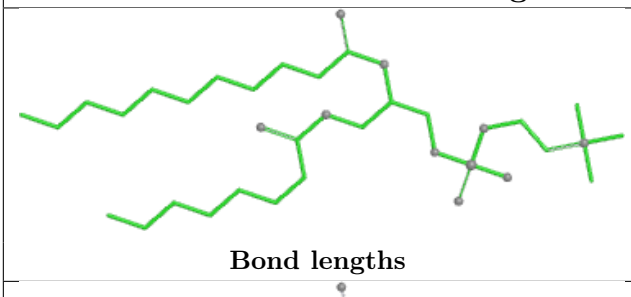


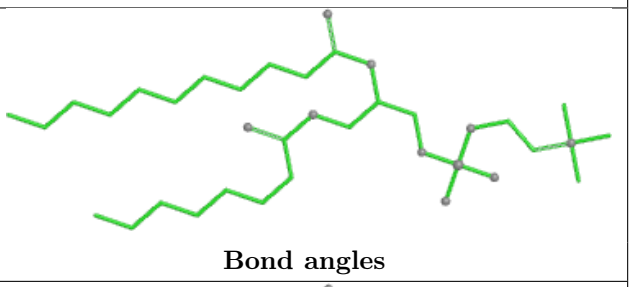
Torsions

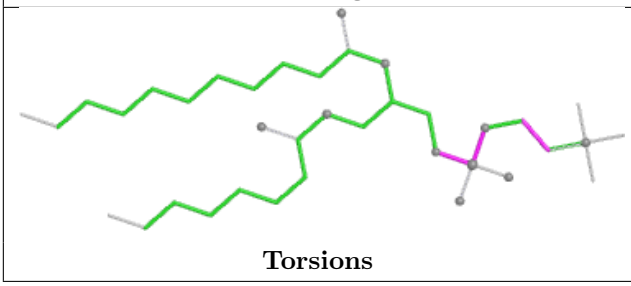


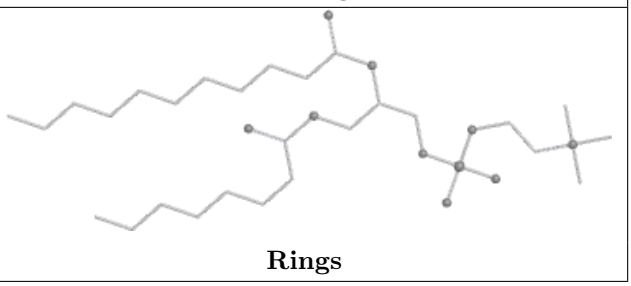
Rings

Ligand PC1 AM 201

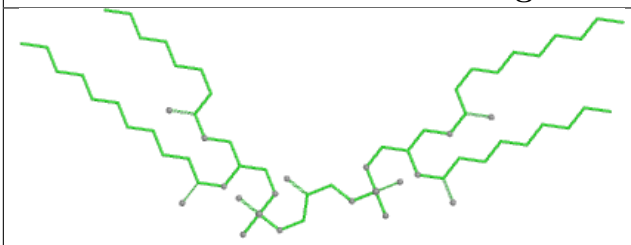

Bond lengths

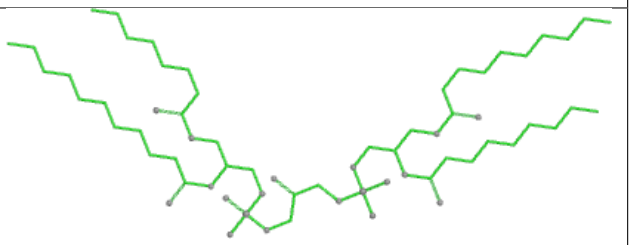

Bond angles

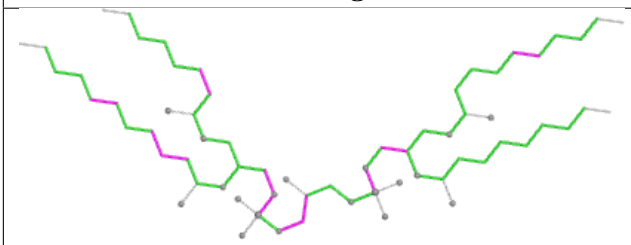

Torsions

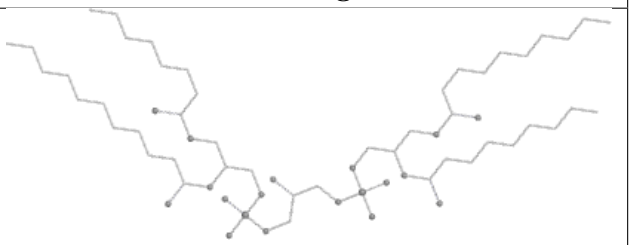

Rings

Ligand CDL B5 202

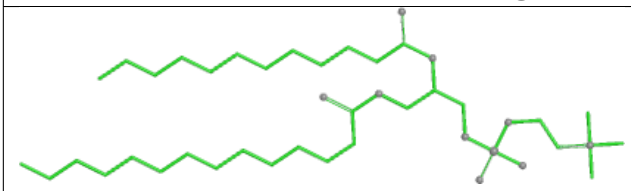

Bond lengths

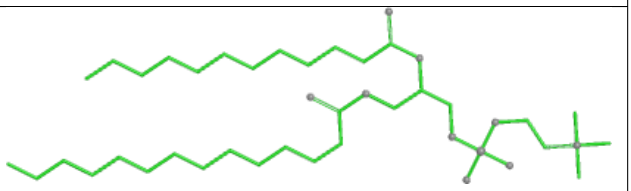

Bond angles

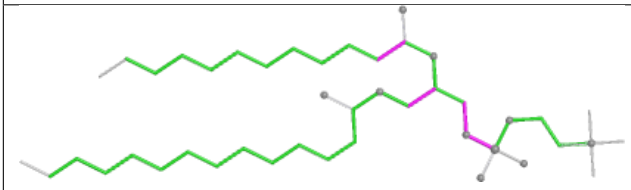

Torsions

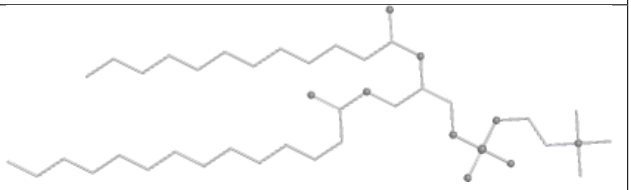

Rings

Ligand PC1 AN 202

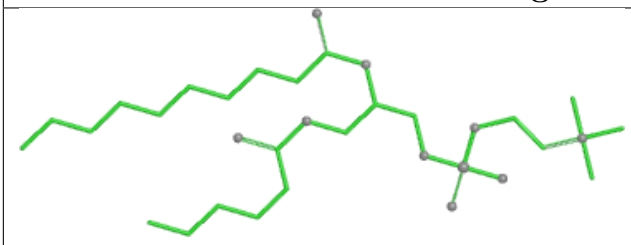

Bond lengths


Bond angles

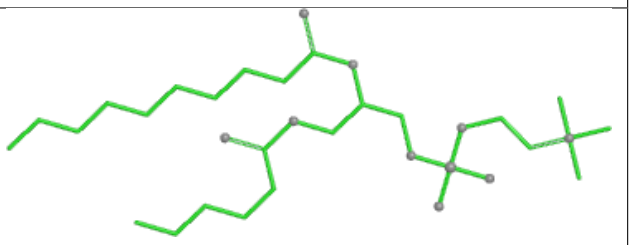

Torsions


Rings

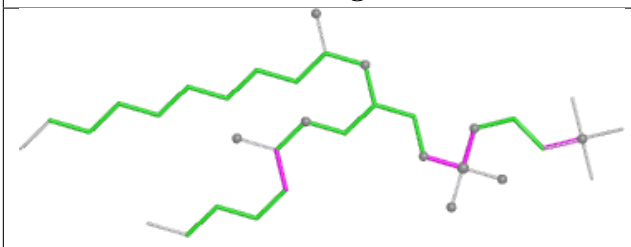
Ligand PC1 5 606



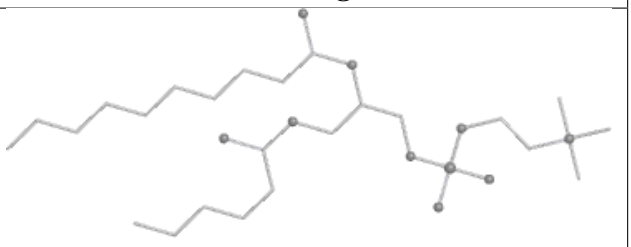
Bond lengths



Bond angles

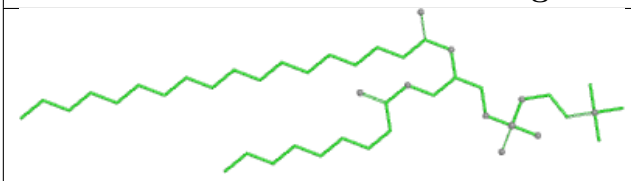


Torsions

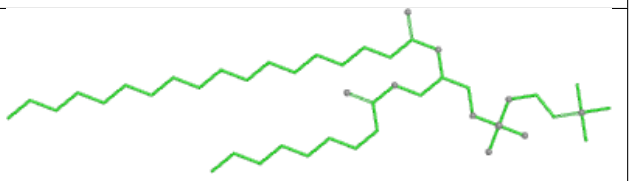


Rings

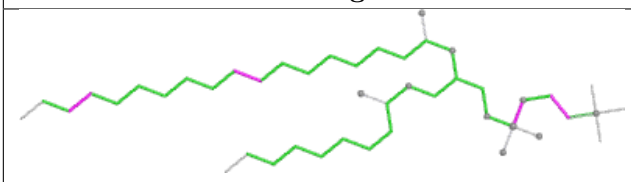
Ligand PC1 2 402



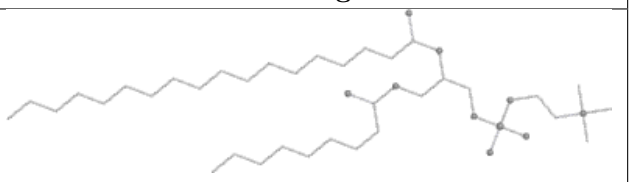
Bond lengths



Bond angles

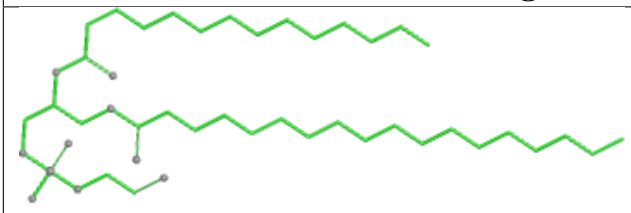


Torsions



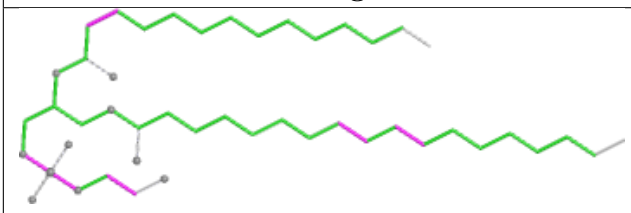
Rings

Ligand 3PE B4 201

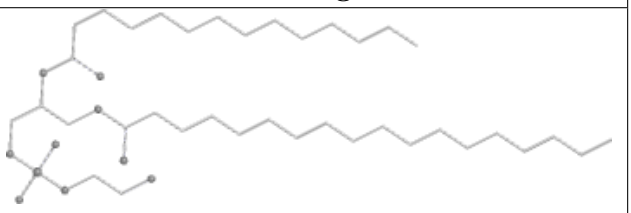


Bond lengths

Bond angles

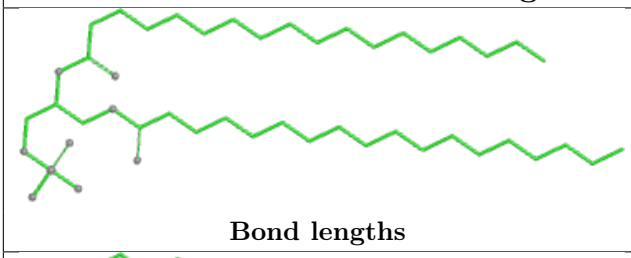


Torsions

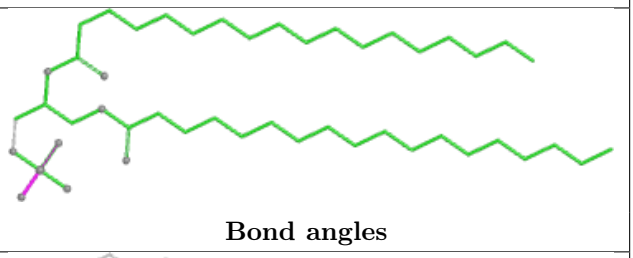


Rings

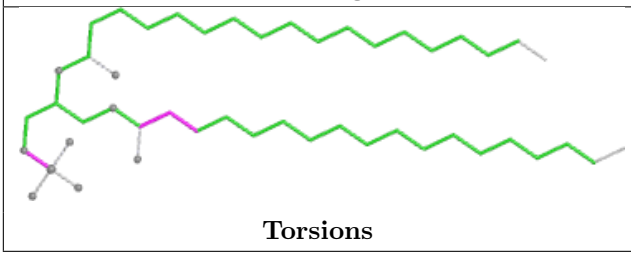
Ligand 3PE B6 201



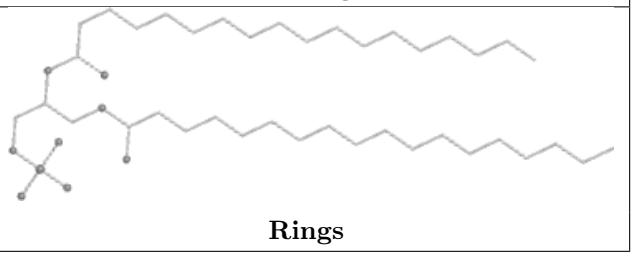
Bond lengths



Bond angles

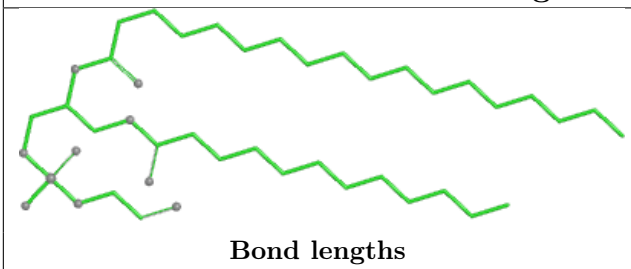


Torsions

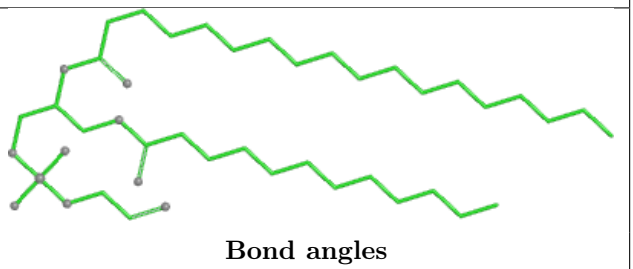


Rings

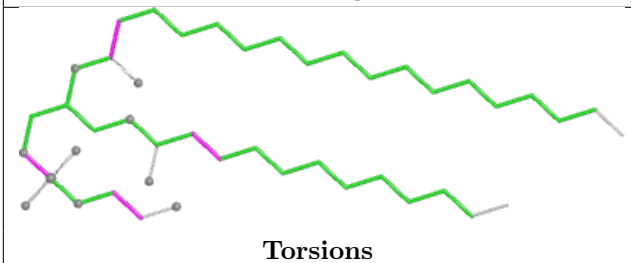
Ligand 3PE 4 503



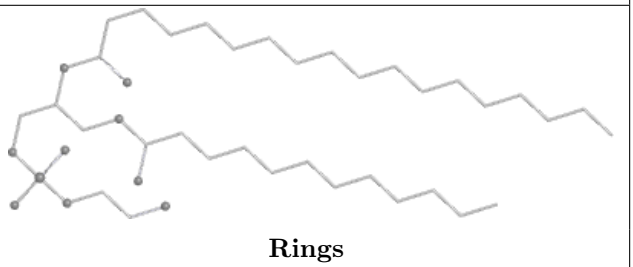
Bond lengths



Bond angles

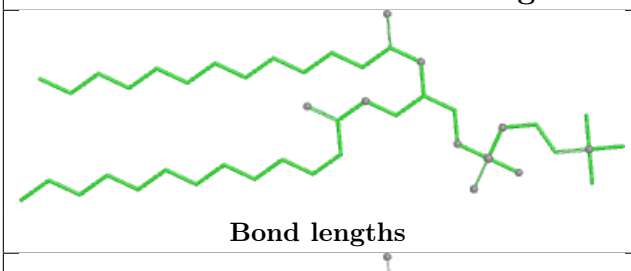


Torsions

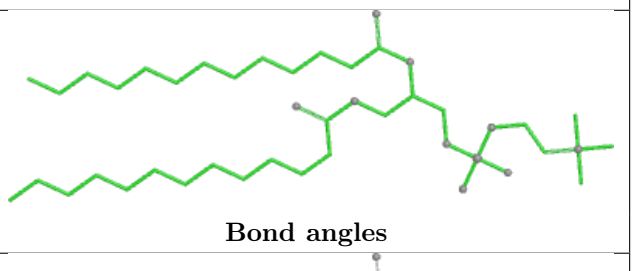


Rings

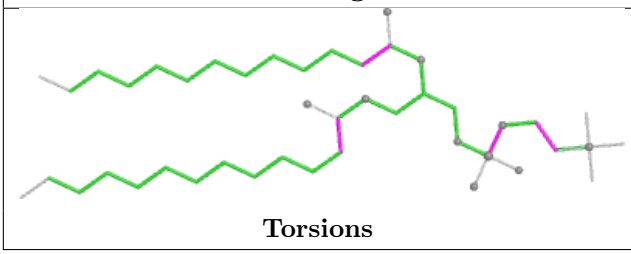
Ligand PC1 A9 501



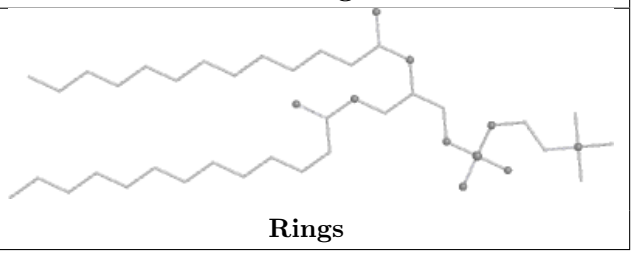
Bond lengths



Bond angles

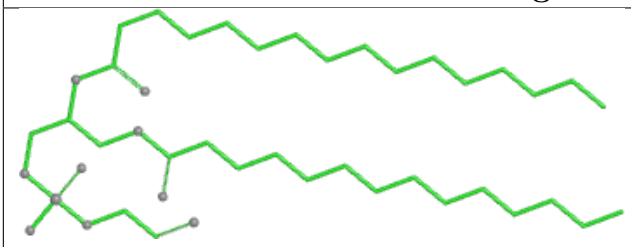


Torsions

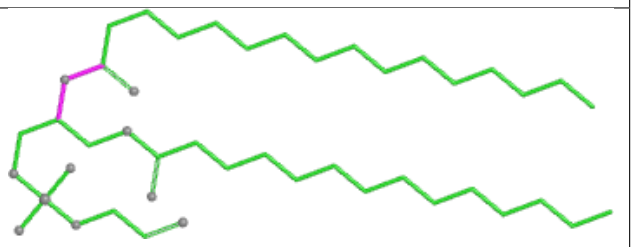


Rings

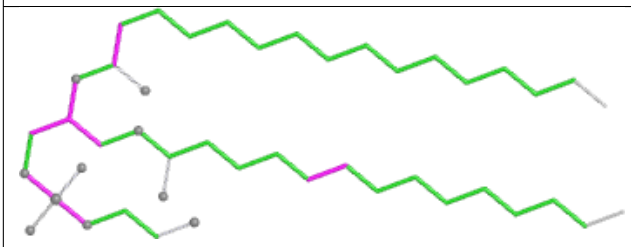
Ligand 3PE 5 608



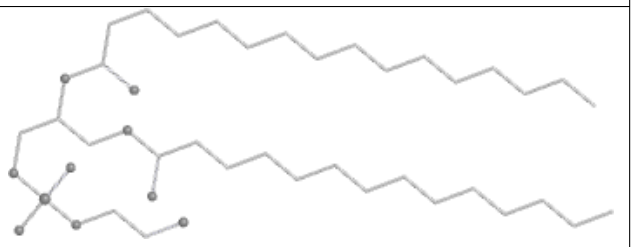
Bond lengths



Bond angles

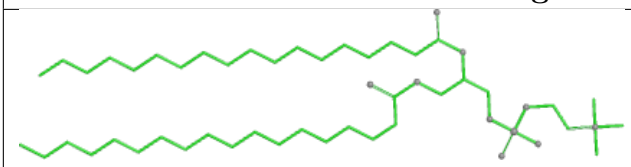


Torsions

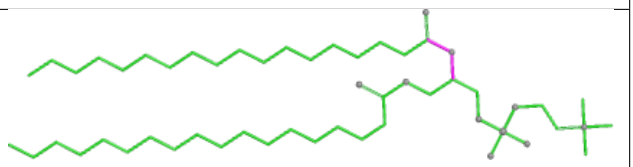


Rings

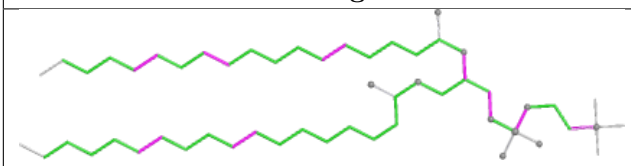
Ligand PC1 1 401



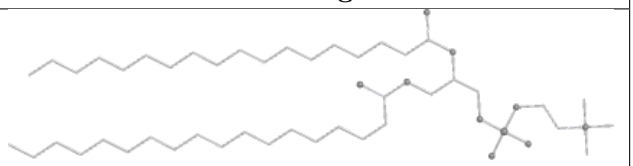
Bond lengths



Bond angles

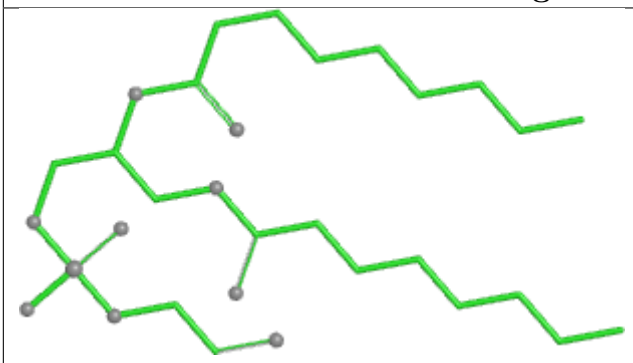


Torsions

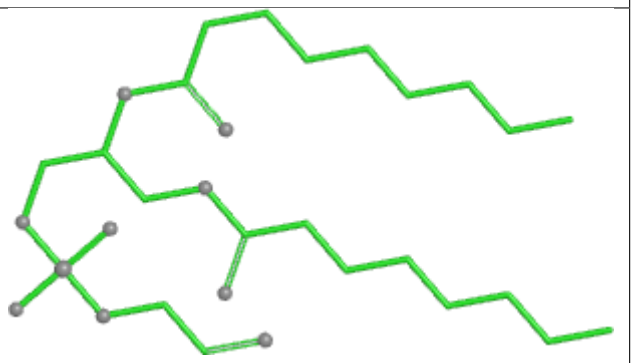


Rings

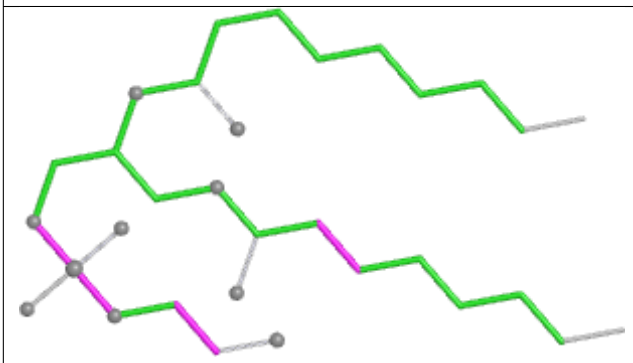
Ligand 3PE 4 502



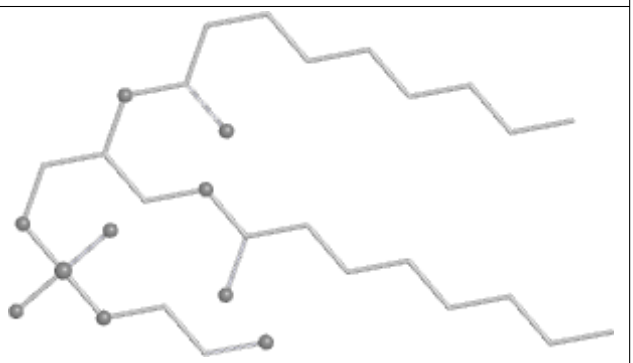
Bond lengths



Bond angles

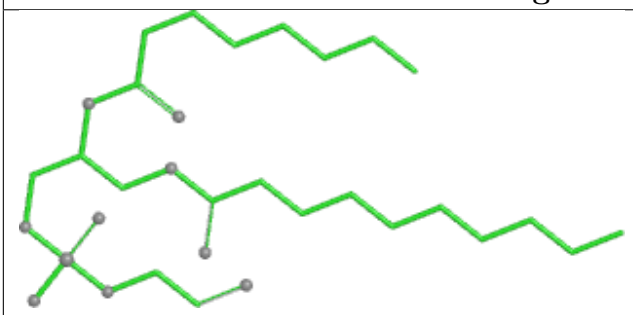


Torsions

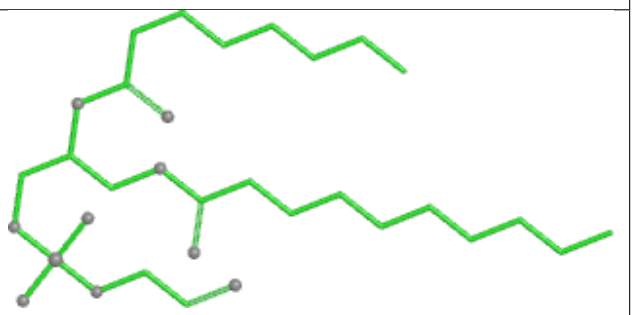


Rings

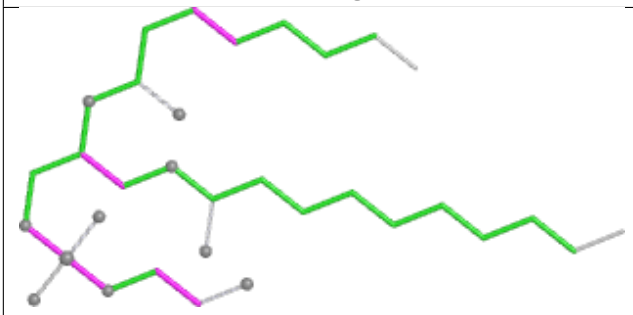
Ligand 3PE 5 605



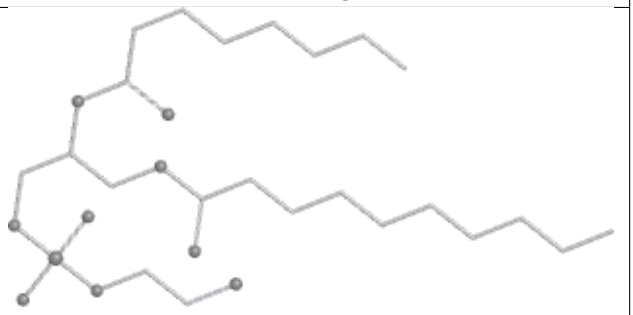
Bond lengths



Bond angles

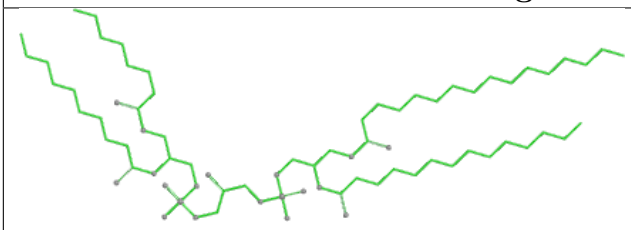


Torsions

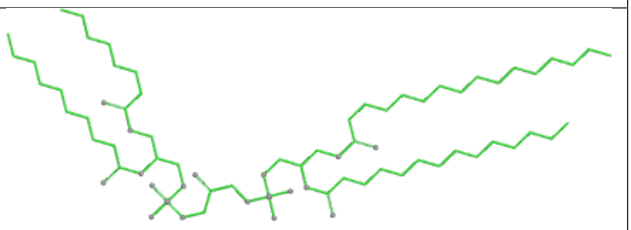


Rings

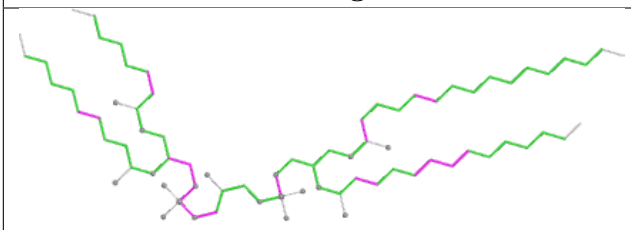
Ligand CDL B5 201



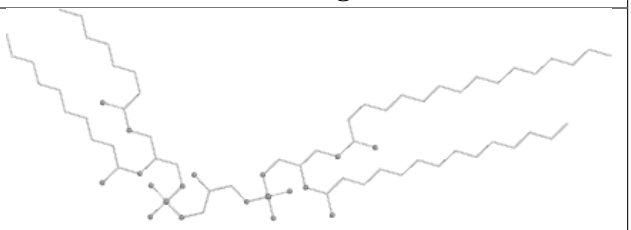
Bond lengths



Bond angles

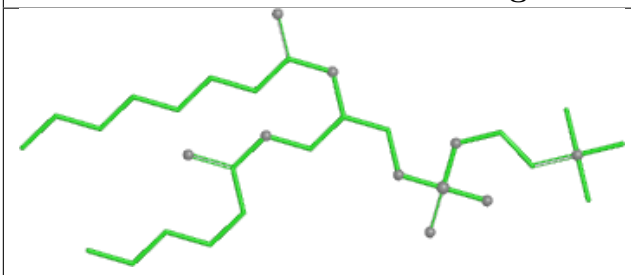


Torsions

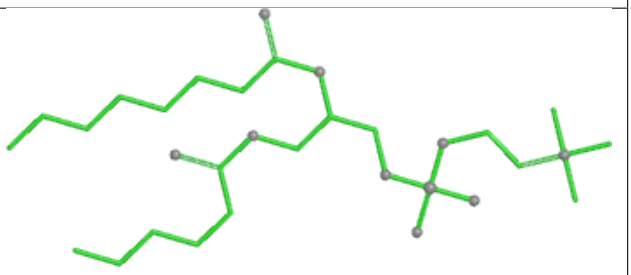


Rings

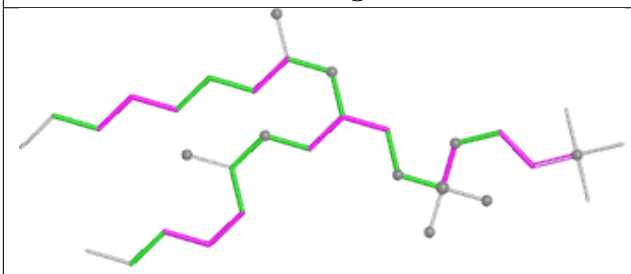
Ligand PC1 AM 206



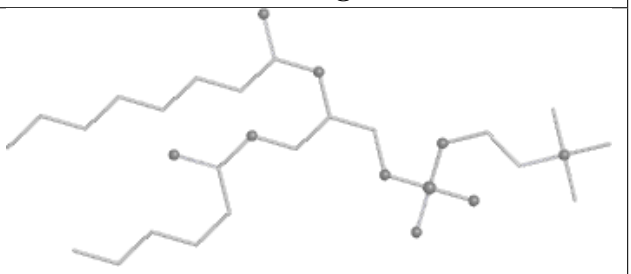
Bond lengths



Bond angles

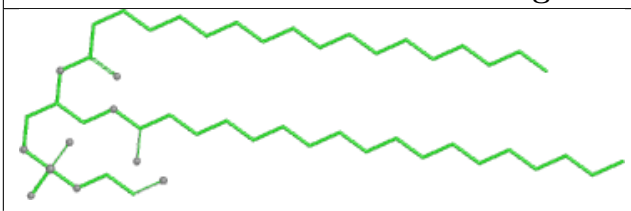


Torsions

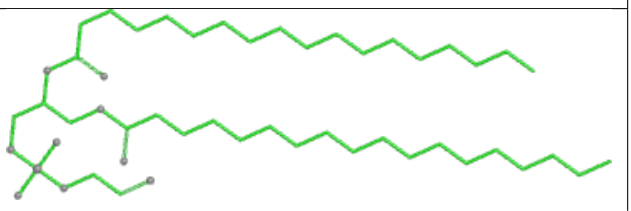


Rings

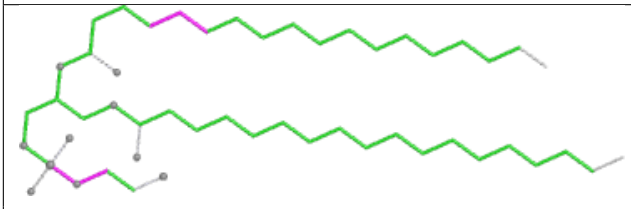
Ligand 3PE 5 602



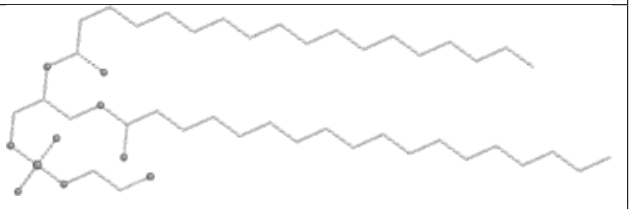
Bond lengths



Bond angles

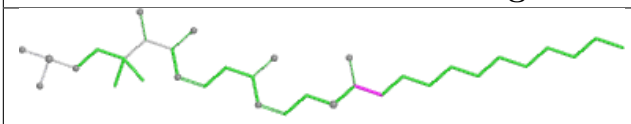


Torsions

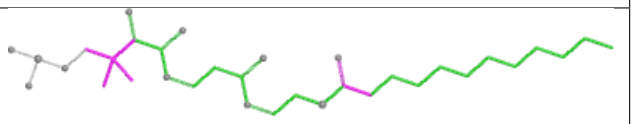


Rings

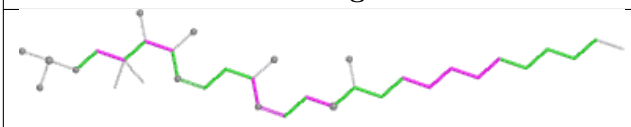
Ligand ZMP AC 201



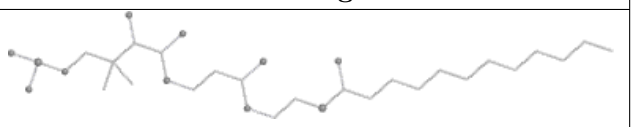
Bond lengths



Bond angles

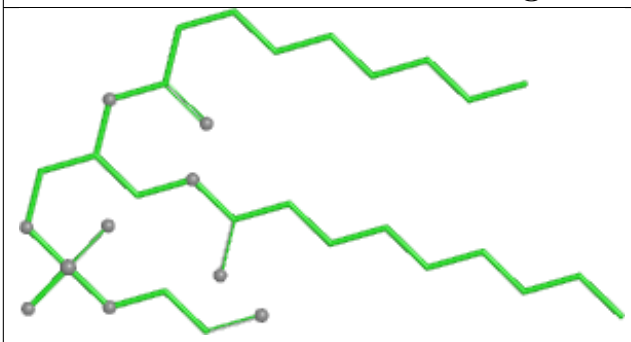


Torsions

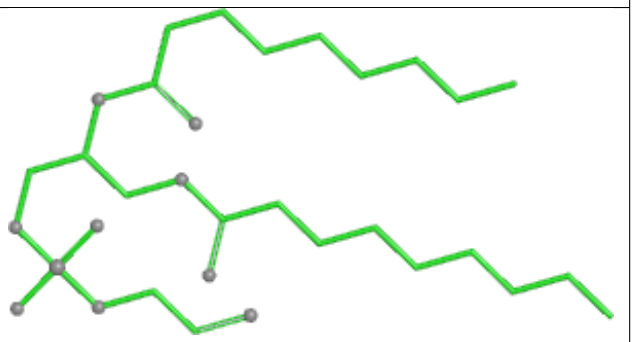


Rings

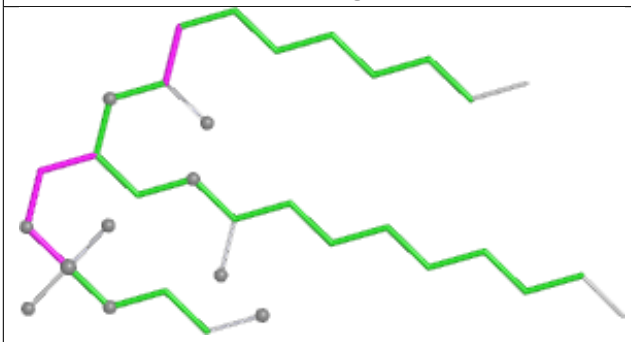
Ligand 3PE S7 303



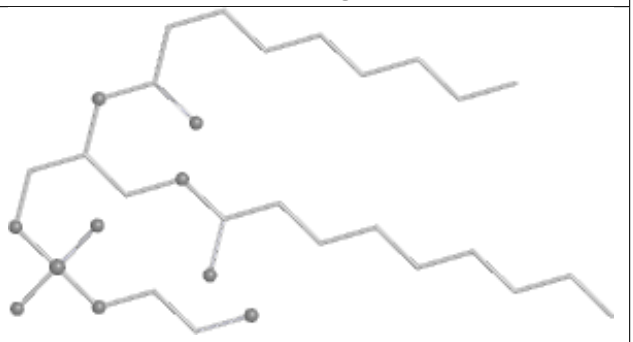
Bond lengths



Bond angles

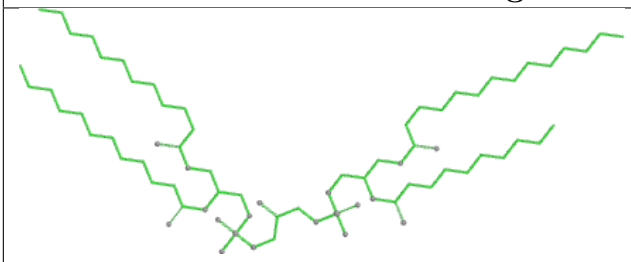


Torsions

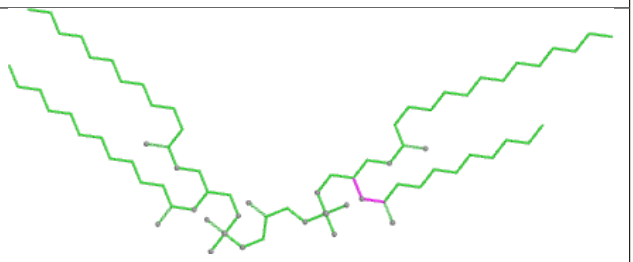


Rings

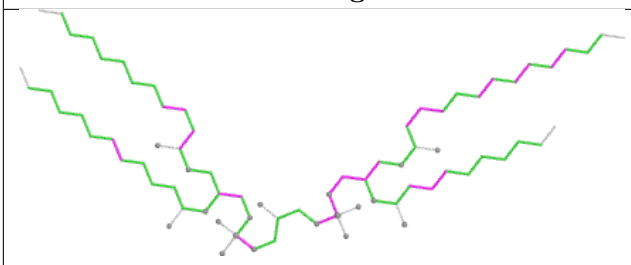
Ligand CDL AM 204



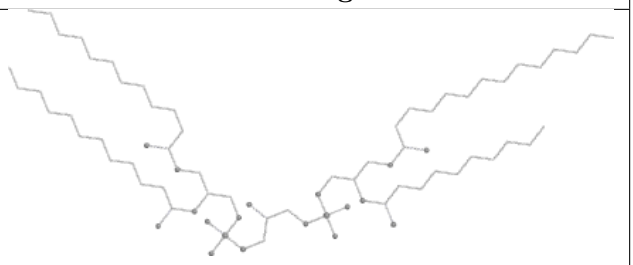
Bond lengths



Bond angles

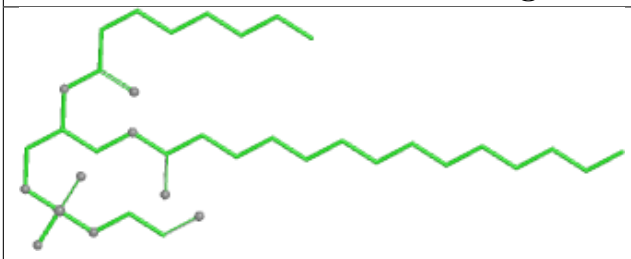


Torsions

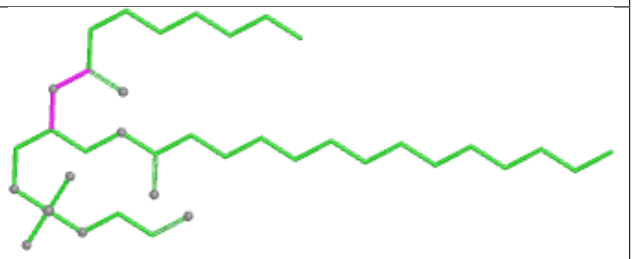


Rings

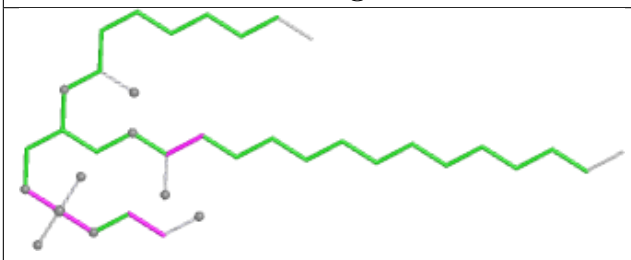
Ligand 3PE B1 103



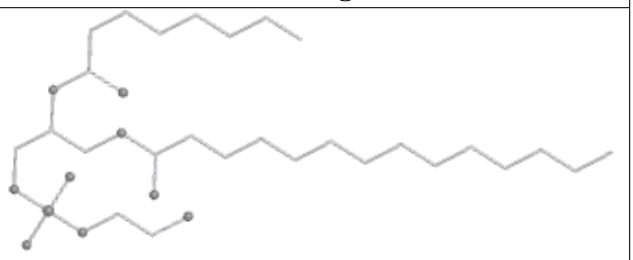
Bond lengths



Bond angles

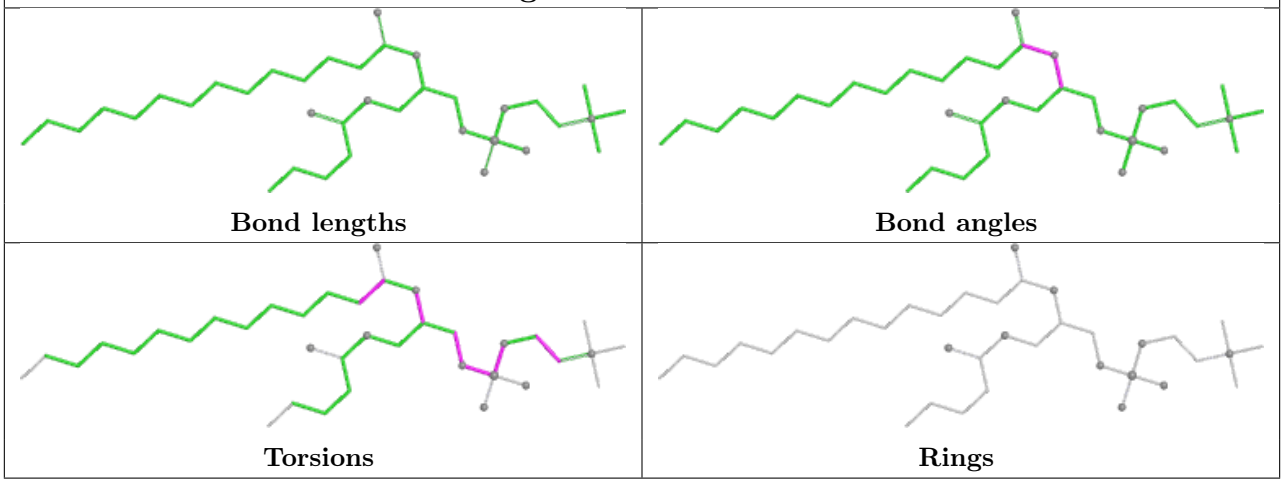


Torsions

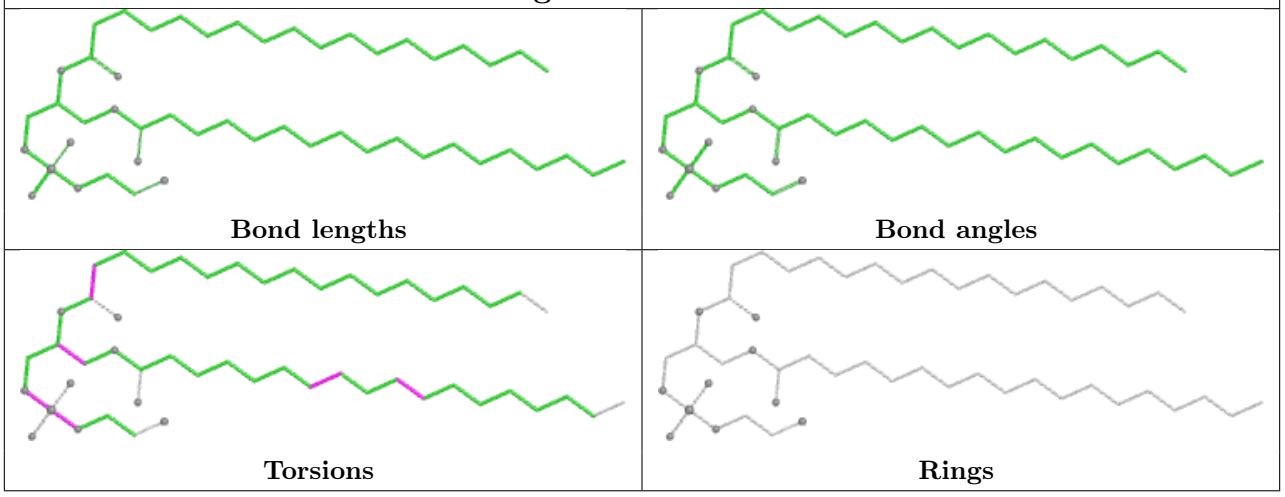


Rings

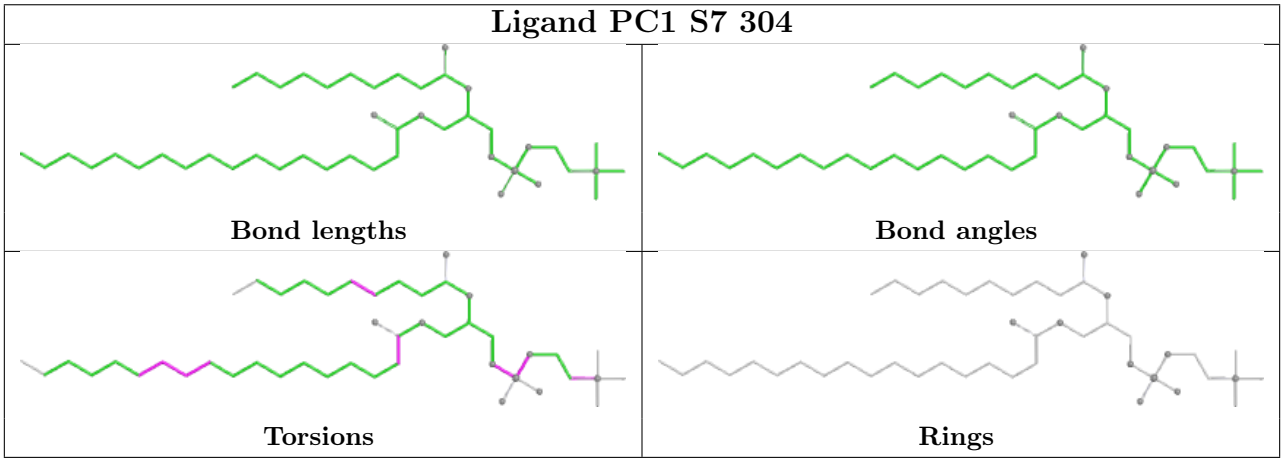
Ligand PC1 B6 202



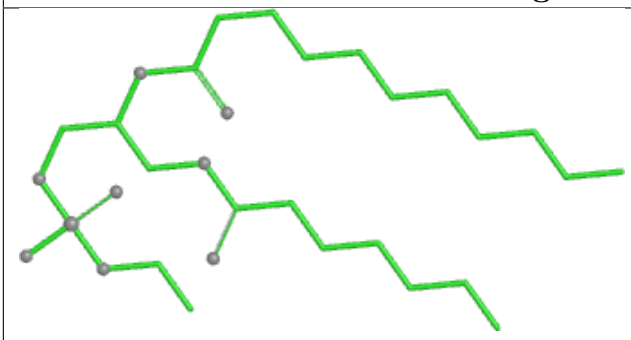
Ligand 3PE 5 607



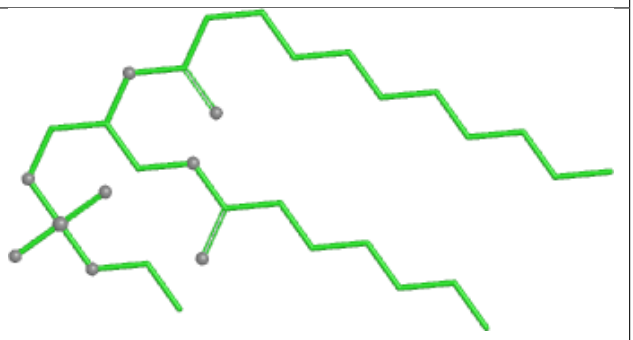
Ligand PC1 S7 304



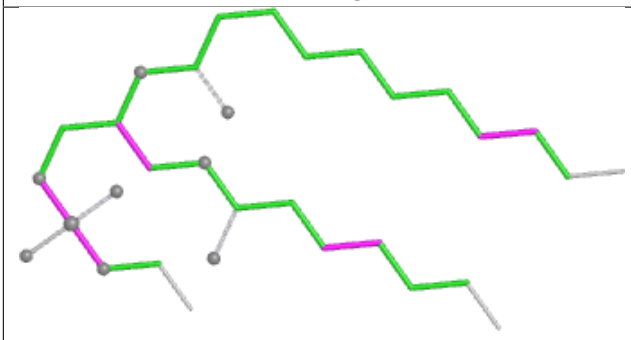
Ligand 3PE 5 601



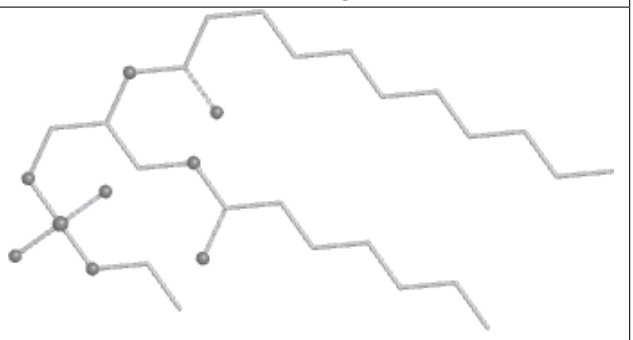
Bond lengths



Bond angles

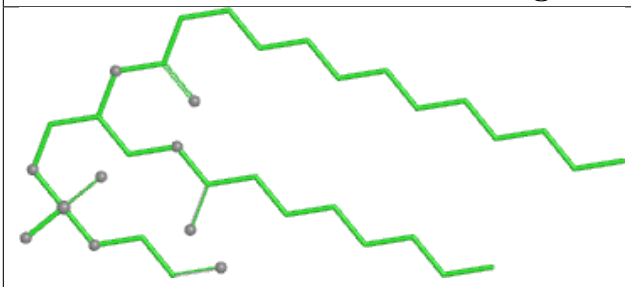


Torsions

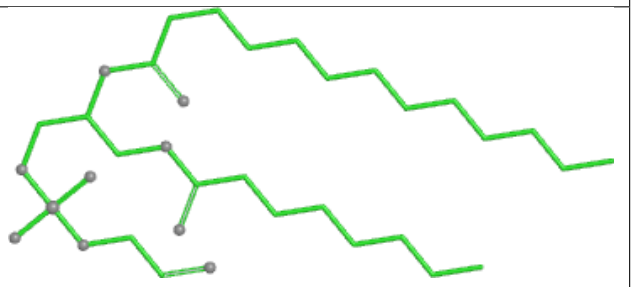


Rings

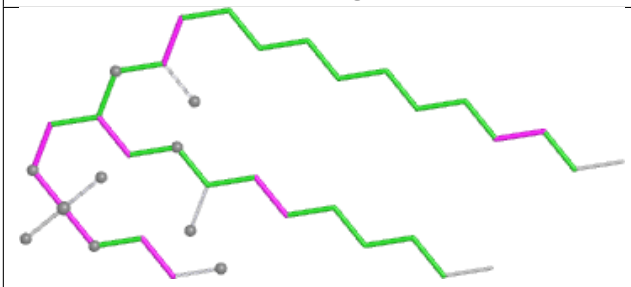
Ligand 3PE 4 504



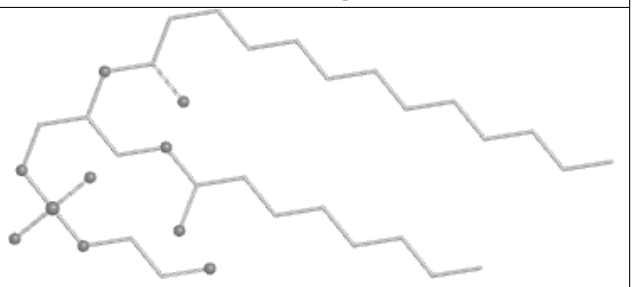
Bond lengths



Bond angles

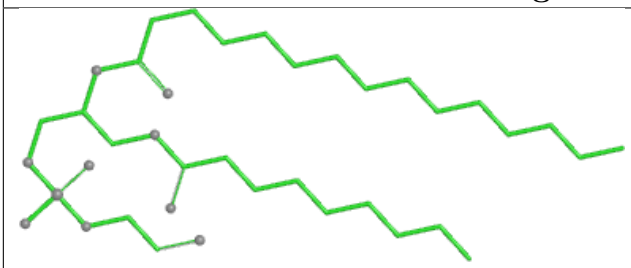


Torsions

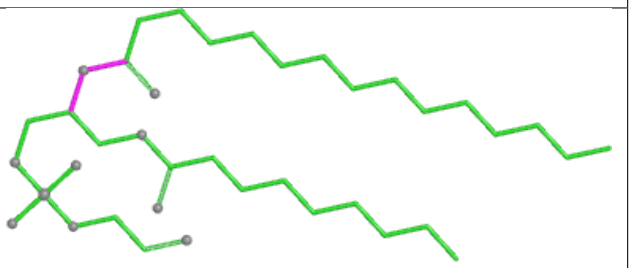


Rings

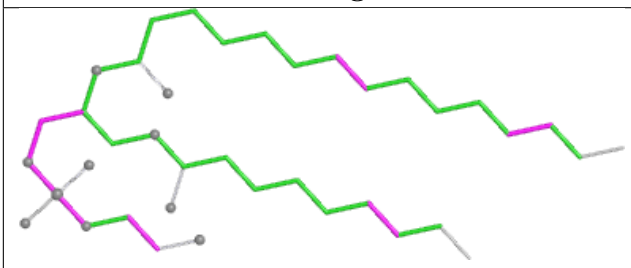
Ligand 3PE 4 506



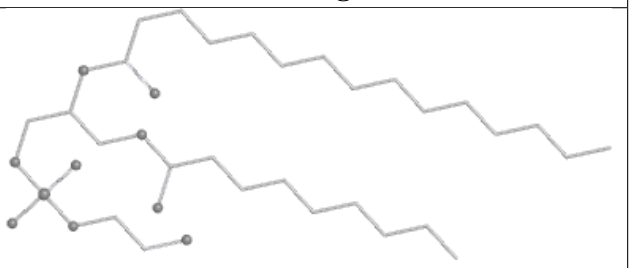
Bond lengths



Bond angles

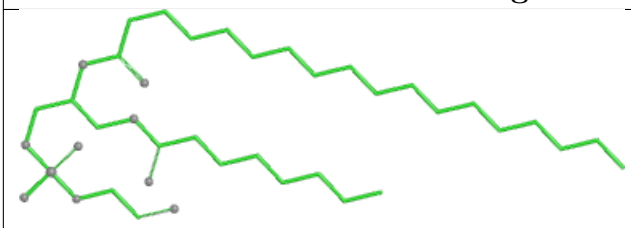


Torsions



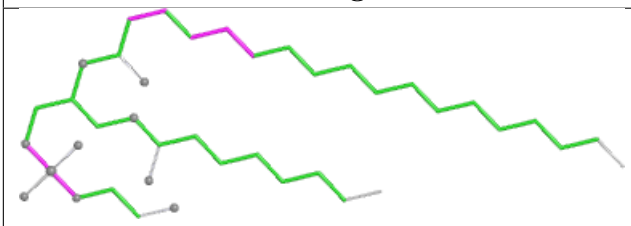
Rings

Ligand 3PE AM 202

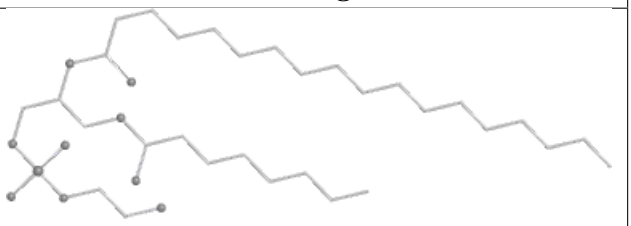


Bond lengths

Bond angles

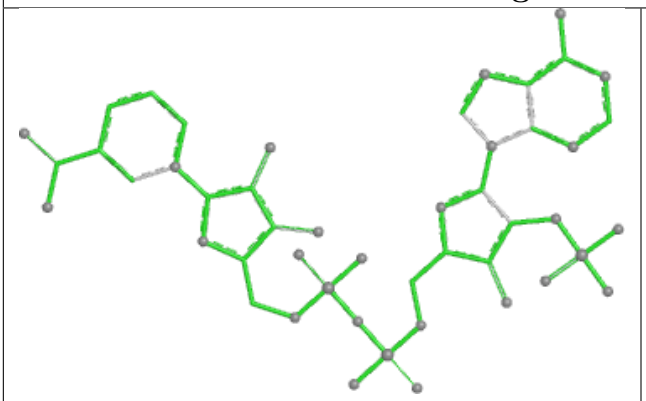


Torsions

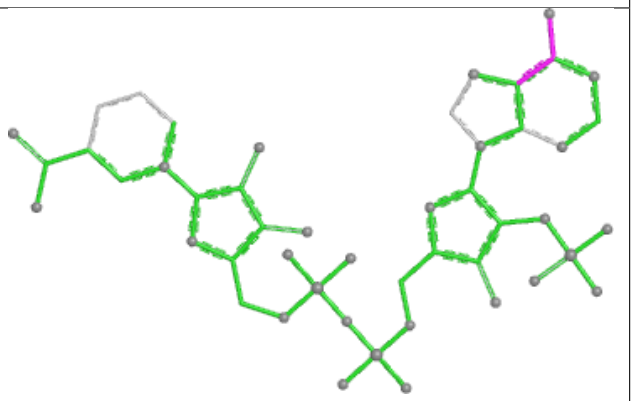


Rings

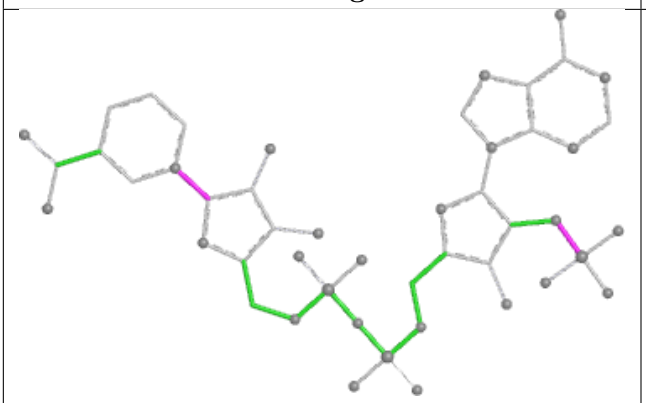
Ligand NDP A9 502



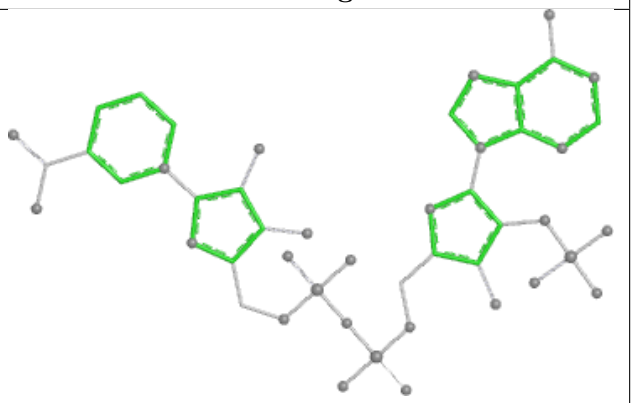
Bond lengths



Bond angles

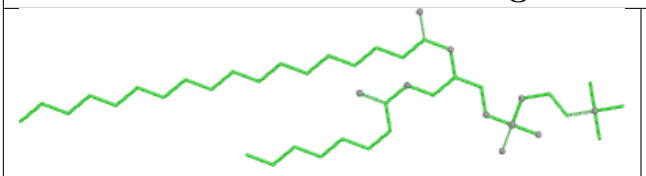


Torsions

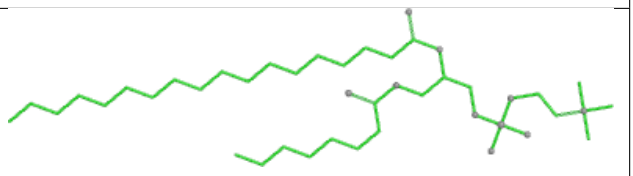


Rings

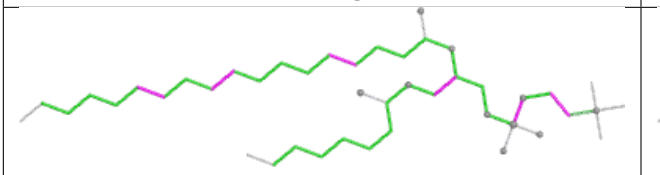
Ligand PC1 AM 205



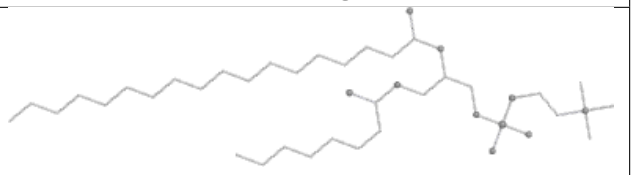
Bond lengths



Bond angles

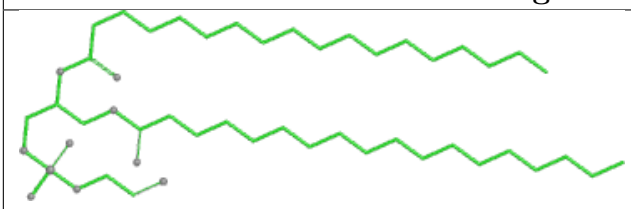


Torsions

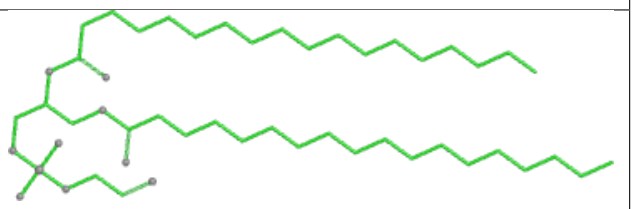


Rings

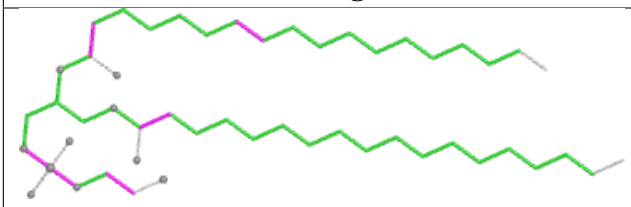
Ligand 3PE 1 403



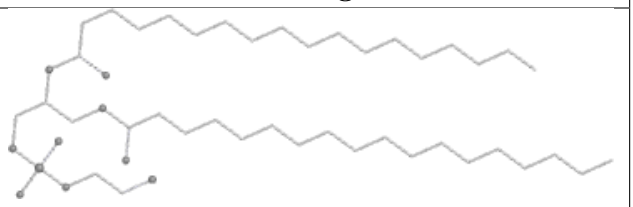
Bond lengths



Bond angles

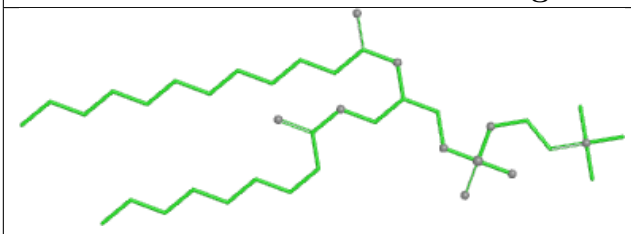


Torsions

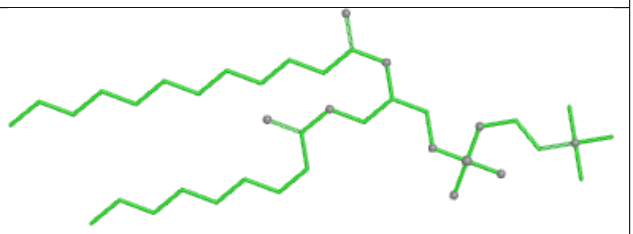


Rings

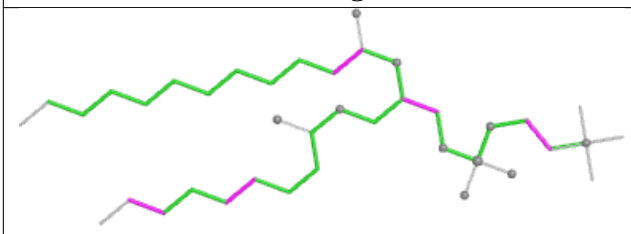
Ligand PC1 4 505



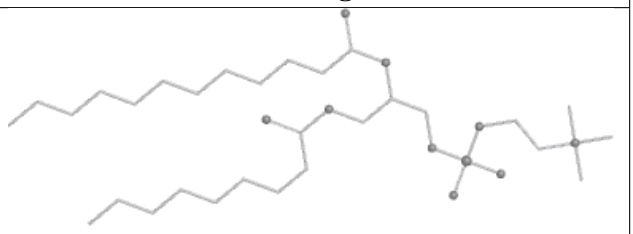
Bond lengths



Bond angles

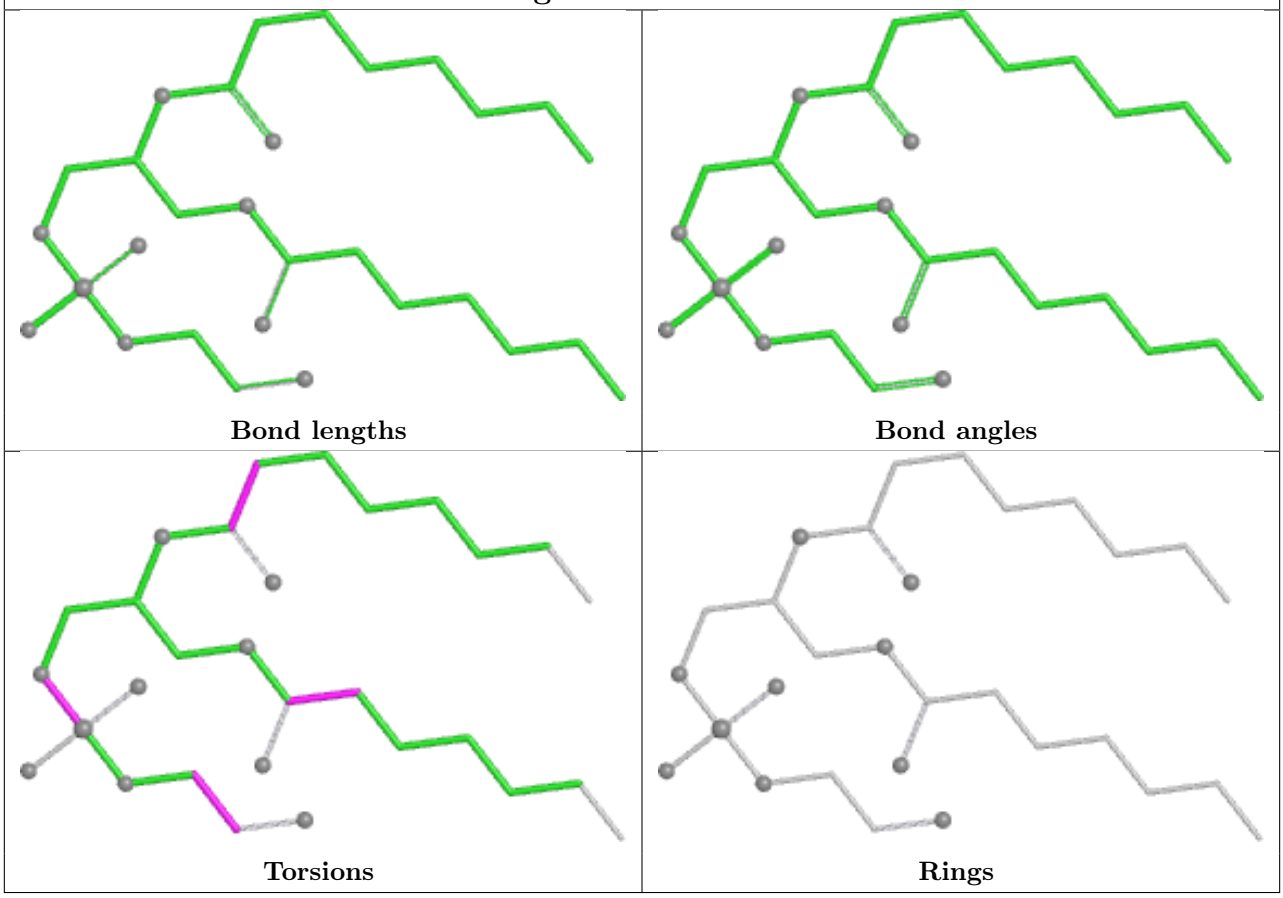


Torsions

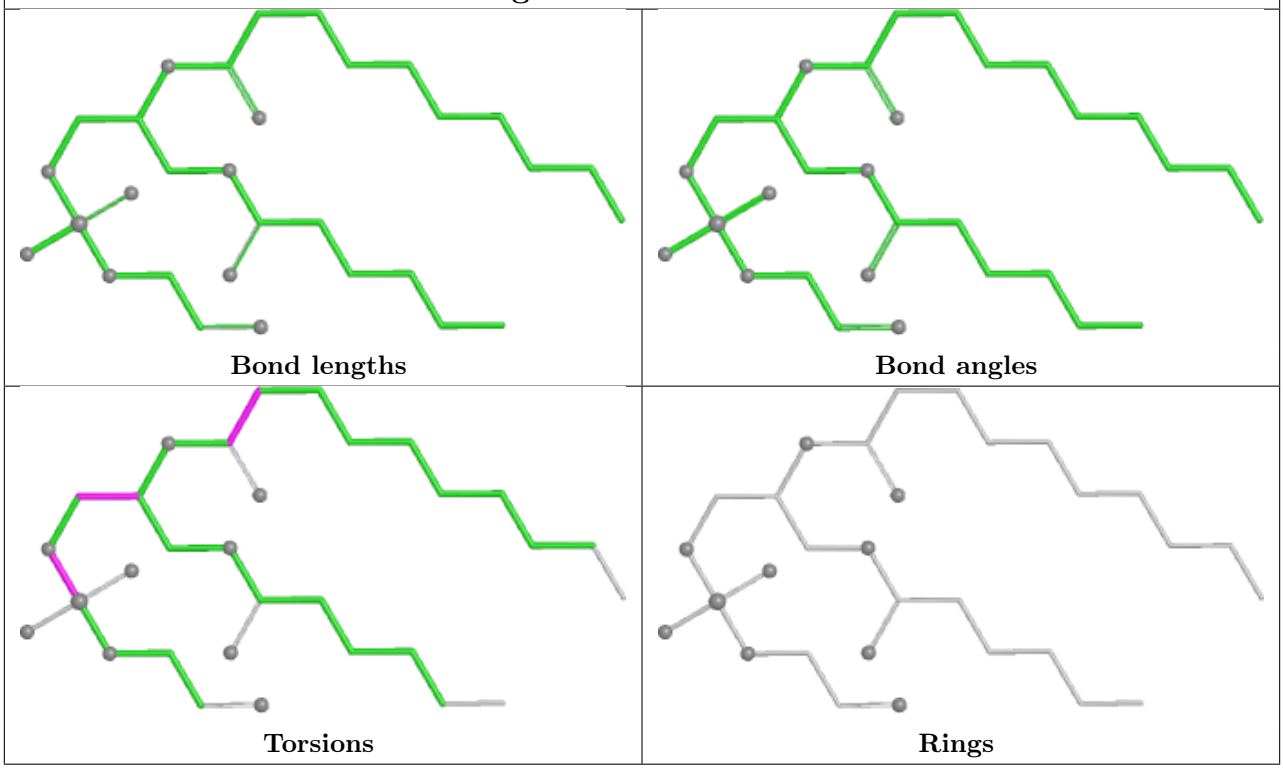


Rings

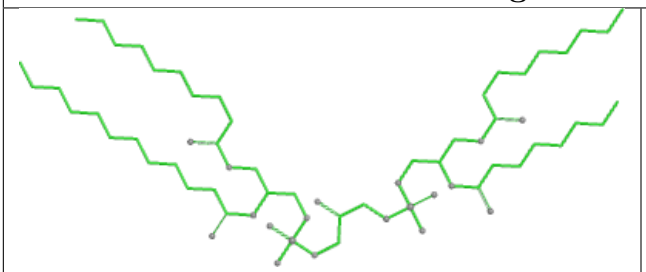
Ligand 3PE 5 604



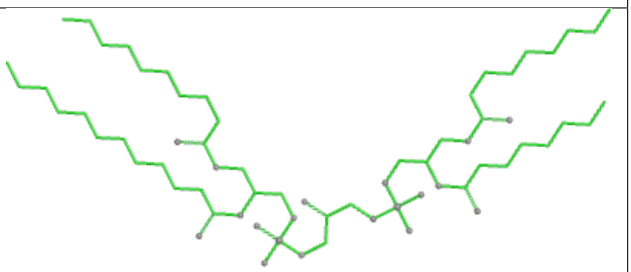
Ligand 3PE AM 203



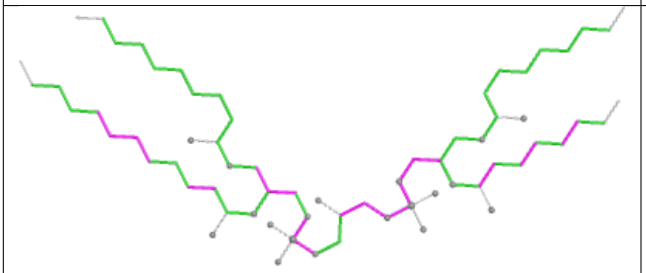
Ligand CDL AN 201



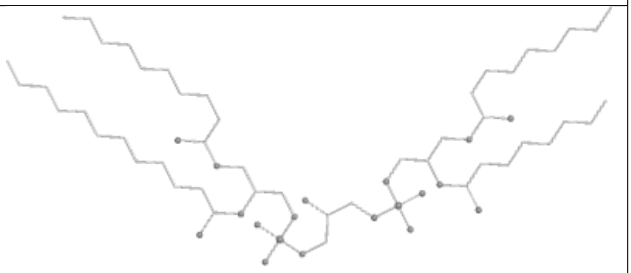
Bond lengths



Bond angles

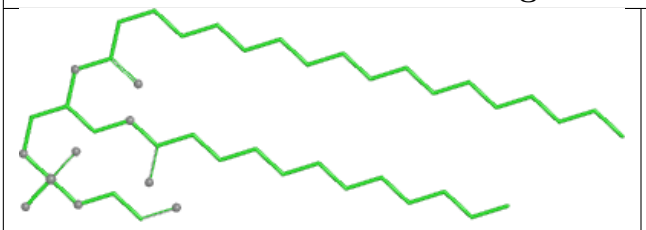


Torsions



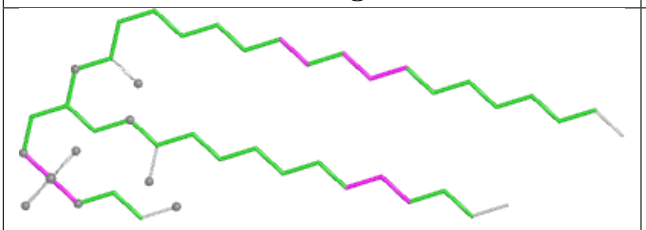
Rings

Ligand 3PE C2 201

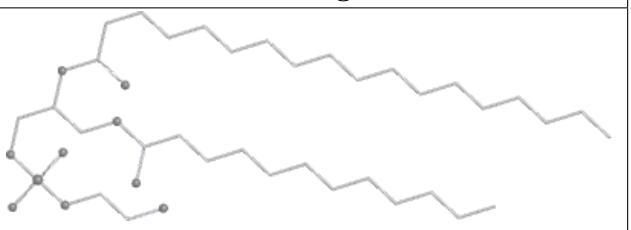


Bond lengths

Bond angles

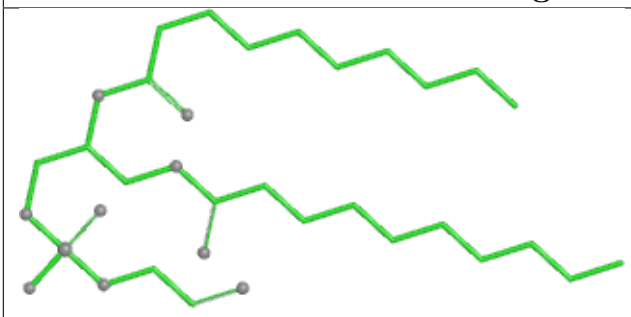


Torsions

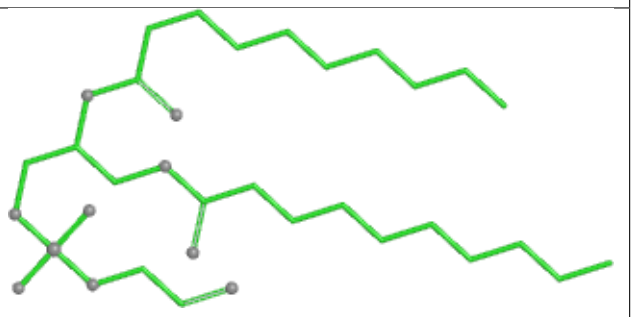


Rings

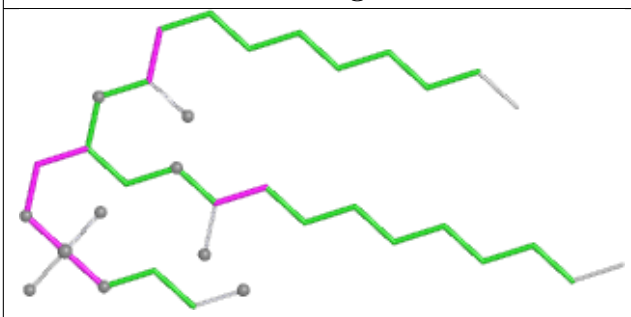
Ligand 3PE 6 202



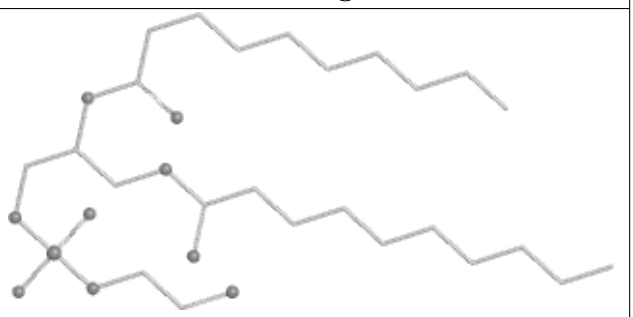
Bond lengths



Bond angles

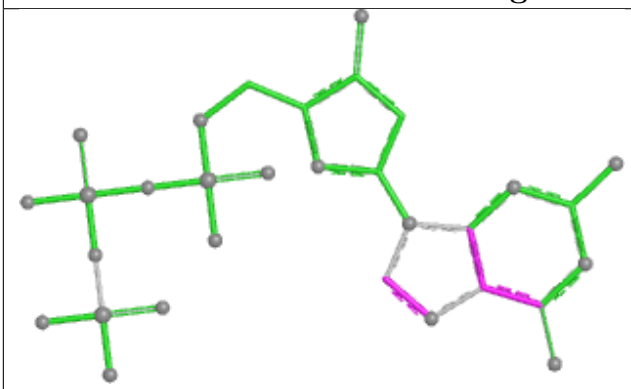


Torsions

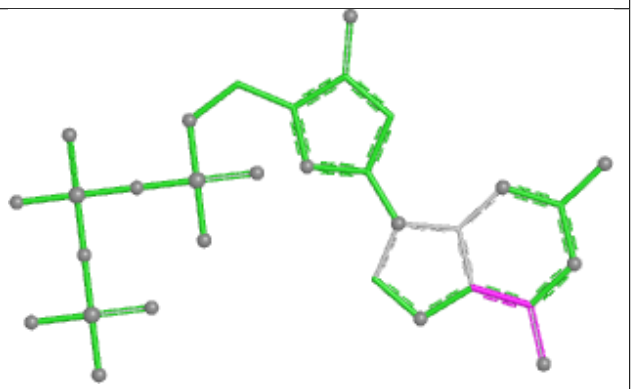


Rings

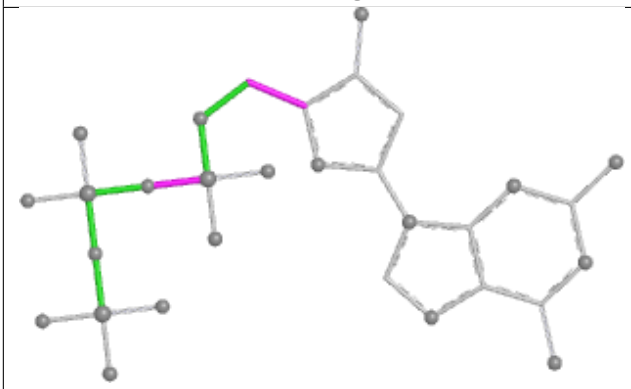
Ligand DGT AL 501



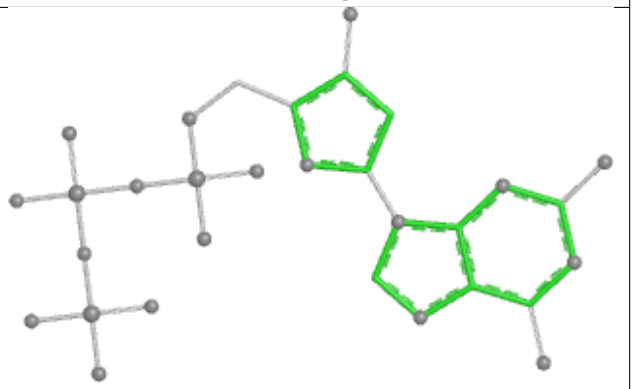
Bond lengths



Bond angles

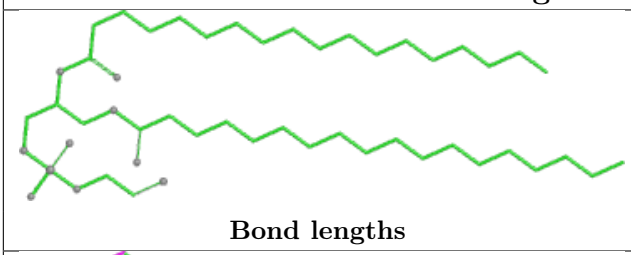


Torsions

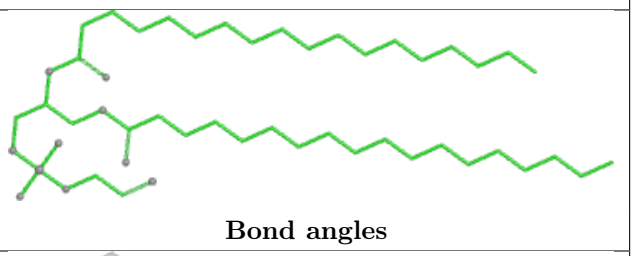


Rings

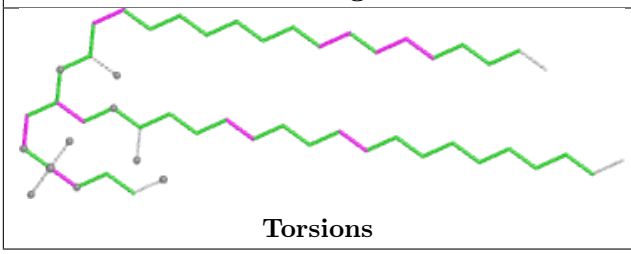
Ligand 3PE 3 202



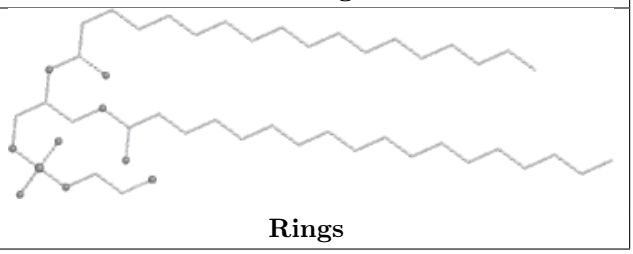
Bond lengths



Bond angles

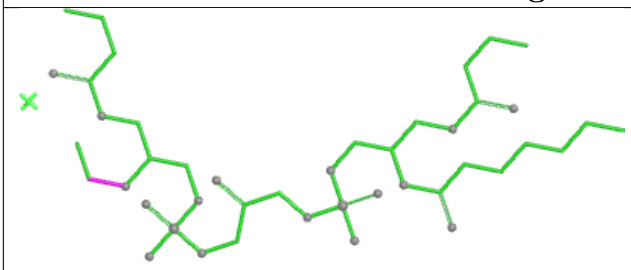


Torsions

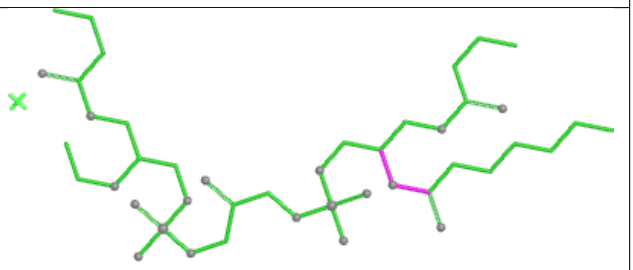


Rings

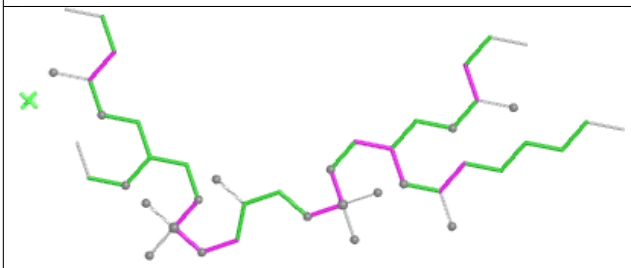
Ligand CDL 2 403



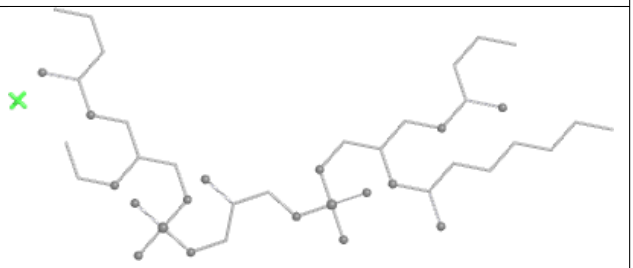
Bond lengths



Bond angles

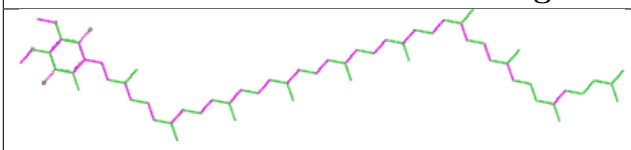


Torsions

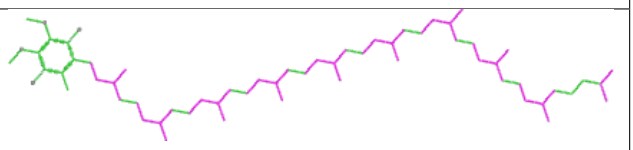


Rings

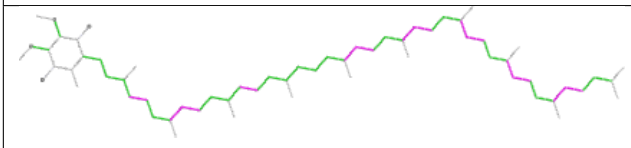
Ligand U10 1 402



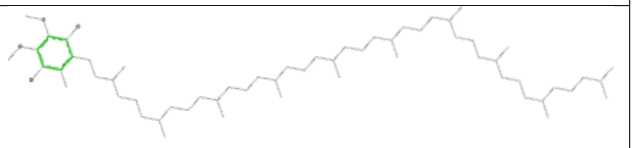
Bond lengths



Bond angles

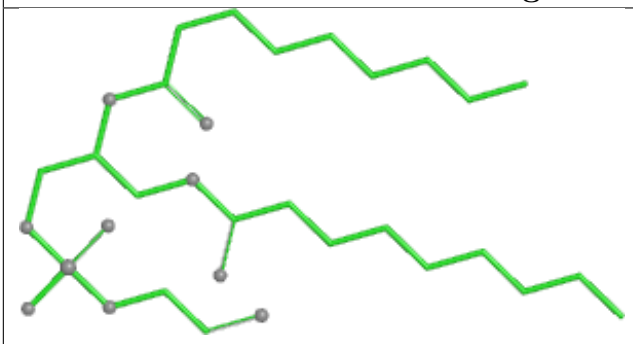


Torsions

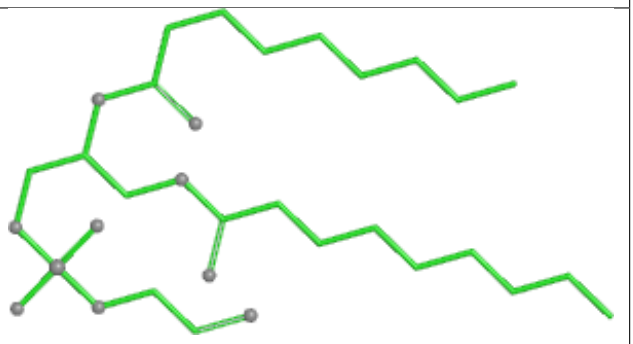


Rings

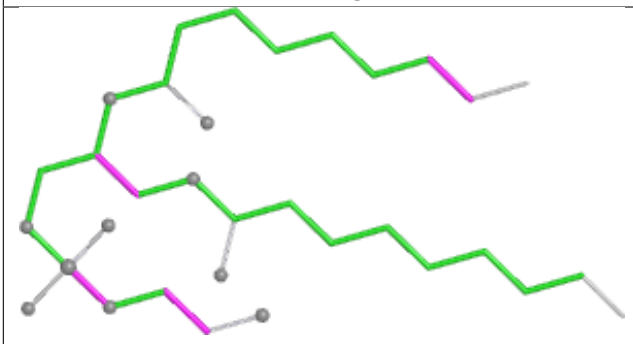
Ligand 3PE S7 302



Bond lengths



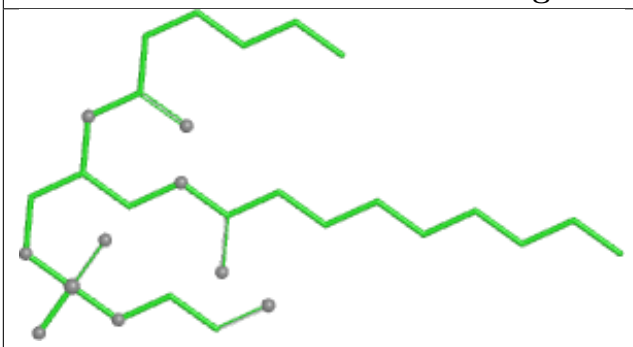
Bond angles



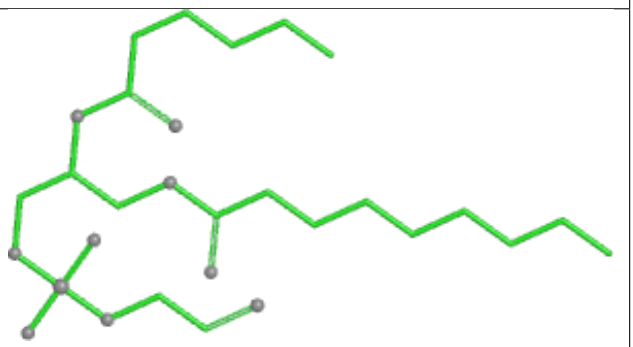
Torsions

Rings

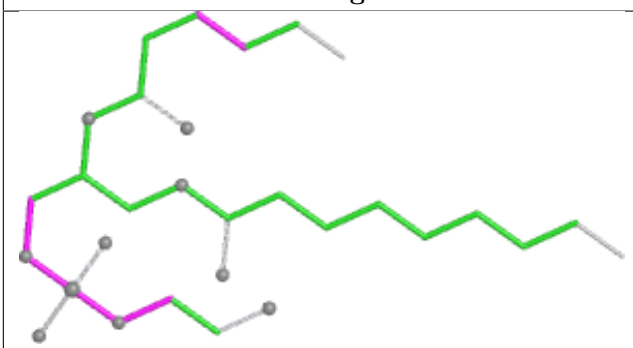
Ligand 3PE 2 401



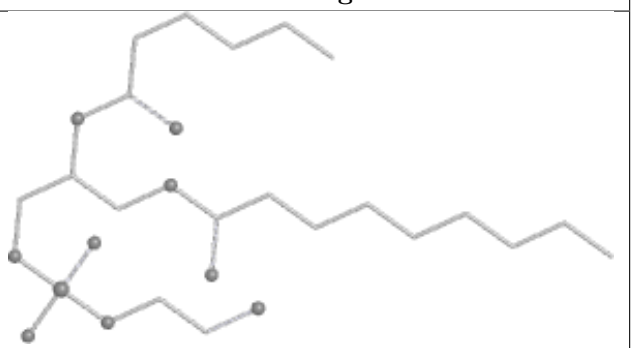
Bond lengths



Bond angles

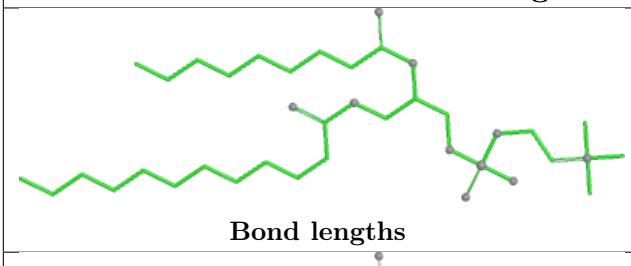


Torsions

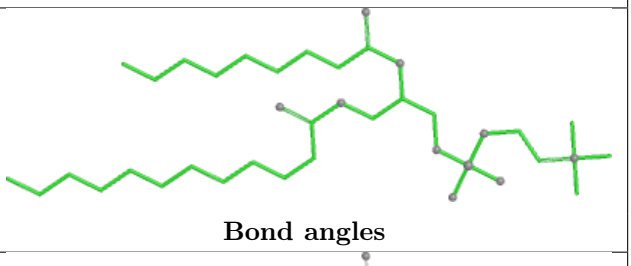


Rings

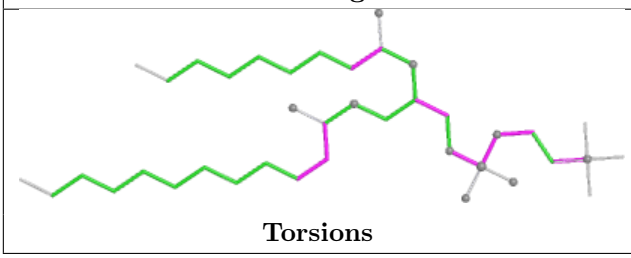
Ligand PC1 4 501



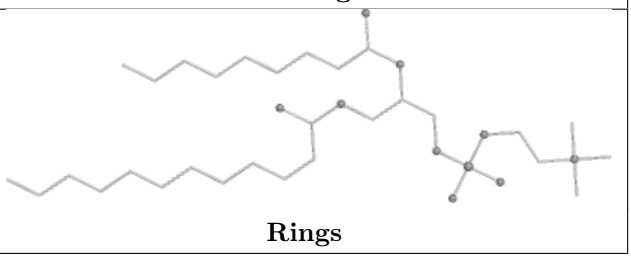
Bond lengths



Bond angles

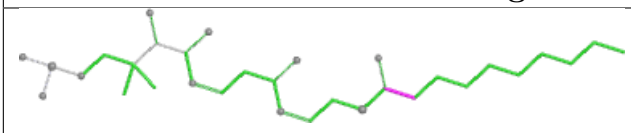


Torsions

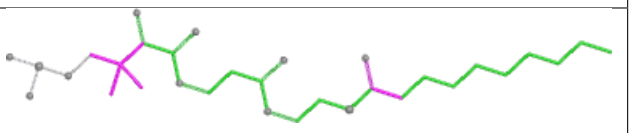


Rings

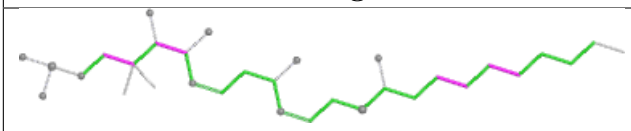
Ligand ZMP AB 201



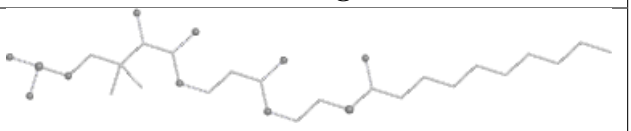
Bond lengths



Bond angles



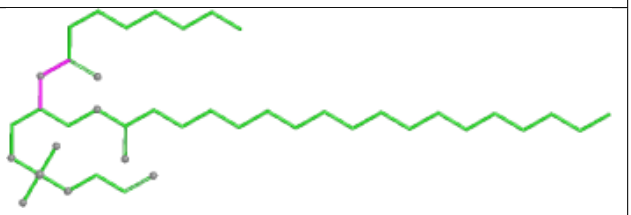
Torsions



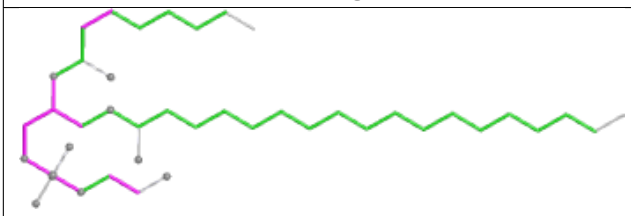
Rings

Ligand 3PE 3 203

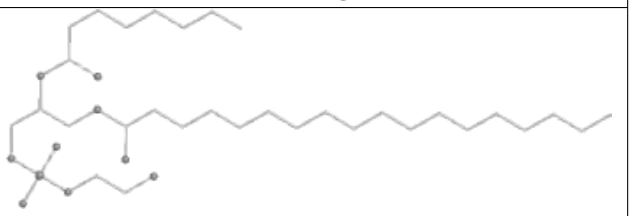
Bond lengths



Bond angles

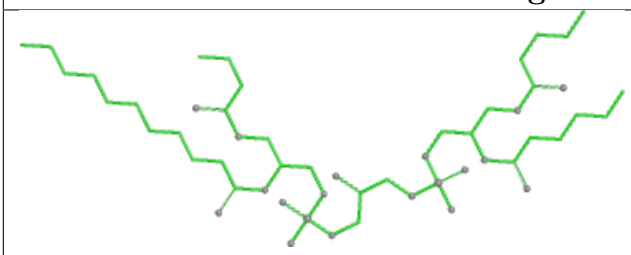


Torsions

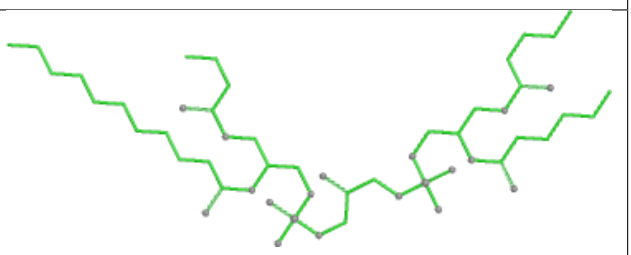


Rings

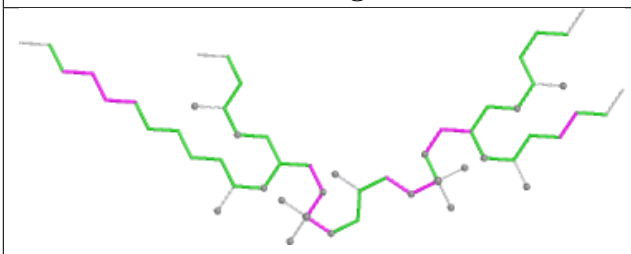
Ligand CDL 3 201



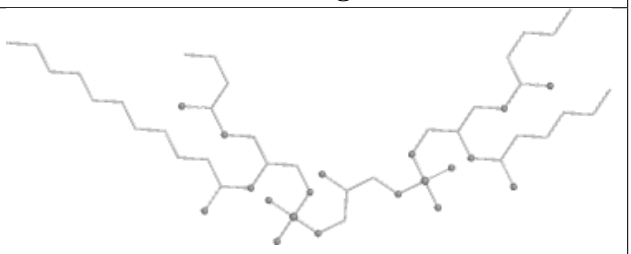
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

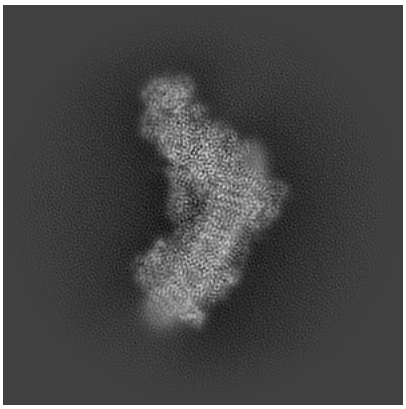
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-28582. These allow visual inspection of the internal detail of the map and identification of artifacts.

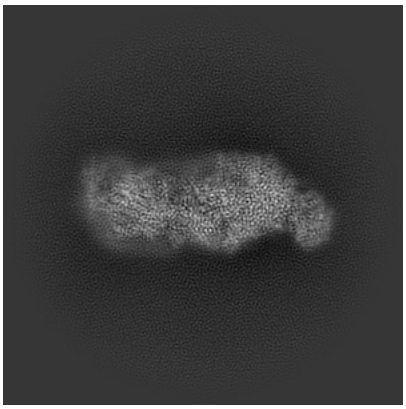
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

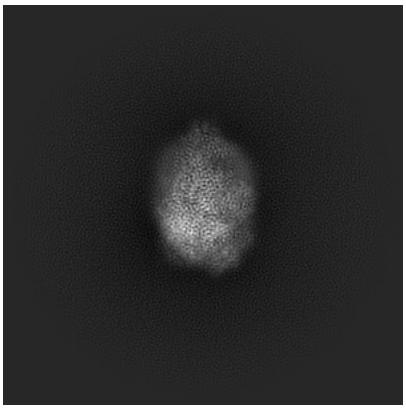
6.1.1 Primary map



X

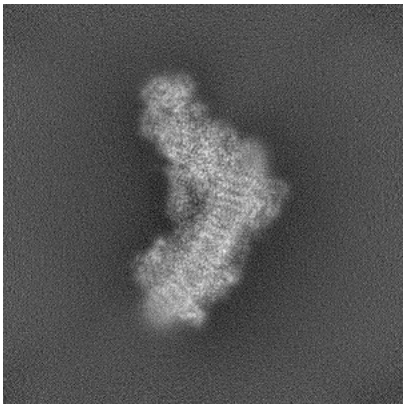


Y

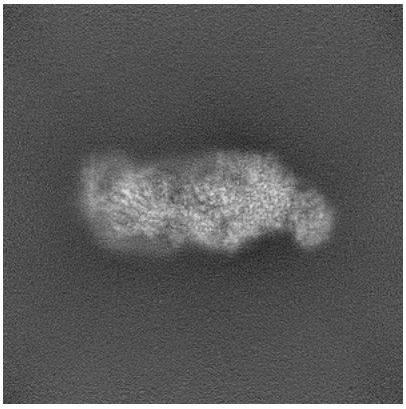


Z

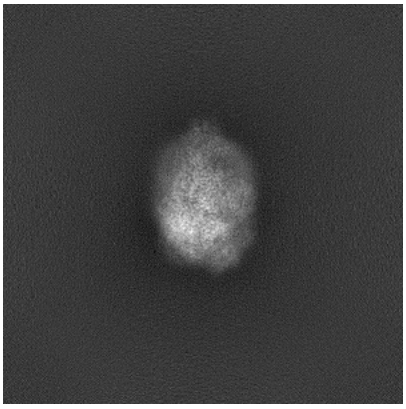
6.1.2 Raw map



X



Y

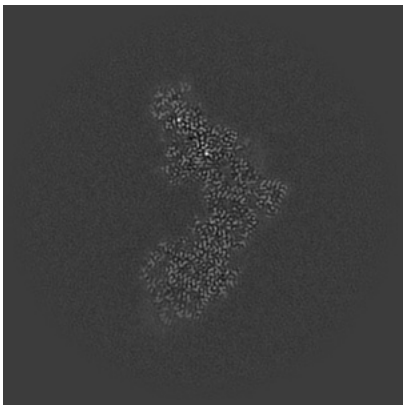


Z

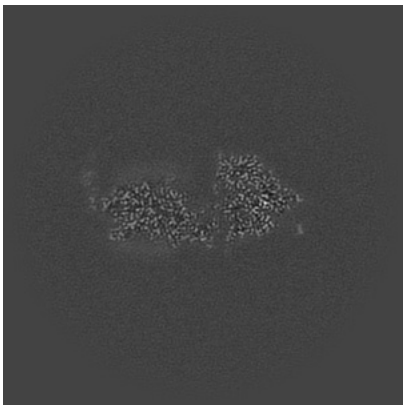
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

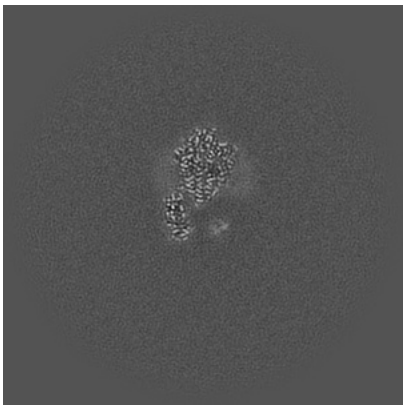
6.2.1 Primary map



X Index: 256

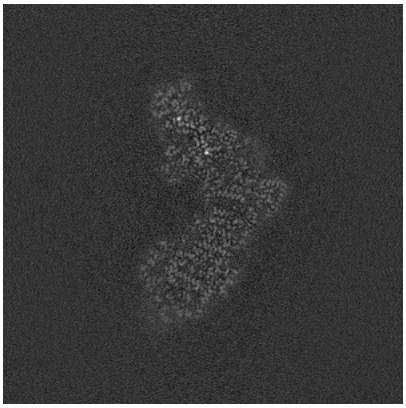


Y Index: 256

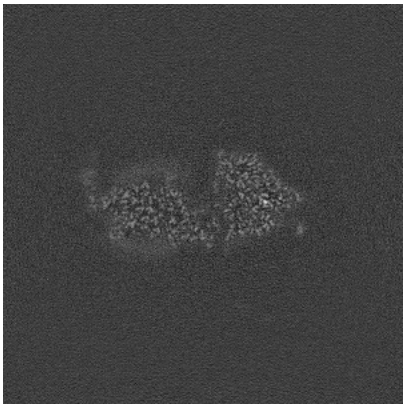


Z Index: 256

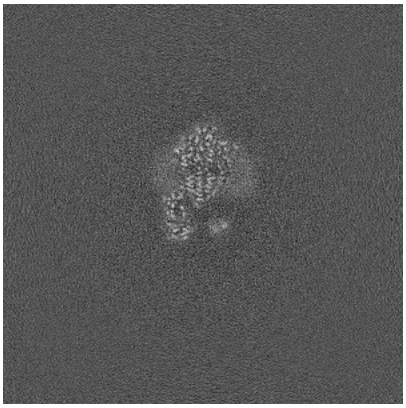
6.2.2 Raw map



X Index: 256



Y Index: 256

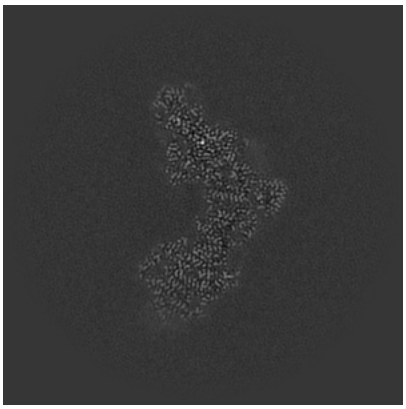


Z Index: 256

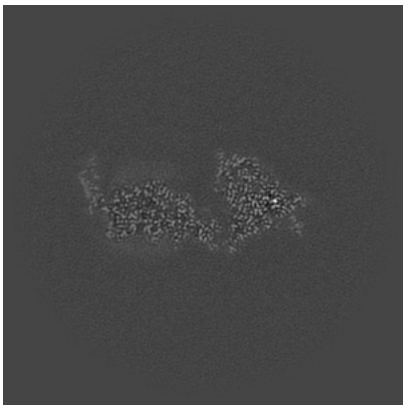
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

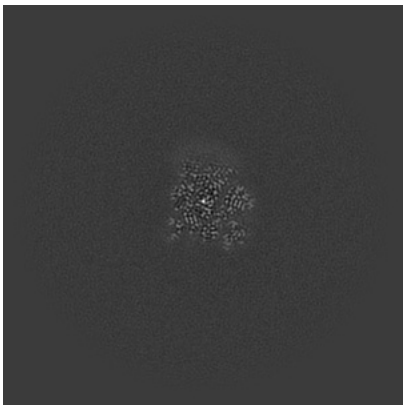
6.3.1 Primary map



X Index: 258

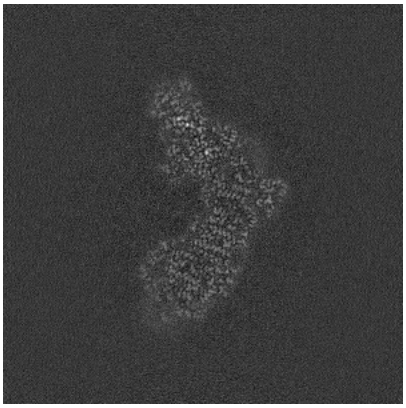


Y Index: 251

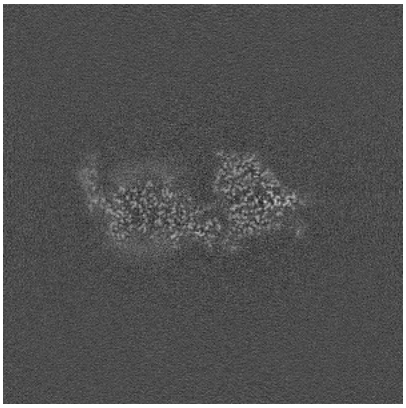


Z Index: 321

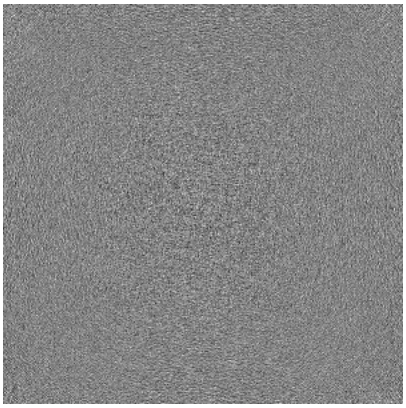
6.3.2 Raw map



X Index: 255



Y Index: 253

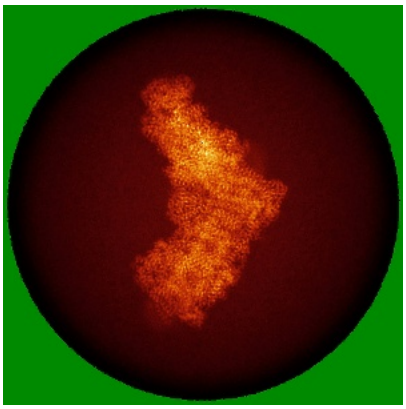


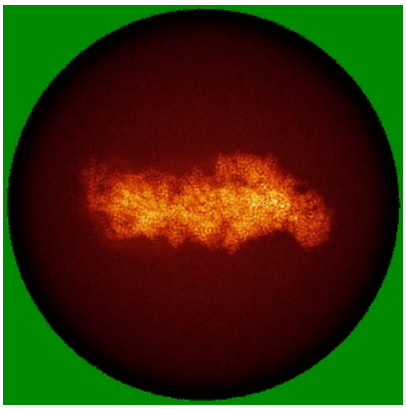
Z Index: 0

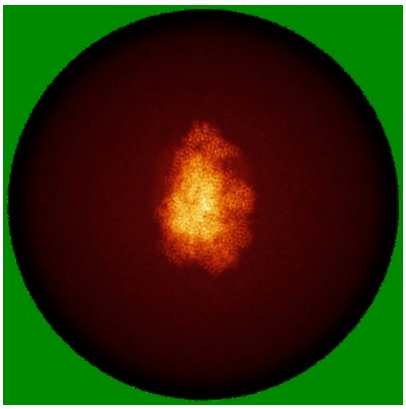
The images above show the largest variance slices of the map in three orthogonal directions.

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

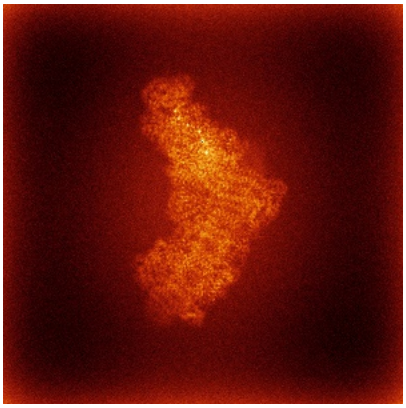
6.4.1 Primary map

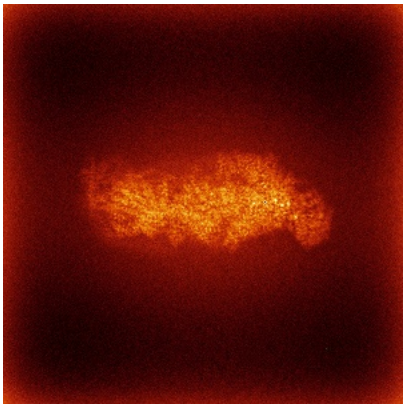

X

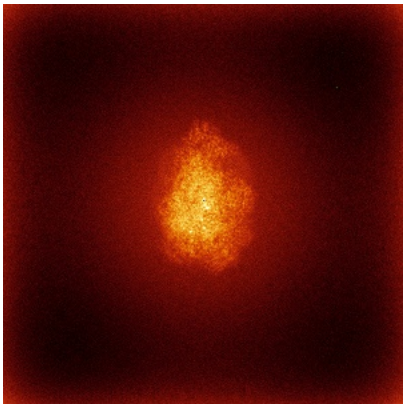

Y


Z

6.4.2 Raw map


X

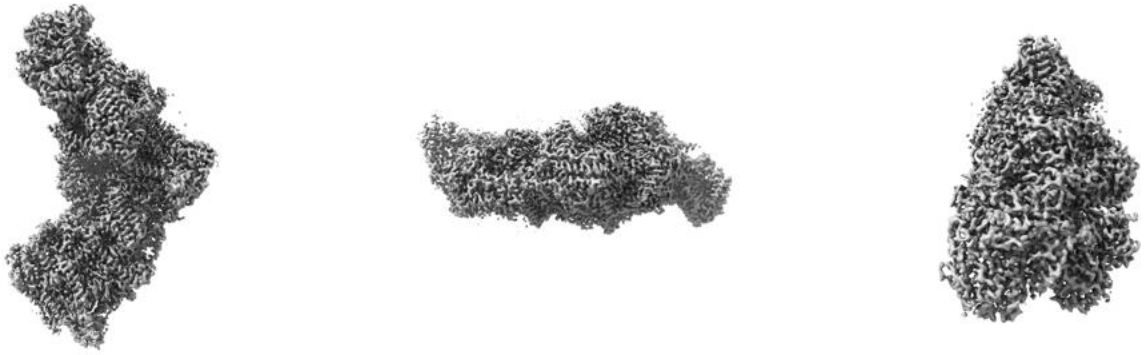

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

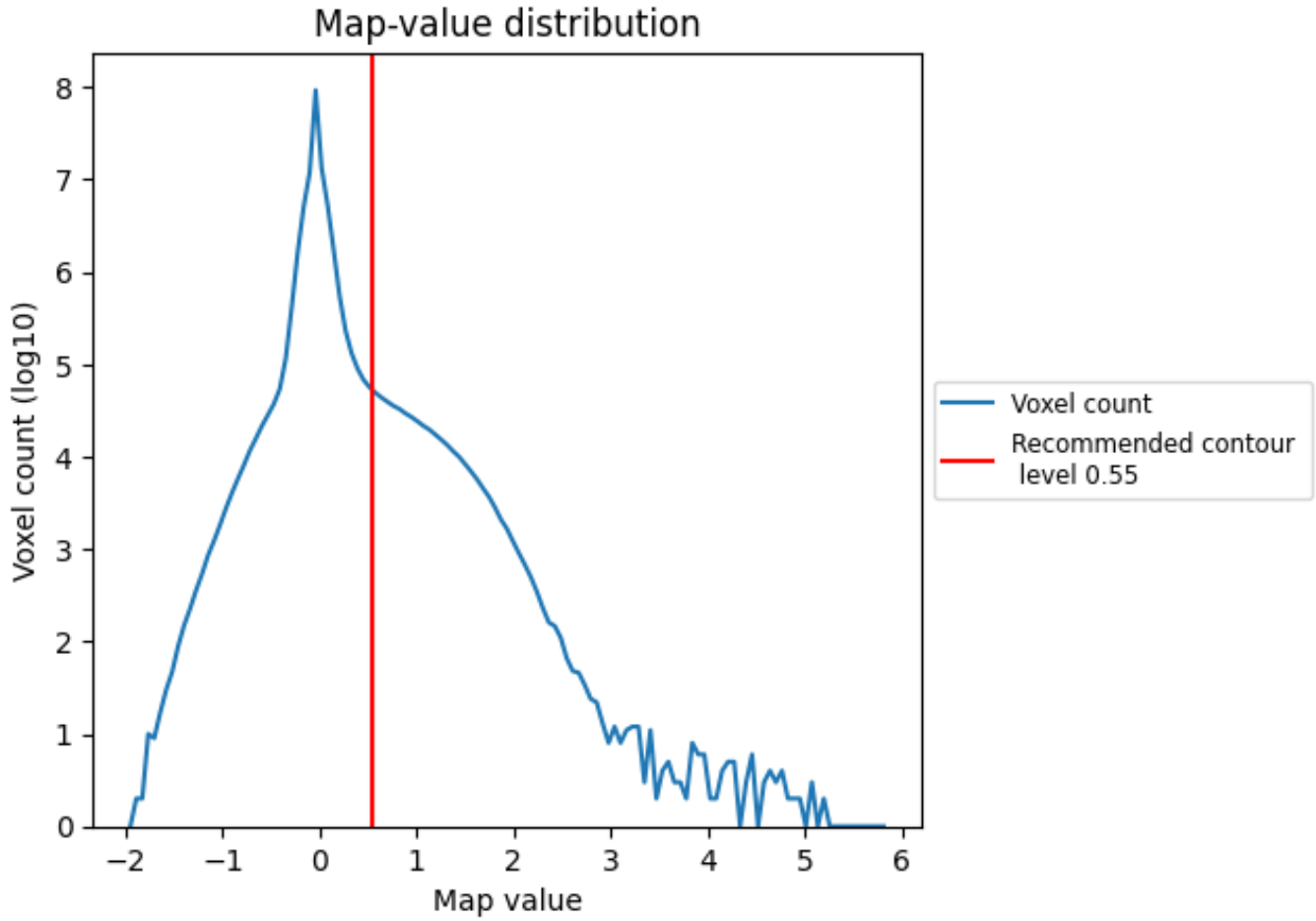
6.6 Mask visualisation (i)

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

7 Map analysis

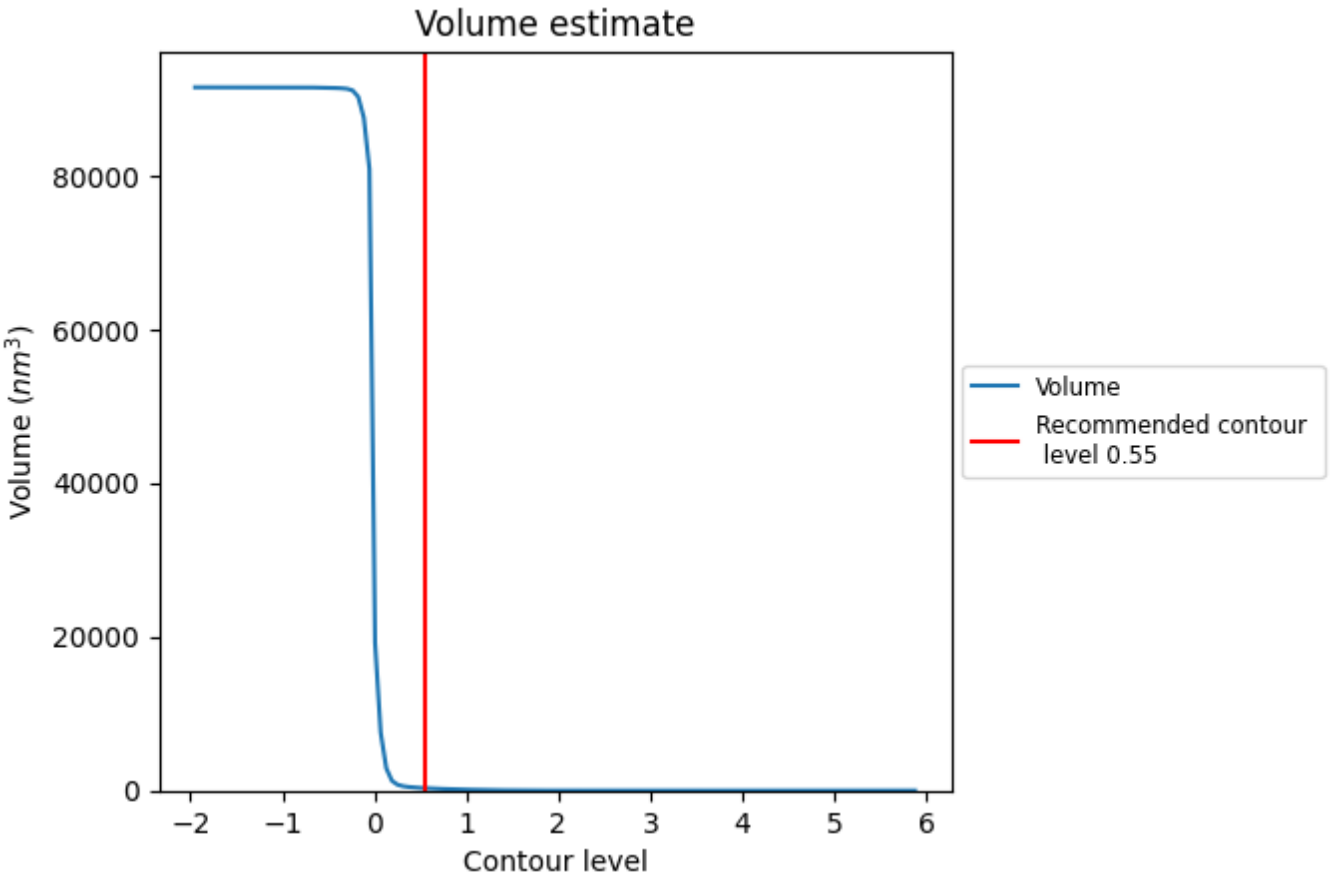
This section contains the results of statistical analysis of the map.

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.

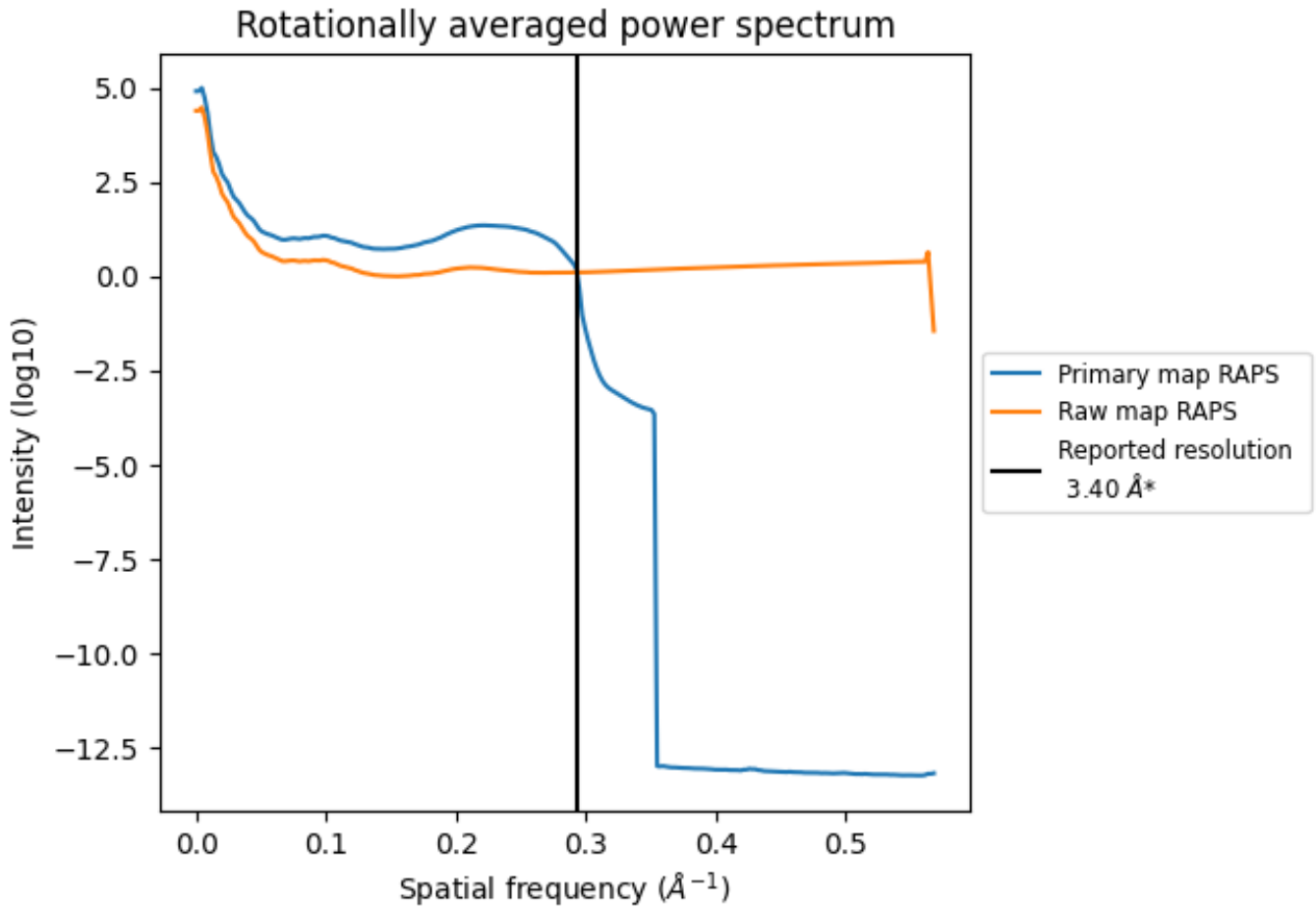
7.2 Volume estimate



The volume at the recommended contour level is 311 nm^3; this corresponds to an approximate mass of 281 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)

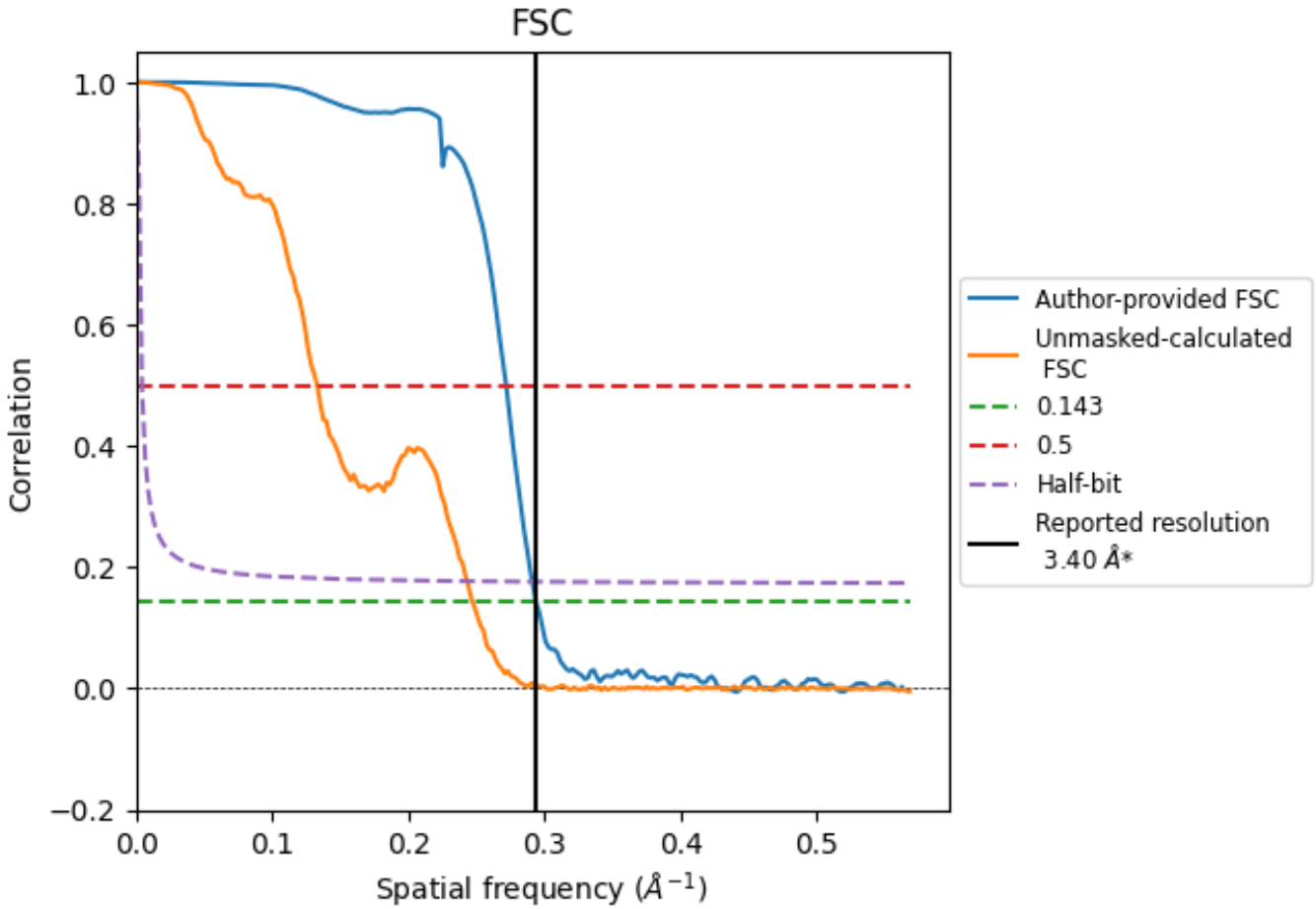


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

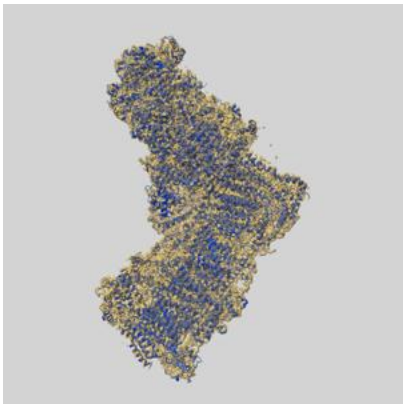
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	3.68	3.44
Unmasked-calculated*	4.05	7.52	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.05 differs from the reported value 3.4 by more than 10 %

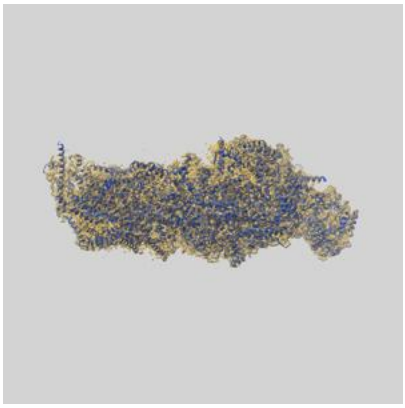
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-28582 and PDB model 8ESZ. Per-residue inclusion information can be found in section 3 on page 22.

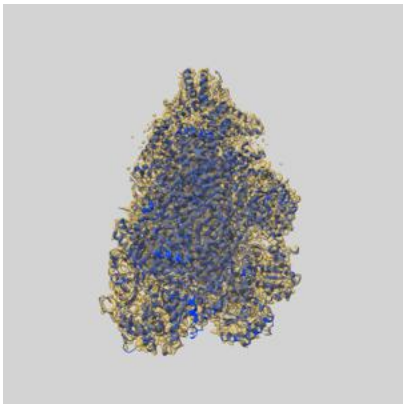
9.1 Map-model overlay



X



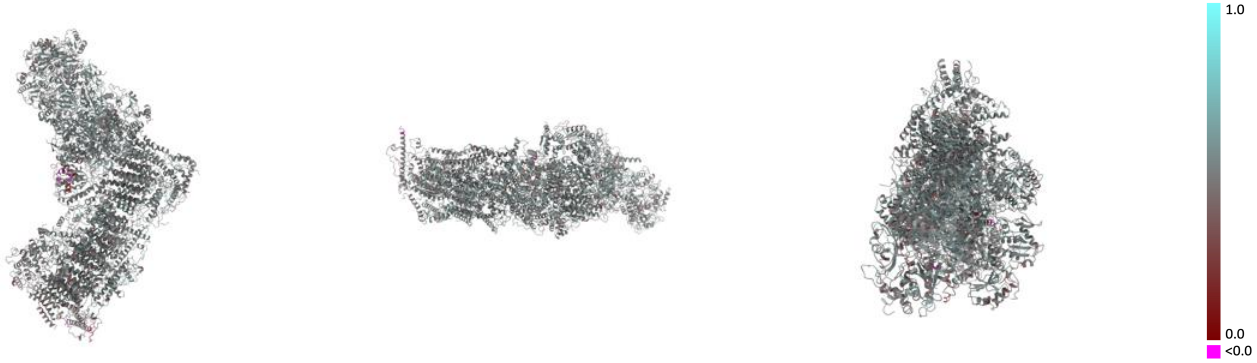
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

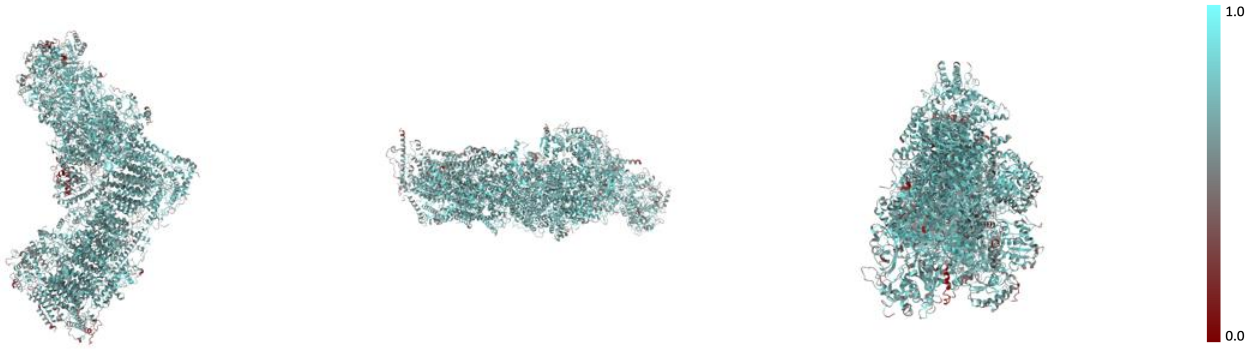
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

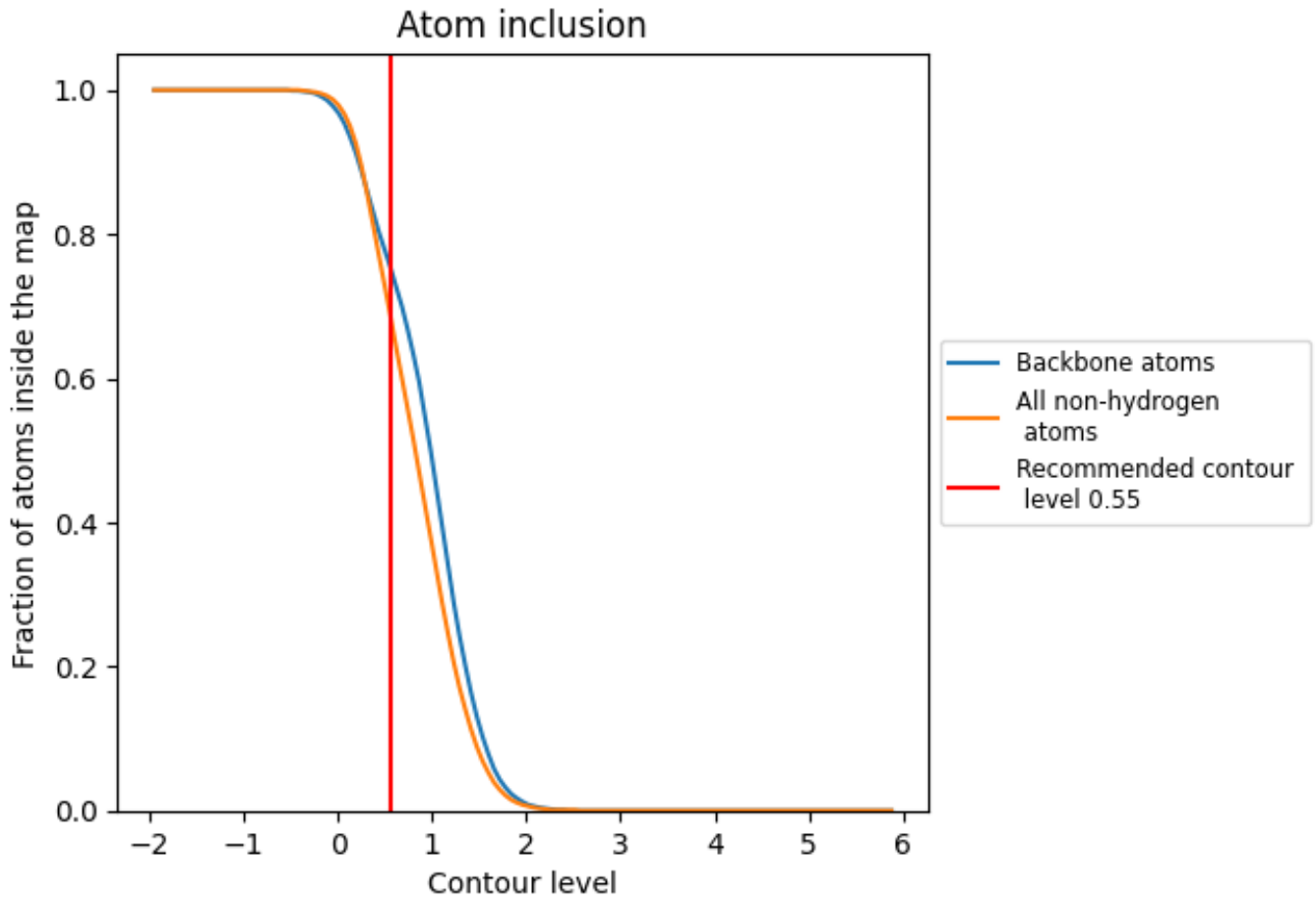
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.55).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 69% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6920	0.4980
1	0.7330	0.5050
2	0.7390	0.5110
3	0.6850	0.4990
4	0.7440	0.5130
4L	0.7090	0.4980
5	0.6680	0.4840
6	0.6760	0.4990
A1	0.7160	0.4930
A3	0.6920	0.5070
A5	0.6810	0.5030
A6	0.6790	0.4900
A7	0.6730	0.5000
A8	0.6810	0.4930
A9	0.7240	0.5140
AB	0.3060	0.3330
AC	0.5680	0.4610
AL	0.7260	0.5090
AM	0.5800	0.4840
AN	0.6500	0.4960
AO	0.7240	0.5040
B1	0.5950	0.4860
B2	0.5740	0.4560
B3	0.5400	0.4410
B4	0.6930	0.4910
B5	0.7390	0.5250
B6	0.6420	0.4920
B7	0.5390	0.4190
B8	0.6740	0.4870
B9	0.6740	0.4870
BL	0.7320	0.5060
BM	0.6830	0.4900
C2	0.7030	0.5130
S1	0.7020	0.5040
S2	0.7440	0.5120

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
S3	0.7680	0.5300
S4	0.6750	0.5070
S5	0.7370	0.5150
S6	0.7240	0.5330
S7	0.7450	0.5060
S8	0.7760	0.5190
V1	0.6850	0.4880
V2	0.6370	0.4870
V3	0.1480	0.3400