Full wwPDB EM Validation Report

Aug 12, 2026 – 10:49 PM JST

PDB ID	:	9J6H / pdb_00009j6h
EMDB ID	:	EMD-61173
Title	:	Complex I from respirasome closed state 1 bound by metformin and CoQ10 (SC-MetC1-iv)
Authors	:	Teng, F.; He, Z.X.; Hu, Y.Q.; Xu, C.Y.; Guo, R.Y.; Zhou, L.
Deposited on	:	2024-08-16
Resolution	:	2.92 Å(reported)

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

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

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

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

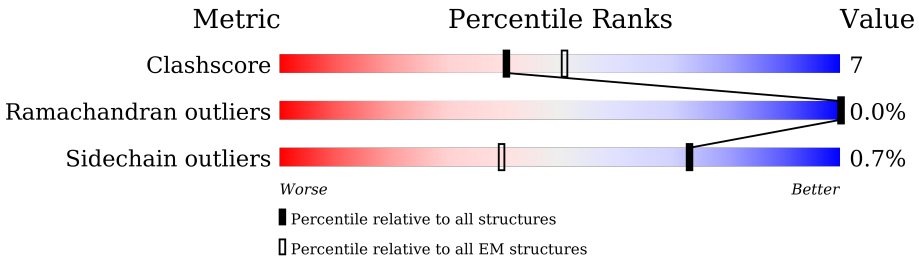
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

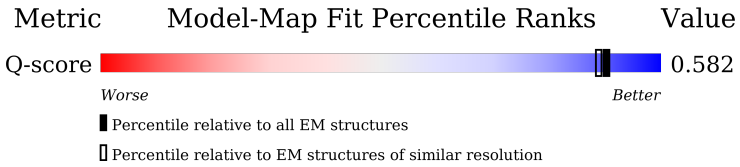
1 Overall quality at a glance

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

The reported resolution of this entry is 2.92 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13007 (2.42 - 3.42)

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	4L	98	77% 23%
2	A1	70	87% 13%
3	A2	85	5% 87% 13%
4	A3	83	90% 10%

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Mol	Chain	Length	Quality of chain
5	A5	112	90% 10%
6	A6	114	89% 11%
7	A7	112	9% 79% 7% 13%
8	A8	171	86% 14%
9	A9	341	85% 15%
10	AB	87	10% 74% 15% 11%
10	AC	87	82% 17%
11	AK	321	5% 84% 15%
12	AL	140	89% 11%
13	AM	144	6% 88% 11%
14	AN	142	88% 12%
15	B1	56	14% 80% 20%
16	B2	67	6% 85% 15%
17	B3	80	11% 84% 16%
18	B4	128	93% 7%
19	B5	138	91% 9%
20	B6	126	10% 65% 17% 18%
21	B7	125	6% 88% 12%
22	B8	156	94% 6%
23	B9	178	87% 13%
24	BK	176	82% 16%
25	BL	102	82% 14%
26	CA	49	94% 6%
27	CB	121	87% 13%
28	N1	318	74% 26%

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Mol	Chain	Length	Quality of chain
29	N2	347	79% 21%
30	N3	115	83% 17%
31	N4	459	77% 22%
32	N5	603	78% 22%
33	N6	174	9% 80% 18%
34	S1	689	78% 22%
35	S2	430	76% 23%
36	S3	208	88% 12%
37	S4	124	6% 87% 13%
38	S5	105	90% 10%
39	S6	96	5% 88% 12%
40	S7	156	77% 22%
41	S8	176	77% 23%
42	V1	431	77% 22%
43	V2	217	84% 15%
44	V3	42	74% 26%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 68554 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	4L	98	748	493	113	128	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A1	70	562	361	101	94	6	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A2	85	686	431	128	125	2	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A3	83	643	417	110	115	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A5	112	910	588	154	165	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A6	114	Total	C	N	O	S	0	0
			967	617	178	167	5		

- Molecule 7 is a protein called Complex I-B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A7	97	Total	C	N	O	S	0	0
			780	491	147	139	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A8	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A9	341	Total	C	N	O	S	0	0
			2743	1777	480	477	9		

- Molecule 10 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AB	77	Total	C	N	O	S	0	0
			624	402	93	124	5		
10	AC	87	Total	C	N	O	S	0	0
			702	452	103	142	5		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	321	Total	C	N	O	S	0	0
			2601	1655	444	492	10		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

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

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

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

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	142	Total	C	N	O	S	0	0
			1173	755	203	206	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	B1	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	B2	67	Total	C	N	O	S	0	0
			584	385	95	103	1		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	B3	80	Total	C	N	O	S	0	0
			641	418	108	114	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	B4	128	Total	C	N	O	0	0
			1062	691	182	189		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	B5	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B6	103	Total	C	N	O	S	0	0
			882	577	156	148	1		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B7	125	Total	C	N	O	S	0	0
			1068	663	204	190	11		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	B8	156	Total	C	N	O	S	0	0
			1315	853	213	241	8		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B9	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BK	174	Total	C	N	O	S	0	0
			1456	913	264	271	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BL	99	Total	C	N	O	S	0	0
			828	531	137	156	4		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	CA	49	Total	C	N	O	0	0
			417	276	71	70		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	CB	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

- Molecule 28 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	N1	318	Total	C	N	O	S	0	0
			2508	1678	385	424	21		

- Molecule 29 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	N2	347	Total	C	N	O	S	0	0
			2710	1782	420	462	46		

- Molecule 30 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	N3	115	Total	C	N	O	S	0	0
			914	615	134	158	7		

- Molecule 31 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	N4	459	Total	C	N	O	S	0	0
			3631	2412	572	609	38		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	N5	603	Total	C	N	O	S	0	0
			4785	3173	741	820	51		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	N6	174	Total	C	N	O	S	0	0
			1329	892	189	236	12		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	S1	689	Total	C	N	O	S	0	0
			5290	3317	922	1012	39		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	S2	430	Total	C	N	O	S	0	0
			3459	2212	594	629	24		

- Molecule 36 is a protein called Complex I-30kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	S3	208	Total	C	N	O	S	0	0
			1738	1124	298	314	2		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	S4	124	Total	C	N	O	S	0	0
			1007	637	179	188	3		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	S5	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	S6	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	S7	156	Total	C	N	O	S	0	0
			1248	794	227	213	14		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	S8	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	V1	431	Total	C	N	O	S	0	0
			3316	2092	592	612	20		

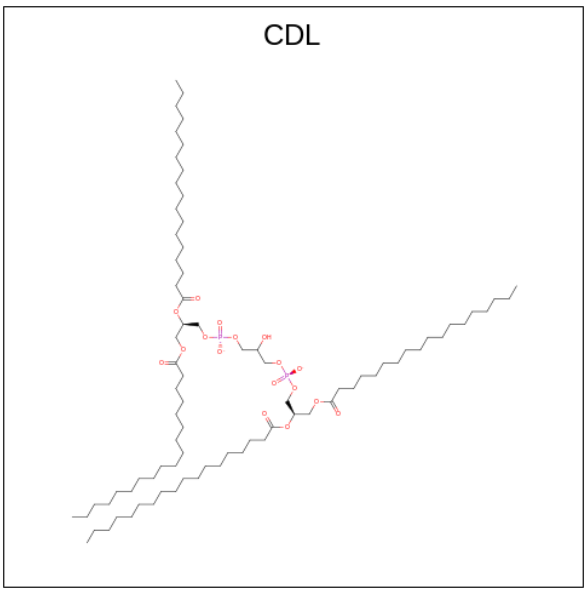
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	V2	217	Total	C	N	O	S	0	0
			1671	1065	281	315	10		

- Molecule 44 is a protein called NADH:ubiquinone oxidoreductase subunit V3.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	V3	42	Total	C	N	O	S	0	0
			355	219	67	68	1		

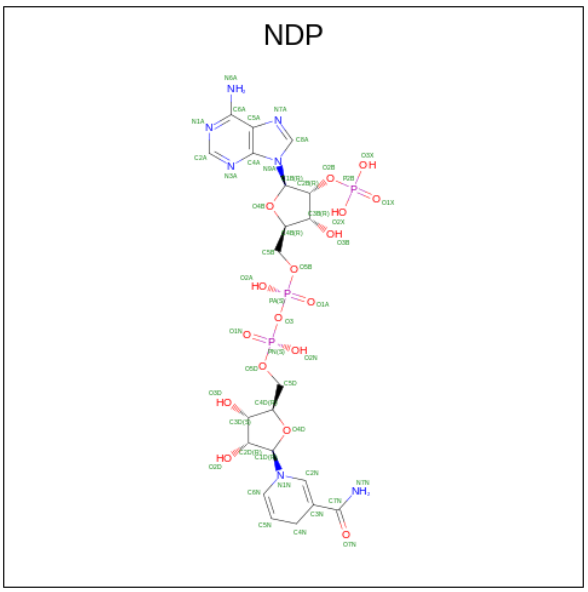
- Molecule 45 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
45	4L	1	Total	C	O	P	0
			92	73	17	2	
45	A7	1	Total	C	O	P	0
			51	32	17	2	
45	A8	1	Total	C	O	P	0
			83	64	17	2	
45	AK	1	Total	C	O	P	0
			68	49	17	2	
45	AL	1	Total	C	O	P	0
			94	75	17	2	
45	B4	1	Total	C	O	P	0
			80	61	17	2	
45	B5	1	Total	C	O	P	0
			100	81	17	2	
45	N1	1	Total	C	O	P	0
			78	59	17	2	
45	N4	1	Total	C	O	P	0
			100	81	17	2	
45	N4	1	Total	C	O	P	0
			62	43	17	2	
45	N5	1	Total	C	O	P	0
			89	70	17	2	
45	N5	1	Total	C	O	P	0
			100	81	17	2	

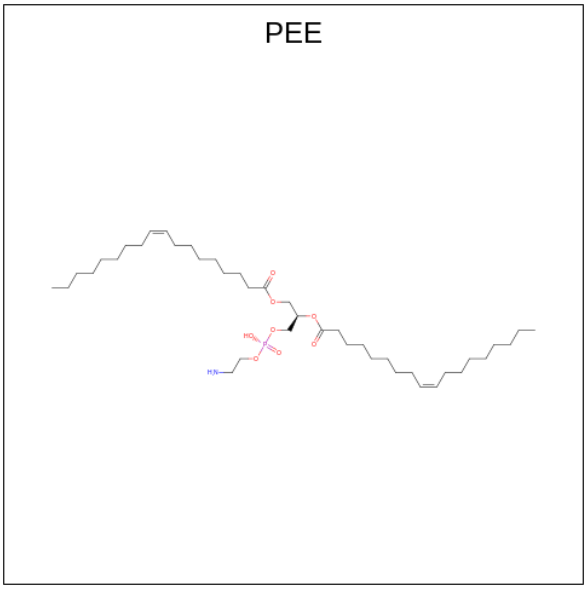
- Molecule 46 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

- Molecule 47 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
47	A9	1	Total	C	N	O	P	0
			39	29	1	8	1	

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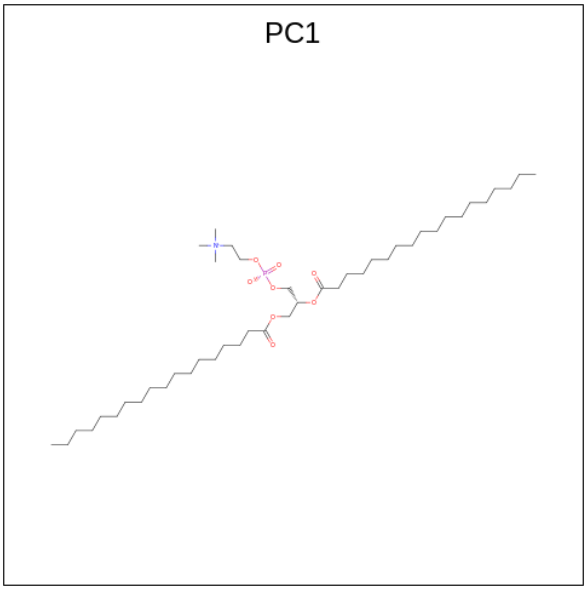
Mol	Chain	Residues	Atoms					AltConf
47	N1	1	Total	C	N	O	P	0
			31	21	1	8	1	
47	N3	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	N4	1	Total	C	N	O	P	0
			49	39	1	8	1	
47	N5	1	Total	C	N	O	P	0
			46	36	1	8	1	
47	N5	1	Total	C	N	O	P	0
			40	30	1	8	1	
47	N5	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	S2	1	Total	C	N	O	P	0
			48	38	1	8	1	
47	S8	1	Total	C	N	O	P	0
			51	41	1	8	1	

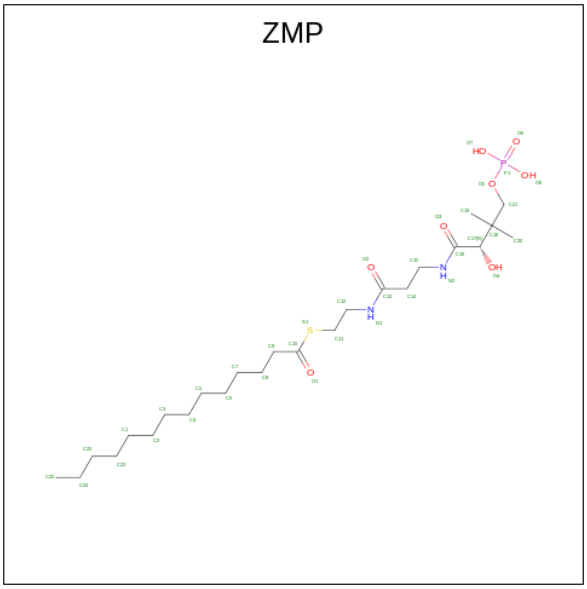
- Molecule 48 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
48	A9	1	Total	C	N	O	P	0
			54	44	1	8	1	
48	N1	1	Total	C	N	O	P	0
			48	38	1	8	1	

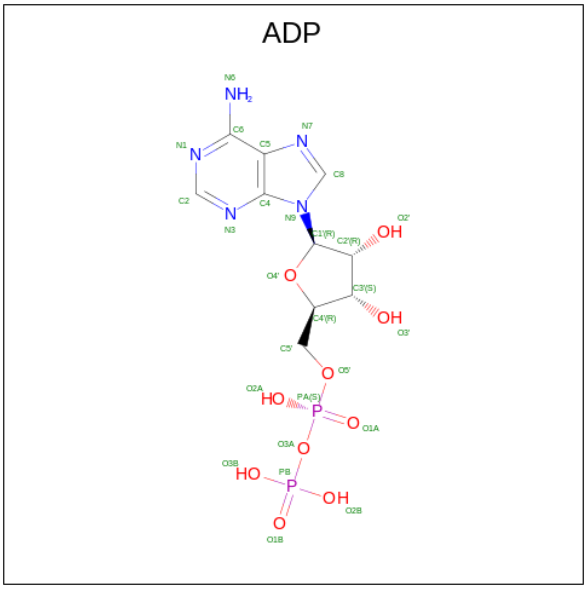
- Molecule 49 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alan

yl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



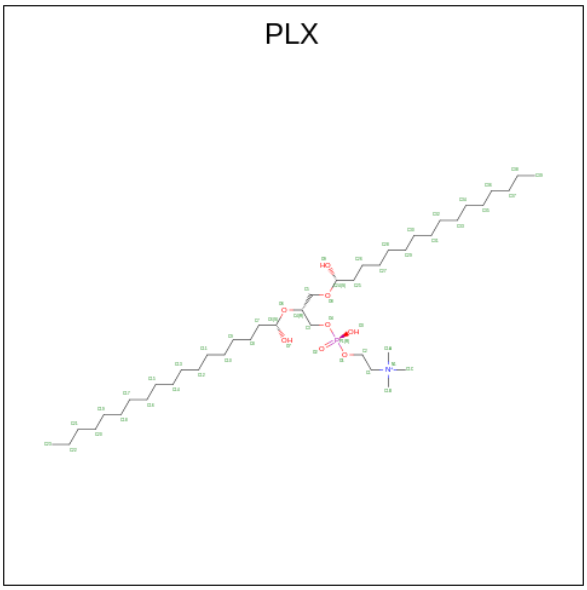
Mol	Chain	Residues	Atoms						AltConf
49	AB	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	
49	AC	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	

- Molecule 50 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



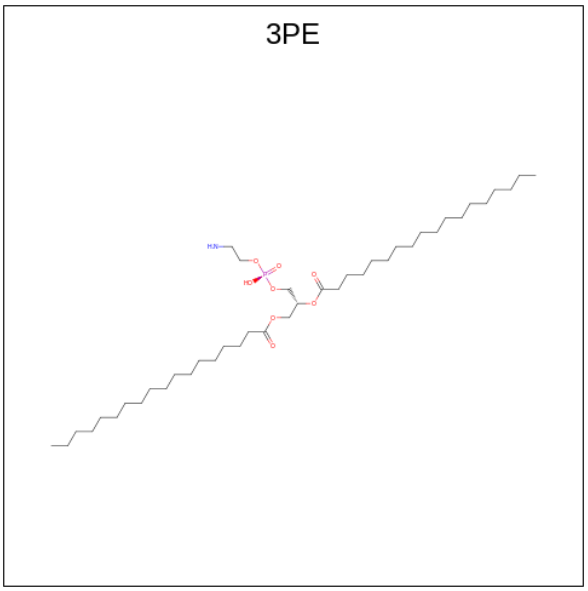
Mol	Chain	Residues	Atoms					AltConf
50	AK	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 51 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: $C_{42}H_{89}NO_8P$).



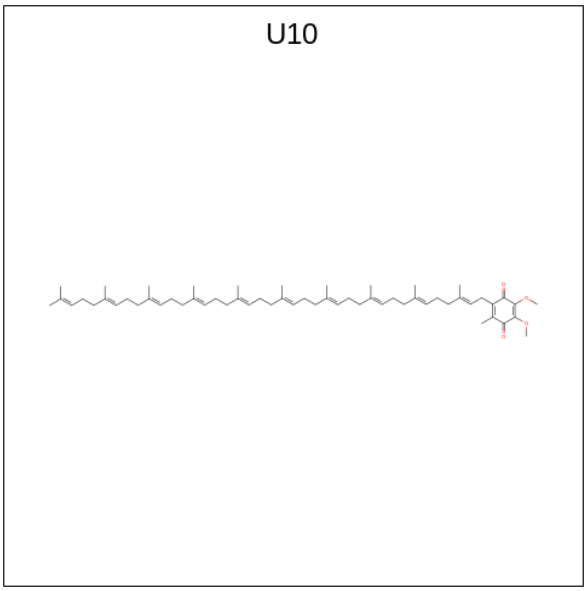
Mol	Chain	Residues	Atoms					AltConf
51	AL	1	Total	C	N	O	P	0
			47	37	1	8	1	
51	AM	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	B1	1	Total	C	N	O	P	0
			52	42	1	8	1	
51	CB	1	Total	C	N	O	P	0
			52	42	1	8	1	
51	N4	1	Total	C	N	O	P	0
			49	39	1	8	1	
51	N6	1	Total	C	N	O	P	0
			52	42	1	8	1	
51	S7	1	Total	C	N	O	P	0
			52	42	1	8	1	

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



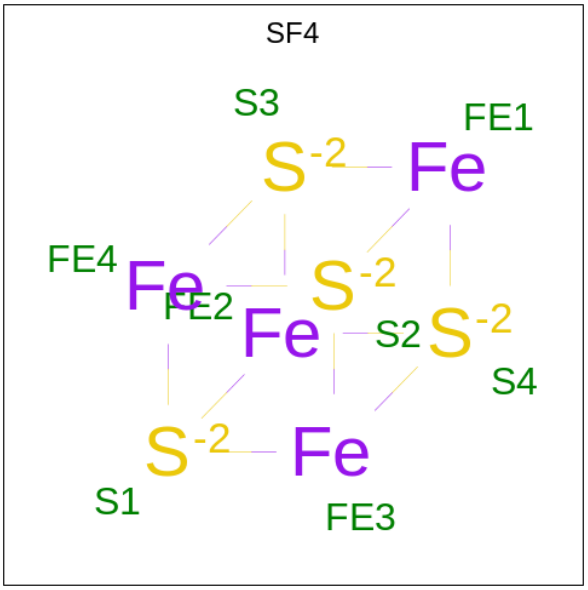
Mol	Chain	Residues	Atoms					AltConf
52	B8	1	Total	C	N	O	P	0
			32	22	1	8	1	
52	CA	1	Total	C	N	O	P	0
			51	41	1	8	1	
52	CB	1	Total	C	N	O	P	0
			46	36	1	8	1	
52	N5	1	Total	C	N	O	P	0
			46	36	1	8	1	
52	S7	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 53 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
53	N1	1	Total	C	O	0
			63	59	4	

- Molecule 54 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
54	S1	1	Total	Fe	S	0
			8	4	4	
54	S1	1	Total	Fe	S	0
			8	4	4	
54	S7	1	Total	Fe	S	0
			8	4	4	

Continued on next page...

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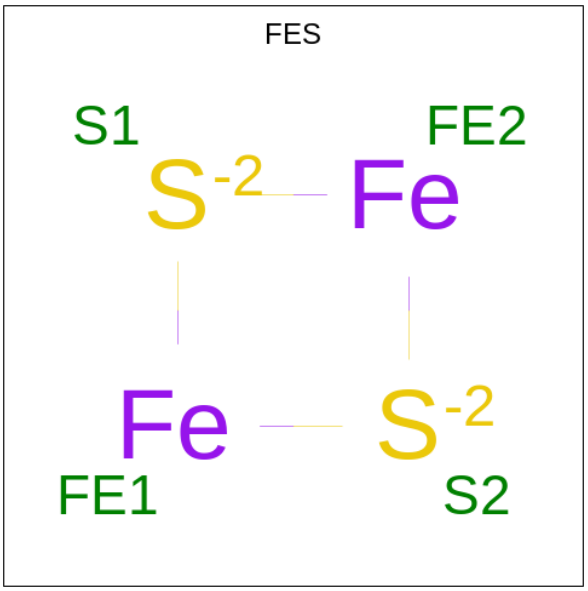
Mol	Chain	Residues	Atoms	AltConf
54	S8	1	Total Fe S 8 4 4	0
54	S8	1	Total Fe S 8 4 4	0
54	V1	1	Total Fe S 8 4 4	0

- Molecule 55 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

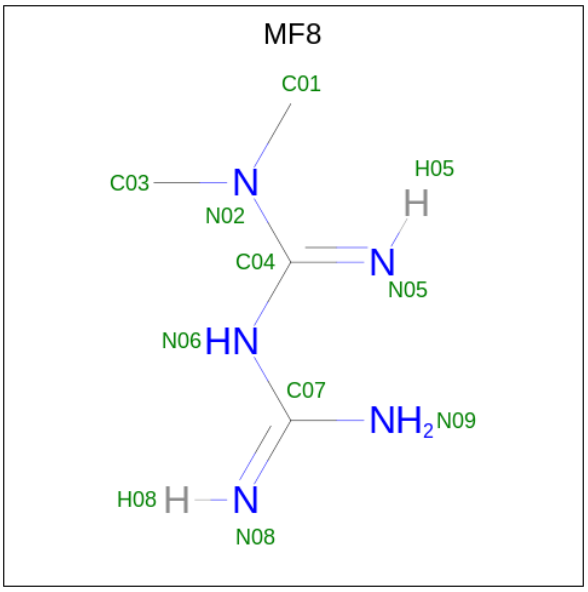


Mol	Chain	Residues	Atoms	AltConf
55	S1	1	Total Fe S 4 2 2	0
55	V2	1	Total Fe S 4 2 2	0

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
56	S1	1	Total Mg 1 1	0

- Molecule 57 is Metformin (CCD ID: MF8) (formula: $C_4H_{11}N_5$) (labeled as "Ligand of Interest" by depositor).

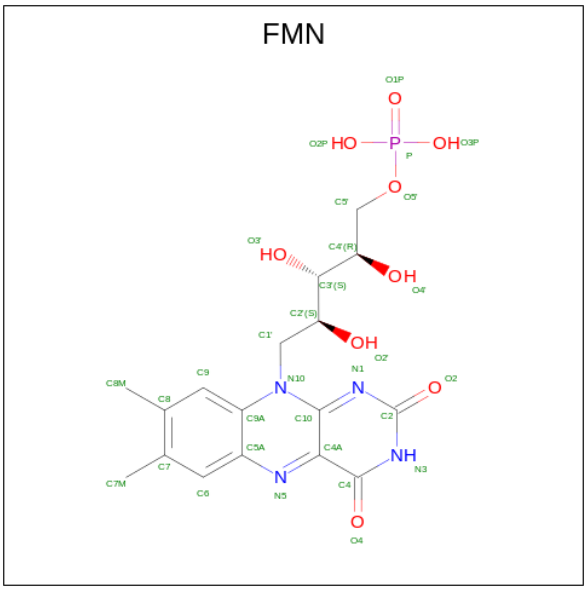


Mol	Chain	Residues	Atoms	AltConf
57	S2	1	Total C N 9 4 5	0

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

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

- Molecule 59 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



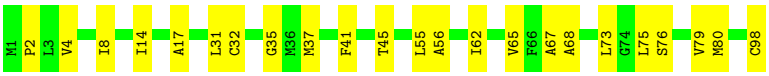
Mol	Chain	Residues	Atoms					AltConf
59	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

3 Residue-property plots (i)

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

• Molecule 1: NADH-ubiquinone oxidoreductase chain 4L

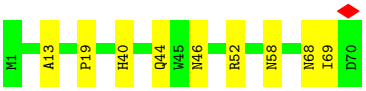
Chain 4L:



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

Chain A1:

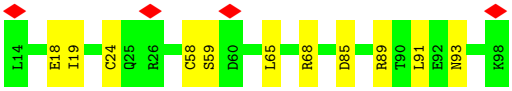




• Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain A2:





• Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain A3:

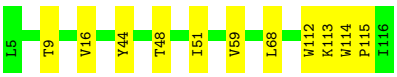




• Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain A5:

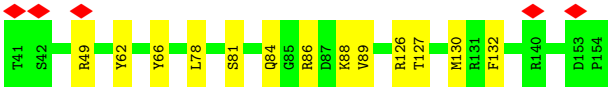




• Molecule 6: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain A6:

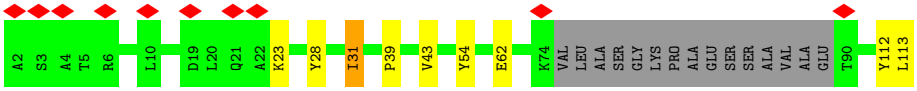




• Molecule 7: Complex I-B14.5a

Chain A7:

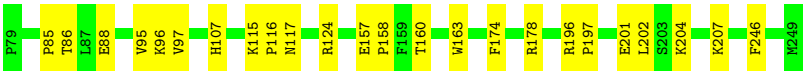




• Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain A8:



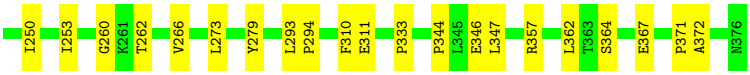


• Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain A9:







• Molecule 10: Acyl carrier protein

Chain AB:

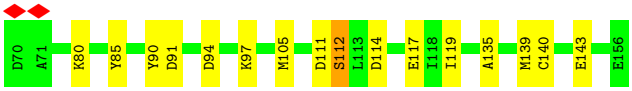




• Molecule 10: Acyl carrier protein

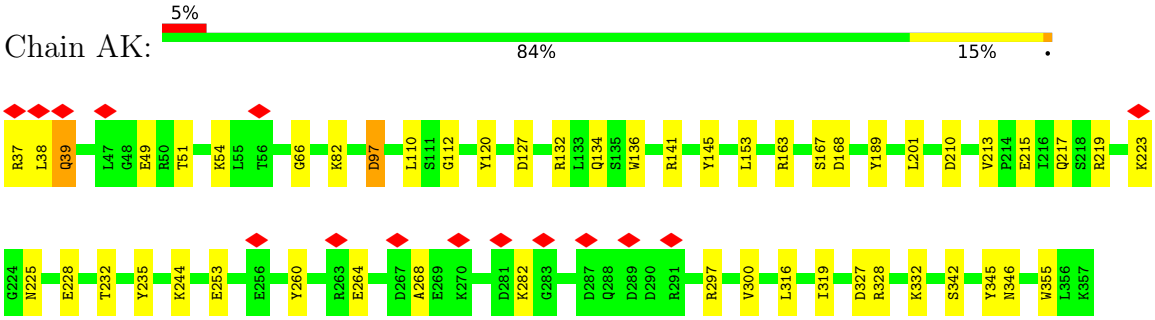
Chain AC:





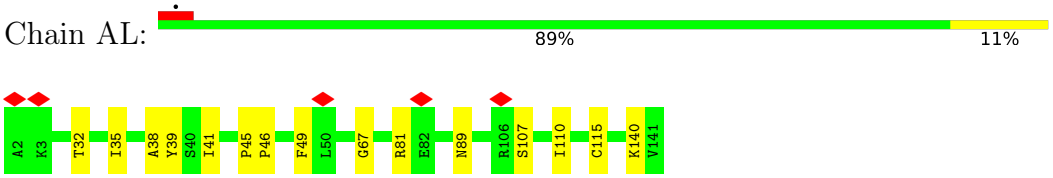
• Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain AK:



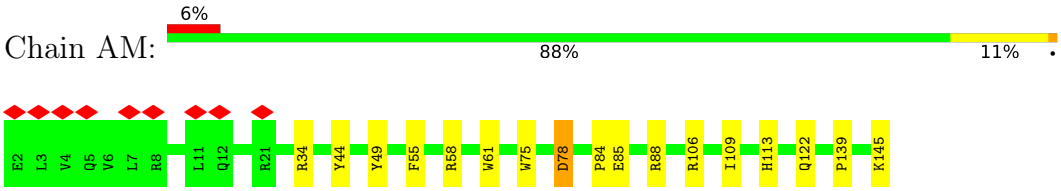
• Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain AL:



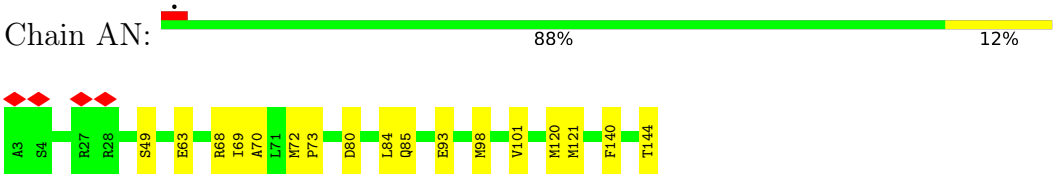
• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain AM:



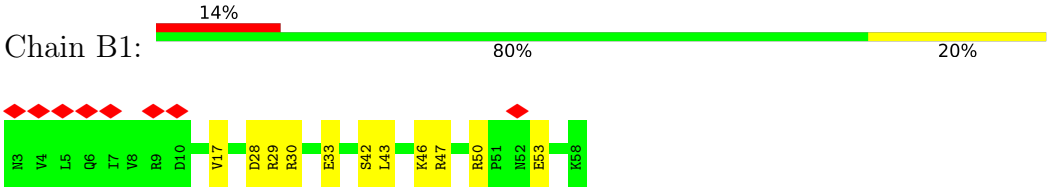
• Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain AN:



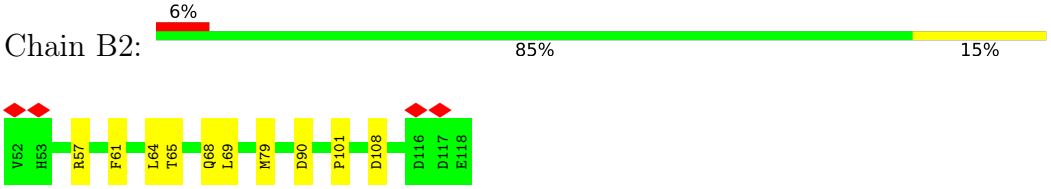
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain B1:



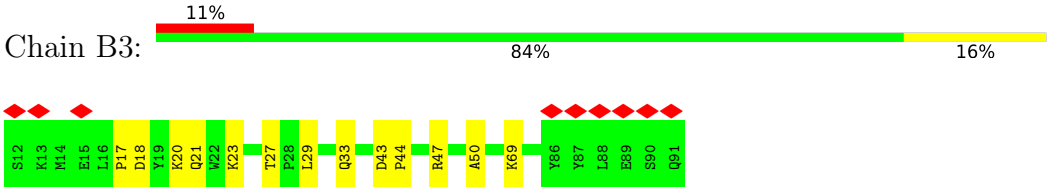
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain B2:



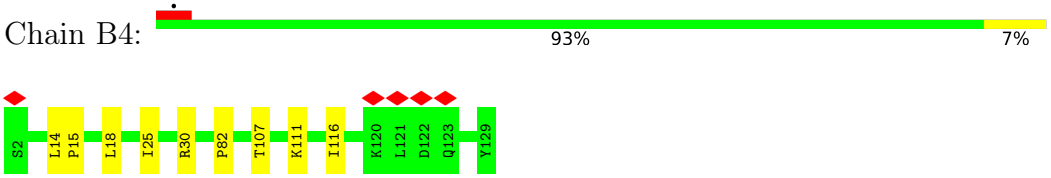
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain B3:



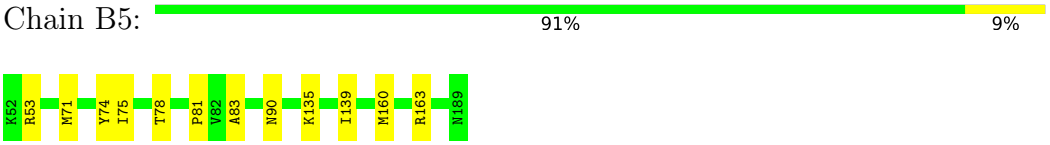
• Molecule 18: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain B4:



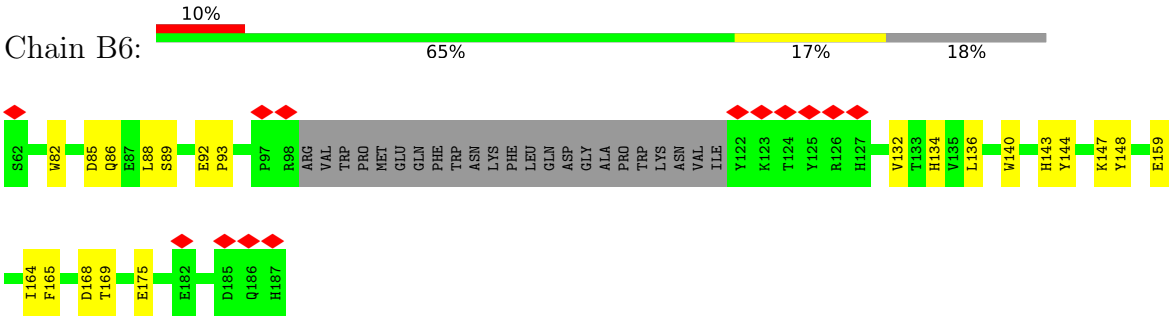
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain B5:



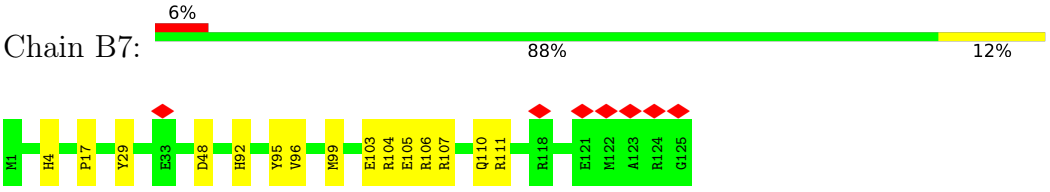
• Molecule 20: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain B6:



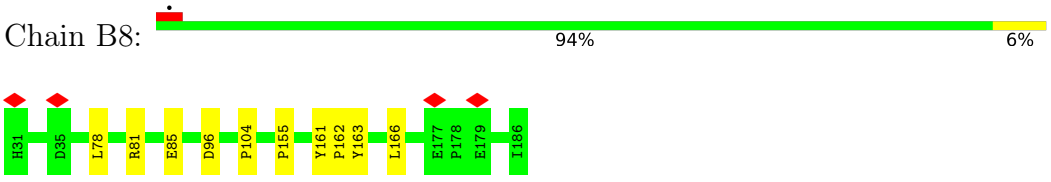
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain B7:



• Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

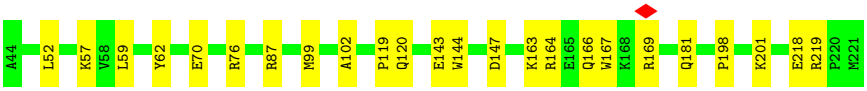
Chain B8:



• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain B9:

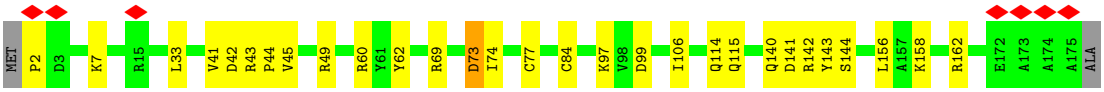




• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain BK:





• Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

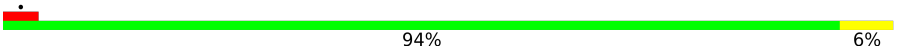
Chain BL:





• Molecule 26: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain CA:

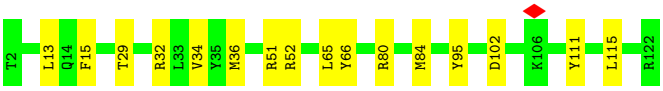




• Molecule 27: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain CB:

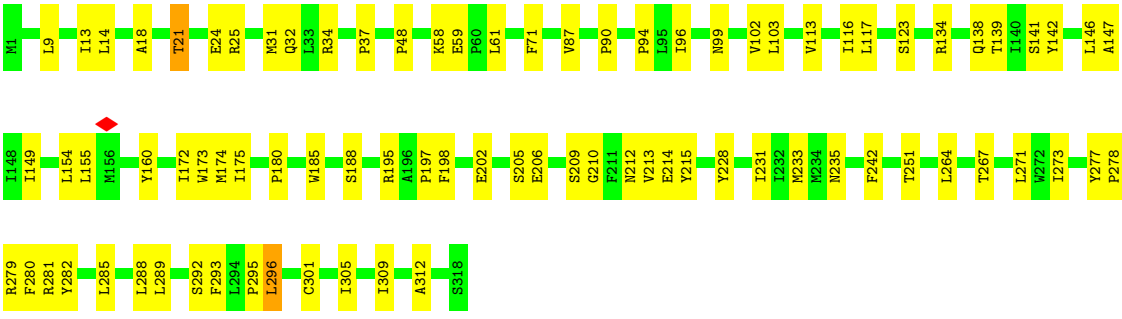




• Molecule 28: NADH-ubiquinone oxidoreductase chain 1

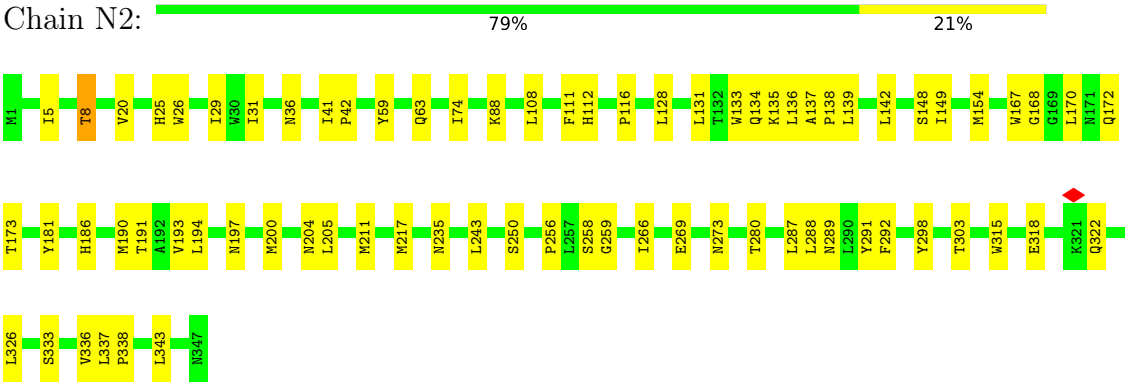
Chain N1:





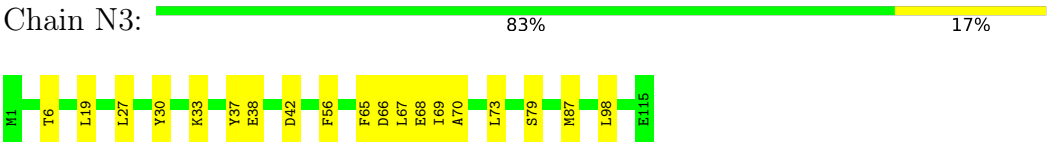
• Molecule 29: NADH-ubiquinone oxidoreductase chain 2

Chain N2:



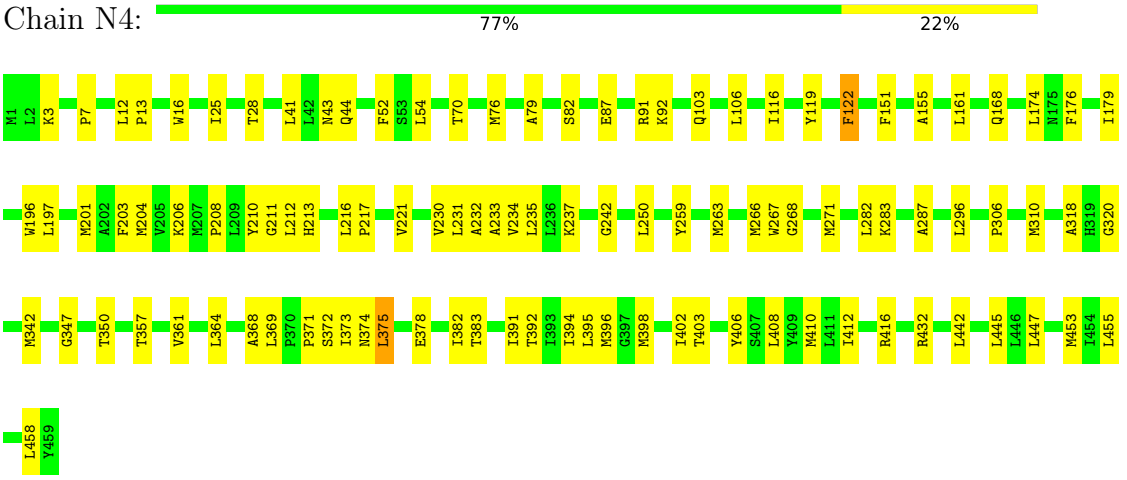
• Molecule 30: NADH-ubiquinone oxidoreductase chain 3

Chain N3:



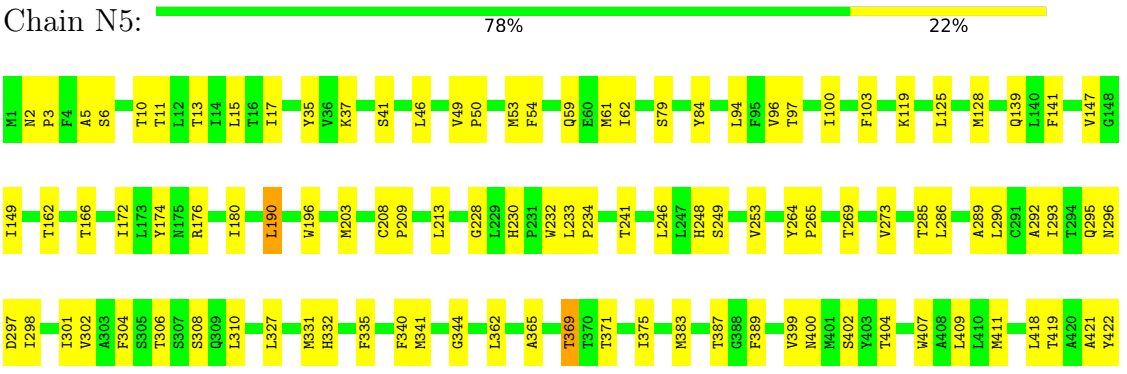
• Molecule 31: NADH-ubiquinone oxidoreductase chain 4

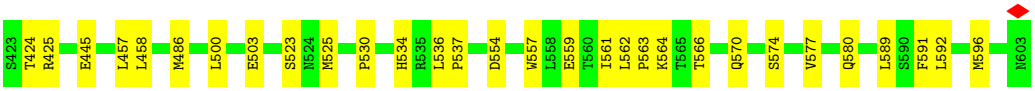
Chain N4:



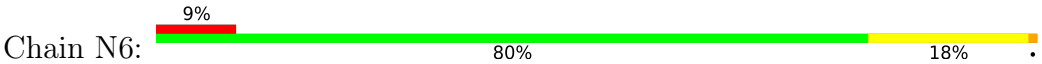
• Molecule 32: NADH-ubiquinone oxidoreductase chain 5

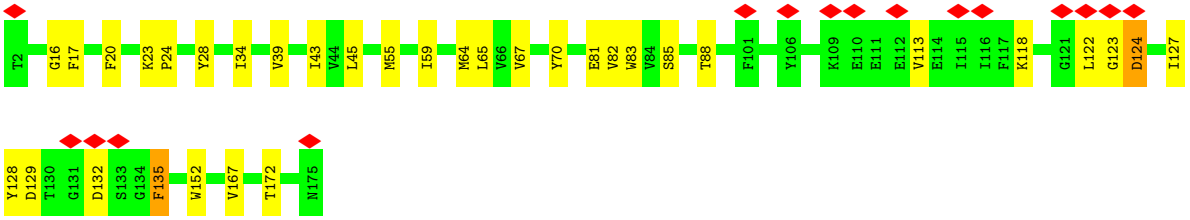
Chain N5:



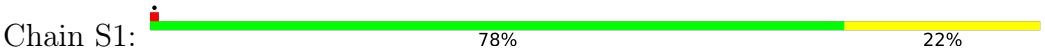


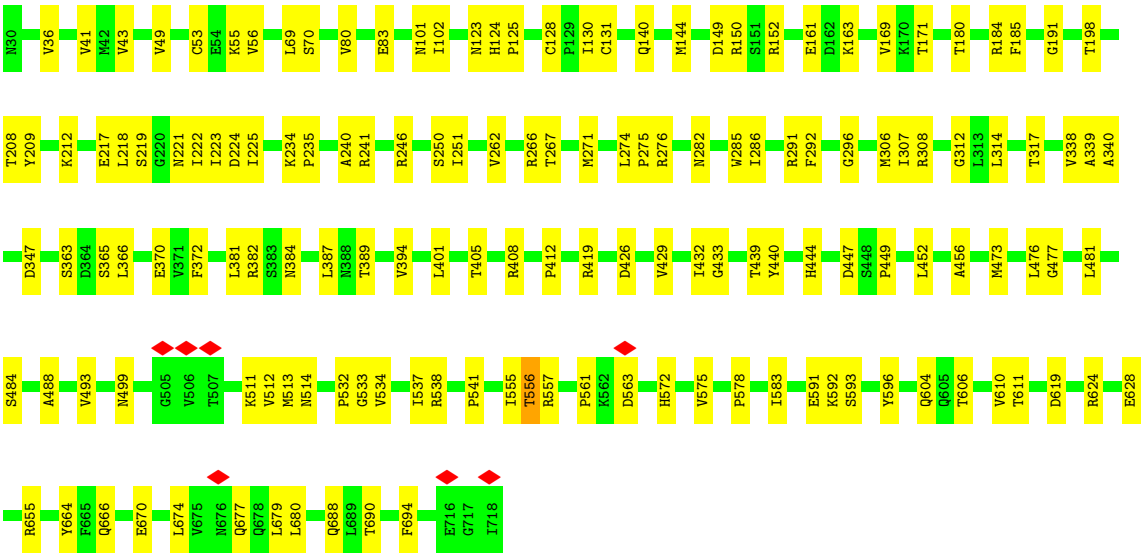
• Molecule 33: NADH-ubiquinone oxidoreductase chain 6



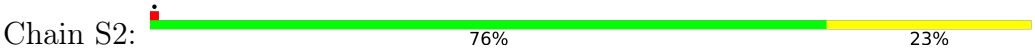


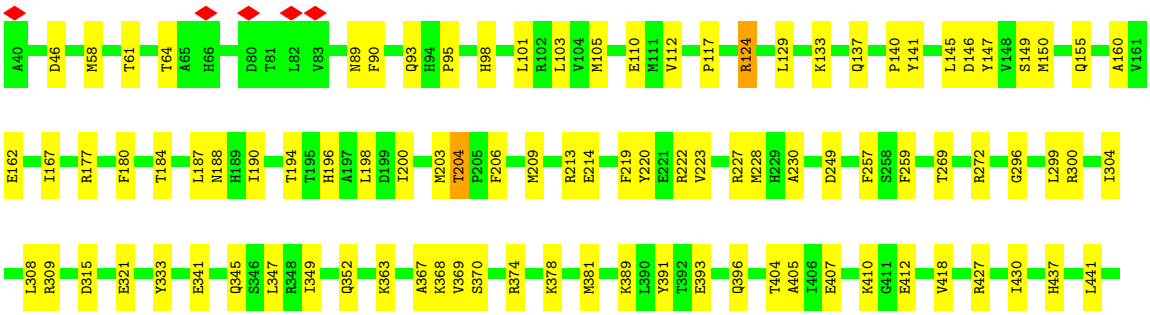
• Molecule 34: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial





• Molecule 35: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial







• Molecule 36: Complex I-30kD

Chain S3:

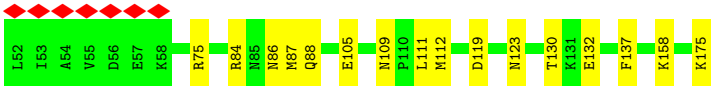




• Molecule 37: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain S4:





• Molecule 38: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain S5:

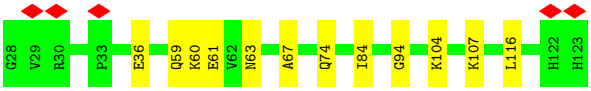




• Molecule 39: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain S6:

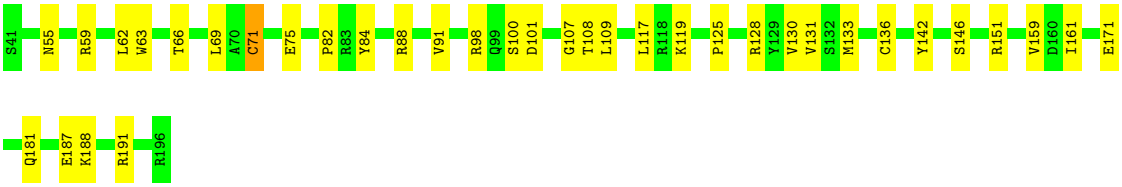




• Molecule 40: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain S7:

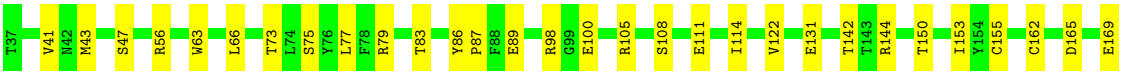


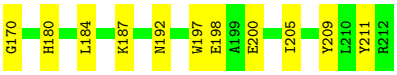


• Molecule 41: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain S8:





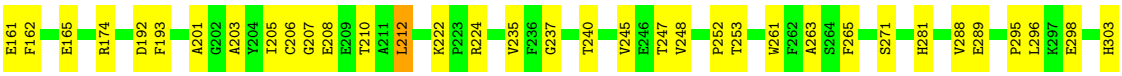


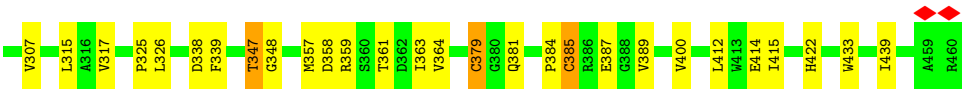
• Molecule 42: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain V1:





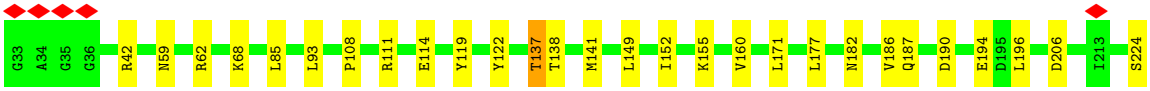




• Molecule 43: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain V2:







• Molecule 44: NADH:ubiquinone oxidoreductase subunit V3

Chain V3:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	269763	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51.9	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	47.538	Depositor
Minimum map value	-25.261	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	1.019	Depositor
Recommended contour level	4.62	Depositor
Map size (Å)	576.0, 576.0, 576.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 2MR, FMN, NDP, PEE, ADP, SF4, MG, FES, 3PE, MF8, CDL, ZN, PC1, PLX, U10, ZMP

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	4L	0.14	0/759	0.30	0/1029
2	A1	0.14	0/577	0.34	0/777
3	A2	0.10	0/697	0.26	0/938
4	A3	0.10	0/664	0.23	0/912
5	A5	0.11	0/929	0.22	0/1258
6	A6	0.13	0/991	0.27	0/1335
7	A7	0.11	0/798	0.25	0/1079
8	A8	0.11	0/1436	0.25	0/1938
9	A9	0.12	0/2820	0.26	0/3823
10	AB	0.08	0/633	0.21	0/851
10	AC	0.12	0/714	0.22	0/965
11	AK	0.11	0/2661	0.27	0/3602
12	AL	0.12	0/1042	0.22	0/1411
13	AM	0.09	0/1245	0.23	0/1694
14	AN	0.13	0/1204	0.26	0/1624
15	B1	0.11	0/491	0.23	0/663
16	B2	0.11	0/610	0.23	0/836
17	B3	0.12	0/660	0.24	0/892
18	B4	0.12	0/1092	0.25	0/1481
19	B5	0.13	0/1184	0.29	0/1603
20	B6	0.14	0/910	0.32	0/1237
21	B7	0.11	0/1092	0.24	0/1459
22	B8	0.12	0/1371	0.25	0/1875
23	B9	0.12	0/1590	0.27	0/2155
24	BK	0.12	0/1489	0.24	0/2008
25	BL	0.13	0/851	0.27	0/1155
26	CA	0.12	0/430	0.23	0/581
27	CB	0.13	0/1031	0.25	0/1394
28	N1	0.17	0/2581	0.34	0/3529
29	N2	0.17	0/2773	0.33	0/3768
30	N3	0.15	0/938	0.27	0/1281
31	N4	0.16	0/3723	0.30	0/5078

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
32	N5	0.15	0/4914	0.33	0/6683
33	N6	0.14	0/1364	0.30	0/1850
34	S1	0.14	0/5378	0.30	0/7287
35	S2	0.16	0/3538	0.29	0/4796
36	S3	0.13	0/1789	0.27	0/2436
37	S4	0.12	0/1030	0.26	0/1391
38	S5	0.11	0/889	0.23	0/1190
39	S6	0.12	0/755	0.27	0/1018
40	S7	0.14	0/1279	0.28	0/1730
41	S8	0.14	0/1443	0.27	0/1952
42	V1	0.14	0/3391	0.30	0/4583
43	V2	0.12	0/1711	0.29	0/2328
44	V3	0.09	0/365	0.25	0/493
All	All	0.14	0/67832	0.28	0/91968

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4L	748	0	799	23	0
2	A1	562	0	557	7	0
3	A2	686	0	699	7	0
4	A3	643	0	642	7	0
5	A5	910	0	950	7	0
6	A6	967	0	972	11	0
7	A7	780	0	808	8	0
8	A8	1398	0	1372	20	0
9	A9	2743	0	2762	31	0
10	AB	624	0	625	8	0
10	AC	702	0	694	12	0
11	AK	2601	0	2566	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	AL	1021	0	1025	13	0
13	AM	1204	0	1162	18	0
14	AN	1173	0	1166	15	0
15	B1	479	0	486	8	0
16	B2	584	0	529	7	0
17	B3	641	0	620	9	0
18	B4	1062	0	1072	6	0
19	B5	1151	0	1164	11	0
20	B6	882	0	899	22	0
21	B7	1068	0	1043	13	0
22	B8	1315	0	1208	6	0
23	B9	1534	0	1470	17	0
24	BK	1456	0	1426	24	0
25	BL	828	0	788	12	0
26	CA	417	0	422	2	0
27	CB	1000	0	994	16	0
28	N1	2508	0	2607	70	0
29	N2	2710	0	2874	50	0
30	N3	914	0	951	21	0
31	N4	3631	0	3839	73	0
32	N5	4785	0	4933	86	0
33	N6	1329	0	1326	33	0
34	S1	5290	0	5321	99	0
35	S2	3459	0	3396	76	0
36	S3	1738	0	1693	18	0
37	S4	1007	0	1008	15	0
38	S5	867	0	871	11	0
39	S6	741	0	701	10	0
40	S7	1248	0	1254	31	0
41	S8	1412	0	1363	34	0
42	V1	3316	0	3272	62	0
43	V2	1671	0	1673	21	0
44	V3	355	0	329	11	0
45	4L	92	0	137	9	0
45	A7	51	0	46	1	0
45	A8	83	0	113	9	0
45	AK	68	0	80	3	0
45	AL	94	0	138	7	0
45	B4	80	0	107	3	0
45	B5	100	0	156	9	0
45	N1	78	0	103	5	0
45	N4	162	0	224	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	N5	189	0	284	10	0
46	A9	48	0	26	1	0
47	A9	39	0	52	4	0
47	N1	31	0	36	3	0
47	N3	51	0	82	4	0
47	N4	49	0	75	6	0
47	N5	137	0	205	9	0
47	S2	48	0	73	6	0
47	S8	51	0	82	8	0
48	A9	54	0	88	2	0
48	N1	48	0	73	2	0
49	AB	36	0	47	2	0
49	AC	36	0	47	2	0
50	AK	27	0	12	4	0
51	AL	47	0	75	1	0
51	AM	51	0	83	4	0
51	B1	52	0	88	2	0
51	CB	52	0	88	5	0
51	N4	49	0	79	6	0
51	N6	52	0	88	3	0
51	S7	52	0	88	5	0
52	B8	32	0	38	0	0
52	CA	51	0	82	2	0
52	CB	46	0	69	1	0
52	N5	46	0	69	1	0
52	S7	51	0	82	1	0
53	N1	63	0	90	10	0
54	S1	16	0	0	1	0
54	S7	8	0	0	0	0
54	S8	16	0	0	1	0
54	V1	8	0	0	0	0
55	S1	4	0	0	0	0
55	V2	4	0	0	0	0
56	S1	1	0	0	0	0
57	S2	9	0	0	0	0
58	S6	1	0	0	0	0
59	V1	31	0	19	1	0
All	All	68554	0	69655	965	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 7.

All (965) 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)
24:BK:140:GLN:O	24:BK:144:SER:HB2	1.73	0.88
49:AC:201:ZMP:H14	23:B9:102:ALA:HB1	1.65	0.78
34:S1:149:ASP:HB2	35:S2:367:ALA:HB3	1.64	0.77
35:S2:222:ARG:NH1	35:S2:249:ASP:OD2	2.19	0.76
20:B6:88:LEU:HD22	20:B6:92:GLU:HG2	1.68	0.76
1:4L:37:MET:HG2	1:4L:67:ALA:HB2	1.65	0.76
45:4L:201:CDL:H521	33:N6:88:THR:HG23	1.67	0.75
42:V1:235:VAL:HG12	42:V1:240:THR:HG21	1.67	0.75
1:4L:68:ALA:HB3	30:N3:67:LEU:HD11	1.66	0.75
29:N2:88:LYS:HG3	29:N2:148:SER:HB3	1.69	0.75
3:A2:59:SER:HB2	34:S1:655:ARG:HD3	1.70	0.73
47:N4:501:PEE:H46	47:S2:501:PEE:H37	1.72	0.71
12:AL:140:LYS:H	29:N2:273:ASN:HD22	1.37	0.71
31:N4:369:LEU:HD21	32:N5:149:ILE:HD13	1.72	0.71
1:4L:14:ILE:HG12	45:4L:201:CDL:H781	1.73	0.71
6:A6:88:LYS:NZ	6:A6:132:PHE:O	2.23	0.71
43:V2:68:LYS:NZ	44:V3:407:SER:OG	2.24	0.70
42:V1:111:LYS:HB2	42:V1:151:ALA:HA	1.71	0.70
11:AK:120:TYR:OH	50:AK:401:ADP:O2'	2.09	0.70
34:S1:433:GLY:HA2	34:S1:447:ASP:HA	1.74	0.70
42:V1:52:ARG:HH21	44:V3:390:GLN:HG2	1.56	0.70
34:S1:124:HIS:HD2	35:S2:381:MET:HE2	1.55	0.70
3:A2:24:CYS:N	3:A2:58:CYS:SG	2.65	0.70
35:S2:308:LEU:HB2	35:S2:407:GLU:HB2	1.73	0.70
42:V1:40:ARG:NH1	42:V1:289:GLU:O	2.25	0.69
28:N1:87:VAL:HG11	30:N3:6:THR:HG21	1.74	0.69
35:S2:90:PHE:HB3	35:S2:103:LEU:HB3	1.75	0.68
41:S8:205:ILE:O	41:S8:209:TYR:HB3	1.93	0.68
42:V1:205:ILE:HG12	42:V1:379:CYS:HB3	1.74	0.68
17:B3:27:THR:HG22	17:B3:29:LEU:H	1.58	0.68
13:AM:34:ARG:NH2	41:S8:89:GLU:OE2	2.28	0.67
53:N1:403:U10:H3M2	40:S7:66:THR:HG22	1.76	0.67
32:N5:3:PRO:HB2	32:N5:53:MET:HE1	1.75	0.67
9:A9:188:GLU:HG3	9:A9:200:ILE:HD13	1.77	0.66
11:AK:120:TYR:HH	50:AK:401:ADP:HO2'	1.41	0.66
34:S1:338:VAL:O	34:S1:365:SER:HB2	1.96	0.66
18:B4:15:PRO:HG2	18:B4:18:LEU:HB2	1.77	0.66
24:BK:2:PRO:O	24:BK:7:LYS:NZ	2.28	0.66
47:N5:701:PEE:H36	45:N5:703:CDL:H231	1.76	0.66
9:A9:346:GLU:HG2	9:A9:371:PRO:HB3	1.78	0.66
35:S2:374:ARG:NH2	41:S8:165:ASP:OD1	2.29	0.65
36:S3:187:ILE:HG23	36:S3:188:LEU:HG	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:N5:5:ALA:HB2	32:N5:61:MET:HE1	1.76	0.65
37:S4:75:ARG:NH1	37:S4:119:ASP:OD1	2.27	0.65
20:B6:132:VAL:O	20:B6:136:LEU:HB3	1.95	0.65
41:S8:63:TRP:HE1	47:S8:303:PEE:H13	1.60	0.65
30:N3:37:TYR:OH	35:S2:93:GLN:NE2	2.30	0.65
31:N4:87:GLU:O	31:N4:92:LYS:NZ	2.30	0.65
9:A9:87:GLU:HG3	9:A9:89:TYR:H	1.61	0.65
12:AL:140:LYS:O	29:N2:273:ASN:ND2	2.30	0.65
11:AK:66:GLY:O	11:AK:163:ARG:NH2	2.28	0.65
40:S7:188:LYS:HB2	40:S7:191:ARG:HB2	1.77	0.65
21:B7:29:TYR:O	21:B7:104:ARG:NH2	2.30	0.64
6:A6:89:VAL:HG22	49:AB:201:ZMP:H2	1.80	0.64
11:AK:134:GLN:HE22	50:AK:401:ADP:HN62	1.46	0.64
34:S1:266:ARG:HD2	34:S1:267:THR:HG23	1.80	0.64
35:S2:155:GLN:NE2	35:S2:315:ASP:OD2	2.31	0.64
45:4L:201:CDL:OB9	33:N6:23:LYS:NZ	2.31	0.64
34:S1:69:LEU:O	37:S4:158:LYS:NZ	2.30	0.64
43:V2:108:PRO:HB2	43:V2:111:ARG:HG2	1.80	0.63
43:V2:182:ASN:HB3	43:V2:194:GLU:HB3	1.79	0.63
45:A8:301:CDL:H112	27:CB:32:ARG:HG2	1.81	0.63
10:AC:114:ASP:OD1	23:B9:87:ARG:NH2	2.31	0.63
25:BL:129:ARG:NH1	25:BL:136:LEU:O	2.30	0.62
35:S2:300:ARG:NH2	35:S2:407:GLU:OE2	2.32	0.62
13:AM:106:ARG:HB2	13:AM:109:ILE:HG13	1.81	0.62
45:B5:201:CDL:H512	47:N5:701:PEE:H14	1.80	0.62
31:N4:391:ILE:HG23	31:N4:394:ILE:HD12	1.82	0.62
32:N5:100:ILE:HG21	32:N5:246:LEU:HB2	1.81	0.62
6:A6:66:TYR:O	6:A6:86:ARG:NH1	2.32	0.62
32:N5:295:GLN:O	32:N5:425:ARG:NH1	2.32	0.62
28:N1:123:SER:HB3	28:N1:214:GLU:HG3	1.80	0.62
35:S2:188:ASN:OD1	35:S2:410:LYS:NZ	2.27	0.62
34:S1:308:ARG:NH1	34:S1:312:GLY:O	2.32	0.62
42:V1:338:ASP:OD1	42:V1:339:PHE:N	2.33	0.62
43:V2:187:GLN:HE21	43:V2:190:ASP:HA	1.64	0.62
10:AB:116:VAL:HG12	10:AB:120:MET:HE2	1.82	0.62
1:4L:31:LEU:HD21	33:N6:67:VAL:HG11	1.82	0.62
37:S4:109:ASN:ND2	37:S4:111:LEU:O	2.33	0.62
15:B1:29:ARG:NH2	51:B1:101:PLX:O2	2.32	0.61
29:N2:108:LEU:HD11	29:N2:191:THR:HG21	1.82	0.61
42:V1:112:TYR:HB2	42:V1:240:THR:HG22	1.81	0.61
34:S1:198:THR:HG21	34:S1:209:TYR:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:N1:102:VAL:HG11	28:N1:154:LEU:HD11	1.82	0.61
6:A6:78:LEU:HD22	6:A6:130:MET:HE3	1.83	0.61
11:AK:145:TYR:OH	11:AK:201:LEU:O	2.16	0.61
28:N1:99:ASN:N	48:N1:402:PC1:O12	2.30	0.61
3:A2:65:LEU:HD11	3:A2:91:LEU:HD13	1.81	0.60
32:N5:249:SER:HA	32:N5:306:THR:HG21	1.83	0.60
25:BL:95:PHE:O	25:BL:99:LEU:HB2	2.00	0.60
32:N5:419:THR:HA	32:N5:422:TYR:CE2	2.36	0.60
29:N2:142:LEU:HB3	29:N2:194:LEU:HD21	1.83	0.60
34:S1:246:ARG:HH22	37:S4:123:ASN:HD21	1.48	0.60
29:N2:289:ASN:HA	29:N2:292:PHE:CE2	2.36	0.60
28:N1:141:SER:HB2	28:N1:289:LEU:HD12	1.83	0.60
9:A9:50:SER:OG	36:S3:225:GLU:OE2	2.19	0.60
12:AL:140:LYS:H	29:N2:273:ASN:ND2	1.99	0.60
19:B5:163:ARG:NH1	27:CB:102:ASP:OD2	2.29	0.60
35:S2:272:ARG:HH11	47:S8:303:PEE:H2	1.66	0.60
20:B6:85:ASP:OD2	23:B9:167:TRP:NE1	2.30	0.60
35:S2:464:PHE:HA	35:S2:467:VAL:HB	1.83	0.60
40:S7:55:ASN:ND2	40:S7:187:GLU:O	2.35	0.60
34:S1:152:ARG:NH1	42:V1:414:GLU:OE1	2.35	0.60
34:S1:282:ASN:ND2	34:S1:285:TRP:O	2.35	0.60
34:S1:456:ALA:O	34:S1:499:ASN:ND2	2.35	0.60
35:S2:61:THR:H	35:S2:64:THR:HG1	1.50	0.59
36:S3:128:ILE:HB	36:S3:145:THR:HG23	1.84	0.59
29:N2:298:TYR:O	29:N2:303:THR:OG1	2.16	0.59
34:S1:401:LEU:HD11	34:S1:432:ILE:HG13	1.83	0.59
32:N5:362:LEU:HA	32:N5:365:ALA:HB3	1.83	0.59
28:N1:174:MET:HB2	28:N1:242:PHE:HA	1.85	0.59
34:S1:250:SER:HB2	34:S1:606:THR:HG23	1.84	0.59
35:S2:393:GLU:OE2	35:S2:396:GLN:NE2	2.36	0.59
8:A8:124:ARG:NE	14:AN:80:ASP:OD2	2.35	0.59
9:A9:173:ASP:HB3	9:A9:176:SER:HB2	1.84	0.59
9:A9:204:SER:HB2	9:A9:266:VAL:HG12	1.84	0.59
31:N4:371:PRO:HD2	45:N5:703:CDL:H391	1.85	0.59
34:S1:208:THR:HG21	34:S1:212:LYS:HB3	1.85	0.59
35:S2:90:PHE:HB2	35:S2:105:MET:HE2	1.85	0.59
42:V1:109:ARG:NH1	42:V1:237:GLY:O	2.36	0.59
21:B7:29:TYR:OH	21:B7:111:ARG:NH2	2.36	0.59
51:CB:201:PLX:H171	38:S5:9:ARG:HH22	1.67	0.59
30:N3:38:GLU:HG2	35:S2:89:ASN:HB2	1.85	0.59
41:S8:47:SER:O	41:S8:56:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:N4:41:LEU:O	31:N4:44:GLN:NE2	2.36	0.58
7:A7:112:TYR:HE2	41:S8:43:MET:HE2	1.69	0.58
34:S1:340:ALA:HB3	34:S1:366:LEU:HD23	1.85	0.58
9:A9:212:ARG:NH1	9:A9:311:GLU:OE2	2.37	0.58
31:N4:403:THR:HA	31:N4:406:TYR:CE2	2.39	0.58
37:S4:175:LYS:NZ	42:V1:222:LYS:O	2.37	0.58
19:B5:90:ASN:ND2	45:B5:201:CDL:OA7	2.37	0.58
39:S6:61:GLU:OE2	41:S8:192:ASN:ND2	2.36	0.58
42:V1:55:GLY:O	42:V1:58:SER:OG	2.20	0.58
3:A2:89:ARG:O	3:A2:93:ASN:ND2	2.37	0.58
42:V1:281:HIS:ND1	42:V1:358:ASP:OD1	2.36	0.58
9:A9:344:PRO:HG2	9:A9:347:LEU:HD13	1.85	0.58
13:AM:88:ARG:HD3	41:S8:200:GLU:HG3	1.83	0.58
40:S7:62:LEU:O	40:S7:91:VAL:HA	2.04	0.58
30:N3:70:ALA:HB2	33:N6:59:ILE:HD11	1.85	0.58
1:4L:2:PRO:HG3	33:N6:127:ILE:HD13	1.86	0.57
12:AL:35:ILE:HD12	45:AL:201:CDL:H811	1.86	0.57
14:AN:144:THR:HB	28:N1:96:ILE:HG23	1.84	0.57
34:S1:488:ALA:HB2	34:S1:677:GLN:HG3	1.85	0.57
42:V1:112:TYR:O	42:V1:240:THR:HA	2.04	0.57
42:V1:113:LEU:HD13	42:V1:149:MET:HE1	1.86	0.57
42:V1:263:ALA:HA	42:V1:271:SER:HB3	1.85	0.57
8:A8:107:HIS:HB3	8:A8:197:PRO:HD2	1.84	0.57
2:A1:46:ASN:ND2	33:N6:132:ASP:OD2	2.37	0.57
29:N2:42:PRO:HG2	33:N6:167:VAL:HG22	1.85	0.57
34:S1:419:ARG:NH1	34:S1:439:THR:O	2.34	0.57
28:N1:197:PRO:HB2	28:N1:280:PHE:HD1	1.69	0.57
1:4L:65:VAL:HA	30:N3:67:LEU:HD22	1.87	0.57
32:N5:253:VAL:HG23	32:N5:310:LEU:HD21	1.86	0.57
9:A9:163:LYS:NZ	9:A9:253:ILE:O	2.30	0.57
28:N1:103:LEU:HD13	33:N6:55:MET:HE3	1.87	0.57
34:S1:534:VAL:HG22	34:S1:537:ILE:HB	1.87	0.57
6:A6:62:TYR:OH	10:AB:117:GLU:OE2	2.21	0.57
9:A9:61:ALA:HB3	9:A9:82:VAL:HG13	1.87	0.57
19:B5:74:TYR:O	25:BL:96:SER:OG	2.22	0.57
45:B5:201:CDL:H511	47:N5:701:PEE:H51	1.87	0.57
32:N5:402:SER:HB2	32:N5:404:THR:HG23	1.87	0.57
28:N1:231:ILE:O	28:N1:235:ASN:ND2	2.38	0.56
31:N4:445:LEU:HB3	45:N5:703:CDL:H452	1.86	0.56
9:A9:357:ARG:NH1	9:A9:364:SER:OG	2.38	0.56
31:N4:155:ALA:HB3	47:S2:501:PEE:H38	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:N4:392:THR:O	31:N4:396:MET:HG2	2.05	0.56
32:N5:293:ILE:HD12	45:N5:704:CDL:H521	1.88	0.56
28:N1:173:TRP:HB3	28:N1:175:ILE:HG22	1.87	0.56
45:N4:503:CDL:H251	45:N4:503:CDL:H851	1.86	0.56
34:S1:452:LEU:HD21	34:S1:493:VAL:HG13	1.88	0.56
42:V1:203:ALA:HB3	42:V1:206:CYS:HB2	1.87	0.56
42:V1:296:LEU:HD21	42:V1:317:VAL:HG11	1.88	0.56
29:N2:197:ASN:HD22	29:N2:200:MET:HG2	1.69	0.56
6:A6:81:SER:OG	9:A9:367:GLU:OE2	2.24	0.56
24:BK:142:ARG:NH1	24:BK:143:TYR:OH	2.39	0.56
31:N4:318:ALA:HB2	31:N4:373:ILE:HG13	1.88	0.56
51:N4:502:PLX:H192	45:N5:703:CDL:H611	1.87	0.56
23:B9:52:LEU:O	23:B9:57:LYS:NZ	2.38	0.55
16:B2:108:ASP:OD1	21:B7:107:ARG:NH1	2.39	0.55
28:N1:31:MET:HG2	41:S8:77:LEU:HB2	1.88	0.55
32:N5:103:PHE:HB2	32:N5:341:MET:HE3	1.88	0.55
13:AM:145:LYS:HE2	34:S1:563:ASP:HA	1.88	0.55
24:BK:73:ASP:OD1	24:BK:73:ASP:N	2.37	0.55
42:V1:113:LEU:O	42:V1:154:ALA:HA	2.06	0.55
34:S1:163:LYS:O	34:S1:171:THR:OG1	2.23	0.55
34:S1:275:PRO:HG3	34:S1:286:ILE:HG12	1.87	0.55
45:A8:301:CDL:H572	45:A8:301:CDL:H532	1.89	0.55
29:N2:131:LEU:O	29:N2:135:LYS:HG2	2.07	0.55
15:B1:28:ASP:OD2	31:N4:3:LYS:NZ	2.38	0.55
15:B1:47:ARG:NH2	15:B1:53:GLU:OE2	2.39	0.55
45:N1:401:CDL:H331	45:N1:401:CDL:H181	1.88	0.55
9:A9:198:ALA:O	9:A9:260:GLY:HA2	2.06	0.55
30:N3:68:GLU:HG3	30:N3:98:LEU:HD13	1.88	0.55
31:N4:394:ILE:HG12	52:N5:706:3PE:H362	1.89	0.55
34:S1:251:ILE:HG21	34:S1:604:GLN:HB3	1.89	0.55
41:S8:142:THR:O	41:S8:187:LYS:NZ	2.39	0.55
42:V1:162:PHE:HB3	42:V1:165:GLU:HB2	1.89	0.55
34:S1:405:THR:HB	34:S1:477:GLY:HA3	1.88	0.55
24:BK:114:GLN:HG3	32:N5:203:MET:HG2	1.89	0.55
28:N1:134:ARG:NH2	35:S2:110:GLU:OE2	2.36	0.55
30:N3:79:SER:HA	30:N3:87:MET:HE2	1.89	0.55
11:AK:210:ASP:OD1	11:AK:244:LYS:NZ	2.34	0.54
24:BK:60:ARG:NH1	24:BK:62:TYR:OH	2.40	0.54
29:N2:170:LEU:HD11	29:N2:288:LEU:HD22	1.90	0.54
45:AK:402:CDL:H342	45:AK:402:CDL:H142	1.89	0.54
31:N4:447:LEU:HD11	51:N4:502:PLX:H381	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:S1:389:THR:HG21	34:S1:473:MET:HE2	1.90	0.54
34:S1:83:GLU:HB2	34:S1:101:ASN:HB3	1.88	0.54
5:A5:48:THR:HA	5:A5:51:ILE:HG12	1.89	0.54
34:S1:493:VAL:HG23	34:S1:513:MET:HE1	1.89	0.54
9:A9:206:ILE:HG13	46:A9:401:NDP:H42N	1.90	0.54
29:N2:280:THR:HG21	47:N4:501:PEE:H19	1.90	0.54
31:N4:196:TRP:CD1	31:N4:250:LEU:HB3	2.43	0.54
33:N6:17:PHE:HA	33:N6:20:PHE:CE2	2.42	0.54
7:A7:62:GLU:OE2	36:S3:44:ARG:NH1	2.37	0.54
17:B3:69:LYS:HZ3	32:N5:371:THR:HB	1.72	0.54
10:AC:105:MET:HE3	10:AC:139:MET:HE1	1.88	0.54
20:B6:147:LYS:HE3	20:B6:148:TYR:CZ	2.43	0.54
34:S1:666:GLN:NE2	34:S1:670:GLU:OE2	2.40	0.54
42:V1:364:VAL:HG12	42:V1:400:VAL:HG12	1.89	0.54
5:A5:44:TYR:O	5:A5:48:THR:HG22	2.08	0.54
43:V2:149:LEU:HD11	43:V2:160:VAL:HG23	1.91	0.53
31:N4:310:MET:HB3	31:N4:455:LEU:HD22	1.89	0.53
35:S2:378:LYS:NZ	39:S6:94:GLY:O	2.37	0.53
33:N6:113:VAL:HG13	33:N6:118:LYS:HG2	1.88	0.53
34:S1:433:GLY:O	34:S1:444:HIS:NE2	2.36	0.53
35:S2:162:GLU:OE2	35:S2:177:ARG:NH2	2.39	0.53
42:V1:138:LEU:HD13	42:V1:245:VAL:HG13	1.90	0.53
4:A3:151:VAL:O	8:A8:207:LYS:NZ	2.29	0.53
19:B5:139:ILE:HG23	31:N4:54:LEU:HD23	1.90	0.53
28:N1:295:PRO:HB3	47:N3:201:PEE:H26	1.90	0.53
45:N4:504:CDL:H362	45:N4:504:CDL:H122	1.90	0.53
32:N5:228:GLY:H	32:N5:230:HIS:HD2	1.56	0.53
35:S2:145:LEU:HD13	35:S2:430:ILE:HG21	1.88	0.53
11:AK:342:SER:O	11:AK:346:ASN:ND2	2.42	0.53
14:AN:98:MET:HE3	14:AN:101:VAL:HG21	1.90	0.53
31:N4:383:THR:HG21	32:N5:190:LEU:HD22	1.91	0.53
32:N5:2:ASN:ND2	32:N5:59:GLN:OE1	2.42	0.53
27:CB:13:LEU:HD21	38:S5:4:PHE:HB3	1.90	0.53
28:N1:154:LEU:HD13	28:N1:160:TYR:HD1	1.73	0.53
28:N1:209:SER:OG	28:N1:212:ASN:OD1	2.26	0.53
32:N5:97:THR:HG21	32:N5:125:LEU:HD22	1.90	0.53
34:S1:688:GLN:HE21	34:S1:694:PHE:HA	1.73	0.53
39:S6:74:GLN:HG3	41:S8:108:SER:HB2	1.90	0.53
11:AK:260:TYR:HB3	11:AK:264:GLU:HB2	1.91	0.53
23:B9:143:GLU:O	23:B9:164:ARG:NH2	2.42	0.53
28:N1:21:THR:HG21	53:N1:403:U10:H28	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:N1:273:ILE:HD13	47:S8:303:PEE:H59	1.91	0.53
29:N2:167:TRP:HB3	32:N5:574:SER:HA	1.91	0.53
31:N4:266:MET:HB3	31:N4:395:LEU:HD13	1.91	0.53
34:S1:43:VAL:HG12	34:S1:55:LYS:HD2	1.91	0.53
8:A8:202:LEU:HD13	14:AN:70:ALA:HB2	1.91	0.53
32:N5:248:HIS:O	32:N5:253:VAL:HG22	2.09	0.53
35:S2:214:GLU:OE2	35:S2:227:ARG:NH2	2.41	0.53
13:AM:75:TRP:HE1	51:AM:201:PLX:H11	1.74	0.53
18:B4:14:LEU:HD12	18:B4:15:PRO:HD2	1.90	0.53
28:N1:58:LYS:NZ	40:S7:101:ASP:OD1	2.31	0.53
1:4L:55:LEU:H	38:S5:25:GLN:HE22	1.57	0.53
32:N5:562:LEU:HB3	32:N5:563:PRO:HD3	1.91	0.53
45:4L:201:CDL:H231	12:AL:41:ILE:HD12	1.90	0.52
31:N4:16:TRP:CE2	45:N4:503:CDL:H272	2.44	0.52
32:N5:293:ILE:HD13	32:N5:418:LEU:HD22	1.91	0.52
35:S2:269:THR:O	35:S2:333:TYR:OH	2.25	0.52
11:AK:82:LYS:HZ2	11:AK:268:ALA:HB3	1.74	0.52
28:N1:281:ARG:NH1	35:S2:452:ASP:OD1	2.42	0.52
29:N2:112:HIS:O	29:N2:116:PRO:HD2	2.08	0.52
32:N5:561:ILE:HG23	47:N5:702:PEE:H61	1.91	0.52
34:S1:387:LEU:HD12	34:S1:514:ASN:HB3	1.90	0.52
34:S1:476:LEU:HD21	34:S1:481:LEU:HD21	1.91	0.52
35:S2:124:2MR:O	40:S7:146:SER:OG	2.18	0.52
35:S2:410:LYS:HE2	35:S2:463:VAL:HG23	1.89	0.52
1:4L:98:CYS:HB3	32:N5:580:GLN:HB2	1.92	0.52
32:N5:15:LEU:HD11	32:N5:94:LEU:HD21	1.90	0.52
34:S1:389:THR:OG1	34:S1:511:LYS:O	2.26	0.52
34:S1:593:SER:HA	34:S1:606:THR:O	2.10	0.52
45:4L:201:CDL:H181	32:N5:589:LEU:HD11	1.92	0.52
24:BK:115:GLN:HG2	32:N5:62:ILE:HG12	1.91	0.52
30:N3:56:PHE:O	33:N6:70:TYR:OH	2.27	0.52
28:N1:139:THR:HA	28:N1:142:TYR:CE2	2.44	0.52
28:N1:25:ARG:HD3	28:N1:37:PRO:HG2	1.90	0.52
31:N4:233:ALA:HA	31:N4:320:GLY:HA2	1.91	0.52
33:N6:124:ASP:OD1	33:N6:124:ASP:N	2.42	0.52
28:N1:18:ALA:HB1	28:N1:48:PRO:HB3	1.91	0.52
42:V1:94:PRO:HB2	42:V1:97:LEU:HB2	1.91	0.52
44:V3:386:TYR:CZ	44:V3:388:ASN:HB3	2.44	0.52
1:4L:37:MET:HG2	1:4L:67:ALA:CB	2.36	0.52
45:AL:201:CDL:H401	45:AL:201:CDL:H771	1.92	0.52
28:N1:288:LEU:HD11	47:S8:303:PEE:H8	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:V1:295:PRO:HG2	42:V1:298:GLU:HB2	1.92	0.52
28:N1:34:ARG:HG2	40:S7:82:PRO:HA	1.92	0.52
28:N1:58:LYS:HE2	40:S7:125:PRO:HG2	1.92	0.51
32:N5:119:LYS:NZ	45:N5:703:CDL:OA3	2.35	0.51
30:N3:30:TYR:OH	40:S7:128:ARG:NH2	2.34	0.51
31:N4:382:ILE:HG12	31:N4:396:MET:HG3	1.92	0.51
11:AK:232:THR:HG23	11:AK:235:TYR:H	1.75	0.51
21:B7:103:GLU:O	21:B7:107:ARG:HG2	2.10	0.51
34:S1:128:CYS:SG	34:S1:140:GLN:NE2	2.83	0.51
11:AK:213:VAL:HG12	11:AK:217:GLN:HE21	1.75	0.51
35:S2:321:GLU:O	35:S2:352:GLN:NE2	2.42	0.51
3:A2:18:GLU:HG2	3:A2:68:ARG:HB3	1.92	0.51
35:S2:129:LEU:O	35:S2:133:LYS:HG2	2.11	0.51
37:S4:112:MET:HG3	41:S8:184:LEU:HD23	1.91	0.51
13:AM:44:TYR:OH	13:AM:113:HIS:N	2.35	0.51
40:S7:69:LEU:HB2	40:S7:107:GLY:HA3	1.93	0.51
1:4L:73:LEU:HD21	29:N2:41:ILE:HG13	1.93	0.51
11:AK:327:ASP:OD1	31:N4:91:ARG:NH2	2.39	0.51
28:N1:61:LEU:HD23	40:S7:125:PRO:HB3	1.93	0.51
30:N3:33:LYS:O	40:S7:98:ARG:NH1	2.38	0.51
31:N4:12:LEU:HB2	31:N4:13:PRO:HD3	1.92	0.51
9:A9:293:LEU:HD12	9:A9:294:PRO:HD2	1.93	0.51
35:S2:140:PRO:HB2	40:S7:142:TYR:CE2	2.46	0.51
35:S2:194:THR:HB	35:S2:206:PHE:HA	1.93	0.51
28:N1:24:GLU:HA	28:N1:271:LEU:HD13	1.93	0.51
34:S1:408:ARG:HD2	34:S1:439:THR:HG23	1.92	0.51
35:S2:101:LEU:HB2	35:S2:464:PHE:CZ	2.45	0.51
14:AN:49:SER:HB2	28:N1:172:ILE:HD13	1.93	0.51
18:B4:107:THR:HG22	18:B4:111:LYS:HE2	1.93	0.51
34:S1:338:VAL:HB	34:S1:363:SER:HB2	1.92	0.50
35:S2:230:ALA:O	41:S8:98:ARG:NH2	2.43	0.50
43:V2:85:LEU:HD13	44:V3:400:LEU:HD22	1.92	0.50
32:N5:6:SER:O	32:N5:10:THR:OG1	2.21	0.50
20:B6:165:PHE:O	20:B6:168:ASP:HB2	2.12	0.50
28:N1:309:ILE:HD11	30:N3:87:MET:HE1	1.94	0.50
29:N2:20:VAL:HG13	29:N2:29:ILE:HG23	1.94	0.50
40:S7:84:TYR:CE1	40:S7:171:GLU:HG3	2.46	0.50
8:A8:201:GLU:HA	8:A8:204:LYS:HD3	1.93	0.50
20:B6:164:ILE:HB	21:B7:48:ASP:HB3	1.92	0.50
34:S1:274:LEU:HD21	37:S4:87:MET:HE2	1.94	0.50
43:V2:155:LYS:NZ	43:V2:206:ASP:OD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A8:115:LYS:HB3	8:A8:116:PRO:HD3	1.94	0.50
8:A8:174:PHE:HB3	8:A8:178:ARG:HH12	1.75	0.50
28:N1:113:VAL:HG13	28:N1:139:THR:HG21	1.94	0.50
32:N5:399:VAL:HG12	32:N5:409:LEU:HD13	1.93	0.50
1:4L:75:LEU:O	1:4L:79:VAL:HG13	2.12	0.50
16:B2:65:THR:HB	16:B2:68:GLN:HG2	1.93	0.50
16:B2:90:ASP:N	16:B2:90:ASP:OD1	2.44	0.50
21:B7:17:PRO:HB3	21:B7:105:GLU:HG2	1.93	0.50
25:BL:89:VAL:HG21	31:N4:25:ILE:HG23	1.93	0.50
31:N4:119:TYR:CZ	31:N4:161:LEU:HB2	2.47	0.50
34:S1:251:ILE:HD13	34:S1:604:GLN:HB2	1.93	0.50
45:4L:201:CDL:HA61	12:AL:49:PHE:HA	1.93	0.50
4:A3:163:LEU:HD23	4:A3:166:LEU:HD23	1.94	0.50
20:B6:143:HIS:HD2	24:BK:45:VAL:HG21	1.76	0.50
43:V2:93:LEU:HD12	43:V2:122:TYR:HB3	1.94	0.50
25:BL:150:PRO:HG3	27:CB:115:LEU:HD22	1.93	0.50
28:N1:32:GLN:HG2	35:S2:204:THR:HG23	1.92	0.50
31:N4:267:TRP:O	31:N4:271:MET:HG2	2.12	0.50
42:V1:325:PRO:HG3	42:V1:433:TRP:HB3	1.92	0.50
19:B5:71:MET:HE3	31:N4:442:LEU:HD11	1.94	0.49
29:N2:26:TRP:HB3	29:N2:74:ILE:HD13	1.94	0.49
30:N3:66:ASP:O	30:N3:69:ILE:HG13	2.12	0.49
8:A8:246:PHE:HE1	45:A8:301:CDL:H341	1.77	0.49
10:AC:117:GLU:OE2	23:B9:62:TYR:OH	2.29	0.49
21:B7:107:ARG:HA	21:B7:110:GLN:HG2	1.94	0.49
36:S3:89:HIS:CG	36:S3:90:PRO:HD2	2.48	0.49
9:A9:64:PHE:O	9:A9:67:ARG:HG2	2.12	0.49
11:AK:297:ARG:HA	11:AK:300:VAL:HG22	1.94	0.49
45:AK:402:CDL:H382	29:N2:133:TRP:HZ3	1.77	0.49
45:B5:201:CDL:H822	31:N4:442:LEU:HD22	1.93	0.49
20:B6:143:HIS:CD2	24:BK:45:VAL:HG21	2.47	0.49
36:S3:132:LEU:HB2	36:S3:141:ILE:HG22	1.93	0.49
12:AL:32:THR:HG23	45:AL:201:CDL:H781	1.94	0.49
25:BL:72:ASP:OD1	25:BL:72:ASP:N	2.35	0.49
32:N5:421:ALA:O	32:N5:424:THR:OG1	2.27	0.49
9:A9:220:MET:HG2	47:A9:402:PEE:H17	1.95	0.49
10:AC:112:SER:HB2	23:B9:59:LEU:HD21	1.94	0.49
20:B6:85:ASP:O	23:B9:163:LYS:NZ	2.45	0.49
27:CB:36:MET:HE1	51:CB:201:PLX:H393	1.95	0.49
31:N4:408:LEU:HD12	32:N5:172:ILE:HG21	1.94	0.49
35:S2:167:ILE:HD13	35:S2:369:VAL:HG11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A9:223:PHE:HB3	47:A9:402:PEE:H28	1.95	0.49
14:AN:85:GLN:OE1	38:S5:105:ARG:NH1	2.39	0.49
35:S2:149:SER:HA	35:S2:184:THR:HG22	1.95	0.49
41:S8:100:GLU:O	41:S8:170:GLY:N	2.36	0.49
8:A8:160:THR:HA	8:A8:163:TRP:CD1	2.47	0.49
11:AK:168:ASP:OD2	11:AK:189:TYR:OH	2.30	0.49
16:B2:101:PRO:HD2	21:B7:99:MET:HE1	1.95	0.49
29:N2:42:PRO:HG3	33:N6:167:VAL:HG13	1.94	0.49
31:N4:369:LEU:HD23	45:N5:703:CDL:H362	1.95	0.49
34:S1:262:VAL:HG23	34:S1:276:ARG:HB2	1.95	0.49
35:S2:418:VAL:HB	35:S2:427:ARG:HB3	1.94	0.49
34:S1:49:VAL:HG13	34:S1:102:ILE:HD13	1.94	0.49
42:V1:288:VAL:HG21	42:V1:303:HIS:CD2	2.47	0.49
12:AL:67:GLY:HA2	45:AL:201:CDL:H221	1.93	0.49
31:N4:70:THR:HA	31:N4:103:GLN:HE21	1.77	0.49
35:S2:412:GLU:OE2	36:S3:140:ARG:NH2	2.46	0.49
1:4L:35:GLY:HA3	33:N6:20:PHE:CZ	2.48	0.49
2:A1:69:ILE:HG23	8:A8:97:VAL:HG13	1.94	0.49
8:A8:196:ARG:NH2	14:AN:63:GLU:OE2	2.45	0.49
33:N6:82:VAL:HG12	33:N6:85:SER:HB2	1.95	0.49
35:S2:296:GLY:HA2	35:S2:300:ARG:HH21	1.77	0.49
32:N5:530:PRO:O	32:N5:534:HIS:HB2	2.12	0.48
32:N5:559:GLU:O	32:N5:564:LYS:HB2	2.13	0.48
34:S1:307:ILE:HG23	34:S1:317:THR:HG21	1.94	0.48
34:S1:426:ASP:OD2	44:V3:418:ARG:NH2	2.46	0.48
37:S4:130:THR:HG22	37:S4:132:GLU:H	1.77	0.48
43:V2:59:ASN:OD1	43:V2:62:ARG:NH1	2.46	0.48
20:B6:89:SER:HB2	20:B6:92:GLU:HB2	1.95	0.48
32:N5:536:LEU:HB3	32:N5:537:PRO:HD3	1.96	0.48
34:S1:149:ASP:OD2	34:S1:150:ARG:NH2	2.46	0.48
35:S2:137:GLN:O	40:S7:142:TYR:OH	2.31	0.48
37:S4:112:MET:O	41:S8:144:ARG:NH1	2.42	0.48
42:V1:110:PRO:HB3	42:V1:152:ARG:HD3	1.94	0.48
42:V1:118:ASP:HB3	42:V1:207:GLY:HA2	1.93	0.48
45:4L:201:CDL:H252	12:AL:38:ALA:HB2	1.95	0.48
29:N2:211:MET:HG2	29:N2:333:SER:HB2	1.96	0.48
31:N4:216:LEU:HB3	31:N4:217:PRO:HD3	1.94	0.48
34:S1:217:GLU:HG3	34:S1:412:PRO:HB3	1.94	0.48
35:S2:227:ARG:NH1	40:S7:75:GLU:OE1	2.46	0.48
32:N5:369:THR:OG1	32:N5:445:GLU:OE1	2.29	0.48
35:S2:190:ILE:HG23	35:S2:209:MET:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S2:190:ILE:HG21	35:S2:213:ARG:HG3	1.95	0.48
28:N1:213:VAL:HG13	28:N1:214:GLU:HG2	1.95	0.48
32:N5:241:THR:HG21	32:N5:344:GLY:HA3	1.95	0.48
32:N5:383:MET:O	32:N5:389:PHE:HB2	2.14	0.48
35:S2:391:TYR:HD1	41:S8:122:VAL:HG21	1.78	0.48
36:S3:145:THR:OG1	36:S3:146:TYR:N	2.47	0.48
11:AK:141:ARG:NH2	50:AK:401:ADP:N7	2.61	0.48
31:N4:211:GLY:H	31:N4:213:HIS:HD2	1.62	0.48
42:V1:357:MET:HB3	42:V1:361:THR:HG21	1.95	0.48
7:A7:39:PRO:HG3	41:S8:211:TYR:CZ	2.49	0.48
8:A8:85:PRO:HG2	14:AN:84:LEU:HD13	1.95	0.48
28:N1:90:PRO:HB3	28:N1:94:PRO:HD3	1.96	0.48
28:N1:146:LEU:HG	28:N1:188:SER:HB3	1.96	0.48
42:V1:384:PRO:HG2	42:V1:422:HIS:O	2.13	0.48
36:S3:118:ASP:OD2	36:S3:125:ARG:NH2	2.44	0.48
45:A8:301:CDL:H381	29:N2:256:PRO:HB2	1.96	0.48
11:AK:355:TRP:H	11:AK:355:TRP:CD1	2.32	0.48
45:B5:201:CDL:H672	51:N4:502:PLX:H181	1.94	0.48
27:CB:52:ARG:NH1	29:N2:318:GLU:OE1	2.46	0.48
28:N1:154:LEU:HD13	28:N1:160:TYR:CD1	2.48	0.48
32:N5:290:LEU:O	32:N5:523:SER:OG	2.31	0.48
32:N5:400:ASN:HB3	32:N5:486:MET:HE3	1.96	0.48
44:V3:420:SER:HB3	44:V3:423:HIS:ND1	2.29	0.48
53:N1:403:U10:H3M3	35:S2:95:PRO:HA	1.95	0.47
30:N3:30:TYR:HH	40:S7:128:ARG:HH22	1.58	0.47
34:S1:449:PRO:HB2	34:S1:679:LEU:HD13	1.96	0.47
35:S2:187:LEU:HD23	35:S2:213:ARG:HG2	1.96	0.47
31:N4:221:VAL:HA	31:N4:283:LYS:HD3	1.96	0.47
51:N6:201:PLX:H22	51:N6:201:PLX:H1C2	1.63	0.47
34:S1:394:VAL:HA	34:S1:473:MET:HE1	1.96	0.47
36:S3:119:VAL:HG12	36:S3:121:THR:HG22	1.96	0.47
40:S7:59:ARG:HG3	40:S7:181:GLN:HB3	1.96	0.47
6:A6:78:LEU:HD23	6:A6:126:ARG:HD3	1.97	0.47
9:A9:217:PHE:HA	9:A9:220:MET:HE2	1.97	0.47
19:B5:53:ARG:NH2	20:B6:89:SER:O	2.47	0.47
19:B5:75:ILE:HD12	45:B5:201:CDL:H871	1.97	0.47
32:N5:331:MET:HB3	32:N5:387:THR:HG22	1.97	0.47
34:S1:185:PHE:CZ	34:S1:221:ASN:HB2	2.49	0.47
12:AL:81:ARG:HH11	12:AL:89:ASN:HD21	1.63	0.47
17:B3:33:GLN:NE2	17:B3:43:ASP:OD1	2.47	0.47
31:N4:76:MET:SD	31:N4:230:VAL:HB	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:N4:375:LEU:HD11	32:N5:141:PHE:HE2	1.79	0.47
34:S1:512:VAL:O	34:S1:514:ASN:ND2	2.48	0.47
39:S6:36:GLU:OE2	39:S6:60:LYS:NZ	2.37	0.47
45:AL:201:CDL:H532	32:N5:577:VAL:HG22	1.96	0.47
32:N5:190:LEU:HB2	32:N5:196:TRP:NE1	2.30	0.47
34:S1:338:VAL:HB	34:S1:363:SER:CB	2.44	0.47
41:S8:75:SER:O	41:S8:79:ARG:HG3	2.15	0.47
41:S8:150:THR:HG21	41:S8:180:HIS:CD2	2.49	0.47
8:A8:86:THR:OG1	8:A8:88:GLU:OE1	2.26	0.47
11:AK:342:SER:HB2	11:AK:345:TYR:HD2	1.79	0.47
21:B7:103:GLU:OE2	21:B7:106:ARG:NH2	2.41	0.47
29:N2:36:ASN:OD1	29:N2:134:GLN:NE2	2.33	0.47
29:N2:291:TYR:HD2	31:N4:151:PHE:CE2	2.31	0.47
34:S1:49:VAL:HG11	34:S1:80:VAL:HG21	1.97	0.47
40:S7:88:ARG:HD2	41:S8:83:THR:HG21	1.95	0.47
6:A6:66:TYR:CE2	6:A6:86:ARG:HD3	2.50	0.47
22:B8:78:LEU:HD11	22:B8:104:PRO:HB2	1.97	0.47
45:A8:301:CDL:H372	29:N2:337:LEU:HD23	1.96	0.47
9:A9:129:LEU:HD23	9:A9:167:ILE:HG13	1.96	0.47
49:AC:201:ZMP:H22	49:AC:201:ZMP:H25B	1.49	0.47
14:AN:68:ARG:O	14:AN:72:MET:HG3	2.15	0.47
14:AN:93:GLU:HG3	38:S5:98:HIS:CD2	2.49	0.47
16:B2:79:MET:SD	32:N5:375:ILE:HG12	2.55	0.47
43:V2:111:ARG:NH1	43:V2:114:GLU:OE2	2.48	0.47
13:AM:139:PRO:HG3	34:S1:306:MET:HE1	1.95	0.47
34:S1:556:THR:OG1	34:S1:557:ARG:N	2.48	0.47
42:V1:141:GLY:HA2	42:V1:252:PRO:HD3	1.97	0.47
45:A8:301:CDL:H192	27:CB:34:VAL:HG12	1.97	0.46
11:AK:316:LEU:HB2	11:AK:319:ILE:HG12	1.96	0.46
29:N2:139:LEU:HD13	29:N2:190:MET:HE1	1.97	0.46
32:N5:96:VAL:O	32:N5:100:ILE:HG12	2.15	0.46
32:N5:295:GLN:HB2	32:N5:301:ILE:HG12	1.97	0.46
34:S1:240:ALA:HB2	34:S1:271:MET:HE2	1.96	0.46
41:S8:153:ILE:HG12	54:S8:302:SF4:S1	2.55	0.46
8:A8:160:THR:HA	8:A8:163:TRP:NE1	2.30	0.46
10:AC:94:ASP:HB3	10:AC:97:LYS:HG2	1.97	0.46
52:CA:101:3PE:H292	52:CA:101:3PE:H2D2	1.97	0.46
34:S1:144:MET:HG3	35:S2:389:LYS:HG3	1.96	0.46
34:S1:296:GLY:O	34:S1:572:HIS:NE2	2.38	0.46
35:S2:194:THR:HG21	35:S2:209:MET:HB2	1.97	0.46
11:AK:37:ARG:C	11:AK:39:GLN:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AN:121:MET:HG3	33:N6:128:TYR:HB2	1.98	0.46
20:B6:159:GLU:HG3	32:N5:61:MET:HG2	1.97	0.46
34:S1:70:SER:O	34:S1:184:ARG:NH1	2.48	0.46
1:4L:76:SER:O	1:4L:79:VAL:HG22	2.15	0.46
4:A3:135:PRO:HB2	14:AN:69:ILE:HD11	1.97	0.46
48:A9:403:PC1:H3I2	47:N1:404:PEE:H57	1.98	0.46
23:B9:120:GLN:OE1	32:N5:296:ASN:ND2	2.46	0.46
41:S8:63:TRP:HB3	41:S8:66:LEU:HD12	1.98	0.46
5:A5:59:VAL:HG23	5:A5:68:LEU:HD21	1.96	0.46
53:N1:403:U10:H303	40:S7:63:TRP:HH2	1.81	0.46
31:N4:210:TYR:CG	31:N4:268:GLY:HA3	2.51	0.46
1:4L:32:CYS:HA	33:N6:20:PHE:HE1	1.81	0.46
13:AM:55:PHE:CE1	13:AM:58:ARG:HG3	2.51	0.46
45:B5:201:CDL:H251	45:B5:201:CDL:H211	1.97	0.46
28:N1:289:LEU:HA	28:N1:293:PHE:HB2	1.97	0.46
34:S1:592:LYS:NZ	34:S1:619:ASP:OD2	2.37	0.46
42:V1:129:GLU:OE2	42:V1:132:ARG:NH2	2.49	0.46
27:CB:51:ARG:CZ	29:N2:322:GLN:HG2	2.46	0.46
32:N5:162:THR:O	32:N5:166:THR:HG23	2.16	0.46
34:S1:534:VAL:HG23	34:S1:537:ILE:HD12	1.98	0.46
35:S2:341:GLU:O	35:S2:345:GLN:HG2	2.16	0.46
35:S2:363:LYS:HD3	35:S2:370:SER:HB2	1.97	0.46
10:AC:85:TYR:OH	17:B3:17:PRO:O	2.29	0.46
11:AK:97:ASP:N	11:AK:97:ASP:OD1	2.48	0.46
51:AL:202:PLX:H1A2	51:AL:202:PLX:H21	1.59	0.46
26:CA:55:TRP:O	26:CA:59:ILE:HG12	2.15	0.46
51:CB:201:PLX:H271	51:CB:201:PLX:H302	1.71	0.46
28:N1:160:TYR:OH	30:N3:73:LEU:O	2.34	0.46
29:N2:287:LEU:HD12	47:S2:501:PEE:H64	1.98	0.46
31:N4:79:ALA:O	31:N4:82:SER:HB3	2.16	0.46
34:S1:347:ASP:OD1	34:S1:347:ASP:N	2.47	0.46
20:B6:148:TYR:CE1	24:BK:49:ARG:HG2	2.51	0.46
29:N2:197:ASN:HB2	29:N2:269:GLU:HG2	1.98	0.46
32:N5:327:LEU:O	32:N5:331:MET:HG2	2.16	0.46
35:S2:184:THR:OG1	35:S2:220:TYR:OH	2.31	0.46
40:S7:109:LEU:HD13	40:S7:117:LEU:HD13	1.97	0.46
27:CB:15:PHE:O	27:CB:80:ARG:NH1	2.48	0.45
28:N1:296:LEU:HD13	47:S8:303:PEE:H19	1.98	0.45
34:S1:124:HIS:CG	34:S1:125:PRO:HD2	2.51	0.45
34:S1:219:SER:O	34:S1:222:ILE:HG12	2.16	0.45
34:S1:123:ASN:ND2	42:V1:387:GLU:OE1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:S1:130:ILE:HG23	41:S8:114:ILE:HD12	1.99	0.45
35:S2:405:ALA:HB1	35:S2:412:GLU:HG3	1.98	0.45
42:V1:141:GLY:HA3	42:V1:248:VAL:O	2.16	0.45
7:A7:54:TYR:CZ	35:S2:368:LYS:HD2	2.52	0.45
11:AK:38:LEU:O	11:AK:39:GLN:HG2	2.16	0.45
11:AK:51:THR:HG21	11:AK:153:LEU:HD22	1.98	0.45
32:N5:375:ILE:HD12	32:N5:458:LEU:HD11	1.98	0.45
42:V1:201:ALA:HB3	43:V2:119:TYR:CD1	2.51	0.45
42:V1:412:LEU:HD12	42:V1:415:ILE:HD11	1.98	0.45
6:A6:127:THR:HG23	36:S3:219:VAL:O	2.17	0.45
11:AK:110:LEU:HD21	11:AK:332:LYS:HD3	1.97	0.45
51:AM:201:PLX:H82	51:S7:302:PLX:H72	1.99	0.45
47:N1:404:PEE:H55	30:N3:19:LEU:HD11	1.99	0.45
29:N2:111:PHE:HA	32:N5:591:PHE:CE1	2.51	0.45
32:N5:174:TYR:HD2	32:N5:232:TRP:HB3	1.81	0.45
34:S1:222:ILE:HA	34:S1:225:ILE:HG12	1.98	0.45
34:S1:476:LEU:HD22	34:S1:493:VAL:HG21	1.99	0.45
35:S2:309:ARG:HG3	35:S2:407:GLU:HB3	1.99	0.45
52:S7:303:3PE:H342	52:S7:303:3PE:H281	1.96	0.45
1:4L:62:ILE:HG21	29:N2:31:ILE:HD11	1.99	0.45
11:AK:328:ARG:HH21	25:BL:58:ASP:CG	2.24	0.45
17:B3:47:ARG:HA	17:B3:50:ALA:HB3	1.97	0.45
53:N1:403:U10:H303	40:S7:63:TRP:CH2	2.52	0.45
32:N5:285:THR:HA	32:N5:308:SER:HA	1.98	0.45
35:S2:98:HIS:HB2	35:S2:464:PHE:HE2	1.81	0.45
15:B1:17:VAL:HG13	31:N4:7:PRO:HB3	1.97	0.45
28:N1:180:PRO:HB3	47:S8:303:PEE:H21	1.97	0.45
31:N4:197:LEU:HB3	47:N4:501:PEE:H29	1.98	0.45
34:S1:538:ARG:HG2	34:S1:555:ILE:HD11	1.99	0.45
34:S1:541:PRO:HB3	34:S1:561:PRO:HD3	1.98	0.45
37:S4:84:ARG:NH1	37:S4:88:GLN:O	2.49	0.45
2:A1:40:HIS:N	2:A1:44:GLN:OE1	2.50	0.45
4:A3:160:GLY:HA3	8:A8:204:LYS:HE3	1.98	0.45
45:AK:402:CDL:H162	45:AK:402:CDL:H361	1.98	0.45
24:BK:141:ASP:O	24:BK:162:ARG:NH2	2.50	0.45
31:N4:232:ALA:O	31:N4:237:LYS:NZ	2.50	0.45
31:N4:282:LEU:HD11	31:N4:410:MET:HG3	1.99	0.45
32:N5:49:VAL:HB	32:N5:50:PRO:HD3	1.99	0.45
36:S3:157:VAL:HG21	36:S3:182:PRO:HD3	1.98	0.45
40:S7:108:THR:HA	40:S7:136:CYS:HB3	1.99	0.45
42:V1:131:ILE:HD13	42:V1:158:ILE:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BL:109:LEU:HD22	31:N4:43:ASN:HB2	1.98	0.45
45:N1:401:CDL:H752	45:N1:401:CDL:H532	1.99	0.45
31:N4:201:MET:HE1	31:N4:212:LEU:HD11	1.98	0.45
31:N4:347:GLY:O	31:N4:350:THR:HG22	2.16	0.45
34:S1:169:VAL:HG22	34:S1:223:ILE:HD11	1.98	0.45
11:AK:253:GLU:O	11:AK:282:LYS:NZ	2.48	0.45
29:N2:235:ASN:O	29:N2:315:TRP:NE1	2.48	0.45
32:N5:292:ALA:HB2	32:N5:304:PHE:HB3	1.99	0.45
34:S1:484:SER:HB2	34:S1:680:LEU:HD11	1.99	0.45
1:4L:4:VAL:O	1:4L:8:ILE:HG12	2.17	0.45
13:AM:34:ARG:HH12	13:AM:58:ARG:HB3	1.82	0.45
33:N6:24:PRO:HG3	33:N6:83:TRP:CE2	2.51	0.45
34:S1:161:GLU:OE2	43:V2:42:ARG:NH1	2.50	0.45
39:S6:67:ALA:HB2	41:S8:111:GLU:HG3	1.99	0.45
42:V1:119:GLU:HA	59:V1:502:FMN:HM71	1.99	0.45
7:A7:113:LEU:HD12	41:S8:41:VAL:HA	1.99	0.44
16:B2:57:ARG:NH1	16:B2:61:PHE:O	2.50	0.44
30:N3:65:PHE:O	30:N3:69:ILE:HG23	2.17	0.44
32:N5:298:ILE:O	32:N5:302:VAL:HG23	2.16	0.44
32:N5:332:HIS:HA	32:N5:335:PHE:CZ	2.52	0.44
35:S2:190:ILE:HD11	35:S2:257:PHE:CZ	2.53	0.44
10:AB:104:PHE:HD1	10:AB:108:LEU:HD12	1.81	0.44
51:CB:201:PLX:H131	51:CB:201:PLX:H101	1.75	0.44
31:N4:176:PHE:HA	31:N4:179:ILE:HG12	1.98	0.44
42:V1:347:THR:HG22	42:V1:348:GLY:H	1.83	0.44
2:A1:19:PRO:HB3	28:N1:9:LEU:HD12	1.98	0.44
7:A7:28:TYR:CZ	13:AM:55:PHE:HB3	2.52	0.44
9:A9:246:SER:O	9:A9:250:ILE:HG12	2.17	0.44
10:AB:93:ILE:HD12	10:AB:108:LEU:HD13	1.99	0.44
13:AM:55:PHE:CZ	13:AM:58:ARG:HG3	2.52	0.44
20:B6:140:TRP:HD1	24:BK:41:VAL:HG13	1.83	0.44
22:B8:81:ARG:NH1	22:B8:85:GLU:OE1	2.43	0.44
31:N4:357:THR:O	31:N4:361:VAL:HG23	2.18	0.44
32:N5:592:LEU:HD11	32:N5:596:MET:HE3	1.98	0.44
9:A9:279:TYR:HB2	9:A9:372:ALA:HB2	2.00	0.44
11:AK:39:GLN:HE21	11:AK:39:GLN:HA	1.83	0.44
26:CA:47:THR:HG23	27:CB:65:LEU:HD22	1.99	0.44
31:N4:122:PHE:HE2	31:N4:206:LYS:HG3	1.83	0.44
32:N5:566:THR:O	32:N5:570:GLN:HG2	2.17	0.44
34:S1:224:ASP:OD2	34:S1:291:ARG:NH2	2.48	0.44
34:S1:575:VAL:C	34:S1:578:PRO:HD2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:V1:326:LEU:HD22	42:V1:363:ILE:HD11	1.98	0.44
32:N5:213:LEU:HB3	32:N5:273:VAL:HG11	2.00	0.44
47:N5:705:PEE:H54	47:N5:705:PEE:H48	1.75	0.44
43:V2:137:THR:HG22	43:V2:138:THR:H	1.82	0.44
13:AM:58:ARG:HD2	41:S8:89:GLU:OE1	2.18	0.44
28:N1:14:LEU:HB3	53:N1:403:U10:H412	2.00	0.44
29:N2:25:HIS:HB2	38:S5:15:ASP:HB2	2.00	0.44
31:N4:412:ILE:HG12	31:N4:416:ARG:HD2	1.99	0.44
45:N4:503:CDL:OB9	45:N4:503:CDL:O1	2.33	0.44
35:S2:299:LEU:HD22	35:S2:304:ILE:HD12	2.00	0.44
35:S2:430:ILE:HB	35:S2:469:ARG:HD2	1.98	0.44
47:S2:501:PEE:H76	47:S2:501:PEE:H71	1.70	0.44
23:B9:166:GLN:HG2	23:B9:169:ARG:HH22	1.82	0.44
24:BK:33:LEU:HD13	32:N5:49:VAL:HG13	2.00	0.44
28:N1:117:LEU:HD11	33:N6:65:LEU:HD12	1.99	0.44
28:N1:233:MET:HE3	28:N1:233:MET:HB3	1.87	0.44
29:N2:217:MET:HE2	29:N2:326:LEU:HB2	2.00	0.44
31:N4:82:SER:HB2	31:N4:432:ARG:NH1	2.33	0.44
31:N4:282:LEU:HD13	31:N4:342:MET:HG3	1.99	0.44
35:S2:150:MET:SD	35:S2:228:MET:HB2	2.57	0.44
8:A8:157:GLU:HB2	8:A8:158:PRO:HD3	2.00	0.44
47:N3:201:PEE:H22	47:N3:201:PEE:H27	1.66	0.44
35:S2:146:ASP:OD2	35:S2:149:SER:OG	2.35	0.44
8:A8:246:PHE:HD2	31:N4:116:ILE:HG23	1.82	0.44
28:N1:138:GLN:HG3	28:N1:285:LEU:HD21	2.00	0.44
28:N1:301:CYS:O	28:N1:305:ILE:HG13	2.18	0.44
31:N4:231:LEU:HD23	31:N4:235:LEU:HD12	1.99	0.44
45:N4:503:CDL:H422	45:N4:503:CDL:H812	2.00	0.44
32:N5:11:THR:HG22	32:N5:46:LEU:HB3	1.99	0.44
34:S1:191:GLY:HA3	34:S1:439:THR:HB	2.00	0.44
42:V1:118:ASP:HA	42:V1:159:ARG:HB3	2.00	0.44
49:AB:201:ZMP:H25A	49:AB:201:ZMP:H22	1.74	0.43
15:B1:30:ARG:O	15:B1:33:GLU:HG2	2.18	0.43
20:B6:82:TRP:O	20:B6:86:GLN:HG2	2.18	0.43
23:B9:70:GLU:OE2	23:B9:76:ARG:NH1	2.42	0.43
53:N1:403:U10:H171	53:N1:403:U10:H151	1.52	0.43
29:N2:193:VAL:HG21	29:N2:266:ILE:HG12	2.00	0.43
31:N4:398:MET:O	31:N4:402:ILE:HG13	2.17	0.43
2:A1:52:ARG:NH1	2:A1:58:ASN:OD1	2.50	0.43
11:AK:215:GLU:HG3	11:AK:219:ARG:HD2	1.98	0.43
20:B6:132:VAL:O	20:B6:136:LEU:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B7:92:HIS:O	21:B7:96:VAL:HG13	2.18	0.43
25:BL:77:ASP:OD1	25:BL:78:LYS:N	2.51	0.43
27:CB:13:LEU:HD11	38:S5:6:VAL:HG12	2.00	0.43
29:N2:149:ILE:HD13	29:N2:154:MET:HE3	2.00	0.43
47:N4:501:PEE:H15	47:N4:501:PEE:H8	2.00	0.43
32:N5:297:ASP:O	32:N5:301:ILE:HG13	2.19	0.43
32:N5:341:MET:SD	32:N5:457:LEU:HD12	2.57	0.43
34:S1:131:CYS:O	34:S1:241:ARG:NH1	2.34	0.43
35:S2:160:ALA:HA	35:S2:404:THR:HG21	2.00	0.43
35:S2:203:MET:O	35:S2:206:PHE:HB3	2.18	0.43
42:V1:112:TYR:CD1	42:V1:153:ALA:HB3	2.53	0.43
43:V2:137:THR:O	43:V2:141:MET:N	2.47	0.43
21:B7:4:HIS:NE2	22:B8:155:PRO:HD3	2.33	0.43
45:N1:401:CDL:H791	33:N6:16:GLY:HA2	2.01	0.43
31:N4:203:PHE:CE1	31:N4:242:GLY:HA3	2.54	0.43
33:N6:39:VAL:O	33:N6:43:ILE:HG13	2.19	0.43
36:S3:209:GLU:OE1	40:S7:151:ARG:NH1	2.51	0.43
43:V2:152:ILE:HG21	43:V2:171:LEU:HD13	2.00	0.43
51:CB:201:PLX:H22	51:CB:201:PLX:H1C3	1.72	0.43
29:N2:59:TYR:O	29:N2:63:GLN:HG2	2.19	0.43
34:S1:372:PHE:H	34:S1:532:PRO:HB2	1.83	0.43
42:V1:85:LEU:HD21	42:V1:247:THR:HG23	2.00	0.43
43:V2:224:SER:OG	43:V2:226:GLU:OE1	2.31	0.43
45:A7:201:CDL:HA61	45:A7:201:CDL:H521	2.00	0.43
9:A9:310:PHE:CE2	48:A9:403:PC1:H11	2.53	0.43
11:AK:49:GLU:OE2	11:AK:54:LYS:NZ	2.49	0.43
13:AM:109:ILE:HG12	41:S8:198:GLU:HB3	1.99	0.43
28:N1:205:SER:HB2	28:N1:279:ARG:HH12	1.83	0.43
29:N2:137:ALA:HB3	29:N2:138:PRO:HD3	2.01	0.43
33:N6:28:TYR:HB3	33:N6:83:TRP:CH2	2.54	0.43
42:V1:161:GLU:HG2	43:V2:177:LEU:HD22	1.99	0.43
1:4L:55:LEU:HD23	1:4L:55:LEU:HA	1.87	0.43
5:A5:112:TRP:CE2	36:S3:87:PHE:HB3	2.54	0.43
10:AC:90:TYR:CE1	17:B3:44:PRO:HB2	2.54	0.43
13:AM:122:GLN:HA	39:S6:59:GLN:HG2	2.00	0.43
25:BL:106:VAL:HG13	31:N4:453:MET:HE3	1.99	0.43
34:S1:246:ARG:HH12	37:S4:123:ASN:HD22	1.67	0.43
41:S8:153:ILE:HG13	41:S8:155:CYS:HB3	1.99	0.43
1:4L:56:ALA:HA	38:S5:18:MET:HE3	2.00	0.43
10:AC:140:CYS:HB3	10:AC:143:GLU:HG3	2.01	0.43
12:AL:107:SER:HB3	12:AL:110:ILE:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B8:162:PRO:HB2	22:B8:163:TYR:CD2	2.53	0.43
28:N1:113:VAL:O	28:N1:116:ILE:HG12	2.19	0.43
28:N1:288:LEU:O	28:N1:292:SER:HB2	2.19	0.43
34:S1:611:THR:HG21	37:S4:105:GLU:HA	2.01	0.43
9:A9:126:VAL:HG23	9:A9:161:VAL:HG11	2.01	0.43
51:AM:201:PLX:H271	51:S7:302:PLX:H111	2.00	0.43
28:N1:59:GLU:HG3	30:N3:27:LEU:HD13	2.00	0.43
32:N5:37:LYS:HE2	32:N5:37:LYS:HB3	1.87	0.43
32:N5:213:LEU:HD23	32:N5:213:LEU:HA	1.78	0.43
51:N6:201:PLX:H182	51:N6:201:PLX:H212	1.81	0.43
34:S1:180:THR:N	54:S1:802:SF4:S4	2.85	0.43
35:S2:198:LEU:HD13	35:S2:203:MET:HB3	2.01	0.43
42:V1:235:VAL:H	42:V1:240:THR:HG21	1.84	0.43
5:A5:113:LYS:O	36:S3:122:ARG:NH2	2.50	0.43
10:AB:140:CYS:HB2	10:AB:143:GLU:HG3	2.01	0.43
28:N1:142:TYR:CD1	28:N1:142:TYR:C	2.97	0.43
53:N1:403:U10:H351	53:N1:403:U10:H371	1.67	0.43
32:N5:407:TRP:O	32:N5:411:MET:HG2	2.19	0.43
33:N6:24:PRO:O	33:N6:81:GLU:HB2	2.18	0.43
33:N6:152:TRP:HZ3	51:N6:201:PLX:H142	1.84	0.43
34:S1:251:ILE:HD11	34:S1:596:TYR:HB2	2.01	0.43
34:S1:381:LEU:HD13	34:S1:664:TYR:HB3	2.01	0.43
34:S1:382:ARG:C	34:S1:384:ASN:H	2.26	0.43
42:V1:51:TRP:NE1	44:V3:390:GLN:OE1	2.41	0.43
11:AK:127:ASP:O	11:AK:132:ARG:NH1	2.51	0.43
17:B3:18:ASP:O	17:B3:21:GLN:HG2	2.19	0.43
19:B5:83:ALA:HA	45:B5:201:CDL:H162	2.00	0.43
28:N1:267:THR:O	28:N1:271:LEU:HG	2.19	0.43
47:N4:501:PEE:H43	45:N4:504:CDL:H412	2.00	0.43
33:N6:34:ILE:HG13	33:N6:64:MET:HG3	2.01	0.43
34:S1:591:GLU:HG2	34:S1:610:VAL:HG23	2.01	0.43
35:S2:257:PHE:HD2	35:S2:347:LEU:HD11	1.84	0.43
40:S7:75:GLU:HB2	40:S7:133:MET:HE1	2.01	0.43
3:A2:85:ASP:OD1	3:A2:85:ASP:N	2.52	0.42
18:B4:82:PRO:HB2	45:B4:201:CDL:HB4	2.00	0.42
20:B6:144:TYR:OH	24:BK:49:ARG:NH1	2.52	0.42
23:B9:218:GLU:HG2	23:B9:219:ARG:HG2	2.01	0.42
31:N4:168:GLN:HB2	31:N4:174:LEU:HG	2.01	0.42
31:N4:211:GLY:H	31:N4:213:HIS:CD2	2.37	0.42
32:N5:289:ALA:O	32:N5:293:ILE:HG23	2.19	0.42
34:S1:624:ARG:NH1	34:S1:628:GLU:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:V1:51:TRP:CD1	44:V3:388:ASN:HD22	2.37	0.42
43:V2:245:VAL:HG13	43:V2:249:LEU:HD13	2.01	0.42
9:A9:64:PHE:HZ	9:A9:208:GLY:HA3	1.83	0.42
9:A9:219:SER:HB3	47:A9:402:PEE:H1	2.01	0.42
10:AB:78:ALA:HA	10:AB:81:ASP:OD2	2.20	0.42
34:S1:306:MET:HB2	34:S1:583:ILE:HB	2.01	0.42
42:V1:41:ILE:HG12	42:V1:253:THR:HG21	2.00	0.42
9:A9:192:ARG:HH12	9:A9:198:ALA:HB3	1.82	0.42
14:AN:120:MET:HE2	14:AN:120:MET:HB3	1.83	0.42
14:AN:140:PHE:CZ	48:N1:402:PC1:H151	2.54	0.42
45:B4:201:CDL:H1	45:B4:201:CDL:H512	2.00	0.42
20:B6:147:LYS:NZ	24:BK:42:ASP:OD1	2.52	0.42
51:N4:502:PLX:H1A3	47:N5:701:PEE:H3	2.00	0.42
32:N5:174:TYR:CD2	32:N5:232:TRP:HB3	2.53	0.42
32:N5:176:ARG:O	32:N5:180:ILE:HG13	2.19	0.42
34:S1:370:GLU:O	34:S1:533:GLY:N	2.53	0.42
36:S3:83:GLU:OE1	36:S3:142:ARG:NH2	2.33	0.42
1:4L:17:ALA:HB2	45:4L:201:CDL:H821	2.01	0.42
4:A3:127:ALA:HB2	28:N1:312:ALA:HA	2.01	0.42
45:A8:301:CDL:HB61	27:CB:29:THR:HB	2.02	0.42
9:A9:235:THR:HB	9:A9:273:LEU:HB2	2.01	0.42
10:AC:119:ILE:HG21	10:AC:135:ALA:HB1	2.01	0.42
45:AL:201:CDL:H322	45:AL:201:CDL:H352	1.89	0.42
20:B6:89:SER:H	20:B6:92:GLU:HB2	1.85	0.42
32:N5:233:LEU:HB3	32:N5:234:PRO:HD3	2.00	0.42
34:S1:306:MET:HE2	34:S1:314:LEU:HB3	2.01	0.42
35:S2:374:ARG:NH1	41:S8:162:CYS:O	2.48	0.42
35:S2:437:HIS:O	35:S2:460:GLN:NE2	2.53	0.42
35:S2:448:HIS:HB3	35:S2:452:ASP:HB2	2.01	0.42
42:V1:385:CYS:O	42:V1:389:VAL:HB	2.19	0.42
43:V2:237:PRO:HA	43:V2:238:PRO:HD3	1.94	0.42
10:AC:80:LYS:HE3	10:AC:80:LYS:HB3	1.86	0.42
25:BL:90:VAL:HG22	31:N4:28:THR:HG21	2.00	0.42
53:N1:403:U10:H372	53:N1:403:U10:H411	1.75	0.42
31:N4:372:SER:HB3	45:N5:703:CDL:H382	2.01	0.42
32:N5:79:SER:O	32:N5:139:GLN:NE2	2.52	0.42
33:N6:129:ASP:HB2	38:S5:32:ARG:NH1	2.35	0.42
34:S1:36:VAL:HG11	34:S1:56:VAL:HG21	2.02	0.42
34:S1:246:ARG:HH12	37:S4:123:ASN:ND2	2.17	0.42
18:B4:25:ILE:HG21	18:B4:30:ARG:CZ	2.50	0.42
29:N2:190:MET:HG2	29:N2:204:ASN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:N4:204:MET:O	31:N4:208:PRO:HA	2.20	0.42
32:N5:534:HIS:CD2	47:N5:705:PEE:H16	2.54	0.42
33:N6:24:PRO:HG2	33:N6:28:TYR:HB2	2.00	0.42
35:S2:180:PHE:CZ	35:S2:223:VAL:HG11	2.54	0.42
39:S6:104:LYS:HG2	39:S6:107:LYS:HG2	2.01	0.42
47:A9:402:PEE:H32	47:A9:402:PEE:H26	1.88	0.42
11:AK:225:ASN:HB3	11:AK:228:GLU:HG2	2.01	0.42
15:B1:50:ARG:HB2	15:B1:53:GLU:HG2	2.00	0.42
19:B5:135:LYS:NZ	31:N4:52:PHE:O	2.52	0.42
24:BK:74:ILE:O	27:CB:111:TYR:HB2	2.20	0.42
28:N1:202:GLU:HA	28:N1:210:GLY:HA3	2.02	0.42
32:N5:128:MET:HE2	32:N5:147:VAL:HG11	2.00	0.42
33:N6:122:LEU:HG	33:N6:123:GLY:H	1.85	0.42
34:S1:339:ALA:HA	34:S1:365:SER:HB2	2.02	0.42
35:S2:112:VAL:HG21	35:S2:453:VAL:HG21	2.02	0.42
51:S7:302:PLX:H92	51:S7:302:PLX:H261	2.02	0.42
42:V1:146:GLY:HA3	42:V1:193:PHE:CE1	2.53	0.42
7:A7:31:ILE:H	7:A7:31:ILE:HG13	1.61	0.42
9:A9:362:LEU:HD23	9:A9:362:LEU:HA	1.94	0.42
34:S1:217:GLU:HG2	34:S1:218:LEU:HG	2.02	0.42
34:S1:688:GLN:NE2	34:S1:694:PHE:HA	2.34	0.42
43:V2:248:GLY:O	43:V2:249:LEU:HD23	2.20	0.42
45:4L:201:CDL:H191	45:4L:201:CDL:H152	2.00	0.42
51:AM:201:PLX:H1A2	51:AM:201:PLX:H22	1.79	0.42
16:B2:64:LEU:HD13	16:B2:69:LEU:HD21	2.02	0.42
23:B9:99:MET:HE2	23:B9:99:MET:HA	2.01	0.42
32:N5:264:TYR:CG	32:N5:265:PRO:HD3	2.55	0.42
34:S1:429:VAL:HG11	34:S1:440:TYR:HE1	1.85	0.42
42:V1:315:LEU:HB2	42:V1:359:ARG:HA	2.02	0.42
9:A9:176:SER:O	9:A9:182:ARG:NE	2.53	0.42
20:B6:134:HIS:NE2	32:N5:35:TYR:OH	2.34	0.42
31:N4:368:ALA:HB1	31:N4:375:LEU:HD12	2.02	0.42
35:S2:345:GLN:O	35:S2:349:ILE:HG13	2.20	0.42
36:S3:120:PRO:HB3	37:S4:137:PHE:CE1	2.55	0.42
40:S7:130:VAL:HB	40:S7:159:VAL:HA	2.02	0.42
42:V1:44:ASN:ND2	42:V1:133:HIS:O	2.53	0.42
42:V1:222:LYS:HD3	42:V1:381:GLN:HB2	2.01	0.42
28:N1:155:LEU:HD21	28:N1:305:ILE:HA	2.01	0.41
28:N1:228:TYR:HA	28:N1:231:ILE:HD12	2.02	0.41
29:N2:186:HIS:O	29:N2:190:MET:HG3	2.20	0.41
31:N4:119:TYR:HA	31:N4:122:PHE:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:N4:296:LEU:HD21	31:N4:378:GLU:HG3	2.02	0.41
32:N5:265:PRO:O	32:N5:269:THR:HG23	2.20	0.41
34:S1:53:CYS:HA	34:S1:56:VAL:HG22	2.01	0.41
36:S3:75:GLN:HB3	36:S3:87:PHE:CD1	2.55	0.41
38:S5:95:PRO:HG2	38:S5:98:HIS:HB2	2.01	0.41
41:S8:86:TYR:CG	41:S8:87:PRO:HA	2.55	0.41
42:V1:65:THR:O	42:V1:69:LEU:HG	2.19	0.41
42:V1:98:LYS:O	42:V1:101:PHE:HB2	2.20	0.41
44:V3:383:ASN:O	44:V3:383:ASN:ND2	2.53	0.41
51:B1:101:PLX:H1A3	51:B1:101:PLX:H22	1.75	0.41
20:B6:92:GLU:HB3	20:B6:93:PRO:HD3	2.01	0.41
28:N1:58:LYS:NZ	40:S7:100:SER:O	2.52	0.41
28:N1:277:TYR:CD2	47:S8:303:PEE:H57	2.55	0.41
31:N4:455:LEU:HD23	31:N4:455:LEU:HA	1.93	0.41
47:N4:501:PEE:H47	47:N4:501:PEE:H40	1.63	0.41
33:N6:135:PHE:HD1	33:N6:135:PHE:HA	1.72	0.41
35:S2:196:HIS:O	35:S2:200:ILE:HG12	2.20	0.41
39:S6:63:ASN:OD1	41:S8:105:ARG:NH2	2.53	0.41
39:S6:116:LEU:HD23	39:S6:116:LEU:HA	1.91	0.41
42:V1:261:TRP:NE1	42:V1:265:PHE:HE2	2.18	0.41
2:A1:68:ASN:ND2	8:A8:96:LYS:HB3	2.35	0.41
6:A6:88:LYS:HD2	6:A6:88:LYS:HA	1.83	0.41
47:N1:404:PEE:H58	47:N1:404:PEE:H53	1.81	0.41
31:N4:106:LEU:HD13	31:N4:234:VAL:HG11	2.02	0.41
33:N6:82:VAL:HG22	33:N6:83:TRP:H	1.86	0.41
42:V1:99:TRP:N	42:V1:99:TRP:CD1	2.87	0.41
42:V1:412:LEU:HD23	42:V1:439:ILE:HD11	2.02	0.41
1:4L:41:PHE:O	1:4L:45:THR:HG22	2.19	0.41
1:4L:80:MET:SD	33:N6:172:THR:HA	2.59	0.41
5:A5:9:THR:HG23	5:A5:16:VAL:HG22	2.03	0.41
12:AL:39:TYR:CZ	45:AL:201:CDL:H592	2.55	0.41
24:BK:144:SER:H	24:BK:158:LYS:NZ	2.19	0.41
29:N2:168:GLY:O	29:N2:172:GLN:HG2	2.19	0.41
30:N3:87:MET:HE3	30:N3:87:MET:HB3	1.98	0.41
31:N4:318:ALA:HB1	31:N4:374:ASN:CG	2.46	0.41
42:V1:192:ASP:HB3	44:V3:411:MET:SD	2.61	0.41
17:B3:20:LYS:O	17:B3:23:LYS:NZ	2.54	0.41
23:B9:144:TRP:HA	23:B9:147:ASP:OD2	2.20	0.41
24:BK:99:ASP:OD2	24:BK:142:ARG:NH1	2.53	0.41
28:N1:195:ARG:HD3	28:N1:231:ILE:HD11	2.01	0.41
28:N1:197:PRO:HB3	28:N1:278:PRO:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:N5:172:ILE:O	32:N5:176:ARG:HG2	2.20	0.41
4:A3:111:GLY:HA3	47:N3:201:PEE:H41	2.02	0.41
13:AM:85:GLU:H	13:AM:85:GLU:CD	2.28	0.41
45:B4:201:CDL:H812	32:N5:557:TRP:HB3	2.02	0.41
21:B7:95:TYR:CD2	21:B7:99:MET:HE2	2.56	0.41
24:BK:43:ARG:HB2	24:BK:44:PRO:HD3	2.02	0.41
24:BK:97:LYS:HE3	24:BK:97:LYS:HB3	1.90	0.41
47:N3:201:PEE:H36	47:N3:201:PEE:H30	1.67	0.41
34:S1:291:ARG:HD2	34:S1:292:PHE:CE2	2.56	0.41
35:S2:219:PHE:O	35:S2:223:VAL:HG22	2.20	0.41
6:A6:81:SER:HB3	6:A6:84:GLN:HG3	2.03	0.41
10:AB:137:LYS:HE3	10:AB:137:LYS:HB2	1.93	0.41
20:B6:169:THR:HA	20:B6:175:GLU:O	2.21	0.41
23:B9:201:LYS:HE3	23:B9:201:LYS:HB2	1.88	0.41
47:S2:501:PEE:H16	47:S2:501:PEE:H22	1.94	0.41
42:V1:118:ASP:O	42:V1:120:GLY:N	2.53	0.41
8:A8:117:ASN:HB3	14:AN:73:PRO:HG2	2.03	0.41
13:AM:84:PRO:HB3	41:S8:197:TRP:CE3	2.56	0.41
24:BK:77:CYS:SG	24:BK:84:CYS:HB3	2.61	0.41
28:N1:37:PRO:HA	40:S7:88:ARG:HA	2.01	0.41
29:N2:5:ILE:O	29:N2:8:THR:HG22	2.21	0.41
45:N4:503:CDL:OA9	45:N4:503:CDL:H712	2.20	0.41
35:S2:117:PRO:HG3	35:S2:441:LEU:HD23	2.03	0.41
47:S2:501:PEE:H34	47:S2:501:PEE:H27	1.70	0.41
42:V1:174:ARG:HA	44:V3:406:LEU:HD21	2.02	0.41
42:V1:210:THR:HB	42:V1:224:ARG:H	1.85	0.41
45:A8:301:CDL:H352	29:N2:338:PRO:HG3	2.02	0.41
10:AB:115:GLN:O	10:AB:119:ILE:HG12	2.21	0.41
12:AL:45:PRO:HA	12:AL:46:PRO:HD3	1.92	0.41
15:B1:42:SER:O	15:B1:46:LYS:HB2	2.20	0.41
15:B1:43:LEU:O	24:BK:69:ARG:HD2	2.21	0.41
45:B5:201:CDL:H191	45:B5:201:CDL:H762	2.03	0.41
28:N1:147:ALA:HB1	30:N3:69:ILE:HD13	2.02	0.41
45:N1:401:CDL:H752	45:N1:401:CDL:H782	1.83	0.41
45:N1:401:CDL:H721	45:N1:401:CDL:H341	2.03	0.41
53:N1:403:U10:H251	53:N1:403:U10:H271	1.63	0.41
29:N2:136:LEU:HD12	29:N2:205:LEU:HD21	2.02	0.41
29:N2:173:THR:HG22	35:S2:58:MET:HG2	2.02	0.41
51:N4:502:PLX:H191	45:N5:703:CDL:H211	2.03	0.41
51:N4:502:PLX:H101	51:N4:502:PLX:H71	1.95	0.41
32:N5:208:CYS:HA	32:N5:209:PRO:HD3	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:V1:208:GLU:O	42:V1:212:LEU:HB2	2.21	0.41
1:4L:35:GLY:HA3	33:N6:20:PHE:HZ	1.86	0.41
7:A7:23:LYS:HG3	35:S2:259:PHE:CD1	2.56	0.41
45:A8:301:CDL:H782	52:CB:202:3PE:H281	2.03	0.41
21:B7:96:VAL:HA	21:B7:99:MET:HE3	2.03	0.41
24:BK:74:ILE:HG23	24:BK:156:LEU:HD22	2.02	0.41
24:BK:106:ILE:HD11	25:BL:136:LEU:HD13	2.03	0.41
28:N1:149:ILE:HG21	28:N1:185:TRP:HB2	2.02	0.41
28:N1:273:ILE:HG23	28:N1:277:TYR:CD2	2.56	0.41
31:N4:216:LEU:HD23	31:N4:287:ALA:HB1	2.02	0.41
31:N4:364:LEU:HD22	31:N4:369:LEU:HD22	2.02	0.41
47:N5:701:PEE:H35	47:N5:701:PEE:H29	1.84	0.41
35:S2:147:TYR:CB	40:S7:71:CYS:HB3	2.51	0.41
51:S7:302:PLX:H21	51:S7:302:PLX:H1C2	1.74	0.41
43:V2:186:VAL:HG22	43:V2:196:LEU:HD11	2.03	0.41
3:A2:19:ILE:HD13	3:A2:91:LEU:HD11	2.03	0.40
5:A5:114:TRP:CD2	5:A5:115:PRO:HA	2.56	0.40
9:A9:262:THR:O	9:A9:333:PRO:HD2	2.21	0.40
11:AK:112:GLY:HA2	11:AK:136:TRP:CD2	2.56	0.40
11:AK:223:LYS:HE2	11:AK:223:LYS:HB2	1.92	0.40
13:AM:49:TYR:HB2	13:AM:61:TRP:CE2	2.56	0.40
28:N1:71:PHE:O	28:N1:215:TYR:OH	2.35	0.40
28:N1:198:PHE:CD1	28:N1:285:LEU:HD13	2.56	0.40
35:S2:141:TYR:O	35:S2:145:LEU:HG	2.20	0.40
37:S4:75:ARG:HA	37:S4:75:ARG:HD2	1.86	0.40
39:S6:84:ILE:HD12	39:S6:84:ILE:HA	1.91	0.40
40:S7:131:VAL:HG22	40:S7:161:ILE:HB	2.03	0.40
51:S7:302:PLX:H393	51:S7:302:PLX:H362	1.90	0.40
41:S8:131:GLU:HB2	41:S8:144:ARG:HB3	2.02	0.40
2:A1:13:ALA:HB2	28:N1:264:LEU:HD11	2.02	0.40
27:CB:80:ARG:O	27:CB:84:MET:HG2	2.21	0.40
28:N1:13:ILE:HD13	28:N1:13:ILE:HA	1.87	0.40
28:N1:134:ARG:NH1	28:N1:206:GLU:OE1	2.34	0.40
31:N4:306:PRO:HB3	31:N4:458:LEU:HD12	2.03	0.40
32:N5:13:THR:O	32:N5:17:ILE:HG13	2.21	0.40
33:N6:124:ASP:O	33:N6:127:ILE:HG12	2.21	0.40
1:4L:55:LEU:HD13	38:S5:17:TRP:HE3	1.86	0.40
8:A8:95:VAL:HG12	8:A8:97:VAL:HG22	2.03	0.40
13:AM:78:ASP:OD1	13:AM:78:ASP:N	2.53	0.40
22:B8:96:ASP:OD1	22:B8:96:ASP:N	2.51	0.40
23:B9:119:PRO:HB3	32:N5:525:MET:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:CA:101:3PE:H262	27:CB:66:TYR:CE1	2.57	0.40
29:N2:243:LEU:HD23	45:N4:503:CDL:H351	2.03	0.40
29:N2:258:SER:OG	29:N2:336:VAL:HG22	2.21	0.40
32:N5:54:PHE:CZ	32:N5:84:TYR:HB2	2.57	0.40
35:S2:46:ASP:OD1	35:S2:46:ASP:N	2.54	0.40
10:AC:105:MET:HE2	10:AC:111:ASP:C	2.46	0.40
19:B5:78:THR:C	19:B5:81:PRO:HD2	2.47	0.40
19:B5:160:MET:HE2	27:CB:95:TYR:HB2	2.04	0.40
22:B8:161:TYR:HB3	22:B8:166:LEU:HG	2.02	0.40
23:B9:181:GLN:NE2	23:B9:198:PRO:O	2.48	0.40
28:N1:277:TYR:OH	41:S8:66:LEU:HB3	2.21	0.40
4:A3:110:ILE:HD11	47:S8:303:PEE:H36	2.03	0.40
10:AC:91:ASP:HB2	17:B3:44:PRO:HB3	2.04	0.40
18:B4:116:ILE:HD13	18:B4:116:ILE:HA	1.96	0.40
29:N2:168:GLY:HA3	29:N2:181:TYR:CE1	2.56	0.40
29:N2:250:SER:O	29:N2:259:GLY:HA3	2.20	0.40
30:N3:42:ASP:OD1	40:S7:119:LYS:NZ	2.55	0.40
31:N4:259:TYR:O	31:N4:263:MET:HG2	2.21	0.40
32:N5:500:LEU:HB2	45:N5:704:CDL:H551	2.02	0.40
47:N5:705:PEE:H19	47:N5:705:PEE:H26	1.79	0.40
34:S1:234:LYS:HB3	34:S1:235:PRO:HD3	2.03	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	4L	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
2	A1	68/70 (97%)	68 (100%)	0	0	100	100
3	A2	83/85 (98%)	78 (94%)	5 (6%)	0	100	100
4	A3	81/83 (98%)	78 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	A5	110/112 (98%)	108 (98%)	2 (2%)	0	100	100
6	A6	112/114 (98%)	108 (96%)	3 (3%)	1 (1%)	14	40
7	A7	93/112 (83%)	91 (98%)	2 (2%)	0	100	100
8	A8	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
9	A9	339/341 (99%)	330 (97%)	9 (3%)	0	100	100
10	AB	75/87 (86%)	75 (100%)	0	0	100	100
10	AC	85/87 (98%)	85 (100%)	0	0	100	100
11	AK	319/321 (99%)	309 (97%)	10 (3%)	0	100	100
12	AL	138/140 (99%)	138 (100%)	0	0	100	100
13	AM	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
14	AN	140/142 (99%)	131 (94%)	9 (6%)	0	100	100
15	B1	54/56 (96%)	54 (100%)	0	0	100	100
16	B2	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
17	B3	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
18	B4	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
19	B5	136/138 (99%)	134 (98%)	2 (2%)	0	100	100
20	B6	99/126 (79%)	95 (96%)	4 (4%)	0	100	100
21	B7	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
22	B8	154/156 (99%)	151 (98%)	3 (2%)	0	100	100
23	B9	176/178 (99%)	173 (98%)	3 (2%)	0	100	100
24	BK	172/176 (98%)	169 (98%)	3 (2%)	0	100	100
25	BL	97/102 (95%)	89 (92%)	8 (8%)	0	100	100
26	CA	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
27	CB	119/121 (98%)	117 (98%)	2 (2%)	0	100	100
28	N1	316/318 (99%)	307 (97%)	9 (3%)	0	100	100
29	N2	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
30	N3	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
31	N4	457/459 (100%)	451 (99%)	6 (1%)	0	100	100
32	N5	601/603 (100%)	577 (96%)	24 (4%)	0	100	100
33	N6	172/174 (99%)	161 (94%)	11 (6%)	0	100	100
34	S1	687/689 (100%)	660 (96%)	27 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	S2	427/430 (99%)	412 (96%)	15 (4%)	0	100	100
36	S3	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
37	S4	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
38	S5	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
39	S6	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
40	S7	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
41	S8	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
42	V1	429/431 (100%)	413 (96%)	16 (4%)	0	100	100
43	V2	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
44	V3	40/42 (95%)	38 (95%)	2 (5%)	0	100	100
All	All	8151/8299 (98%)	7911 (97%)	239 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A6	49	ARG

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	4L	85/85 (100%)	85 (100%)	0	100	100
2	A1	58/58 (100%)	58 (100%)	0	100	100
3	A2	76/76 (100%)	76 (100%)	0	100	100
4	A3	69/69 (100%)	69 (100%)	0	100	100
5	A5	99/99 (100%)	99 (100%)	0	100	100
6	A6	107/107 (100%)	107 (100%)	0	100	100
7	A7	87/97 (90%)	85 (98%)	2 (2%)	44	74
8	A8	153/153 (100%)	153 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	A9	295/295 (100%)	293 (99%)	2 (1%)	76 91
10	AB	71/80 (89%)	71 (100%)	0	100 100
10	AC	80/80 (100%)	79 (99%)	1 (1%)	61 84
11	AK	284/284 (100%)	281 (99%)	3 (1%)	65 86
12	AL	101/101 (100%)	100 (99%)	1 (1%)	68 87
13	AM	130/130 (100%)	129 (99%)	1 (1%)	73 89
14	AN	123/123 (100%)	123 (100%)	0	100 100
15	B1	53/53 (100%)	53 (100%)	0	100 100
16	B2	62/62 (100%)	62 (100%)	0	100 100
17	B3	62/62 (100%)	62 (100%)	0	100 100
18	B4	113/113 (100%)	113 (100%)	0	100 100
19	B5	121/121 (100%)	121 (100%)	0	100 100
20	B6	98/119 (82%)	98 (100%)	0	100 100
21	B7	112/112 (100%)	112 (100%)	0	100 100
22	B8	141/141 (100%)	141 (100%)	0	100 100
23	B9	159/159 (100%)	159 (100%)	0	100 100
24	BK	155/156 (99%)	154 (99%)	1 (1%)	78 92
25	BL	91/94 (97%)	89 (98%)	2 (2%)	45 75
26	CA	45/45 (100%)	45 (100%)	0	100 100
27	CB	108/108 (100%)	108 (100%)	0	100 100
28	N1	275/275 (100%)	271 (98%)	4 (2%)	57 82
29	N2	311/311 (100%)	308 (99%)	3 (1%)	68 87
30	N3	100/100 (100%)	100 (100%)	0	100 100
31	N4	410/410 (100%)	408 (100%)	2 (0%)	81 93
32	N5	537/537 (100%)	530 (99%)	7 (1%)	61 84
33	N6	140/140 (100%)	137 (98%)	3 (2%)	47 76
34	S1	579/579 (100%)	575 (99%)	4 (1%)	76 91
35	S2	370/370 (100%)	369 (100%)	1 (0%)	86 95
36	S3	190/190 (100%)	189 (100%)	1 (0%)	81 93
37	S4	112/112 (100%)	111 (99%)	1 (1%)	70 88
38	S5	93/93 (100%)	93 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
39	S6	79/79 (100%)	79 (100%)	0	100 100
40	S7	132/132 (100%)	131 (99%)	1 (1%)	73 89
41	S8	151/151 (100%)	149 (99%)	2 (1%)	61 84
42	V1	344/344 (100%)	339 (98%)	5 (2%)	57 82
43	V2	183/183 (100%)	181 (99%)	2 (1%)	65 86
44	V3	41/41 (100%)	41 (100%)	0	100 100
All	All	7185/7229 (99%)	7136 (99%)	49 (1%)	73 91

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	A7	31	ILE
7	A7	43	VAL
9	A9	129	LEU
9	A9	132	ARG
10	AC	112	SER
11	AK	39	GLN
11	AK	97	ASP
11	AK	167	SER
12	AL	115	CYS
13	AM	78	ASP
24	BK	73	ASP
25	BL	72	ASP
25	BL	83	ASP
28	N1	21	THR
28	N1	251	THR
28	N1	282	TYR
28	N1	296	LEU
29	N2	8	THR
29	N2	128	LEU
29	N2	343	LEU
31	N4	122	PHE
31	N4	375	LEU
32	N5	41	SER
32	N5	190	LEU
32	N5	286	LEU
32	N5	340	PHE
32	N5	369	THR
32	N5	503	GLU
32	N5	554	ASP

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Mol	Chain	Res	Type
33	N6	45	LEU
33	N6	124	ASP
33	N6	135	PHE
34	S1	41	VAL
34	S1	556	THR
34	S1	674	LEU
34	S1	690	THR
35	S2	204	THR
36	S3	145	THR
37	S4	86	ASN
40	S7	71	CYS
41	S8	73	THR
41	S8	169	GLU
42	V1	212	LEU
42	V1	307	VAL
42	V1	347	THR
42	V1	379	CYS
42	V1	385	CYS
43	V2	137	THR
43	V2	249	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
1	4L	7	ASN
1	4L	57	ASN
2	A1	27	HIS
2	A1	61	HIS
3	A2	25	GLN
5	A5	71	GLN
5	A5	86	ASN
5	A5	110	ASN
6	A6	84	GLN
7	A7	9	GLN
7	A7	21	GLN
7	A7	25	GLN
8	A8	107	HIS
8	A8	141	ASN
8	A8	142	GLN
9	A9	38	HIS
9	A9	72	HIS
9	A9	122	HIS

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Mol	Chain	Res	Type
9	A9	154	GLN
9	A9	215	ASN
11	AK	39	GLN
11	AK	87	HIS
11	AK	134	GLN
11	AK	217	GLN
11	AK	221	GLN
11	AK	325	GLN
12	AL	79	GLN
12	AL	89	ASN
13	AM	112	ASN
14	AN	24	ASN
14	AN	61	GLN
15	B1	3	ASN
15	B1	6	GLN
16	B2	63	GLN
16	B2	71	GLN
17	B3	33	GLN
18	B4	50	GLN
19	B5	189	ASN
20	B6	143	HIS
21	B7	76	ASN
21	B7	85	HIS
21	B7	110	GLN
22	B8	56	ASN
22	B8	115	ASN
23	B9	93	HIS
23	B9	104	GLN
23	B9	117	GLN
24	BK	55	GLN
24	BK	107	GLN
24	BK	124	ASN
24	BK	149	HIS
25	BL	115	GLN
25	BL	140	ASN
26	CA	61	GLN
26	CA	62	HIS
26	CA	73	ASN
28	N1	138	GLN
28	N1	317	GLN
29	N2	49	ASN
29	N2	83	GLN

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Mol	Chain	Res	Type
29	N2	112	HIS
29	N2	144	GLN
29	N2	186	HIS
29	N2	273	ASN
29	N2	322	GLN
30	N3	26	GLN
30	N3	82	ASN
31	N4	81	GLN
31	N4	83	HIS
31	N4	213	HIS
31	N4	279	GLN
31	N4	304	GLN
31	N4	338	HIS
31	N4	415	GLN
32	N5	23	ASN
32	N5	139	GLN
32	N5	230	HIS
32	N5	248	HIS
32	N5	447	ASN
32	N5	470	ASN
32	N5	471	ASN
32	N5	524	ASN
32	N5	540	HIS
32	N5	580	GLN
34	S1	39	GLN
34	S1	142	GLN
34	S1	260	ASN
34	S1	278	HIS
34	S1	282	ASN
34	S1	331	GLN
34	S1	336	ASN
34	S1	425	ASN
34	S1	498	GLN
34	S1	604	GLN
34	S1	652	ASN
34	S1	677	GLN
34	S1	688	GLN
35	S2	93	GLN
35	S2	98	HIS
35	S2	168	GLN
35	S2	189	HIS
35	S2	229	HIS

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Mol	Chain	Res	Type
35	S2	239	HIS
36	S3	75	GLN
36	S3	77	GLN
36	S3	123	GLN
36	S3	196	HIS
37	S4	123	ASN
37	S4	163	ASN
38	S5	25	GLN
38	S5	45	HIS
39	S6	74	GLN
39	S6	117	GLN
42	V1	220	GLN
42	V1	270	ASN
42	V1	277	ASN
42	V1	303	HIS
42	V1	344	GLN
42	V1	393	ASN
42	V1	456	GLN
43	V2	74	HIS
43	V2	87	GLN
43	V2	153	GLN
43	V2	187	GLN
43	V2	189	ASN
43	V2	246	GLN
44	V3	388	ASN
44	V3	419	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	2MR	S2	124	35	10,12,13	2.43	2 (20%)	5,13,15	0.95	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
35	2MR	S2	124	35	-	3/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	S2	124	2MR	CZ-NE	5.14	1.45	1.34
35	S2	124	2MR	CZ-NH2	5.07	1.44	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	S2	124	2MR	NE-CD-CG-CB
35	S2	124	2MR	CA-CB-CG-CD
35	S2	124	2MR	CG-CD-NE-CZ

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	S2	124	2MR	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 52 ligands modelled in this entry, 2 are monoatomic - leaving 50 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	$\#\|Z\| > 2$
54	SF4	S1	801	34	0,12,12	-	-	-		
48	PC1	N1	402	-	47,47,53	0.30	0	53,55,61	0.31	0
54	SF4	S1	802	34	0,12,12	-	-	-		
47	PEE	N5	705	-	50,50,50	1.32	5 (10%)	53,55,55	1.16	4 (7%)
57	MF8	S2	502	-	7,8,8	0.87	0	7,10,10	1.44	1 (14%)
55	FES	S1	803	34	0,4,4	-	-	-		
52	3PE	B8	201	-	31,31,50	0.37	0	34,36,55	0.35	0
53	U10	N1	403	-	63,63,63	2.16	21 (33%)	76,79,79	1.68	21 (27%)
50	ADP	AK	401	-	27,29,29	1.35	4 (14%)	42,45,45	1.94	10 (23%)
47	PEE	N5	702	-	39,39,50	1.49	5 (12%)	41,44,55	1.23	3 (7%)
45	CDL	N5	703	-	88,88,99	0.31	0	94,100,111	0.31	0
54	SF4	V1	501	42	0,12,12	-	-	-		
47	PEE	A9	402	-	38,38,50	1.49	5 (13%)	41,43,55	1.24	3 (7%)
51	PLX	AL	202	-	46,46,51	1.15	4 (8%)	50,54,59	0.87	1 (2%)
52	3PE	S7	303	-	50,50,50	0.31	0	53,55,55	0.46	0
45	CDL	N1	401	-	77,77,99	0.34	0	83,89,111	0.30	0
47	PEE	N5	701	-	45,45,50	1.39	5 (11%)	48,50,55	1.18	4 (8%)
52	3PE	N5	706	-	45,45,50	0.32	0	48,50,55	0.28	0
51	PLX	B1	101	-	51,51,51	1.11	4 (7%)	55,59,59	0.89	1 (1%)
52	3PE	CA	101	-	50,50,50	0.31	0	53,55,55	0.29	0
55	FES	V2	301	43	0,4,4	-	-	-		
59	FMN	V1	502	-	33,33,33	0.23	0	48,50,50	0.40	0
46	NDP	A9	401	-	49,52,52	0.33	0	66,80,80	0.33	0
47	PEE	S8	303	-	50,50,50	1.32	5 (10%)	53,55,55	1.22	3 (5%)
49	ZMP	AC	201	10	29,35,36	0.64	1 (3%)	34,42,45	0.70	0
49	ZMP	AB	201	10	29,35,36	0.65	1 (3%)	34,42,45	0.74	0
45	CDL	N4	503	-	99,99,99	0.29	0	105,111,111	0.28	0
51	PLX	N6	201	-	51,51,51	1.11	4 (7%)	55,59,59	0.86	1 (1%)
52	3PE	CB	202	-	45,45,50	0.32	0	48,50,55	0.30	0
45	CDL	B5	201	-	99,99,99	0.30	0	105,111,111	0.31	0
54	SF4	S8	301	41	0,12,12	-	-	-		
45	CDL	A7	201	-	50,50,99	0.40	0	56,62,111	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
47	PEE	N1	404	-	30,30,50	1.28	3 (10%)	33,35,55	1.18	2 (6%)
48	PC1	A9	403	-	53,53,53	0.30	0	59,61,61	0.31	0
47	PEE	N4	501	-	48,48,50	1.34	5 (10%)	51,53,55	1.21	4 (7%)
51	PLX	CB	201	-	51,51,51	1.10	3 (5%)	55,59,59	0.89	1 (1%)
45	CDL	N4	504	-	61,61,99	0.37	0	67,73,111	0.35	0
51	PLX	S7	302	-	51,51,51	1.10	3 (5%)	55,59,59	0.88	1 (1%)
45	CDL	AK	402	-	67,67,99	0.36	0	73,79,111	0.38	0
54	SF4	S8	302	41	0,12,12	-	-	-		
47	PEE	S2	501	-	47,47,50	1.35	5 (10%)	50,52,55	1.19	3 (6%)
45	CDL	AL	201	-	93,93,99	0.31	0	99,105,111	0.31	0
51	PLX	N4	502	-	48,48,51	1.13	4 (8%)	52,56,59	0.88	1 (1%)
45	CDL	N5	704	-	99,99,99	0.30	0	105,111,111	0.28	0
51	PLX	AM	201	-	50,50,51	1.11	4 (8%)	54,58,59	0.86	1 (1%)
45	CDL	4L	201	-	91,91,99	0.32	0	97,103,111	0.37	0
45	CDL	A8	301	-	82,82,99	0.32	0	88,94,111	0.33	0
45	CDL	B4	201	-	79,79,99	0.33	0	85,91,111	0.29	0
54	SF4	S7	301	40	0,12,12	-	-	-		
47	PEE	N3	201	-	50,50,50	1.32	5 (10%)	53,55,55	1.15	4 (7%)

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
54	SF4	S1	801	34	-	-	0/6/5/5
48	PC1	N1	402	-	-	14/51/51/57	-
54	SF4	S1	802	34	-	-	0/6/5/5
47	PEE	N5	705	-	-	20/54/54/54	-
57	MF8	S2	502	-	-	5/8/8/8	-
55	FES	S1	803	34	-	-	0/1/1/1
52	3PE	B8	201	-	-	8/35/35/54	-
53	U10	N1	403	-	-	18/63/87/87	0/1/1/1
50	ADP	AK	401	-	-	5/16/32/32	0/3/3/3
47	PEE	N5	702	-	-	22/43/43/54	-
45	CDL	N5	703	-	-	28/99/99/110	-
54	SF4	V1	501	42	-	-	0/6/5/5
47	PEE	A9	402	-	-	27/42/42/54	-
51	PLX	AL	202	-	-	21/50/50/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	3PE	S7	303	-	-	11/54/54/54	-
45	CDL	N1	401	-	-	16/88/88/110	-
47	PEE	N5	701	-	-	26/49/49/54	-
52	3PE	N5	706	-	-	8/49/49/54	-
51	PLX	B1	101	-	-	17/55/55/55	-
52	3PE	CA	101	-	-	11/54/54/54	-
55	FES	V2	301	43	-	-	0/1/1/1
59	FMN	V1	502	-	-	0/18/18/18	0/3/3/3
46	NDP	A9	401	-	-	5/34/77/77	0/5/5/5
47	PEE	S8	303	-	-	27/54/54/54	-
49	ZMP	AC	201	10	-	20/40/42/43	-
49	ZMP	AB	201	10	-	11/40/42/43	-
45	CDL	N4	503	-	-	26/110/110/110	-
51	PLX	N6	201	-	-	23/55/55/55	-
52	3PE	CB	202	-	-	10/49/49/54	-
45	CDL	B5	201	-	-	24/110/110/110	-
54	SF4	S8	301	41	-	-	0/6/5/5
45	CDL	A7	201	-	-	8/61/61/110	-
47	PEE	N1	404	-	-	20/34/34/54	-
48	PC1	A9	403	-	-	15/57/57/57	-
47	PEE	N4	501	-	-	32/52/52/54	-
51	PLX	CB	201	-	-	26/55/55/55	-
45	CDL	N4	504	-	-	21/72/72/110	-
51	PLX	S7	302	-	-	24/55/55/55	-
45	CDL	AK	402	-	-	14/78/78/110	-
54	SF4	S8	302	41	-	-	0/6/5/5
47	PEE	S2	501	-	-	33/51/51/54	-
45	CDL	AL	201	-	-	25/104/104/110	-
51	PLX	N4	502	-	-	19/52/52/55	-
45	CDL	N5	704	-	-	20/110/110/110	-
51	PLX	AM	201	-	-	24/54/54/55	-
45	CDL	4L	201	-	-	19/102/102/110	-
45	CDL	A8	301	-	-	25/93/93/110	-
45	CDL	B4	201	-	-	20/90/90/110	-
54	SF4	S7	301	40	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	PEE	N3	201	-	-	25/54/54/54	-

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	N1	403	U10	C6-C1	10.28	1.54	1.35
50	AK	401	ADP	C5-C4	4.44	1.47	1.39
53	N1	403	U10	C4-C3	4.26	1.53	1.36
47	N5	705	PEE	C18-C19	4.05	1.55	1.31
47	N3	201	PEE	C18-C19	4.05	1.55	1.31
47	N5	702	PEE	C18-C19	4.05	1.55	1.31
47	N5	701	PEE	C18-C19	4.04	1.55	1.31
47	S2	501	PEE	C18-C19	4.03	1.55	1.31
47	A9	402	PEE	C18-C19	4.03	1.55	1.31
47	S8	303	PEE	C18-C19	4.03	1.55	1.31
47	N4	501	PEE	C18-C19	4.00	1.54	1.31
47	N5	702	PEE	C39-C38	3.95	1.54	1.31
47	S8	303	PEE	C39-C38	3.95	1.54	1.31
47	N4	501	PEE	C39-C38	3.95	1.54	1.31
47	N3	201	PEE	C39-C38	3.94	1.54	1.31
47	S2	501	PEE	C39-C38	3.93	1.54	1.31
47	N5	701	PEE	C39-C38	3.93	1.54	1.31
47	N5	705	PEE	C39-C38	3.91	1.54	1.31
47	A9	402	PEE	C39-C38	3.88	1.54	1.28
47	N5	701	PEE	O3-C30	3.30	1.43	1.33
47	N5	702	PEE	O3-C30	3.28	1.42	1.33
47	N3	201	PEE	O3-C30	3.27	1.42	1.33
47	N1	404	PEE	O3-C30	3.27	1.42	1.33
47	S2	501	PEE	O3-C30	3.22	1.42	1.33
47	A9	402	PEE	O3-C30	3.22	1.42	1.33
47	S8	303	PEE	O3-C30	3.21	1.42	1.33
47	N4	501	PEE	O3-C30	3.16	1.42	1.33
47	N5	705	PEE	O3-C30	3.16	1.42	1.33
53	N1	403	U10	C41-C39	3.02	1.57	1.51
51	CB	201	PLX	O6-C4	-3.01	1.40	1.44
51	S7	302	PLX	O6-C4	-2.95	1.40	1.44
51	B1	101	PLX	O6-C4	-2.94	1.40	1.44
51	N4	502	PLX	O6-C4	-2.93	1.40	1.44
51	AL	202	PLX	O6-C4	-2.92	1.40	1.44
53	N1	403	U10	C7-C8	2.85	1.54	1.50
51	N6	201	PLX	O6-C4	-2.84	1.40	1.44
51	AM	201	PLX	O6-C4	-2.84	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	N1	403	U10	C26-C24	2.74	1.57	1.51
47	S8	303	PEE	O2-C10	2.74	1.42	1.34
47	N5	705	PEE	O2-C10	2.67	1.41	1.34
47	N5	702	PEE	O2-C10	2.66	1.41	1.34
50	AK	401	ADP	C5-C6	2.65	1.48	1.41
47	N5	701	PEE	O2-C10	2.63	1.41	1.34
53	N1	403	U10	C31-C29	2.62	1.56	1.51
53	N1	403	U10	C21-C19	2.62	1.56	1.51
47	N3	201	PEE	O2-C10	2.61	1.41	1.34
47	A9	402	PEE	O2-C10	2.58	1.41	1.34
47	S2	501	PEE	O2-C10	2.57	1.41	1.34
47	N1	404	PEE	O2-C10	2.57	1.41	1.34
47	N4	501	PEE	O2-C2	-2.55	1.40	1.46
47	S2	501	PEE	O2-C2	-2.53	1.40	1.46
47	N1	404	PEE	O2-C2	-2.53	1.40	1.46
53	N1	403	U10	C7-C6	2.52	1.55	1.51
47	N5	705	PEE	O2-C2	-2.51	1.40	1.46
49	AB	201	ZMP	C9-C10	-2.50	1.48	1.50
53	N1	403	U10	O5-C5	-2.49	1.18	1.23
47	N4	501	PEE	O2-C10	2.49	1.41	1.34
47	N3	201	PEE	O2-C2	-2.48	1.40	1.46
47	A9	402	PEE	O2-C2	-2.48	1.40	1.46
47	N5	702	PEE	O2-C2	-2.46	1.40	1.46
53	N1	403	U10	C36-C34	2.46	1.56	1.51
47	N5	701	PEE	O2-C2	-2.46	1.40	1.46
53	N1	403	U10	C11-C9	2.40	1.56	1.51
49	AC	201	ZMP	C9-C10	-2.39	1.48	1.50
50	AK	401	ADP	C8-N7	2.38	1.36	1.31
53	N1	403	U10	C51-C49	2.36	1.56	1.51
47	S8	303	PEE	O2-C2	-2.36	1.40	1.46
53	N1	403	U10	C46-C44	2.35	1.56	1.51
53	N1	403	U10	O3-C3M	-2.26	1.40	1.45
53	N1	403	U10	C16-C14	2.25	1.56	1.51
53	N1	403	U10	C6-C5	2.22	1.52	1.46
53	N1	403	U10	O2-C2	-2.21	1.18	1.23
50	AK	401	ADP	C5-N7	-2.18	1.34	1.39
51	N6	201	PLX	C1B-N1	-2.17	1.43	1.50
51	N4	502	PLX	C1B-N1	-2.17	1.43	1.50
51	B1	101	PLX	C1B-N1	-2.16	1.43	1.50
53	N1	403	U10	C27-C28	2.16	1.57	1.50
51	AL	202	PLX	C1B-N1	-2.13	1.43	1.50
51	S7	302	PLX	C1B-N1	-2.12	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	N1	403	U10	C42-C43	2.11	1.57	1.50
51	CB	201	PLX	C1B-N1	-2.10	1.43	1.50
51	AM	201	PLX	C1B-N1	-2.09	1.43	1.50
53	N1	403	U10	C22-C23	2.07	1.57	1.50
51	AM	201	PLX	P1-O4	2.06	1.67	1.59
53	N1	403	U10	O4-C4M	-2.06	1.40	1.45
51	S7	302	PLX	C1A-N1	-2.05	1.44	1.50
51	B1	101	PLX	P1-O4	2.04	1.67	1.59
51	CB	201	PLX	C1A-N1	-2.04	1.44	1.50
51	N6	201	PLX	C1A-N1	-2.04	1.44	1.50
51	N6	201	PLX	P1-O4	2.03	1.67	1.59
51	N4	502	PLX	P1-O4	2.03	1.67	1.59
51	N4	502	PLX	C1A-N1	-2.03	1.44	1.50
51	AL	202	PLX	P1-O4	2.03	1.67	1.59
51	AM	201	PLX	C7-C6	2.01	1.55	1.50
51	B1	101	PLX	C1A-N1	-2.01	1.44	1.50
51	AL	202	PLX	C1A-N1	-2.01	1.44	1.50

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	AK	401	ADP	C5-C4-N3	-6.19	118.67	126.75
50	AK	401	ADP	N3-C4-N9	4.88	135.12	127.08
47	S8	303	PEE	O2-C10-C11	4.62	121.46	111.50
53	N1	403	U10	C7-C8-C9	-4.32	119.60	126.79
47	N5	702	PEE	O2-C10-C11	4.14	120.42	111.50
47	N1	404	PEE	O2-C10-C11	4.02	120.16	111.50
47	A9	402	PEE	O2-C10-C11	3.98	120.07	111.50
47	N5	705	PEE	O2-C10-C11	3.94	119.98	111.50
47	N4	501	PEE	O2-C10-C11	3.93	119.97	111.50
47	N5	701	PEE	O2-C10-C11	3.93	119.97	111.50
47	N3	201	PEE	O2-C10-C11	3.92	119.96	111.50
50	AK	401	ADP	C2-N3-C4	3.89	120.93	111.75
47	S2	501	PEE	O2-C10-C11	3.84	119.79	111.50
57	S2	502	MF8	C07-N06-C04	3.35	131.88	124.55
53	N1	403	U10	C17-C18-C19	-3.25	119.83	127.66
50	AK	401	ADP	C4-C5-N7	-3.19	106.74	110.62
50	AK	401	ADP	N3-C2-N1	-3.16	123.66	128.60
50	AK	401	ADP	PA-O3A-PB	-3.14	122.04	132.83
53	N1	403	U10	C40-C39-C41	3.12	120.52	115.27
53	N1	403	U10	C10-C9-C11	3.10	120.48	115.27
53	N1	403	U10	C32-C33-C34	-2.96	120.54	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	N1	403	U10	C37-C38-C39	-2.93	120.59	127.66
53	N1	403	U10	C50-C49-C51	2.83	120.03	115.27
53	N1	403	U10	C15-C14-C16	2.79	119.97	115.27
53	N1	403	U10	C45-C44-C46	2.79	119.97	115.27
53	N1	403	U10	C20-C19-C21	2.73	119.87	115.27
47	N4	501	PEE	O3-C30-C31	2.72	120.43	111.91
47	S2	501	PEE	O3-C30-C31	2.71	120.43	111.91
50	AK	401	ADP	C5-N7-C8	2.71	107.36	103.51
53	N1	403	U10	C35-C34-C36	2.69	119.80	115.27
53	N1	403	U10	C12-C13-C14	-2.68	121.21	127.66
53	N1	403	U10	C42-C43-C44	-2.67	121.22	127.66
47	N1	404	PEE	O3-C30-C31	2.66	120.25	111.91
53	N1	403	U10	C47-C48-C49	-2.64	121.30	127.66
50	AK	401	ADP	C4-N9-C8	2.63	108.58	105.73
47	N3	201	PEE	O3-C30-C31	2.62	120.12	111.91
53	N1	403	U10	C30-C29-C31	2.62	119.67	115.27
47	A9	402	PEE	O3-C30-C31	2.60	120.06	111.91
47	N5	702	PEE	O3-C30-C31	2.57	119.96	111.91
53	N1	403	U10	C25-C24-C26	2.56	119.58	115.27
47	S8	303	PEE	O3-C30-C31	2.55	119.92	111.91
53	N1	403	U10	C22-C23-C24	-2.55	121.52	127.66
47	A9	402	PEE	C37-C38-C39	-2.51	109.78	126.84
47	N5	701	PEE	O3-C30-C31	2.46	119.64	111.91
47	N5	705	PEE	O3-C30-C31	2.45	119.61	111.91
53	N1	403	U10	C27-C28-C29	-2.40	121.88	127.66
53	N1	403	U10	C1M-C1-C6	-2.36	120.56	124.40
53	N1	403	U10	C56-C54-C55	2.32	119.73	114.60
51	CB	201	PLX	O3-P1-O2	-2.27	101.03	112.24
51	AM	201	PLX	O3-P1-O2	-2.25	101.14	112.24
51	B1	101	PLX	O3-P1-O2	-2.24	101.16	112.24
51	N6	201	PLX	O3-P1-O2	-2.22	101.25	112.24
51	N4	502	PLX	O3-P1-O2	-2.21	101.31	112.24
51	AL	202	PLX	O3-P1-O2	-2.20	101.37	112.24
51	S7	302	PLX	O3-P1-O2	-2.19	101.43	112.24
50	AK	401	ADP	C6-C5-N7	2.15	136.03	132.02
53	N1	403	U10	C52-C53-C54	-2.09	120.61	127.75
47	N5	705	PEE	C37-C38-C39	-2.09	108.71	124.73
47	S8	303	PEE	C17-C18-C19	-2.09	108.72	124.73
47	N4	501	PEE	C20-C19-C18	-2.06	108.94	124.73
50	AK	401	ADP	N9-C8-N7	-2.04	111.12	113.91
47	N5	701	PEE	C37-C38-C39	-2.03	109.13	124.73
47	S2	501	PEE	C20-C19-C18	-2.02	109.20	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	N5	701	PEE	C20-C19-C18	-2.02	109.20	124.73
47	N3	201	PEE	C37-C38-C39	-2.02	109.24	124.73
47	N5	702	PEE	C37-C38-C39	-2.01	109.28	124.73
47	N5	705	PEE	C17-C18-C19	-2.01	109.30	124.73
47	N4	501	PEE	C17-C18-C19	-2.01	109.32	124.73
47	N3	201	PEE	C20-C19-C18	-2.00	109.37	124.73

There are no chirality outliers.

All (773) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	4L	201	CDL	CA2-OA2-PA1-OA3
45	4L	201	CDL	CA2-OA2-PA1-OA4
45	4L	201	CDL	CA3-OA5-PA1-OA3
45	4L	201	CDL	CB2-OB2-PB2-OB4
45	A7	201	CDL	CB3-OB5-PB2-OB4
45	A8	301	CDL	CA2-OA2-PA1-OA3
45	A8	301	CDL	CA2-OA2-PA1-OA4
45	A8	301	CDL	CA3-OA5-PA1-OA4
45	A8	301	CDL	CB3-OB5-PB2-OB4
45	AK	402	CDL	CA2-OA2-PA1-OA4
45	AK	402	CDL	CA3-OA5-PA1-OA3
45	AK	402	CDL	CA3-OA5-PA1-OA4
45	AK	402	CDL	CB2-OB2-PB2-OB3
45	AK	402	CDL	CB2-OB2-PB2-OB4
45	AK	402	CDL	CB2-OB2-PB2-OB5
45	AL	201	CDL	C1-CA2-OA2-PA1
45	AL	201	CDL	CA2-OA2-PA1-OA3
45	AL	201	CDL	CB2-OB2-PB2-OB4
45	AL	201	CDL	CB3-OB5-PB2-OB4
45	B4	201	CDL	CA3-OA5-PA1-OA2
45	B4	201	CDL	CA3-OA5-PA1-OA3
45	B4	201	CDL	CB2-OB2-PB2-OB3
45	B5	201	CDL	CA2-OA2-PA1-OA3
45	B5	201	CDL	CB3-OB5-PB2-OB3
45	N1	401	CDL	CB2-OB2-PB2-OB4
45	N1	401	CDL	CB3-OB5-PB2-OB2
45	N4	503	CDL	CA2-OA2-PA1-OA4
45	N4	503	CDL	CA3-OA5-PA1-OA4
45	N4	504	CDL	CA2-OA2-PA1-OA3
45	N5	703	CDL	CA2-OA2-PA1-OA3
45	N5	703	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
45	N5	703	CDL	CA2-OA2-PA1-OA5
45	N5	703	CDL	CA3-OA5-PA1-OA3
45	N5	703	CDL	CB2-OB2-PB2-OB3
45	N5	703	CDL	CB2-OB2-PB2-OB4
45	N5	703	CDL	CB3-OB5-PB2-OB3
45	N5	704	CDL	CB2-OB2-PB2-OB4
47	A9	402	PEE	C4-O4P-P-O3P
47	A9	402	PEE	C4-O4P-P-O2P
47	A9	402	PEE	C4-O4P-P-O1P
47	N1	404	PEE	C1-O3P-P-O2P
47	N1	404	PEE	C4-O4P-P-O3P
47	N1	404	PEE	C4-O4P-P-O2P
47	N1	404	PEE	C4-O4P-P-O1P
47	N3	201	PEE	C17-C18-C19-C20
47	N3	201	PEE	C1-O3P-P-O2P
47	N3	201	PEE	C1-O3P-P-O1P
47	N3	201	PEE	C1-O3P-P-O4P
47	N4	501	PEE	C1-O3P-P-O2P
47	N4	501	PEE	C1-O3P-P-O1P
47	N4	501	PEE	C4-O4P-P-O2P
47	N4	501	PEE	C4-O4P-P-O1P
47	N4	501	PEE	O4P-C4-C5-N
47	N5	701	PEE	C4-O4P-P-O3P
47	N5	701	PEE	C4-O4P-P-O1P
47	N5	702	PEE	O4-C10-O2-C2
47	N5	702	PEE	C1-O3P-P-O2P
47	N5	702	PEE	C1-O3P-P-O4P
47	N5	702	PEE	C31-C30-O3-C3
47	S2	501	PEE	O4-C10-O2-C2
47	S2	501	PEE	C1-O3P-P-O2P
47	S2	501	PEE	C1-O3P-P-O1P
47	S2	501	PEE	C4-O4P-P-O3P
47	S2	501	PEE	C4-O4P-P-O2P
47	S2	501	PEE	C4-O4P-P-O1P
47	S8	303	PEE	O4-C10-O2-C2
47	S8	303	PEE	O3P-C1-C2-O2
47	S8	303	PEE	C1-O3P-P-O1P
48	A9	403	PC1	C1-O11-P-O12
48	A9	403	PC1	C1-O11-P-O14
48	A9	403	PC1	C1-O11-P-O13
48	N1	402	PC1	C11-O13-P-O12
48	N1	402	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
49	AC	201	ZMP	C17-C18-C21-O5
49	AC	201	ZMP	O1-C10-S1-C11
49	AC	201	ZMP	C9-C10-S1-C11
49	AC	201	ZMP	C7-C8-C9-C10
50	AK	401	ADP	C5'-O5'-PA-O2A
50	AK	401	ADP	C5'-O5'-PA-O3A
51	AL	202	PLX	O7-C6-C7-C8
51	AL	202	PLX	O7-C6-O6-C4
51	AL	202	PLX	C3-O4-P1-O2
51	AL	202	PLX	O9-C24-C25-C26
51	AM	201	PLX	O7-C6-O6-C4
51	AM	201	PLX	C3-O4-P1-O2
51	AM	201	PLX	C2-O1-P1-O4
51	AM	201	PLX	C2-O1-P1-O2
51	B1	101	PLX	O7-C6-O6-C4
51	B1	101	PLX	C3-O4-P1-O1
51	B1	101	PLX	C3-O4-P1-O2
51	B1	101	PLX	C3-O4-P1-O3
51	CB	201	PLX	C3-C4-O6-C6
51	CB	201	PLX	O9-C24-O8-C5
51	N4	502	PLX	O7-C6-O6-C4
51	N4	502	PLX	C3-O4-P1-O2
51	N4	502	PLX	C3-O4-P1-O3
51	N4	502	PLX	C25-C24-O8-C5
51	N6	201	PLX	O7-C6-O6-C4
51	N6	201	PLX	N1-C1-C2-O1
51	S7	302	PLX	O6-C6-C7-C8
51	S7	302	PLX	C2-O1-P1-O2
51	S7	302	PLX	O9-C24-C25-C26
52	B8	201	3PE	O13-C11-C12-N
52	CA	101	3PE	C11-O13-P-O11
52	CA	101	3PE	C11-O13-P-O14
52	CB	202	3PE	C1-O11-P-O12
52	CB	202	3PE	C1-O11-P-O14
52	CB	202	3PE	C11-O13-P-O11
52	CB	202	3PE	C11-O13-P-O12
52	CB	202	3PE	C11-O13-P-O14
52	N5	706	3PE	C1-O11-P-O12
52	N5	706	3PE	C11-O13-P-O14
52	S7	303	3PE	C2-C1-O11-P
52	S7	303	3PE	O13-C11-C12-N
53	N1	403	U10	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
53	N1	403	U10	C23-C24-C26-C27
53	N1	403	U10	C25-C24-C26-C27
53	N1	403	U10	C33-C34-C36-C37
53	N1	403	U10	C35-C34-C36-C37
53	N1	403	U10	C34-C36-C37-C38
47	N3	201	PEE	O5-C30-O3-C3
47	N4	501	PEE	O5-C30-O3-C3
47	N5	702	PEE	O5-C30-O3-C3
47	N3	201	PEE	C31-C30-O3-C3
47	N1	404	PEE	O5-C30-O3-C3
47	N4	501	PEE	C31-C30-O3-C3
47	N5	702	PEE	C11-C10-O2-C2
47	S2	501	PEE	C11-C10-O2-C2
47	S8	303	PEE	C11-C10-O2-C2
47	N1	404	PEE	C31-C30-O3-C3
47	N4	501	PEE	C17-C18-C19-C20
47	N4	501	PEE	C37-C38-C39-C40
47	N5	701	PEE	C17-C18-C19-C20
47	N5	705	PEE	C37-C38-C39-C40
47	S8	303	PEE	C37-C38-C39-C40
45	A7	201	CDL	O1-C1-CA2-OA2
47	A9	402	PEE	C31-C30-O3-C3
47	A9	402	PEE	C11-C10-O2-C2
47	N5	705	PEE	C11-C10-O2-C2
47	A9	402	PEE	O4-C10-O2-C2
47	N5	705	PEE	O4-C10-O2-C2
53	N1	403	U10	C13-C14-C16-C17
47	A9	402	PEE	O5-C30-O3-C3
53	N1	403	U10	C14-C16-C17-C18
53	N1	403	U10	C29-C31-C32-C33
53	N1	403	U10	C44-C46-C47-C48
53	N1	403	U10	C49-C51-C52-C53
47	S2	501	PEE	C31-C30-O3-C3
45	A8	301	CDL	CA2-C1-CB2-OB2
45	B4	201	CDL	CB2-C1-CA2-OA2
47	N5	702	PEE	O3P-C1-C2-O2
45	A8	301	CDL	O1-C1-CB2-OB2
45	B4	201	CDL	O1-C1-CA2-OA2
47	N3	201	PEE	C22-C23-C24-C25
47	N1	404	PEE	C30-C31-C32-C33
47	N5	702	PEE	C30-C31-C32-C33
52	CB	202	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
53	N1	403	U10	C19-C21-C22-C23
53	N1	403	U10	C24-C26-C27-C28
53	N1	403	U10	C39-C41-C42-C43
45	N1	401	CDL	O1-C1-CB2-OB2
47	N5	705	PEE	C33-C34-C35-C36
47	S2	501	PEE	O5-C30-O3-C3
47	N5	701	PEE	C37-C38-C39-C40
47	S8	303	PEE	C17-C18-C19-C20
45	4L	201	CDL	CA2-OA2-PA1-OA5
45	4L	201	CDL	CA3-OA5-PA1-OA2
45	4L	201	CDL	CB2-OB2-PB2-OB5
45	A7	201	CDL	CB3-OB5-PB2-OB2
45	A8	301	CDL	CA2-OA2-PA1-OA5
45	A8	301	CDL	CB2-OB2-PB2-OB5
45	A8	301	CDL	CB3-OB5-PB2-OB2
45	AK	402	CDL	CA2-OA2-PA1-OA5
45	AK	402	CDL	CA3-OA5-PA1-OA2
45	AL	201	CDL	CA2-OA2-PA1-OA5
45	AL	201	CDL	CB2-OB2-PB2-OB5
45	B4	201	CDL	CA2-OA2-PA1-OA5
45	B5	201	CDL	CA3-OA5-PA1-OA2
45	N1	401	CDL	CB2-OB2-PB2-OB5
45	N4	503	CDL	CA2-OA2-PA1-OA5
45	N4	503	CDL	CA3-OA5-PA1-OA2
45	N4	503	CDL	CB3-OB5-PB2-OB2
45	N4	504	CDL	CA2-OA2-PA1-OA5
45	N4	504	CDL	CA3-OA5-PA1-OA2
45	N4	504	CDL	CB2-OB2-PB2-OB5
45	N5	703	CDL	CA3-OA5-PA1-OA2
45	N5	703	CDL	CB2-OB2-PB2-OB5
45	N5	703	CDL	CB3-OB5-PB2-OB2
47	N1	404	PEE	C1-O3P-P-O4P
47	N3	201	PEE	C4-O4P-P-O3P
47	N4	501	PEE	C1-O3P-P-O4P
47	N4	501	PEE	C4-O4P-P-O3P
47	S2	501	PEE	C1-O3P-P-O4P
48	A9	403	PC1	C11-O13-P-O11
48	N1	402	PC1	C11-O13-P-O11
48	N1	402	PC1	C1-O11-P-O13
51	AL	202	PLX	C3-O4-P1-O1
51	N6	201	PLX	C3-O4-P1-O1
51	S7	302	PLX	C2-O1-P1-O4

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Mol	Chain	Res	Type	Atoms
52	CB	202	3PE	C1-O11-P-O13
52	N5	706	3PE	C1-O11-P-O13
52	S7	303	3PE	C1-O11-P-O13
47	N3	201	PEE	C11-C12-C13-C14
47	N1	404	PEE	C10-C11-C12-C13
45	A7	201	CDL	CB2-C1-CA2-OA2
45	N1	401	CDL	CA2-C1-CB2-OB2
47	S8	303	PEE	C31-C30-O3-C3
51	N6	201	PLX	O8-C24-C25-C26
51	S7	302	PLX	O8-C24-C25-C26
45	N4	503	CDL	C32-C33-C34-C35
45	N4	503	CDL	C78-C79-C80-C81
47	S8	303	PEE	C14-C15-C16-C17
47	S8	303	PEE	C33-C34-C35-C36
49	AB	201	ZMP	C1-C2-C3-C4
51	S7	302	PLX	C7-C8-C9-C10
52	CA	101	3PE	C23-C24-C25-C26
47	N1	404	PEE	C12-C13-C14-C15
47	N5	701	PEE	C14-C15-C16-C17
47	N5	702	PEE	C14-C15-C16-C17
47	N5	702	PEE	C12-C13-C14-C15
49	AC	201	ZMP	C1-C22-C23-C24
47	N5	702	PEE	C11-C12-C13-C14
51	N6	201	PLX	C35-C36-C37-C38
47	A9	402	PEE	C17-C18-C19-C20
48	A9	403	PC1	C23-C24-C25-C26
45	N5	704	CDL	C22-C23-C24-C25
45	N1	401	CDL	C76-C77-C78-C79
49	AB	201	ZMP	C3-C4-C5-C6
49	AC	201	ZMP	C6-C7-C8-C9
51	N6	201	PLX	C34-C35-C36-C37
45	N4	503	CDL	C61-C62-C63-C64
47	N5	701	PEE	C31-C32-C33-C34
51	AL	202	PLX	C29-C30-C31-C32
51	S7	302	PLX	C13-C14-C15-C16
45	4L	201	CDL	C39-C40-C41-C42
51	AL	202	PLX	C7-C8-C9-C10
45	N5	704	CDL	C72-C73-C74-C75
47	N4	501	PEE	C23-C24-C25-C26
47	N4	501	PEE	C11-C10-O2-C2
45	N5	703	CDL	C60-C61-C62-C63
47	A9	402	PEE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
47	N3	201	PEE	C32-C33-C34-C35
47	N3	201	PEE	C33-C34-C35-C36
47	N5	705	PEE	C21-C22-C23-C24
51	N4	502	PLX	C12-C13-C14-C15
47	N3	201	PEE	C21-C22-C23-C24
47	N5	701	PEE	O4P-C4-C5-N
47	S2	501	PEE	O4P-C4-C5-N
45	N4	503	CDL	C38-C39-C40-C41
49	AB	201	ZMP	C5-C6-C7-C8
51	CB	201	PLX	C7-C8-C9-C10
47	N3	201	PEE	C10-C11-C12-C13
45	AL	201	CDL	C52-C53-C54-C55
45	N1	401	CDL	C12-C13-C14-C15
47	S2	501	PEE	C34-C35-C36-C37
47	N4	501	PEE	C22-C23-C24-C25
45	B4	201	CDL	C32-C33-C34-C35
47	N5	701	PEE	C21-C22-C23-C24
47	N5	701	PEE	C11-C12-C13-C14
51	AM	201	PLX	C31-C32-C33-C34
51	AL	202	PLX	C3-C4-C5-O8
47	N5	701	PEE	C32-C33-C34-C35
51	CB	201	PLX	C31-C32-C33-C34
47	A9	402	PEE	C11-C12-C13-C14
47	N5	701	PEE	C33-C34-C35-C36
47	N1	404	PEE	C33-C34-C35-C36
51	AM	201	PLX	O9-C24-C25-C26
51	B1	101	PLX	O9-C24-C25-C26
51	S7	302	PLX	O7-C6-C7-C8
47	N4	501	PEE	C39-C40-C41-C42
47	N5	701	PEE	C15-C16-C17-C18
47	N5	705	PEE	C35-C36-C37-C38
47	S2	501	PEE	C35-C36-C37-C38
47	S8	303	PEE	C15-C16-C17-C18
47	S8	303	PEE	C35-C36-C37-C38
47	A9	402	PEE	C10-C11-C12-C13
49	AB	201	ZMP	C22-C23-C24-C25
48	N1	402	PC1	C37-C38-C39-C3A
49	AB	201	ZMP	C2-C1-C22-C23
47	S8	303	PEE	O5-C30-O3-C3
47	N4	501	PEE	O4-C10-O2-C2
51	S7	302	PLX	C32-C33-C34-C35
47	A9	402	PEE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
47	N5	701	PEE	C12-C13-C14-C15
47	S2	501	PEE	C13-C14-C15-C16
51	N4	502	PLX	C34-C35-C36-C37
45	4L	201	CDL	CA5-C11-C12-C13
52	S7	303	3PE	C21-C22-C23-C24
47	N5	702	PEE	C18-C19-C20-C21
51	N6	201	PLX	C28-C29-C30-C31
47	N5	702	PEE	C37-C38-C39-C40
45	AL	201	CDL	C33-C34-C35-C36
47	N4	501	PEE	C35-C36-C37-C38
51	S7	302	PLX	C27-C28-C29-C30
47	N1	404	PEE	C11-C12-C13-C14
45	B5	201	CDL	C17-C18-C19-C20
49	AC	201	ZMP	C22-C23-C24-C25
52	CA	101	3PE	C35-C36-C37-C38
47	N4	501	PEE	C11-C12-C13-C14
47	N5	702	PEE	C10-C11-C12-C13
47	N5	701	PEE	C11-C10-O2-C2
47	N5	705	PEE	O3P-C1-C2-O2
51	CB	201	PLX	O4-C3-C4-O6
45	N4	503	CDL	O1-C1-CA2-OA2
45	A8	301	CDL	OB6-CB4-CB6-OB8
47	A9	402	PEE	O2-C2-C3-O3
51	AL	202	PLX	O6-C4-C5-O8
52	S7	303	3PE	O21-C2-C3-O31
47	S8	303	PEE	C22-C23-C24-C25
47	S2	501	PEE	C42-C43-C44-C45
51	S7	302	PLX	C14-C15-C16-C17
47	A9	402	PEE	C35-C36-C37-C38
47	N5	702	PEE	C35-C36-C37-C38
47	S2	501	PEE	C19-C20-C21-C22
45	N4	504	CDL	CA7-C31-C32-C33
47	S8	303	PEE	C42-C43-C44-C45
45	N4	503	CDL	C77-C78-C79-C80
47	N5	701	PEE	O4-C10-O2-C2
47	N5	702	PEE	C33-C34-C35-C36
47	S2	501	PEE	C16-C17-C18-C19
47	S2	501	PEE	C38-C39-C40-C41
45	B4	201	CDL	CB2-OB2-PB2-OB5
45	B5	201	CDL	CA2-OA2-PA1-OA5
47	S8	303	PEE	C1-O3P-P-O4P
51	AM	201	PLX	C3-O4-P1-O1

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Mol	Chain	Res	Type	Atoms
51	N4	502	PLX	C3-O4-P1-O1
47	S2	501	PEE	C20-C21-C22-C23
48	N1	402	PC1	C2-C1-O11-P
51	CB	201	PLX	C11-C12-C13-C14
45	AL	201	CDL	OB5-CB3-CB4-CB6
47	N5	702	PEE	O3P-C1-C2-C3
49	AC	201	ZMP	C1-C2-C3-C4
51	CB	201	PLX	C17-C18-C19-C20
47	N3	201	PEE	C30-C31-C32-C33
45	B5	201	CDL	CB2-C1-CA2-OA2
51	AM	201	PLX	C25-C26-C27-C28
45	AK	402	CDL	C53-C54-C55-C56
47	N3	201	PEE	C23-C24-C25-C26
45	A8	301	CDL	CB3-CB4-CB6-OB8
45	N4	503	CDL	CB3-CB4-CB6-OB8
45	N4	504	CDL	CA3-CA4-CA6-OA8
47	N1	404	PEE	C1-C2-C3-O3
47	N4	501	PEE	C1-C2-C3-O3
47	N5	701	PEE	C1-C2-C3-O3
51	B1	101	PLX	C3-C4-C5-O8
52	S7	303	3PE	C1-C2-C3-O31
45	N5	703	CDL	C52-C53-C54-C55
45	N5	704	CDL	C59-C60-C61-C62
47	S2	501	PEE	C43-C44-C45-C46
47	N4	501	PEE	C24-C25-C26-C27
49	AC	201	ZMP	C2-C3-C4-C5
51	AL	202	PLX	O6-C6-C7-C8
51	AM	201	PLX	O6-C6-C7-C8
51	N6	201	PLX	O6-C6-C7-C8
49	AB	201	ZMP	O3-C16-C17-O4
49	AC	201	ZMP	O3-C16-C17-O4
47	S2	501	PEE	C33-C34-C35-C36
51	AL	202	PLX	C14-C15-C16-C17
47	N3	201	PEE	C35-C36-C37-C38
47	N5	701	PEE	C35-C36-C37-C38
47	S2	501	PEE	C15-C16-C17-C18
45	N4	503	CDL	C62-C63-C64-C65
51	AL	202	PLX	C32-C33-C34-C35
49	AC	201	ZMP	C22-C1-C2-C3
45	A8	301	CDL	OA5-CA3-CA4-OA6
45	N4	503	CDL	OA5-CA3-CA4-OA6
49	AC	201	ZMP	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
51	N4	502	PLX	C31-C32-C33-C34
45	N1	401	CDL	C75-C76-C77-C78
51	N4	502	PLX	O6-C4-C5-O8
45	N5	704	CDL	C17-C18-C19-C20
49	AB	201	ZMP	C6-C7-C8-C9
45	4L	201	CDL	C15-C16-C17-C18
51	AM	201	PLX	C12-C13-C14-C15
47	S2	501	PEE	C18-C19-C20-C21
45	B5	201	CDL	OB5-CB3-CB4-CB6
47	A9	402	PEE	O3P-C1-C2-C3
47	N4	501	PEE	O3P-C1-C2-C3
47	N5	701	PEE	O3P-C1-C2-C3
47	N5	705	PEE	O3P-C1-C2-C3
47	S8	303	PEE	O3P-C1-C2-C3
51	CB	201	PLX	O4-C3-C4-C5
52	S7	303	3PE	O11-C1-C2-C3
45	A8	301	CDL	C11-C12-C13-C14
45	N4	503	CDL	CB5-C51-C52-C53
45	N4	503	CDL	C33-C34-C35-C36
47	N5	705	PEE	C14-C15-C16-C17
45	N4	504	CDL	C13-C14-C15-C16
47	A9	402	PEE	C34-C35-C36-C37
48	A9	403	PC1	C32-C33-C34-C35
47	N4	501	PEE	C10-C11-C12-C13
47	S8	303	PEE	C12-C13-C14-C15
47	S8	303	PEE	C34-C35-C36-C37
45	B5	201	CDL	CB4-CB3-OB5-PB2
47	N3	201	PEE	C38-C39-C40-C41
47	S8	303	PEE	C1-C2-C3-O3
51	AM	201	PLX	C3-C4-C5-O8
51	N4	502	PLX	C3-C4-C5-O8
51	N6	201	PLX	C3-C4-C5-O8
45	A8	301	CDL	C17-C18-C19-C20
49	AB	201	ZMP	C4-C5-C6-C7
45	AL	201	CDL	CB3-OB5-PB2-OB2
45	N5	704	CDL	CB2-OB2-PB2-OB5
47	N5	702	PEE	C4-O4P-P-O3P
51	B1	101	PLX	C5-C4-O6-C6
51	N4	502	PLX	C3-C4-O6-C6
51	N4	502	PLX	C5-C4-O6-C6
51	N6	201	PLX	C5-C4-O6-C6
45	B4	201	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
51	N6	201	PLX	O9-C24-C25-C26
45	B4	201	CDL	C74-C75-C76-C77
45	AL	201	CDL	OB5-CB3-CB4-OB6
45	B4	201	CDL	OB5-CB3-CB4-OB6
45	N4	504	CDL	OB5-CB3-CB4-OB6
51	AM	201	PLX	O4-C3-C4-O6
47	N5	705	PEE	C24-C25-C26-C27
51	N4	502	PLX	C29-C30-C31-C32
45	AL	201	CDL	OB6-CB4-CB6-OB8
47	N4	501	PEE	O2-C2-C3-O3
47	N4	501	PEE	C32-C33-C34-C35
47	S2	501	PEE	C12-C13-C14-C15
51	B1	101	PLX	C29-C30-C31-C32
47	S2	501	PEE	C21-C22-C23-C24
47	S8	303	PEE	C13-C14-C15-C16
51	B1	101	PLX	C25-C26-C27-C28
45	N4	504	CDL	C1-CA2-OA2-PA1
45	N4	504	CDL	CB4-CB3-OB5-PB2
47	S2	501	PEE	C2-C1-O3P-P
45	B4	201	CDL	C73-C74-C75-C76
45	N4	503	CDL	C12-C13-C14-C15
51	N6	201	PLX	C7-C8-C9-C10
47	N5	701	PEE	C22-C23-C24-C25
47	A9	402	PEE	C31-C32-C33-C34
51	AL	202	PLX	C30-C31-C32-C33
45	N1	401	CDL	C32-C33-C34-C35
51	CB	201	PLX	C15-C16-C17-C18
51	CB	201	PLX	C16-C17-C18-C19
45	4L	201	CDL	OB5-CB3-CB4-CB6
45	A8	301	CDL	OA5-CA3-CA4-CA6
45	A8	301	CDL	OB5-CB3-CB4-CB6
51	AM	201	PLX	O4-C3-C4-C5
51	N6	201	PLX	O4-C3-C4-C5
47	A9	402	PEE	C15-C16-C17-C18
51	CB	201	PLX	C29-C30-C31-C32
49	AC	201	ZMP	N2-C16-C17-O4
51	AM	201	PLX	C27-C28-C29-C30
45	B4	201	CDL	C80-C81-C82-C83
47	N5	705	PEE	C22-C23-C24-C25
51	N6	201	PLX	C29-C30-C31-C32
47	S8	303	PEE	C3-C2-O2-C10
52	B8	201	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
47	N5	701	PEE	C30-C31-C32-C33
45	B5	201	CDL	CB3-CB4-CB6-OB8
45	N5	704	CDL	CA4-CA3-OA5-PA1
47	N1	404	PEE	C14-C15-C16-C17
45	4L	201	CDL	OB5-CB3-CB4-OB6
45	A8	301	CDL	OB5-CB3-CB4-OB6
45	AK	402	CDL	OA5-CA3-CA4-OA6
47	A9	402	PEE	O3P-C1-C2-O2
51	N4	502	PLX	C9-C10-C11-C12
57	S2	502	MF8	N06-C04-N02-C01
52	N5	706	3PE	C22-C23-C24-C25
51	AL	202	PLX	C28-C29-C30-C31
47	S8	303	PEE	O2-C2-C3-O3
51	S7	302	PLX	C15-C16-C17-C18
45	A8	301	CDL	C38-C39-C40-C41
45	N5	704	CDL	CB5-C51-C52-C53
51	S7	302	PLX	C6-C7-C8-C9
45	A7	201	CDL	CA2-OA2-PA1-OA5
45	B5	201	CDL	CB3-OB5-PB2-OB2
51	B1	101	PLX	C2-O1-P1-O4
51	N6	201	PLX	C2-O1-P1-O4
51	S7	302	PLX	C3-O4-P1-O1
52	B8	201	3PE	C1-O11-P-O13
52	N5	706	3PE	C11-O13-P-O11
51	CB	201	PLX	C9-C10-C11-C12
45	N5	703	CDL	C1-CB2-OB2-PB2
50	AK	401	ADP	C4'-C5'-O5'-PA
48	N1	402	PC1	C27-C28-C29-C2A
45	4L	201	CDL	CA3-OA5-PA1-OA4
45	A8	301	CDL	CB2-OB2-PB2-OB3
45	AK	402	CDL	CA2-OA2-PA1-OA3
45	AL	201	CDL	CA2-OA2-PA1-OA4
45	AL	201	CDL	CB3-OB5-PB2-OB3
45	B4	201	CDL	CA2-OA2-PA1-OA3
45	B4	201	CDL	CB2-OB2-PB2-OB4
45	B5	201	CDL	CA3-OA5-PA1-OA3
45	B5	201	CDL	CA3-OA5-PA1-OA4
45	N1	401	CDL	CB2-OB2-PB2-OB3
45	N1	401	CDL	CB3-OB5-PB2-OB3
45	N4	503	CDL	CB3-OB5-PB2-OB3
45	N4	504	CDL	CA2-OA2-PA1-OA4
45	N4	504	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
45	N5	703	CDL	CA3-OA5-PA1-OA4
45	N5	703	CDL	CB3-OB5-PB2-OB4
45	N5	704	CDL	CB2-OB2-PB2-OB3
47	N1	404	PEE	C1-O3P-P-O1P
47	N3	201	PEE	C4-O4P-P-O2P
47	N5	702	PEE	C1-O3P-P-O1P
47	N5	705	PEE	C4-O4P-P-O1P
47	S8	303	PEE	C4-O4P-P-O2P
48	A9	403	PC1	C11-O13-P-O14
48	N1	402	PC1	C11-O13-P-O14
51	AL	202	PLX	C3-O4-P1-O3
51	AL	202	PLX	C2-O1-P1-O3
51	N6	201	PLX	C3-O4-P1-O2
51	N6	201	PLX	C3-O4-P1-O3
52	N5	706	3PE	C11-O13-P-O12
52	S7	303	3PE	C1-O11-P-O14
47	N1	404	PEE	C13-C14-C15-C16
51	N4	502	PLX	C13-C14-C15-C16
45	N4	504	CDL	OB5-CB3-CB4-CB6
47	N3	201	PEE	C5-C4-O4P-P
51	AL	202	PLX	C25-C24-O8-C5
51	N6	201	PLX	C25-C24-O8-C5
51	S7	302	PLX	C25-C24-O8-C5
52	CB	202	3PE	C12-C11-O13-P
48	A9	403	PC1	C28-C29-C2A-C2B
52	CB	202	3PE	C39-C3A-C3B-C3C
51	AM	201	PLX	C14-C15-C16-C17
47	N4	501	PEE	O3P-C1-C2-O2
47	N5	701	PEE	O3P-C1-C2-O2
45	B5	201	CDL	O1-C1-CA2-OA2
48	N1	402	PC1	C11-C12-N-C15
47	N4	501	PEE	C34-C35-C36-C37
51	N4	502	PLX	C33-C34-C35-C36
47	N5	705	PEE	C1-C2-C3-O3
48	A9	403	PC1	O13-C11-C12-N
51	AM	201	PLX	N1-C1-C2-O1
51	CB	201	PLX	C3-C4-C5-O8
45	B5	201	CDL	OB6-CB4-CB6-OB8
45	N4	503	CDL	OB6-CB4-CB6-OB8
45	N4	504	CDL	OA6-CA4-CA6-OA8
47	N1	404	PEE	O2-C2-C3-O3
47	N5	701	PEE	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
47	N5	705	PEE	O2-C2-C3-O3
51	AM	201	PLX	O6-C4-C5-O8
51	B1	101	PLX	O6-C4-C5-O8
51	CB	201	PLX	O6-C4-C5-O8
51	N6	201	PLX	O6-C4-C5-O8
45	N4	503	CDL	CB4-CB3-OB5-PB2
51	S7	302	PLX	C25-C26-C27-C28
45	4L	201	CDL	C23-C24-C25-C26
45	AL	201	CDL	C52-C51-CB5-OB6
51	AL	202	PLX	O8-C24-C25-C26
51	CB	201	PLX	O8-C24-C25-C26
51	CB	201	PLX	O7-C6-C7-C8
51	CB	201	PLX	O9-C24-C25-C26
47	N5	705	PEE	C19-C20-C21-C22
51	AL	202	PLX	C33-C34-C35-C36
49	AC	201	ZMP	C20-C18-C21-O5
45	N1	401	CDL	C13-C14-C15-C16
47	S2	501	PEE	C40-C41-C42-C43
45	4L	201	CDL	CA6-CA4-OA6-CA5
52	CA	101	3PE	C29-C2A-C2B-C2C
45	N4	503	CDL	C21-C22-C23-C24
47	A9	402	PEE	C2-C1-O3P-P
51	N6	201	PLX	O4-C3-C4-O6
51	S7	302	PLX	O4-C3-C4-O6
48	N1	402	PC1	C11-C12-N-C14
46	A9	401	NDP	O4D-C1D-N1N-C6N
45	AL	201	CDL	C36-C37-C38-C39
49	AC	201	ZMP	C14-C15-N2-C16
45	A7	201	CDL	CB2-OB2-PB2-OB5
45	AL	201	CDL	CA3-OA5-PA1-OA2
45	N1	401	CDL	CA2-OA2-PA1-OA5
45	N5	704	CDL	CA3-OA5-PA1-OA2
51	CB	201	PLX	C2-O1-P1-O4
51	N4	502	PLX	C2-O1-P1-O4
45	N5	703	CDL	C33-C34-C35-C36
47	N5	702	PEE	C32-C33-C34-C35
47	N4	501	PEE	C12-C13-C14-C15
47	A9	402	PEE	C1-C2-C3-O3
45	N4	504	CDL	C72-C71-CB7-OB8
45	N4	504	CDL	C72-C71-CB7-OB9
46	A9	401	NDP	PN-O3-PA-O1A
51	AM	201	PLX	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
45	B5	201	CDL	C1-CA2-OA2-PA1
45	N5	704	CDL	C1-CA2-OA2-PA1
57	S2	502	MF8	N08-C07-N06-C04
51	AL	202	PLX	C11-C10-C9-C8
52	CA	101	3PE	C24-C25-C26-C27
47	N5	705	PEE	C18-C19-C20-C21
48	A9	403	PC1	C38-C39-C3A-C3B
47	S8	303	PEE	C21-C22-C23-C24
47	S8	303	PEE	O4P-C4-C5-N
45	N5	703	CDL	OA5-CA3-CA4-OA6
45	N1	401	CDL	C73-C74-C75-C76
57	S2	502	MF8	N06-C04-N02-C03
53	N1	403	U10	C50-C49-C51-C52
51	N6	201	PLX	C10-C11-C12-C13
49	AB	201	ZMP	O3-C16-C17-C18
45	AK	402	CDL	C1-CA2-OA2-PA1
45	N4	504	CDL	CA4-CA3-OA5-PA1
49	AC	201	ZMP	S1-C11-C12-N1
46	A9	401	NDP	C2D-C1D-N1N-C6N
51	AM	201	PLX	C7-C8-C9-C10
51	S7	302	PLX	C12-C13-C14-C15
45	N4	503	CDL	C81-C82-C83-C84
45	N5	704	CDL	C15-C16-C17-C18
51	B1	101	PLX	C24-C25-C26-C27
45	N5	703	CDL	CA3-CA4-CA6-OA8
45	N5	704	CDL	CB3-CB4-CB6-OB8
49	AC	201	ZMP	C19-C18-C21-O5
45	N5	703	CDL	C36-C37-C38-C39
49	AB	201	ZMP	N2-C16-C17-C18
47	S8	303	PEE	C19-C20-C21-C22
51	N6	201	PLX	C26-C27-C28-C29
45	AK	402	CDL	CA6-CA4-OA6-CA5
47	N4	501	PEE	C1-C2-O2-C10
52	S7	303	3PE	C1-C2-O21-C21
48	N1	402	PC1	C11-C12-N-C13
47	N3	201	PEE	C40-C41-C42-C43
47	N5	702	PEE	C36-C37-C38-C39
51	AM	201	PLX	C5-C4-O6-C6
57	S2	502	MF8	N05-C04-N02-C01
47	N3	201	PEE	C41-C42-C43-C44
47	N5	702	PEE	C34-C35-C36-C37
51	N4	502	PLX	C4-C3-O4-P1

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Mol	Chain	Res	Type	Atoms
45	N5	704	CDL	C42-C43-C44-C45
51	S7	302	PLX	O4-C3-C4-C5
48	A9	403	PC1	C29-C2A-C2B-C2C
51	B1	101	PLX	C11-C12-C13-C14
49	AB	201	ZMP	C12-C11-S1-C10
49	AC	201	ZMP	C12-C11-S1-C10
45	N5	704	CDL	OB6-CB4-CB6-OB8
51	B1	101	PLX	C20-C21-C22-C23
45	N1	401	CDL	C78-C79-C80-C81
45	B5	201	CDL	CA2-C1-CB2-OB2
53	N1	403	U10	C48-C49-C51-C52
47	A9	402	PEE	C18-C19-C20-C21
45	4L	201	CDL	C17-C18-C19-C20
52	CB	202	3PE	C26-C27-C28-C29
45	N4	503	CDL	C72-C71-CB7-OB8
45	N5	704	CDL	C12-C11-CA5-OA6
47	N5	701	PEE	C16-C17-C18-C19
48	A9	403	PC1	C22-C23-C24-C25
53	N1	403	U10	C45-C44-C46-C47
51	S7	302	PLX	C19-C20-C21-C22
51	B1	101	PLX	C4-C5-O8-C24
45	N5	703	CDL	C53-C54-C55-C56
49	AC	201	ZMP	S1-C10-C9-C8
49	AC	201	ZMP	O1-C10-C9-C8
51	AM	201	PLX	O8-C24-C25-C26
51	CB	201	PLX	C2-C1-N1-C1C
51	CB	201	PLX	C36-C37-C38-C39
51	S7	302	PLX	C11-C10-C9-C8
45	B4	201	CDL	OB5-CB3-CB4-CB6
45	N4	503	CDL	OA5-CA3-CA4-CA6
45	4L	201	CDL	C52-C51-CB5-OB6
53	N1	403	U10	C9-C11-C12-C13
45	A8	301	CDL	C33-C34-C35-C36
45	B4	201	CDL	C12-C11-CA5-OA6
45	N5	703	CDL	OA6-CA4-CA6-OA8
45	N5	704	CDL	OA6-CA4-CA6-OA8
51	CB	201	PLX	C11-C10-C9-C8
45	A8	301	CDL	C32-C31-CA7-OA8
51	B1	101	PLX	C13-C14-C15-C16
48	A9	403	PC1	C3A-C3B-C3C-C3D
45	A8	301	CDL	C22-C23-C24-C25
45	AL	201	CDL	CA6-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
45	B5	201	CDL	CB6-CB4-OB6-CB5
45	N4	504	CDL	CB6-CB4-OB6-CB5
45	N5	703	CDL	C12-C11-CA5-OA6
47	N3	201	PEE	C36-C37-C38-C39
47	N4	501	PEE	C40-C41-C42-C43
45	AL	201	CDL	CB3-CB4-CB6-OB8
51	AL	202	PLX	C7-C6-O6-C4
52	N5	706	3PE	C1-C2-C3-O31
51	N4	502	PLX	C17-C18-C19-C20
47	N1	404	PEE	O2-C10-C11-C12
48	N1	402	PC1	O21-C21-C22-C23
51	CB	201	PLX	C28-C29-C30-C31
46	A9	401	NDP	O4B-C4B-C5B-O5B
47	N5	705	PEE	C11-C12-C13-C14
45	A7	201	CDL	C72-C71-CB7-OB8
45	B5	201	CDL	O1-C1-CB2-OB2
45	N5	703	CDL	OB5-CB3-CB4-CB6
45	B5	201	CDL	C80-C81-C82-C83
47	S8	303	PEE	C11-C12-C13-C14
45	N5	703	CDL	C72-C71-CB7-OB8
47	N4	501	PEE	O2-C10-C11-C12
47	N5	701	PEE	O2-C10-C11-C12
47	S2	501	PEE	O2-C10-C11-C12
47	S2	501	PEE	C44-C45-C46-C47
45	B5	201	CDL	C21-C22-C23-C24
46	A9	401	NDP	C5D-O5D-PN-O3
45	B4	201	CDL	C32-C31-CA7-OA8
45	N5	703	CDL	C52-C51-CB5-OB6
45	A8	301	CDL	C32-C31-CA7-OA9
45	B5	201	CDL	C22-C23-C24-C25
47	N5	705	PEE	C31-C32-C33-C34
50	AK	401	ADP	O4'-C4'-C5'-O5'
45	AL	201	CDL	C32-C31-CA7-OA8
48	N1	402	PC1	O22-C21-C22-C23
47	A9	402	PEE	O2-C10-C11-C12
48	A9	403	PC1	C26-C27-C28-C29
51	S7	302	PLX	C29-C30-C31-C32
52	CA	101	3PE	C31-C32-C33-C34
52	B8	201	3PE	O21-C21-C22-C23
51	AM	201	PLX	C26-C27-C28-C29
45	N4	503	CDL	CA5-C11-C12-C13
45	N5	703	CDL	C52-C51-CB5-OB7

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Mol	Chain	Res	Type	Atoms
47	N1	404	PEE	O4-C10-C11-C12
47	N3	201	PEE	C24-C25-C26-C27
47	S2	501	PEE	C11-C12-C13-C14
52	CA	101	3PE	C2B-C2C-C2D-C2E
45	A7	201	CDL	C72-C71-CB7-OB9
45	N5	703	CDL	C12-C11-CA5-OA7
47	N4	501	PEE	O4-C10-C11-C12
45	4L	201	CDL	CB3-OB5-PB2-OB3
45	A8	301	CDL	CA3-OA5-PA1-OA3
45	B5	201	CDL	CA2-OA2-PA1-OA4
45	N1	401	CDL	CA3-OA5-PA1-OA3
45	N4	503	CDL	CB2-OB2-PB2-OB3
45	N4	504	CDL	CA3-OA5-PA1-OA3
45	N4	504	CDL	CB3-OB5-PB2-OB3
45	N5	704	CDL	CB3-OB5-PB2-OB3
47	A9	402	PEE	C1-O3P-P-O1P
47	N5	705	PEE	C1-O3P-P-O1P
50	AK	401	ADP	C5'-O5'-PA-O1A
51	AM	201	PLX	C3-O4-P1-O3
51	B1	101	PLX	C2-O1-P1-O2
51	CB	201	PLX	C2-O1-P1-O2
51	CB	201	PLX	C2-C1-N1-C1B
51	N6	201	PLX	C2-O1-P1-O2
51	S7	302	PLX	C3-O4-P1-O2
52	B8	201	3PE	C1-O11-P-O12
45	B4	201	CDL	C12-C11-CA5-OA7
47	A9	402	PEE	O4-C10-C11-C12
47	N5	701	PEE	O4-C10-C11-C12
45	AL	201	CDL	C12-C11-CA5-OA6
51	S7	302	PLX	C17-C18-C19-C20
52	CA	101	3PE	C36-C37-C38-C39
47	A9	402	PEE	O4P-C4-C5-N
52	CA	101	3PE	C2A-C2B-C2C-C2D
57	S2	502	MF8	N09-C07-N06-C04
47	N3	201	PEE	O2-C10-C11-C12
45	AL	201	CDL	CA3-CA4-OA6-CA5
45	N4	504	CDL	CB3-CB4-OB6-CB5
47	A9	402	PEE	C5-C4-O4P-P
47	N1	404	PEE	C5-C4-O4P-P
47	N4	501	PEE	C3-C2-O2-C10
47	N5	701	PEE	C5-C4-O4P-P
51	AM	201	PLX	C1-C2-O1-P1

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Mol	Chain	Res	Type	Atoms
52	CA	101	3PE	C12-C11-O13-P
52	S7	303	3PE	C12-C11-O13-P
45	B4	201	CDL	C32-C31-CA7-OA9
45	4L	201	CDL	C12-C11-CA5-OA6
47	S2	501	PEE	C14-C15-C16-C17
51	CB	201	PLX	C2-C1-N1-C1A
45	B5	201	CDL	C12-C11-CA5-OA6
45	A8	301	CDL	C54-C55-C56-C57
45	N5	704	CDL	C72-C71-CB7-OB8
45	N5	703	CDL	C72-C71-CB7-OB9
47	S2	501	PEE	O4-C10-C11-C12
45	AL	201	CDL	CB4-CB3-OB5-PB2
52	B8	201	3PE	C2-C1-O11-P
51	CB	201	PLX	C24-C25-C26-C27
45	AL	201	CDL	C32-C31-CA7-OA9
48	N1	402	PC1	C2F-C2G-C2H-C2I
45	AK	402	CDL	C72-C71-CB7-OB8
47	N5	705	PEE	O2-C10-C11-C12
47	S2	501	PEE	C36-C37-C38-C39
45	AL	201	CDL	C12-C11-CA5-OA7
45	N5	704	CDL	C72-C71-CB7-OB9
52	S7	303	3PE	C3B-C3C-C3D-C3E
47	N3	201	PEE	C15-C16-C17-C18
48	A9	403	PC1	C3B-C3C-C3D-C3E
45	B5	201	CDL	C12-C11-CA5-OA7
52	N5	706	3PE	C23-C24-C25-C26
52	B8	201	3PE	O22-C21-C22-C23
52	B8	201	3PE	C25-C26-C27-C28

There are no ring outliers.

42 monomers are involved in 148 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	N1	402	PC1	2	0
54	S1	802	SF4	1	0
47	N5	705	PEE	3	0
53	N1	403	U10	10	0
50	AK	401	ADP	4	0
47	N5	702	PEE	1	0
45	N5	703	CDL	8	0
47	A9	402	PEE	4	0
51	AL	202	PLX	1	0

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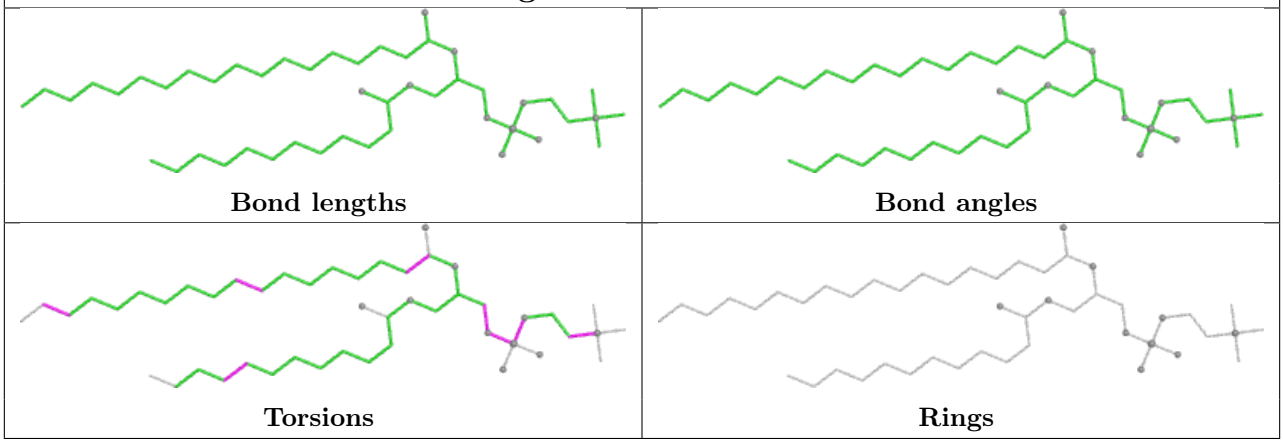
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	S7	303	3PE	1	0
45	N1	401	CDL	5	0
47	N5	701	PEE	5	0
52	N5	706	3PE	1	0
51	B1	101	PLX	2	0
52	CA	101	3PE	2	0
59	V1	502	FMN	1	0
46	A9	401	NDP	1	0
47	S8	303	PEE	8	0
49	AC	201	ZMP	2	0
49	AB	201	ZMP	2	0
45	N4	503	CDL	6	0
51	N6	201	PLX	3	0
52	CB	202	3PE	1	0
45	B5	201	CDL	9	0
45	A7	201	CDL	1	0
47	N1	404	PEE	3	0
48	A9	403	PC1	2	0
47	N4	501	PEE	6	0
51	CB	201	PLX	5	0
45	N4	504	CDL	2	0
51	S7	302	PLX	5	0
45	AK	402	CDL	3	0
54	S8	302	SF4	1	0
47	S2	501	PEE	6	0
45	AL	201	CDL	7	0
51	N4	502	PLX	6	0
45	N5	704	CDL	2	0
51	AM	201	PLX	4	0
45	4L	201	CDL	9	0
45	A8	301	CDL	9	0
45	B4	201	CDL	3	0
47	N3	201	PEE	4	0

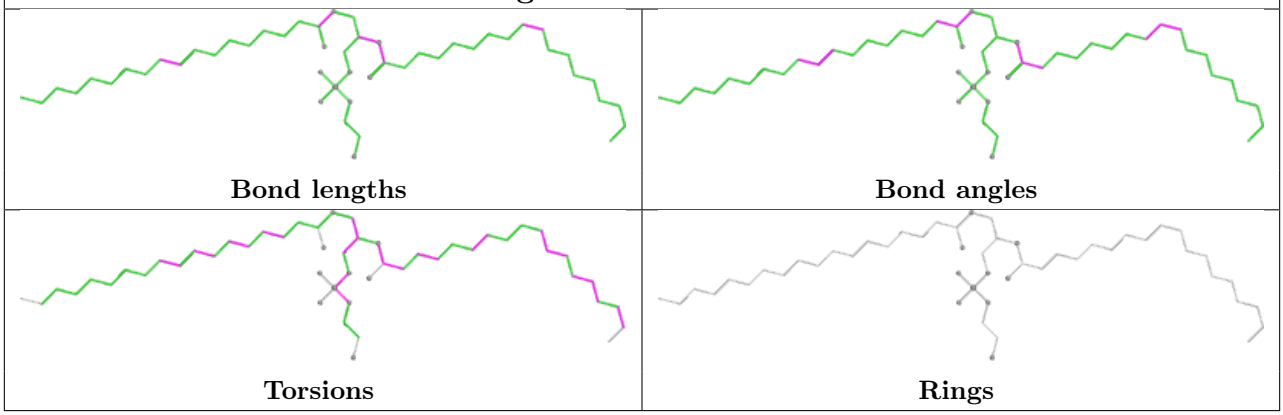
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

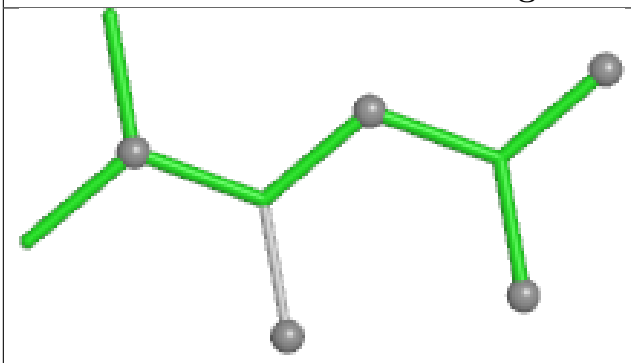
Ligand PC1 N1 402



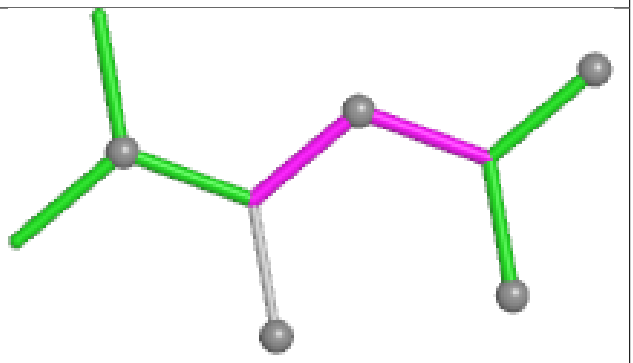
Ligand PEE N5 705



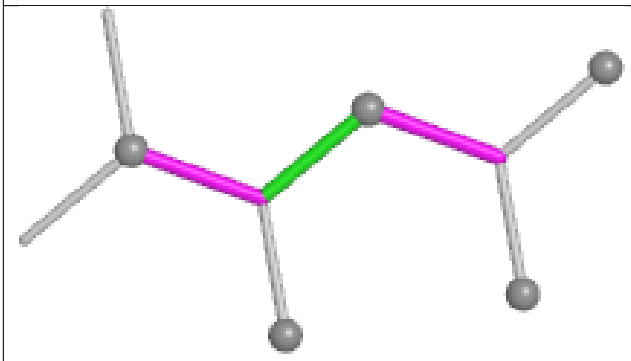
Ligand MF8 S2 502



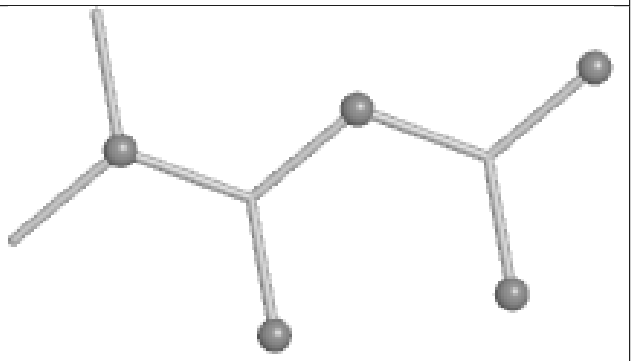
Bond lengths



Bond angles

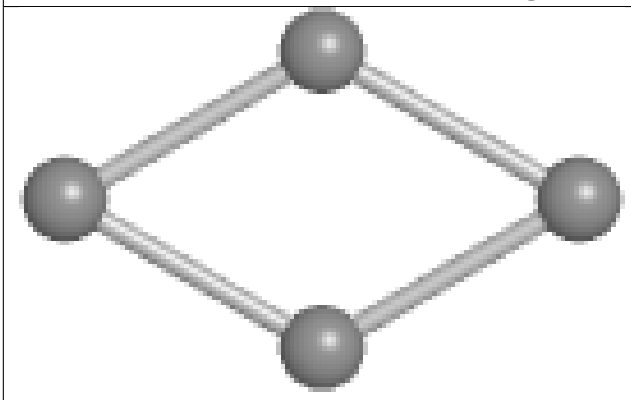


Torsions

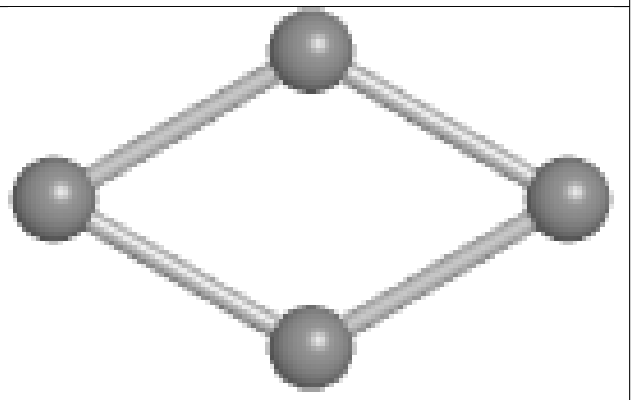


Rings

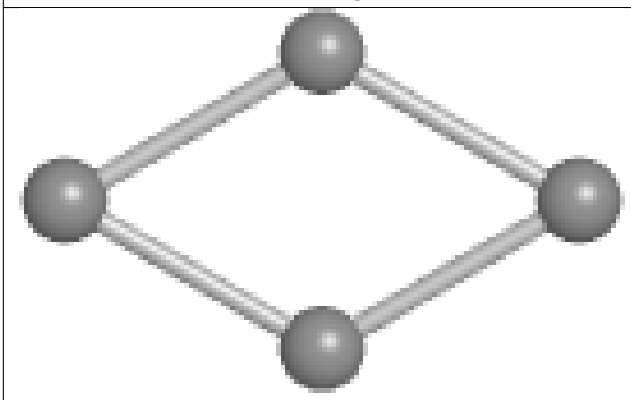
Ligand FES S1 803



Bond lengths



Bond angles



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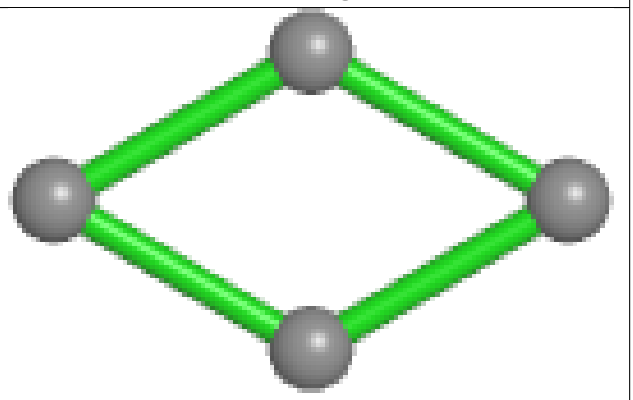
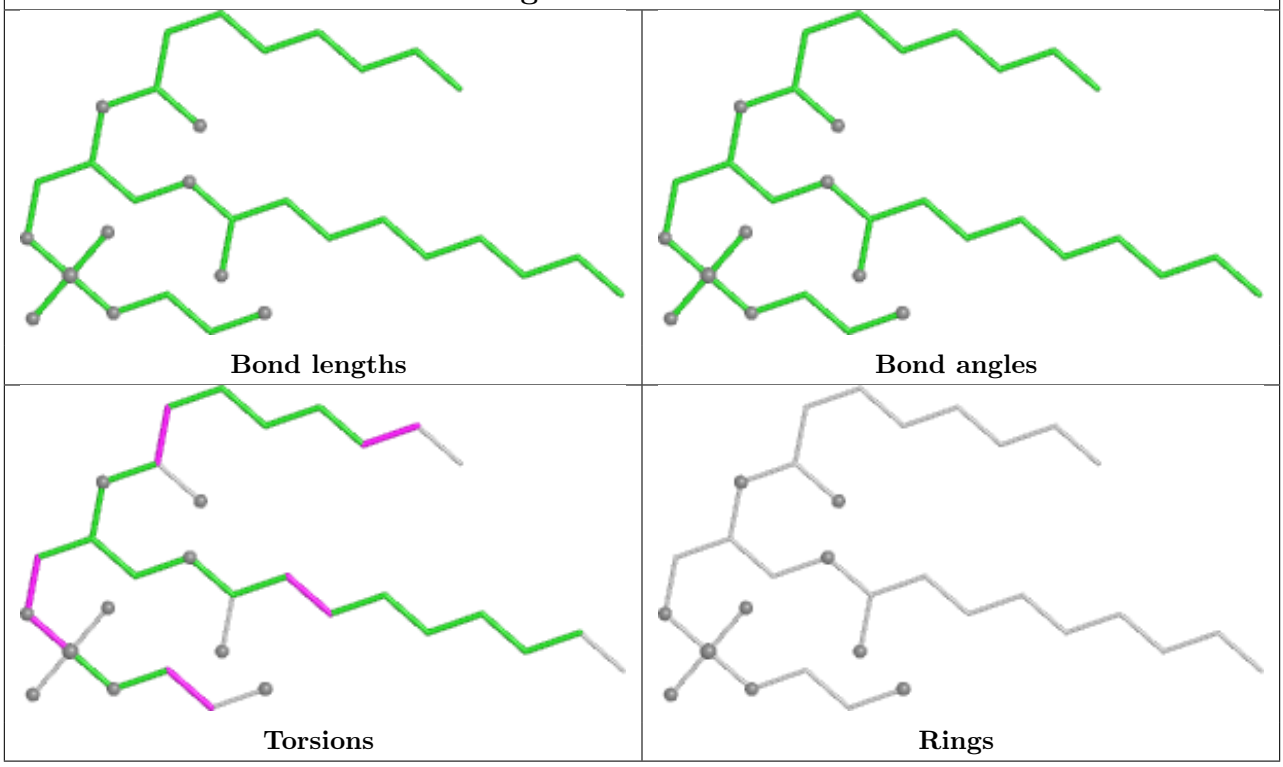
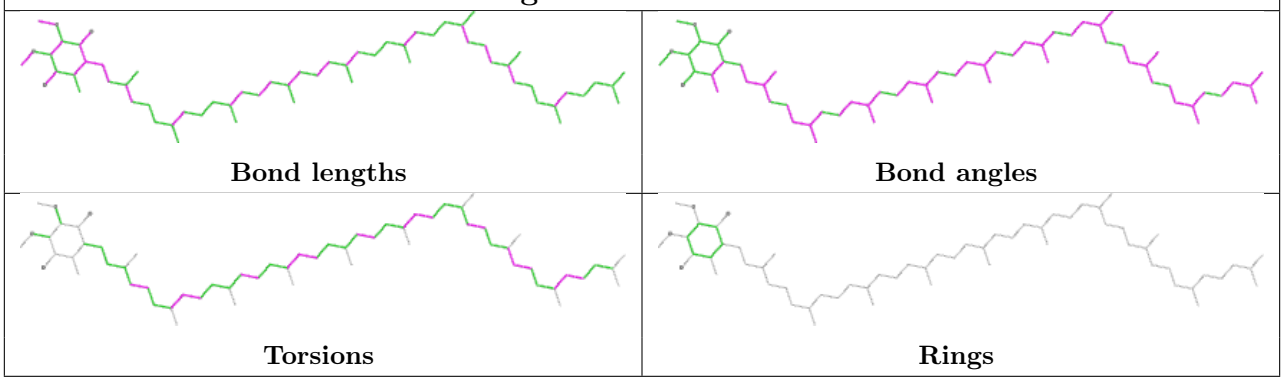


Rings

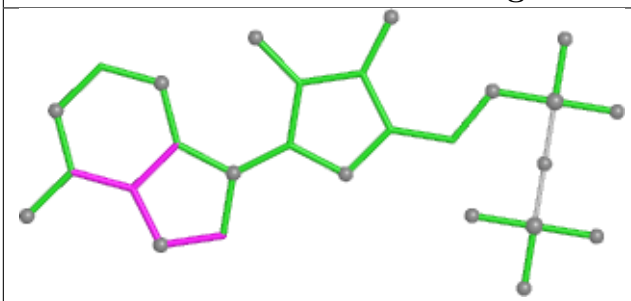
Ligand 3PE B8 201



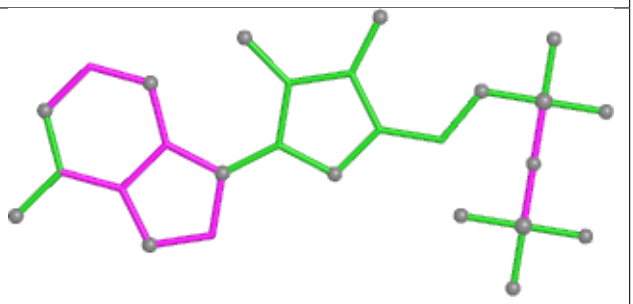
Ligand U10 N1 403



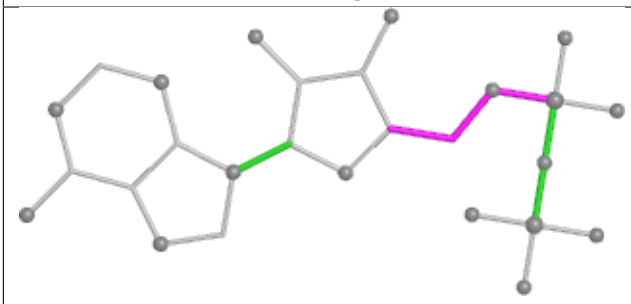
Ligand ADP AK 401



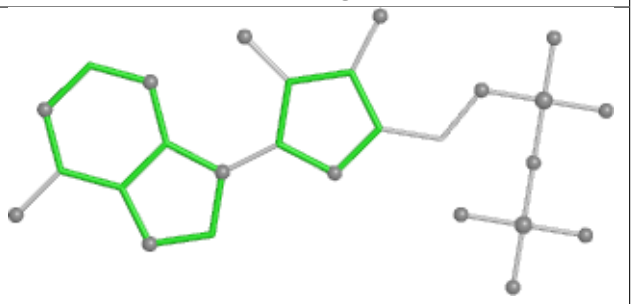
Bond lengths



Bond angles

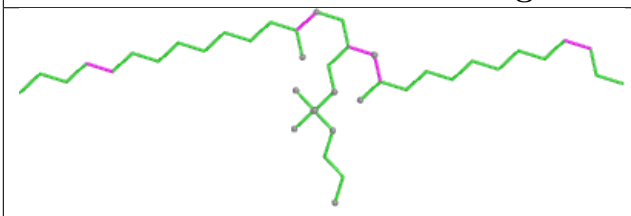


Torsions

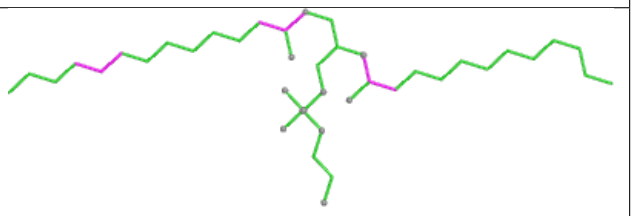


Rings

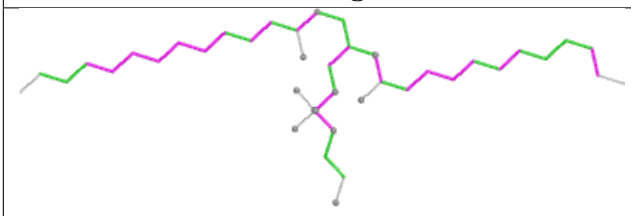
Ligand PEE N5 702



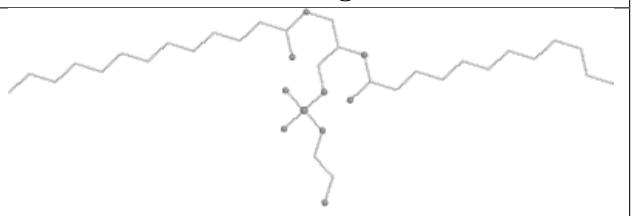
Bond lengths



Bond angles

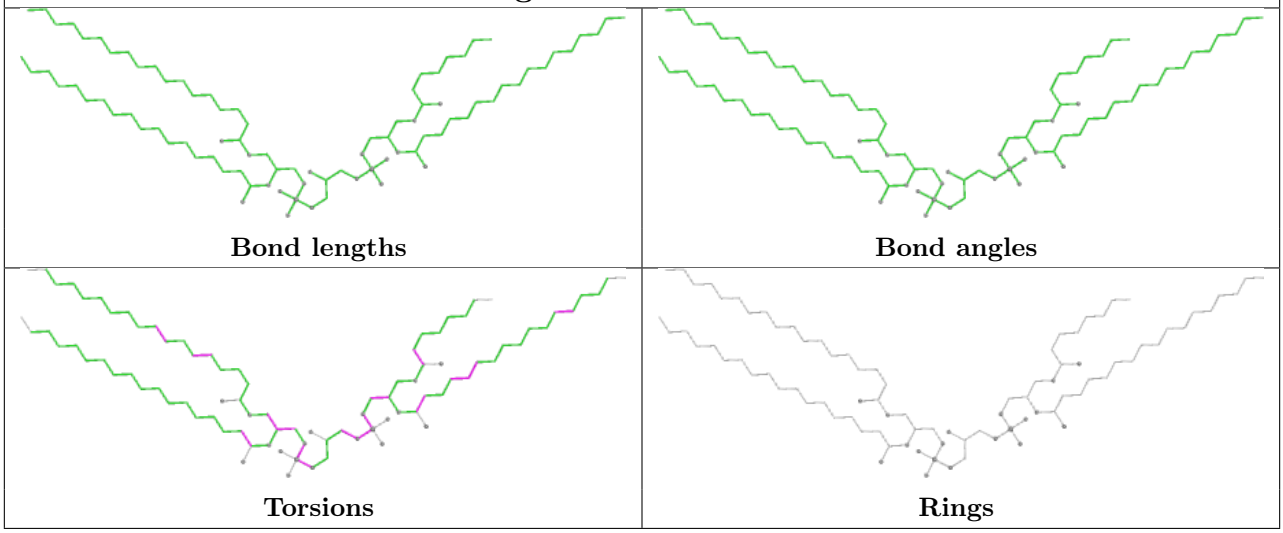


Torsions

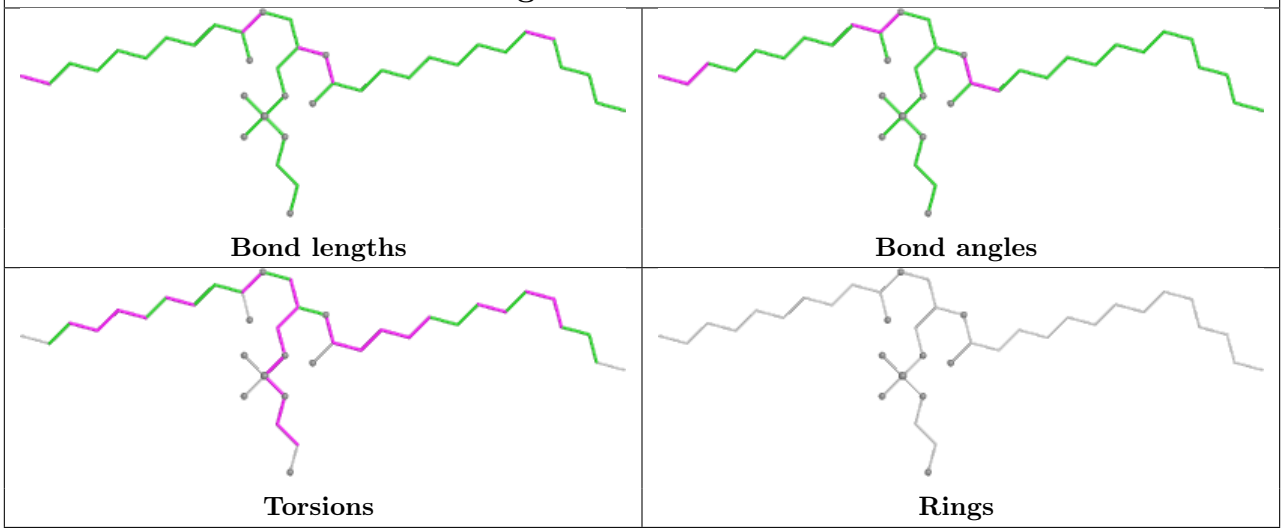


Rings

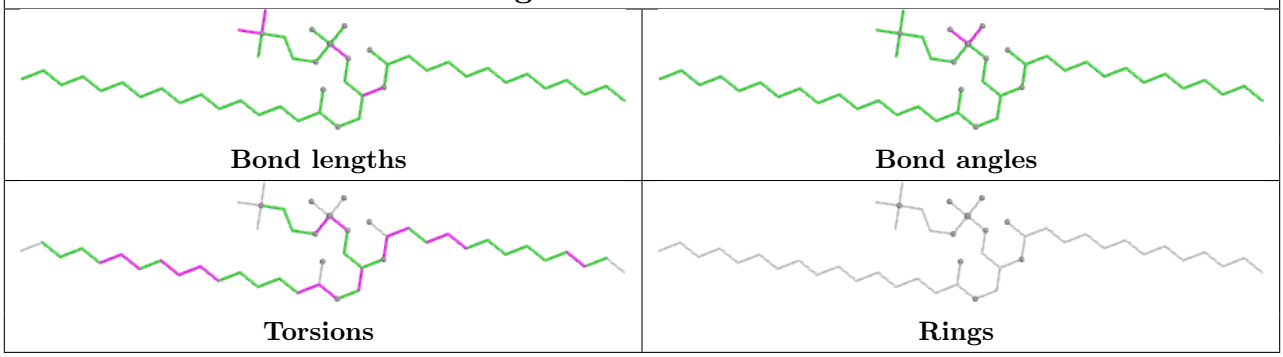
Ligand CDL N5 703



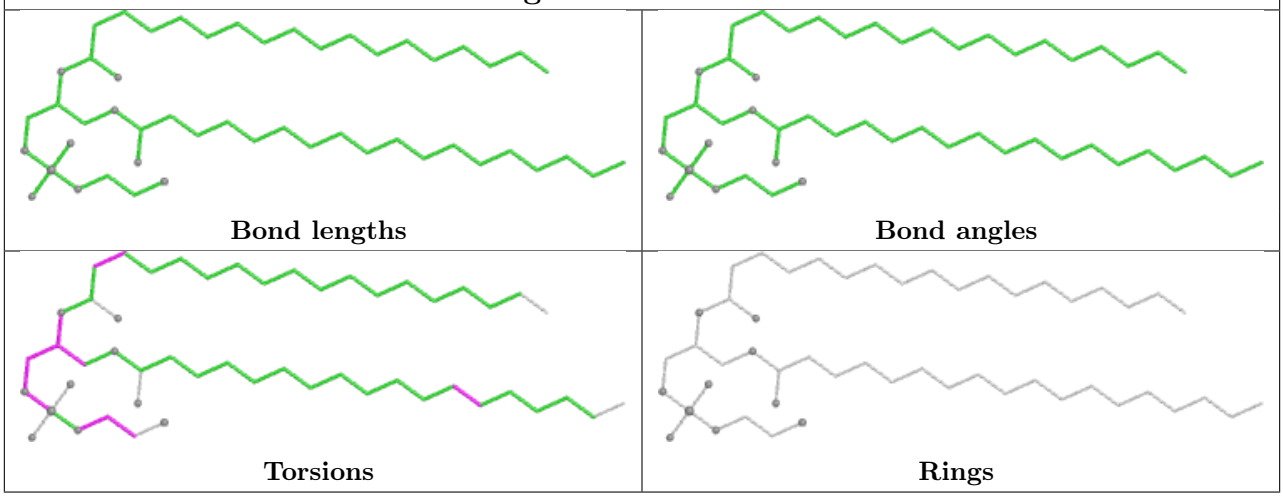
Ligand PEE A9 402



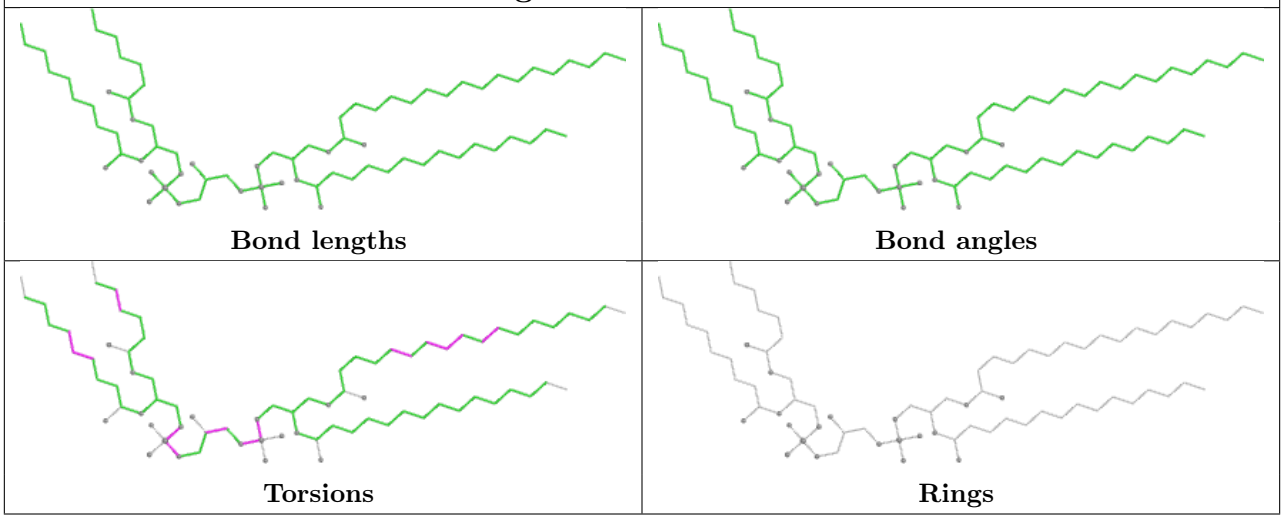
Ligand PLX AL 202



Ligand 3PE S7 303



Ligand CDL N1 401



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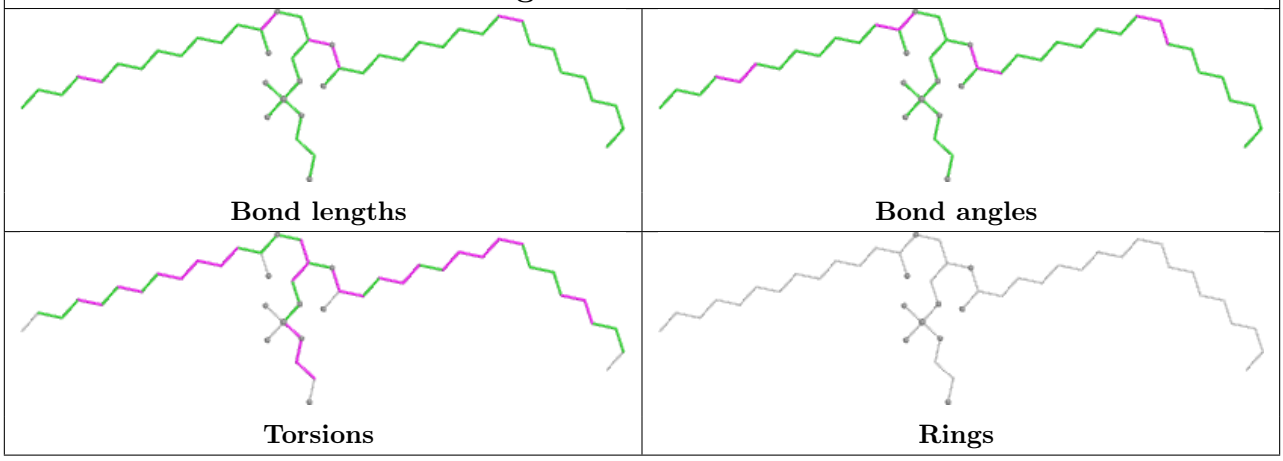

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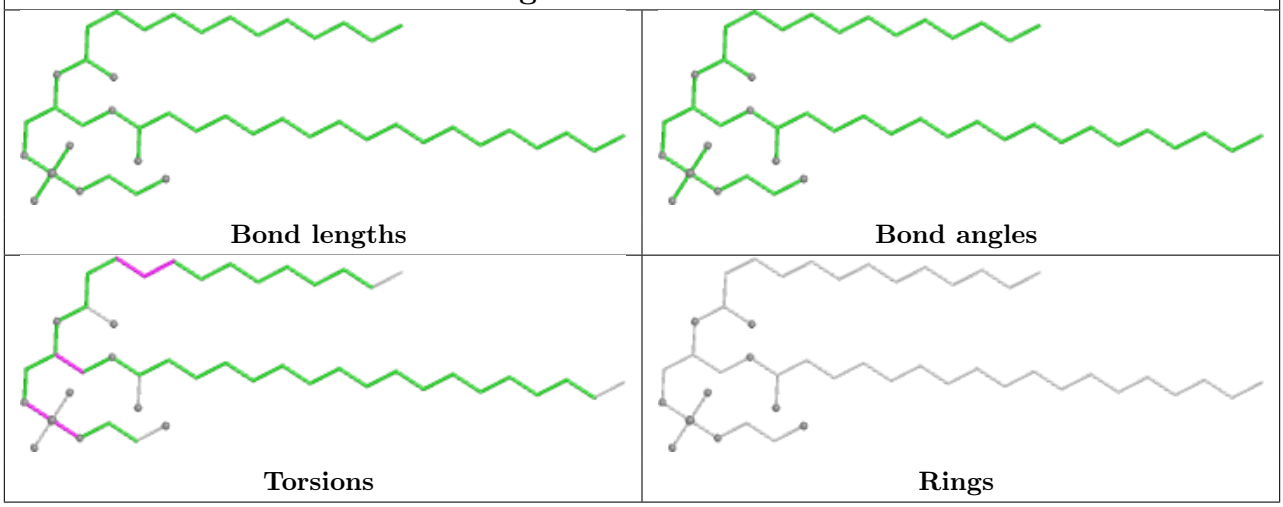
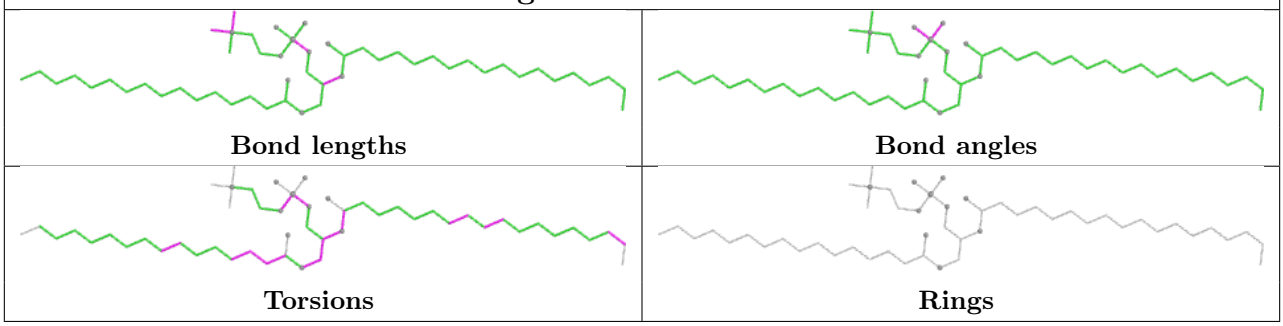
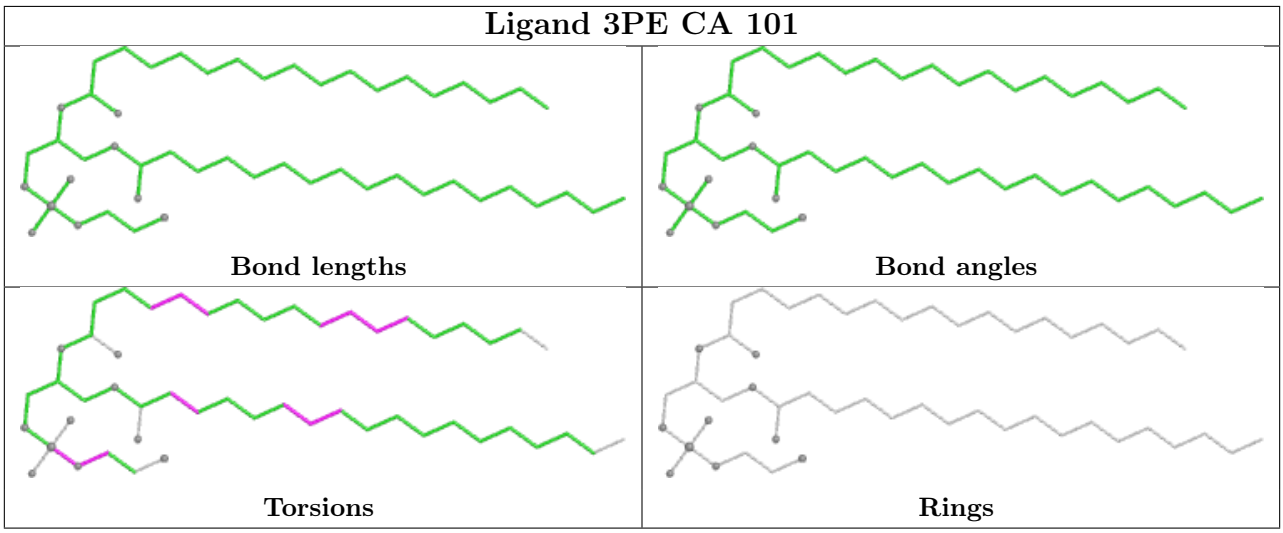


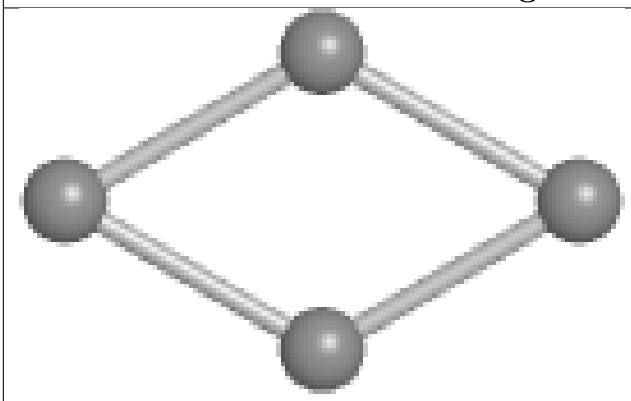
Ligand PLX B1 101



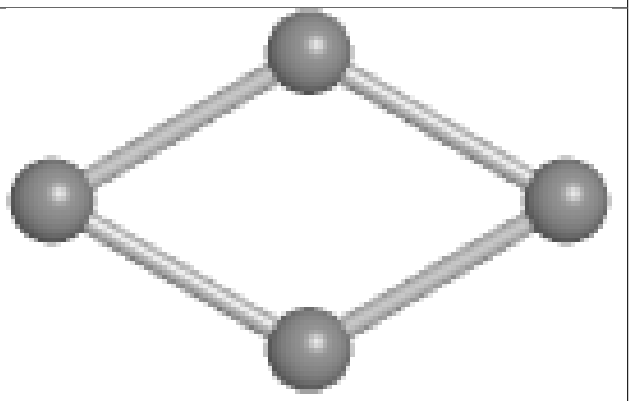
Ligand 3PE CA 101



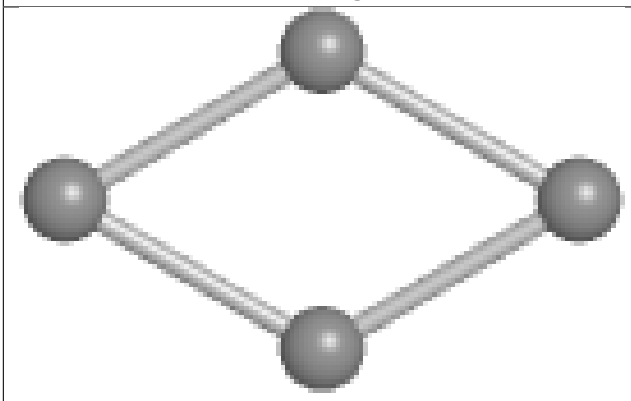
Ligand FES V2 301



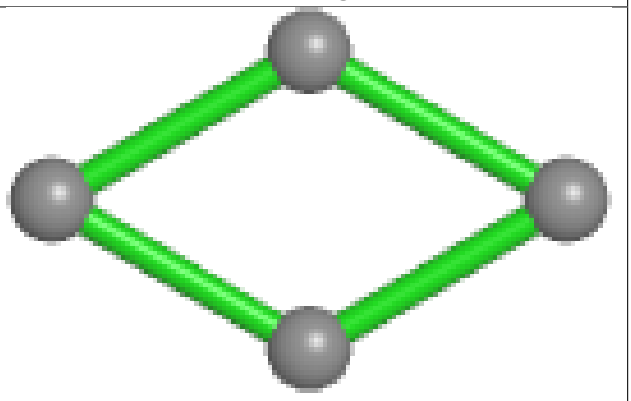
Bond lengths



Bond angles

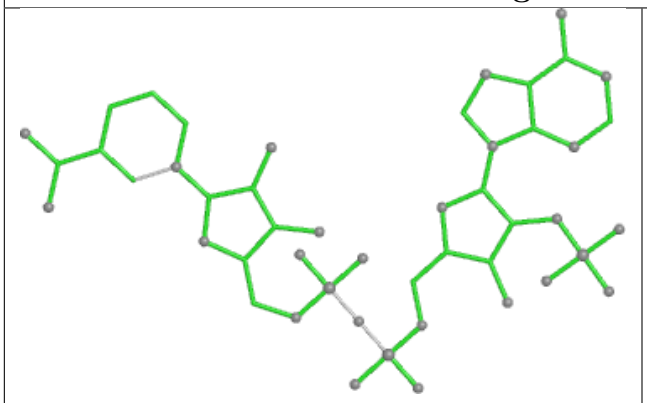


Torsions

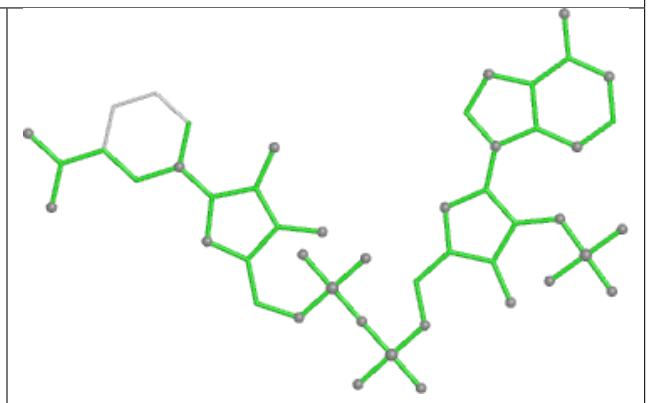


Rings

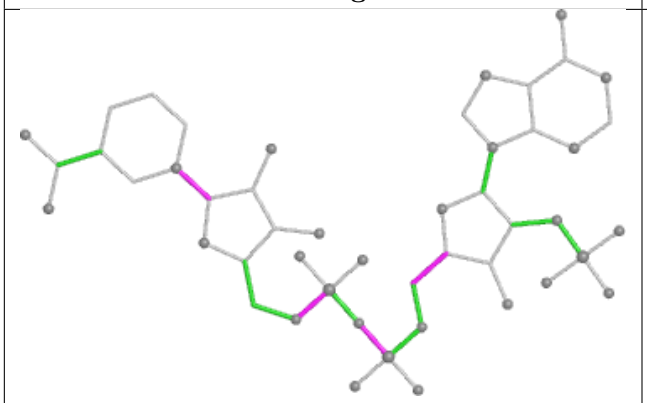
Ligand NDP A9 401



Bond lengths



Bond angles



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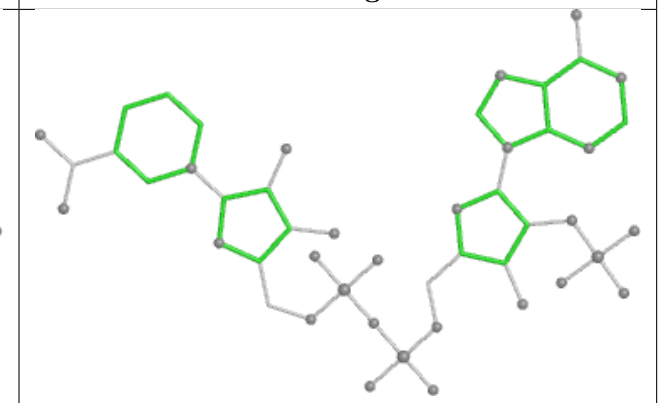
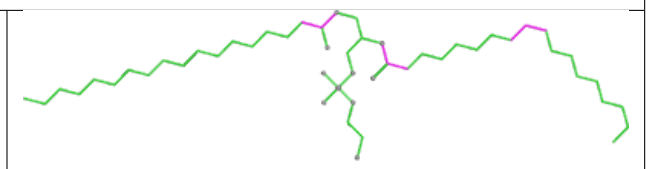


Rings

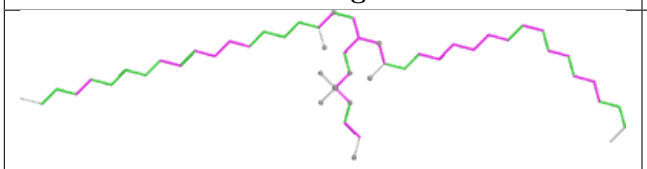
Ligand PEE S8 303



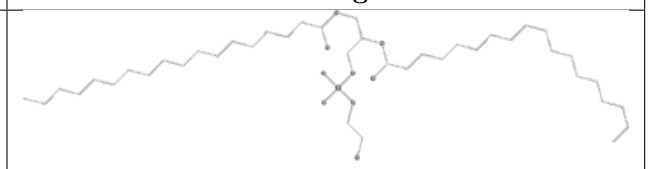
Bond lengths



Bond angles

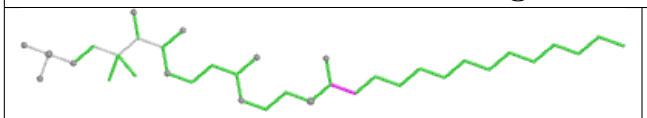


Torsions

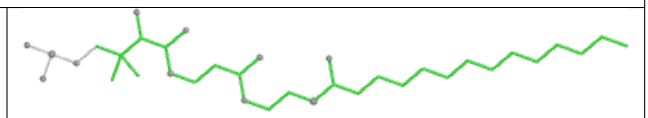


Rings

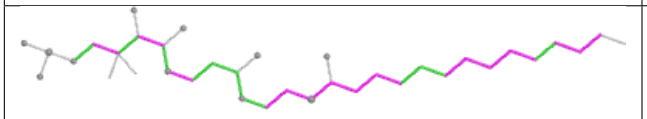
Ligand ZMP AC 201



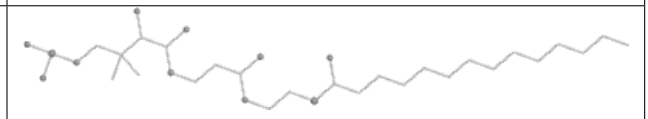
Bond lengths



Bond angles

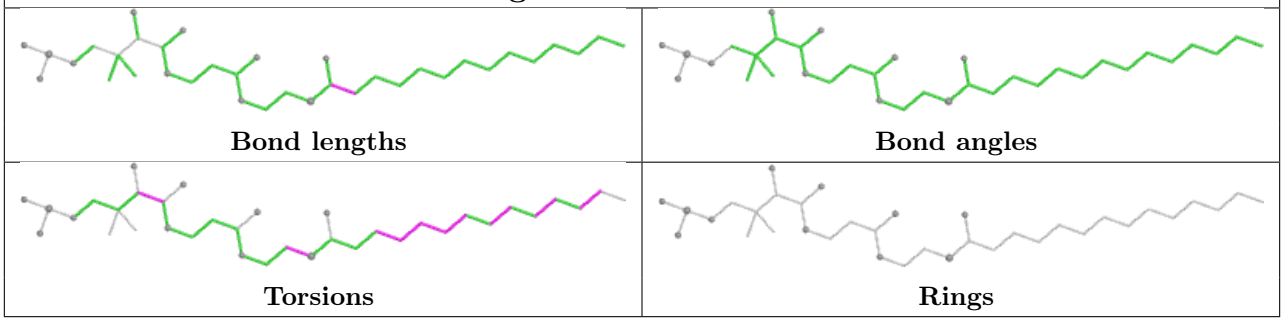


Torsions

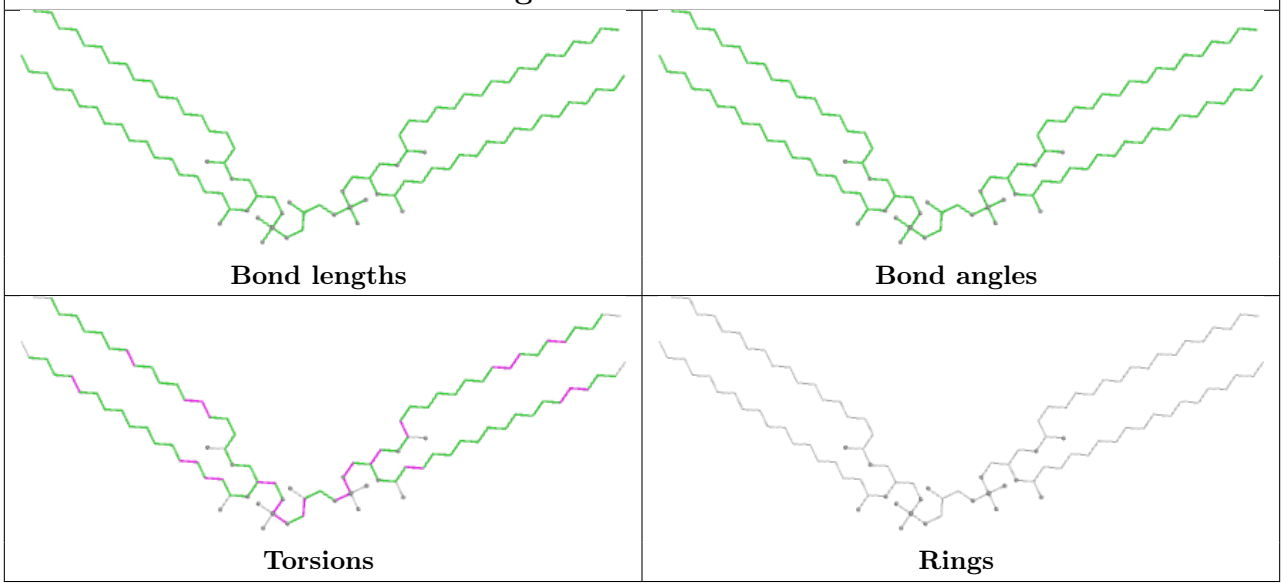


Rings

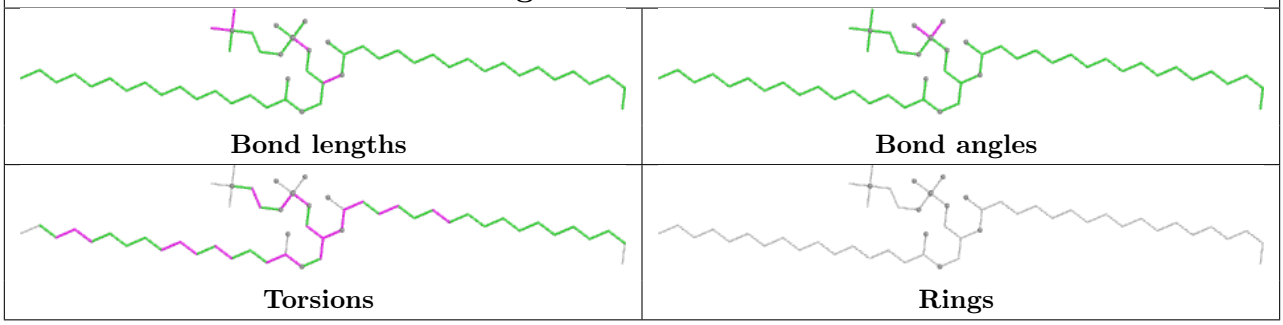
Ligand ZMP AB 201



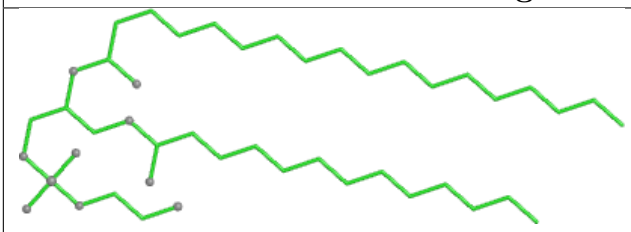
Ligand CDL N4 503



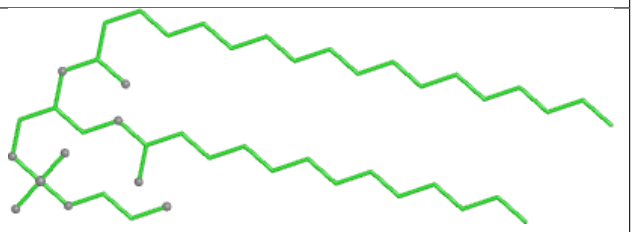
Ligand PLX N6 201



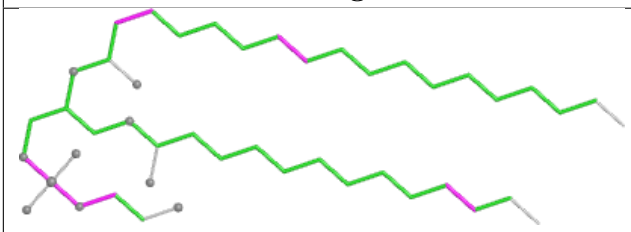
Ligand 3PE CB 202



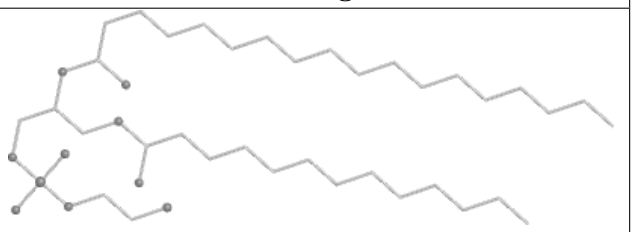
Bond lengths



Bond angles

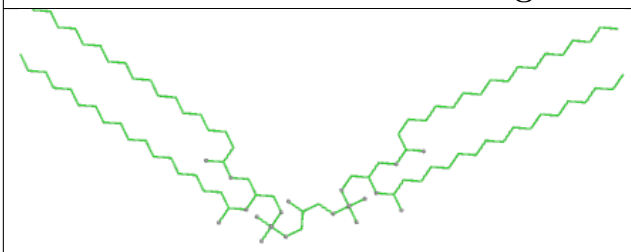


Torsions

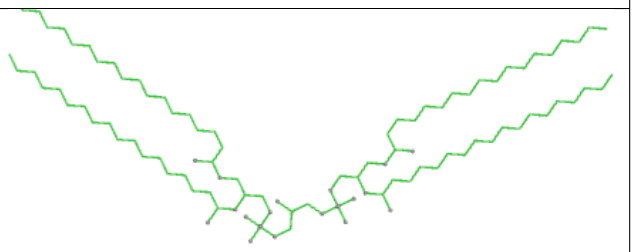


Rings

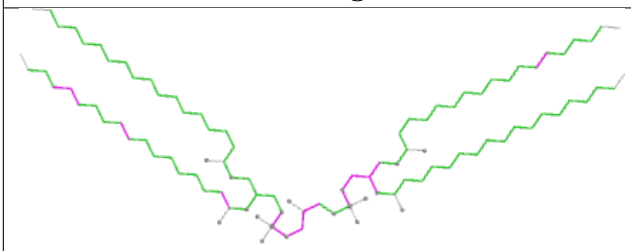
Ligand CDL B5 201



Bond lengths



Bond angles



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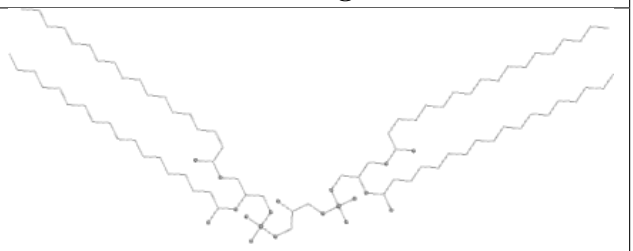
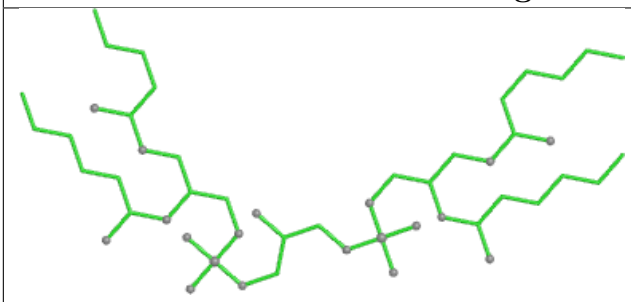
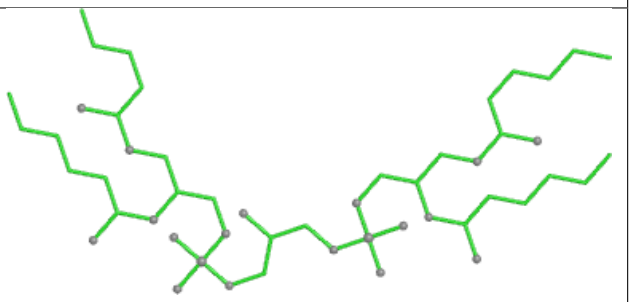


Rings

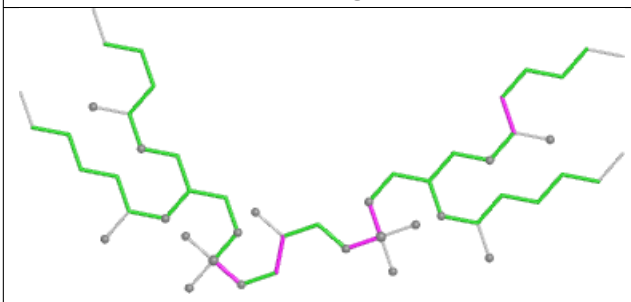
Ligand CDL A7 201



Bond lengths



Bond angles



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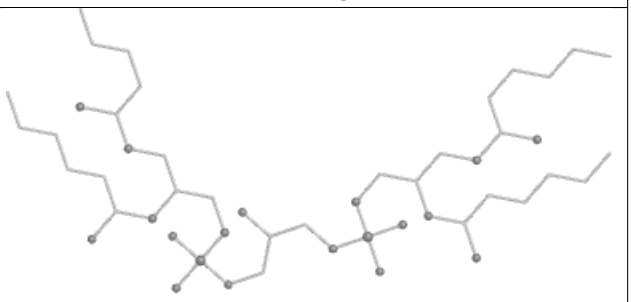
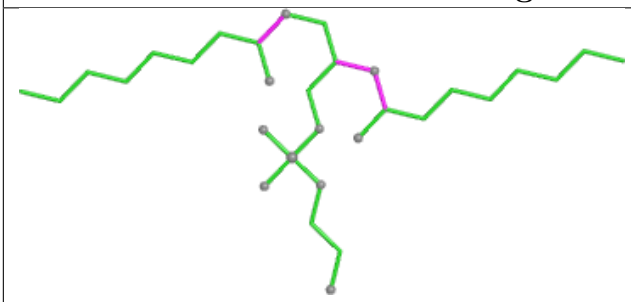
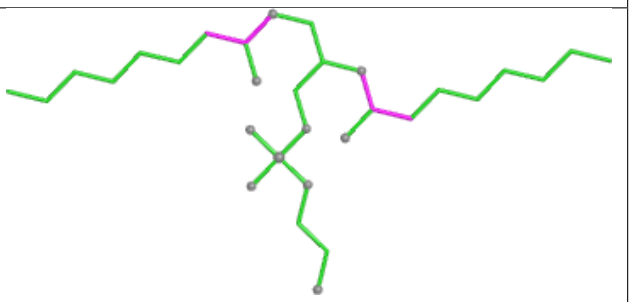


Rings

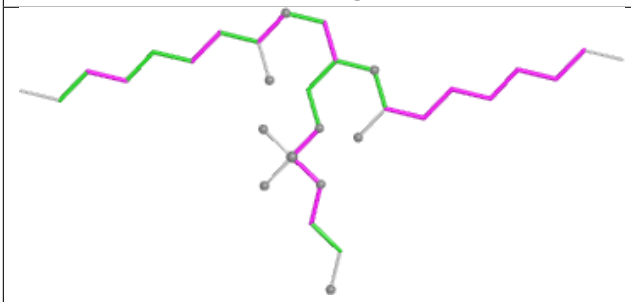
Ligand PEE N1 404



Bond lengths



Bond angles



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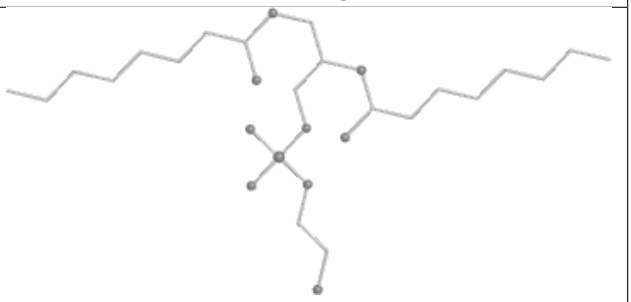
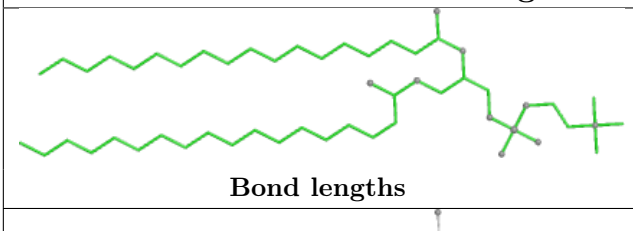
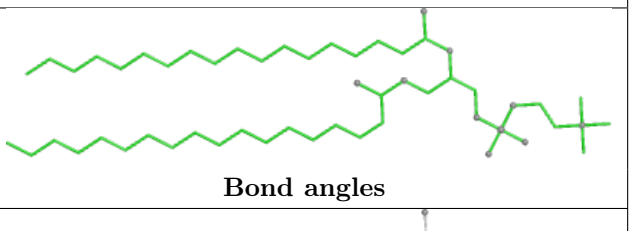


Rings

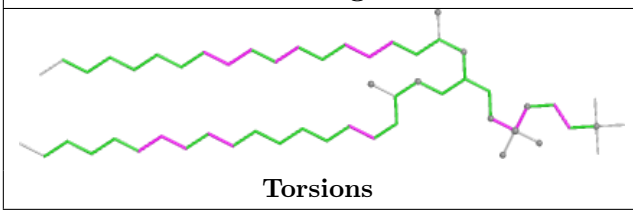
Ligand PC1 A9 403



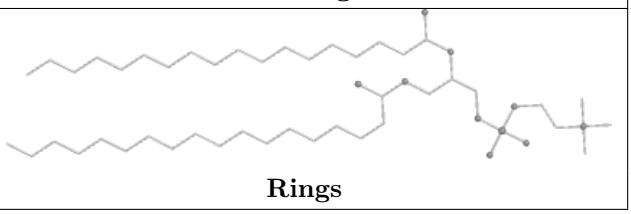
Bond lengths



Bond angles

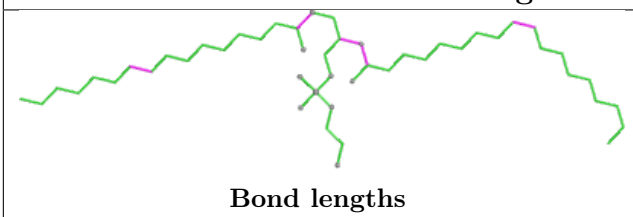


Torsions

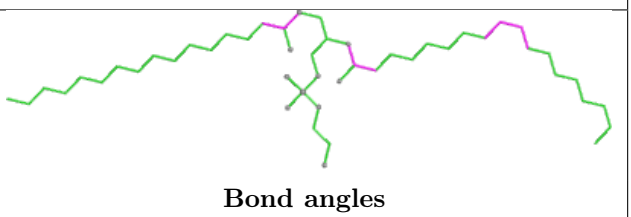


Rings

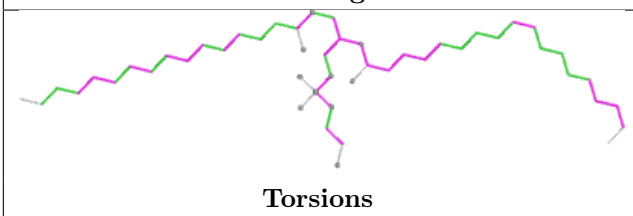
Ligand PEE N4 501



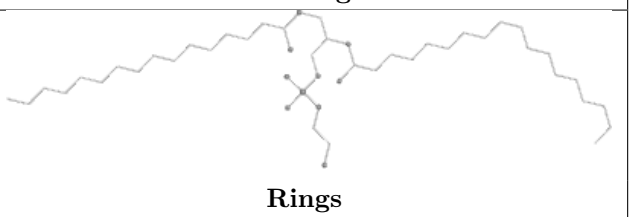
Bond lengths



Bond angles

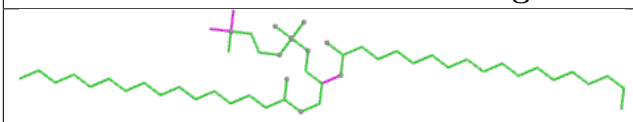


Torsions

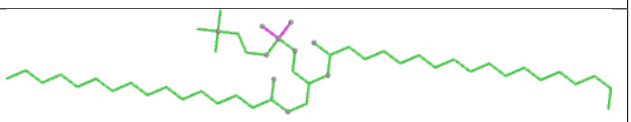


Rings

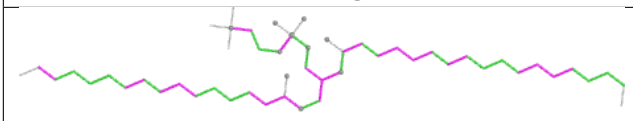
Ligand PLX CB 201



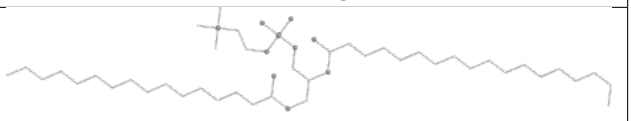
Bond lengths



Bond angles

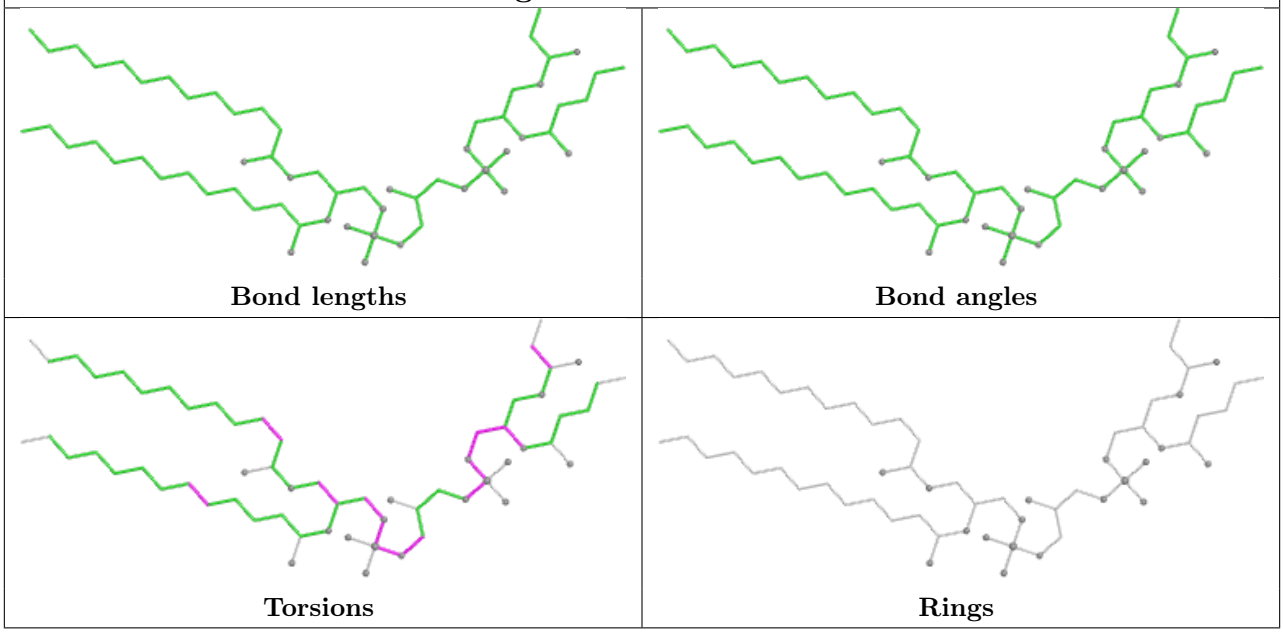


Torsions

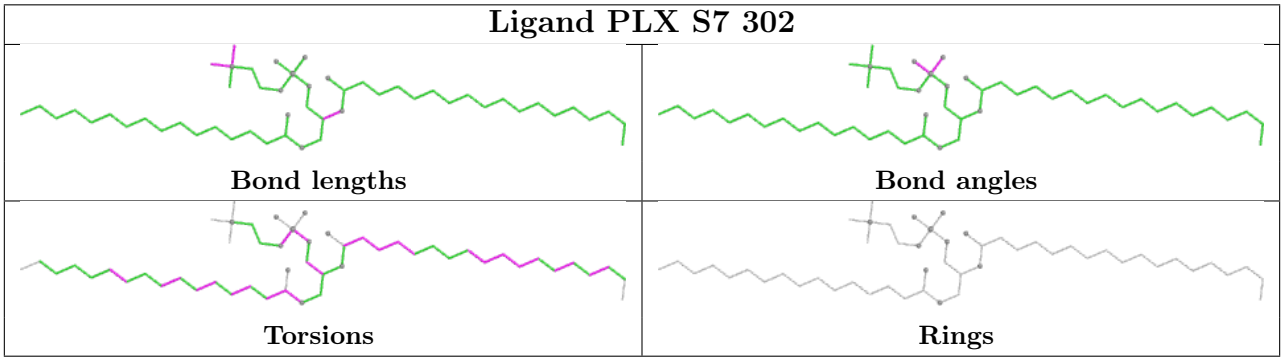


Rings

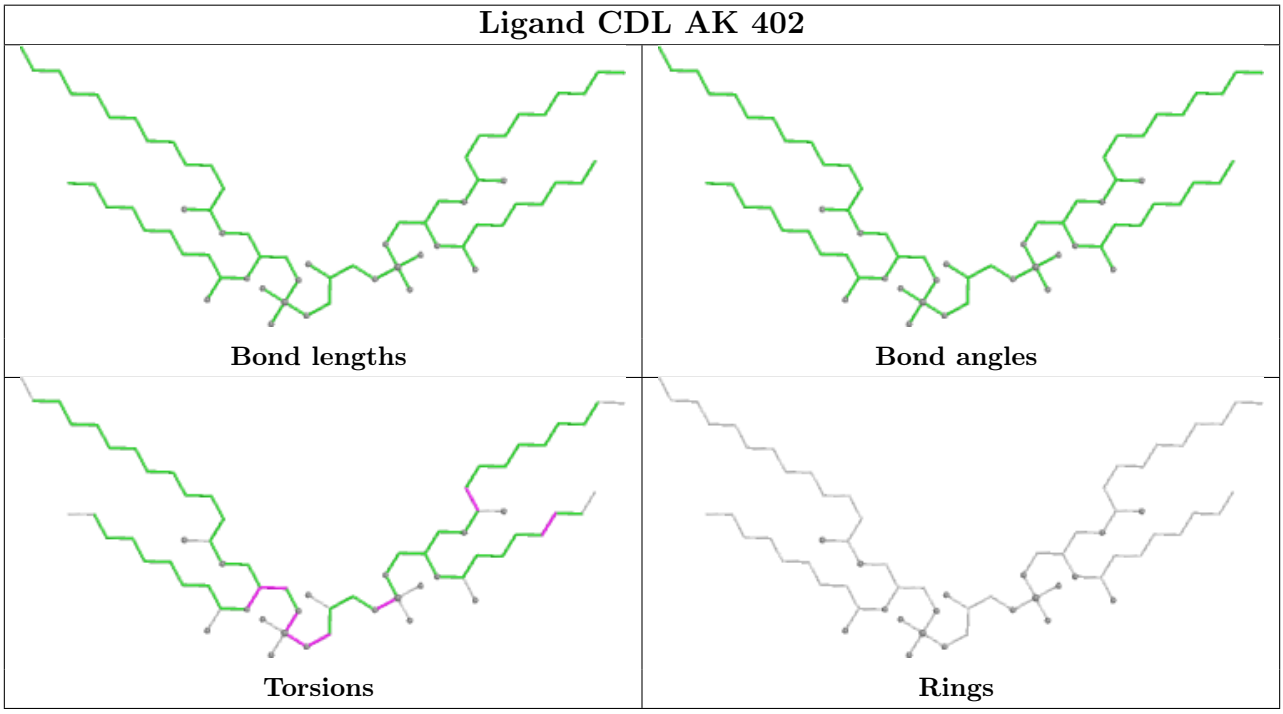
Ligand CDL N4 504



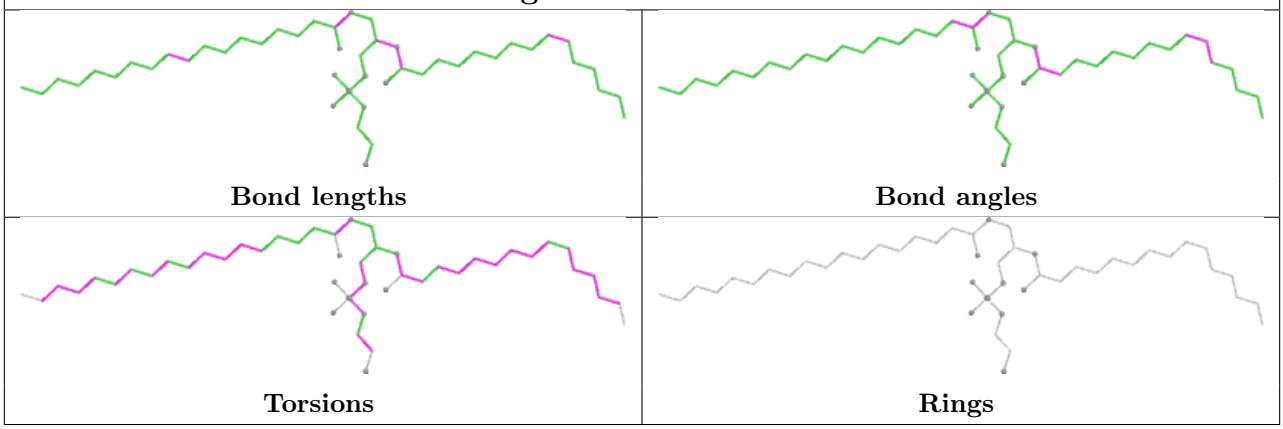
Ligand PLX S7 302



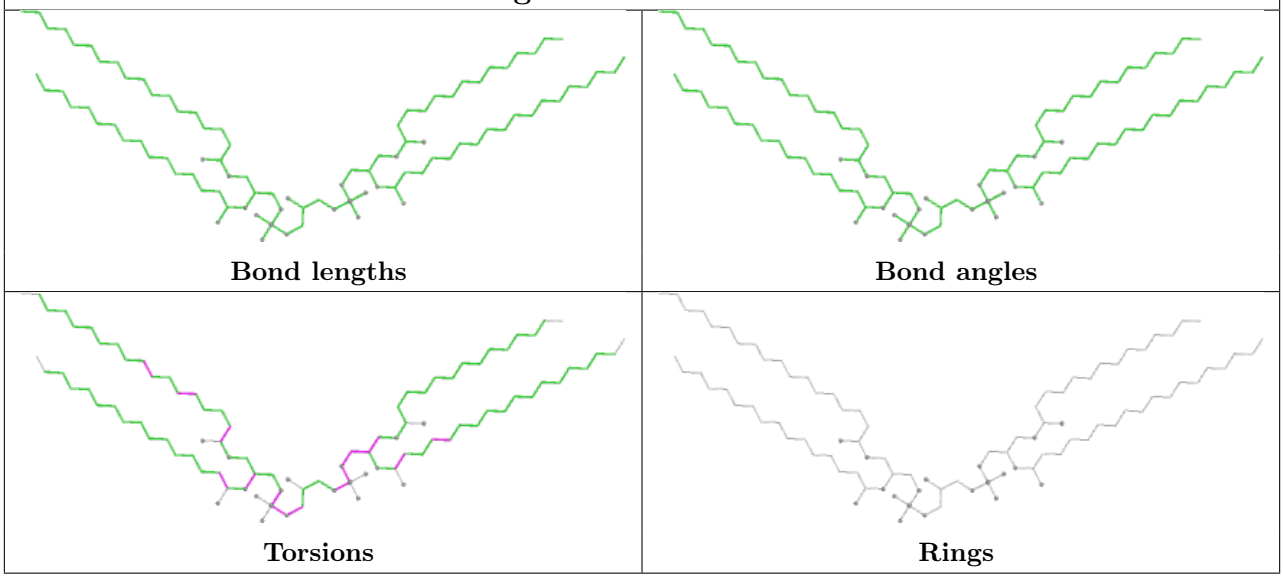
Ligand CDL AK 402



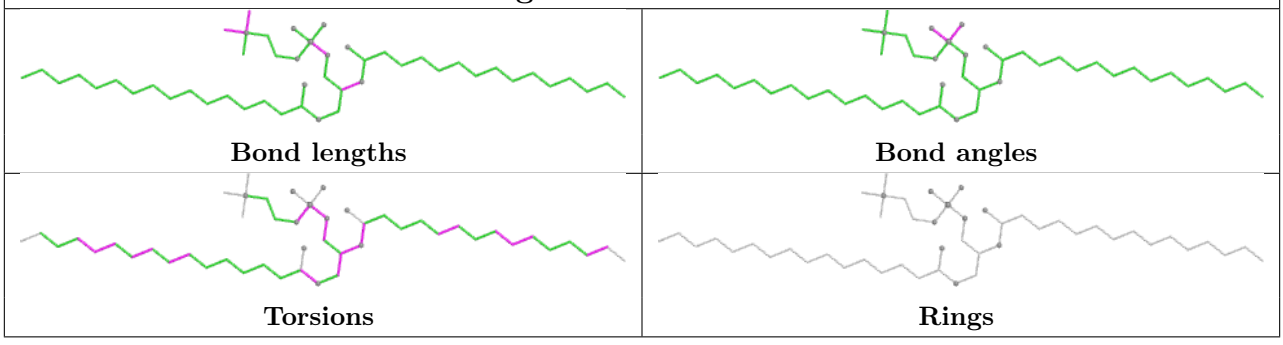
Ligand PEE S2 501



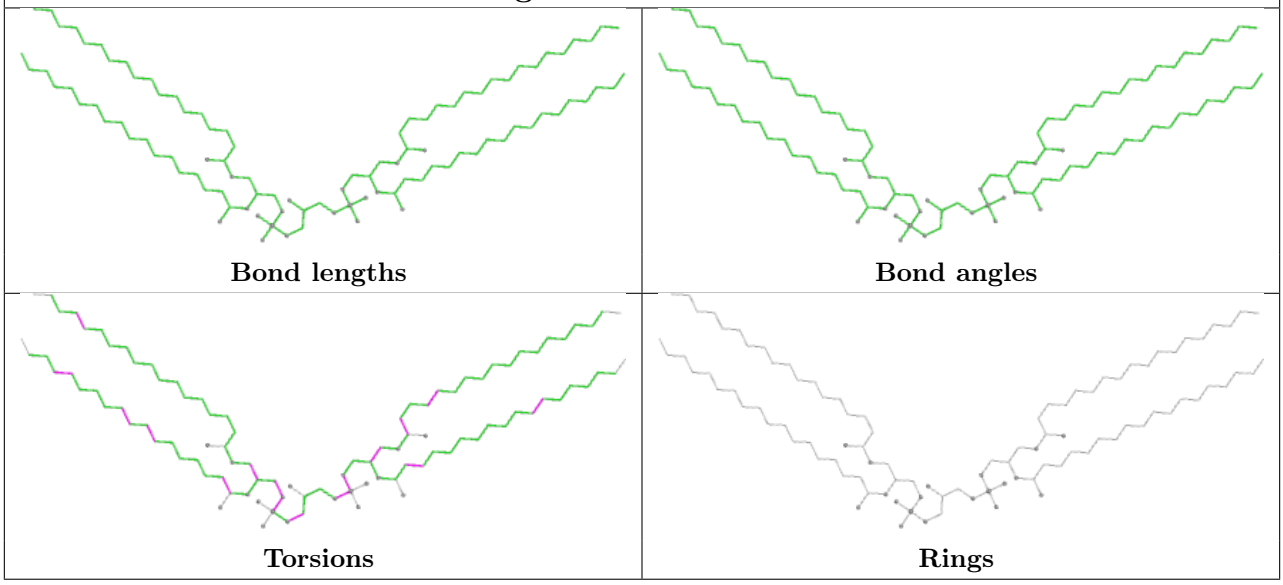
Ligand CDL AL 201



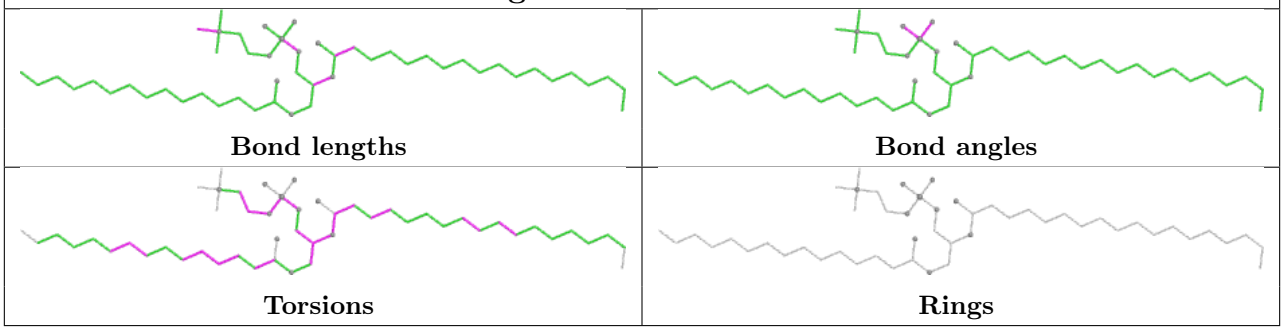
Ligand PLX N4 502



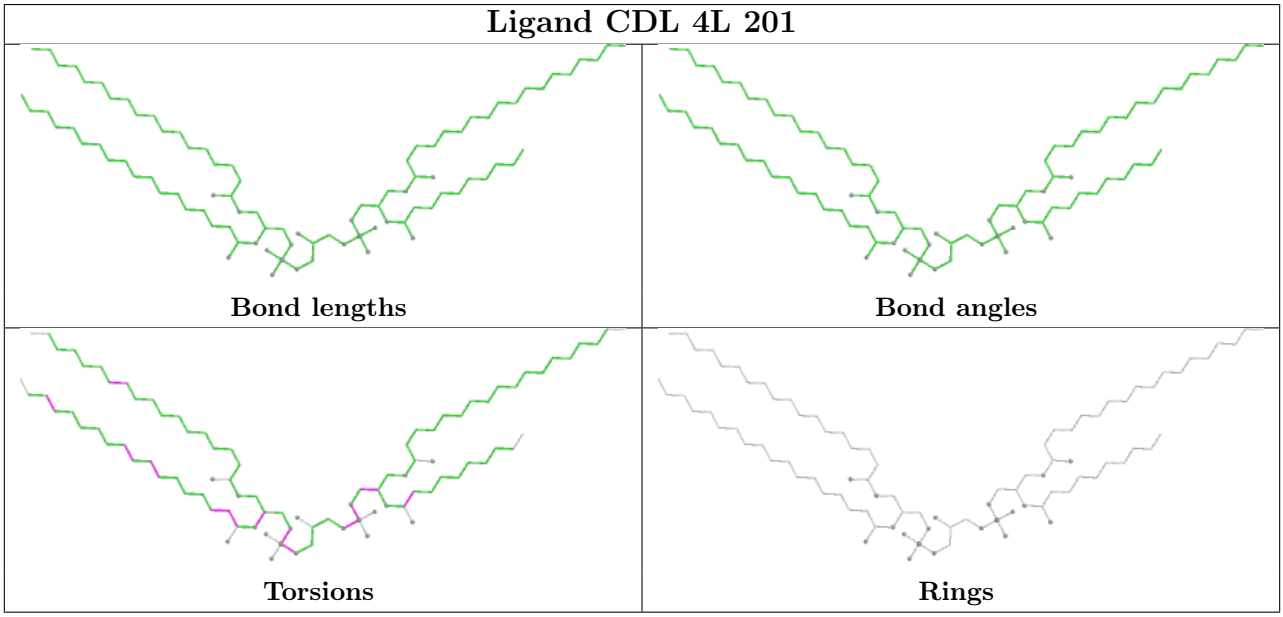
Ligand CDL N5 704



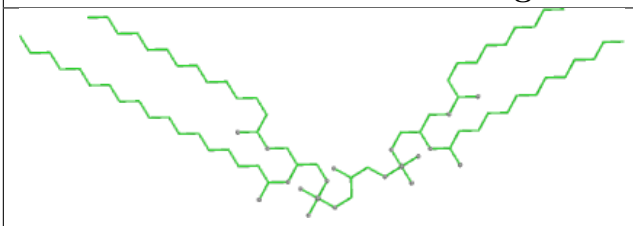
Ligand PLX AM 201



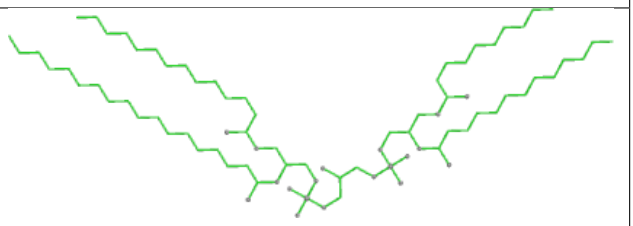
Ligand CDL 4L 201



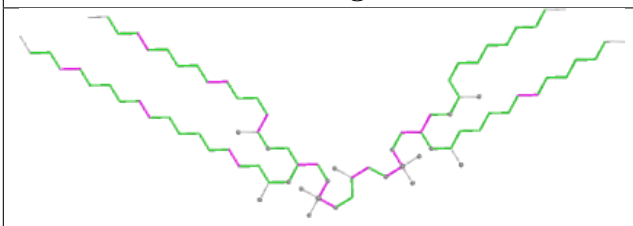
Ligand CDL A8 301



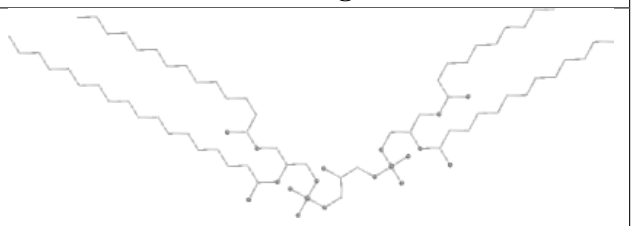
Bond lengths



Bond angles

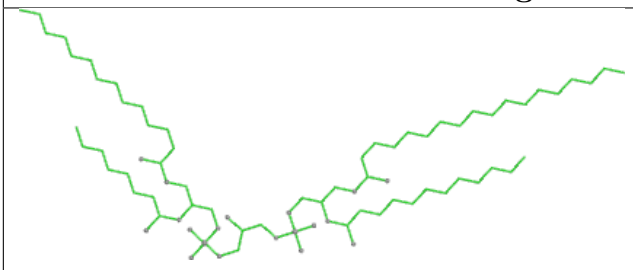


Torsions

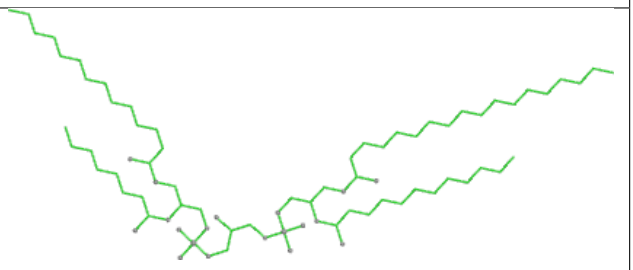


Rings

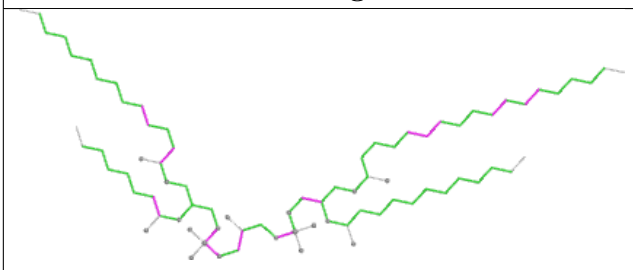
Ligand CDL B4 201



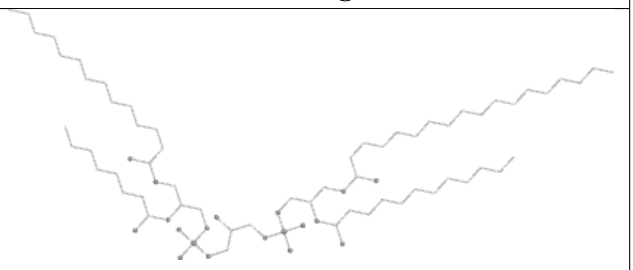
Bond lengths



Bond angles



Torsions

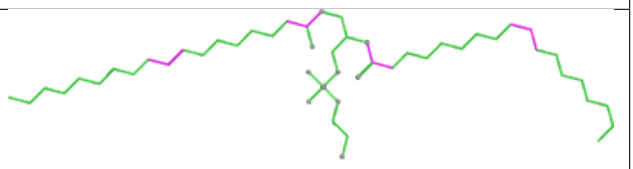


Rings

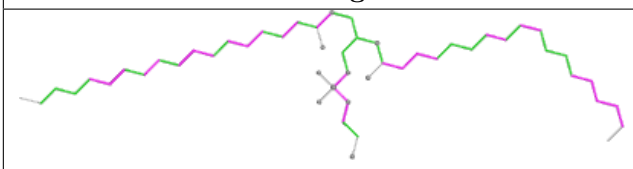
Ligand PEE N3 201



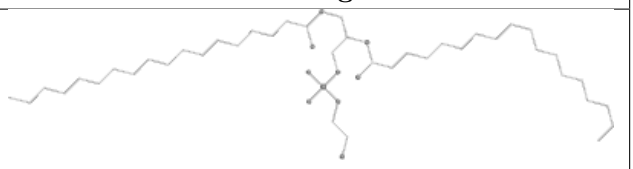
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

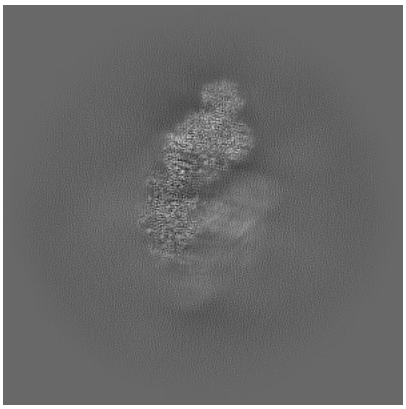
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-61173. These allow visual inspection of the internal detail of the map and identification of artifacts.

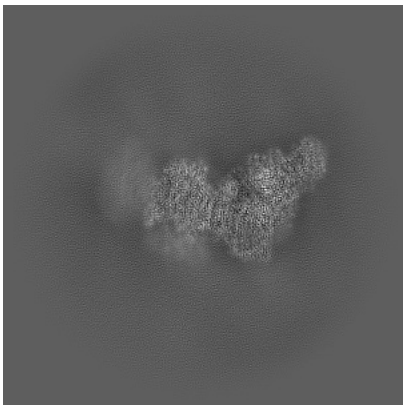
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

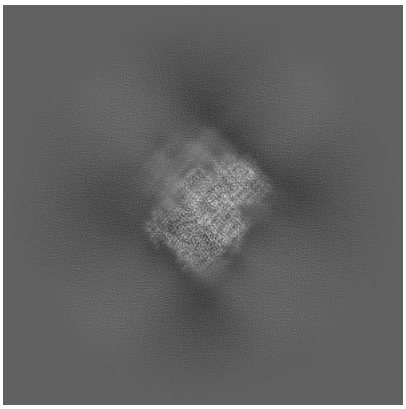
6.1.1 Primary map



X

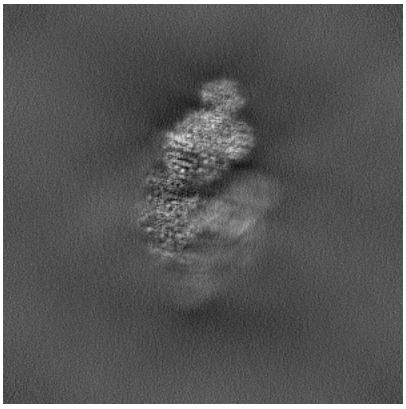


Y

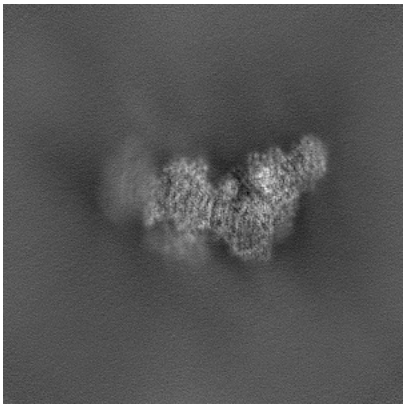


Z

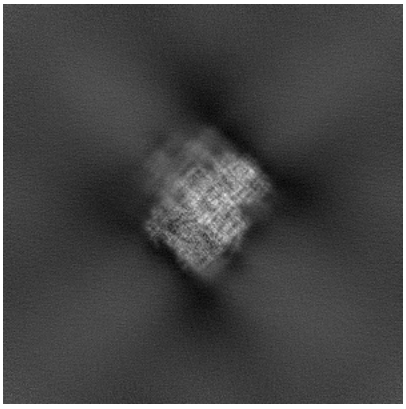
6.1.2 Raw map



X



Y

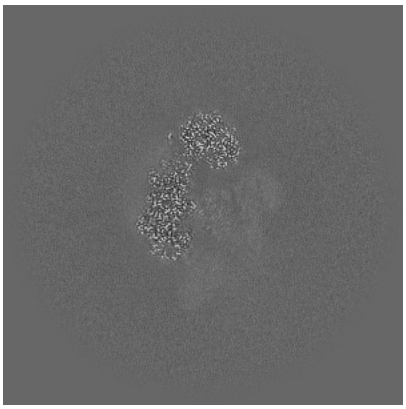


Z

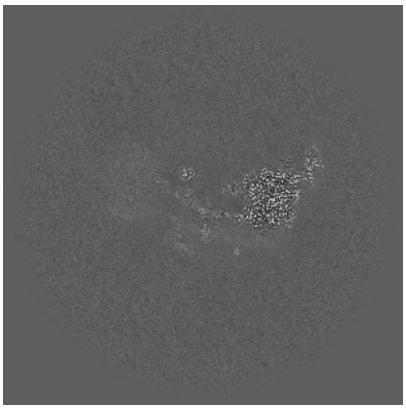
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

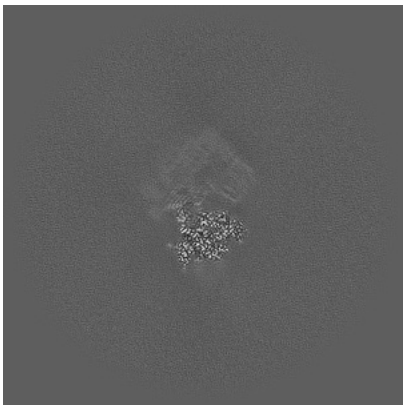
6.2.1 Primary map



X Index: 240

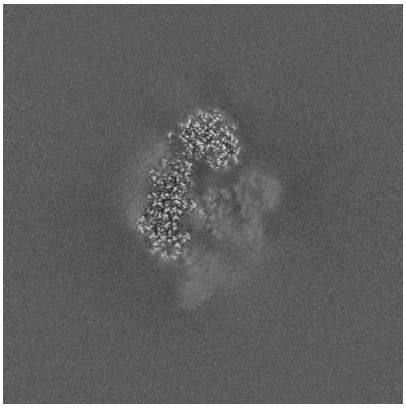


Y Index: 240

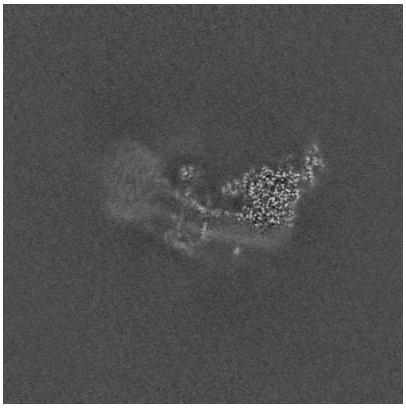


Z Index: 240

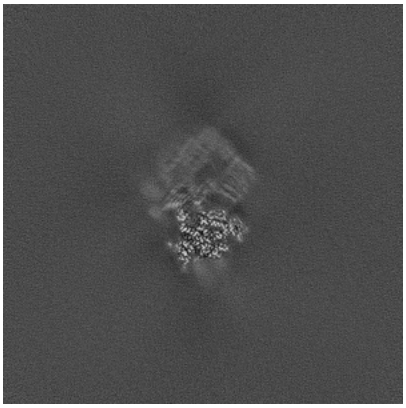
6.2.2 Raw map



X Index: 240



Y Index: 240

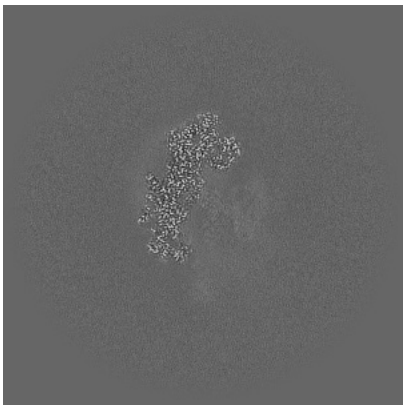


Z Index: 240

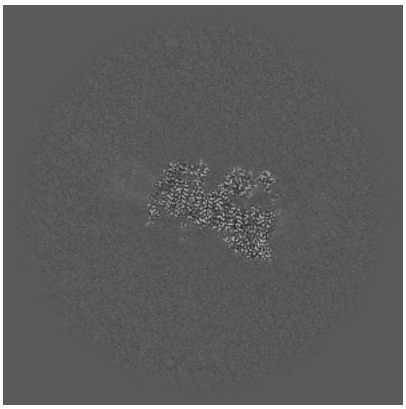
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

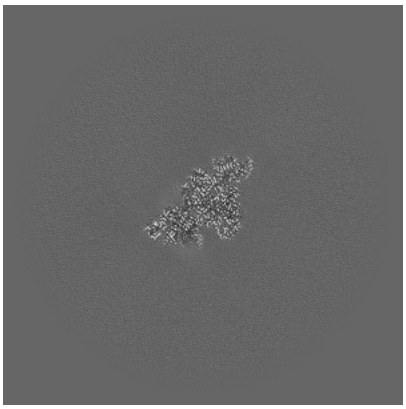
6.3.1 Primary map



X Index: 229

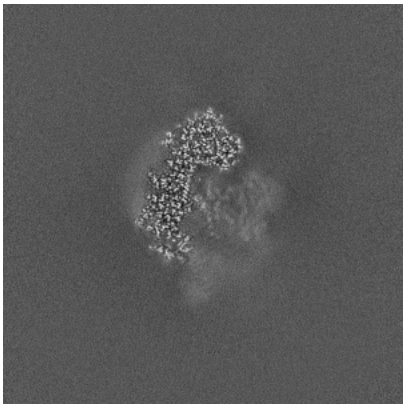


Y Index: 206

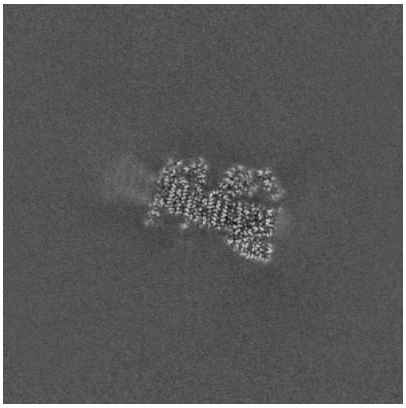


Z Index: 314

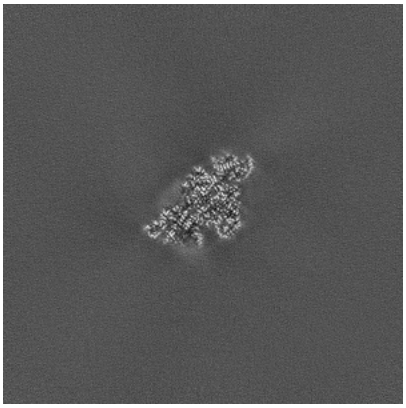
6.3.2 Raw map



X Index: 235



Y Index: 208

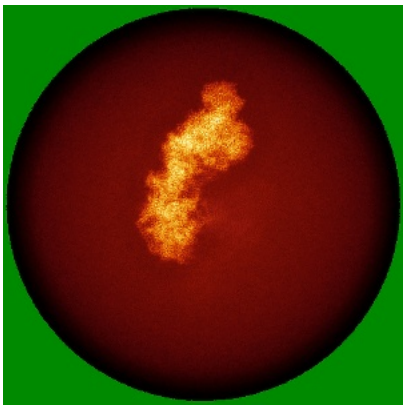


Z Index: 314

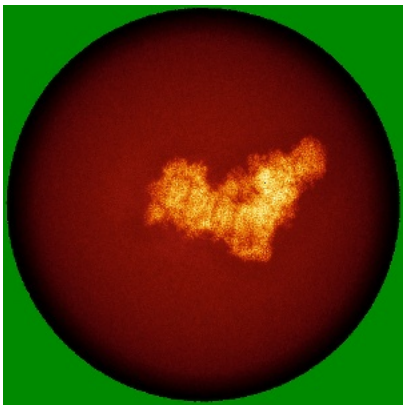
The images above show the largest variance slices of the map in three orthogonal directions.

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

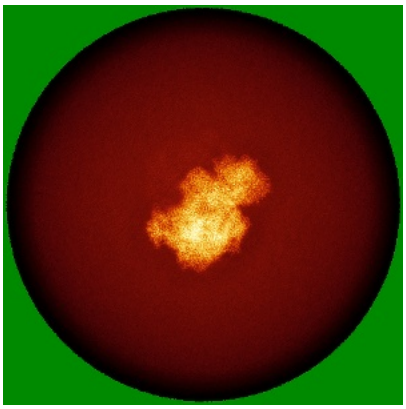
6.4.1 Primary map



X

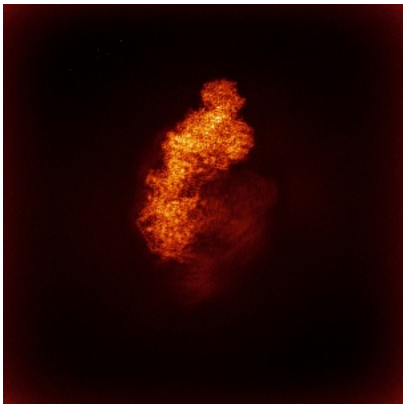


Y

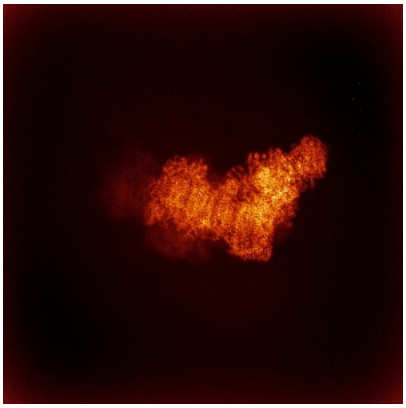


Z

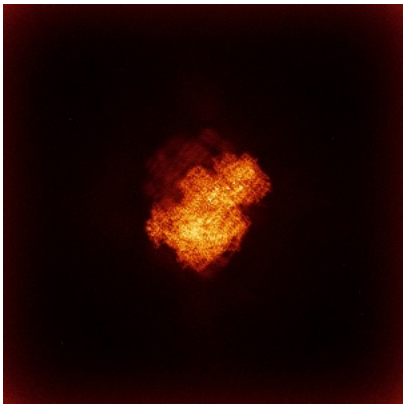
6.4.2 Raw map



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 4.62. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

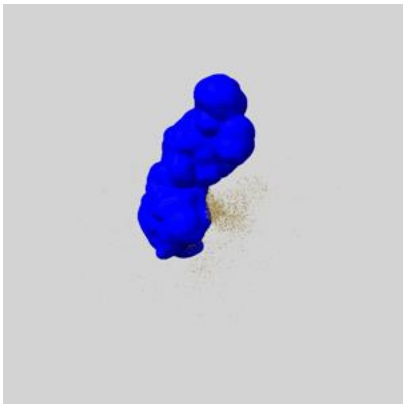
6.6 Mask visualisation

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

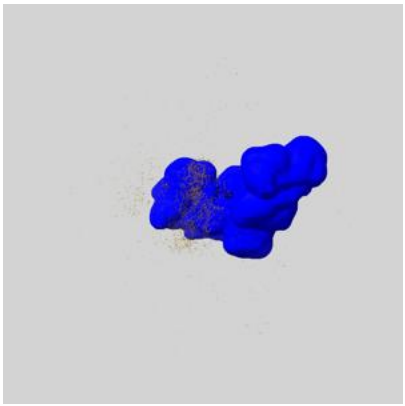
A mask typically either:

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

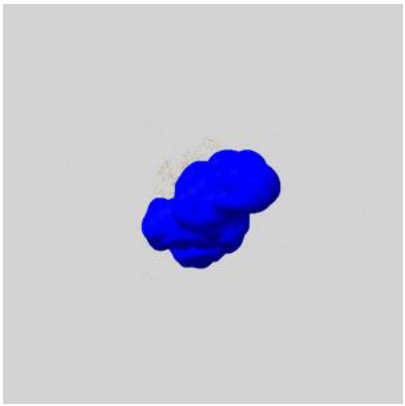
6.6.1 emd_61173_msk_1.map



X



Y

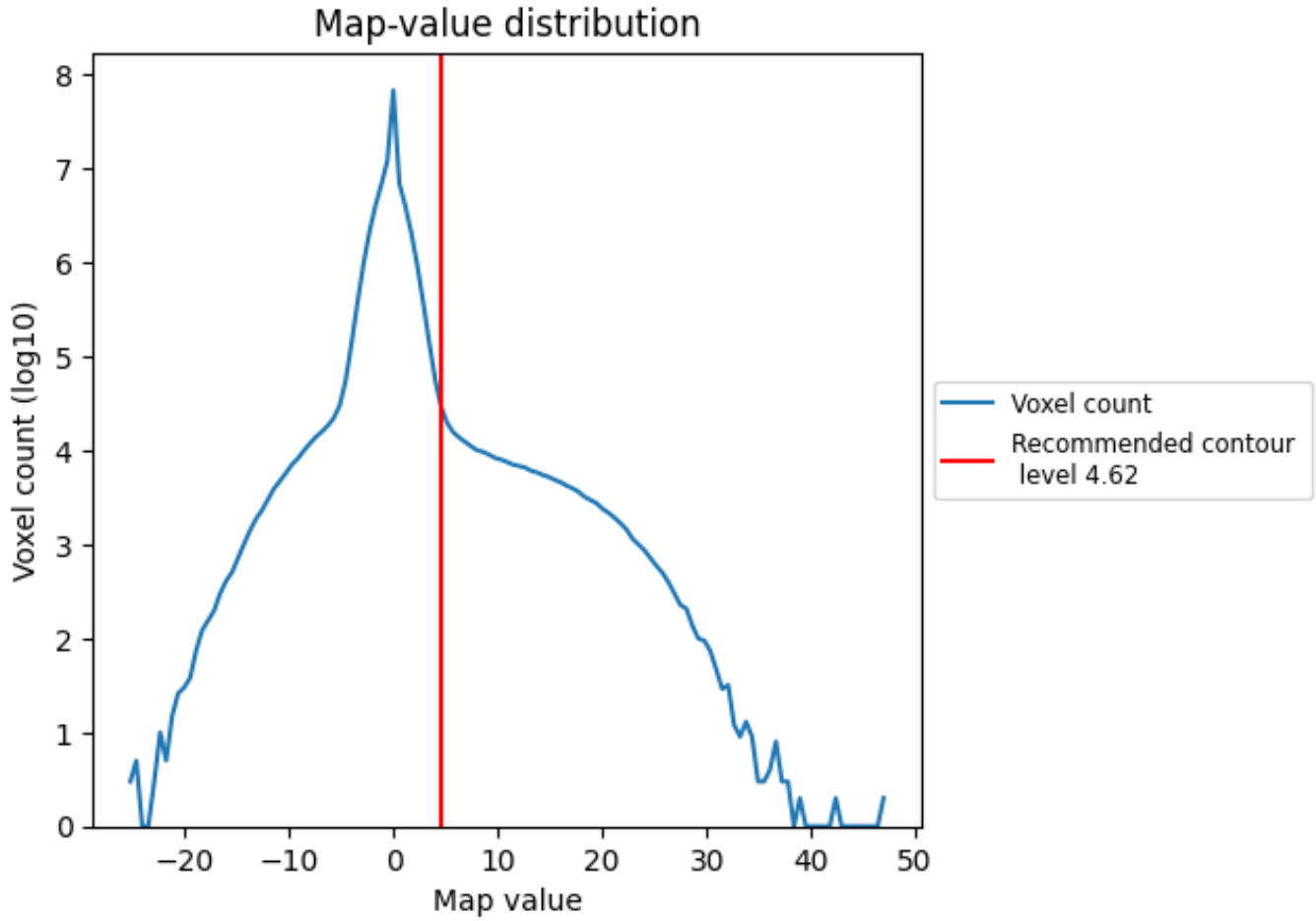


Z

7 Map analysis

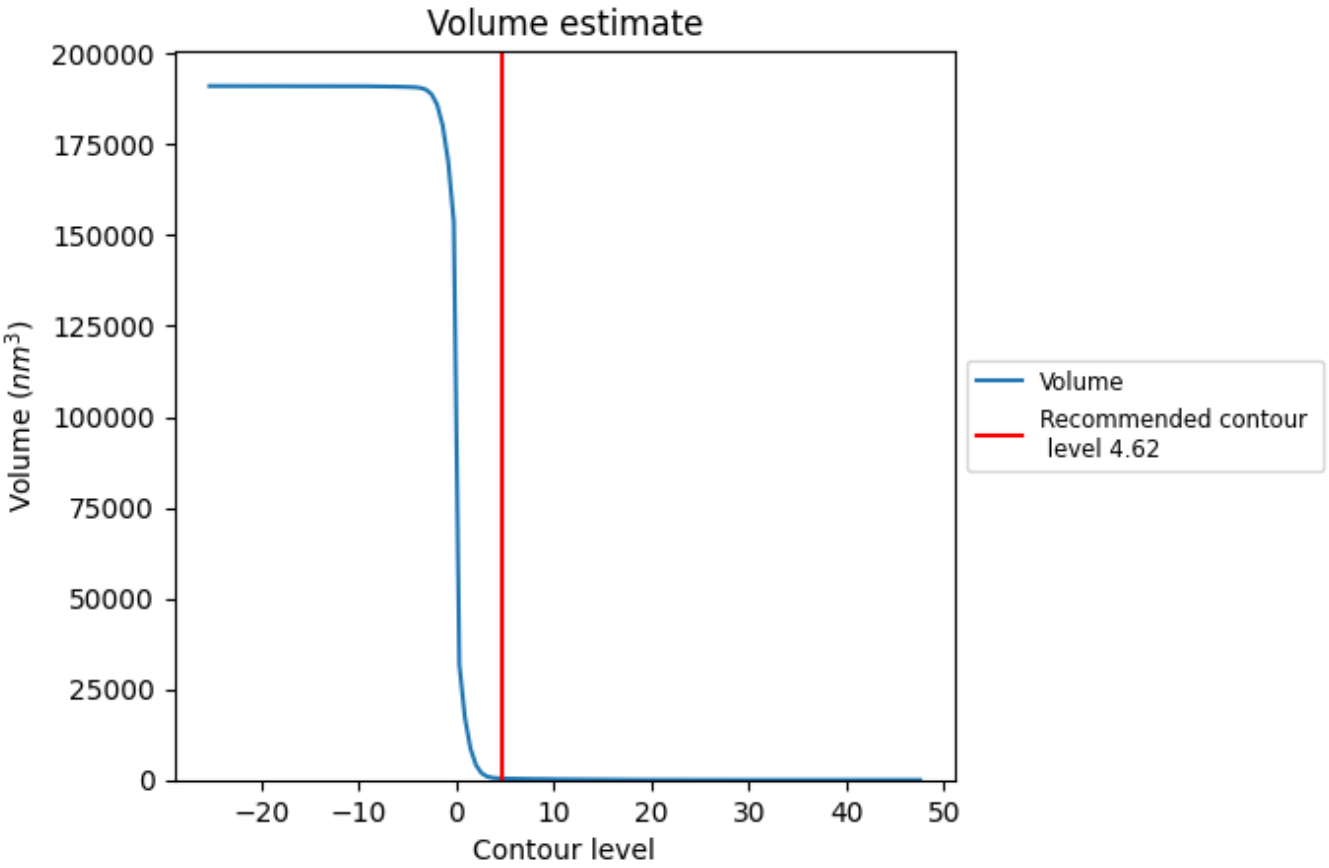
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

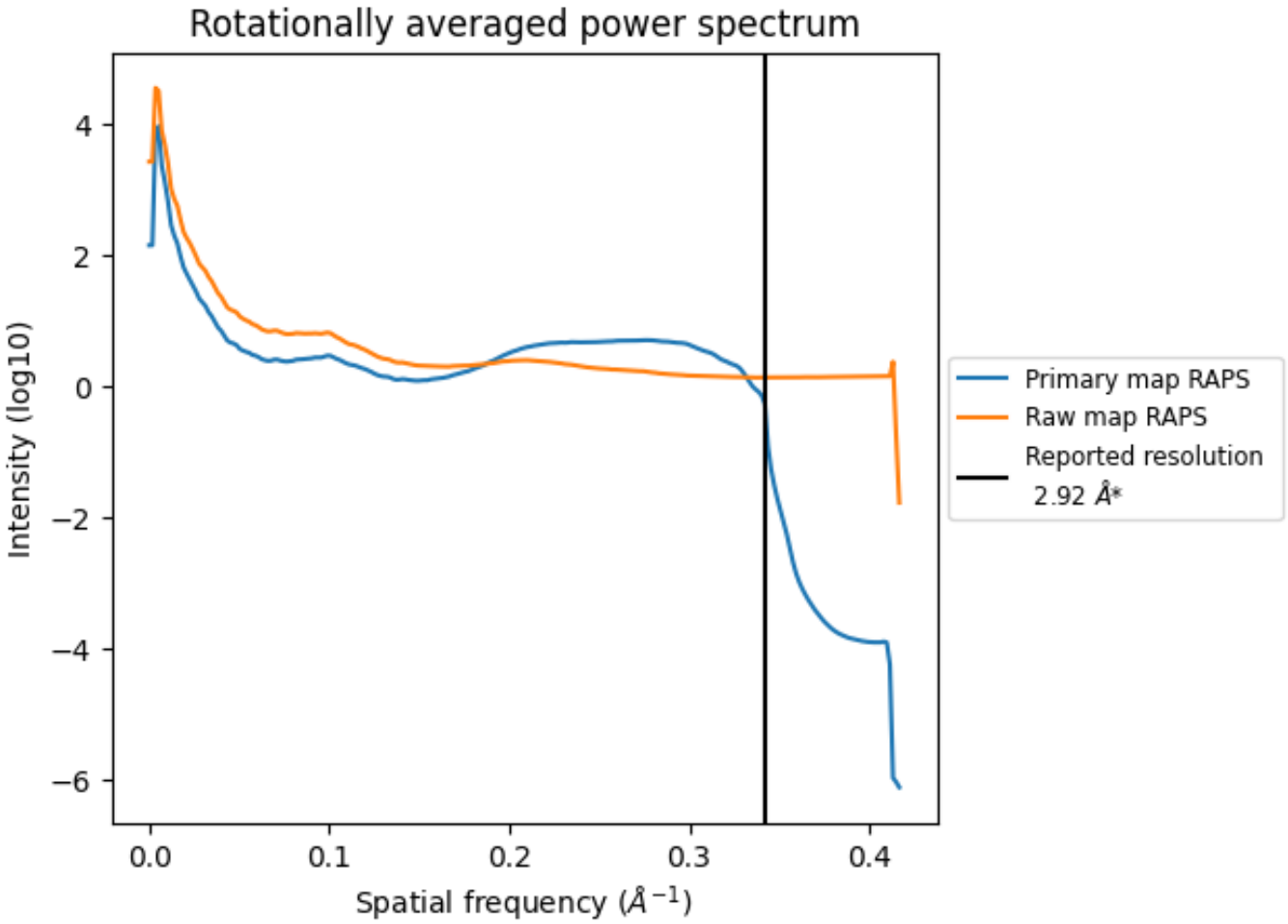
7.2 Volume estimate



The volume at the recommended contour level is 419 nm^3; this corresponds to an approximate mass of 379 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)

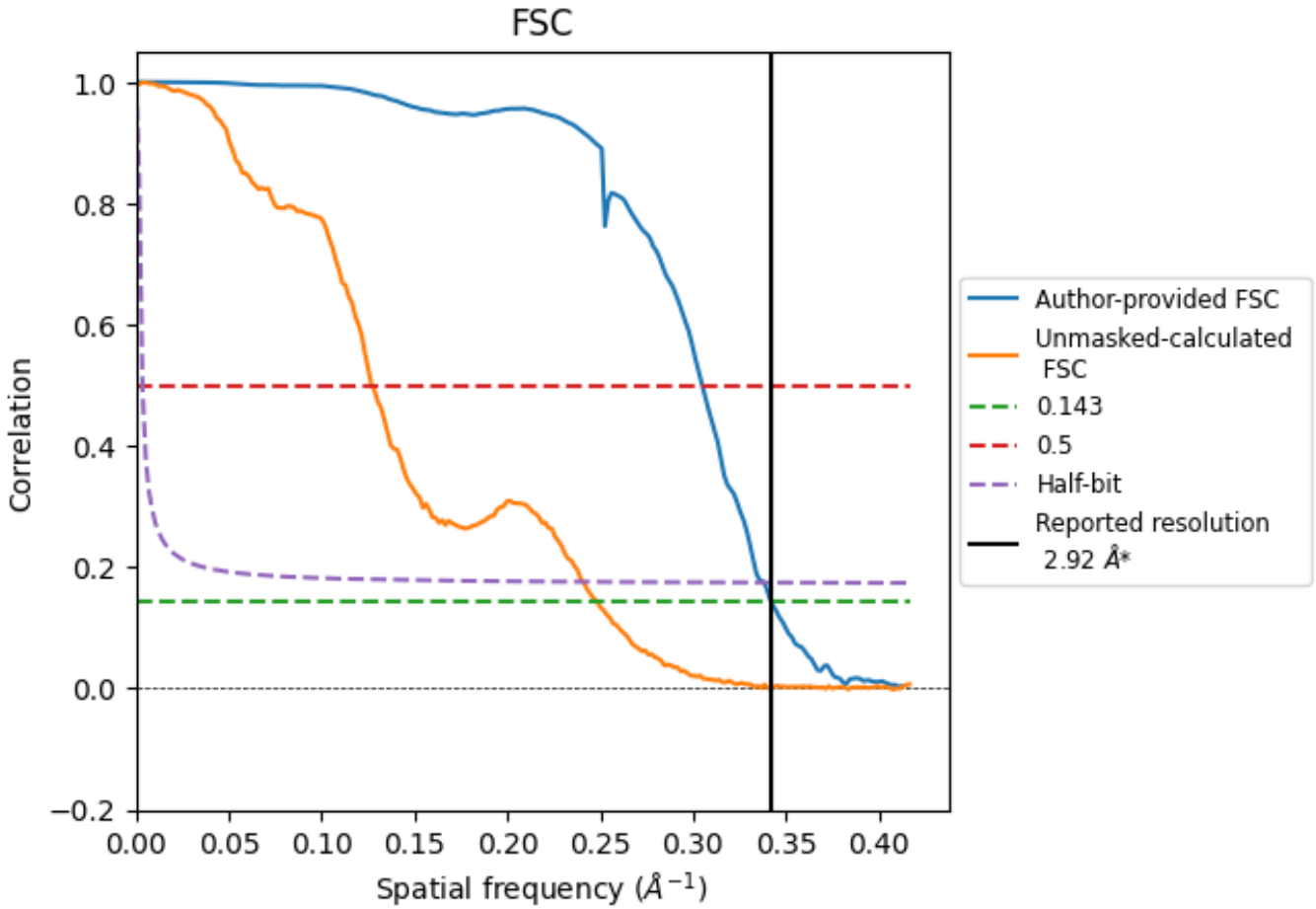


*Reported resolution corresponds to spatial frequency of 0.342 Å^{-1}

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 0.342 Å^{-1}

8.2 Resolution estimates (i)

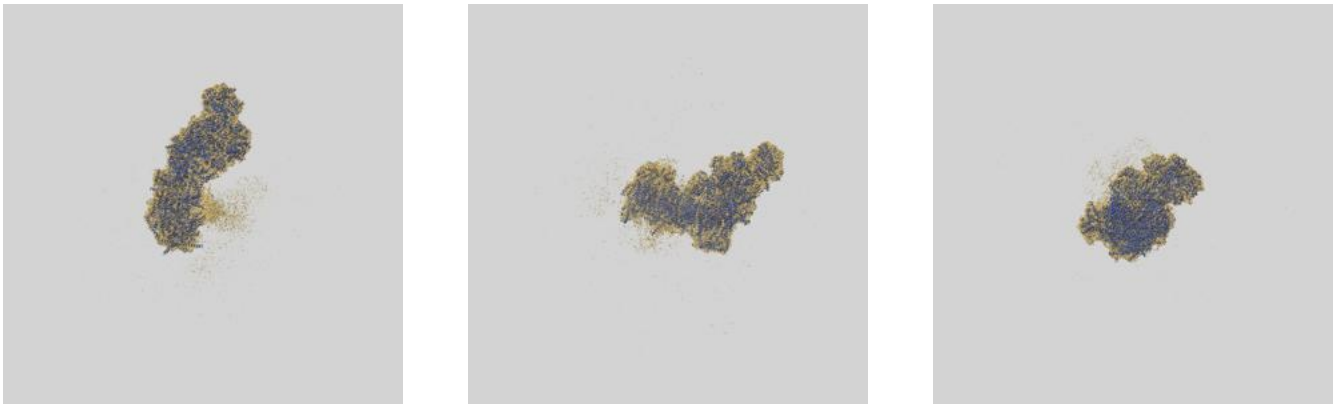
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	2.92	3.28	2.96
Unmasked-calculated*	4.03	7.87	4.15

*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 4.03 differs from the reported value 2.92 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-61173 and PDB model 9J6H. Per-residue inclusion information can be found in section 3 on page 22.

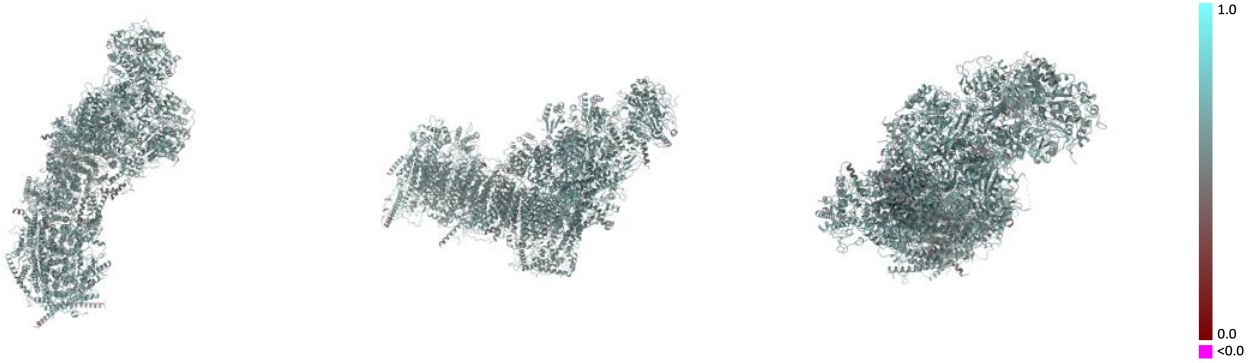
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.62 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.

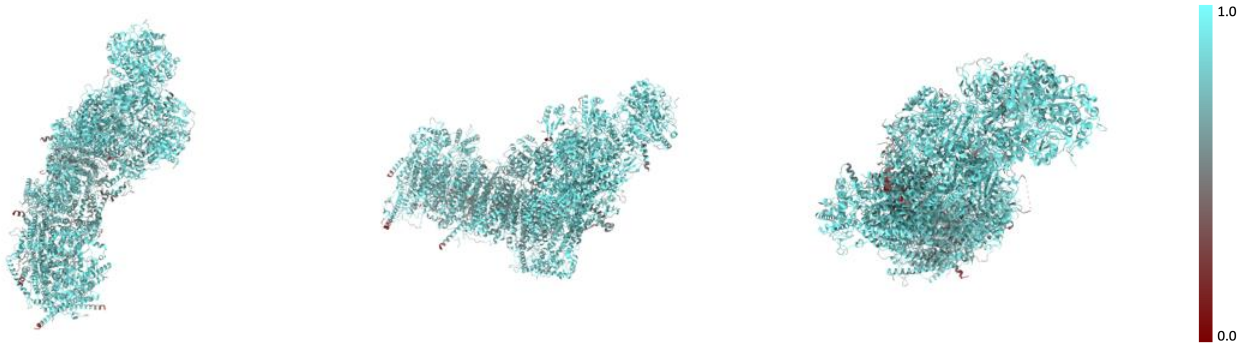
9.2 Q-score mapped to coordinate model (i)



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.

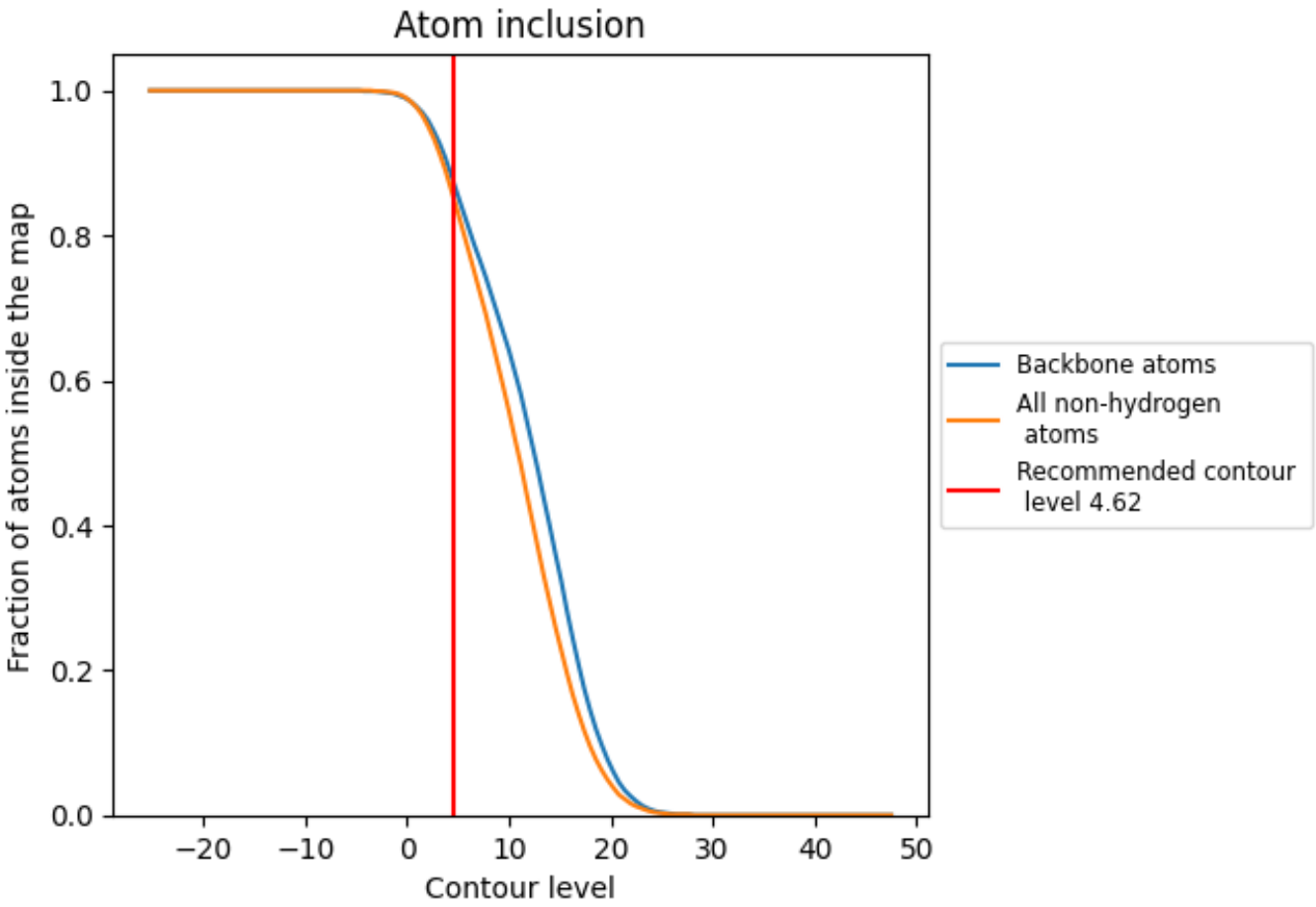
9.3 Atom inclusion mapped to coordinate model (i)



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 (4.62).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 85% 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 (4.62) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8490	0.5820
4L	0.8500	0.5950
A1	0.8980	0.5900
A2	0.8080	0.5600
A3	0.8490	0.5750
A5	0.8450	0.5860
A6	0.8340	0.5780
A7	0.7390	0.5630
A8	0.8710	0.5840
A9	0.8800	0.5940
AB	0.6730	0.4910
AC	0.8470	0.5890
AK	0.7830	0.5550
AL	0.7850	0.5660
AM	0.7580	0.5770
AN	0.8580	0.5760
B1	0.7420	0.5610
B2	0.8100	0.5720
B3	0.7490	0.5490
B4	0.7880	0.5700
B5	0.8730	0.5980
B6	0.7530	0.5500
B7	0.8110	0.5630
B8	0.8470	0.5860
B9	0.8680	0.5850
BK	0.8270	0.5770
BL	0.8200	0.5730
CA	0.7800	0.5580
CB	0.8530	0.5880
N1	0.8710	0.5860
N2	0.8840	0.5950
N3	0.8750	0.5940
N4	0.8700	0.5940
N5	0.8620	0.5920
N6	0.7740	0.5500



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Chain	Atom inclusion	Q-score
S1	0.8690	0.5810
S2	0.9000	0.6020
S3	0.9200	0.6140
S4	0.8440	0.5920
S5	0.8110	0.5690
S6	0.8210	0.5810
S7	0.9010	0.6050
S8	0.9400	0.6160
V1	0.8680	0.5740
V2	0.8420	0.5660
V3	0.8370	0.5700