Full wwPDB EM Validation Report (i)

Aug 6, 2026 – 12:32 PM JST

PDB ID	:	7W2K / pdb_00007w2k
EMDB ID	:	EMD-32263
Title	:	Deactive state CI from Rotenone-NADH dataset, Subclass 1
Authors	:	Gu, J.K.; Yang, M.J.
Deposited on	:	2021-11-24
Resolution	:	2.90 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 (i) 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 (i)) were used in the production of this report:

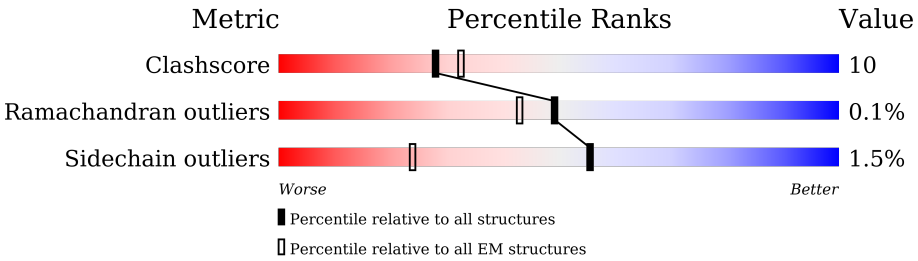
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

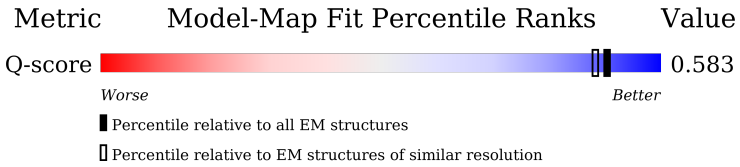
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	A	431	74% 26%
2	B	176	74% 25%
3	C	156	78% 21%
4	E	115	10% 83% 17%

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Mol	Chain	Length	Quality of chain
5	F	86	13% 66% 34%
6	G	88	52% 63% 38%
6	X	88	6% 66% 33%
7	H	112	5% 68% 31%
8	I	112	9% 69% 16% 13%
9	J	342	10% 68% 19% 13%
10	K	42	14% 62% 36%
11	L	125	6% 82% 18%
12	M	690	82% 18%
13	N	144	7% 75% 25%
14	O	217	10% 75% 23%
15	P	208	79% 21%
16	Q	430	76% 22%
17	S	70	84% 16%
18	T	96	8% 93% 7%
19	U	83	7% 82% 17%
20	V	140	24% 81% 18%
21	W	142	5% 78% 22%
22	Y	70	19% 77% 21%
23	Z	84	29% 83% 17%
24	a	140	86% 14%
25	b	126	14% 66% 14% 18%
26	c	156	8% 72% 25%
27	d	175	7% 75% 25%
28	e	107	13% 79% 21%

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Mol	Chain	Length	Quality of chain
29	f	42	19% 76% 24%
30	g	121	85% 15%
31	h	105	83% 17%
32	i	347	78% 21%
33	j	113	12% 67% 20% 12%
34	k	98	7% 73% 27%
35	l	603	74% 25%
36	m	175	9% 55% 17% 26%
37	n	56	23% 80% 20%
38	o	128	6% 86% 13%
39	p	178	80% 19%
40	r	459	74% 25%
41	s	318	72% 23% 5%
42	u	171	79% 21%
43	v	131	18% 63% 32% 5%
44	w	320	8% 78% 22%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	A	501	-	-	X	-
45	SF4	C	301	-	-	X	-

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 66522 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	431	3318	2095	591	612	20	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	156	1235	788	221	212	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	115	965	616	176	168	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	86	688	433	129	124	2	0	0

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	88	693	447	102	139	5	0	0
6	X	88	696	449	103	139	5	0	0

- Molecule 7 is a protein called Complex I subunit B13.

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

- Molecule 8 is a protein called Complex I-B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	97	762	479	144	136	3	0	0

- Molecule 9 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	297	2352	1511	420	413	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	377	VAL	ILE	conflict	UNP F1SL07

- Molecule 10 is a protein called Complex I-9kD.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	690	5293	3319	923	1012	39	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	217	1648	1054	277	308	9	0	0

- Molecule 15 is a protein called Complex I-30kD.

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

- Molecule 16 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	419	3364	2153	574	613	24	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	S	70	567	364	104	94	5	0	0

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

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

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

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

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

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

- Molecule 21 is a protein called Complex I-B16.6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W	142	1161	749	197	206	9	0	0

- Molecule 22 is a protein called Complex I-AGGG.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Y	70	583	386	98	98	1	0	0

- Molecule 23 is a protein called Complex I-B12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Z	84	674	437	116	120	1	0	0

- Molecule 24 is a protein called Complex I-SGDH.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	a	140	1152	754	196	199	3	0	0

- Molecule 25 is a protein called Complex I-B17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	b	103	875	571	158	145	1	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	e	107	890	568	145	173	4	0	0

- Molecule 29 is a protein called Complex I-KFYI.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	f	42	342	225	58	59	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	i	347	2706	1779	419	462	46	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	j	99	800	545	118	132	5	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	l	603	4782	3171	741	820	50	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	m	129	948	636	138	166	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	n	56	456	295	83	77	1	0	0

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	o	128	1058	688	181	189	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	s	303	2394	1607	369	397	21	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	v	124	1020	637	189	185	9	0	0

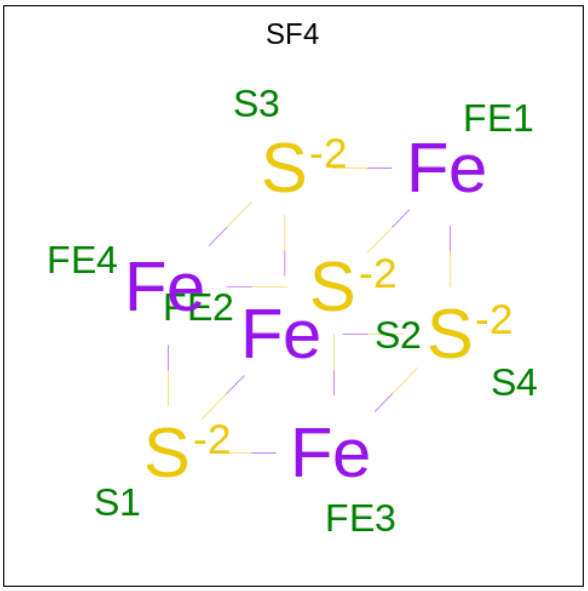
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	1	MYR	-	acetylation	UNP F1SCH1
v	126	ALA	GLN	conflict	UNP F1SCH1
v	128	ALA	PRO	conflict	UNP F1SCH1
v	130	ALA	GLU	conflict	UNP F1SCH1
v	131	ALA	VAL	conflict	UNP F1SCH1

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

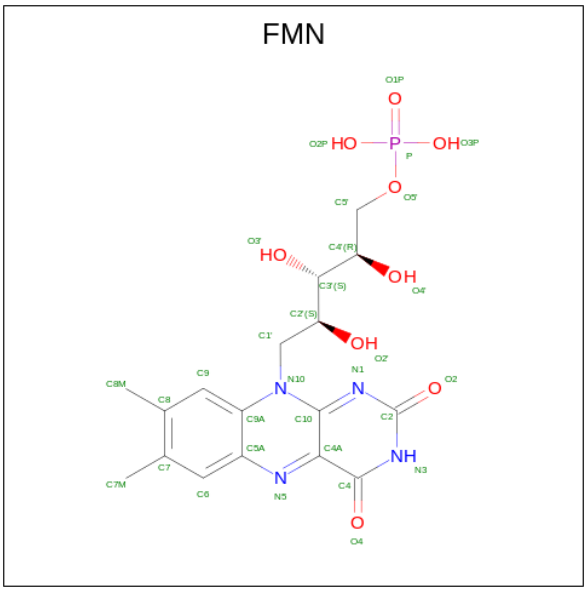
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	w	320	2574	1638	437	489	10	0	0

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



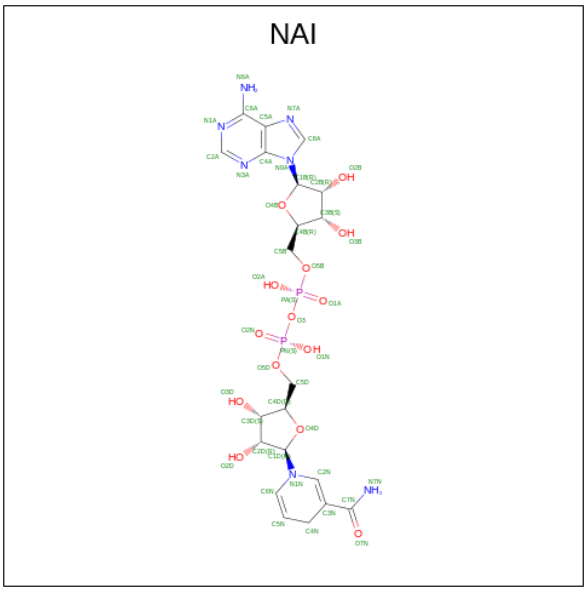
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	A	1	8	4	4	0
45	B	1	8	4	4	0
45	B	1	8	4	4	0
45	C	1	8	4	4	0
45	M	1	8	4	4	0
45	M	1	8	4	4	0

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



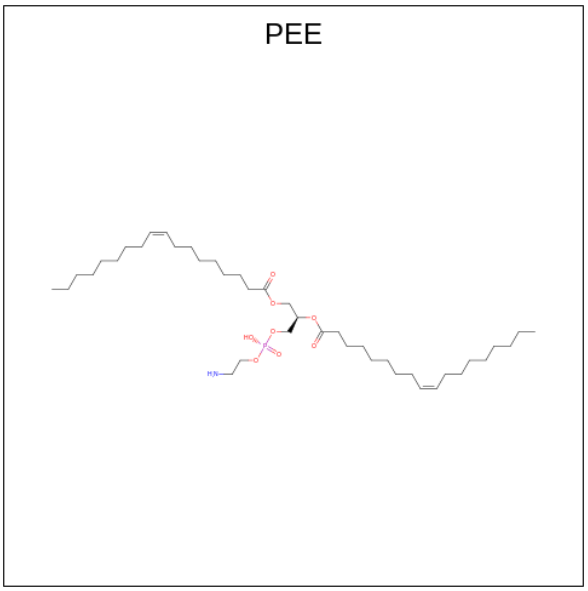
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	A	1	31	17	4	9	1	0

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



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

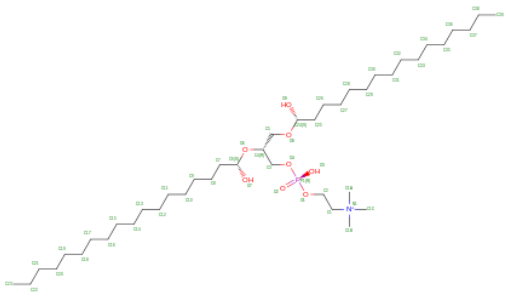
- Molecule 48 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	B	1	51	41	1	8	1	0
			Total	C	N	O	P	
48	C	1	47	37	1	8	1	0
			Total	C	N	O	P	
48	Q	1	47	37	1	8	1	0
			Total	C	N	O	P	
48	b	1	46	36	1	8	1	0
			Total	C	N	O	P	
48	j	1	51	41	1	8	1	0
			Total	C	N	O	P	
48	l	1	46	36	1	8	1	0
			Total	C	N	O	P	
48	r	1	51	41	1	8	1	0
			Total	C	N	O	P	
48	s	1	41	31	1	8	1	0

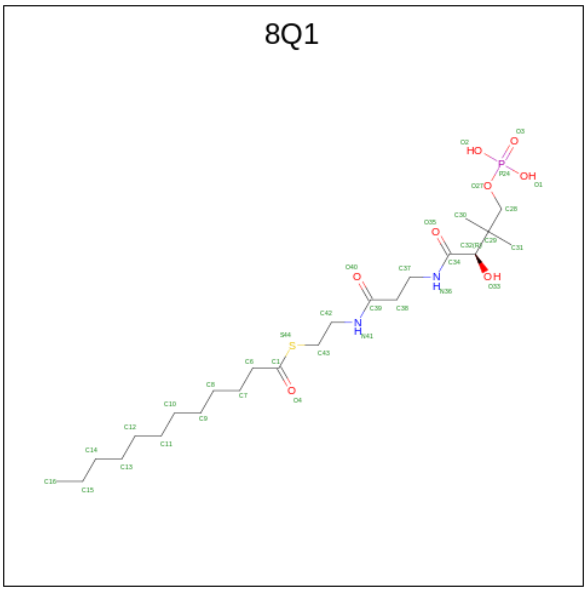
- Molecule 49 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: $C_{42}H_{89}NO_8P$) (labeled as "Ligand of Interest" by depositor).

PLX



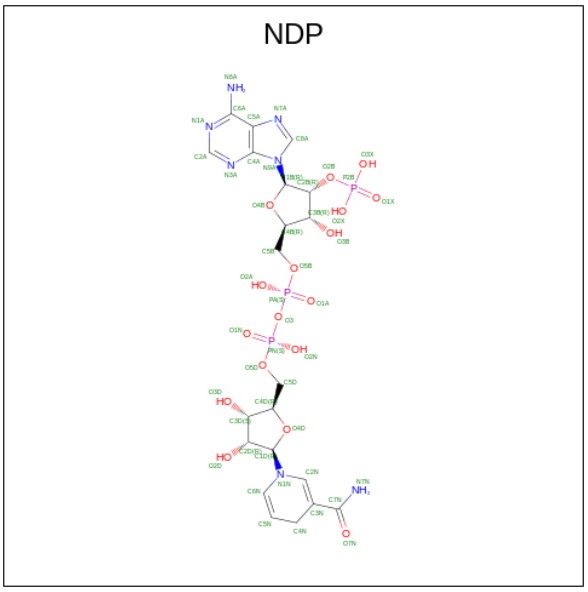
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	C	1	52	42	1	8	1	0
49	a	1	52	42	1	8	1	0
49	e	1	52	42	1	8	1	0
49	g	1	52	42	1	8	1	0
49	j	1	52	42	1	8	1	0
49	r	1	52	42	1	8	1	0

- Molecule 50 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



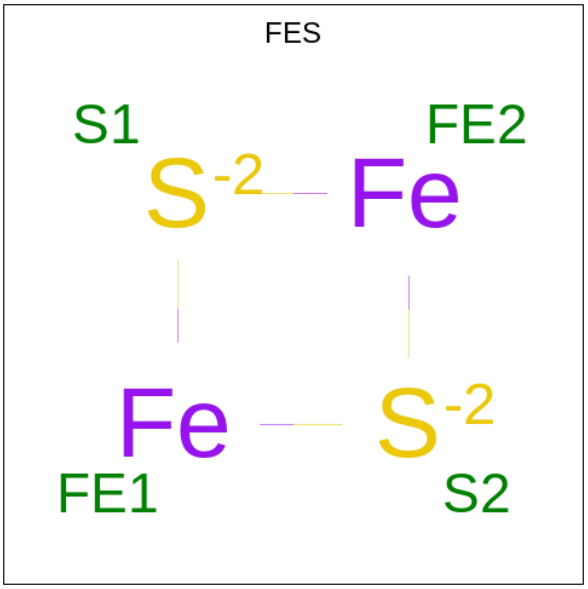
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
50	G	1	35	23	2	8	1	1	0
			Total	C	N	O	P	S	
50	X	1	35	23	2	8	1	1	0

- Molecule 51 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 52 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



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

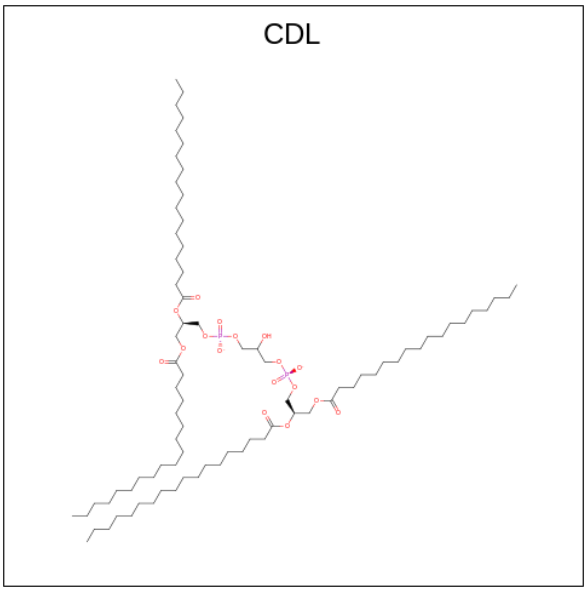
- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

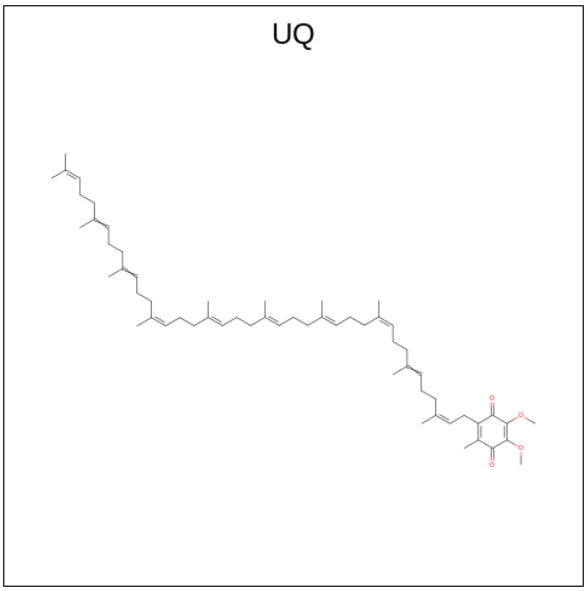
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
54	T	1	1	1	0

- Molecule 55 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



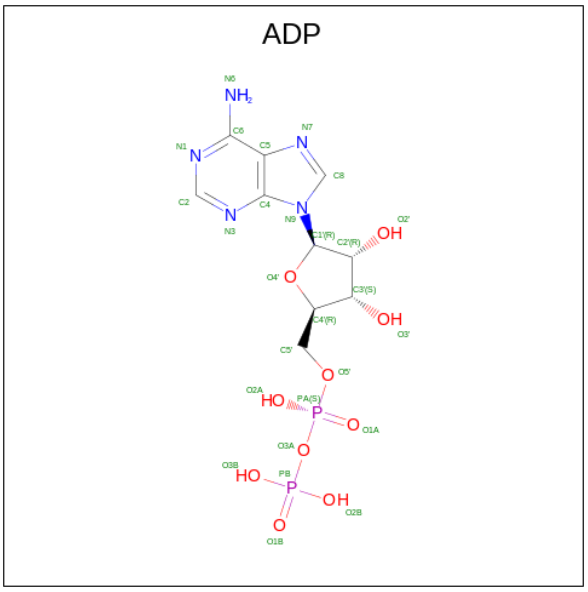
Mol	Chain	Residues	Atoms				AltConf
55	a	1	Total	C	O	P	0
			91	72	17	2	
55	i	1	Total	C	O	P	0
			66	47	17	2	
55	l	1	Total	C	O	P	0
			99	80	17	2	
55	l	1	Total	C	O	P	0
			100	81	17	2	
55	r	1	Total	C	O	P	0
			100	81	17	2	
55	u	1	Total	C	O	P	0
			78	59	17	2	

- Molecule 56 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
56	s	1	28	24	4	0

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



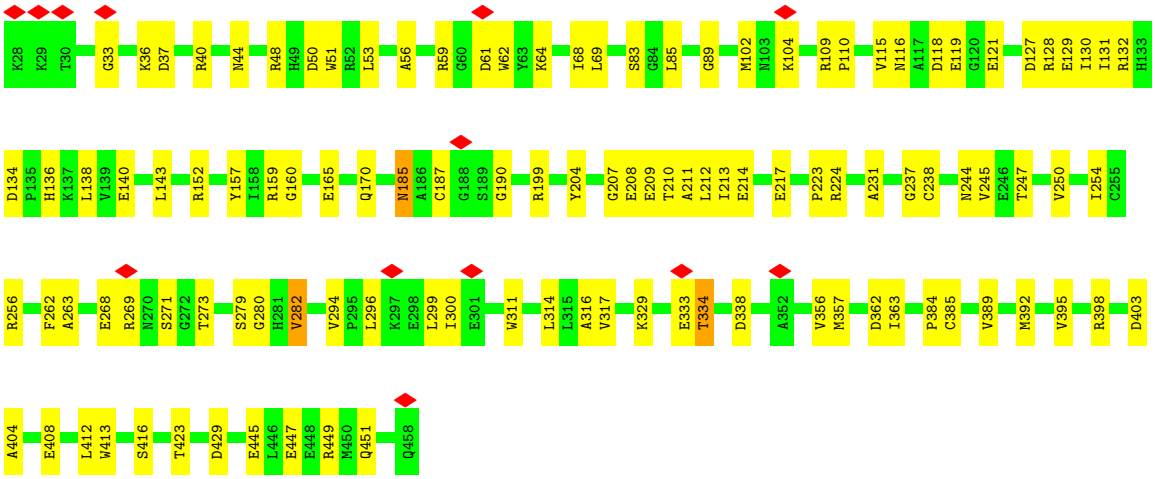
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	w	1	27	10	5	10	2	0

3 Residue-property plots (i)

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

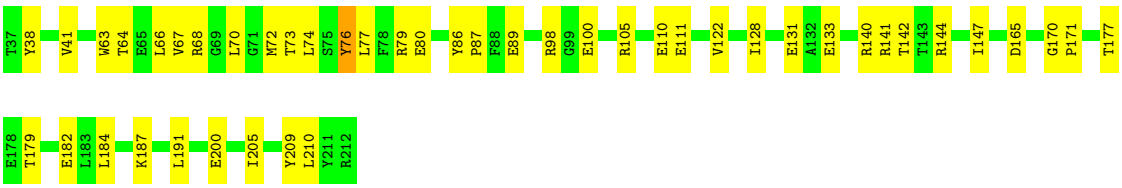
• Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain A: 74% 26%



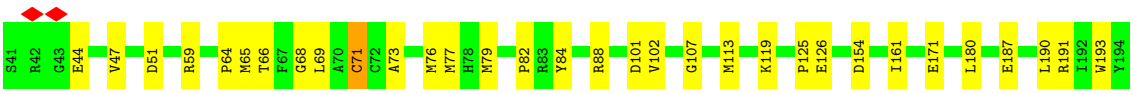
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain B: 74% 25%



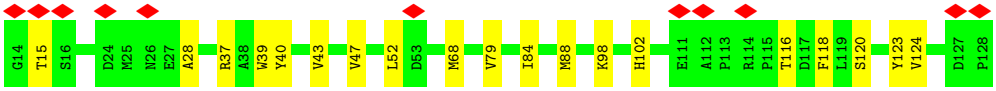
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain C: 78% 21%



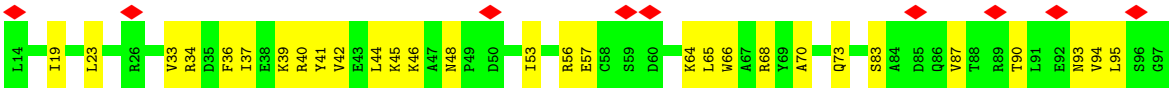
• Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain E:



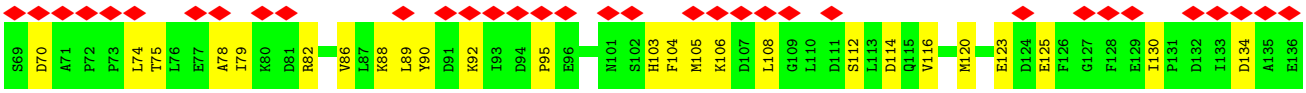
• Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

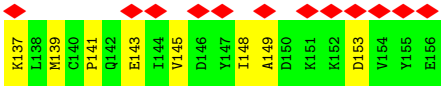
Chain F:



• Molecule 6: Acyl carrier protein

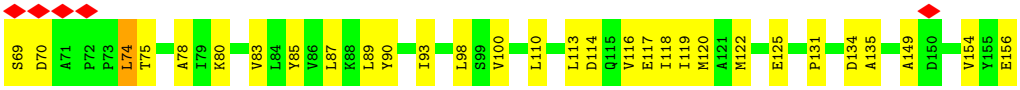
Chain G:





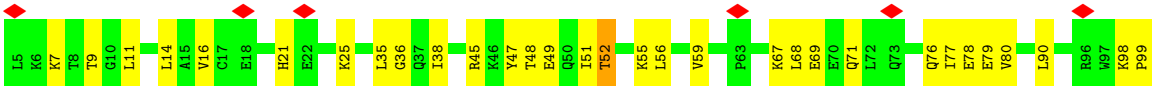
• Molecule 6: Acyl carrier protein

Chain X:



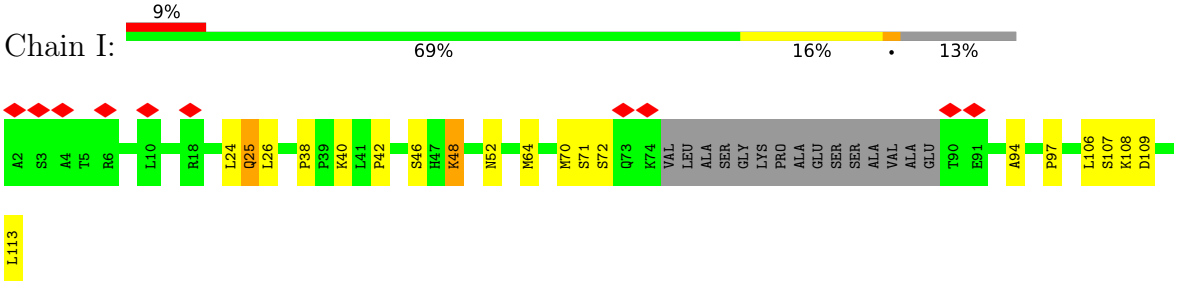
• Molecule 7: Complex I subunit B13

Chain H:



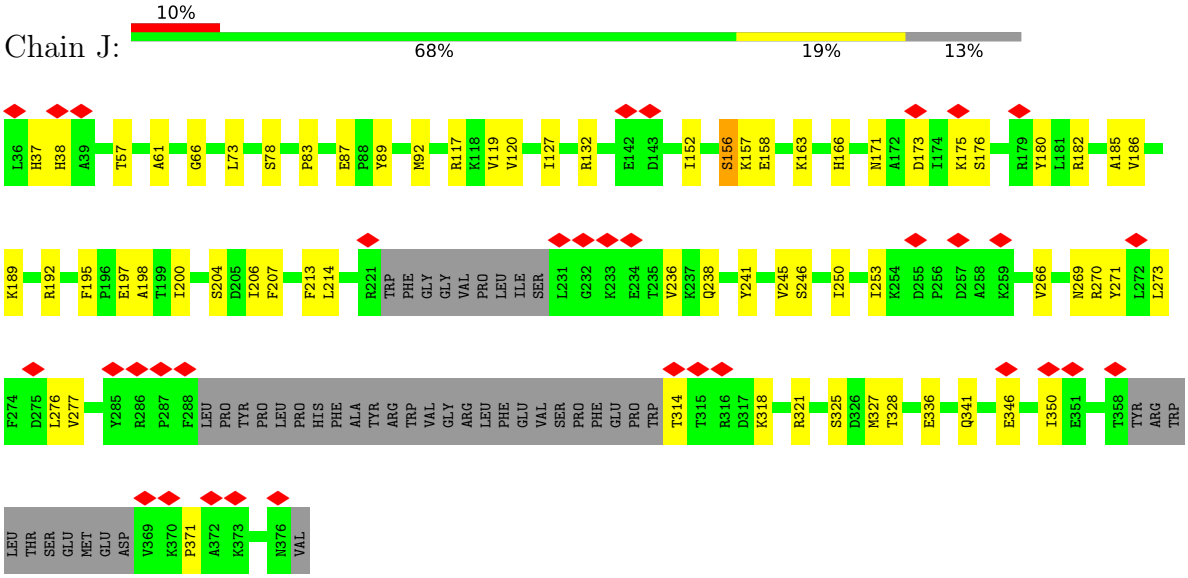
• Molecule 8: Complex I-B14.5a

Chain I:



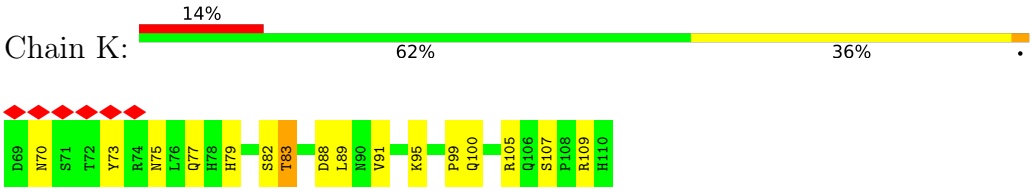
• Molecule 9: NADH:ubiquinone oxidoreductase subunit A9

Chain J:



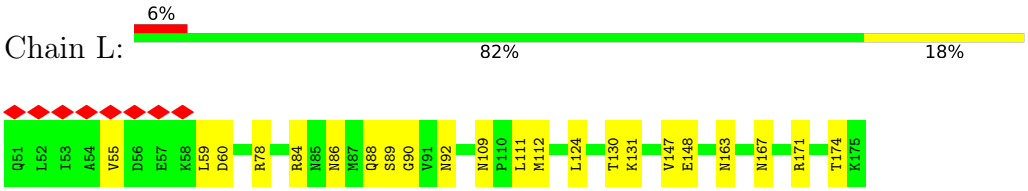
• Molecule 10: Complex I-9kD

Chain K:



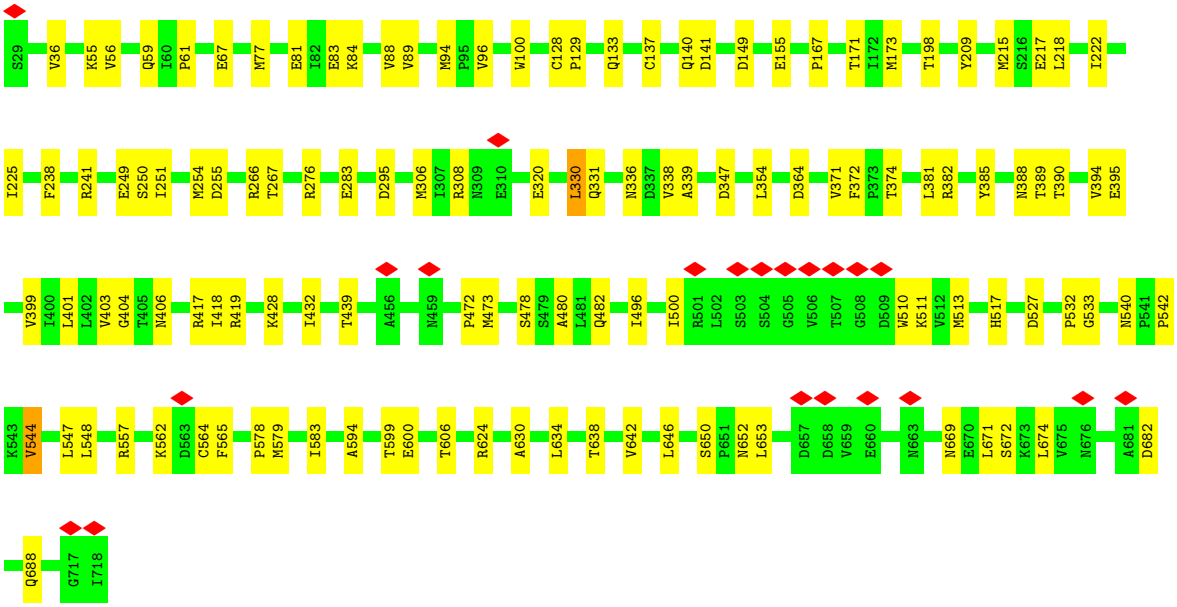
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain L:



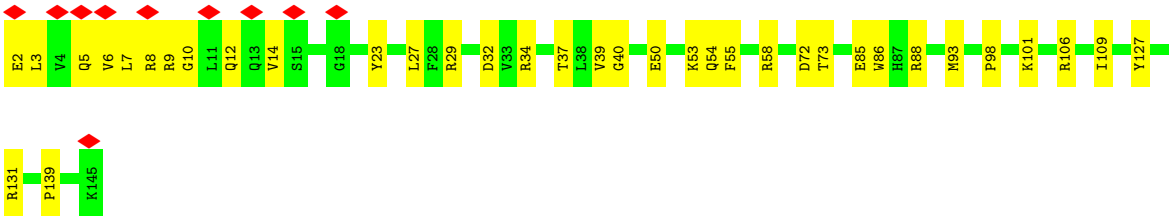
• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain M:



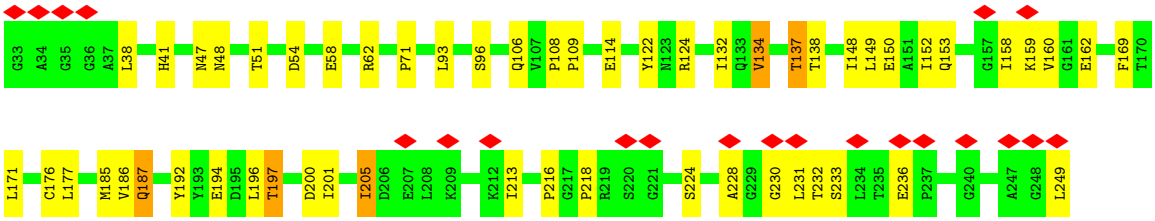
• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain N:



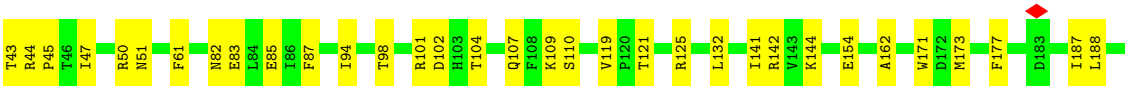
• Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

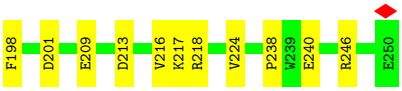
Chain O:



• Molecule 15: Complex I-30kD

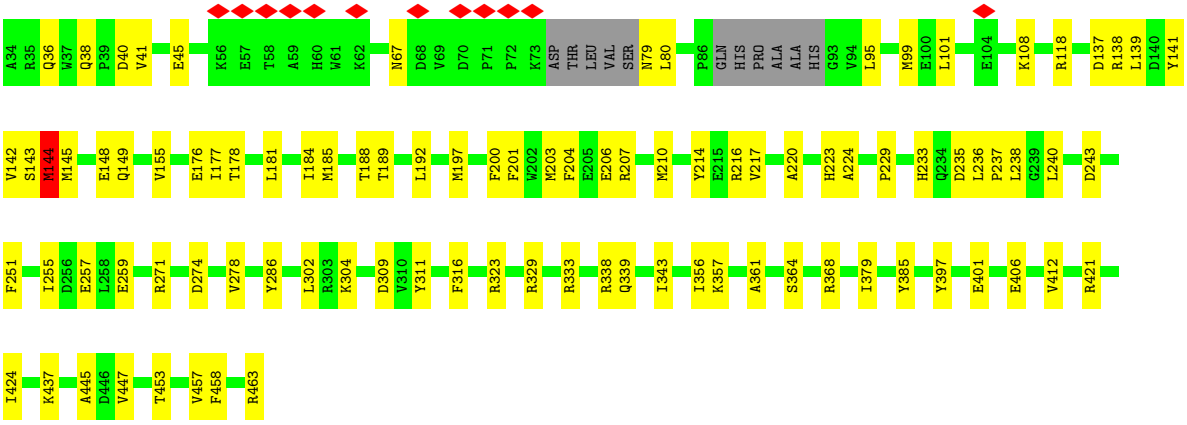
Chain P:





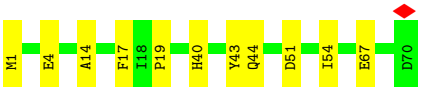
• Molecule 16: Complex I-49kD

Chain Q:



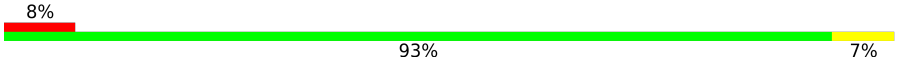
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

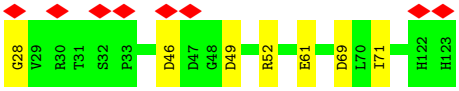
Chain S:



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

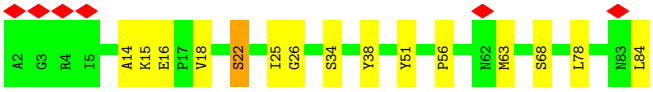
Chain T:





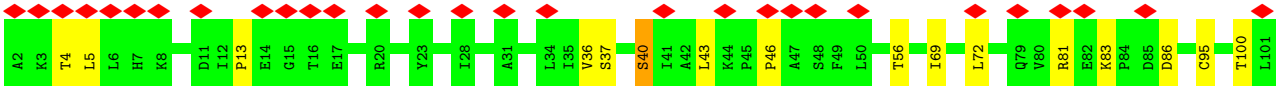
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:



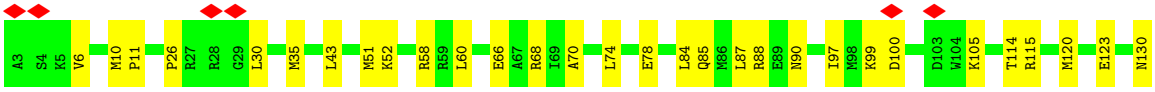
• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

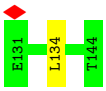
Chain V:



- Molecule 21: Complex I-B16.6

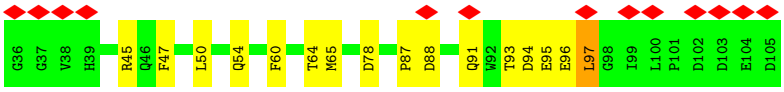
Chain W:





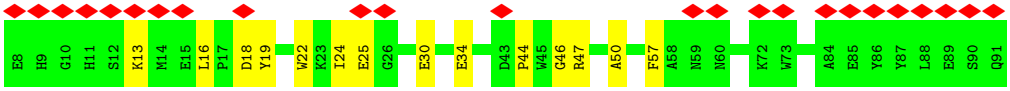
- Molecule 22: Complex I-AGGG

Chain Y:



- Molecule 23: Complex I-B12

Chain Z:

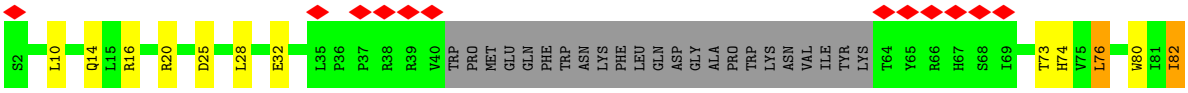


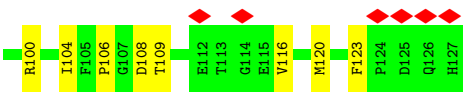
- Molecule 24: Complex I-SGDH

Chain a:

- Molecule 25: Complex I-B17

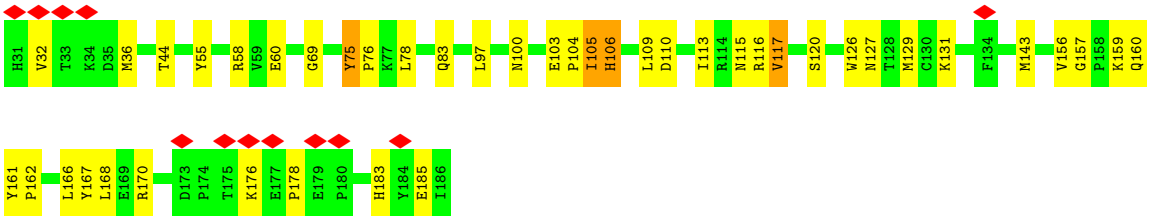
Chain b:





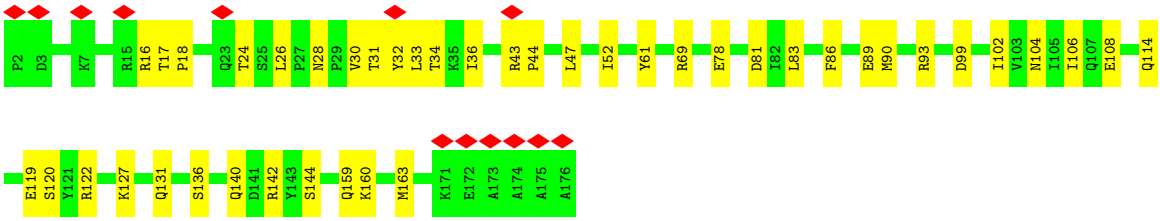
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c:



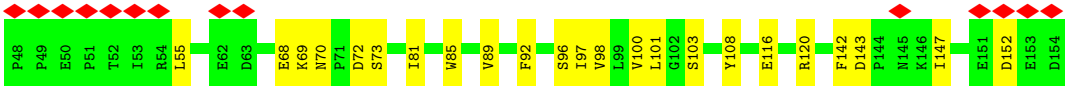
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d:



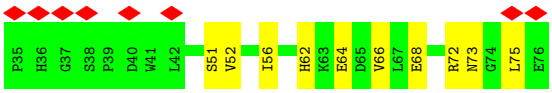
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e:



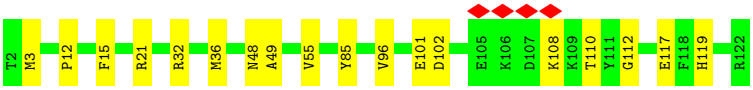
• Molecule 29: Complex I-KFYI

Chain f:



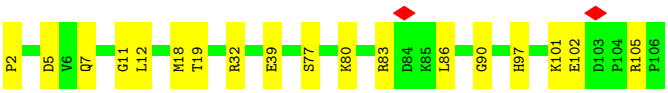
• Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g:



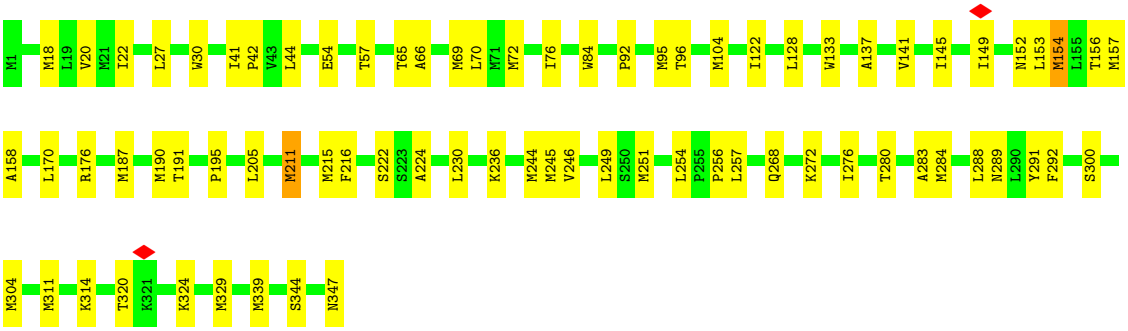
• Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h:



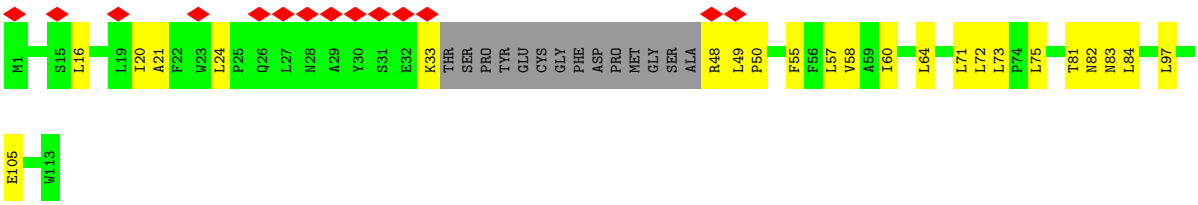
• Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain i:



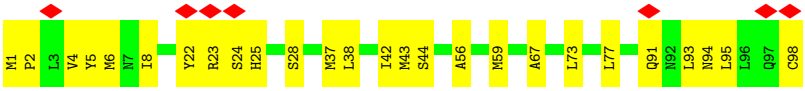
• Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j:



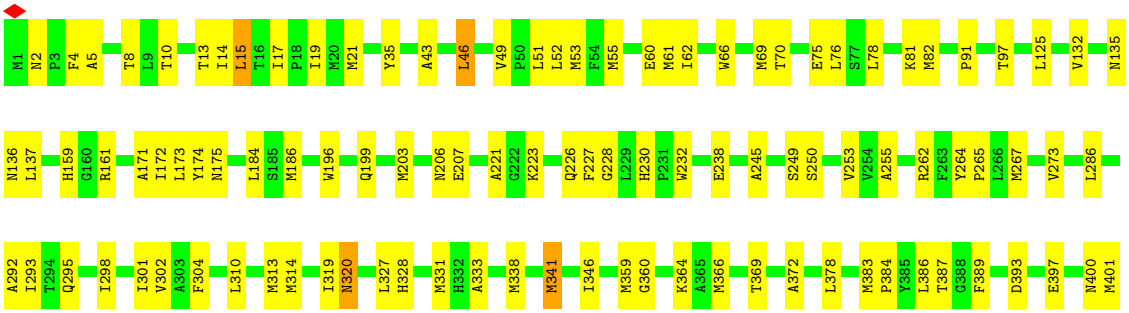
• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

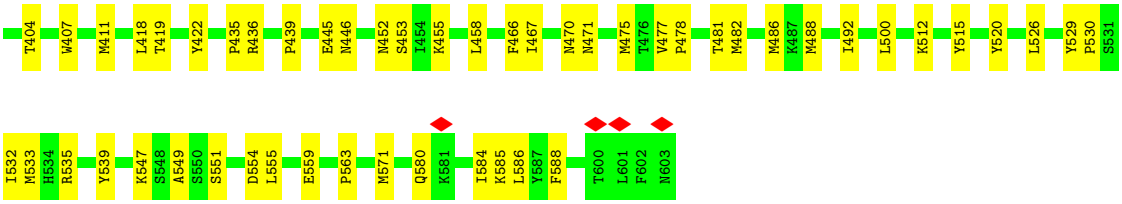
Chain k:



• Molecule 35: NADH-ubiquinone oxidoreductase chain 5

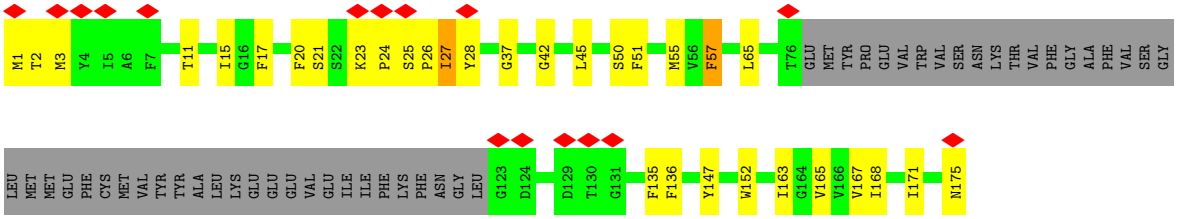
Chain l:





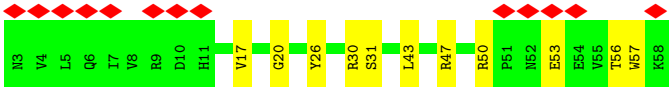
• Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain m:



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

Chain n:

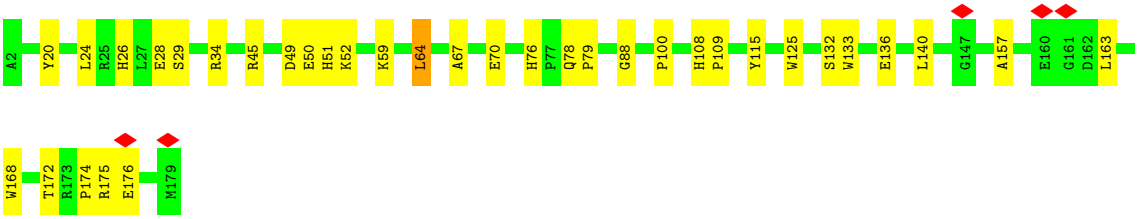


• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o:

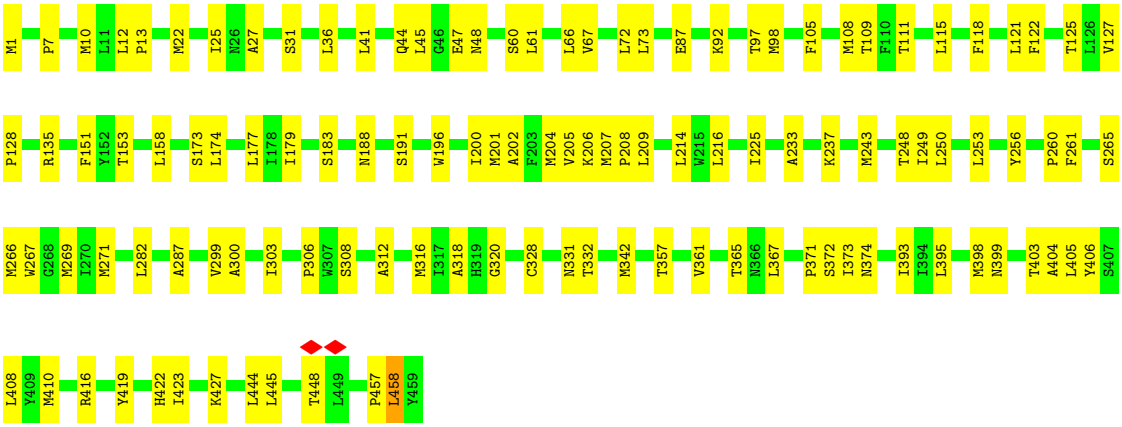
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p:



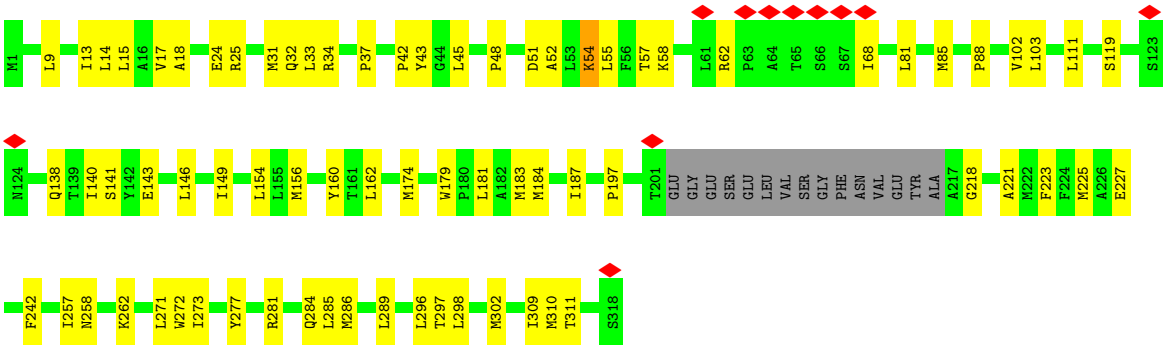
• Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r:



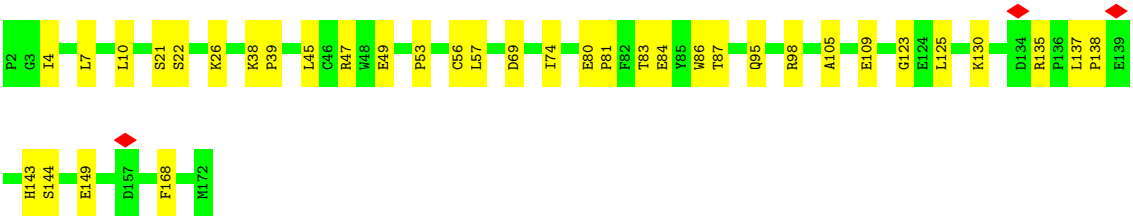
• Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s:



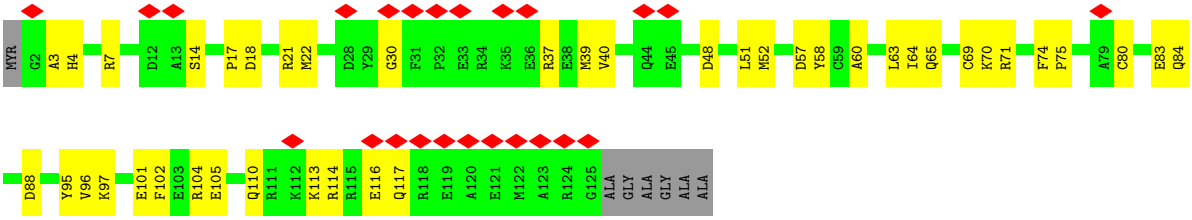
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:



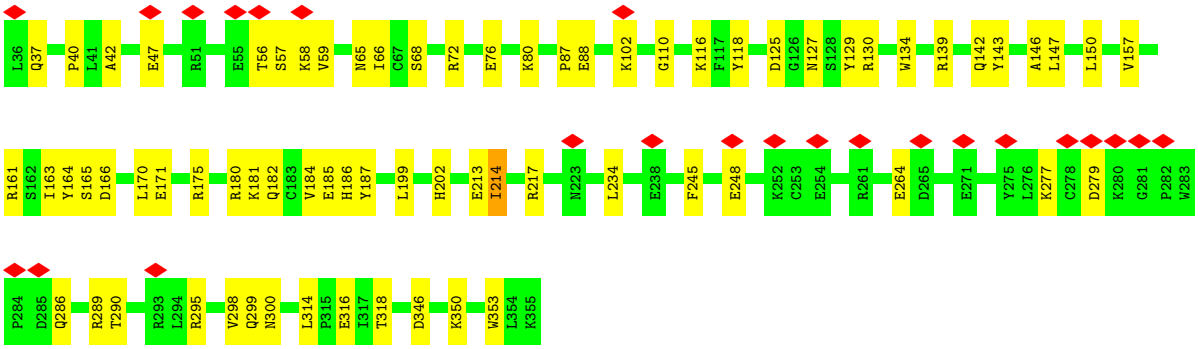
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v:



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

Chain w:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99503	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.196	Depositor
Minimum map value	-0.112	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0279	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	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: 8Q1, ZN, CDL, PLX, MG, UQ, 2MR, PEE, SF4, ADP, FMN, NDP, FES, NAI

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.15	0/3393	0.36	0/4584
2	B	0.13	0/1443	0.30	0/1952
3	C	0.14	0/1266	0.33	0/1715
4	E	0.16	0/989	0.38	0/1333
5	F	0.22	0/699	0.62	2/941 (0.2%)
6	G	0.15	0/705	0.38	0/956
6	X	0.17	0/708	0.39	0/959
7	H	0.13	0/929	0.30	0/1258
8	I	0.14	0/780	0.36	0/1059
9	J	0.14	0/2404	0.33	0/3245
10	K	0.10	0/365	0.30	0/493
11	L	0.10	0/1039	0.29	0/1403
12	M	0.12	0/5381	0.30	0/7291
13	N	0.11	0/1245	0.33	0/1694
14	O	0.18	0/1688	0.50	4/2301 (0.2%)
15	P	0.14	0/1789	0.34	0/2436
16	Q	0.19	0/3437	0.48	5/4656 (0.1%)
17	S	0.14	0/582	0.30	0/783
18	T	0.10	0/755	0.29	0/1018
19	U	0.12	0/664	0.31	0/912
20	V	0.16	0/1042	0.34	1/1411 (0.1%)
21	W	0.13	0/1192	0.27	0/1610
22	Y	0.13	0/609	0.32	0/835
23	Z	0.13	0/695	0.34	0/939
24	a	0.13	0/1185	0.32	0/1606
25	b	0.13	0/902	0.32	0/1227
26	c	0.21	0/1371	0.63	5/1875 (0.3%)
27	d	0.13	0/1494	0.29	0/2015
28	e	0.12	0/916	0.30	0/1246
29	f	0.14	0/350	0.35	0/473
30	g	0.14	0/1031	0.35	0/1394
31	h	0.12	0/889	0.31	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	i	0.15	0/2769	0.36	0/3764
33	j	0.16	0/819	0.35	0/1117
34	k	0.15	0/759	0.36	0/1029
35	l	0.17	0/4911	0.40	3/6680 (0.0%)
36	m	0.17	0/970	0.39	0/1316
37	n	0.11	0/468	0.36	0/633
38	o	0.13	0/1088	0.28	0/1477
39	p	0.14	0/1590	0.34	0/2155
40	r	0.17	0/3723	0.39	0/5078
41	s	0.16	0/2464	0.36	0/3369
42	u	0.11	0/1436	0.32	0/1938
43	v	0.15	0/1044	0.42	0/1403
44	w	0.13	0/2634	0.32	0/3571
All	All	0.15	0/66612	0.37	20/90340 (0.0%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	c	105	ILE	N-CA-C	11.58	122.43	110.62
5	F	39	LYS	N-CA-C	8.79	120.63	111.14
26	c	75	TYR	CA-C-N	8.78	128.71	119.85
26	c	75	TYR	C-N-CA	8.78	128.71	119.85
14	O	230	GLY	N-CA-C	6.25	120.23	112.73
14	O	224	SER	N-CA-C	6.15	120.13	111.52
14	O	228	ALA	N-CA-C	5.87	117.67	111.28
16	Q	144	MET	N-CA-C	5.86	117.67	111.28
5	F	40	ARG	N-CA-C	5.78	121.09	112.94
16	Q	67	ASN	N-CA-C	-5.73	100.37	109.76
14	O	232	THR	N-CA-C	5.56	117.34	111.28
16	Q	236	LEU	CA-C-N	5.42	125.36	119.78
16	Q	236	LEU	C-N-CA	5.42	125.36	119.78
35	l	2	ASN	CA-C-N	5.36	125.03	119.56
35	l	2	ASN	C-N-CA	5.36	125.03	119.56
26	c	105	ILE	CA-C-N	5.34	131.75	121.54
26	c	105	ILE	C-N-CA	5.34	131.75	121.54
20	V	13	PRO	CA-N-CD	-5.24	104.66	112.00
35	l	547	LYS	N-CA-C	5.20	117.03	111.36
16	Q	233	HIS	N-CA-C	5.05	116.87	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3318	0	3280	97	0
2	B	1412	0	1363	36	0
3	C	1235	0	1229	25	0
4	E	965	0	964	17	0
5	F	688	0	702	38	0
6	G	693	0	671	28	0
6	X	696	0	680	35	0
7	H	910	0	950	27	0
8	I	762	0	766	17	0
9	J	2352	0	2394	42	0
10	K	355	0	329	13	0
11	L	1016	0	1016	16	0
12	M	5293	0	5324	89	0
13	N	1204	0	1162	26	0
14	O	1648	0	1635	36	0
15	P	1738	0	1693	32	0
16	Q	3364	0	3292	72	0
17	S	567	0	565	10	0
18	T	741	0	702	6	0
19	U	643	0	642	11	0
20	V	1021	0	1027	15	0
21	W	1161	0	1144	34	0
22	Y	583	0	525	11	0
23	Z	674	0	643	13	0
24	a	1152	0	1154	18	0
25	b	875	0	895	21	0
26	c	1315	0	1208	39	0
27	d	1461	0	1429	30	0
28	e	890	0	837	19	0
29	f	342	0	341	6	0
30	g	1000	0	994	17	0
31	h	867	0	871	15	0
32	i	2706	0	2863	56	0
33	j	800	0	855	19	0
34	k	748	0	799	23	0
35	l	4782	0	4926	123	0
36	m	948	0	960	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	n	456	0	433	9	0
38	o	1058	0	1061	15	0
39	p	1534	0	1470	27	0
40	r	3631	0	3839	91	0
41	s	2394	0	2508	54	0
42	u	1398	0	1380	29	0
43	v	1020	0	957	39	0
44	w	2574	0	2516	50	0
45	A	8	0	0	2	0
45	B	16	0	0	0	0
45	C	8	0	0	2	0
45	M	16	0	0	0	0
46	A	31	0	19	2	0
47	A	44	0	27	5	0
48	B	51	0	82	9	0
48	C	47	0	71	4	0
48	Q	47	0	71	4	0
48	b	46	0	69	0	0
48	j	51	0	82	2	0
48	l	46	0	69	2	0
48	r	51	0	82	7	0
48	s	41	0	59	1	0
49	C	52	0	88	3	0
49	a	52	0	88	3	0
49	e	52	0	88	4	0
49	g	52	0	88	6	0
49	j	52	0	88	5	0
49	r	52	0	88	3	0
50	G	35	0	0	1	0
50	X	35	0	0	3	0
51	J	48	0	24	1	0
52	M	4	0	0	0	0
52	O	4	0	0	1	0
53	M	1	0	0	0	0
54	T	1	0	0	0	0
55	a	91	0	132	6	0
55	i	66	0	76	3	0
55	l	199	0	307	15	0
55	r	100	0	156	9	0
55	u	78	0	103	6	0
56	s	28	0	31	7	0
57	w	27	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	66522	0	66993	1285	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 10.

All (1285) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:74:LEU:CD1	6:X:154:VAL:HG11	1.52	1.37
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.23
1:A:210:THR:CG2	1:A:224:ARG:H	1.51	1.22
1:A:210:THR:CG2	1:A:224:ARG:HG2	1.69	1.21
51:J:401:NDP:O4D	51:J:401:NDP:C4D	1.68	1.20
5:F:48:ASN:OD1	5:F:95:LEU:HD21	1.44	1.15
35:l:5:ALA:HB2	35:l:61:MET:HE1	1.24	1.14
16:Q:188:THR:CG2	16:Q:200:PHE:HA	1.77	1.13
40:r:10:MET:HE2	40:r:10:MET:HA	1.30	1.12
1:A:210:THR:HG23	1:A:224:ARG:CG	1.82	1.10
1:A:210:THR:HG22	1:A:224:ARG:H	1.18	1.09
6:X:74:LEU:HD11	6:X:154:VAL:HG11	1.20	1.08
6:X:74:LEU:HD11	6:X:154:VAL:CG1	1.84	1.06
16:Q:188:THR:HG21	16:Q:200:PHE:HA	1.08	1.05
26:c:78:LEU:HB2	26:c:106:HIS:HD2	1.24	1.02
6:X:74:LEU:CD1	6:X:154:VAL:CG1	2.37	1.02
14:O:148:ILE:HG23	14:O:201:ILE:HG13	1.40	1.01
6:X:80:LYS:HZ1	6:X:100:VAL:HG21	1.23	1.00
6:X:80:LYS:NZ	6:X:100:VAL:HG21	1.75	0.99
1:A:210:THR:HG21	1:A:224:ARG:H	1.30	0.95
1:A:210:THR:CG2	1:A:224:ARG:CG	2.42	0.94
16:Q:144:MET:CE	16:Q:214:TYR:CE2	2.51	0.94
1:A:210:THR:HG23	1:A:224:ARG:HG2	0.97	0.94
9:J:213:PHE:HZ	9:J:276:LEU:HD21	1.33	0.93
16:Q:188:THR:HG21	16:Q:200:PHE:CA	1.99	0.92
1:A:210:THR:CG2	1:A:224:ARG:N	2.33	0.92
45:C:301:SF4:S4	16:Q:223:HIS:CD2	2.63	0.91
26:c:162:PRO:HG3	43:v:39:MET:HE3	1.53	0.90
1:A:210:THR:HG21	1:A:224:ARG:N	1.87	0.89
26:c:100:ASN:HB2	26:c:103:GLU:HG3	1.54	0.88
26:c:78:LEU:HB2	26:c:106:HIS:CD2	2.10	0.85
16:Q:188:THR:CG2	16:Q:200:PHE:CA	2.54	0.85
1:A:282:VAL:HG13	1:A:356:VAL:HG21	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:5:ALA:CB	35:l:61:MET:HE1	2.09	0.81
35:l:320:ASN:ND2	35:l:320:ASN:O	2.13	0.81
6:X:74:LEU:HD12	6:X:154:VAL:HG11	1.60	0.80
5:F:48:ASN:OD1	5:F:95:LEU:CD2	2.30	0.79
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.63	0.79
40:r:10:MET:HA	40:r:10:MET:CE	2.11	0.79
30:g:108:LYS:HE3	30:g:108:LYS:HA	1.65	0.79
1:A:33:GLY:HA2	1:A:294:VAL:HG12	1.64	0.78
6:X:80:LYS:NZ	6:X:100:VAL:CG2	2.47	0.78
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.67	0.77
25:b:14:GLN:HE22	39:p:157:ALA:HB3	1.49	0.77
20:V:69:ILE:HG13	20:V:100:THR:HG21	1.66	0.76
16:Q:185:MET:HE3	16:Q:189:THR:HG21	1.65	0.76
1:A:157:TYR:CG	1:A:212:LEU:HD11	2.21	0.76
35:l:5:ALA:HB2	35:l:61:MET:CE	2.11	0.76
40:r:12:LEU:HB2	40:r:13:PRO:HD3	1.65	0.75
32:i:211:MET:HE3	32:i:251:MET:HG2	1.68	0.75
20:V:140:LYS:HG3	20:V:141:VAL:HG13	1.70	0.74
21:W:134:LEU:HD11	36:m:1:MET:HA	1.69	0.73
1:A:157:TYR:CG	1:A:212:LEU:CD1	2.72	0.73
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.22	0.72
16:Q:144:MET:HE2	16:Q:214:TYR:CE2	2.24	0.72
41:s:281:ARG:HB2	41:s:284:GLN:HG3	1.71	0.72
16:Q:144:MET:HE2	16:Q:214:TYR:HE2	1.53	0.72
9:J:213:PHE:CZ	9:J:276:LEU:HD21	2.21	0.72
16:Q:144:MET:HE1	16:Q:214:TYR:CE2	2.24	0.72
6:X:74:LEU:HD12	6:X:74:LEU:O	1.89	0.72
15:P:83:GLU:OE2	15:P:142:ARG:NH2	2.23	0.72
16:Q:177:ILE:HG23	16:Q:210:MET:HE2	1.72	0.72
1:A:185:ASN:HB3	1:A:190:GLY:H	1.54	0.71
2:B:68:ARG:NH2	21:W:26:PRO:O	2.24	0.71
5:F:46:LYS:CE	12:M:674:LEU:HD11	2.20	0.70
5:F:70:ALA:O	5:F:73:GLN:NE2	2.24	0.70
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.73	0.70
1:A:210:THR:HG22	1:A:224:ARG:N	2.01	0.70
25:b:104:ILE:HB	43:v:48:ASP:HB3	1.74	0.70
2:B:177:THR:HG21	2:B:182:GLU:HB2	1.72	0.70
33:j:60:ILE:HG21	36:m:168:ILE:HG21	1.72	0.70
14:O:196:LEU:HD13	14:O:201:ILE:HD11	1.72	0.69
2:B:200:GLU:HG3	13:N:88:ARG:HB2	1.73	0.69
6:X:80:LYS:HZ1	6:X:100:VAL:CG2	2.00	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:181:LEU:HD21	16:Q:210:MET:HB2	1.73	0.69
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.73	0.68
3:C:73:ALA:O	3:C:77:MET:HG3	1.94	0.68
5:F:44:LEU:HD12	5:F:44:LEU:O	1.94	0.68
7:H:51:ILE:HD11	8:I:94:ALA:HB3	1.74	0.68
35:l:250:SER:HB2	35:l:333:ALA:HA	1.75	0.68
44:w:88:GLU:OE2	44:w:161:ARG:NH1	2.26	0.68
16:Q:80:LEU:HD13	33:j:50:PRO:HG3	1.76	0.68
35:l:4:PHE:CE2	35:l:61:MET:HG3	2.28	0.68
6:X:120:MET:HE1	39:p:24:LEU:HB2	1.76	0.68
22:Y:95:GLU:OE2	22:Y:95:GLU:N	2.27	0.68
27:d:24:THR:HG22	27:d:26:LEU:H	1.58	0.67
23:Z:24:ILE:HG22	23:Z:30:GLU:HG2	1.76	0.67
26:c:105:ILE:HG23	26:c:109:LEU:HD22	1.76	0.67
12:M:557:ARG:NH1	12:M:579:MET:O	2.26	0.67
26:c:55:TYR:CE2	26:c:76:PRO:HD3	2.28	0.67
1:A:157:TYR:CB	1:A:212:LEU:HD11	2.25	0.67
8:I:64:MET:HE2	15:P:50:ARG:HH12	1.59	0.66
32:i:280:THR:O	32:i:284:MET:HG2	1.95	0.66
22:Y:60:PHE:O	22:Y:64:THR:HG23	1.95	0.66
1:A:152:ARG:NH2	10:K:99:PRO:O	2.27	0.66
5:F:23:LEU:HD13	5:F:37:ILE:HD12	1.77	0.66
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.28	0.66
11:L:88:GLN:NE2	12:M:141:ASP:OD2	2.29	0.66
12:M:388:ASN:HB3	12:M:511:LYS:HE2	1.78	0.66
14:O:38:LEU:O	14:O:124:ARG:NH2	2.26	0.65
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.78	0.65
1:A:217:GLU:OE1	11:L:171:ARG:NH1	2.28	0.65
9:J:87:GLU:HG3	9:J:89:TYR:H	1.60	0.65
40:r:204:MET:HG3	40:r:209:LEU:HB2	1.78	0.65
35:l:228:GLY:HA3	48:l:703:PEE:H38	1.78	0.65
6:G:105:MET:SD	6:G:105:MET:N	2.69	0.65
44:w:129:TYR:OH	44:w:186:HIS:ND1	2.25	0.65
12:M:171:THR:HG23	12:M:173:MET:HE3	1.77	0.65
48:Q:501:PEE:H37	48:Q:501:PEE:H60	1.77	0.65
26:c:160:GLN:OE1	43:v:37:ARG:NH1	2.29	0.65
39:p:29:SER:HB3	39:p:76:HIS:HD2	1.60	0.65
43:v:39:MET:HE2	43:v:58:TYR:HA	1.78	0.65
2:B:79:ARG:NH1	8:I:25:GLN:OE1	2.30	0.64
6:X:69:SER:OG	6:X:70:ASP:N	2.30	0.64
9:J:270:ARG:NH2	9:J:328:THR:OG1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:139:MET:N	6:G:143:GLU:OE2	2.30	0.64
27:d:30:VAL:O	27:d:34:THR:HG23	1.96	0.64
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.80	0.64
5:F:90:THR:O	5:F:94:VAL:HG23	1.98	0.64
25:b:28:LEU:HD22	25:b:32:GLU:HG2	1.79	0.64
33:j:64:LEU:HD13	36:m:165:VAL:HG22	1.79	0.64
44:w:72:ARG:HH12	44:w:264:GLU:HA	1.62	0.63
9:J:117:ARG:NH1	9:J:158:GLU:OE2	2.32	0.63
40:r:87:GLU:O	40:r:92:LYS:NZ	2.29	0.63
5:F:46:LYS:HE3	12:M:674:LEU:HD11	1.78	0.63
35:l:346:ILE:HG12	35:l:366:MET:HE1	1.80	0.63
35:l:401:MET:HE3	35:l:482:MET:HG3	1.80	0.63
21:W:10:MET:HE3	21:W:11:PRO:HD2	1.80	0.63
21:W:88:ARG:NH2	42:u:7:LEU:O	2.32	0.63
24:a:120:TRP:O	24:a:124:THR:HG22	1.99	0.63
44:w:116:LYS:HG2	44:w:127:ASN:HD22	1.64	0.63
37:n:47:ARG:HH21	37:n:56:THR:HG23	1.64	0.63
1:A:109:ARG:NH1	1:A:237:GLY:O	2.32	0.62
13:N:32:ASP:OD2	13:N:58:ARG:NH2	2.32	0.62
15:P:44:ARG:HB3	15:P:45:PRO:HD3	1.81	0.62
39:p:176:GLU:OE2	39:p:176:GLU:N	2.27	0.62
6:X:74:LEU:HD12	6:X:74:LEU:C	2.24	0.62
55:u:201:CDL:H762	55:u:201:CDL:H121	1.81	0.62
10:K:88:ASP:OD1	14:O:62:ARG:NH1	2.31	0.62
26:c:83:GLN:NE2	26:c:97:LEU:O	2.32	0.62
44:w:125:ASP:O	44:w:130:ARG:NH2	2.33	0.62
18:T:28:GLY:N	18:T:69:ASP:OD2	2.31	0.62
26:c:75:TYR:CG	26:c:76:PRO:HD2	2.35	0.62
32:i:158:ALA:HB2	32:i:191:THR:HG22	1.81	0.62
2:B:76:TYR:HE1	41:s:33:LEU:HB2	1.64	0.62
15:P:43:THR:HA	15:P:47:ILE:HD12	1.82	0.62
35:l:78:LEU:HD11	55:l:701:CDL:H251	1.82	0.61
16:Q:144:MET:CE	16:Q:214:TYR:HE2	2.04	0.61
6:G:88:LYS:HE2	6:G:95:PRO:HB3	1.81	0.61
40:r:282:LEU:HG	40:r:342:MET:HG3	1.81	0.61
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.33	0.61
6:G:103:HIS:ND1	6:G:106:LYS:HG2	2.14	0.61
16:Q:79:ASN:HA	16:Q:101:LEU:O	2.01	0.61
49:g:201:PLX:H301	32:i:347:ASN:HB3	1.82	0.61
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.36	0.61
35:l:10:THR:CG2	35:l:46:LEU:HD11	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:r:503:CDL:H742	55:r:503:CDL:H271	1.82	0.61
1:A:64:LYS:HZ2	14:O:249:LEU:HD23	1.66	0.61
6:X:74:LEU:HD12	6:X:154:VAL:CG1	2.24	0.61
55:a:201:CDL:H422	27:d:44:PRO:HB3	1.83	0.61
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.83	0.61
35:l:51:LEU:HD22	35:l:91:PRO:HG3	1.83	0.61
11:L:109:ASN:ND2	11:L:111:LEU:O	2.34	0.60
12:M:472:PRO:O	12:M:510:TRP:NE1	2.29	0.60
16:Q:274:ASP:OD1	16:Q:323:ARG:NH2	2.31	0.60
1:A:210:THR:HG21	1:A:224:ARG:CG	2.29	0.60
35:l:161:ARG:NH1	35:l:238:GLU:OE1	2.34	0.60
1:A:50:ASP:O	1:A:59:ARG:NH2	2.30	0.60
24:a:130:GLU:O	24:a:134:GLU:HG2	2.01	0.60
12:M:547:LEU:HD11	12:M:579:MET:HE2	1.84	0.60
19:U:26:GLY:HA3	48:j:201:PEE:H37	1.84	0.60
1:A:40:ARG:NH1	14:O:233:SER:OG	2.35	0.60
7:H:67:LYS:O	7:H:71:GLN:HG3	2.01	0.60
6:X:75:THR:HG23	6:X:78:ALA:H	1.66	0.60
1:A:210:THR:HG21	1:A:224:ARG:CA	2.31	0.60
2:B:72:MET:HE3	16:Q:257:GLU:HA	1.82	0.60
16:Q:302:LEU:HD11	16:Q:406:GLU:HG3	1.83	0.60
21:W:120:MET:H	21:W:123:GLU:HG3	1.67	0.60
31:h:32:ARG:HH11	31:h:32:ARG:HG2	1.66	0.60
41:s:184:MET:HE1	41:s:296:LEU:HB3	1.83	0.60
16:Q:188:THR:HG23	16:Q:200:PHE:CA	2.31	0.60
35:l:70:THR:HG23	35:l:75:GLU:HG3	1.83	0.60
40:r:237:LYS:HD2	40:r:316:MET:HB3	1.84	0.60
4:E:37:ARG:HG2	6:G:120:MET:SD	2.41	0.60
9:J:314:THR:HA	9:J:318:LYS:HB3	1.84	0.60
27:d:99:ASP:OD2	27:d:142:ARG:NH1	2.35	0.59
37:n:50:ARG:HB2	37:n:53:GLU:HB2	1.84	0.59
8:I:108:LYS:H	8:I:108:LYS:HD3	1.67	0.59
18:T:46:ASP:O	18:T:52:ARG:NH1	2.34	0.59
6:X:118:ILE:O	6:X:122:MET:HG2	2.02	0.59
31:h:97:HIS:HA	31:h:102:GLU:HB3	1.84	0.59
43:v:4:HIS:HA	43:v:7:ARG:HE	1.67	0.59
6:X:74:LEU:HD13	6:X:154:VAL:HG11	1.73	0.59
30:g:101:GLU:OE2	30:g:101:GLU:N	2.34	0.59
1:A:211:ALA:HB2	1:A:223:PRO:HG3	1.85	0.59
48:B:303:PEE:H64	41:s:273:ILE:HD11	1.85	0.59
36:m:21:SER:O	36:m:23:LYS:NZ	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:65:MET:HE1	35:l:378:LEU:HD12	1.83	0.59
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.84	0.59
55:i:401:CDL:H141	55:i:401:CDL:H371	1.84	0.59
55:a:201:CDL:H772	55:a:201:CDL:H212	1.84	0.59
5:F:45:LYS:HG2	12:M:671:LEU:HD21	1.83	0.59
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.84	0.59
21:W:85:GLN:OE1	31:h:105:ARG:NH1	2.35	0.59
6:X:154:VAL:HG23	6:X:154:VAL:O	2.03	0.59
22:Y:87:PRO:HG3	43:v:96:VAL:HG22	1.85	0.59
24:a:137:MET:HE3	27:d:83:LEU:HD22	1.85	0.59
16:Q:259:GLU:OE1	16:Q:338:ARG:NH2	2.29	0.59
35:l:419:THR:HA	35:l:422:TYR:CE2	2.37	0.59
43:v:80:CYS:HB2	43:v:83:GLU:OE1	2.03	0.59
1:A:317:VAL:HG22	1:A:356:VAL:HG12	1.85	0.58
13:N:72:ASP:OD1	13:N:72:ASP:N	2.36	0.58
35:l:10:THR:HG23	35:l:46:LEU:CD1	2.33	0.58
1:A:210:THR:HG21	1:A:224:ARG:O	2.03	0.58
2:B:77:LEU:HB2	41:s:31:MET:HG3	1.84	0.58
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.85	0.58
26:c:105:ILE:CD1	38:o:65:LEU:HD12	2.33	0.58
43:v:51:LEU:HD21	43:v:64:ILE:HD13	1.85	0.58
1:A:140:GLU:OE1	1:A:256:ARG:NH1	2.35	0.58
1:A:263:ALA:HA	1:A:271:SER:HB3	1.85	0.58
30:g:36:MET:HE2	32:i:339:MET:HE2	1.84	0.58
9:J:192:ARG:NH1	9:J:198:ALA:O	2.36	0.58
32:i:72:MET:HE2	32:i:76:ILE:HG13	1.83	0.58
1:A:138:LEU:HD13	1:A:245:VAL:HG13	1.85	0.58
9:J:336:GLU:OE1	9:J:341:GLN:NE2	2.37	0.58
24:a:166:GLY:O	24:a:170:GLN:NE2	2.36	0.58
4:E:88:MET:HE1	15:P:171:TRP:HZ2	1.68	0.58
23:Z:30:GLU:O	23:Z:34:GLU:HG2	2.04	0.58
24:a:79:GLY:HA3	55:a:201:CDL:H222	1.86	0.58
5:F:90:THR:HA	5:F:93:ASN:ND2	2.18	0.58
11:L:90:GLY:HA3	15:P:238:PRO:HB2	1.85	0.58
22:Y:54:GLN:NE2	35:l:446:ASN:OD1	2.37	0.58
2:B:177:THR:HG22	2:B:179:THR:H	1.68	0.58
35:l:372:ALA:HA	35:l:458:LEU:HD21	1.86	0.58
40:r:403:THR:HA	40:r:406:TYR:CE2	2.39	0.58
2:B:184:LEU:HB3	11:L:112:MET:HE2	1.86	0.57
5:F:23:LEU:O	5:F:57:GLU:HA	2.04	0.57
15:P:125:ARG:NH2	15:P:201:ASP:OD1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:l:701:CDL:H452	40:r:445:LEU:HB3	1.86	0.57
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.86	0.57
32:i:122:ILE:O	32:i:176:ARG:NH1	2.36	0.57
32:i:283:ALA:HB1	40:r:158:LEU:HD13	1.85	0.57
35:l:10:THR:HG23	35:l:46:LEU:HD12	1.85	0.57
1:A:296:LEU:O	1:A:300:ILE:HD12	2.04	0.57
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.44	0.57
27:d:114:GLN:HG3	35:l:203:MET:HG2	1.87	0.57
29:f:68:GLU:OE1	29:f:72:ARG:HG3	2.05	0.57
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.87	0.57
10:K:100:GLN:HB3	14:O:71:PRO:HA	1.86	0.57
12:M:394:VAL:HG22	12:M:473:MET:HE1	1.86	0.57
25:b:32:GLU:HG3	39:p:115:TYR:HA	1.85	0.57
25:b:74:HIS:NE2	35:l:35:TYR:OH	2.31	0.57
37:n:30:ARG:NH1	37:n:30:ARG:HB3	2.19	0.57
35:l:559:GLU:O	35:l:563:PRO:HD2	2.05	0.57
7:H:76:GLN:O	7:H:79:GLU:HG2	2.04	0.57
26:c:78:LEU:HD12	26:c:106:HIS:HA	1.87	0.57
35:l:359:MET:O	35:l:436:ARG:NH2	2.38	0.57
1:A:116:ASN:ND2	1:A:207:GLY:O	2.31	0.57
1:A:209:GLU:O	1:A:213:ILE:HG13	2.05	0.57
6:G:123:GLU:HG2	6:G:130:ILE:HD12	1.87	0.57
40:r:260:PRO:HG2	49:r:502:PLX:H132	1.86	0.57
2:B:111:GLU:O	2:B:141:ARG:NH1	2.38	0.57
3:C:69:LEU:HB2	3:C:107:GLY:HA3	1.87	0.57
13:N:73:THR:HG22	13:N:73:THR:O	2.05	0.57
20:V:4:THR:HG23	20:V:5:LEU:HD12	1.86	0.57
27:d:33:LEU:HD13	35:l:49:VAL:HG13	1.87	0.57
30:g:12:PRO:HB3	31:h:5:ASP:HB3	1.85	0.57
21:W:114:THR:HG1	42:u:143:HIS:HD1	1.52	0.56
6:X:117:GLU:OE1	39:p:45:ARG:NH1	2.38	0.56
1:A:445:GLU:OE1	1:A:445:GLU:N	2.38	0.56
12:M:354:LEU:HD22	12:M:548:LEU:HD22	1.87	0.56
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	1.87	0.56
24:a:163:ARG:NH2	30:g:102:ASP:OD2	2.35	0.56
36:m:57:PHE:CE1	41:s:111:LEU:HD21	2.40	0.56
5:F:36:PHE:CB	5:F:87:VAL:HG21	2.36	0.56
9:J:213:PHE:CD1	9:J:214:LEU:HD12	2.41	0.56
15:P:85:GLU:OE2	15:P:142:ARG:NH1	2.38	0.56
35:l:4:PHE:HB2	35:l:53:MET:CE	2.35	0.56
5:F:36:PHE:CG	5:F:87:VAL:HG21	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:25:GLU:HA	23:Z:30:GLU:OE2	2.05	0.56
35:l:488:MET:O	35:l:492:ILE:HG13	2.05	0.56
7:H:55:LYS:HE3	15:P:104:THR:HG21	1.87	0.56
21:W:114:THR:OG1	42:u:143:HIS:ND1	2.32	0.56
27:d:28:ASN:HD21	27:d:31:THR:HG23	1.71	0.56
44:w:65:ASN:O	44:w:68:SER:OG	2.21	0.56
35:l:549:ALA:HB2	40:r:271:MET:HE3	1.86	0.56
12:M:650:SER:OG	12:M:652:ASN:OD1	2.21	0.56
27:d:26:LEU:HD23	43:v:75:PRO:HB2	1.88	0.56
55:l:701:CDL:H541	55:l:701:CDL:HA62	1.88	0.56
6:G:103:HIS:CE1	6:G:105:MET:HB2	2.41	0.56
12:M:388:ASN:ND2	12:M:513:MET:O	2.32	0.56
40:r:312:ALA:O	40:r:316:MET:HG3	2.05	0.56
27:d:127:LYS:O	27:d:131:GLN:HG3	2.06	0.55
40:r:98:MET:HE3	55:r:503:CDL:H172	1.88	0.55
1:A:159:ARG:NH2	14:O:176:CYS:O	2.38	0.55
19:U:63:MET:O	42:u:130:LYS:NZ	2.38	0.55
33:j:16:LEU:O	33:j:20:ILE:HG23	2.06	0.55
41:s:102:VAL:HG11	41:s:154:LEU:HD11	1.88	0.55
1:A:362:ASP:OD1	1:A:449:ARG:NH2	2.39	0.55
16:Q:142:VAL:CG2	16:Q:457:VAL:HG21	2.37	0.55
35:l:51:LEU:HG	35:l:55:MET:HE3	1.89	0.55
55:l:701:CDL:H432	55:l:701:CDL:H621	1.89	0.55
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.89	0.55
20:V:81:ARG:NH2	20:V:86:ASP:OD2	2.40	0.55
26:c:116:ARG:HG2	48:l:703:PEE:H49	1.88	0.55
1:A:36:LYS:HE2	1:A:36:LYS:H	1.71	0.55
30:g:101:GLU:H	30:g:101:GLU:CD	2.15	0.55
32:i:246:VAL:HG11	55:r:503:CDL:H392	1.88	0.55
41:s:141:SER:HB3	41:s:289:LEU:HD22	1.88	0.55
44:w:139:ARG:NH1	44:w:166:ASP:OD2	2.39	0.55
40:r:398:MET:HA	40:r:398:MET:HE2	1.89	0.55
6:X:93:ILE:HD11	6:X:110:LEU:HD11	1.89	0.55
2:B:63:TRP:O	2:B:67:VAL:HG23	2.07	0.55
14:O:197:THR:H	14:O:200:ASP:HB2	1.71	0.55
6:X:90:TYR:OH	6:X:114:ASP:OD1	2.25	0.55
24:a:91:VAL:HG22	27:d:52:ILE:HD11	1.89	0.55
26:c:100:ASN:HB2	26:c:103:GLU:CG	2.34	0.55
35:l:4:PHE:CD2	35:l:61:MET:HG3	2.41	0.55
6:X:90:TYR:HE1	23:Z:44:PRO:HB2	1.71	0.55
35:l:161:ARG:NH2	39:p:88:GLY:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.40	0.55
12:M:372:PHE:H	12:M:532:PRO:HB2	1.72	0.54
15:P:240:GLU:OE2	15:P:246:ARG:NH1	2.40	0.54
16:Q:145:MET:HG3	16:Q:214:TYR:CE2	2.41	0.54
14:O:134:VAL:HG11	14:O:149:LEU:HD13	1.88	0.54
34:k:44:SER:HB2	34:k:59:MET:HE1	1.89	0.54
2:B:110:GLU:HG3	18:T:71:ILE:HB	1.89	0.54
3:C:196:ARG:NH1	48:C:302:PEE:O1P	2.40	0.54
14:O:194:GLU:HB2	14:O:218:PRO:HB3	1.89	0.54
5:F:23:LEU:CD1	5:F:37:ILE:HD12	2.37	0.54
32:i:133:TRP:HE3	55:i:401:CDL:H391	1.73	0.54
15:P:44:ARG:HB3	15:P:45:PRO:CD	2.38	0.54
34:k:98:CYS:HB2	35:l:580:GLN:HB2	1.88	0.54
1:A:398:ARG:HE	1:A:404:ALA:HB2	1.73	0.54
6:G:112:SER:O	6:G:116:VAL:HG23	2.08	0.54
41:s:62:ARG:HD3	41:s:68:ILE:HD13	1.89	0.54
5:F:33:VAL:O	5:F:37:ILE:HG13	2.08	0.54
5:F:46:LYS:HE2	12:M:674:LEU:CD2	2.38	0.54
7:H:36:GLY:HA2	7:H:45:ARG:HH21	1.71	0.54
21:W:66:GLU:HG2	42:u:125:LEU:HB2	1.89	0.54
32:i:30:TRP:HD1	32:i:70:LEU:HD23	1.73	0.54
40:r:373:ILE:HD11	40:r:444:LEU:HD23	1.89	0.54
15:P:173:MET:HB3	15:P:198:PHE:HB2	1.90	0.54
29:f:68:GLU:HG2	30:g:21:ARG:CZ	2.37	0.54
5:F:46:LYS:HE2	12:M:674:LEU:HD21	1.90	0.53
24:a:134:GLU:HG3	37:n:57:TRP:HE1	1.73	0.53
43:v:51:LEU:HD13	43:v:63:LEU:HD23	1.89	0.53
43:v:113:LYS:HA	43:v:116:GLU:OE1	2.07	0.53
11:L:78:ARG:NH1	11:L:148:GLU:OE1	2.41	0.53
12:M:401:LEU:HD21	12:M:432:ILE:HD12	1.90	0.53
13:N:8:ARG:O	13:N:12:GLN:HG3	2.08	0.53
22:Y:97:LEU:HD12	43:v:104:ARG:HB2	1.90	0.53
23:Z:22:TRP:HB3	23:Z:50:ALA:HB3	1.90	0.53
30:g:48:ASN:HB3	30:g:55:VAL:HA	1.91	0.53
35:l:327:LEU:O	35:l:331:MET:HG2	2.08	0.53
36:m:25:SER:O	36:m:27:ILE:N	2.41	0.53
40:r:188:ASN:OD1	40:r:256:TYR:OH	2.26	0.53
35:l:172:ILE:HG21	40:r:408:LEU:HD12	1.91	0.53
35:l:227:PHE:O	35:l:230:HIS:ND1	2.39	0.53
35:l:526:LEU:HD12	35:l:530:PRO:HG2	1.91	0.53
40:r:41:LEU:O	40:r:44:GLN:NE2	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:141:PRO:O	6:G:145:VAL:HG23	2.09	0.53
25:b:123:PHE:CD1	43:v:40:VAL:HG11	2.43	0.53
6:G:74:LEU:HD13	6:G:79:ILE:HG12	1.90	0.53
12:M:478:SER:O	12:M:482:GLN:HG2	2.09	0.53
22:Y:45:ARG:HG2	35:l:439:PRO:HB3	1.91	0.53
32:i:54:GLU:HG3	34:k:93:LEU:HD22	1.90	0.53
9:J:57:THR:HG21	9:J:120:VAL:HG12	1.91	0.53
12:M:67:GLU:N	12:M:67:GLU:OE2	2.36	0.53
12:M:385:TYR:OH	12:M:527:ASP:OD1	2.21	0.53
15:P:216:VAL:HG23	15:P:218:ARG:HG2	1.91	0.53
16:Q:40:ASP:OD1	16:Q:40:ASP:N	2.37	0.53
41:s:102:VAL:HG21	41:s:154:LEU:HD11	1.90	0.53
9:J:83:PRO:HG3	9:J:119:VAL:HG11	1.91	0.53
12:M:61:PRO:HB2	12:M:77:MET:HG3	1.91	0.53
16:Q:333:ARG:NH2	16:Q:453:THR:O	2.38	0.53
35:l:14:ILE:HD11	35:l:43:ALA:HA	1.91	0.53
40:r:204:MET:SD	40:r:243:MET:HE1	2.48	0.53
55:r:503:CDL:H332	55:r:503:CDL:H202	1.90	0.53
1:A:89:GLY:O	47:A:503:NAI:H2N	2.08	0.53
5:F:87:VAL:HA	5:F:90:THR:HG22	1.89	0.53
7:H:38:ILE:HG13	7:H:100:TRP:CH2	2.43	0.53
33:j:83:ASN:ND2	49:j:202:PLX:O2	2.42	0.53
34:k:1:MET:HE2	34:k:6:MET:HG2	1.92	0.53
37:n:30:ARG:HB3	37:n:30:ARG:HH11	1.73	0.53
40:r:207:MET:HE2	40:r:243:MET:HE3	1.91	0.53
40:r:237:LYS:NZ	40:r:316:MET:O	2.42	0.53
12:M:390:THR:HA	12:M:600:GLU:HG2	1.91	0.52
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.90	0.52
16:Q:188:THR:CG2	16:Q:200:PHE:CB	2.86	0.52
21:W:130:ASN:OD1	36:m:1:MET:N	2.28	0.52
25:b:109:THR:HG22	25:b:116:VAL:HG22	1.91	0.52
43:v:69:CYS:SG	43:v:70:LYS:N	2.82	0.52
4:E:47:VAL:HA	4:E:52:LEU:HD12	1.90	0.52
5:F:23:LEU:HD12	5:F:34:ARG:HG2	1.91	0.52
26:c:105:ILE:CG2	26:c:109:LEU:HD22	2.38	0.52
35:l:136:ASN:OD1	35:l:136:ASN:N	2.42	0.52
35:l:207:GLU:OE1	35:l:207:GLU:N	2.42	0.52
44:w:171:GLU:OE1	44:w:175:ARG:NH2	2.41	0.52
16:Q:206:GLU:O	16:Q:210:MET:HG3	2.09	0.52
15:P:213:ASP:HB3	15:P:216:VAL:HG22	1.91	0.52
16:Q:184:ILE:HG23	16:Q:203:MET:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Q:501:PEE:H27	35:l:563:PRO:HA	1.90	0.52
28:e:68:GLU:HG3	28:e:69:LYS:N	2.24	0.52
36:m:45:LEU:HD23	36:m:50:SER:HA	1.91	0.52
19:U:14:ALA:O	19:U:15:LYS:HG2	2.10	0.52
33:j:84:LEU:HD13	41:s:309:ILE:HG23	1.91	0.52
35:l:8:THR:HB	35:l:82:MET:HE2	1.92	0.52
35:l:245:ALA:O	35:l:249:SER:OG	2.21	0.52
1:A:157:TYR:CD2	1:A:212:LEU:HD13	2.44	0.52
6:X:75:THR:OG1	6:X:156:GLU:O	2.27	0.52
12:M:347:ASP:HB3	12:M:594:ALA:HB1	1.91	0.52
32:i:190:MET:HE2	32:i:205:LEU:HA	1.92	0.52
38:o:56:ARG:NH1	40:r:422:HIS:O	2.40	0.52
3:C:154:ASP:OD1	3:C:154:ASP:N	2.42	0.52
7:H:47:TYR:O	7:H:51:ILE:HG12	2.10	0.52
21:W:90:ASN:ND2	21:W:123:GLU:O	2.43	0.52
6:X:149:ALA:HA	6:X:154:VAL:HG22	1.92	0.52
12:M:406:ASN:ND2	12:M:688:GLN:O	2.34	0.52
17:S:51:ASP:OD2	42:u:22:SER:OG	2.28	0.52
32:i:20:VAL:HG11	32:i:137:ALA:HB1	1.92	0.52
32:i:92:PRO:O	32:i:96:THR:HG23	2.10	0.52
39:p:50:GLU:HG2	39:p:51:HIS:ND1	2.25	0.52
12:M:389:THR:HB	12:M:473:MET:HE3	1.91	0.51
35:l:78:LEU:HD21	55:l:701:CDL:H272	1.91	0.51
41:s:223:PHE:O	41:s:227:GLU:HG2	2.10	0.51
9:J:157:LYS:NZ	9:J:197:GLU:OE1	2.35	0.51
35:l:171:ALA:O	35:l:175:ASN:ND2	2.36	0.51
14:O:153:GLN:HE22	14:O:160:VAL:HG22	1.74	0.51
39:p:64:LEU:HA	39:p:67:ALA:HB3	1.92	0.51
14:O:41:HIS:NE2	14:O:47:ASN:OD1	2.42	0.51
26:c:78:LEU:HD11	26:c:104:PRO:HB2	1.92	0.51
28:e:98:VAL:HG22	40:r:36:LEU:HB2	1.93	0.51
41:s:45:LEU:O	41:s:48:PRO:HD2	2.09	0.51
14:O:132:ILE:HD11	14:O:169:PHE:HD2	1.75	0.51
14:O:152:ILE:HG21	14:O:171:LEU:HD13	1.91	0.51
39:p:100:PRO:HG3	40:r:419:TYR:CE1	2.45	0.51
41:s:221:ALA:O	41:s:225:MET:HG3	2.10	0.51
1:A:127:ASP:HA	1:A:130:ILE:HG12	1.92	0.51
26:c:161:TYR:HB3	26:c:166:LEU:HG	1.92	0.51
4:E:28:ALA:HB1	4:E:79:VAL:HG11	1.92	0.51
12:M:308:ARG:NH2	12:M:578:PRO:O	2.44	0.51
50:X:201:8Q1:O27	50:X:201:8Q1:O33	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:41:ILE:HG13	34:k:73:LEU:HD21	1.93	0.51
35:l:293:ILE:HG13	35:l:418:LEU:HD22	1.93	0.51
41:s:51:ASP:HB3	56:s:402:UQ:H8	1.92	0.51
42:u:83:THR:HA	42:u:86:TRP:CD1	2.46	0.51
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.92	0.51
14:O:201:ILE:HG23	14:O:205:ILE:HD13	1.92	0.51
15:P:94:ILE:O	15:P:98:THR:OG1	2.22	0.51
34:k:25:HIS:O	34:k:28:SER:N	2.36	0.51
1:A:204:TYR:OH	47:A:503:NAI:H5N	2.11	0.51
35:l:397:GLU:OE1	35:l:482:MET:HE1	2.11	0.51
36:m:11:THR:O	36:m:15:ILE:HD12	2.10	0.51
1:A:48:ARG:NH1	10:K:70:ASN:O	2.38	0.51
12:M:306:MET:HB2	12:M:583:ILE:HB	1.93	0.51
21:W:66:GLU:OE2	42:u:123:GLY:N	2.44	0.51
35:l:66:TRP:O	35:l:78:LEU:N	2.41	0.51
39:p:175:ARG:HG2	39:p:176:GLU:OE2	2.09	0.51
6:X:83:VAL:HA	6:X:122:MET:HE1	1.93	0.50
24:a:136:THR:HG21	40:r:48:ASN:HD22	1.76	0.50
44:w:118:TYR:OH	57:w:401:ADP:O2'	2.30	0.50
9:J:171:ASN:HA	9:J:327:MET:HE3	1.93	0.50
10:K:88:ASP:O	10:K:91:VAL:HG12	2.11	0.50
40:r:61:LEU:HB2	40:r:457:PRO:HD3	1.91	0.50
12:M:419:ARG:NH1	12:M:439:THR:O	2.44	0.50
15:P:209:GLU:HG2	15:P:224:VAL:HA	1.92	0.50
16:Q:142:VAL:HG23	16:Q:457:VAL:HG21	1.93	0.50
32:i:128:LEU:HD12	32:i:216:PHE:HB3	1.92	0.50
2:B:131:GLU:HG3	2:B:144:ARG:HD2	1.92	0.50
3:C:51:ASP:OD1	3:C:190:LEU:HB2	2.11	0.50
11:L:78:ARG:NH2	12:M:249:GLU:OE1	2.44	0.50
12:M:389:THR:O	12:M:390:THR:OG1	2.27	0.50
26:c:105:ILE:HD12	38:o:65:LEU:HD12	1.92	0.50
11:L:92:ASN:HB3	15:P:238:PRO:HA	1.93	0.50
1:A:392:MET:HG2	1:A:412:LEU:HD11	1.93	0.50
8:I:46:SER:O	8:I:52:ASN:ND2	2.44	0.50
12:M:167:PRO:HD2	12:M:215:MET:HE1	1.92	0.50
13:N:3:LEU:O	13:N:7:LEU:HG	2.12	0.50
16:Q:41:VAL:O	16:Q:45:GLU:HG2	2.11	0.50
41:s:138:GLN:HA	41:s:286:MET:HE1	1.92	0.50
44:w:180:ARG:NH1	44:w:316:GLU:OE2	2.44	0.50
21:W:97:ILE:HD13	31:h:83:ARG:HB2	1.93	0.50
25:b:100:ARG:HB3	35:l:60:GLU:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:h:32:ARG:HG2	31:h:32:ARG:NH1	2.27	0.50
35:l:475:MET:HB3	43:v:52:MET:HE3	1.94	0.50
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.93	0.50
44:w:353:TRP:H	44:w:353:TRP:CD1	2.30	0.50
30:g:32:ARG:HB3	32:i:339:MET:HE1	1.93	0.50
1:A:357:MET:HE1	1:A:363:ILE:HG13	1.93	0.50
25:b:25:ASP:OD2	39:p:125:TRP:NE1	2.34	0.50
39:p:28:GLU:OE2	39:p:34:ARG:NH1	2.43	0.50
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.46	0.50
1:A:214:GLU:OE2	1:A:224:ARG:NE	2.39	0.49
21:W:105:LYS:HE2	42:u:4:ILE:HD11	1.94	0.49
50:X:201:8Q1:N36	50:X:201:8Q1:O40	2.44	0.49
55:a:201:CDL:H771	28:e:100:VAL:HA	1.94	0.49
35:l:132:VAL:O	35:l:262:ARG:NH2	2.44	0.49
55:l:701:CDL:H601	55:l:701:CDL:H772	1.93	0.49
40:r:191:SER:HB3	48:r:501:PEE:H2	1.94	0.49
1:A:160:GLY:O	1:A:199:ARG:NH2	2.45	0.49
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.40	0.49
6:X:80:LYS:HZ2	6:X:100:VAL:CG2	2.25	0.49
32:i:245:MET:HE1	55:r:503:CDL:H171	1.94	0.49
32:i:256:PRO:HB2	55:u:201:CDL:H601	1.94	0.49
1:A:51:TRP:NE1	10:K:77:GLN:OE1	2.35	0.49
4:E:116:THR:HG22	4:E:116:THR:O	2.13	0.49
17:S:19:PRO:HB3	41:s:9:LEU:HD12	1.93	0.49
6:X:74:LEU:CD1	6:X:74:LEU:C	2.86	0.49
3:C:125:PRO:HB2	41:s:58:LYS:HE3	1.94	0.49
16:Q:139:LEU:HD11	16:Q:424:ILE:HD13	1.93	0.49
43:v:17:PRO:HB3	43:v:105:GLU:OE2	2.12	0.49
5:F:36:PHE:CG	5:F:87:VAL:CG2	2.96	0.49
12:M:331:GLN:NE2	12:M:630:ALA:O	2.44	0.49
27:d:69:ARG:NH1	37:n:43:LEU:O	2.43	0.49
30:g:117:GLU:OE1	30:g:119:HIS:NE2	2.45	0.49
34:k:8:ILE:HG21	34:k:43:MET:HB2	1.94	0.49
35:l:173:LEU:HD12	40:r:405:LEU:HD21	1.93	0.49
3:C:71:CYS:HB3	16:Q:141:TYR:CB	2.42	0.49
14:O:137:THR:HG22	14:O:138:THR:H	1.78	0.49
22:Y:47:PHE:HE2	22:Y:50:LEU:HD11	1.78	0.49
55:a:201:CDL:H192	55:a:201:CDL:H752	1.94	0.49
32:i:246:VAL:HG21	55:r:503:CDL:H361	1.95	0.49
34:k:91:GLN:O	34:k:94:ASN:ND2	2.46	0.49
35:l:393:ASP:O	35:l:397:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:152:ILE:O	9:J:156:SER:OG	2.28	0.49
23:Z:18:ASP:OD1	23:Z:19:TYR:N	2.45	0.49
12:M:198:THR:HG21	12:M:209:TYR:HB2	1.95	0.49
20:V:120:LEU:HD21	48:r:501:PEE:H66	1.95	0.49
26:c:166:LEU:O	26:c:170:ARG:HG3	2.12	0.49
28:e:116:GLU:O	28:e:120:ARG:HG3	2.12	0.49
34:k:4:VAL:O	34:k:8:ILE:HG12	2.13	0.49
35:l:383:MET:SD	35:l:384:PRO:HD2	2.53	0.49
40:r:306:PRO:HA	40:r:458:LEU:HD22	1.95	0.49
1:A:44:ASN:HB3	1:A:134:ASP:OD1	2.13	0.49
1:A:244:ASN:N	46:A:502:FMN:O1P	2.34	0.49
27:d:86:PHE:O	27:d:90:MET:HG2	2.13	0.49
17:S:17:PHE:CZ	41:s:257:ILE:HD13	2.48	0.49
6:X:119:ILE:HG21	6:X:135:ALA:HB1	1.94	0.49
32:i:276:ILE:HG21	48:r:501:PEE:H14	1.95	0.49
44:w:110:GLY:HA2	44:w:134:TRP:CD2	2.48	0.49
1:A:185:ASN:C	1:A:187:CYS:H	2.20	0.48
3:C:190:LEU:HD11	48:C:302:PEE:H13	1.95	0.48
16:Q:188:THR:CG2	16:Q:200:PHE:HB2	2.43	0.48
32:i:54:GLU:OE2	34:k:95:LEU:HB2	2.13	0.48
34:k:22:TYR:O	35:l:585:LYS:NZ	2.46	0.48
39:p:132:SER:OG	39:p:163:LEU:HB2	2.13	0.48
40:r:48:ASN:N	40:r:48:ASN:OD1	2.46	0.48
40:r:208:PRO:HD3	40:r:216:LEU:HD13	1.95	0.48
1:A:294:VAL:HG21	1:A:299:LEU:HD13	1.95	0.48
55:a:201:CDL:H361	25:b:80:TRP:HB3	1.95	0.48
3:C:193:TRP:HB2	48:C:302:PEE:H3	1.95	0.48
16:Q:143:SER:HB2	16:Q:178:THR:HG22	1.95	0.48
27:d:119:GLU:HG2	43:v:52:MET:HA	1.94	0.48
49:e:201:PLX:H382	40:r:67:VAL:HG12	1.95	0.48
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.95	0.48
11:L:84:ARG:NH1	11:L:88:GLN:O	2.46	0.48
26:c:117:VAL:HG21	35:l:539:TYR:HB2	1.94	0.48
35:l:159:HIS:HB3	40:r:416:ARG:HG2	1.95	0.48
44:w:295:ARG:HA	44:w:298:VAL:HG22	1.95	0.48
6:G:82:ARG:O	6:G:86:VAL:HG12	2.14	0.48
6:G:125:GLU:HA	6:G:125:GLU:OE1	2.14	0.48
7:H:69:GLU:HG3	7:H:77:ILE:HG12	1.94	0.48
9:J:273:LEU:O	9:J:277:VAL:HG23	2.14	0.48
11:L:59:LEU:HD12	11:L:60:ASP:N	2.29	0.48
12:M:217:GLU:HG2	12:M:218:LEU:HG	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:249:GLU:HG2	12:M:276:ARG:HD3	1.96	0.48
31:h:18:MET:HE3	34:k:56:ALA:HA	1.95	0.48
32:i:65:THR:O	32:i:69:MET:HG3	2.13	0.48
36:m:175:ASN:OD1	44:w:289:ARG:NH2	2.45	0.48
40:r:371:PRO:O	40:r:448:THR:OG1	2.30	0.48
2:B:89:GLU:OE1	13:N:34:ARG:NH2	2.47	0.48
12:M:394:VAL:HG11	12:M:418:ILE:HG12	1.95	0.48
12:M:517:HIS:HB2	12:M:599:THR:HG22	1.95	0.48
16:Q:99:MET:HE1	16:Q:447:VAL:HG21	1.96	0.48
20:V:102:GLY:O	20:V:106:ARG:N	2.47	0.48
7:H:38:ILE:HG21	7:H:45:ARG:HB2	1.96	0.48
35:l:313:MET:HG3	35:l:328:HIS:HD2	1.79	0.48
38:o:75:ASN:O	38:o:79:ASN:ND2	2.45	0.48
40:r:12:LEU:HB2	40:r:13:PRO:CD	2.39	0.48
40:r:300:ALA:O	40:r:308:SER:HB3	2.13	0.48
43:v:51:LEU:O	43:v:52:MET:HG2	2.14	0.48
3:C:59:ARG:NH1	49:C:303:PLX:O3	2.47	0.48
7:H:106:GLU:OE2	8:I:72:SER:OG	2.29	0.48
9:J:37:HIS:CE1	18:T:49:ASP:HA	2.48	0.48
9:J:166:HIS:HB3	9:J:200:ILE:HD13	1.96	0.48
55:u:201:CDL:H741	55:u:201:CDL:H712	1.62	0.48
12:M:173:MET:HE2	12:M:173:MET:HA	1.94	0.48
24:a:140:LEU:HD21	40:r:177:LEU:HB3	1.96	0.48
26:c:156:VAL:HG11	43:v:95:TYR:CZ	2.49	0.48
32:i:222:SER:O	32:i:224:ALA:N	2.46	0.48
40:r:153:THR:HG23	40:r:206:LYS:NZ	2.29	0.48
14:O:48:ASN:OD1	14:O:51:THR:OG1	2.27	0.48
36:m:25:SER:O	36:m:28:TYR:N	2.43	0.48
40:r:269:MET:HE3	40:r:399:ASN:HB2	1.96	0.48
1:A:385:CYS:O	1:A:389:VAL:HB	2.14	0.47
13:N:29:ARG:NH2	13:N:73:THR:O	2.47	0.47
5:F:45:LYS:HG2	12:M:671:LEU:CD2	2.45	0.47
10:K:105:ARG:NH1	11:L:167:ASN:O	2.45	0.47
35:l:62:ILE:HD13	35:l:81:LYS:HA	1.95	0.47
1:A:102:MET:O	1:A:102:MET:HG3	2.14	0.47
1:A:119:GLU:OE2	1:A:127:ASP:N	2.46	0.47
1:A:398:ARG:HG2	1:A:403:ASP:HB3	1.96	0.47
5:F:83:SER:O	5:F:87:VAL:HG13	2.15	0.47
12:M:255:ASP:N	12:M:255:ASP:OD1	2.46	0.47
13:N:40:GLY:HA3	13:N:86:TRP:CH2	2.50	0.47
35:l:298:ILE:O	35:l:302:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:357:THR:O	40:r:361:VAL:HG23	2.14	0.47
11:L:174:THR:HG21	14:O:114:GLU:OE2	2.14	0.47
14:O:185:MET:HB3	14:O:194:GLU:HA	1.95	0.47
20:V:81:ARG:NH2	20:V:83:LYS:HD2	2.29	0.47
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.79	0.47
55:l:702:CDL:H591	55:l:702:CDL:H622	1.49	0.47
1:A:329:LYS:O	1:A:333:GLU:HG2	2.14	0.47
14:O:194:GLU:O	14:O:218:PRO:HA	2.15	0.47
26:c:167:TYR:CD2	26:c:178:PRO:HG3	2.49	0.47
26:c:176:LYS:HD2	26:c:176:LYS:HA	1.72	0.47
32:i:249:LEU:HD22	32:i:254:LEU:HD12	1.95	0.47
35:l:15:LEU:HD21	35:l:125:LEU:HG	1.97	0.47
38:o:25:ILE:HD12	38:o:30:ARG:HH21	1.79	0.47
40:r:115:LEU:HD12	40:r:174:LEU:HD22	1.95	0.47
4:E:88:MET:HE1	15:P:171:TRP:CZ2	2.47	0.47
6:G:75:THR:HG23	6:G:78:ALA:H	1.80	0.47
9:J:204:SER:OG	9:J:238:GLN:O	2.29	0.47
30:g:15:PHE:HD1	49:g:201:PLX:H71	1.80	0.47
43:v:60:ALA:O	43:v:64:ILE:HG12	2.15	0.47
1:A:129:GLU:OE1	1:A:132:ARG:NH2	2.44	0.47
2:B:105:ARG:HH21	2:B:191:LEU:HD22	1.80	0.47
4:E:15:THR:OG1	11:L:55:VAL:O	2.32	0.47
5:F:46:LYS:HE2	12:M:674:LEU:CD1	2.45	0.47
9:J:92:MET:HE2	9:J:92:MET:HA	1.97	0.47
12:M:250:SER:OG	12:M:251:ILE:N	2.43	0.47
12:M:371:VAL:HG22	12:M:533:GLY:HA2	1.97	0.47
15:P:162:ALA:HB2	16:Q:286:TYR:C	2.40	0.47
16:Q:137:ASP:OD2	16:Q:148:GLU:OE1	2.33	0.47
25:b:120:MET:HG2	43:v:40:VAL:HG12	1.97	0.47
33:j:83:ASN:HD21	49:j:202:PLX:H1A2	1.80	0.47
34:k:23:ARG:HG2	36:m:23:LYS:HE2	1.96	0.47
35:l:295:GLN:HB2	35:l:301:ILE:HG12	1.96	0.47
1:A:311:TRP:NE1	1:A:333:GLU:OE2	2.34	0.47
35:l:515:TYR:OH	39:p:70:GLU:OE2	2.33	0.47
42:u:80:GLU:HB2	42:u:81:PRO:HD3	1.97	0.47
1:A:447:GLU:O	1:A:451:GLN:HG3	2.15	0.47
15:P:87:PHE:CE2	15:P:144:LYS:HD2	2.50	0.47
17:S:43:TYR:CZ	21:W:68:ARG:HG3	2.50	0.47
20:V:36:VAL:O	20:V:40:SER:OG	2.33	0.47
20:V:37:SER:OG	20:V:56:THR:HA	2.14	0.47
28:e:143:ASP:OD1	28:e:143:ASP:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:320:THR:OG1	44:w:300:ASN:HB2	2.15	0.47
35:l:10:THR:CG2	35:l:46:LEU:CD1	2.91	0.47
35:l:383:MET:HB3	35:l:386:LEU:HD12	1.97	0.47
44:w:37:GLN:NE2	44:w:299:GLN:OE1	2.48	0.47
44:w:214:ILE:HD12	44:w:234:LEU:HD13	1.96	0.47
4:E:68:MET:HA	4:E:68:MET:HE2	1.96	0.47
9:J:213:PHE:HD1	9:J:214:LEU:HD12	1.80	0.47
16:Q:176:GLU:OE2	16:Q:311:TYR:OH	2.25	0.47
36:m:3:MET:N	36:m:3:MET:SD	2.88	0.47
41:s:140:ILE:HA	41:s:143:GLU:HG2	1.97	0.47
41:s:156:MET:HG2	41:s:174:MET:HE1	1.97	0.47
55:u:201:CDL:H171	55:u:201:CDL:H201	1.77	0.47
43:v:114:ARG:O	43:v:117:GLN:HG3	2.15	0.47
1:A:268:GLU:HG2	1:A:269:ARG:CZ	2.44	0.46
16:Q:397:TYR:OH	16:Q:406:GLU:OE2	2.33	0.46
40:r:105:PHE:O	40:r:109:THR:OG1	2.23	0.46
4:E:98:LYS:HB3	4:E:102:HIS:HB2	1.97	0.46
6:G:145:VAL:HA	6:G:148:ILE:HD12	1.97	0.46
8:I:97:PRO:HD3	15:P:61:PHE:CE1	2.51	0.46
9:J:206:ILE:HG12	9:J:245:VAL:HG21	1.97	0.46
32:i:268:GLN:NE2	32:i:272:LYS:HE2	2.30	0.46
38:o:59:VAL:HG22	40:r:423:ILE:HG12	1.97	0.46
44:w:181:LYS:O	44:w:184:VAL:HG22	2.15	0.46
48:B:303:PEE:H34	19:U:25:ILE:HD11	1.97	0.46
7:H:35:LEU:HD13	7:H:49:GLU:HG3	1.95	0.46
11:L:163:ASN:O	11:L:171:ARG:HA	2.15	0.46
12:M:81:GLU:HB3	12:M:88:VAL:HG12	1.97	0.46
26:c:185:GLU:HG3	43:v:37:ARG:HG2	1.97	0.46
35:l:554:ASP:O	40:r:214:LEU:HD11	2.15	0.46
41:s:149:ILE:HG13	41:s:297:THR:HG23	1.96	0.46
3:C:88:ARG:HA	41:s:37:PRO:HA	1.97	0.46
7:H:21:HIS:O	7:H:25:LYS:HG3	2.16	0.46
9:J:175:LYS:HA	9:J:175:LYS:HD3	1.82	0.46
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.96	0.46
26:c:160:GLN:HG2	26:c:183:HIS:ND1	2.30	0.46
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.97	0.46
35:l:223:LYS:HG2	35:l:255:ALA:HB3	1.98	0.46
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.50	0.46
55:l:701:CDL:H582	55:l:701:CDL:H551	1.62	0.46
39:p:59:LYS:HE2	39:p:59:LYS:HB2	1.59	0.46
5:F:19:ILE:HG22	5:F:53:ILE:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:231:LEU:HD22	14:O:231:LEU:N	2.31	0.46
26:c:157:GLY:HA2	43:v:22:MET:HE2	1.97	0.46
29:f:73:ASN:HB3	29:f:75:LEU:HD23	1.97	0.46
32:i:311:MET:HE3	32:i:314:LYS:HB2	1.98	0.46
33:j:49:LEU:N	33:j:50:PRO:HD2	2.31	0.46
40:r:118:PHE:O	40:r:122:PHE:HB3	2.15	0.46
1:A:157:TYR:HB2	1:A:212:LEU:HD11	1.96	0.46
2:B:74:LEU:HB2	41:s:272:TRP:CZ2	2.51	0.46
3:C:79:MET:HB3	3:C:79:MET:HE2	1.72	0.46
49:C:303:PLX:H21	49:C:303:PLX:H1C3	1.60	0.46
21:W:99:LYS:HD2	21:W:100:ASP:N	2.31	0.46
32:i:149:ILE:HD11	32:i:195:PRO:HG3	1.97	0.46
32:i:153:LEU:O	32:i:157:MET:HG3	2.15	0.46
35:l:384:PRO:HA	35:l:389:PHE:CD1	2.50	0.46
55:l:702:CDL:H541	55:l:702:CDL:H572	1.64	0.46
40:r:299:VAL:O	40:r:303:ILE:HG12	2.16	0.46
42:u:105:ALA:O	42:u:109:GLU:HG2	2.16	0.46
2:B:98:ARG:NH2	16:Q:224:ALA:O	2.41	0.46
5:F:44:LEU:HD12	5:F:44:LEU:C	2.41	0.46
12:M:336:ASN:HD21	12:M:540:ASN:HD22	1.64	0.46
15:P:119:VAL:HG12	15:P:121:THR:HG22	1.96	0.46
25:b:106:PRO:HG2	25:b:120:MET:HE3	1.98	0.46
34:k:28:SER:HB3	36:m:23:LYS:HG2	1.97	0.46
41:s:52:ALA:HB2	56:s:402:UQ:H112	1.97	0.46
3:C:187:GLU:HB2	9:J:87:GLU:OE2	2.16	0.46
28:e:70:ASN:O	28:e:73:SER:HB2	2.16	0.46
32:i:57:THR:HA	34:k:77:LEU:HD13	1.98	0.46
35:l:292:ALA:HB2	35:l:304:PHE:HB3	1.97	0.46
36:m:1:MET:SD	36:m:2:THR:N	2.89	0.46
35:l:452:ASN:HA	35:l:455:LYS:HE3	1.97	0.46
1:A:157:TYR:CD2	1:A:212:LEU:CD1	2.98	0.46
12:M:557:ARG:NH2	12:M:564:CYS:O	2.49	0.46
16:Q:445:ALA:HB3	41:s:281:ARG:HD2	1.97	0.46
22:Y:78:ASP:OD1	22:Y:78:ASP:N	2.49	0.46
55:l:701:CDL:H321	55:l:701:CDL:H351	1.54	0.46
40:r:202:ALA:O	40:r:205:VAL:HG12	2.16	0.46
1:A:37:ASP:HB3	14:O:236:GLU:HG2	1.97	0.45
3:C:64:PRO:HB3	3:C:102:VAL:HG13	1.98	0.45
12:M:562:LYS:HA	12:M:562:LYS:HD3	1.85	0.45
21:W:70:ALA:HB2	42:u:125:LEU:HD13	1.97	0.45
28:e:152:ASP:OD1	28:e:152:ASP:N	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:361:VAL:O	40:r:365:THR:HG23	2.15	0.45
41:s:149:ILE:HG12	41:s:181:LEU:HD22	1.98	0.45
3:C:161:ILE:HG13	3:C:180:LEU:HB2	1.97	0.45
20:V:118:MET:HE2	20:V:118:MET:HB3	1.83	0.45
28:e:92:PHE:O	28:e:96:SER:HB2	2.15	0.45
49:j:202:PLX:H132	36:m:152:TRP:HZ3	1.81	0.45
35:l:19:ILE:HG21	55:l:701:CDL:H852	1.98	0.45
35:l:62:ILE:HD11	35:l:81:LYS:HG3	1.98	0.45
40:r:97:THR:HG21	55:r:503:CDL:H242	1.97	0.45
20:V:114:ALA:O	20:V:118:MET:HB2	2.16	0.45
26:c:58:ARG:NH2	26:c:60:GLU:OE1	2.49	0.45
49:e:201:PLX:H121	49:e:201:PLX:H152	1.77	0.45
32:i:41:ILE:HG22	36:m:171:ILE:HD11	1.98	0.45
32:i:72:MET:HA	32:i:72:MET:HE3	1.98	0.45
35:l:69:MET:HE3	35:l:76:LEU:HD12	1.99	0.45
39:p:45:ARG:O	39:p:49:ASP:HB2	2.16	0.45
44:w:213:GLU:OE1	44:w:217:ARG:NE	2.42	0.45
5:F:45:LYS:CG	12:M:671:LEU:HD21	2.46	0.45
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.50	0.45
24:a:152:LYS:HD3	30:g:96:VAL:HG21	1.98	0.45
25:b:16:ARG:HG3	25:b:20:ARG:HD2	1.96	0.45
27:d:159:GLN:O	27:d:163:MET:HG2	2.16	0.45
35:l:466:PHE:O	35:l:470:ASN:ND2	2.46	0.45
36:m:23:LYS:N	36:m:24:PRO:HD3	2.32	0.45
39:p:20:TYR:CZ	39:p:24:LEU:HD11	2.51	0.45
41:s:285:LEU:HD12	41:s:286:MET:HE2	1.97	0.45
1:A:338:ASP:OD1	1:A:338:ASP:N	2.49	0.45
9:J:173:ASP:OD1	9:J:176:SER:HB2	2.16	0.45
16:Q:220:ALA:HB3	16:Q:224:ALA:HA	1.99	0.45
16:Q:304:LYS:NZ	16:Q:316:PHE:O	2.47	0.45
25:b:10:LEU:O	25:b:14:GLN:HG3	2.16	0.45
26:c:126:TRP:HA	26:c:129:MET:HE2	1.99	0.45
35:l:369:THR:N	35:l:445:GLU:OE1	2.38	0.45
40:r:200:ILE:HG23	40:r:204:MET:HE2	1.98	0.45
6:G:103:HIS:NE2	6:G:105:MET:SD	2.89	0.45
16:Q:251:PHE:O	16:Q:255:ILE:HG13	2.17	0.45
6:X:89:LEU:HD12	23:Z:47:ARG:HB2	1.99	0.45
35:l:206:ASN:HB3	35:l:207:GLU:OE1	2.17	0.45
35:l:400:ASN:HB3	35:l:486:MET:HE3	1.99	0.45
36:m:17:PHE:HA	36:m:20:PHE:CD2	2.52	0.45
38:o:45:ARG:NH2	39:p:140:LEU:HD22	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:59:VAL:HG12	44:w:202:HIS:HD2	1.82	0.45
1:A:250:VAL:O	1:A:254:ILE:HG12	2.16	0.45
2:B:133:GLU:OE2	13:N:131:ARG:NH2	2.50	0.45
48:B:303:PEE:H26	48:B:303:PEE:H31	1.73	0.45
49:C:303:PLX:H212	49:C:303:PLX:H181	1.80	0.45
9:J:185:ALA:O	9:J:189:LYS:HG2	2.16	0.45
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.99	0.45
12:M:395:GLU:OE2	12:M:417:ARG:NH1	2.46	0.45
13:N:6:VAL:HG12	13:N:9:ARG:NH2	2.32	0.45
17:S:4:GLU:OE2	41:s:43:TYR:CE2	2.69	0.45
26:c:167:TYR:HD2	26:c:168:LEU:HD23	1.81	0.45
44:w:57:SER:HB3	44:w:150:LEU:HD21	1.98	0.45
7:H:48:THR:O	7:H:52:THR:OG1	2.26	0.45
7:H:77:ILE:O	7:H:80:VAL:HG22	2.17	0.45
21:W:85:GLN:HG3	42:u:10:LEU:HD22	1.97	0.45
27:d:160:LYS:HE2	28:e:147:ILE:HG23	1.99	0.45
30:g:49:ALA:HB2	55:r:503:CDL:H712	1.98	0.45
40:r:108:MET:HB3	40:r:121:LEU:HD13	1.99	0.45
42:u:80:GLU:O	42:u:84:GLU:HG3	2.17	0.45
43:v:114:ARG:HG3	43:v:114:ARG:HH11	1.81	0.45
1:A:128:ARG:O	1:A:132:ARG:HG2	2.17	0.45
2:B:66:LEU:HD13	48:B:303:PEE:H59	1.98	0.45
14:O:150:GLU:HA	14:O:153:GLN:HG3	1.99	0.45
17:S:54:ILE:HD11	42:u:21:SER:HA	1.97	0.45
19:U:56:PRO:HG2	42:u:45:LEU:HB2	1.99	0.45
25:b:123:PHE:HD1	43:v:40:VAL:HG11	1.80	0.45
26:c:69:GLY:HA3	38:o:86:THR:HG21	1.98	0.45
55:l:701:CDL:H382	40:r:372:SER:HB3	1.98	0.45
38:o:114:LYS:HB3	38:o:114:LYS:HE3	1.61	0.45
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.79	0.45
5:F:64:LYS:HB2	5:F:64:LYS:HE2	1.66	0.45
22:Y:93:THR:HG23	22:Y:96:GLU:H	1.82	0.45
28:e:97:ILE:O	28:e:101:LEU:HB2	2.17	0.45
49:j:202:PLX:H322	49:j:202:PLX:H351	1.55	0.45
35:l:467:ILE:O	35:l:471:ASN:HB2	2.17	0.45
2:B:100:GLU:O	2:B:170:GLY:N	2.45	0.44
4:E:39:TRP:O	4:E:43:VAL:HG23	2.17	0.44
9:J:61:ALA:HA	9:J:66:GLY:HA3	1.98	0.44
12:M:89:VAL:HB	12:M:94:MET:HE3	1.99	0.44
19:U:38:TYR:HB2	41:s:310:MET:O	2.17	0.44
49:a:202:PLX:H351	49:a:202:PLX:H381	1.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:110:ASP:OD1	26:c:110:ASP:N	2.50	0.44
42:u:38:LYS:HB3	42:u:39:PRO:HD3	2.00	0.44
55:u:201:CDL:H752	55:u:201:CDL:H781	1.56	0.44
3:C:84:TYR:CE1	3:C:171:GLU:HG3	2.52	0.44
5:F:41:TYR:CE2	12:M:381:LEU:HD21	2.53	0.44
13:N:2:GLU:N	13:N:5:GLN:HG3	2.32	0.44
16:Q:36:GLN:NE2	40:r:135:ARG:O	2.49	0.44
32:i:236:LYS:HB2	32:i:311:MET:HE2	1.98	0.44
40:r:45:LEU:HD13	40:r:47:GLU:HB2	2.00	0.44
44:w:170:LEU:HD22	44:w:187:TYR:CD1	2.52	0.44
1:A:413:TRP:O	1:A:416:SER:OG	2.33	0.44
2:B:64:THR:HG21	21:W:35:MET:HE1	1.98	0.44
9:J:182:ARG:O	9:J:186:VAL:HG23	2.18	0.44
12:M:306:MET:HE1	13:N:139:PRO:HG3	1.99	0.44
13:N:85:GLU:HB2	13:N:98:PRO:HB3	1.99	0.44
26:c:129:MET:HE3	35:l:532:ILE:HD11	1.98	0.44
40:r:201:MET:HE1	40:r:261:PHE:CE1	2.52	0.44
41:s:32:GLN:OE1	41:s:34:ARG:NH2	2.45	0.44
41:s:103:LEU:HD23	41:s:103:LEU:HA	1.86	0.44
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.52	0.44
9:J:173:ASP:OD1	9:J:173:ASP:N	2.50	0.44
35:l:137:LEU:HD13	35:l:186:MET:HG2	1.99	0.44
35:l:314:MET:HE3	35:l:314:MET:HB3	1.90	0.44
39:p:108:HIS:CD2	39:p:109:PRO:HD2	2.53	0.44
41:s:13:ILE:O	41:s:17:VAL:HG13	2.17	0.44
1:A:210:THR:HG21	1:A:224:ARG:C	2.42	0.44
2:B:70:LEU:HD11	48:B:303:PEE:H65	2.00	0.44
2:B:171:PRO:HB2	13:N:93:MET:HE1	2.00	0.44
3:C:191:ARG:O	3:C:195:ARG:HG3	2.18	0.44
9:J:269:ASN:HB2	9:J:271:TYR:CE1	2.53	0.44
13:N:34:ARG:NH1	13:N:54:GLN:OE1	2.39	0.44
29:f:64:GLU:OE1	29:f:64:GLU:N	2.51	0.44
32:i:268:GLN:HG3	42:u:168:PHE:HZ	1.82	0.44
40:r:267:TRP:O	40:r:271:MET:HG2	2.18	0.44
1:A:115:VAL:HG11	1:A:138:LEU:HD11	2.00	0.44
48:B:303:PEE:H52	41:s:187:ILE:HD12	1.98	0.44
5:F:46:LYS:CE	12:M:674:LEU:CD1	2.93	0.44
9:J:204:SER:OG	9:J:204:SER:O	2.35	0.44
16:Q:145:MET:HG3	16:Q:214:TYR:CZ	2.53	0.44
16:Q:192:LEU:HD13	16:Q:197:MET:HA	1.99	0.44
34:k:2:PRO:HD2	34:k:5:TYR:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:174:TYR:CD2	35:l:232:TRP:HB3	2.53	0.44
40:r:248:THR:HG23	40:r:249:ILE:HG23	2.00	0.44
5:F:46:LYS:HE2	12:M:674:LEU:HD11	2.00	0.44
7:H:38:ILE:CG2	7:H:45:ARG:HB2	2.48	0.44
10:K:109:ARG:NH2	14:O:106:GLN:O	2.43	0.44
16:Q:155:VAL:HB	16:Q:229:PRO:HB3	2.00	0.44
21:W:84:LEU:HD12	42:u:57:LEU:HD21	1.98	0.44
32:i:152:ASN:O	32:i:156:THR:OG1	2.26	0.44
35:l:14:ILE:O	35:l:17:ILE:HG12	2.18	0.44
40:r:1:MET:O	40:r:1:MET:HG3	2.18	0.44
44:w:42:ALA:HB1	44:w:47:GLU:HG3	1.99	0.44
3:C:65:MET:HE2	3:C:65:MET:HB2	1.75	0.44
12:M:638:THR:O	12:M:642:VAL:HG23	2.17	0.44
13:N:127:TYR:OH	18:T:61:GLU:O	2.25	0.44
21:W:60:LEU:HD13	42:u:98:ARG:HD3	1.99	0.44
23:Z:57:PHE:CG	35:l:435:PRO:HG3	2.52	0.44
55:i:401:CDL:HB62	44:w:40:PRO:HB2	2.00	0.44
35:l:331:MET:HB3	35:l:387:THR:HG22	2.00	0.44
39:p:26:HIS:CD2	39:p:79:PRO:HB3	2.53	0.44
40:r:233:ALA:HA	40:r:320:GLY:HA2	2.00	0.44
43:v:21:ARG:HB3	43:v:21:ARG:NH1	2.33	0.44
6:G:90:TYR:OH	6:G:114:ASP:OD1	2.33	0.44
16:Q:192:LEU:HD12	16:Q:197:MET:HB3	1.98	0.44
28:e:103:SER:HA	49:e:201:PLX:H271	2.00	0.44
30:g:85:TYR:CZ	32:i:344:SER:HB3	2.53	0.44
40:r:216:LEU:HD23	40:r:287:ALA:HB1	2.00	0.44
44:w:277:LYS:HA	44:w:277:LYS:HD2	1.81	0.44
44:w:295:ARG:O	44:w:299:GLN:HG2	2.18	0.44
1:A:85:LEU:HD21	1:A:247:THR:HG23	1.99	0.43
7:H:56:LEU:HA	7:H:59:VAL:HG12	1.99	0.43
9:J:127:ILE:HD11	9:J:253:ILE:HD11	2.00	0.43
12:M:496:ILE:O	12:M:500:ILE:HD12	2.18	0.43
16:Q:38:GLN:HG3	32:i:304:MET:HE2	1.98	0.43
21:W:99:LYS:NZ	21:W:100:ASP:OD2	2.42	0.43
27:d:43:ARG:O	27:d:47:LEU:HG	2.17	0.43
35:l:320:ASN:ND2	35:l:320:ASN:C	2.74	0.43
42:u:47:ARG:NH2	42:u:53:PRO:HG3	2.33	0.43
1:A:170:GLN:HB3	10:K:89:LEU:HD13	1.99	0.43
2:B:41:VAL:HA	8:I:113:LEU:HB3	1.99	0.43
17:S:40:HIS:N	17:S:44:GLN:OE1	2.47	0.43
19:U:51:TYR:HB3	36:m:136:PHE:HE2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:104:ILE:HD13	27:d:18:PRO:HG3	2.00	0.43
35:l:551:SER:HA	35:l:555:LEU:HB2	2.00	0.43
37:n:17:VAL:HG13	40:r:7:PRO:HB3	2.00	0.43
7:H:90:LEU:HB2	15:P:102:ASP:HB3	1.99	0.43
9:J:157:LYS:HE2	9:J:195:PHE:CD2	2.54	0.43
6:X:87:LEU:HD13	6:X:98:LEU:HD11	2.00	0.43
24:a:147:ALA:HB2	40:r:173:SER:HB2	2.00	0.43
28:e:85:TRP:O	28:e:89:VAL:HG22	2.19	0.43
35:l:338:MET:HE2	35:l:338:MET:HB3	1.70	0.43
35:l:549:ALA:CB	40:r:271:MET:HE3	2.47	0.43
35:l:571:MET:HE2	35:l:571:MET:HB3	1.89	0.43
44:w:87:PRO:O	44:w:142:GLN:NE2	2.47	0.43
1:A:118:ASP:O	1:A:159:ARG:HD2	2.17	0.43
1:A:314:LEU:O	1:A:329:LYS:HD3	2.19	0.43
1:A:316:ALA:HB3	1:A:357:MET:HE2	2.01	0.43
48:B:303:PEE:H21	48:B:303:PEE:H16	1.72	0.43
32:i:154:MET:HE2	32:i:191:THR:CG2	2.48	0.43
35:l:267:MET:HE1	35:l:273:VAL:HG12	1.99	0.43
38:o:84:PRO:O	38:o:88:LEU:HB2	2.19	0.43
40:r:12:LEU:HD22	40:r:97:THR:HG23	2.00	0.43
56:s:402:UQ:HM53	56:s:402:UQ:H72	1.71	0.43
1:A:64:LYS:O	1:A:68:ILE:HG13	2.19	0.43
1:A:110:PRO:O	1:A:238:CYS:HB3	2.18	0.43
9:J:73:LEU:O	9:J:78:SER:OG	2.33	0.43
14:O:58:GLU:H	14:O:58:GLU:CD	2.26	0.43
14:O:177:LEU:N	52:O:301:FES:S1	2.82	0.43
14:O:196:LEU:HD13	14:O:201:ILE:CD1	2.46	0.43
27:d:78:GLU:HB2	27:d:81:ASP:HB2	1.99	0.43
32:i:215:MET:HE1	32:i:244:MET:HG3	2.01	0.43
35:l:221:ALA:HA	35:l:226:GLN:HG2	2.00	0.43
36:m:51:PHE:CZ	36:m:55:MET:HE3	2.53	0.43
40:r:72:LEU:HD12	40:r:72:LEU:HA	1.81	0.43
12:M:338:VAL:HG12	12:M:544:VAL:HG13	2.00	0.43
12:M:404:GLY:HA3	12:M:480:ALA:HB2	2.00	0.43
15:P:51:ASN:HB3	15:P:82:ASN:HD21	1.84	0.43
17:S:1:MET:HE3	17:S:1:MET:HB3	1.75	0.43
26:c:113:ILE:C	26:c:115:ASN:H	2.27	0.43
31:h:12:LEU:HD23	31:h:12:LEU:HA	1.91	0.43
33:j:81:THR:C	33:j:83:ASN:H	2.27	0.43
35:l:8:THR:CG2	35:l:82:MET:HE2	2.48	0.43
38:o:107:THR:O	38:o:111:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:367:LEU:HG	40:r:404:ALA:HA	2.01	0.43
44:w:165:SER:HB3	44:w:245:PHE:CE1	2.53	0.43
1:A:131:ILE:CD1	1:A:245:VAL:HG11	2.49	0.43
8:I:24:LEU:HD23	8:I:24:LEU:HA	1.89	0.43
12:M:133:GLN:O	12:M:137:CYS:HB2	2.19	0.43
12:M:251:ILE:HB	12:M:606:THR:HG22	2.00	0.43
12:M:399:VAL:HG23	12:M:428:LYS:HG2	2.01	0.43
25:b:82:ILE:HD11	35:l:13:THR:HG21	2.01	0.43
34:k:23:ARG:HD3	36:m:23:LYS:HB2	2.01	0.43
35:l:319:ILE:HG22	35:l:404:THR:HG21	2.01	0.43
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.53	0.43
37:n:26:TYR:CE2	37:n:30:ARG:HD2	2.54	0.43
1:A:329:LYS:HE3	1:A:329:LYS:HB3	1.64	0.43
7:H:9:THR:O	7:H:76:GLN:NE2	2.49	0.43
9:J:246:SER:O	9:J:250:ILE:HG12	2.19	0.43
12:M:83:GLU:HG2	12:M:84:LYS:HG3	1.99	0.43
25:b:14:GLN:NE2	39:p:157:ALA:HB3	2.27	0.43
27:d:89:GLU:O	27:d:93:ARG:HG2	2.19	0.43
40:r:427:LYS:HA	40:r:427:LYS:HD3	1.82	0.43
49:r:502:PLX:H91	49:r:502:PLX:H121	1.69	0.43
43:v:22:MET:HE1	43:v:102:PHE:HA	2.01	0.43
44:w:147:LEU:HD23	44:w:147:LEU:HA	1.89	0.43
44:w:182:GLN:HB3	44:w:314:LEU:HD21	1.99	0.43
4:E:40:TYR:CD1	6:G:120:MET:HE1	2.53	0.43
7:H:98:LYS:HG3	7:H:100:TRP:CZ2	2.54	0.43
10:K:73:TYR:CZ	10:K:75:ASN:HB3	2.54	0.43
12:M:249:GLU:HG2	12:M:276:ARG:CD	2.49	0.43
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.49	0.43
13:N:27:LEU:HD21	41:s:42:PRO:HB3	2.00	0.43
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.54	0.43
6:X:113:LEU:O	6:X:116:VAL:HG12	2.19	0.43
24:a:78:THR:OG1	28:e:96:SER:HB3	2.19	0.43
49:j:202:PLX:H342	49:j:202:PLX:H372	1.77	0.43
35:l:21:MET:HE2	35:l:21:MET:HB3	1.78	0.43
40:r:121:LEU:O	40:r:125:THR:HG23	2.19	0.43
43:v:18:ASP:OD1	43:v:18:ASP:C	2.61	0.43
9:J:207:PHE:HB2	9:J:214:LEU:HD13	2.01	0.42
12:M:55:LYS:NZ	12:M:55:LYS:HB3	2.34	0.42
13:N:14:VAL:HA	13:N:23:TYR:CD1	2.54	0.42
25:b:108:ASP:OD1	43:v:71:ARG:NH2	2.52	0.42
35:l:184:LEU:HB2	40:r:393:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:102:LYS:NZ	44:w:102:LYS:HB3	2.33	0.42
44:w:314:LEU:O	44:w:318:THR:HG22	2.19	0.42
1:A:279:SER:OG	1:A:280:GLY:N	2.52	0.42
12:M:36:VAL:HB	12:M:56:VAL:HG21	2.01	0.42
14:O:158:ILE:HB	14:O:162:GLU:HB2	2.00	0.42
19:U:14:ALA:C	19:U:16:GLU:H	2.27	0.42
21:W:74:LEU:O	21:W:78:GLU:HG3	2.19	0.42
26:c:127:ASN:O	26:c:131:LYS:HG3	2.19	0.42
30:g:55:VAL:HG11	55:r:503:CDL:H711	2.00	0.42
32:i:66:ALA:HB2	32:i:104:MET:HG2	2.01	0.42
40:r:328:CYS:O	40:r:332:THR:HG23	2.19	0.42
43:v:97:LYS:HB2	43:v:97:LYS:HE2	1.84	0.42
43:v:110:GLN:HA	43:v:110:GLN:OE1	2.19	0.42
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.54	0.42
7:H:7:LYS:HA	7:H:16:VAL:HG21	2.01	0.42
8:I:48:LYS:H	8:I:48:LYS:HG3	1.65	0.42
9:J:204:SER:HB3	9:J:266:VAL:HG12	2.01	0.42
11:L:131:LYS:HD2	11:L:147:VAL:HG11	2.02	0.42
12:M:544:VAL:HA	12:M:565:PHE:O	2.18	0.42
14:O:186:VAL:HG23	14:O:196:LEU:HD12	2.02	0.42
16:Q:237:PRO:HD2	16:Q:240:LEU:HD22	2.02	0.42
18:T:52:ARG:HG3	18:T:52:ARG:HH11	1.84	0.42
21:W:115:ARG:HH12	31:h:39:GLU:HG3	1.83	0.42
28:e:55:LEU:HB3	44:w:318:THR:HG23	2.01	0.42
39:p:76:HIS:O	39:p:78:GLN:N	2.53	0.42
44:w:277:LYS:HG3	44:w:279:ASP:OD1	2.19	0.42
8:I:42:PRO:HD3	21:W:6:VAL:HG13	2.01	0.42
10:K:95:LYS:HE3	10:K:95:LYS:HB3	1.93	0.42
15:P:101:ARG:O	15:P:109:LYS:NZ	2.52	0.42
20:V:95:CYS:HA	20:V:115:CYS:HA	2.02	0.42
23:Z:18:ASP:OD1	23:Z:18:ASP:C	2.62	0.42
32:i:141:VAL:O	32:i:145:ILE:HG12	2.20	0.42
32:i:170:LEU:HD11	32:i:288:LEU:HD22	2.01	0.42
33:j:55:PHE:O	33:j:58:VAL:HG12	2.20	0.42
35:l:341:MET:HE1	35:l:453:SER:HB2	2.00	0.42
40:r:201:MET:HE1	40:r:261:PHE:HE1	1.83	0.42
44:w:76:GLU:HG3	44:w:80:LYS:HE2	2.01	0.42
44:w:182:GLN:HA	44:w:185:GLU:OE2	2.19	0.42
2:B:38:TYR:CZ	8:I:106:LEU:HD13	2.54	0.42
5:F:68:ARG:NH2	12:M:364:ASP:OD2	2.51	0.42
12:M:347:ASP:OD1	12:M:347:ASP:N	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:78:LEU:HD12	26:c:106:HIS:CA	2.48	0.42
27:d:104:ASN:O	27:d:108:GLU:HG3	2.19	0.42
36:m:42:GLY:HA2	48:s:401:PEE:H23	2.01	0.42
38:o:88:LEU:HD12	38:o:88:LEU:HA	1.83	0.42
41:s:174:MET:HB3	41:s:242:PHE:HA	2.01	0.42
44:w:59:VAL:HG23	44:w:157:VAL:HG23	2.00	0.42
3:C:66:THR:OG1	3:C:76:MET:HE3	2.20	0.42
5:F:19:ILE:HD12	5:F:66:TRP:O	2.20	0.42
5:F:36:PHE:HB2	5:F:87:VAL:HG21	2.01	0.42
6:G:70:ASP:N	6:G:70:ASP:OD1	2.52	0.42
7:H:99:PRO:HD2	7:H:100:TRP:CZ3	2.54	0.42
12:M:128:CYS:SG	12:M:140:GLN:NE2	2.84	0.42
12:M:129:PRO:O	12:M:241:ARG:NH2	2.52	0.42
21:W:30:LEU:HD12	21:W:30:LEU:HA	1.85	0.42
35:l:378:LEU:HD23	35:l:378:LEU:HA	1.86	0.42
35:l:520:TYR:CE2	55:l:702:CDL:HB22	2.55	0.42
7:H:112:TRP:CE2	15:P:87:PHE:HB3	2.55	0.42
14:O:93:LEU:HD12	14:O:122:TYR:HB3	2.02	0.42
16:Q:235:ASP:N	16:Q:356:ILE:HD13	2.35	0.42
17:S:51:ASP:CG	42:u:22:SER:HG	2.27	0.42
6:X:90:TYR:CE1	23:Z:44:PRO:HB2	2.53	0.42
49:a:202:PLX:H132	49:a:202:PLX:H101	1.74	0.42
49:a:202:PLX:H72	49:a:202:PLX:H252	2.02	0.42
27:d:16:ARG:NH2	43:v:48:ASP:OD2	2.52	0.42
49:g:201:PLX:H361	49:g:201:PLX:H332	1.89	0.42
31:h:7:GLN:O	31:h:11:GLY:N	2.50	0.42
35:l:584:ILE:O	35:l:588:PHE:HD1	2.02	0.42
41:s:88:PRO:O	41:s:162:LEU:HD12	2.19	0.42
2:B:142:THR:O	2:B:187:LYS:NZ	2.52	0.42
4:E:68:MET:HE1	50:G:201:8Q1:C30	2.50	0.42
6:G:103:HIS:CE1	6:G:106:LYS:H	2.36	0.42
9:J:163:LYS:NZ	9:J:253:ILE:O	2.43	0.42
15:P:217:LYS:HE2	33:j:33:LYS:HE3	2.00	0.42
21:W:52:LYS:HD2	21:W:52:LYS:HA	1.86	0.42
50:X:201:8Q1:C30	39:p:52:LYS:HG3	2.49	0.42
27:d:32:TYR:O	27:d:36:ILE:HD12	2.19	0.42
35:l:61:MET:HB3	35:l:61:MET:HE3	1.76	0.42
35:l:76:LEU:HD21	35:l:196:TRP:HE3	1.85	0.42
35:l:253:VAL:HB	35:l:310:LEU:HD11	2.02	0.42
35:l:286:LEU:HD13	35:l:411:MET:SD	2.60	0.42
40:r:196:TRP:HB2	40:r:253:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:26:LYS:NZ	42:u:95:GLN:O	2.43	0.42
1:A:334:THR:O	1:A:334:THR:OG1	2.30	0.42
5:F:23:LEU:HD22	5:F:37:ILE:HD11	2.02	0.42
6:G:90:TYR:CE2	6:G:92:LYS:HB2	2.55	0.42
13:N:101:LYS:HE3	13:N:101:LYS:HB3	1.79	0.42
20:V:124:LEU:HD11	48:r:501:PEE:H64	2.02	0.42
23:Z:24:ILE:HD11	23:Z:46:GLY:C	2.45	0.42
29:f:62:HIS:O	29:f:66:VAL:HG23	2.19	0.42
49:g:201:PLX:H22	49:g:201:PLX:H1C3	1.75	0.42
32:i:230:LEU:HD11	32:i:244:MET:CE	2.50	0.42
39:p:133:TRP:HA	39:p:136:GLU:HG2	2.01	0.42
40:r:318:ALA:HB1	40:r:374:ASN:CG	2.44	0.42
44:w:72:ARG:NH1	44:w:264:GLU:HA	2.30	0.42
1:A:83:SER:HB2	1:A:262:PHE:HD2	1.84	0.42
4:E:118:PHE:CD1	4:E:118:PHE:C	2.97	0.42
6:G:88:LYS:HD2	6:G:88:LYS:HA	1.83	0.42
12:M:682:ASP:OD1	12:M:682:ASP:N	2.51	0.42
16:Q:216:ARG:HH12	16:Q:243:ASP:CG	2.27	0.42
48:Q:501:PEE:H42	48:Q:501:PEE:H35	1.72	0.42
32:i:18:MET:O	32:i:22:ILE:HG12	2.20	0.42
35:l:62:ILE:HD12	35:l:135:ASN:ND2	2.35	0.42
55:l:701:CDL:H401	40:r:445:LEU:HD22	2.02	0.42
42:u:149:GLU:H	42:u:149:GLU:CD	2.22	0.42
44:w:58:LYS:HA	44:w:202:HIS:CD2	2.54	0.42
44:w:245:PHE:O	44:w:248:GLU:HG2	2.20	0.42
1:A:69:LEU:HD11	1:A:143:LEU:HD21	2.02	0.41
5:F:45:LYS:HA	5:F:45:LYS:HD2	1.81	0.41
8:I:40:LYS:HB3	21:W:6:VAL:HA	2.02	0.41
11:L:89:SER:O	12:M:59:GLN:NE2	2.52	0.41
13:N:39:VAL:HG21	13:N:50:GLU:HB3	2.02	0.41
6:X:125:GLU:OE1	35:l:439:PRO:HG2	2.20	0.41
27:d:102:ILE:O	27:d:106:ILE:HG12	2.20	0.41
31:h:101:LYS:H	31:h:101:LYS:HG2	1.75	0.41
33:j:21:ALA:HB1	41:s:218:GLY:HA3	2.01	0.41
37:n:20:GLY:HA3	40:r:10:MET:HG3	2.01	0.41
40:r:127:VAL:HB	40:r:128:PRO:HD3	2.01	0.41
40:r:266:MET:HB3	40:r:395:LEU:HD13	2.02	0.41
41:s:14:LEU:HD22	41:s:225:MET:HE3	2.02	0.41
44:w:171:GLU:OE2	44:w:171:GLU:HA	2.20	0.41
1:A:62:TRP:HA	1:A:140:GLU:OE2	2.21	0.41
3:C:68:GLY:HA2	3:C:73:ALA:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:C:302:PEE:H62	33:j:24:LEU:HD11	2.02	0.41
6:G:104:PHE:HA	6:G:108:LEU:HD12	2.01	0.41
13:N:53:LYS:HD3	13:N:53:LYS:HA	1.82	0.41
6:X:131:PRO:HG2	6:X:134:ASP:HB2	2.02	0.41
26:c:159:LYS:NZ	43:v:57:ASP:OD2	2.52	0.41
27:d:114:GLN:OE1	35:l:199:GLN:HG3	2.20	0.41
31:h:39:GLU:OE1	42:u:144:SER:OG	2.27	0.41
40:r:207:MET:CE	40:r:243:MET:HE3	2.50	0.41
1:A:429:ASP:N	1:A:429:ASP:OD1	2.51	0.41
6:G:89:LEU:HD23	6:G:89:LEU:HA	1.88	0.41
6:G:149:ALA:O	6:G:153:ASP:N	2.53	0.41
7:H:11:LEU:HD12	7:H:14:LEU:HD22	2.01	0.41
7:H:59:VAL:HG23	7:H:68:LEU:HD21	2.02	0.41
9:J:241:TYR:O	9:J:245:VAL:HG23	2.20	0.41
10:K:79:HIS:ND1	14:O:216:PRO:HD2	2.36	0.41
14:O:159:LYS:HB2	14:O:162:GLU:HG3	2.00	0.41
27:d:159:GLN:NE2	28:e:142:PHE:O	2.41	0.41
34:k:37:MET:HG3	34:k:67:ALA:CB	2.50	0.41
40:r:201:MET:HG3	48:r:501:PEE:H33	2.02	0.41
3:C:119:LYS:HB3	3:C:119:LYS:HE3	1.76	0.41
5:F:33:VAL:O	5:F:37:ILE:N	2.41	0.41
10:K:82:SER:OG	10:K:83:THR:N	2.54	0.41
48:Q:501:PEE:H47	48:r:501:PEE:H40	2.02	0.41
21:W:51:MET:SD	41:s:311:THR:HB	2.61	0.41
27:d:140:GLN:O	27:d:144:SER:HB2	2.21	0.41
30:g:3:MET:HB2	30:g:3:MET:HE3	1.83	0.41
34:k:23:ARG:HG3	34:k:24:SER:H	1.86	0.41
35:l:477:VAL:HA	35:l:478:PRO:HD3	1.92	0.41
35:l:500:LEU:HD23	35:l:500:LEU:HA	1.97	0.41
40:r:445:LEU:O	40:r:448:THR:HG22	2.19	0.41
41:s:55:LEU:HD13	41:s:221:ALA:HB2	2.01	0.41
43:v:3:ALA:O	43:v:7:ARG:HG3	2.20	0.41
1:A:395:VAL:HG11	1:A:412:LEU:HD13	2.02	0.41
2:B:80:GLU:HB3	8:I:26:LEU:HD11	2.03	0.41
48:B:303:PEE:H54	41:s:197:PRO:HG3	2.02	0.41
4:E:43:VAL:O	4:E:47:VAL:HG23	2.21	0.41
6:G:134:ASP:HA	6:G:137:LYS:HE3	2.02	0.41
15:P:125:ARG:HH22	15:P:201:ASP:CG	2.26	0.41
20:V:43:LEU:HA	35:l:586:LEU:HB3	2.02	0.41
24:a:106:VAL:HA	24:a:107:PRO:HD3	1.95	0.41
28:e:108:TYR:CE1	49:e:201:PLX:H1B2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:g:201:PLX:H152	49:g:201:PLX:H121	1.60	0.41
41:s:298:LEU:O	41:s:302:MET:HG3	2.21	0.41
1:A:385:CYS:HB3	45:A:501:SF4:S2	2.60	0.41
2:B:205:ILE:O	2:B:209:TYR:HB3	2.20	0.41
4:E:84:ILE:HD13	15:P:177:PHE:CE1	2.56	0.41
13:N:10:GLY:O	13:N:14:VAL:HG23	2.21	0.41
16:Q:142:VAL:HG21	16:Q:457:VAL:HG21	2.02	0.41
6:X:85:TYR:CD2	23:Z:16:LEU:HD23	2.55	0.41
25:b:73:THR:HG23	25:b:74:HIS:ND1	2.35	0.41
26:c:109:LEU:O	26:c:113:ILE:HG23	2.21	0.41
29:f:52:VAL:HG12	29:f:56:ILE:HD12	2.01	0.41
32:i:291:TYR:HA	40:r:151:PHE:HZ	1.85	0.41
33:j:71:LEU:O	36:m:147:TYR:OH	2.36	0.41
48:j:201:PEE:H59	48:j:201:PEE:H64	1.70	0.41
34:k:22:TYR:O	35:l:585:LYS:HG2	2.19	0.41
38:o:25:ILE:HD12	38:o:30:ARG:NH2	2.35	0.41
39:p:29:SER:HB3	39:p:76:HIS:CD2	2.46	0.41
44:w:146:ALA:HB1	44:w:157:VAL:HG21	2.01	0.41
1:A:104:LYS:HE2	1:A:231:ALA:O	2.21	0.41
9:J:180:TYR:HB3	9:J:321:ARG:HD3	2.03	0.41
9:J:236:VAL:HG12	9:J:270:ARG:HH11	1.85	0.41
12:M:669:ASN:O	12:M:672:SER:OG	2.36	0.41
14:O:108:PRO:HA	14:O:109:PRO:HD3	1.96	0.41
19:U:18:VAL:O	19:U:22:SER:OG	2.35	0.41
32:i:276:ILE:HG21	48:r:501:PEE:H7	2.01	0.41
33:j:84:LEU:HD23	33:j:84:LEU:HA	1.81	0.41
35:l:512:LYS:HE2	35:l:512:LYS:HB2	1.70	0.41
40:r:410:MET:HB3	40:r:410:MET:HE3	1.86	0.41
49:r:502:PLX:H51	49:r:502:PLX:H6	1.41	0.41
41:s:81:LEU:O	41:s:85:MET:HG3	2.20	0.41
41:s:258:ASN:O	41:s:262:LYS:HG3	2.21	0.41
56:s:402:UQ:H103	56:s:402:UQ:H71	1.83	0.41
55:u:201:CDL:H602	55:u:201:CDL:H572	1.81	0.41
1:A:53:LEU:HD13	1:A:136:HIS:CE1	2.56	0.41
1:A:56:ALA:HB1	1:A:61:ASP:HB2	2.01	0.41
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.86	0.41
5:F:19:ILE:HD12	5:F:19:ILE:HA	1.84	0.41
5:F:56:ARG:NH1	12:M:382:ARG:HG3	2.35	0.41
12:M:646:LEU:HD22	12:M:653:LEU:HD13	2.01	0.41
13:N:55:PHE:CZ	13:N:58:ARG:HG3	2.56	0.41
24:a:96:ALA:HB2	27:d:61:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:137:MET:HE2	24:a:137:MET:HB3	1.98	0.41
35:l:482:MET:HE2	35:l:482:MET:HB2	1.86	0.41
35:l:549:ALA:HB2	40:r:271:MET:CE	2.50	0.41
40:r:27:ALA:O	40:r:31:SER:OG	2.30	0.41
41:s:25:ARG:HD2	56:s:402:UQ:HM21	2.02	0.41
43:v:101:GLU:HA	43:v:101:GLU:OE1	2.21	0.41
2:B:70:LEU:HG	41:s:277:TYR:OH	2.21	0.41
2:B:128:ILE:HG12	2:B:147:ILE:HG12	2.03	0.41
45:C:301:SF4:S2	16:Q:138:ARG:HG2	2.61	0.41
6:G:90:TYR:HE2	6:G:92:LYS:HB2	1.85	0.41
6:G:137:LYS:HE2	6:G:137:LYS:HB3	1.82	0.41
7:H:59:VAL:HA	7:H:68:LEU:HD11	2.03	0.41
12:M:254:MET:HB3	12:M:254:MET:HE3	1.77	0.41
21:W:10:MET:HE3	21:W:10:MET:HB3	1.92	0.41
21:W:58:ARG:HD2	21:W:58:ARG:HA	1.83	0.41
21:W:120:MET:N	21:W:123:GLU:HG3	2.34	0.41
25:b:76:LEU:HD12	25:b:76:LEU:HA	1.89	0.41
26:c:32:VAL:HA	26:c:36:MET:HE2	2.02	0.41
27:d:122:ARG:HA	27:d:122:ARG:HD3	1.88	0.41
30:g:110:THR:HG22	30:g:112:GLY:H	1.85	0.41
49:g:201:PLX:H1C2	31:h:2:PRO:HD2	2.03	0.41
31:h:19:THR:HA	32:i:84:TRP:HB2	2.03	0.41
33:j:48:ARG:HB2	33:j:49:LEU:H	1.49	0.41
33:j:72:LEU:HD22	33:j:75:LEU:HD11	2.03	0.41
33:j:73:LEU:O	41:s:160:TYR:OH	2.39	0.41
34:k:38:LEU:HD21	36:m:37:GLY:HA2	2.03	0.41
35:l:292:ALA:HB2	35:l:304:PHE:CB	2.51	0.41
35:l:529:TYR:CZ	35:l:533:MET:HG3	2.56	0.41
36:m:163:ILE:HD13	36:m:163:ILE:HA	1.91	0.41
40:r:225:ILE:HD13	40:r:331:ASN:HB2	2.02	0.41
41:s:18:ALA:HB2	56:s:402:UQ:H152	2.03	0.41
12:M:624:ARG:HA	12:M:634:LEU:HD12	2.02	0.41
14:O:187:GLN:HG3	14:O:192:TYR:CE1	2.55	0.41
14:O:213:ILE:HD12	14:O:213:ILE:O	2.20	0.41
16:Q:339:GLN:O	16:Q:343:ILE:HG13	2.21	0.41
19:U:78:LEU:HD22	42:u:123:GLY:HA3	2.03	0.41
27:d:43:ARG:HB2	27:d:44:PRO:HD3	2.03	0.41
32:i:27:LEU:HD13	34:k:59:MET:HG2	2.03	0.41
34:k:42:ILE:HD13	34:k:42:ILE:HA	1.89	0.41
55:l:702:CDL:H382	55:l:702:CDL:H351	1.81	0.41
41:s:143:GLU:HA	41:s:146:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:37:GLN:OE1	44:w:37:GLN:HA	2.21	0.41
2:B:210:LEU:HD12	8:I:38:PRO:HB3	2.02	0.40
4:E:120:SER:O	4:E:124:VAL:HG22	2.20	0.40
16:Q:238:LEU:HD23	16:Q:238:LEU:HA	1.79	0.40
19:U:84:LEU:HD23	19:U:84:LEU:HA	1.94	0.40
24:a:66:ARG:NH1	28:e:72:ASP:HB2	2.36	0.40
32:i:44:LEU:HD22	32:i:122:ILE:HG21	2.03	0.40
44:w:59:VAL:HG12	44:w:202:HIS:CD2	2.55	0.40
44:w:72:ARG:HE	44:w:72:ARG:HB3	1.70	0.40
44:w:346:ASP:N	44:w:346:ASP:OD1	2.54	0.40
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.56	0.40
48:B:303:PEE:H72	41:s:183:MET:HG2	2.03	0.40
3:C:113:MET:O	3:C:113:MET:HG3	2.21	0.40
9:J:189:LYS:HA	9:J:189:LYS:HD3	1.94	0.40
12:M:96:VAL:HG23	12:M:100:TRP:HE3	1.86	0.40
12:M:140:GLN:HG2	16:Q:379:ILE:HG12	2.02	0.40
12:M:330:LEU:HD22	12:M:330:LEU:HA	1.95	0.40
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.45	0.40
16:Q:278:VAL:HG12	16:Q:329:ARG:HH21	1.85	0.40
16:Q:357:LYS:HD3	16:Q:364:SER:HB3	2.03	0.40
26:c:55:TYR:CZ	26:c:76:PRO:HD3	2.56	0.40
26:c:143:MET:HB3	35:l:407:TRP:CD2	2.56	0.40
31:h:86:LEU:O	31:h:90:GLY:N	2.50	0.40
33:j:81:THR:O	33:j:82:ASN:HB2	2.22	0.40
35:l:52:LEU:HD12	43:v:74:PHE:HZ	1.85	0.40
35:l:535:ARG:NH1	38:o:11:LEU:O	2.54	0.40
38:o:108:ASP:OD1	38:o:108:ASP:C	2.64	0.40
44:w:199:LEU:HD11	44:w:286:GLN:HG3	2.04	0.40
3:C:82:PRO:HG3	16:Q:201:PHE:HB3	2.03	0.40
6:G:79:ILE:HG22	6:G:145:VAL:HG13	2.02	0.40
7:H:76:GLN:O	7:H:78:GLU:N	2.54	0.40
12:M:266:ARG:HG2	12:M:267:THR:HG23	2.03	0.40
12:M:339:ALA:HB3	12:M:542:PRO:HG3	2.03	0.40
13:N:3:LEU:O	13:N:6:VAL:HG22	2.21	0.40
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	2.01	0.40
20:V:126:LYS:HA	20:V:126:LYS:HD2	1.88	0.40
3:C:44:GLU:HA	3:C:47:VAL:HG22	2.03	0.40
3:C:101:ASP:OD2	41:s:54:LYS:HE2	2.21	0.40
8:I:70:MET:HE2	8:I:71:SER:C	2.47	0.40
15:P:107:GLN:HE21	15:P:107:GLN:HB3	1.74	0.40
17:S:14:ALA:O	17:S:17:PHE:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:95:MET:HE1	32:i:145:ILE:HD12	2.04	0.40
32:i:95:MET:HE2	32:i:149:ILE:HG22	2.03	0.40
39:p:168:TRP:O	39:p:172:THR:OG1	2.33	0.40
40:r:265:SER:O	40:r:269:MET:HG2	2.22	0.40
56:s:402:UQ:H203	56:s:402:UQ:H171	1.81	0.40
43:v:84:GLN:NE2	43:v:88:ASP:OD2	2.51	0.40
44:w:65:ASN:OD1	44:w:66:ILE:N	2.44	0.40
44:w:143:TYR:OH	44:w:199:LEU:O	2.31	0.40
44:w:350:LYS:HD2	44:w:350:LYS:HA	1.84	0.40
1:A:208:GLU:O	1:A:212:LEU:N	2.46	0.40
47:A:503:NAI:H6N	47:A:503:NAI:H2D	1.82	0.40
8:I:107:SER:C	8:I:109:ASP:H	2.30	0.40
16:Q:108:LYS:HE2	16:Q:108:LYS:HB3	1.85	0.40
16:Q:271:ARG:HA	16:Q:271:ARG:HD2	1.85	0.40
21:W:87:LEU:HD23	21:W:87:LEU:HA	1.94	0.40
22:Y:88:ASP:OD2	22:Y:91:GLN:HG2	2.21	0.40
23:Z:13:LYS:HA	23:Z:13:LYS:HD2	1.78	0.40
24:a:78:THR:HG21	28:e:96:SER:O	2.22	0.40
40:r:22:MET:HE3	40:r:22:MET:HB3	1.84	0.40
40:r:31:SER:HB3	40:r:73:LEU:HD23	2.04	0.40
42:u:69:ASP:OD1	42:u:69:ASP:N	2.53	0.40
43:v:30:GLY:H	43:v:104:ARG:HH22	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	415 (97%)	14 (3%)	0	100	100
2	B	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
3	C	154/156 (99%)	148 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
5	F	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
6	G	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
6	X	86/88 (98%)	86 (100%)	0	0	100	100
7	H	110/112 (98%)	103 (94%)	7 (6%)	0	100	100
8	I	93/112 (83%)	83 (89%)	10 (11%)	0	100	100
9	J	289/342 (84%)	281 (97%)	7 (2%)	1 (0%)	36	65
10	K	40/42 (95%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	666 (97%)	21 (3%)	1 (0%)	48	77
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
15	P	206/208 (99%)	194 (94%)	12 (6%)	0	100	100
16	Q	412/430 (96%)	398 (97%)	14 (3%)	0	100	100
17	S	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
18	T	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
19	U	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
20	V	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	18	48
21	W	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
22	Y	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
23	Z	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
24	a	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
25	b	99/126 (79%)	93 (94%)	6 (6%)	0	100	100
26	c	154/156 (99%)	145 (94%)	8 (5%)	1 (1%)	21	51
27	d	173/175 (99%)	172 (99%)	1 (1%)	0	100	100
28	e	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
29	f	40/42 (95%)	38 (95%)	2 (5%)	0	100	100
30	g	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
32	i	345/347 (99%)	336 (97%)	9 (3%)	0	100	100
33	j	95/113 (84%)	87 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	k	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
35	l	601/603 (100%)	573 (95%)	27 (4%)	1 (0%)	43	72
36	m	125/175 (71%)	112 (90%)	12 (10%)	1 (1%)	16	44
37	n	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
38	o	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
39	p	176/178 (99%)	166 (94%)	9 (5%)	1 (1%)	21	51
40	r	457/459 (100%)	446 (98%)	11 (2%)	0	100	100
41	s	299/318 (94%)	290 (97%)	9 (3%)	0	100	100
42	u	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
43	v	122/131 (93%)	114 (93%)	8 (7%)	0	100	100
44	w	318/320 (99%)	305 (96%)	13 (4%)	0	100	100
All	All	8029/8316 (96%)	7731 (96%)	291 (4%)	7 (0%)	49	77

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	38	HIS
12	M	283	GLU
26	c	106	HIS
20	V	46	PRO
35	l	15	LEU
36	m	26	PRO
39	p	174	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/345 (100%)	341 (99%)	4 (1%)	63	86
2	B	151/151 (100%)	149 (99%)	2 (1%)	61	86
3	C	129/132 (98%)	127 (98%)	2 (2%)	55	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	106/107 (99%)	106 (100%)	0	100	100
5	F	75/76 (99%)	73 (97%)	2 (3%)	39	73
6	G	76/81 (94%)	76 (100%)	0	100	100
6	X	77/81 (95%)	76 (99%)	1 (1%)	61	86
7	H	99/99 (100%)	98 (99%)	1 (1%)	68	89
8	I	82/97 (84%)	80 (98%)	2 (2%)	43	75
9	J	253/296 (86%)	249 (98%)	4 (2%)	55	83
10	K	41/41 (100%)	39 (95%)	2 (5%)	22	54
11	L	113/113 (100%)	110 (97%)	3 (3%)	39	73
12	M	579/580 (100%)	574 (99%)	5 (1%)	70	90
13	N	130/130 (100%)	129 (99%)	1 (1%)	73	90
14	O	176/183 (96%)	169 (96%)	7 (4%)	28	62
15	P	190/190 (100%)	188 (99%)	2 (1%)	65	88
16	Q	358/370 (97%)	355 (99%)	3 (1%)	73	90
17	S	58/58 (100%)	57 (98%)	1 (2%)	53	82
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	69/69 (100%)	66 (96%)	3 (4%)	26	60
20	V	101/101 (100%)	99 (98%)	2 (2%)	48	78
21	W	121/123 (98%)	121 (100%)	0	100	100
22	Y	58/63 (92%)	56 (97%)	2 (3%)	32	66
23	Z	65/65 (100%)	65 (100%)	0	100	100
24	a	119/122 (98%)	118 (99%)	1 (1%)	73	90
25	b	97/119 (82%)	95 (98%)	2 (2%)	47	77
26	c	141/141 (100%)	138 (98%)	3 (2%)	47	77
27	d	155/155 (100%)	152 (98%)	3 (2%)	50	79
28	e	99/99 (100%)	98 (99%)	1 (1%)	68	89
29	f	35/38 (92%)	34 (97%)	1 (3%)	37	71
30	g	108/108 (100%)	108 (100%)	0	100	100
31	h	93/93 (100%)	91 (98%)	2 (2%)	45	77
32	i	310/311 (100%)	303 (98%)	7 (2%)	44	76
33	j	88/99 (89%)	85 (97%)	3 (3%)	32	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	536/537 (100%)	531 (99%)	5 (1%)	70	90
36	m	98/141 (70%)	94 (96%)	4 (4%)	27	61
37	n	46/53 (87%)	45 (98%)	1 (2%)	45	77
38	o	112/113 (99%)	109 (97%)	3 (3%)	39	73
39	p	159/159 (100%)	158 (99%)	1 (1%)	78	93
40	r	410/410 (100%)	404 (98%)	6 (2%)	57	84
41	s	263/275 (96%)	259 (98%)	4 (2%)	57	84
42	u	153/153 (100%)	150 (98%)	3 (2%)	48	78
43	v	103/111 (93%)	101 (98%)	2 (2%)	50	79
44	w	279/283 (99%)	274 (98%)	5 (2%)	51	80
All	All	7020/7235 (97%)	6914 (98%)	106 (2%)	55	84

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	ASN
1	A	273	THR
1	A	282	VAL
1	A	334	THR
2	B	73	THR
2	B	76	TYR
3	C	71	CYS
3	C	126	GLU
5	F	42	VAL
5	F	65	LEU
7	H	52	THR
8	I	25	GLN
8	I	48	LYS
9	J	132	ARG
9	J	156	SER
9	J	325	SER
9	J	350	ILE
10	K	83	THR
10	K	107	SER
11	L	86	ASN
11	L	124	LEU
11	L	130	THR

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Mol	Chain	Res	Type
12	M	295	ASP
12	M	330	LEU
12	M	374	THR
12	M	403	VAL
12	M	544	VAL
13	N	37	THR
14	O	54	ASP
14	O	96	SER
14	O	134	VAL
14	O	137	THR
14	O	187	GLN
14	O	197	THR
14	O	205	ILE
15	P	110	SER
15	P	154	GLU
16	Q	144	MET
16	Q	217	VAL
16	Q	437	LYS
17	S	67	GLU
19	U	22	SER
19	U	34	SER
19	U	68	SER
20	V	40	SER
20	V	72	LEU
6	X	74	LEU
22	Y	94	ASP
22	Y	97	LEU
24	a	160	MET
25	b	76	LEU
25	b	82	ILE
26	c	44	THR
26	c	117	VAL
26	c	120	SER
27	d	17	THR
27	d	120	SER
27	d	136	SER
28	e	81	ILE
29	f	51	SER
31	h	77	SER
31	h	80	LYS
32	i	154	MET
32	i	187	MET

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Mol	Chain	Res	Type
32	i	211	MET
32	i	257	LEU
32	i	300	SER
32	i	324	LYS
32	i	329	MET
33	j	57	LEU
33	j	97	LEU
33	j	105	GLU
35	l	46	LEU
35	l	320	ASN
35	l	341	MET
35	l	364	LYS
35	l	481	THR
36	m	27	ILE
36	m	57	PHE
36	m	65	LEU
36	m	135	PHE
37	n	31	SER
38	o	9	SER
38	o	41	SER
38	o	108	ASP
39	p	64	LEU
40	r	60	SER
40	r	66	LEU
40	r	111	THR
40	r	179	ILE
40	r	183	SER
40	r	458	LEU
41	s	15	LEU
41	s	54	LYS
41	s	57	THR
41	s	119	SER
42	u	56	CYS
42	u	74	ILE
42	u	87	THR
43	v	14	SER
43	v	65	GLN
44	w	56	THR
44	w	163	ILE
44	w	164	TYR
44	w	214	ILE
44	w	290	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	ASN
1	A	393	ASN
4	E	45	ASN
4	E	126	HIS
5	F	86	GLN
9	J	79	GLN
9	J	122	HIS
9	J	376	ASN
11	L	71	HIS
12	M	205	GLN
12	M	300	GLN
12	M	453	GLN
12	M	495	ASN
12	M	540	ASN
13	N	12	GLN
13	N	17	HIS
14	O	182	ASN
15	P	107	GLN
15	P	196	HIS
15	P	228	GLN
16	Q	160	ASN
16	Q	182	ASN
16	Q	183	HIS
16	Q	190	HIS
21	W	24	ASN
21	W	76	GLN
22	Y	83	HIS
25	b	14	GLN
25	b	127	HIS
26	c	56	ASN
26	c	100	ASN
32	i	83	GLN
32	i	289	ASN
33	j	108	GLN
34	k	25	HIS
34	k	92	ASN
35	l	59	GLN
35	l	72	GLN
35	l	135	ASN
35	l	199	GLN
35	l	354	GLN

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Mol	Chain	Res	Type
35	l	447	ASN
35	l	546	GLN
36	m	46	ASN
37	n	40	ASN
39	p	75	GLN
39	p	76	HIS
41	s	317	GLN
43	v	85	HIS
44	w	92	HIS
44	w	132	GLN
44	w	202	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	2MR	Q	118	16	10,12,13	1.98	1 (10%)	5,13,15	6.05	3 (60%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	2MR	Q	118	16	-	3/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.64	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Q	118	2MR	NE-CZ-NH2	12.39	130.84	119.48
16	Q	118	2MR	CD-NE-CZ	4.37	131.60	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.01	130.51	123.86

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 2 are monoatomic - leaving 35 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	$\#\|Z\| > 2$
50	8Q1	G	201	6	31,34,34	1.69	6 (19%)	40,43,43	1.52	6 (15%)
48	PEE	s	401	-	40,40,50	1.15	5 (12%)	43,45,55	1.01	2 (4%)
52	FES	O	301	14	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
48	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	0.97	2 (3%)
56	UQ	s	402	-	28,28,63	3.27	7 (25%)	34,37,79	2.79	10 (29%)
49	PLX	g	201	-	51,51,51	1.14	3 (5%)	55,59,59	0.61	1 (1%)
48	PEE	C	302	-	46,46,50	1.21	6 (13%)	49,51,55	0.94	2 (4%)
48	PEE	Q	501	-	46,46,50	1.21	6 (13%)	49,51,55	1.00	2 (4%)
47	NAI	A	503	-	45,48,48	3.91	20 (44%)	60,73,73	1.77	12 (20%)
55	CDL	l	701	-	98,98,99	1.09	8 (8%)	104,110,111	0.88	4 (3%)
55	CDL	l	702	-	99,99,99	1.09	9 (9%)	105,111,111	0.85	4 (3%)
49	PLX	e	201	-	51,51,51	1.14	4 (7%)	55,59,59	0.60	1 (1%)
45	SF4	B	302	2	0,12,12	-	-	-		
45	SF4	M	802	12	0,12,12	-	-	-		
48	PEE	B	303	-	50,50,50	1.16	6 (12%)	53,55,55	0.98	2 (3%)
50	8Q1	X	201	-	31,34,34	1.71	6 (19%)	40,43,43	1.60	6 (15%)
57	ADP	w	401	-	27,29,29	2.96	8 (29%)	42,45,45	1.99	9 (21%)
55	CDL	u	201	-	77,77,99	1.20	9 (11%)	83,89,111	0.95	4 (4%)
48	PEE	b	201	-	45,45,50	1.22	6 (13%)	48,50,55	0.98	2 (4%)
55	CDL	i	401	-	65,65,99	1.28	8 (12%)	71,77,111	0.97	4 (5%)
49	PLX	j	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.59	1 (1%)
48	PEE	j	201	-	50,50,50	1.16	6 (12%)	53,55,55	0.95	2 (3%)
51	NDP	J	401	-	49,52,52	4.40	23 (46%)	66,80,80	2.24	14 (21%)
52	FES	M	803	12	0,4,4	-	-	-		
46	FMN	A	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.21	8 (16%)
49	PLX	r	502	-	51,51,51	1.14	4 (7%)	55,59,59	0.62	1 (1%)
55	CDL	r	503	-	99,99,99	1.09	8 (8%)	105,111,111	0.85	4 (3%)
55	CDL	a	201	-	90,90,99	1.14	8 (8%)	96,102,111	0.92	4 (4%)
45	SF4	C	301	16,3	0,12,12	-	-	-		
49	PLX	a	202	-	51,51,51	1.14	4 (7%)	55,59,59	0.60	1 (1%)
49	PLX	C	303	-	51,51,51	1.15	4 (7%)	55,59,59	0.59	1 (1%)
45	SF4	M	801	12	0,12,12	-	-	-		
45	SF4	B	301	2	0,12,12	-	-	-		
48	PEE	l	703	-	45,45,50	1.23	6 (13%)	48,50,55	0.99	2 (4%)
45	SF4	A	501	1	0,12,12	-	-	-		

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
50	8Q1	G	201	6	-	18/41/41/41	-
48	PEE	s	401	-	-	16/44/44/54	-
52	FES	O	301	14	-	-	0/1/1/1
48	PEE	r	501	-	-	23/54/54/54	-
56	UQ	s	402	-	-	8/21/45/87	0/1/1/1
49	PLX	g	201	-	-	28/55/55/55	-
48	PEE	C	302	-	-	24/50/50/54	-
48	PEE	Q	501	-	-	25/50/50/54	-
47	NAI	A	503	-	-	7/29/72/72	0/5/5/5
55	CDL	l	701	-	-	50/109/109/110	-
55	CDL	l	702	-	-	58/110/110/110	-
49	PLX	e	201	-	-	33/55/55/55	-
45	SF4	B	302	2	-	-	0/6/5/5
45	SF4	M	802	12	-	-	0/6/5/5
48	PEE	B	303	-	-	22/54/54/54	-
50	8Q1	X	201	-	-	20/41/41/41	-
57	ADP	w	401	-	-	3/16/32/32	0/3/3/3
55	CDL	u	201	-	-	41/88/88/110	-
48	PEE	b	201	-	-	22/49/49/54	-
55	CDL	i	401	-	-	35/76/76/110	-
49	PLX	j	202	-	-	32/55/55/55	-
48	PEE	j	201	-	-	21/54/54/54	-
51	NDP	J	401	-	-	7/34/77/77	0/4/5/5
55	CDL	r	503	-	-	71/110/110/110	-
46	FMN	A	502	-	-	8/18/18/18	0/3/3/3
49	PLX	r	502	-	-	21/55/55/55	-
52	FES	M	803	12	-	-	0/1/1/1
55	CDL	a	201	-	-	49/101/101/110	-
45	SF4	C	301	16,3	-	-	0/6/5/5
49	PLX	a	202	-	-	31/55/55/55	-
49	PLX	C	303	-	-	24/55/55/55	-
45	SF4	M	801	12	-	-	0/6/5/5
45	SF4	B	301	2	-	-	0/6/5/5
48	PEE	l	703	-	-	21/49/49/54	-
45	SF4	A	501	1	-	-	0/6/5/5

All (192) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	J	401	NDP	C3B-C2B	-12.77	1.24	1.52
51	J	401	NDP	C6N-C5N	12.54	1.55	1.33
51	J	401	NDP	O4D-C4D	10.71	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.25	1.26	1.53
51	J	401	NDP	C3D-C4D	-9.84	1.27	1.53
56	s	402	UQ	C13-C14	9.24	1.55	1.33
47	A	503	NAI	O4B-C1B	9.15	1.63	1.42
56	s	402	UQ	C8-C9	8.94	1.54	1.33
57	w	401	ADP	C3'-C4'	-8.85	1.30	1.53
47	A	503	NAI	O4B-C4B	-8.29	1.26	1.45
56	s	402	UQ	C18-C19	8.23	1.56	1.32
51	J	401	NDP	O4B-C4B	-7.97	1.27	1.45
57	w	401	ADP	O4'-C4'	7.74	1.62	1.45
47	A	503	NAI	C2D-C1D	-7.58	1.29	1.53
51	J	401	NDP	C2N-C3N	7.35	1.55	1.34
47	A	503	NAI	C2B-C1B	-7.23	1.30	1.53
47	A	503	NAI	O4D-C4D	7.03	1.60	1.45
51	J	401	NDP	C6A-N6A	5.96	1.49	1.34
47	A	503	NAI	C2D-C3D	5.92	1.69	1.53
51	J	401	NDP	P2B-O2B	5.77	1.70	1.59
47	A	503	NAI	C7N-N7N	5.74	1.48	1.33
57	w	401	ADP	C6-N6	5.53	1.48	1.34
47	A	503	NAI	O4D-C1D	5.50	1.55	1.42
50	X	201	8Q1	C34-N36	5.49	1.45	1.33
51	J	401	NDP	C3B-C4B	5.48	1.67	1.53
50	G	201	8Q1	C34-N36	5.43	1.45	1.33
50	X	201	8Q1	C39-N41	5.42	1.45	1.33
50	G	201	8Q1	C39-N41	5.29	1.45	1.33
47	A	503	NAI	C6A-N6A	5.22	1.47	1.34
47	A	503	NAI	C4N-C3N	-5.06	1.40	1.49
51	J	401	NDP	O4D-C1D	-4.88	1.30	1.42
51	J	401	NDP	C6N-N1N	4.78	1.49	1.37
47	A	503	NAI	O2B-C2B	4.54	1.53	1.43
51	J	401	NDP	C1B-N9A	-4.47	1.33	1.46
51	J	401	NDP	O4B-C1B	4.46	1.52	1.42
57	w	401	ADP	O4'-C1'	-4.40	1.31	1.42
51	J	401	NDP	C7N-N7N	4.20	1.44	1.33
51	J	401	NDP	O2D-C2D	-4.15	1.33	1.43
47	A	503	NAI	C6N-C5N	3.94	1.40	1.33
46	A	502	FMN	C4A-N5	3.86	1.38	1.30
48	C	302	PEE	C18-C19	3.75	1.53	1.31
48	s	401	PEE	C18-C19	3.74	1.53	1.31
48	B	303	PEE	C18-C19	3.74	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	l	703	PEE	C18-C19	3.74	1.53	1.31
48	r	501	PEE	C18-C19	3.73	1.53	1.31
48	Q	501	PEE	C18-C19	3.72	1.53	1.31
48	j	201	PEE	C18-C19	3.71	1.53	1.31
48	b	201	PEE	C18-C19	3.71	1.53	1.31
48	b	201	PEE	C39-C38	3.65	1.52	1.31
48	C	302	PEE	C39-C38	3.65	1.52	1.31
48	r	501	PEE	C39-C38	3.65	1.52	1.31
48	j	201	PEE	C39-C38	3.65	1.52	1.31
48	l	703	PEE	C39-C38	3.64	1.52	1.31
48	Q	501	PEE	C39-C38	3.64	1.52	1.31
48	B	303	PEE	C39-C38	3.64	1.52	1.31
47	A	503	NAI	C7N-C3N	3.62	1.56	1.48
55	i	401	CDL	OA8-CA7	3.47	1.43	1.33
55	u	201	CDL	OA8-CA7	3.46	1.43	1.33
55	l	702	CDL	OA8-CA7	3.45	1.43	1.33
55	a	201	CDL	OA8-CA7	3.43	1.43	1.33
55	r	503	CDL	OA8-CA7	3.40	1.43	1.33
55	l	701	CDL	OA8-CA7	3.37	1.43	1.33
57	w	401	ADP	O2'-C2'	-3.34	1.35	1.43
47	A	503	NAI	C4N-C5N	-3.31	1.40	1.48
57	w	401	ADP	C8-N9	-3.13	1.31	1.37
55	r	503	CDL	OB6-CB5	3.11	1.43	1.34
51	J	401	NDP	O3D-C3D	3.10	1.50	1.43
57	w	401	ADP	O3'-C3'	3.10	1.50	1.43
55	l	701	CDL	OB6-CB5	3.05	1.42	1.34
55	i	401	CDL	OB8-CB7	3.05	1.42	1.33
55	i	401	CDL	OB6-CB5	3.05	1.42	1.34
55	a	201	CDL	OB6-CB5	3.04	1.42	1.34
55	l	702	CDL	OB6-CB5	3.04	1.42	1.34
51	J	401	NDP	C8A-N9A	-3.04	1.32	1.37
51	J	401	NDP	C7N-C3N	3.02	1.55	1.48
55	u	201	CDL	OB6-CB5	3.01	1.42	1.34
55	u	201	CDL	OB8-CB7	3.01	1.42	1.33
55	l	702	CDL	OB8-CB7	3.00	1.42	1.33
55	a	201	CDL	OB8-CB7	3.00	1.42	1.33
55	r	503	CDL	OB8-CB7	3.00	1.42	1.33
55	a	201	CDL	OA6-CA5	2.99	1.42	1.34
55	l	702	CDL	OA6-CA5	2.97	1.42	1.34
51	J	401	NDP	C5A-N7A	-2.96	1.33	1.39
55	i	401	CDL	OA6-CA5	2.95	1.42	1.34
55	l	701	CDL	OB8-CB7	2.94	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	u	201	CDL	OA6-CA5	2.94	1.42	1.34
55	r	503	CDL	OA6-CA5	2.92	1.42	1.34
55	l	701	CDL	OA6-CA5	2.91	1.42	1.34
49	C	303	PLX	O6-C4	-2.77	1.40	1.44
49	g	201	PLX	O6-C4	-2.73	1.41	1.44
49	e	201	PLX	O6-C4	-2.72	1.41	1.44
56	s	402	UQ	C6-C1	2.66	1.54	1.46
49	a	202	PLX	O6-C4	-2.62	1.41	1.44
49	j	202	PLX	O6-C4	-2.56	1.41	1.44
48	C	302	PEE	O3-C30	2.51	1.40	1.33
48	Q	501	PEE	O3-C30	2.49	1.40	1.33
47	A	503	NAI	C8A-N9A	-2.48	1.33	1.37
46	A	502	FMN	C10-N1	2.48	1.38	1.33
48	b	201	PEE	O3-C30	2.48	1.40	1.33
48	j	201	PEE	O3-C30	2.47	1.40	1.33
47	A	503	NAI	PN-O5D	2.47	1.69	1.59
47	A	503	NAI	O3B-C3B	-2.46	1.37	1.43
55	r	503	CDL	OA6-CA4	-2.45	1.40	1.46
55	l	701	CDL	OA6-CA4	-2.45	1.40	1.46
48	r	501	PEE	O3-C30	2.44	1.40	1.33
48	B	303	PEE	O3-C30	2.43	1.40	1.33
51	J	401	NDP	O2B-C2B	2.43	1.52	1.44
48	j	201	PEE	O2-C2	-2.43	1.40	1.46
49	r	502	PLX	C7-C6	2.43	1.55	1.50
55	a	201	CDL	OA6-CA4	-2.43	1.40	1.46
48	l	703	PEE	O3-C30	2.42	1.40	1.33
48	Q	501	PEE	O2-C2	-2.42	1.40	1.46
55	u	201	CDL	OA6-CA4	-2.41	1.40	1.46
50	X	201	8Q1	C1-S44	2.41	1.82	1.76
48	s	401	PEE	O3-C30	2.41	1.40	1.33
55	i	401	CDL	OA6-CA4	-2.40	1.40	1.46
48	r	501	PEE	O2-C2	-2.40	1.40	1.46
48	B	303	PEE	O2-C2	-2.39	1.40	1.46
51	J	401	NDP	C2D-C3D	2.39	1.59	1.53
50	G	201	8Q1	C6-C1	2.38	1.53	1.50
48	l	703	PEE	O2-C2	-2.38	1.40	1.46
49	j	202	PLX	C7-C6	2.38	1.55	1.50
48	C	302	PEE	O2-C10	2.38	1.41	1.34
48	l	703	PEE	O2-C10	2.37	1.41	1.34
50	G	201	8Q1	C1-S44	2.37	1.81	1.76
48	C	302	PEE	O2-C2	-2.36	1.40	1.46
49	C	303	PLX	C7-C6	2.35	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	s	401	PEE	O2-C10	2.35	1.40	1.34
48	b	201	PEE	O2-C2	-2.35	1.40	1.46
49	e	201	PLX	C7-C6	2.34	1.55	1.50
55	l	702	CDL	OA6-CA4	-2.33	1.40	1.46
49	a	202	PLX	C7-C6	2.32	1.55	1.50
48	b	201	PEE	O2-C10	2.32	1.40	1.34
57	w	401	ADP	C5-N7	-2.28	1.34	1.39
48	s	401	PEE	O2-C2	-2.28	1.40	1.46
47	A	503	NAI	C5B-C4B	2.28	1.58	1.51
49	g	201	PLX	C7-C6	2.27	1.55	1.50
48	r	501	PEE	O2-C10	2.26	1.40	1.34
48	j	201	PEE	O2-C10	2.26	1.40	1.34
48	Q	501	PEE	O2-C10	2.25	1.40	1.34
48	B	303	PEE	O2-C10	2.25	1.40	1.34
50	X	201	8Q1	O35-C34	-2.25	1.18	1.23
50	G	201	8Q1	O35-C34	-2.24	1.18	1.23
55	i	401	CDL	OB6-CB4	-2.22	1.41	1.46
50	G	201	8Q1	O40-C39	-2.21	1.18	1.23
55	a	201	CDL	PB2-OB2	2.21	1.68	1.59
55	l	702	CDL	PB2-OB2	2.20	1.68	1.59
55	r	503	CDL	PB2-OB5	2.20	1.68	1.59
55	l	701	CDL	PB2-OB5	2.20	1.68	1.59
55	i	401	CDL	PB2-OB2	2.20	1.68	1.59
55	r	503	CDL	PB2-OB2	2.19	1.68	1.59
55	u	201	CDL	PB2-OB5	2.19	1.68	1.59
55	l	702	CDL	PB2-OB5	2.18	1.68	1.59
49	r	502	PLX	O6-C4	-2.18	1.41	1.44
50	X	201	8Q1	O40-C39	-2.18	1.18	1.23
50	X	201	8Q1	C6-C1	2.17	1.53	1.50
56	s	402	UQ	O4-C4	-2.17	1.18	1.23
55	u	201	CDL	PB2-OB2	2.17	1.68	1.59
55	a	201	CDL	PB2-OB5	2.17	1.68	1.59
55	l	701	CDL	PB2-OB2	2.16	1.68	1.59
55	a	201	CDL	OB6-CB4	-2.16	1.41	1.46
55	u	201	CDL	OB6-CB4	-2.16	1.41	1.46
56	s	402	UQ	C7-C8	2.16	1.53	1.50
49	a	202	PLX	P1-O4	2.15	1.68	1.59
49	j	202	PLX	P1-O4	2.15	1.68	1.59
55	i	401	CDL	PB2-OB5	2.15	1.68	1.59
49	g	201	PLX	P1-O4	2.14	1.68	1.59
49	r	502	PLX	P1-O4	2.14	1.68	1.59
48	r	501	PEE	O3-C3	-2.13	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	l	702	CDL	OB6-CB4	-2.13	1.41	1.46
48	B	303	PEE	O3-C3	-2.13	1.40	1.45
49	C	303	PLX	P1-O4	2.13	1.67	1.59
55	l	701	CDL	OB6-CB4	-2.12	1.41	1.46
48	l	703	PEE	O3-C3	-2.12	1.40	1.45
51	J	401	NDP	O7N-C7N	-2.11	1.19	1.24
56	s	402	UQ	O1-C1	-2.11	1.18	1.23
51	J	401	NDP	PA-O5B	2.09	1.67	1.59
48	b	201	PEE	O3-C3	-2.09	1.40	1.45
49	e	201	PLX	P1-O4	2.08	1.67	1.59
48	j	201	PEE	O3-C3	-2.08	1.40	1.45
48	s	401	PEE	O3-C3	-2.07	1.40	1.45
49	j	202	PLX	P1-O1	2.07	1.67	1.59
48	C	302	PEE	O3-C3	-2.07	1.40	1.45
48	Q	501	PEE	O3-C3	-2.07	1.40	1.45
49	a	202	PLX	P1-O1	2.05	1.67	1.59
49	r	502	PLX	P1-O1	2.04	1.67	1.59
55	r	503	CDL	OB6-CB4	-2.03	1.41	1.46
49	e	201	PLX	P1-O1	2.03	1.67	1.59
49	C	303	PLX	P1-O1	2.02	1.67	1.59
47	A	503	NAI	C2N-C3N	2.02	1.40	1.34
55	u	201	CDL	C11-CA5	2.01	1.56	1.50
55	l	702	CDL	C11-CA5	2.01	1.56	1.50

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	s	402	UQ	C7-C8-C9	-9.19	111.50	126.79
51	J	401	NDP	C3N-C2N-N1N	-9.10	110.12	123.10
51	J	401	NDP	C1D-N1N-C2N	-6.61	110.11	121.11
50	X	201	8Q1	C6-C1-S44	6.17	120.64	113.46
56	s	402	UQ	C12-C13-C14	-5.94	113.36	127.66
51	J	401	NDP	C5A-C4A-N3A	-5.89	119.07	126.75
47	A	503	NAI	C5A-C4A-N3A	-5.77	119.22	126.75
57	w	401	ADP	C5-C4-N3	-5.75	119.25	126.75
50	G	201	8Q1	C6-C1-S44	5.71	120.11	113.46
51	J	401	NDP	C1D-N1N-C6N	-5.08	109.89	120.83
56	s	402	UQ	C11-C9-C8	-4.72	111.56	121.12
57	w	401	ADP	N3-C2-N1	-4.43	121.68	128.60
56	s	402	UQ	C10-C9-C8	-4.41	112.36	123.68
57	w	401	ADP	N3-C4-N9	4.41	134.34	127.08
56	s	402	UQ	C15-C14-C13	-4.31	112.61	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	s	402	UQ	C16-C14-C13	-4.31	112.39	121.12
47	A	503	NAI	N3A-C2A-N1A	-4.29	121.89	128.60
56	s	402	UQ	C17-C18-C19	-4.18	113.47	127.75
51	J	401	NDP	N3A-C4A-N9A	4.16	133.94	127.08
55	a	201	CDL	OA6-CA5-C11	4.16	120.47	111.50
55	l	701	CDL	OA6-CA5-C11	4.11	120.37	111.50
55	a	201	CDL	OB6-CB5-C51	4.10	120.35	111.50
48	B	303	PEE	O2-C10-C11	4.09	120.31	111.50
48	s	401	PEE	O2-C10-C11	4.08	120.30	111.50
55	r	503	CDL	OB6-CB5-C51	4.03	120.20	111.50
55	l	702	CDL	OA6-CA5-C11	4.03	120.18	111.50
47	A	503	NAI	N3A-C4A-N9A	4.02	133.70	127.08
48	r	501	PEE	O2-C10-C11	4.00	120.13	111.50
55	u	201	CDL	OB6-CB5-C51	3.99	120.10	111.50
48	Q	501	PEE	O2-C10-C11	3.97	120.06	111.50
51	J	401	NDP	N3A-C2A-N1A	-3.96	122.40	128.60
55	l	701	CDL	OB6-CB5-C51	3.93	119.98	111.50
48	l	703	PEE	O2-C10-C11	3.91	119.94	111.50
48	b	201	PEE	O2-C10-C11	3.91	119.92	111.50
55	l	702	CDL	OB6-CB5-C51	3.90	119.90	111.50
55	u	201	CDL	OA6-CA5-C11	3.89	119.89	111.50
55	r	503	CDL	OA6-CA5-C11	3.86	119.82	111.50
47	A	503	NAI	C2A-N3A-C4A	3.84	120.82	111.75
55	i	401	CDL	OA6-CA5-C11	3.81	119.71	111.50
48	j	201	PEE	O2-C10-C11	3.80	119.69	111.50
48	C	302	PEE	O2-C10-C11	3.73	119.53	111.50
51	J	401	NDP	C2A-N3A-C4A	3.72	120.55	111.75
57	w	401	ADP	C2-N3-C4	3.71	120.51	111.75
47	A	503	NAI	C5A-N7A-C8A	3.67	108.72	103.51
55	i	401	CDL	OB6-CB5-C51	3.58	119.22	111.50
57	w	401	ADP	N9-C8-N7	-3.57	109.03	113.91
50	X	201	8Q1	O4-C1-C6	-3.56	119.78	123.99
56	s	402	UQ	C21-C19-C18	-3.42	112.75	122.65
47	A	503	NAI	N9A-C8A-N7A	-3.41	109.25	113.91
57	w	401	ADP	C5-N7-C8	3.40	108.34	103.51
50	X	201	8Q1	C37-C38-C39	3.32	117.88	112.36
51	J	401	NDP	C5A-N7A-C8A	3.24	108.11	103.51
47	A	503	NAI	C4A-C5A-N7A	-3.22	106.70	110.62
50	G	201	8Q1	O4-C1-C6	-3.15	120.27	123.99
47	A	503	NAI	C3D-C2D-C1D	3.13	107.37	101.43
51	J	401	NDP	N9A-C8A-N7A	-3.13	109.64	113.91
56	s	402	UQ	C20-C19-C18	-3.09	113.71	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	A	502	FMN	C4-N3-C2	-3.04	120.03	125.64
57	w	401	ADP	C4-N9-C8	3.01	108.99	105.73
56	s	402	UQ	CM5-C5-C6	-2.94	119.60	124.40
51	J	401	NDP	C4A-C5A-N7A	-2.93	107.05	110.62
50	G	201	8Q1	C37-C38-C39	2.80	117.01	112.36
47	A	503	NAI	C4D-O4D-C1D	-2.79	103.32	109.47
57	w	401	ADP	C4-C5-N7	-2.78	107.23	110.62
47	A	503	NAI	C2D-C3D-C4D	2.75	107.98	102.64
48	l	703	PEE	O3-C30-C31	2.71	120.42	111.91
55	i	401	CDL	OA8-CA7-C31	2.69	120.35	111.91
48	B	303	PEE	O3-C30-C31	2.68	120.32	111.91
55	a	201	CDL	OB8-CB7-C71	2.68	120.32	111.91
46	A	502	FMN	C4A-C4-N3	2.66	119.94	113.19
55	l	701	CDL	OB8-CB7-C71	2.65	120.22	111.91
51	J	401	NDP	C2B-C3B-C4B	2.65	107.75	101.99
55	i	401	CDL	OB8-CB7-C71	2.65	120.21	111.91
57	w	401	ADP	PA-O3A-PB	-2.64	123.77	132.83
55	u	201	CDL	OB8-CB7-C71	2.63	120.17	111.91
48	Q	501	PEE	O3-C30-C31	2.63	120.16	111.91
48	j	201	PEE	O3-C30-C31	2.61	120.11	111.91
55	l	702	CDL	OB8-CB7-C71	2.60	120.05	111.91
48	r	501	PEE	O3-C30-C31	2.59	120.05	111.91
51	J	401	NDP	PN-O3-PA	-2.59	123.93	132.83
48	s	401	PEE	O3-C30-C31	2.59	120.02	111.91
55	u	201	CDL	OA8-CA7-C31	2.57	119.97	111.91
55	l	702	CDL	OA8-CA7-C31	2.56	119.94	111.91
55	a	201	CDL	OA8-CA7-C31	2.54	119.89	111.91
48	C	302	PEE	O3-C30-C31	2.53	119.86	111.91
49	e	201	PLX	C1A-N1-C1	2.53	120.28	109.92
48	b	201	PEE	O3-C30-C31	2.52	119.81	111.91
47	A	503	NAI	PN-O3-PA	-2.51	124.23	132.83
55	l	701	CDL	OA8-CA7-C31	2.50	119.77	111.91
55	r	503	CDL	OB8-CB7-C71	2.47	119.66	111.91
46	A	502	FMN	O4-C4-C4A	-2.46	120.07	126.60
55	r	503	CDL	OA8-CA7-C31	2.46	119.62	111.91
46	A	502	FMN	C4A-C10-N10	2.44	120.05	116.48
49	g	201	PLX	C1A-N1-C1	2.44	119.91	109.92
50	G	201	8Q1	C38-C39-N41	2.38	120.44	116.42
49	r	502	PLX	C1A-N1-C1	2.37	119.61	109.92
49	j	202	PLX	C1A-N1-C1	2.35	119.52	109.92
50	X	201	8Q1	O4-C1-S44	-2.34	119.57	122.61
47	A	503	NAI	C4A-N9A-C8A	2.33	108.25	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	G	201	8Q1	O4-C1-S44	-2.30	119.62	122.61
51	J	401	NDP	C4A-N9A-C8A	2.30	108.22	105.73
49	C	303	PLX	C1A-N1-C1	2.29	119.27	109.92
49	a	202	PLX	C1A-N1-C1	2.26	119.14	109.92
46	A	502	FMN	C9A-C5A-N5	-2.25	119.99	122.43
46	A	502	FMN	C10-C4A-N5	-2.22	120.15	124.86
50	X	201	8Q1	C38-C39-N41	2.19	120.12	116.42
46	A	502	FMN	C4A-C10-N1	-2.18	119.66	124.73
50	G	201	8Q1	C43-S44-C1	2.16	108.60	101.87
50	X	201	8Q1	C43-S44-C1	2.15	108.56	101.87
46	A	502	FMN	C5A-C9A-N10	2.11	120.13	117.95
51	J	401	NDP	C2B-C1B-N9A	-2.10	110.00	113.53

There are no chirality outliers.

All (718) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C1'-C2'-C3'-O3'
46	A	502	FMN	C3'-C4'-C5'-O5'
47	A	503	NAI	C5D-O5D-PN-O3
48	C	302	PEE	C1-O3P-P-O1P
48	C	302	PEE	O4P-C4-C5-N
48	Q	501	PEE	C11-C10-O2-C2
48	b	201	PEE	C1-O3P-P-O1P
48	b	201	PEE	C37-C38-C39-C40
48	l	703	PEE	C11-C10-O2-C2
48	l	703	PEE	O3P-C1-C2-O2
48	l	703	PEE	C4-O4P-P-O2P
48	r	501	PEE	C17-C18-C19-C20
48	r	501	PEE	O3P-C1-C2-O2
48	s	401	PEE	C11-C10-O2-C2
49	C	303	PLX	C3-O4-P1-O3
49	C	303	PLX	N1-C1-C2-O1
49	a	202	PLX	O7-C6-C7-C8
49	a	202	PLX	O7-C6-O6-C4
49	a	202	PLX	O4-C3-C4-O6
49	a	202	PLX	C3-O4-P1-O1
49	a	202	PLX	C3-O4-P1-O2
49	a	202	PLX	C2-O1-P1-O2
49	a	202	PLX	C2-O1-P1-O3

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Mol	Chain	Res	Type	Atoms
49	a	202	PLX	C25-C24-O8-C5
49	e	201	PLX	C3-O4-P1-O1
49	e	201	PLX	C3-O4-P1-O2
49	e	201	PLX	C3-O4-P1-O3
49	e	201	PLX	O9-C24-O8-C5
49	e	201	PLX	O9-C24-C25-C26
49	g	201	PLX	O7-C6-C7-C8
49	g	201	PLX	O7-C6-O6-C4
49	g	201	PLX	O9-C24-C25-C26
49	j	202	PLX	O7-C6-C7-C8
49	j	202	PLX	C3-O4-P1-O3
49	r	502	PLX	O7-C6-O6-C4
49	r	502	PLX	C5-C4-O6-C6
49	r	502	PLX	O9-C24-C25-C26
50	G	201	8Q1	O27-C28-C29-C31
50	G	201	8Q1	O27-C28-C29-C32
50	G	201	8Q1	N36-C37-C38-C39
50	G	201	8Q1	N41-C42-C43-S44
50	G	201	8Q1	C42-C43-S44-C1
50	G	201	8Q1	C28-O27-P24-O1
50	X	201	8Q1	O4-C1-S44-C43
50	X	201	8Q1	C6-C1-S44-C43
50	X	201	8Q1	C28-C29-C32-C34
50	X	201	8Q1	C28-C29-C32-O33
50	X	201	8Q1	C30-C29-C32-C34
50	X	201	8Q1	C30-C29-C32-O33
50	X	201	8Q1	N36-C37-C38-C39
50	X	201	8Q1	C42-C43-S44-C1
50	X	201	8Q1	C28-O27-P24-O2
50	X	201	8Q1	C28-O27-P24-O1
51	J	401	NDP	C5B-O5B-PA-O1A
51	J	401	NDP	C2B-O2B-P2B-O1X
55	a	201	CDL	CA3-OA5-PA1-OA4
55	a	201	CDL	CB2-OB2-PB2-OB3
55	a	201	CDL	CB3-OB5-PB2-OB3
55	i	401	CDL	CA3-OA5-PA1-OA4
55	i	401	CDL	CB3-OB5-PB2-OB3
55	i	401	CDL	CB3-OB5-PB2-OB4
55	l	701	CDL	O1-C1-CA2-OA2
55	l	701	CDL	O1-C1-CB2-OB2
55	l	701	CDL	CA2-C1-CB2-OB2
55	l	701	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
55	l	702	CDL	O1-C1-CA2-OA2
55	l	702	CDL	CA2-C1-CB2-OB2
55	l	702	CDL	CA2-OA2-PA1-OA3
55	l	702	CDL	CA3-OA5-PA1-OA2
55	l	702	CDL	CB2-OB2-PB2-OB4
55	l	702	CDL	CB2-OB2-PB2-OB5
55	l	702	CDL	OB6-CB4-CB6-OB8
55	r	503	CDL	CA2-OA2-PA1-OA3
55	r	503	CDL	CA2-OA2-PA1-OA4
55	r	503	CDL	CA3-OA5-PA1-OA2
55	r	503	CDL	CA3-OA5-PA1-OA3
55	r	503	CDL	CA3-OA5-PA1-OA4
55	u	201	CDL	CB2-C1-CA2-OA2
55	u	201	CDL	CA3-OA5-PA1-OA3
55	u	201	CDL	CA3-OA5-PA1-OA4
56	s	402	UQ	C7-C8-C9-C10
56	s	402	UQ	C7-C8-C9-C11
56	s	402	UQ	C12-C11-C9-C10
57	w	401	ADP	C5'-O5'-PA-O1A
57	w	401	ADP	C5'-O5'-PA-O2A
57	w	401	ADP	C5'-O5'-PA-O3A
56	s	402	UQ	C17-C18-C19-C21
48	s	401	PEE	O5-C30-O3-C3
55	i	401	CDL	OA9-CA7-OA8-CA6
55	l	701	CDL	OA9-CA7-OA8-CA6
48	C	302	PEE	O4-C10-O2-C2
48	Q	501	PEE	O4-C10-O2-C2
48	l	703	PEE	O4-C10-O2-C2
48	s	401	PEE	O4-C10-O2-C2
55	l	702	CDL	C71-CB7-OB8-CB6
48	C	302	PEE	C11-C10-O2-C2
48	l	703	PEE	O5-C30-O3-C3
49	r	502	PLX	C9-C10-C11-C12
48	b	201	PEE	C31-C30-O3-C3
48	l	703	PEE	C31-C30-O3-C3
48	s	401	PEE	C31-C30-O3-C3
55	i	401	CDL	C31-CA7-OA8-CA6
55	l	701	CDL	C31-CA7-OA8-CA6
48	B	303	PEE	C37-C38-C39-C40
48	j	201	PEE	C17-C18-C19-C20
56	s	402	UQ	C12-C13-C14-C15
55	l	701	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
55	r	503	CDL	OB9-CB7-OB8-CB6
49	a	202	PLX	C10-C11-C12-C13
55	a	201	CDL	O1-C1-CB2-OB2
55	l	702	CDL	O1-C1-CB2-OB2
55	r	503	CDL	O1-C1-CA2-OA2
55	l	702	CDL	OB9-CB7-OB8-CB6
49	g	201	PLX	C7-C8-C9-C10
55	i	401	CDL	C31-C32-C33-C34
55	l	702	CDL	C11-C12-C13-C14
49	j	202	PLX	C28-C29-C30-C31
55	l	702	CDL	C59-C60-C61-C62
55	l	701	CDL	C55-C56-C57-C58
47	A	503	NAI	C3D-C4D-C5D-O5D
51	J	401	NDP	O4B-C4B-C5B-O5B
55	r	503	CDL	C71-CB7-OB8-CB6
48	b	201	PEE	O5-C30-O3-C3
49	g	201	PLX	C12-C13-C14-C15
55	u	201	CDL	C71-C72-C73-C74
48	j	201	PEE	C31-C30-O3-C3
55	l	702	CDL	C75-C76-C77-C78
48	r	501	PEE	C11-C10-O2-C2
55	a	201	CDL	CB2-C1-CA2-OA2
55	a	201	CDL	CA2-C1-CB2-OB2
55	r	503	CDL	CB2-C1-CA2-OA2
55	u	201	CDL	CA2-C1-CB2-OB2
55	l	701	CDL	C71-CB7-OB8-CB6
49	j	202	PLX	C32-C33-C34-C35
55	l	702	CDL	CB7-C71-C72-C73
55	l	702	CDL	C35-C36-C37-C38
55	u	201	CDL	C75-C76-C77-C78
55	i	401	CDL	C14-C15-C16-C17
55	u	201	CDL	O1-C1-CA2-OA2
55	u	201	CDL	O1-C1-CB2-OB2
55	r	503	CDL	C51-CB5-OB6-CB4
49	a	202	PLX	C11-C10-C9-C8
51	J	401	NDP	C2D-C1D-N1N-C6N
48	r	501	PEE	C10-C11-C12-C13
55	a	201	CDL	CA7-C31-C32-C33
55	r	503	CDL	CB5-C51-C52-C53
49	C	303	PLX	C28-C29-C30-C31
55	l	702	CDL	C39-C40-C41-C42
48	C	302	PEE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
55	i	401	CDL	CB5-C51-C52-C53
55	l	701	CDL	CB5-C51-C52-C53
55	l	702	CDL	CB5-C51-C52-C53
55	r	503	CDL	CB7-C71-C72-C73
47	A	503	NAI	O4D-C4D-C5D-O5D
49	e	201	PLX	C2-C1-N1-C1A
55	a	201	CDL	CB7-C71-C72-C73
55	l	701	CDL	OB9-CB7-OB8-CB6
55	i	401	CDL	O1-C1-CA2-OA2
48	r	501	PEE	O4-C10-O2-C2
55	r	503	CDL	OB7-CB5-OB6-CB4
55	r	503	CDL	C74-C75-C76-C77
48	j	201	PEE	O5-C30-O3-C3
49	r	502	PLX	C30-C31-C32-C33
48	b	201	PEE	C17-C18-C19-C20
48	j	201	PEE	C11-C10-O2-C2
48	l	703	PEE	C4-O4P-P-O3P
49	C	303	PLX	C3-O4-P1-O1
49	a	202	PLX	C2-O1-P1-O4
49	e	201	PLX	C2-O1-P1-O4
49	j	202	PLX	C3-O4-P1-O1
55	a	201	CDL	CA2-OA2-PA1-OA5
55	a	201	CDL	CA3-OA5-PA1-OA2
55	a	201	CDL	CB3-OB5-PB2-OB2
55	i	401	CDL	CA3-OA5-PA1-OA2
55	i	401	CDL	CB3-OB5-PB2-OB2
55	l	701	CDL	CA2-OA2-PA1-OA5
55	l	702	CDL	CA2-OA2-PA1-OA5
55	l	702	CDL	CB3-OB5-PB2-OB2
55	r	503	CDL	CA2-OA2-PA1-OA5
55	r	503	CDL	CB2-OB2-PB2-OB5
55	r	503	CDL	CB3-OB5-PB2-OB2
55	u	201	CDL	CA3-OA5-PA1-OA2
55	r	503	CDL	CA7-C31-C32-C33
55	i	401	CDL	CB2-C1-CA2-OA2
55	l	702	CDL	CB2-C1-CA2-OA2
48	j	201	PEE	O4-C10-O2-C2
49	r	502	PLX	C11-C12-C13-C14
49	a	202	PLX	O6-C6-C7-C8
49	e	201	PLX	O8-C24-C25-C26
48	s	401	PEE	C13-C14-C15-C16
49	j	202	PLX	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
55	u	201	CDL	C14-C15-C16-C17
48	b	201	PEE	C12-C13-C14-C15
49	a	202	PLX	C33-C34-C35-C36
49	a	202	PLX	C34-C35-C36-C37
55	l	702	CDL	C72-C73-C74-C75
50	G	201	8Q1	O27-C28-C29-C30
48	b	201	PEE	C33-C34-C35-C36
48	j	201	PEE	C21-C22-C23-C24
48	r	501	PEE	C13-C14-C15-C16
49	C	303	PLX	C33-C34-C35-C36
49	r	502	PLX	C12-C13-C14-C15
55	l	702	CDL	C56-C57-C58-C59
55	r	503	CDL	C17-C18-C19-C20
55	r	503	CDL	C35-C36-C37-C38
48	Q	501	PEE	C10-C11-C12-C13
48	l	703	PEE	C30-C31-C32-C33
55	a	201	CDL	C13-C14-C15-C16
55	l	701	CDL	C56-C57-C58-C59
48	C	302	PEE	C37-C38-C39-C40
48	r	501	PEE	C12-C13-C14-C15
49	a	202	PLX	C28-C29-C30-C31
49	r	502	PLX	C15-C16-C17-C18
49	r	502	PLX	C27-C28-C29-C30
55	a	201	CDL	C72-C73-C74-C75
55	l	701	CDL	C81-C82-C83-C84
55	a	201	CDL	O1-C1-CA2-OA2
49	j	202	PLX	C27-C28-C29-C30
55	r	503	CDL	C41-C42-C43-C44
55	r	503	CDL	OA6-CA4-CA6-OA8
55	a	201	CDL	C71-CB7-OB8-CB6
55	i	401	CDL	C71-CB7-OB8-CB6
49	g	201	PLX	C28-C29-C30-C31
49	j	202	PLX	C13-C14-C15-C16
55	l	702	CDL	C37-C38-C39-C40
55	l	702	CDL	C60-C61-C62-C63
55	r	503	CDL	C12-C13-C14-C15
55	r	503	CDL	C62-C63-C64-C65
55	u	201	CDL	C56-C57-C58-C59
49	g	201	PLX	C9-C10-C11-C12
49	r	502	PLX	C28-C29-C30-C31
50	G	201	8Q1	C12-C13-C14-C15
55	a	201	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
55	r	503	CDL	C63-C64-C65-C66
55	u	201	CDL	C57-C58-C59-C60
55	i	401	CDL	CA7-C31-C32-C33
48	C	302	PEE	C43-C44-C45-C46
49	e	201	PLX	C27-C28-C29-C30
49	g	201	PLX	C25-C26-C27-C28
49	g	201	PLX	C27-C28-C29-C30
55	i	401	CDL	C36-C37-C38-C39
55	i	401	CDL	C52-C53-C54-C55
55	r	503	CDL	C73-C74-C75-C76
49	a	202	PLX	C7-C8-C9-C10
50	X	201	8Q1	C7-C8-C9-C10
55	r	503	CDL	C37-C38-C39-C40
48	Q	501	PEE	C21-C22-C23-C24
55	l	701	CDL	C12-C13-C14-C15
55	l	701	CDL	C35-C36-C37-C38
48	B	303	PEE	C23-C24-C25-C26
48	C	302	PEE	C13-C14-C15-C16
48	s	401	PEE	C11-C12-C13-C14
49	a	202	PLX	C31-C32-C33-C34
49	e	201	PLX	C14-C15-C16-C17
49	e	201	PLX	C28-C29-C30-C31
49	e	201	PLX	C33-C34-C35-C36
49	g	201	PLX	C10-C11-C12-C13
55	r	503	CDL	C75-C76-C77-C78
49	e	201	PLX	C2-C1-N1-C1C
48	Q	501	PEE	C22-C23-C24-C25
48	l	703	PEE	C21-C22-C23-C24
49	C	303	PLX	C16-C17-C18-C19
49	j	202	PLX	C25-C26-C27-C28
55	l	702	CDL	C73-C74-C75-C76
48	s	401	PEE	O4P-C4-C5-N
49	j	202	PLX	C7-C8-C9-C10
55	a	201	CDL	C52-C53-C54-C55
49	j	202	PLX	C9-C10-C11-C12
49	e	201	PLX	C11-C12-C13-C14
46	A	502	FMN	O4'-C4'-C5'-O5'
55	r	503	CDL	C34-C35-C36-C37
55	r	503	CDL	C52-C53-C54-C55
55	r	503	CDL	C55-C56-C57-C58
55	u	201	CDL	C54-C55-C56-C57
48	B	303	PEE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
49	a	202	PLX	C12-C13-C14-C15
49	e	201	PLX	C25-C26-C27-C28
55	r	503	CDL	CB3-CB4-CB6-OB8
48	Q	501	PEE	C37-C38-C39-C40
55	l	701	CDL	C20-C21-C22-C23
55	r	503	CDL	C11-C12-C13-C14
48	r	501	PEE	C30-C31-C32-C33
48	C	302	PEE	C32-C33-C34-C35
49	a	202	PLX	C35-C36-C37-C38
49	C	303	PLX	O7-C6-C7-C8
49	e	201	PLX	O7-C6-C7-C8
49	j	202	PLX	O9-C24-C25-C26
49	e	201	PLX	C29-C30-C31-C32
55	r	503	CDL	C43-C44-C45-C46
55	u	201	CDL	CA7-C31-C32-C33
55	l	702	CDL	C55-C56-C57-C58
48	B	303	PEE	C34-C35-C36-C37
49	j	202	PLX	C34-C35-C36-C37
49	j	202	PLX	C19-C20-C21-C22
55	r	503	CDL	C33-C34-C35-C36
55	r	503	CDL	C56-C57-C58-C59
55	l	701	CDL	CB2-C1-CA2-OA2
48	C	302	PEE	C14-C15-C16-C17
55	r	503	CDL	C71-C72-C73-C74
48	B	303	PEE	C14-C15-C16-C17
49	e	201	PLX	C10-C11-C12-C13
49	j	202	PLX	C18-C19-C20-C21
49	r	502	PLX	C14-C15-C16-C17
50	G	201	8Q1	C11-C12-C13-C14
55	l	701	CDL	C75-C76-C77-C78
49	a	202	PLX	C29-C30-C31-C32
49	g	201	PLX	C15-C16-C17-C18
49	g	201	PLX	C14-C15-C16-C17
55	i	401	CDL	C71-C72-C73-C74
48	B	303	PEE	C12-C13-C14-C15
48	l	703	PEE	C22-C23-C24-C25
49	j	202	PLX	C14-C15-C16-C17
48	Q	501	PEE	C31-C30-O3-C3
49	a	202	PLX	C25-C26-C27-C28
55	a	201	CDL	C42-C43-C44-C45
55	l	702	CDL	C54-C55-C56-C57
55	a	201	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
55	i	401	CDL	OB9-CB7-OB8-CB6
49	a	202	PLX	C9-C10-C11-C12
48	b	201	PEE	C21-C22-C23-C24
48	j	201	PEE	C34-C35-C36-C37
49	C	303	PLX	C31-C32-C33-C34
48	Q	501	PEE	C35-C36-C37-C38
48	B	303	PEE	C30-C31-C32-C33
48	r	501	PEE	C31-C32-C33-C34
48	l	703	PEE	C31-C32-C33-C34
55	a	201	CDL	C21-C22-C23-C24
48	s	401	PEE	C33-C34-C35-C36
55	l	701	CDL	C52-C53-C54-C55
48	B	303	PEE	C10-C11-C12-C13
55	i	401	CDL	CB7-C71-C72-C73
49	r	502	PLX	C16-C17-C18-C19
48	r	501	PEE	C41-C42-C43-C44
55	l	702	CDL	C52-C53-C54-C55
48	b	201	PEE	C11-C10-O2-C2
55	l	701	CDL	C11-CA5-OA6-CA4
55	u	201	CDL	C11-CA5-OA6-CA4
55	i	401	CDL	C35-C36-C37-C38
55	u	201	CDL	C60-C61-C62-C63
48	j	201	PEE	C36-C37-C38-C39
48	b	201	PEE	O4-C10-O2-C2
55	l	701	CDL	OA7-CA5-OA6-CA4
55	u	201	CDL	OA7-CA5-OA6-CA4
55	l	702	CDL	C62-C63-C64-C65
55	l	701	CDL	OB6-CB4-CB6-OB8
55	r	503	CDL	OB6-CB4-CB6-OB8
55	r	503	CDL	C15-C16-C17-C18
49	e	201	PLX	C2-C1-N1-C1B
50	X	201	8Q1	C10-C11-C12-C13
48	Q	501	PEE	C19-C20-C21-C22
48	s	401	PEE	C19-C20-C21-C22
55	l	701	CDL	C58-C59-C60-C61
49	C	303	PLX	C13-C14-C15-C16
48	b	201	PEE	C31-C32-C33-C34
55	l	701	CDL	C77-C78-C79-C80
55	r	503	CDL	C59-C60-C61-C62
48	Q	501	PEE	O5-C30-O3-C3
55	l	701	CDL	C39-C40-C41-C42
55	l	702	CDL	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
48	r	501	PEE	C36-C37-C38-C39
46	A	502	FMN	O2'-C2'-C3'-C4'
48	B	303	PEE	C4-O4P-P-O3P
48	C	302	PEE	C1-O3P-P-O4P
55	a	201	CDL	CB2-OB2-PB2-OB5
49	r	502	PLX	C13-C14-C15-C16
55	a	201	CDL	C73-C74-C75-C76
55	l	701	CDL	C62-C63-C64-C65
55	l	701	CDL	CA7-C31-C32-C33
48	l	703	PEE	O3P-C1-C2-C3
48	r	501	PEE	O3P-C1-C2-C3
55	a	201	CDL	OB5-CB3-CB4-CB6
55	l	701	CDL	CB7-C71-C72-C73
55	l	701	CDL	C14-C15-C16-C17
55	l	702	CDL	C11-CA5-OA6-CA4
55	a	201	CDL	C31-C32-C33-C34
48	Q	501	PEE	C12-C13-C14-C15
48	b	201	PEE	C1-C2-C3-O3
49	a	202	PLX	C3-C4-C5-O8
55	l	702	CDL	CB3-CB4-CB6-OB8
55	r	503	CDL	CA3-CA4-CA6-OA8
55	u	201	CDL	C17-C18-C19-C20
49	C	303	PLX	C7-C8-C9-C10
49	j	202	PLX	C26-C27-C28-C29
49	g	201	PLX	C11-C10-C9-C8
50	G	201	8Q1	C7-C8-C9-C10
55	r	503	CDL	C84-C85-C86-C87
49	j	202	PLX	C15-C16-C17-C18
49	r	502	PLX	O8-C24-C25-C26
48	l	703	PEE	C24-C25-C26-C27
49	g	201	PLX	C18-C19-C20-C21
55	l	701	CDL	C73-C74-C75-C76
49	a	202	PLX	C27-C28-C29-C30
55	i	401	CDL	C11-C12-C13-C14
48	B	303	PEE	C15-C16-C17-C18
48	C	302	PEE	C39-C40-C41-C42
49	C	303	PLX	C14-C15-C16-C17
55	r	503	CDL	C78-C79-C80-C81
48	Q	501	PEE	C24-C25-C26-C27
50	G	201	8Q1	C28-O27-P24-O3
50	X	201	8Q1	C28-O27-P24-O3
49	e	201	PLX	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
55	r	503	CDL	C31-CA7-OA8-CA6
49	g	201	PLX	O4-C3-C4-O6
50	X	201	8Q1	C6-C7-C8-C9
55	i	401	CDL	OB6-CB4-CB6-OB8
56	s	402	UQ	C17-C18-C19-C20
50	X	201	8Q1	C31-C29-C32-O33
48	j	201	PEE	C44-C45-C46-C47
48	r	501	PEE	C22-C23-C24-C25
49	a	202	PLX	C19-C20-C21-C22
49	a	202	PLX	C13-C14-C15-C16
55	l	702	CDL	C64-C65-C66-C67
55	a	201	CDL	C14-C15-C16-C17
48	Q	501	PEE	C32-C33-C34-C35
55	r	503	CDL	C32-C33-C34-C35
48	C	302	PEE	C31-C30-O3-C3
55	a	201	CDL	OA5-CA3-CA4-CA6
55	a	201	CDL	CA5-C11-C12-C13
49	g	201	PLX	C32-C33-C34-C35
55	a	201	CDL	C53-C54-C55-C56
49	g	201	PLX	C11-C12-C13-C14
50	G	201	8Q1	C11-C10-C9-C8
55	l	702	CDL	C31-C32-C33-C34
48	B	303	PEE	C38-C39-C40-C41
48	j	201	PEE	C38-C39-C40-C41
55	a	201	CDL	C60-C61-C62-C63
55	l	701	CDL	C31-C32-C33-C34
55	a	201	CDL	C31-CA7-OA8-CA6
48	r	501	PEE	C1-C2-C3-O3
49	g	201	PLX	C3-C4-C5-O8
55	l	701	CDL	CB3-CB4-CB6-OB8
55	u	201	CDL	CA3-CA4-CA6-OA8
49	j	202	PLX	C33-C34-C35-C36
48	B	303	PEE	C17-C18-C19-C20
49	r	502	PLX	C33-C34-C35-C36
55	l	701	CDL	C74-C75-C76-C77
48	l	703	PEE	C32-C33-C34-C35
49	g	201	PLX	C36-C37-C38-C39
49	C	303	PLX	C9-C10-C11-C12
49	C	303	PLX	C17-C18-C19-C20
48	s	401	PEE	C23-C24-C25-C26
48	b	201	PEE	C1-O3P-P-O4P
49	C	303	PLX	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
55	l	702	CDL	C22-C23-C24-C25
55	u	201	CDL	C76-C77-C78-C79
55	a	201	CDL	OA5-CA3-CA4-OA6
55	l	702	CDL	OA5-CA3-CA4-OA6
48	j	201	PEE	C22-C23-C24-C25
48	r	501	PEE	C15-C16-C17-C18
49	C	303	PLX	C11-C10-C9-C8
55	r	503	CDL	OA9-CA7-OA8-CA6
48	r	501	PEE	O2-C2-C3-O3
49	a	202	PLX	O6-C4-C5-O8
49	j	202	PLX	O6-C4-C5-O8
55	l	702	CDL	OA6-CA4-CA6-OA8
55	r	503	CDL	C31-C32-C33-C34
49	C	303	PLX	C26-C27-C28-C29
48	j	201	PEE	C11-C12-C13-C14
55	l	702	CDL	OA7-CA5-OA6-CA4
55	a	201	CDL	C75-C76-C77-C78
55	u	201	CDL	C79-C80-C81-C82
55	l	701	CDL	C71-C72-C73-C74
49	C	303	PLX	C30-C31-C32-C33
49	a	202	PLX	C14-C15-C16-C17
49	j	202	PLX	C30-C31-C32-C33
55	u	201	CDL	C55-C56-C57-C58
48	C	302	PEE	C18-C19-C20-C21
49	a	202	PLX	C15-C16-C17-C18
55	r	503	CDL	C79-C80-C81-C82
50	G	201	8Q1	O4-C1-S44-C43
55	u	201	CDL	CB7-C71-C72-C73
55	l	702	CDL	C17-C18-C19-C20
49	C	303	PLX	O6-C6-C7-C8
48	B	303	PEE	O3P-C1-C2-C3
48	Q	501	PEE	O3P-C1-C2-C3
49	a	202	PLX	O4-C3-C4-C5
49	g	201	PLX	O4-C3-C4-C5
55	i	401	CDL	OB5-CB3-CB4-CB6
55	a	201	CDL	C59-C60-C61-C62
55	u	201	CDL	C18-C19-C20-C21
55	l	701	CDL	C37-C38-C39-C40
55	l	702	CDL	C14-C15-C16-C17
50	G	201	8Q1	C28-O27-P24-O2
50	X	201	8Q1	O33-C32-C34-N36
48	Q	501	PEE	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	C41-C42-C43-C44
48	s	401	PEE	C3-C2-O2-C10
50	G	201	8Q1	C6-C1-S44-C43
48	j	201	PEE	C12-C13-C14-C15
55	r	503	CDL	C60-C61-C62-C63
48	r	501	PEE	C31-C30-O3-C3
55	r	503	CDL	C44-C45-C46-C47
48	Q	501	PEE	C1-C2-C3-O3
48	Q	501	PEE	C2-C1-O3P-P
49	g	201	PLX	C7-C6-O6-C4
49	j	202	PLX	C3-C4-C5-O8
55	r	503	CDL	CB4-CB3-OB5-PB2
48	C	302	PEE	O5-C30-O3-C3
48	B	303	PEE	O3P-C1-C2-O2
55	a	201	CDL	OB5-CB3-CB4-OB6
50	X	201	8Q1	C31-C29-C32-C34
48	B	303	PEE	C21-C22-C23-C24
49	j	202	PLX	C31-C32-C33-C34
48	b	201	PEE	O2-C2-C3-O3
49	r	502	PLX	O6-C4-C5-O8
55	a	201	CDL	OA9-CA7-OA8-CA6
48	j	201	PEE	C43-C44-C45-C46
49	e	201	PLX	C13-C14-C15-C16
55	a	201	CDL	C38-C39-C40-C41
51	J	401	NDP	C5B-O5B-PA-O3
49	r	502	PLX	C31-C32-C33-C34
49	C	303	PLX	C11-C12-C13-C14
55	l	701	CDL	C36-C37-C38-C39
55	r	503	CDL	C76-C77-C78-C79
55	l	702	CDL	C79-C80-C81-C82
48	r	501	PEE	O5-C30-O3-C3
51	J	401	NDP	C3B-C4B-C5B-O5B
49	e	201	PLX	C12-C13-C14-C15
49	C	303	PLX	C19-C20-C21-C22
50	G	201	8Q1	C6-C7-C8-C9
55	i	401	CDL	C74-C75-C76-C77
49	e	201	PLX	C24-C25-C26-C27
55	u	201	CDL	CA2-OA2-PA1-OA5
55	u	201	CDL	CB2-OB2-PB2-OB5
48	l	703	PEE	C13-C14-C15-C16
47	A	503	NAI	C5D-O5D-PN-O1N
48	B	303	PEE	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
48	C	302	PEE	C1-O3P-P-O2P
48	Q	501	PEE	C1-O3P-P-O1P
48	r	501	PEE	C4-O4P-P-O1P
49	e	201	PLX	C2-O1-P1-O2
49	e	201	PLX	C2-O1-P1-O3
49	j	202	PLX	C3-O4-P1-O2
55	a	201	CDL	CA2-OA2-PA1-OA4
55	a	201	CDL	CB2-OB2-PB2-OB4
55	l	701	CDL	CA2-OA2-PA1-OA3
55	l	701	CDL	CB2-OB2-PB2-OB3
55	l	702	CDL	CB2-OB2-PB2-OB3
55	l	702	CDL	CB3-OB5-PB2-OB3
55	l	702	CDL	CB3-OB5-PB2-OB4
55	r	503	CDL	CB2-OB2-PB2-OB3
55	r	503	CDL	CB2-OB2-PB2-OB4
55	r	503	CDL	CB3-OB5-PB2-OB3
55	u	201	CDL	CB2-OB2-PB2-OB4
55	u	201	CDL	CB3-OB5-PB2-OB4
50	G	201	8Q1	C9-C10-C11-C12
55	l	702	CDL	OA5-CA3-CA4-CA6
49	j	202	PLX	C10-C11-C12-C13
55	l	702	CDL	C80-C81-C82-C83
49	j	202	PLX	C25-C24-O8-C5
49	r	502	PLX	C25-C24-O8-C5
49	j	202	PLX	C16-C17-C18-C19
49	e	201	PLX	C36-C37-C38-C39
48	Q	501	PEE	O3P-C1-C2-O2
49	j	202	PLX	O4-C3-C4-O6
55	i	401	CDL	OB5-CB3-CB4-OB6
49	C	303	PLX	C25-C26-C27-C28
55	a	201	CDL	C22-C23-C24-C25
55	r	503	CDL	CA5-C11-C12-C13
55	l	701	CDL	C51-CB5-OB6-CB4
49	e	201	PLX	C9-C10-C11-C12
55	r	503	CDL	C20-C21-C22-C23
55	a	201	CDL	CB5-C51-C52-C53
46	A	502	FMN	C1'-C2'-C3'-C4'
48	B	303	PEE	C13-C14-C15-C16
49	e	201	PLX	C3-C4-C5-O8
55	i	401	CDL	CB3-CB4-CB6-OB8
55	u	201	CDL	C59-C60-C61-C62
49	e	201	PLX	O6-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
49	g	201	PLX	O6-C4-C5-O8
55	u	201	CDL	OA6-CA4-CA6-OA8
48	B	303	PEE	C33-C34-C35-C36
48	Q	501	PEE	C17-C18-C19-C20
48	j	201	PEE	C37-C38-C39-C40
48	r	501	PEE	C38-C39-C40-C41
49	r	502	PLX	C18-C19-C20-C21
55	a	201	CDL	C32-C31-CA7-OA8
50	G	201	8Q1	C10-C11-C12-C13
49	j	202	PLX	O6-C6-C7-C8
55	i	401	CDL	C33-C34-C35-C36
55	r	503	CDL	C14-C15-C16-C17
48	b	201	PEE	C38-C39-C40-C41
55	l	702	CDL	C32-C33-C34-C35
49	j	202	PLX	O4-C3-C4-C5
55	l	701	CDL	OB7-CB5-OB6-CB4
55	l	702	CDL	C58-C59-C60-C61
48	Q	501	PEE	C30-C31-C32-C33
48	r	501	PEE	C24-C25-C26-C27
49	e	201	PLX	C7-C8-C9-C10
55	u	201	CDL	C19-C20-C21-C22
47	A	503	NAI	O4D-C1D-N1N-C2N
48	r	501	PEE	C33-C34-C35-C36
49	C	303	PLX	C36-C37-C38-C39
46	A	502	FMN	O2'-C2'-C3'-O3'
48	C	302	PEE	C42-C43-C44-C45
55	l	701	CDL	C40-C41-C42-C43
55	l	702	CDL	C43-C44-C45-C46
48	l	703	PEE	C36-C37-C38-C39
48	B	303	PEE	O5-C30-O3-C3
48	Q	501	PEE	O2-C2-C3-O3
48	B	303	PEE	C31-C30-O3-C3
48	C	302	PEE	C4-O4P-P-O3P
49	g	201	PLX	C3-O4-P1-O1
55	i	401	CDL	CA2-OA2-PA1-OA5
55	r	503	CDL	C42-C43-C44-C45
55	a	201	CDL	C43-C44-C45-C46
48	Q	501	PEE	C31-C32-C33-C34
55	i	401	CDL	CA4-CA3-OA5-PA1
55	u	201	CDL	OB9-CB7-OB8-CB6
49	e	201	PLX	C31-C32-C33-C34
55	l	702	CDL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
48	l	703	PEE	C14-C15-C16-C17
49	g	201	PLX	C30-C31-C32-C33
55	u	201	CDL	C71-CB7-OB8-CB6
55	l	701	CDL	C54-C55-C56-C57
48	j	201	PEE	C31-C32-C33-C34
48	l	703	PEE	C11-C12-C13-C14
48	C	302	PEE	C33-C34-C35-C36
48	b	201	PEE	C16-C17-C18-C19
48	C	302	PEE	O3P-C1-C2-C3
49	a	202	PLX	C24-C25-C26-C27
55	l	702	CDL	C53-C54-C55-C56
48	s	401	PEE	C20-C21-C22-C23
48	l	703	PEE	C15-C16-C17-C18
49	C	303	PLX	C18-C19-C20-C21
48	j	201	PEE	C40-C41-C42-C43
49	g	201	PLX	O8-C24-C25-C26
55	l	702	CDL	C51-C52-C53-C54
55	u	201	CDL	CB4-CB3-OB5-PB2
50	X	201	8Q1	N41-C42-C43-S44
48	Q	501	PEE	C36-C37-C38-C39
47	A	503	NAI	C2D-C1D-N1N-C2N
55	i	401	CDL	C32-C33-C34-C35
55	l	702	CDL	CA3-CA4-CA6-OA8
55	r	503	CDL	C40-C41-C42-C43
51	J	401	NDP	O4D-C1D-N1N-C6N
55	u	201	CDL	CB3-OB5-PB2-OB2
49	j	202	PLX	C17-C18-C19-C20
55	i	401	CDL	C15-C16-C17-C18
48	b	201	PEE	C24-C25-C26-C27
48	j	201	PEE	O2-C2-C3-O3
55	r	503	CDL	C64-C65-C66-C67
55	r	503	CDL	C39-C40-C41-C42
49	e	201	PLX	C18-C19-C20-C21
48	l	703	PEE	C37-C38-C39-C40
48	s	401	PEE	O3-C30-C31-C32
55	a	201	CDL	C17-C18-C19-C20
48	b	201	PEE	C18-C19-C20-C21
48	C	302	PEE	C38-C39-C40-C41
49	e	201	PLX	O4-C3-C4-O6
48	b	201	PEE	O4P-C4-C5-N
48	s	401	PEE	C24-C25-C26-C27
50	X	201	8Q1	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
56	s	402	UQ	C15-C14-C16-C17
56	s	402	UQ	C12-C11-C9-C8
55	l	701	CDL	C33-C34-C35-C36
55	l	701	CDL	C18-C19-C20-C21
55	r	503	CDL	C52-C51-CB5-OB6
48	j	201	PEE	C16-C17-C18-C19
48	s	401	PEE	C18-C19-C20-C21
48	b	201	PEE	C30-C31-C32-C33
48	B	303	PEE	C39-C40-C41-C42
49	j	202	PLX	C7-C6-O6-C4
49	r	502	PLX	C3-C4-C5-O8
55	a	201	CDL	CA4-CA3-OA5-PA1
55	l	701	CDL	OA5-CA3-CA4-OA6
48	Q	501	PEE	C38-C39-C40-C41
48	C	302	PEE	C15-C16-C17-C18
55	i	401	CDL	OA5-CA3-CA4-CA6
55	r	503	CDL	C82-C83-C84-C85
48	l	703	PEE	C16-C17-C18-C19
55	l	702	CDL	C32-C31-CA7-OA8
48	j	201	PEE	O3-C30-C31-C32
50	X	201	8Q1	C11-C10-C9-C8
55	u	201	CDL	C77-C78-C79-C80
48	B	303	PEE	C40-C41-C42-C43
48	C	302	PEE	C16-C17-C18-C19
48	s	401	PEE	C16-C17-C18-C19
48	b	201	PEE	C34-C35-C36-C37
49	g	201	PLX	C33-C34-C35-C36
55	u	201	CDL	C72-C71-CB7-OB8
48	C	302	PEE	C36-C37-C38-C39
55	r	503	CDL	C36-C37-C38-C39
55	a	201	CDL	C40-C41-C42-C43
55	a	201	CDL	C20-C21-C22-C23
55	r	503	CDL	C52-C51-CB5-OB7
55	i	401	CDL	CA3-CA4-CA6-OA8
49	r	502	PLX	C25-C26-C27-C28
55	l	701	CDL	CB2-OB2-PB2-OB5
55	r	503	CDL	C57-C58-C59-C60
55	l	702	CDL	C12-C11-CA5-OA6
55	r	503	CDL	CA4-CA3-OA5-PA1
47	A	503	NAI	C5D-O5D-PN-O2N
48	r	501	PEE	C1-O3P-P-O1P
49	g	201	PLX	C3-O4-P1-O2

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	CA3-OA5-PA1-OA3
55	l	702	CDL	CA3-OA5-PA1-OA4
55	u	201	CDL	CB2-OB2-PB2-OB3
55	a	201	CDL	OB6-CB4-CB6-OB8
55	i	401	CDL	C13-C14-C15-C16
55	l	701	CDL	C34-C35-C36-C37
55	u	201	CDL	C73-C74-C75-C76
55	r	503	CDL	C72-C71-CB7-OB8
55	u	201	CDL	C12-C11-CA5-OA6
48	b	201	PEE	C13-C14-C15-C16
49	g	201	PLX	C29-C30-C31-C32
55	r	503	CDL	C80-C81-C82-C83
55	l	702	CDL	C32-C31-CA7-OA9
55	u	201	CDL	C72-C71-CB7-OB9
49	C	303	PLX	C29-C30-C31-C32
55	i	401	CDL	OA5-CA3-CA4-OA6
55	r	503	CDL	OB5-CB3-CB4-OB6
55	l	701	CDL	C42-C43-C44-C45
55	l	702	CDL	C12-C11-CA5-OA7
55	l	701	CDL	C72-C71-CB7-OB8
48	j	201	PEE	O5-C30-C31-C32

There are no ring outliers.

29 monomers are involved in 116 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	G	201	8Q1	1	0
48	s	401	PEE	1	0
52	O	301	FES	1	0
48	r	501	PEE	7	0
56	s	402	UQ	7	0
49	g	201	PLX	6	0
48	C	302	PEE	4	0
48	Q	501	PEE	4	0
47	A	503	NAI	5	0
55	l	701	CDL	11	0
55	l	702	CDL	4	0
49	e	201	PLX	4	0
48	B	303	PEE	9	0
50	X	201	8Q1	3	0
57	w	401	ADP	1	0
55	u	201	CDL	6	0

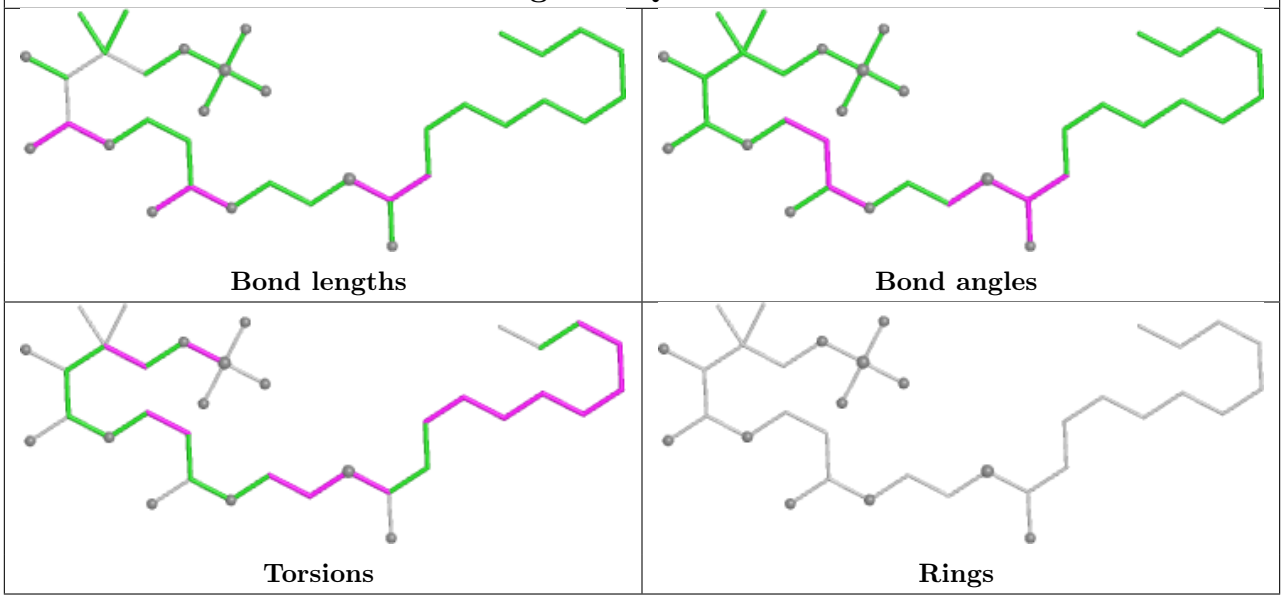
Continued on next page...

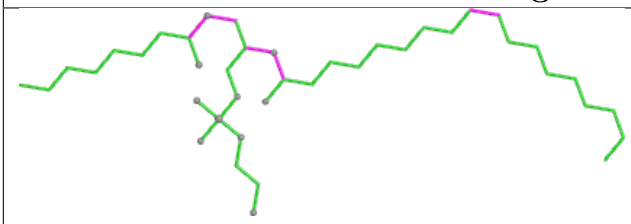
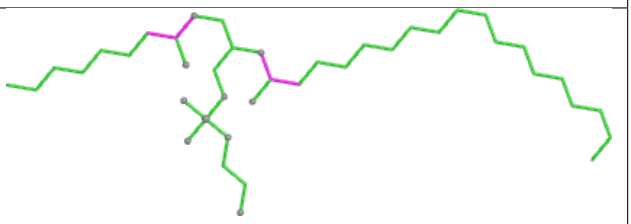
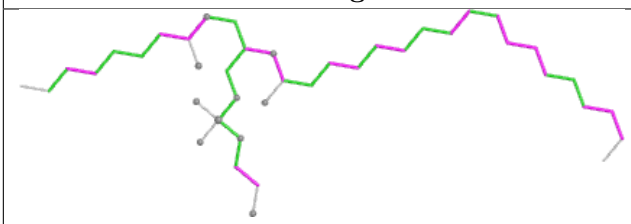
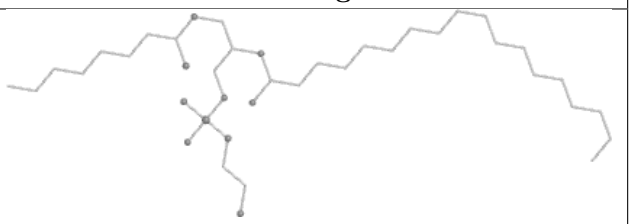
Continued from previous page...

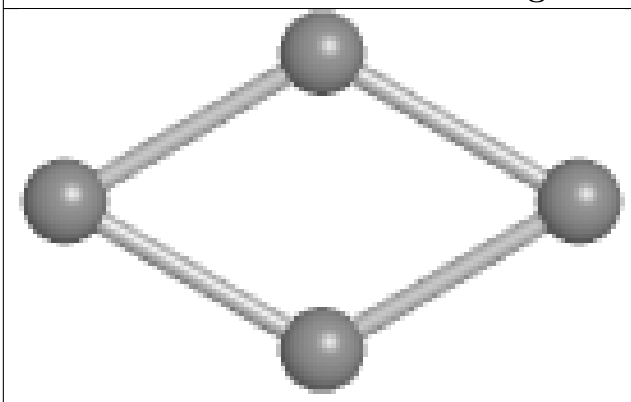
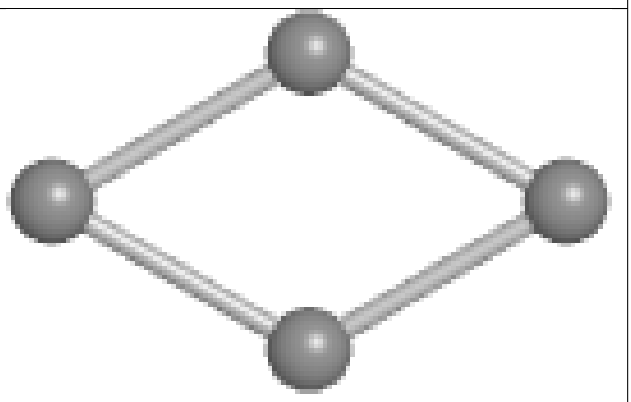
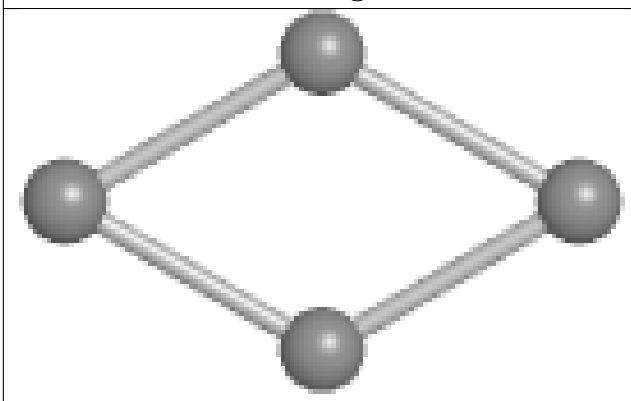
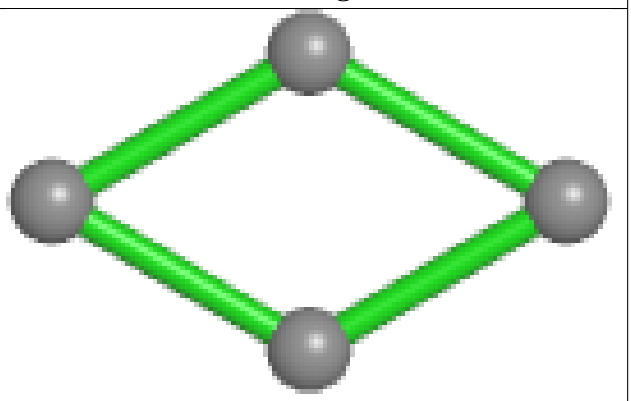
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	i	401	CDL	3	0
49	j	202	PLX	5	0
48	j	201	PEE	2	0
51	J	401	NDP	1	0
46	A	502	FMN	2	0
49	r	502	PLX	3	0
55	r	503	CDL	9	0
55	a	201	CDL	6	0
45	C	301	SF4	2	0
49	a	202	PLX	3	0
49	C	303	PLX	3	0
48	l	703	PEE	2	0
45	A	501	SF4	2	0

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

Ligand 8Q1 G 201



Ligand PEE s 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FES O 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

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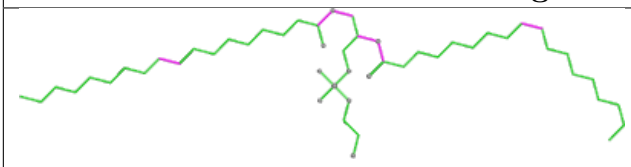
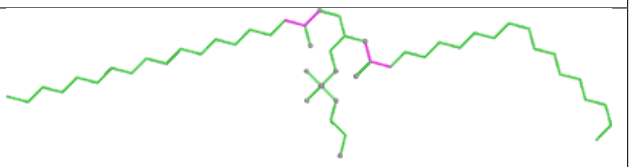
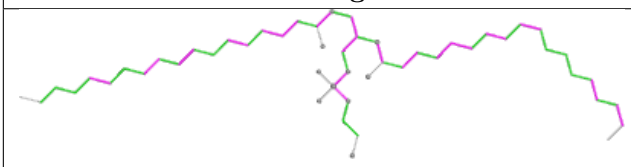
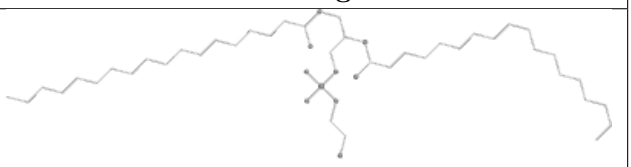
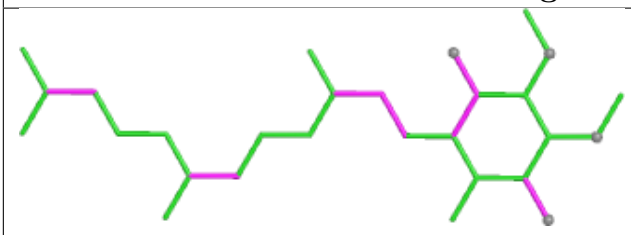
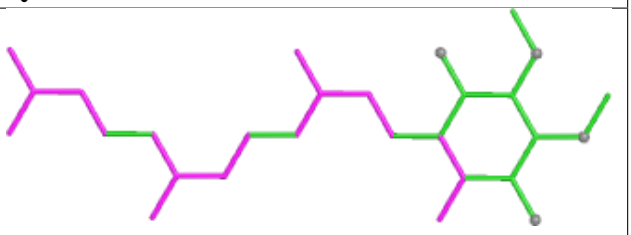
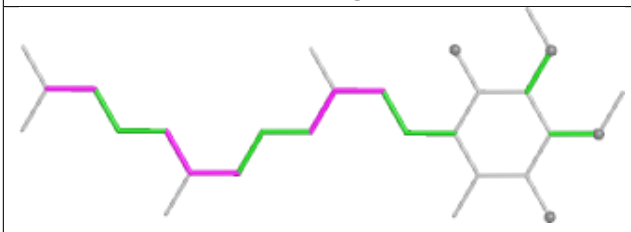
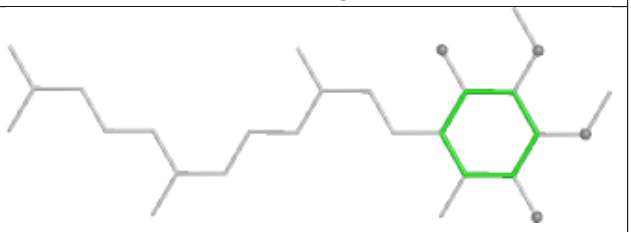
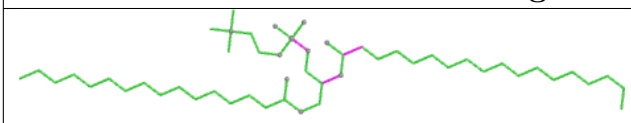
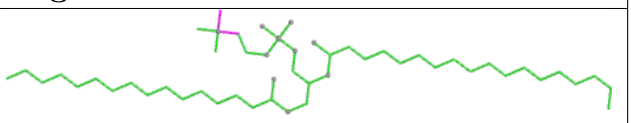
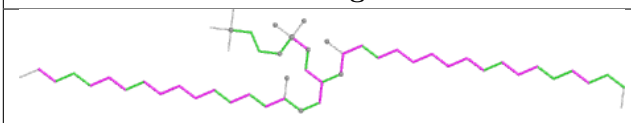
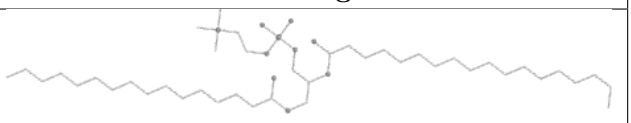
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UQ s 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLX g 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

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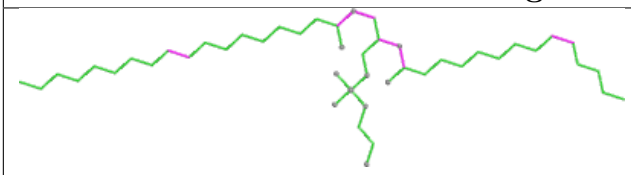
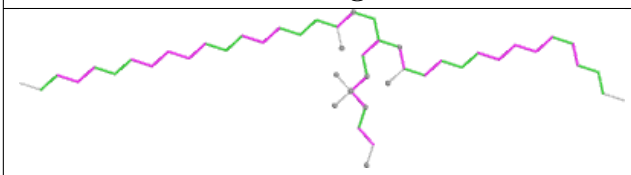
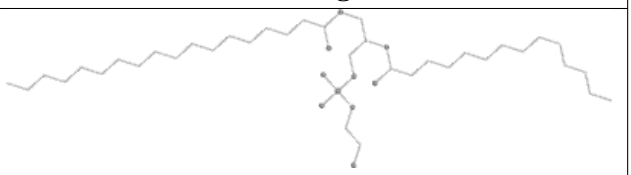
 Bond lengths	Bond angles
 Torsions	 Rings

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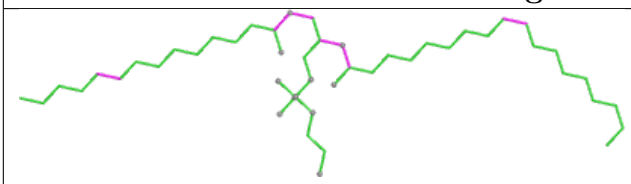
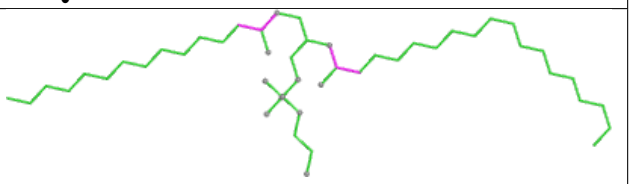
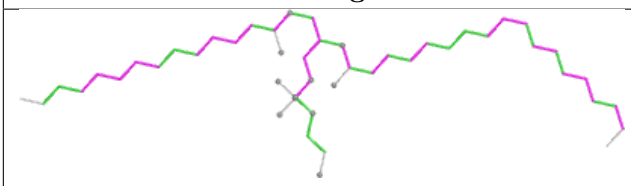
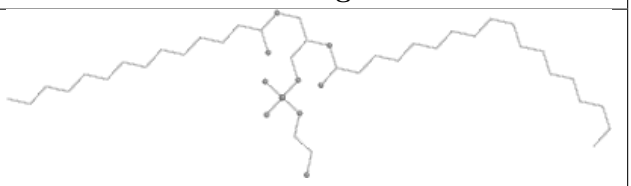
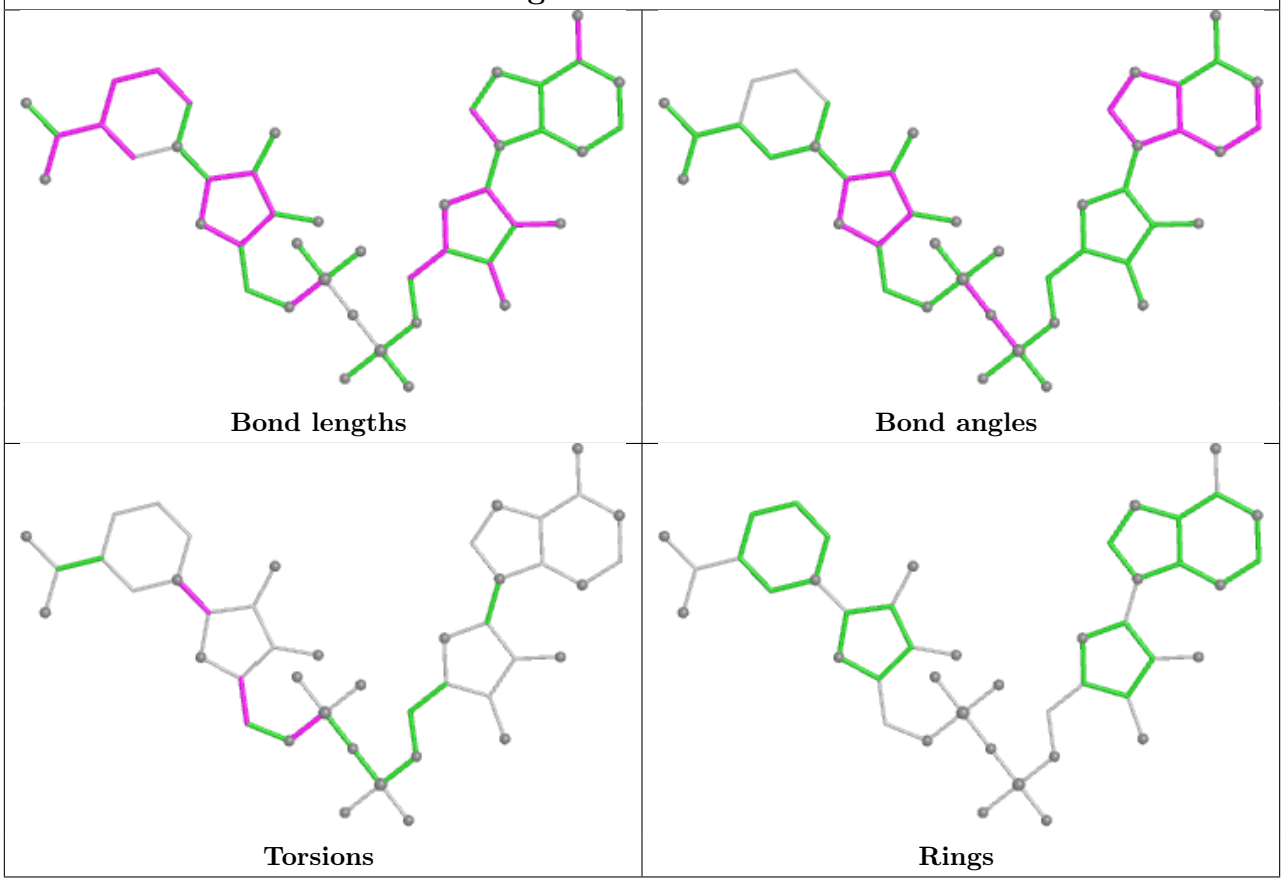
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAI A 503



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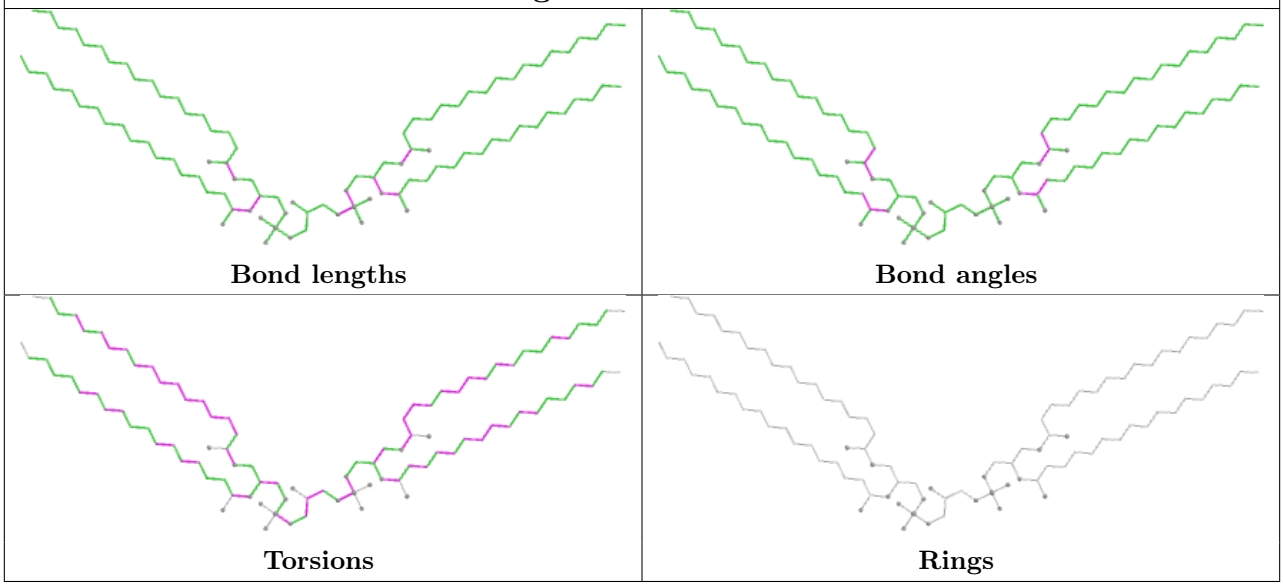

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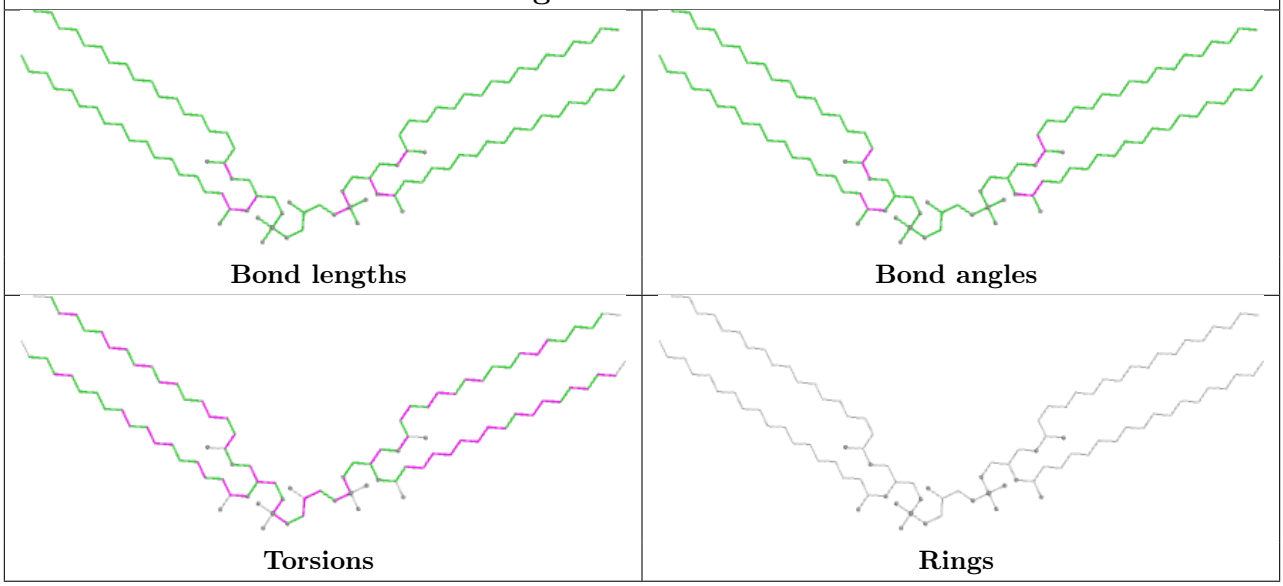
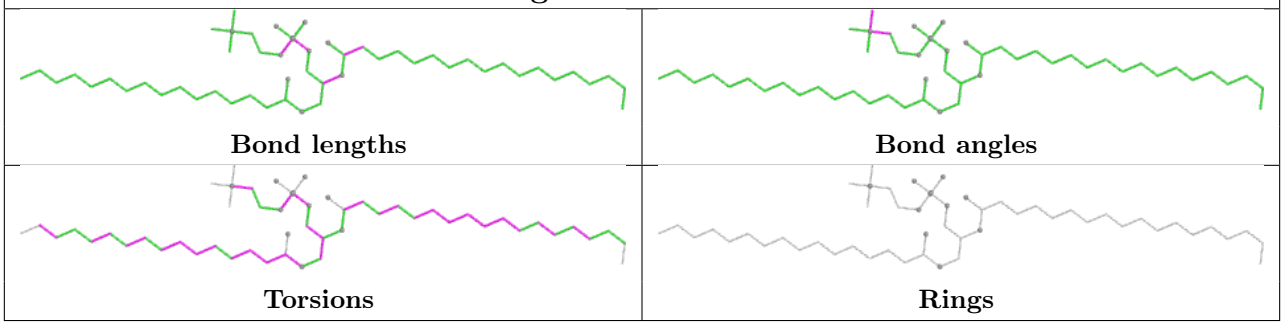
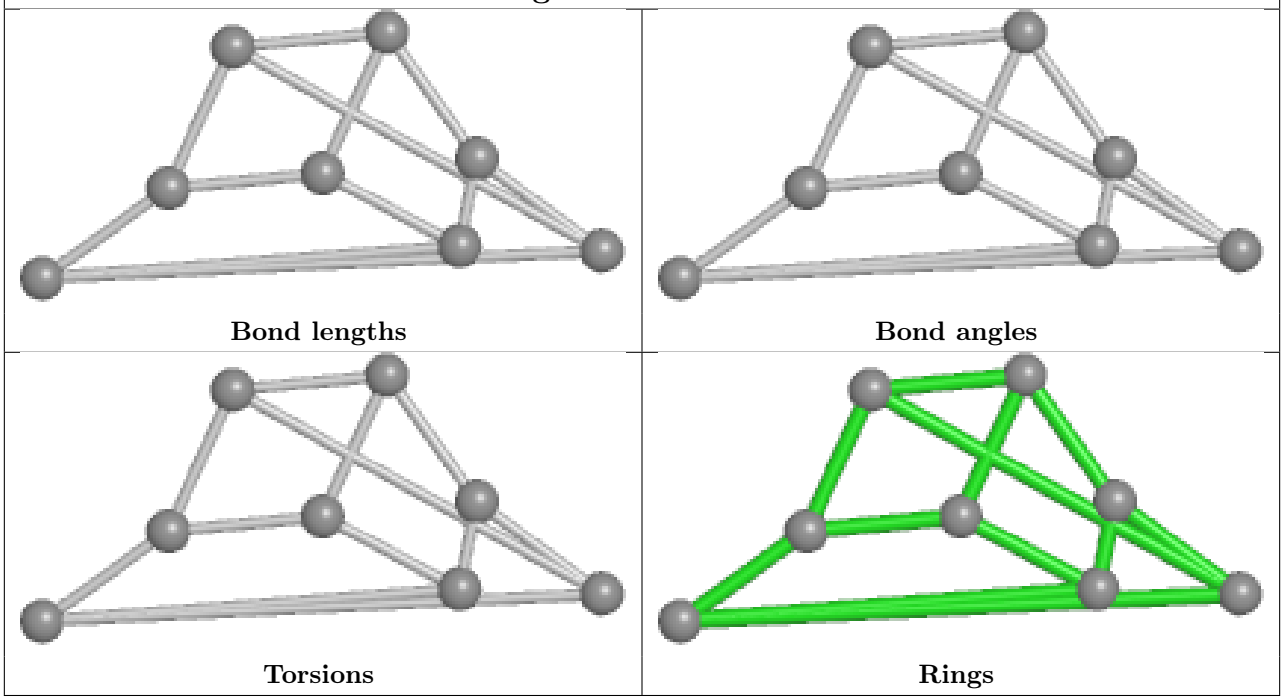


Ligand PLX e 201



Ligand SF4 B 302



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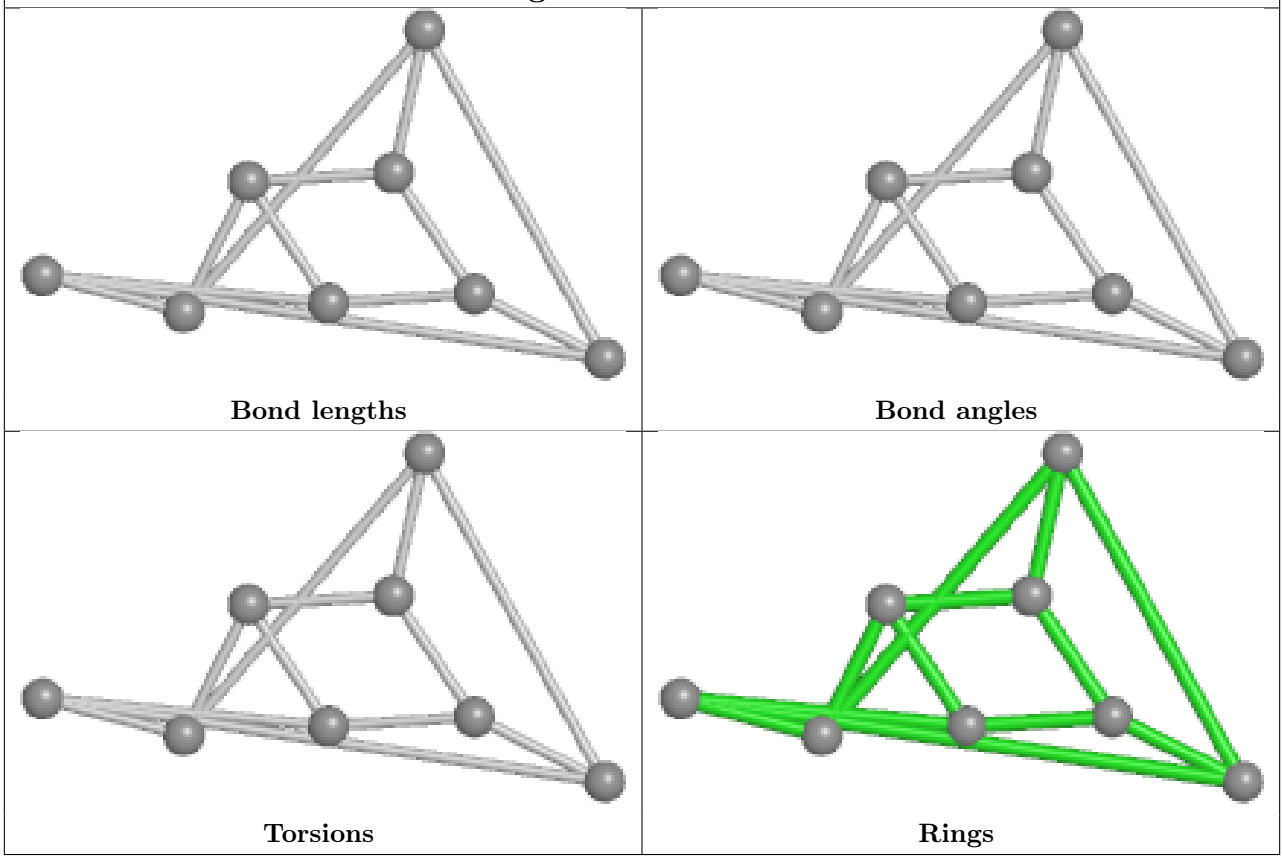

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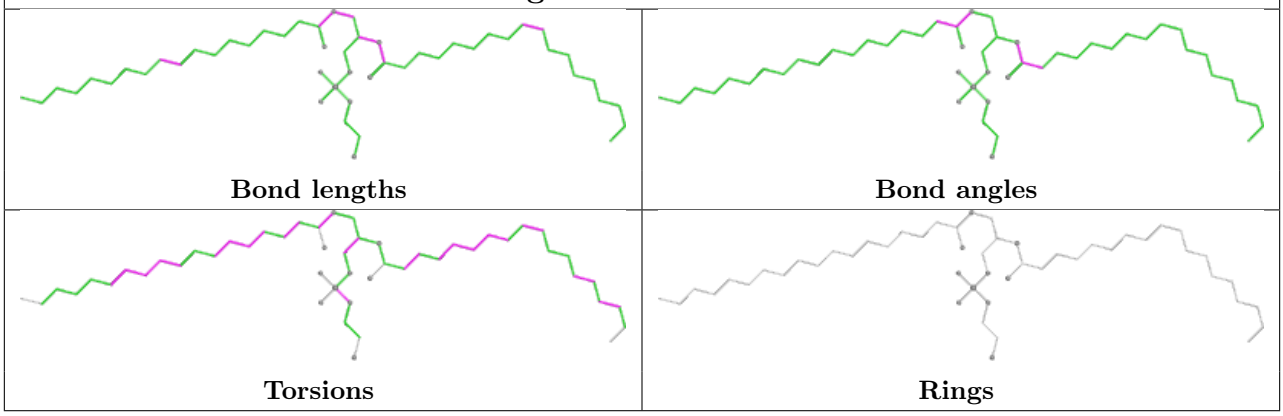
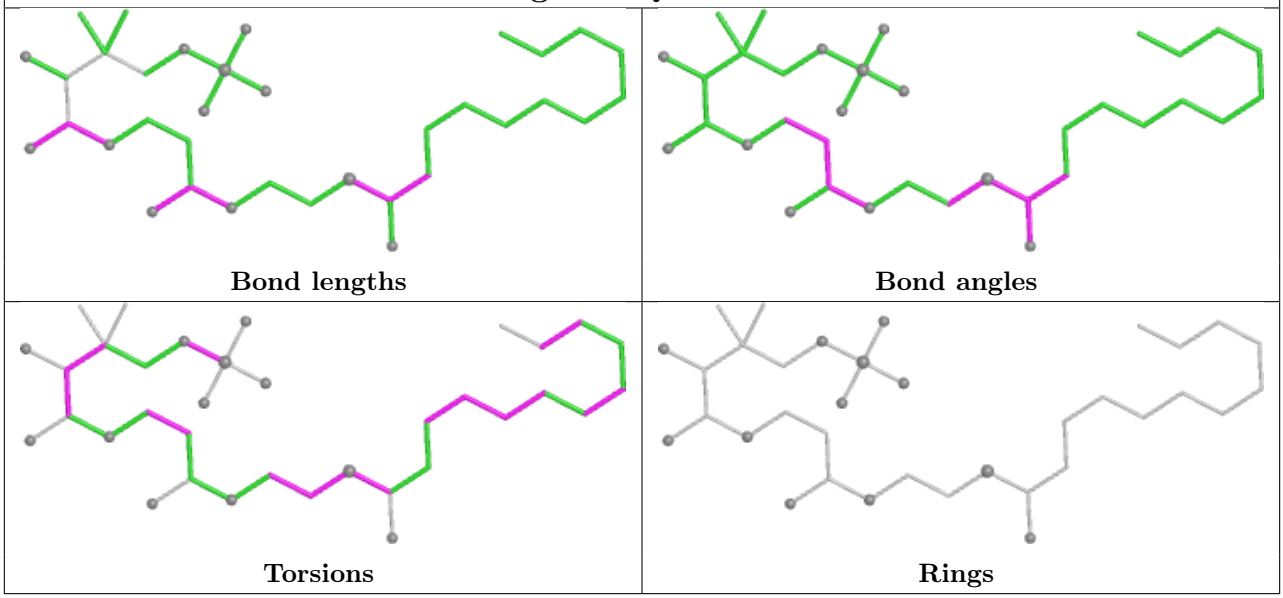
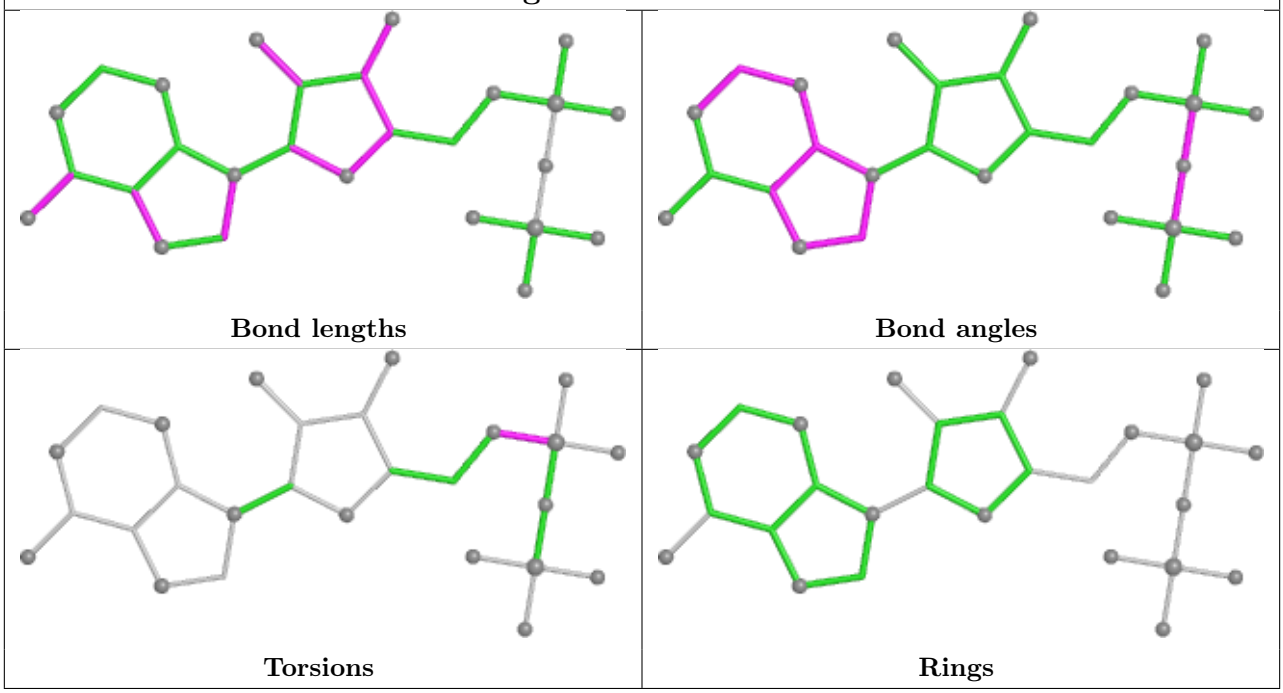


Ligand 8Q1 X 201



Ligand ADP w 401



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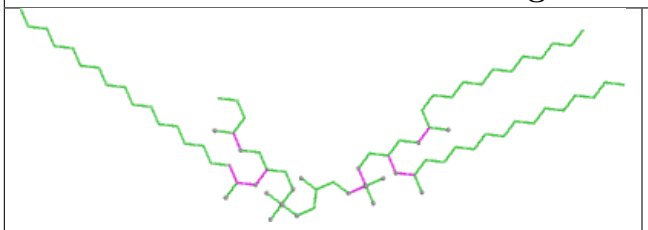
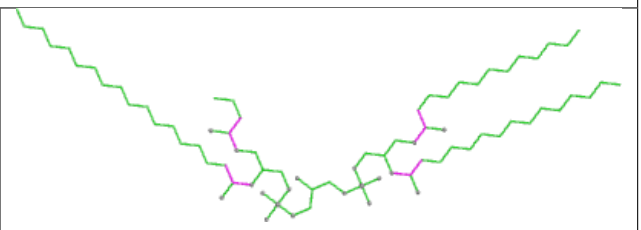
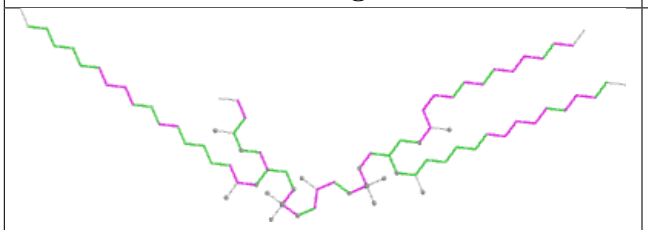


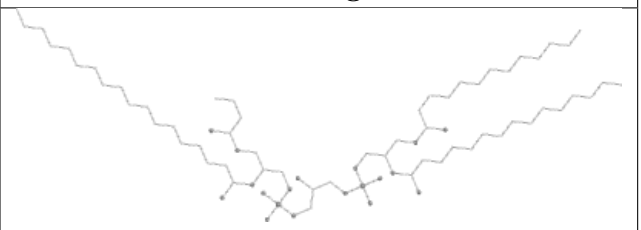
Bond lengths



Bond angles

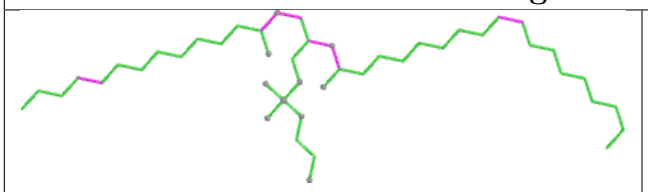


Torsions



Rings

Ligand PEE b 201



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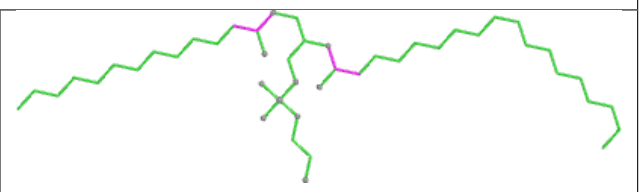

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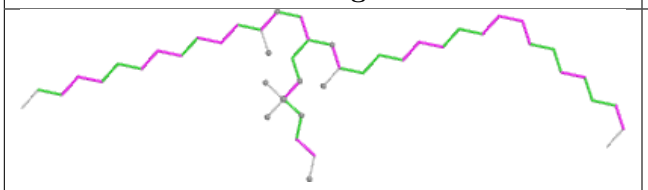

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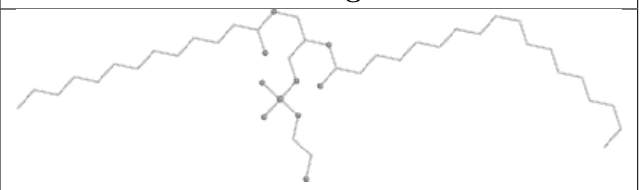
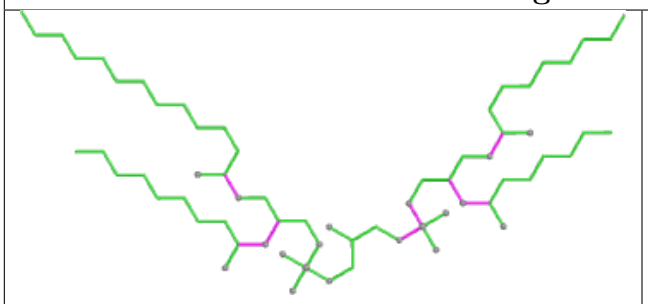
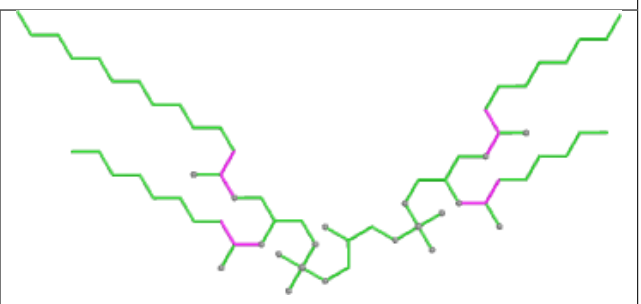


Rings

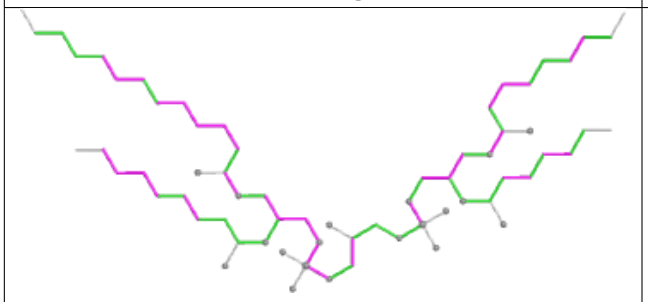
Ligand CDL i 401



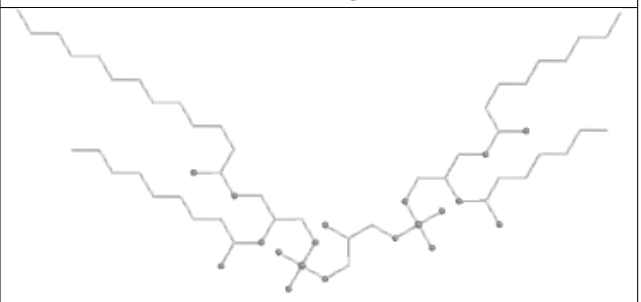
Bond lengths



Bond angles

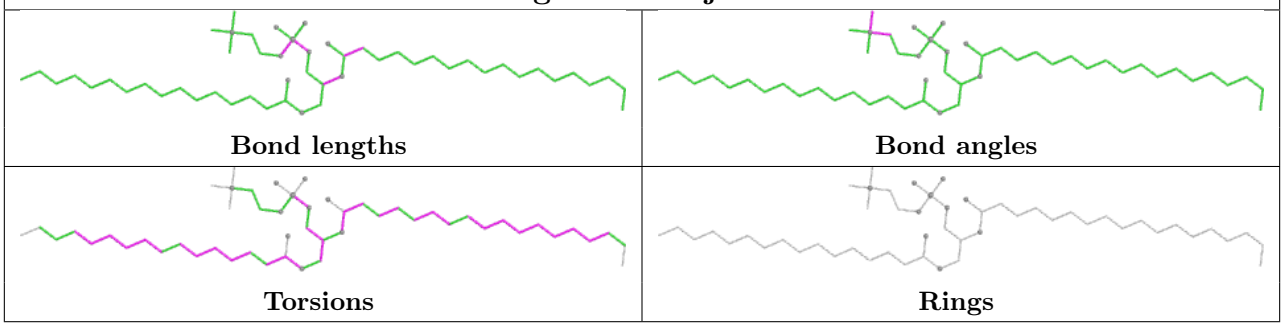


Torsions



Rings

Ligand PLX j 202



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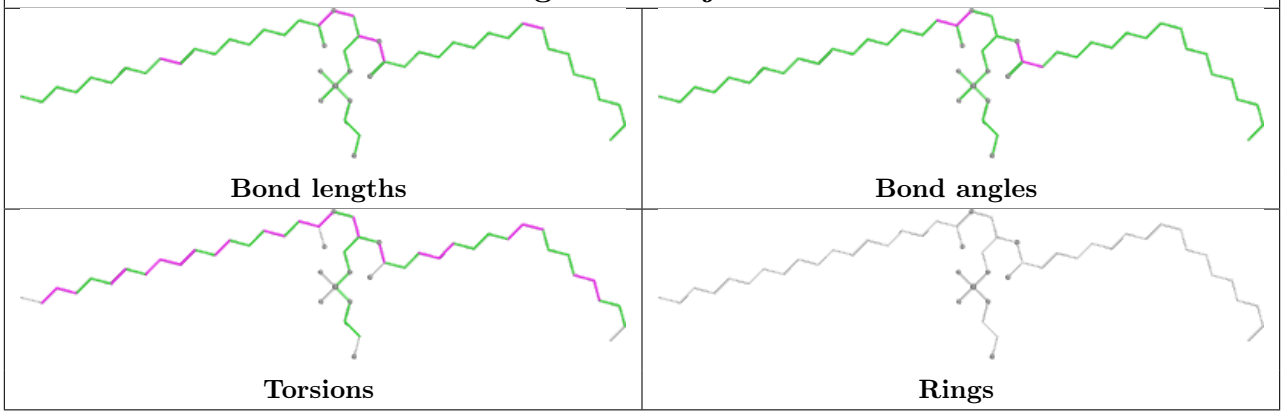
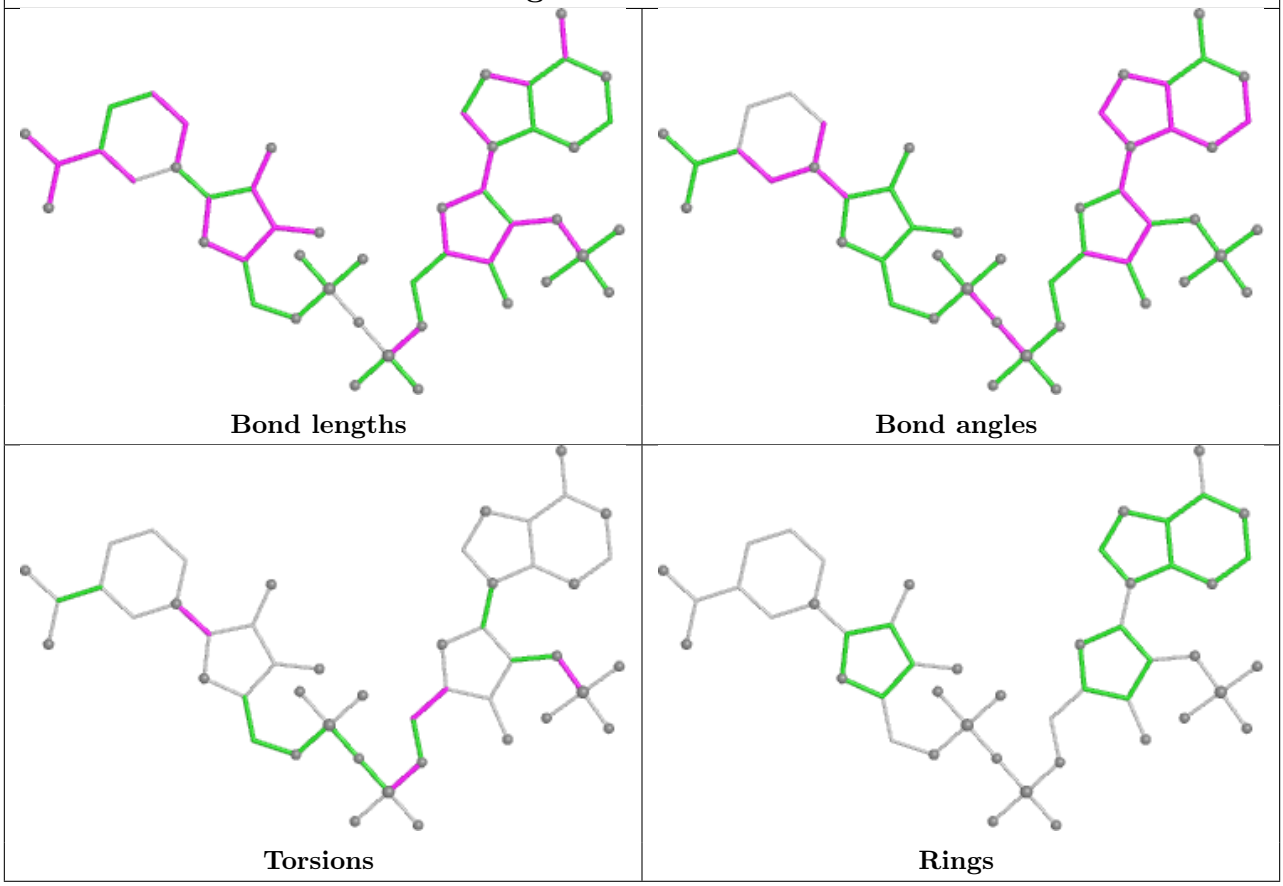
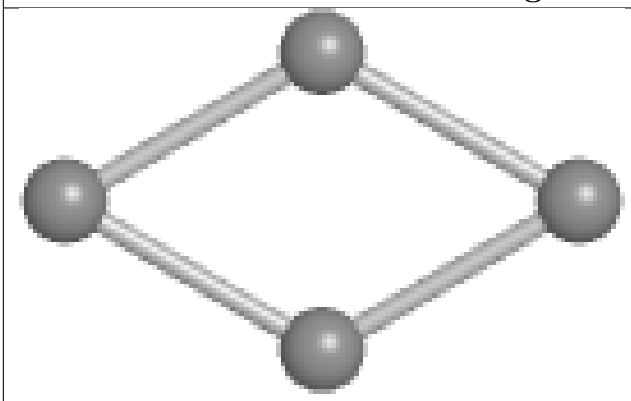
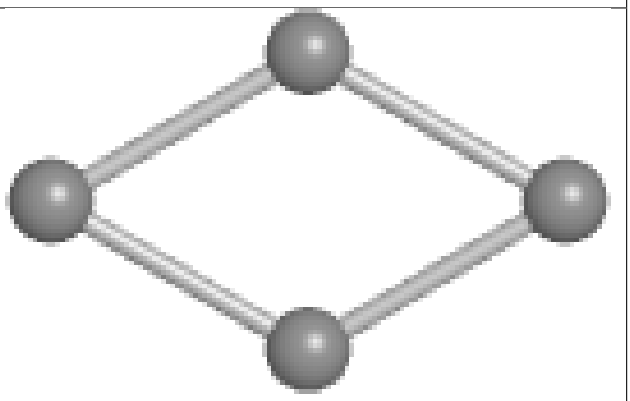
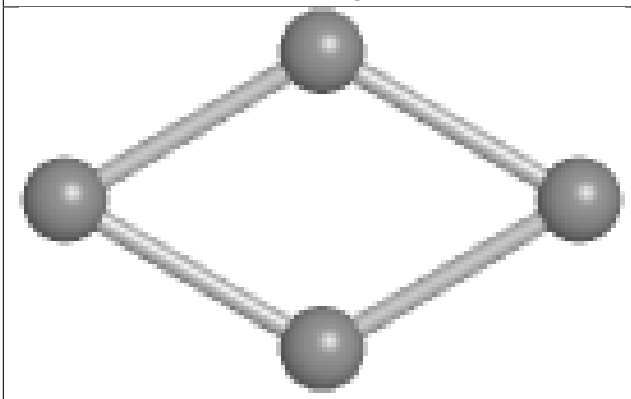
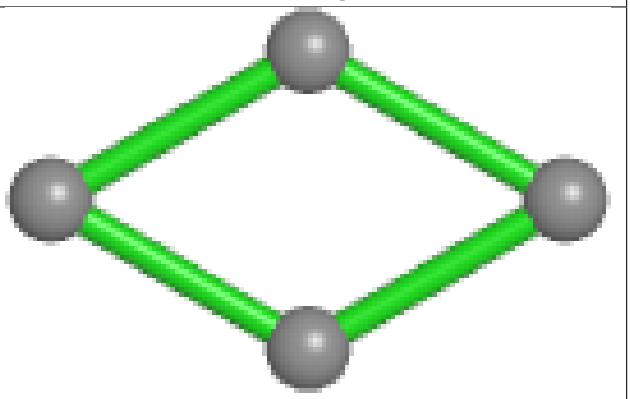
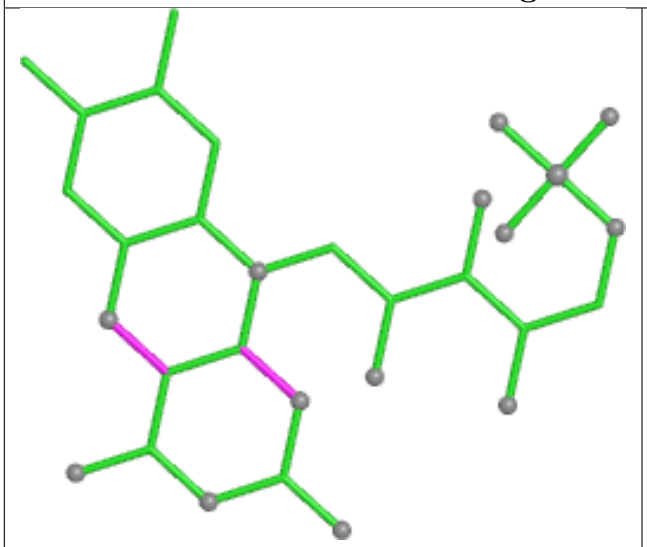


Ligand NDP J 401

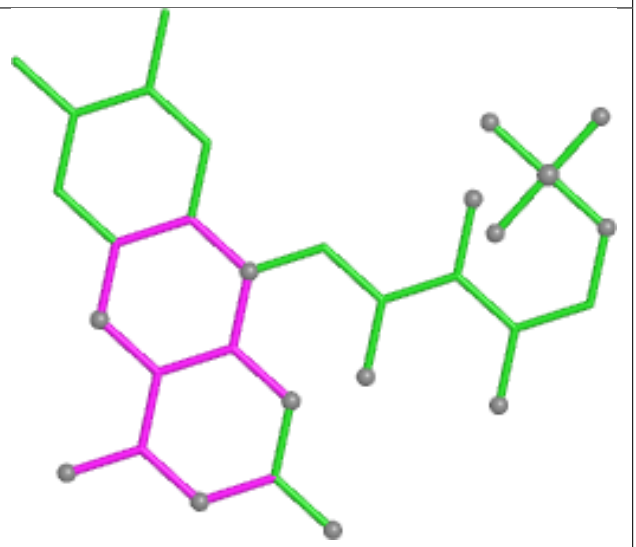


Ligand FES M 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

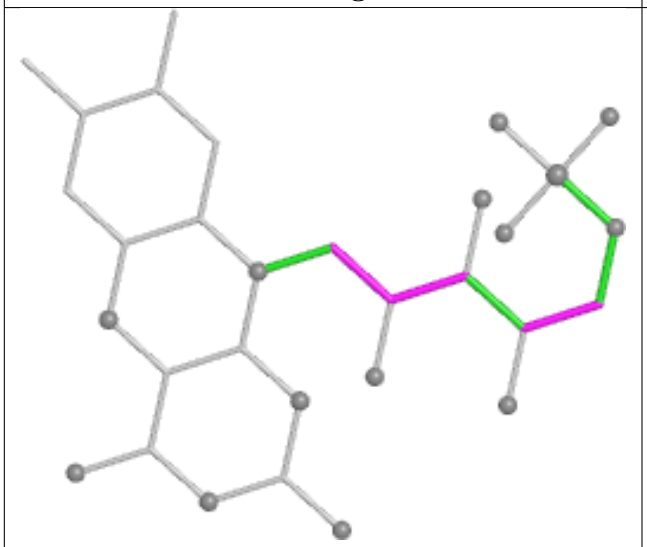
Ligand FMN A 502



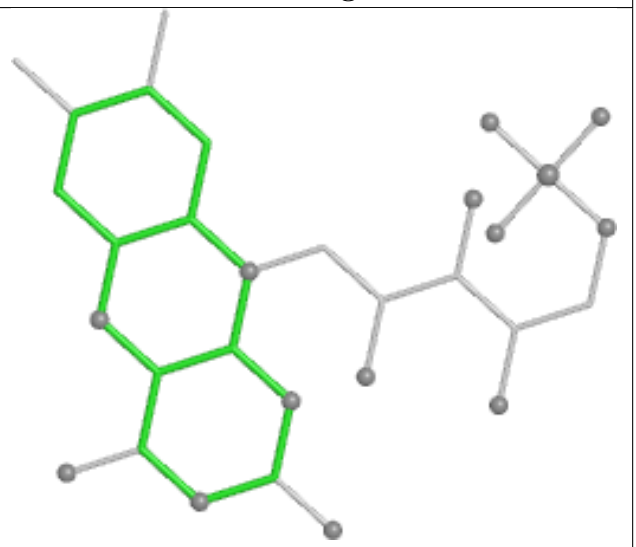
Bond lengths



Bond angles

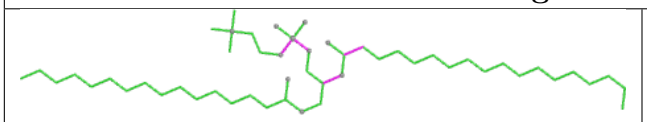


Torsions

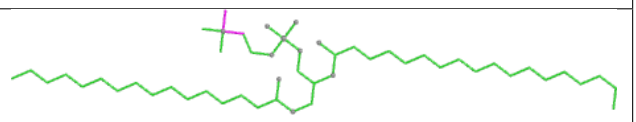


Rings

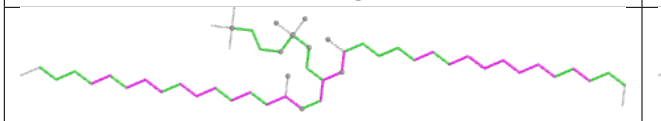
Ligand PLX r 502



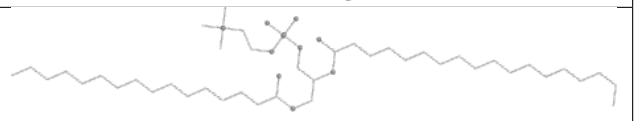
Bond lengths



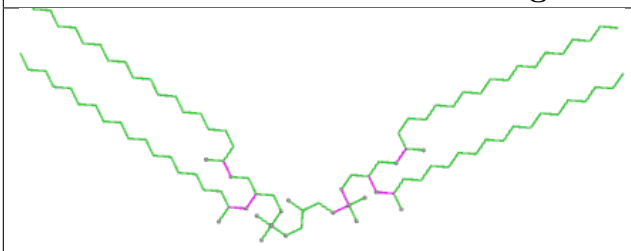
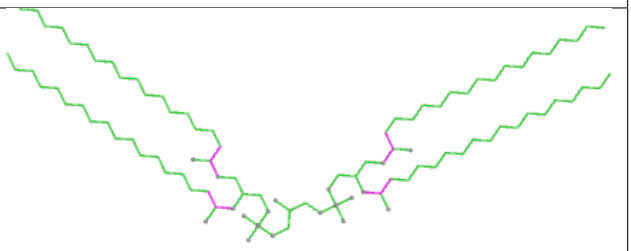
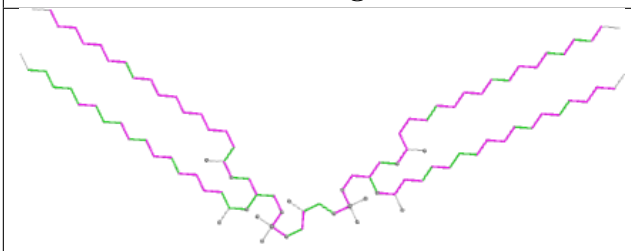
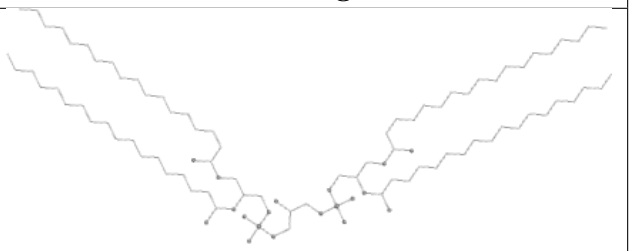
Bond angles

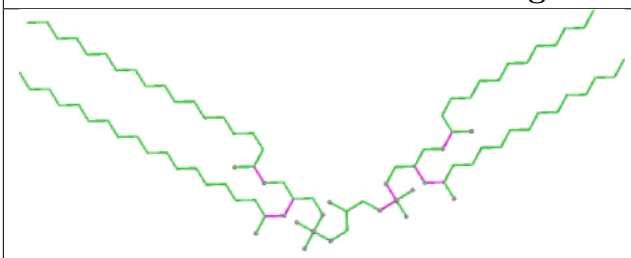
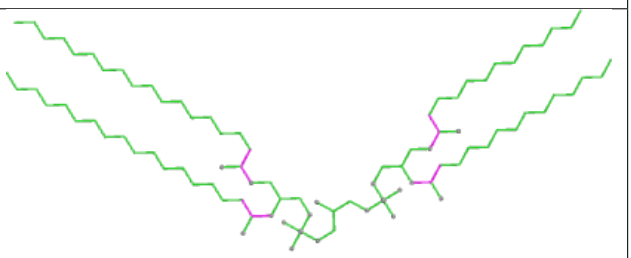
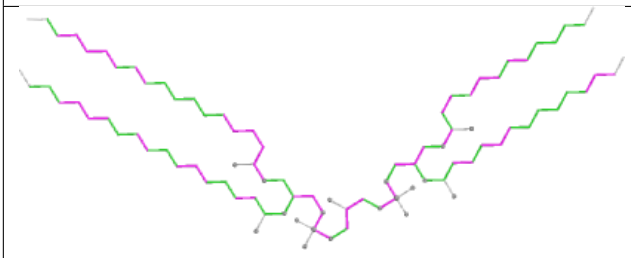
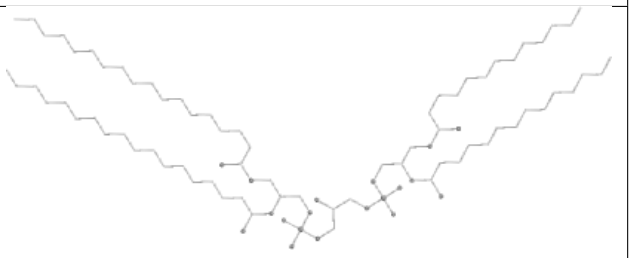


Torsions

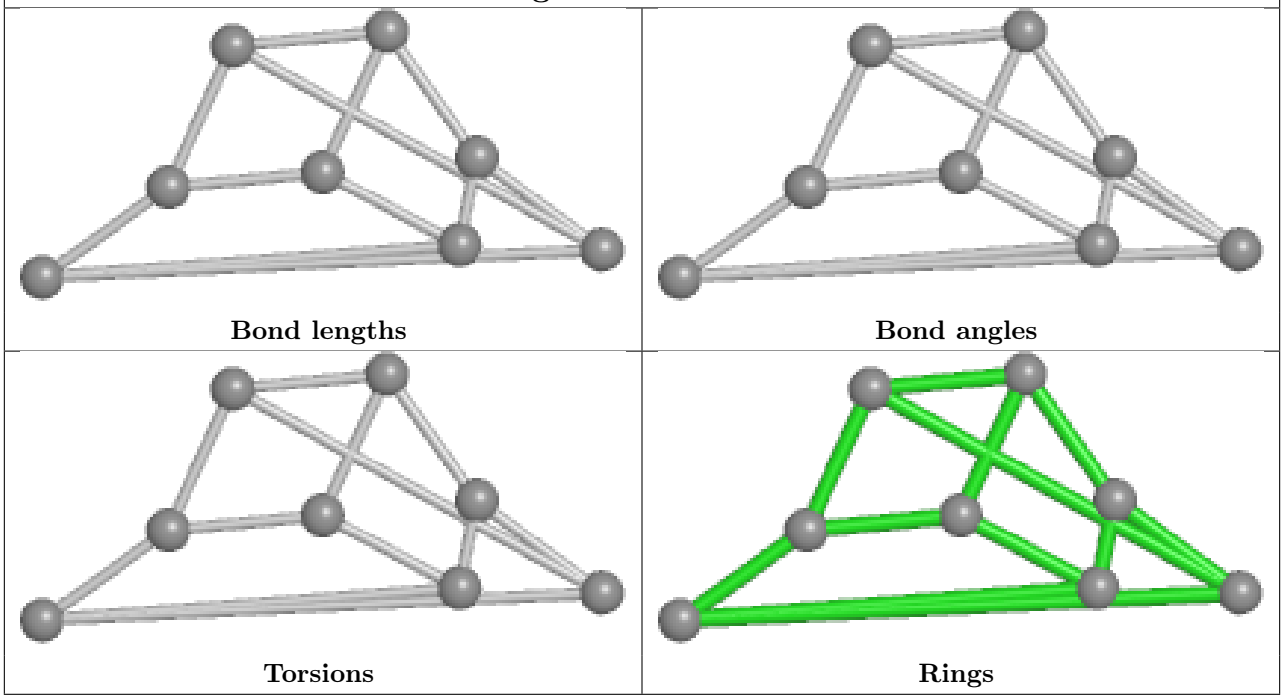


Rings

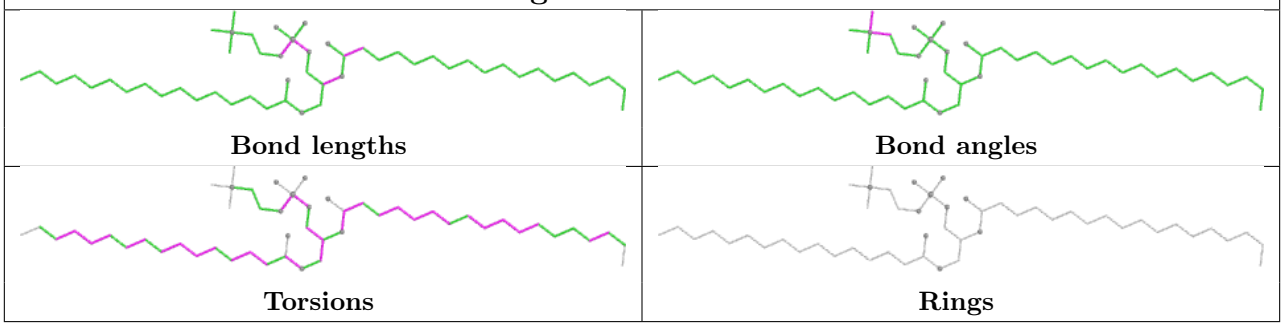
Ligand CDL r 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL a 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

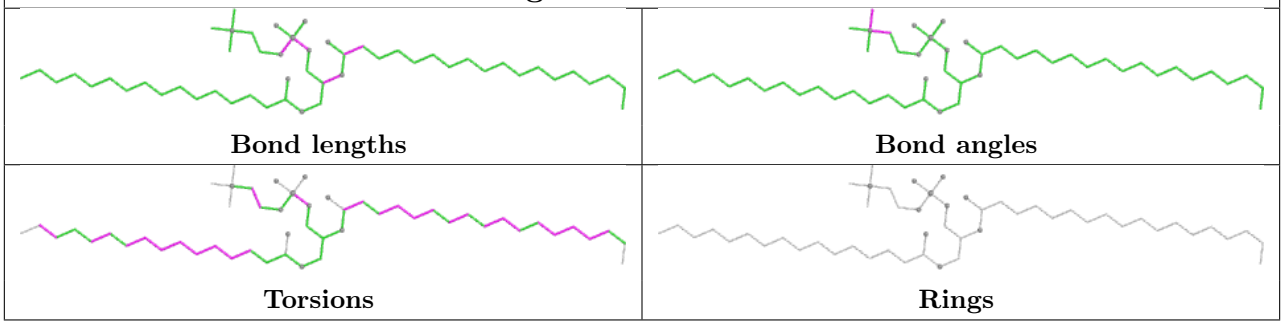
Ligand SF4 C 301



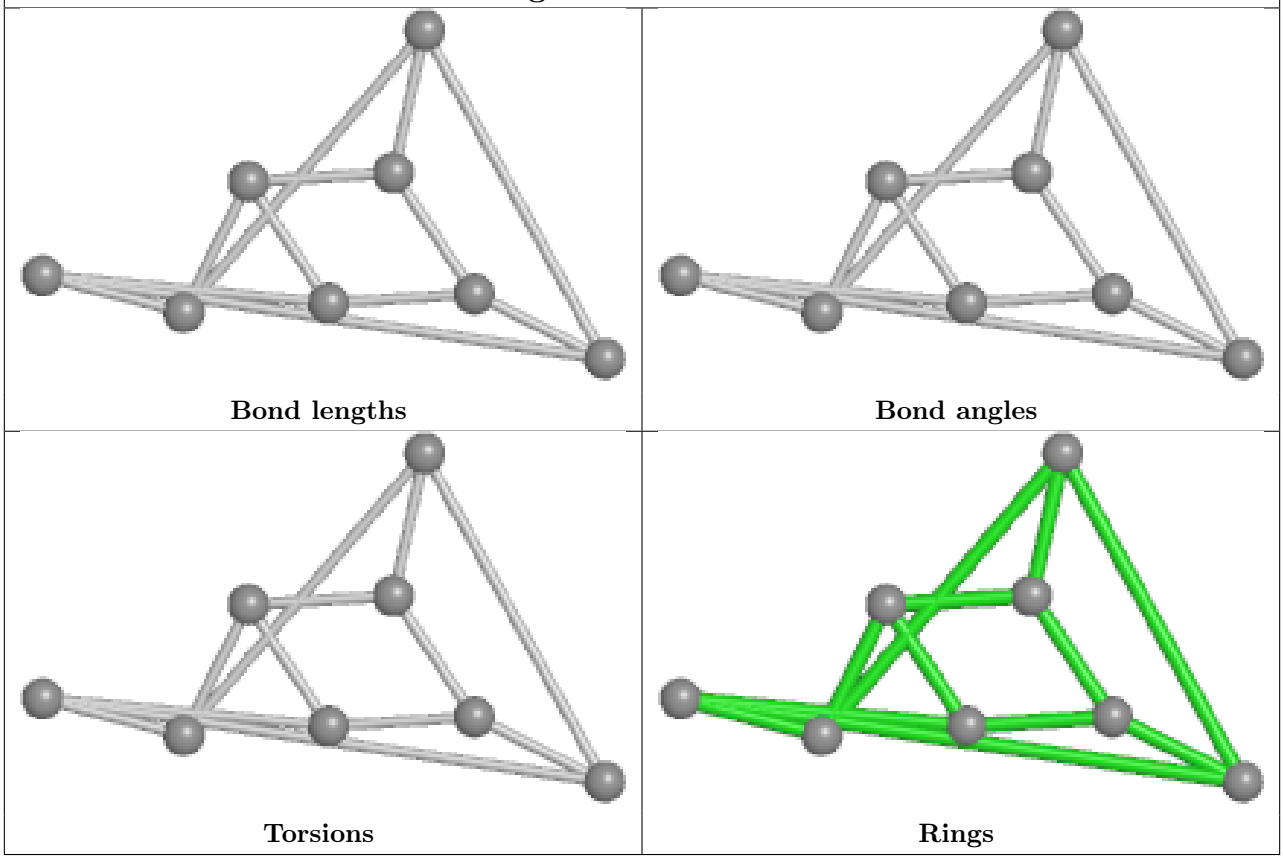
Ligand PLX a 202



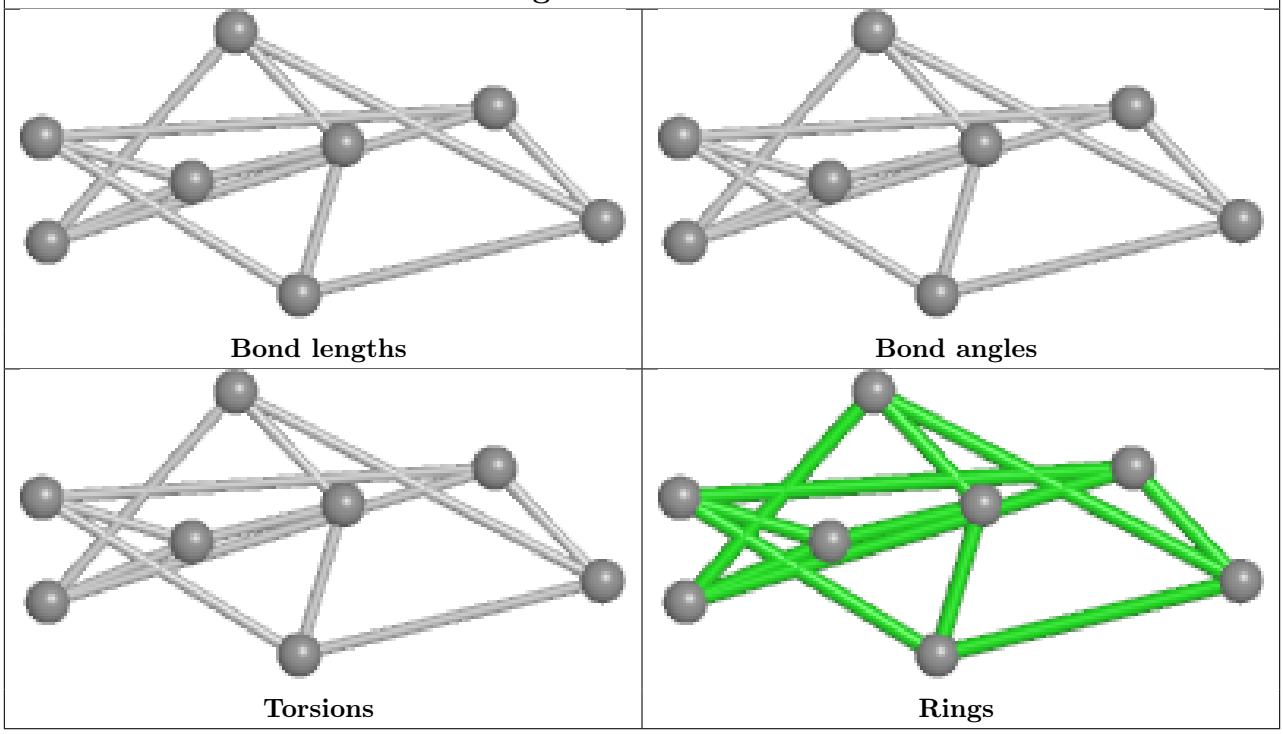
Ligand PLX C 303

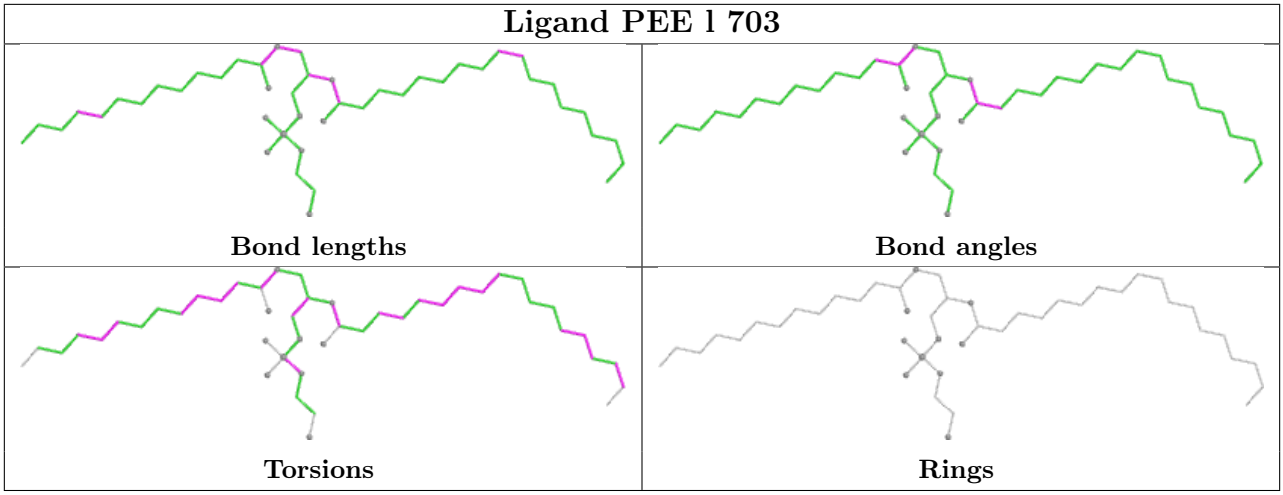


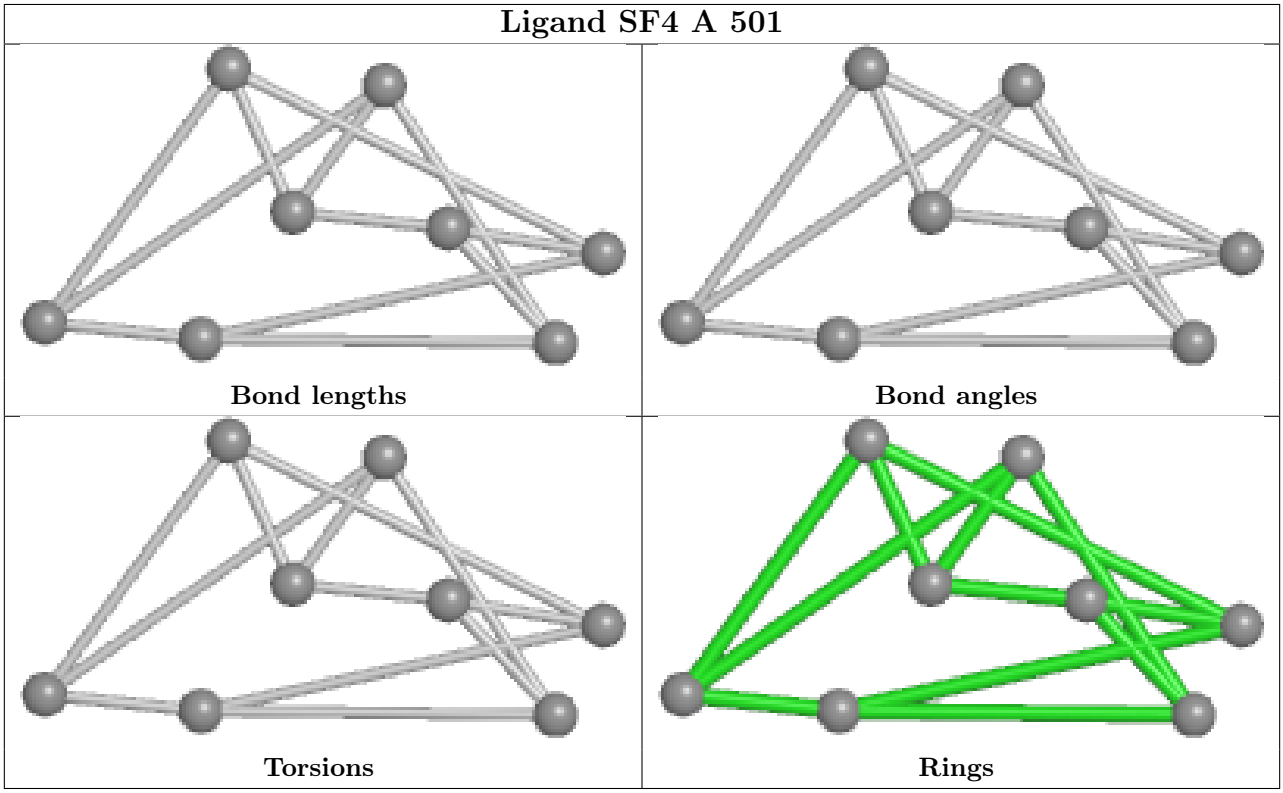
Ligand SF4 M 801



Ligand SF4 B 301







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.

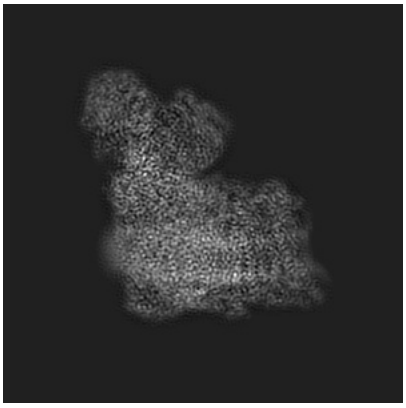
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-32263. These allow visual inspection of the internal detail of the map and identification of artifacts.

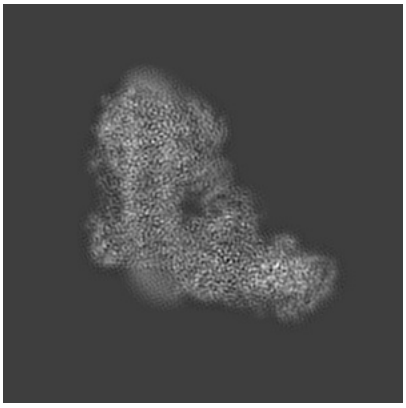
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

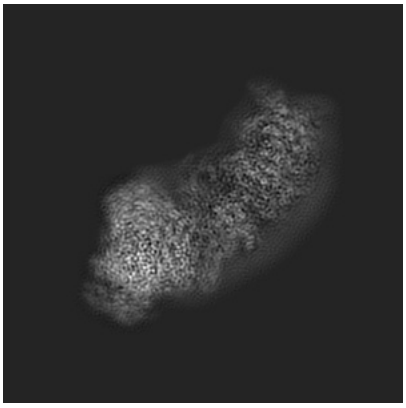
6.1.1 Primary map



X



Y

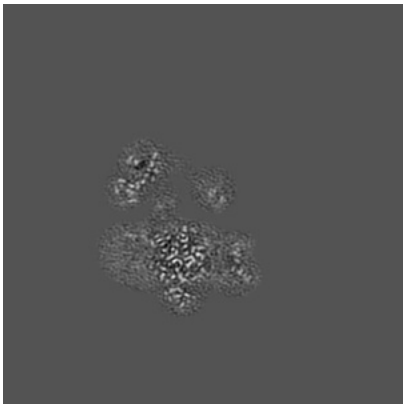


Z

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

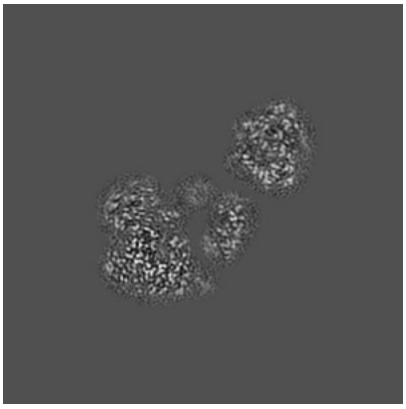
6.2 Central slices (i)

6.2.1 Primary map



X Index: 155

Y Index: 155



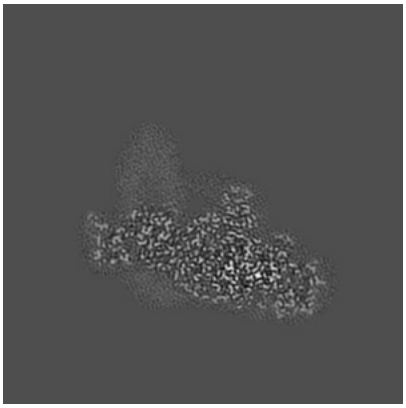
Z Index: 155

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

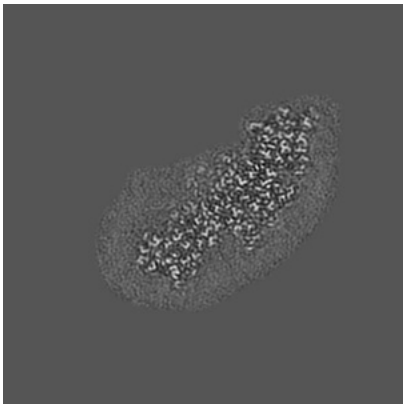
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 106



Y Index: 109

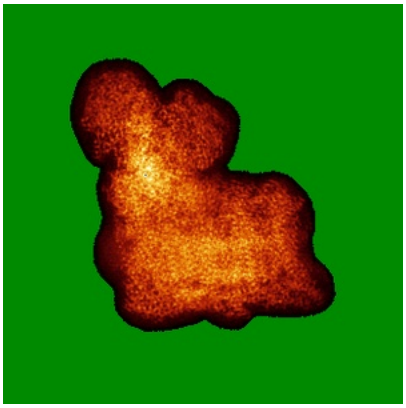


Z Index: 120

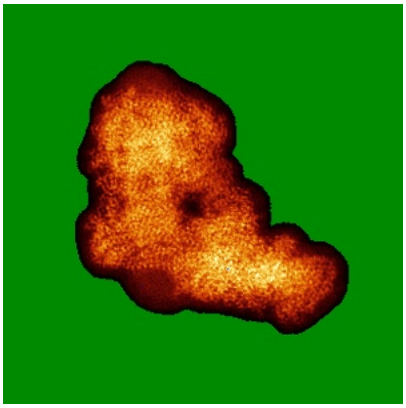
The images above show the largest variance slices of the map in three orthogonal directions.

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

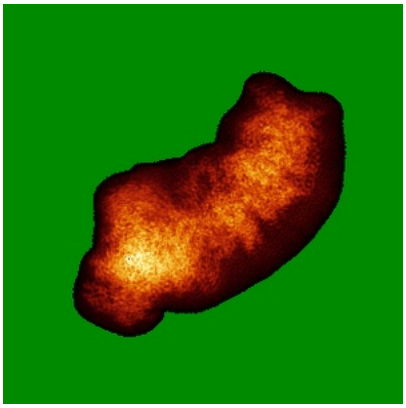
6.4.1 Primary map



X



Y

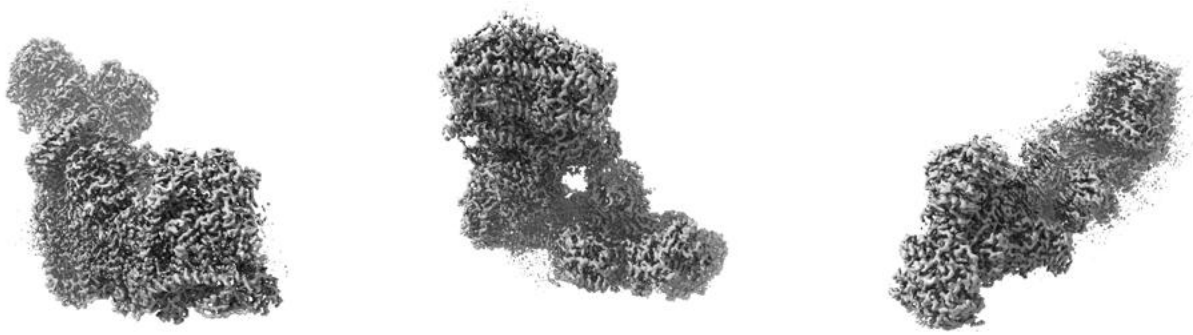


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0279. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

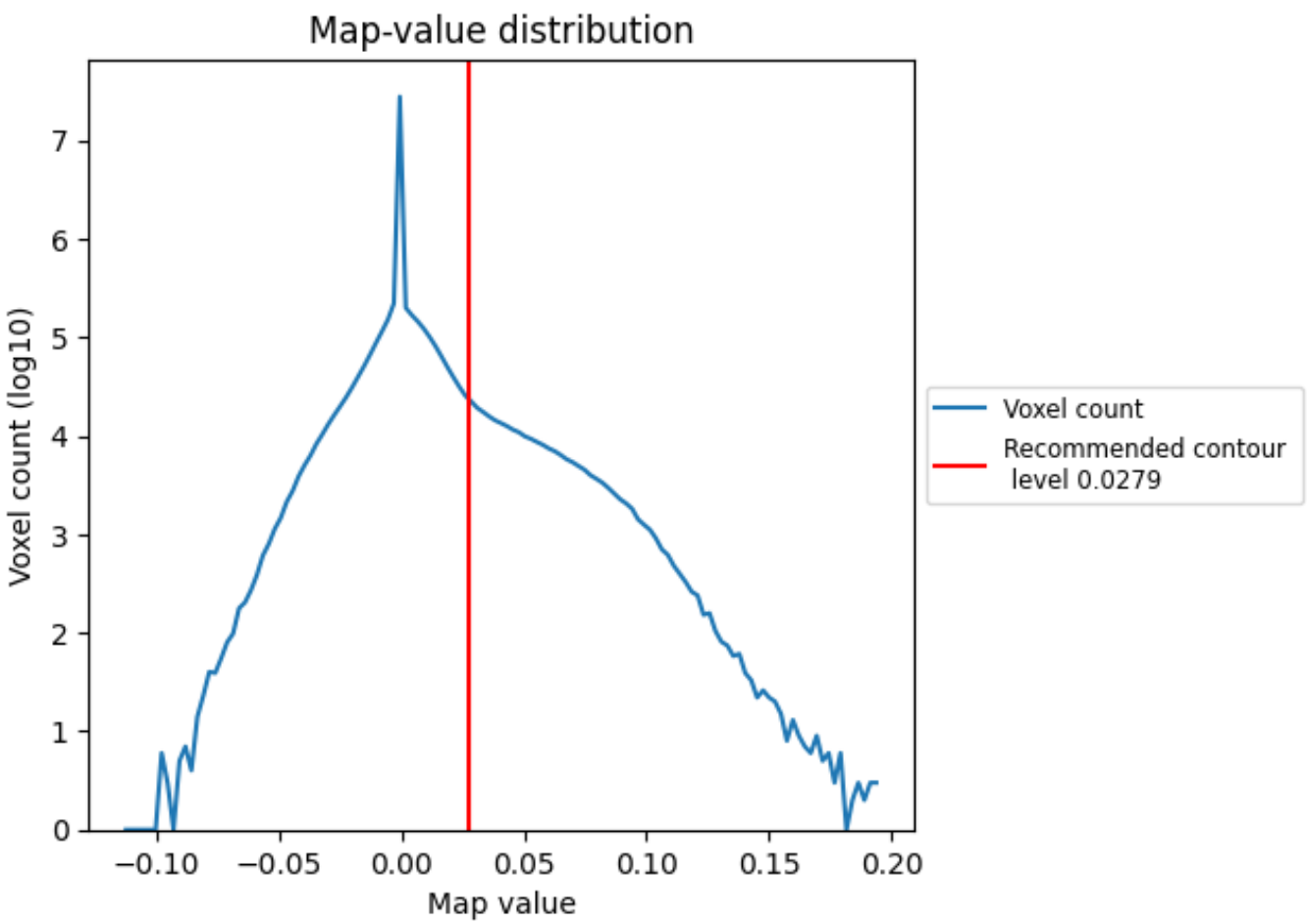
6.6 Mask visualisation (i)

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

7 Map analysis (i)

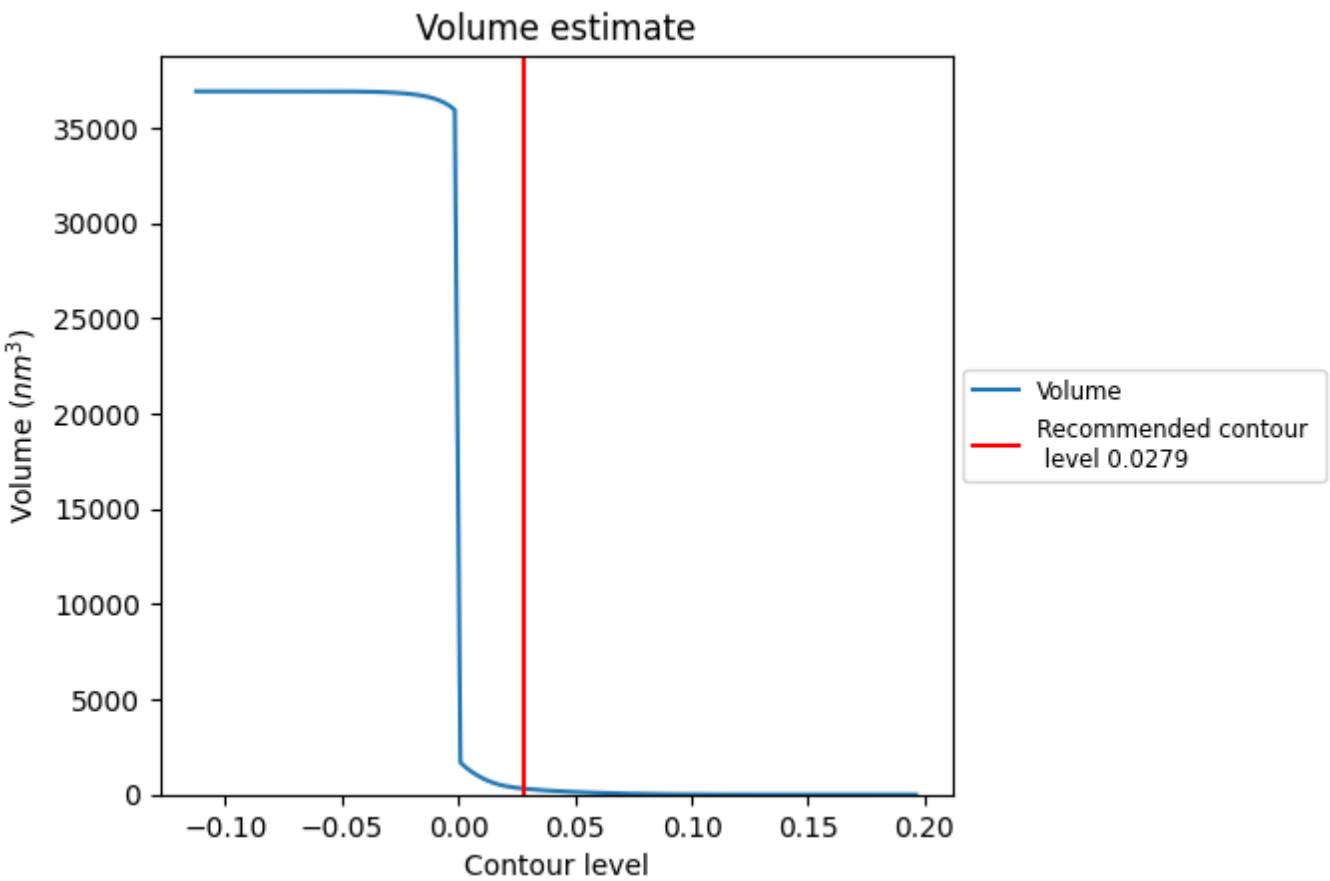
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

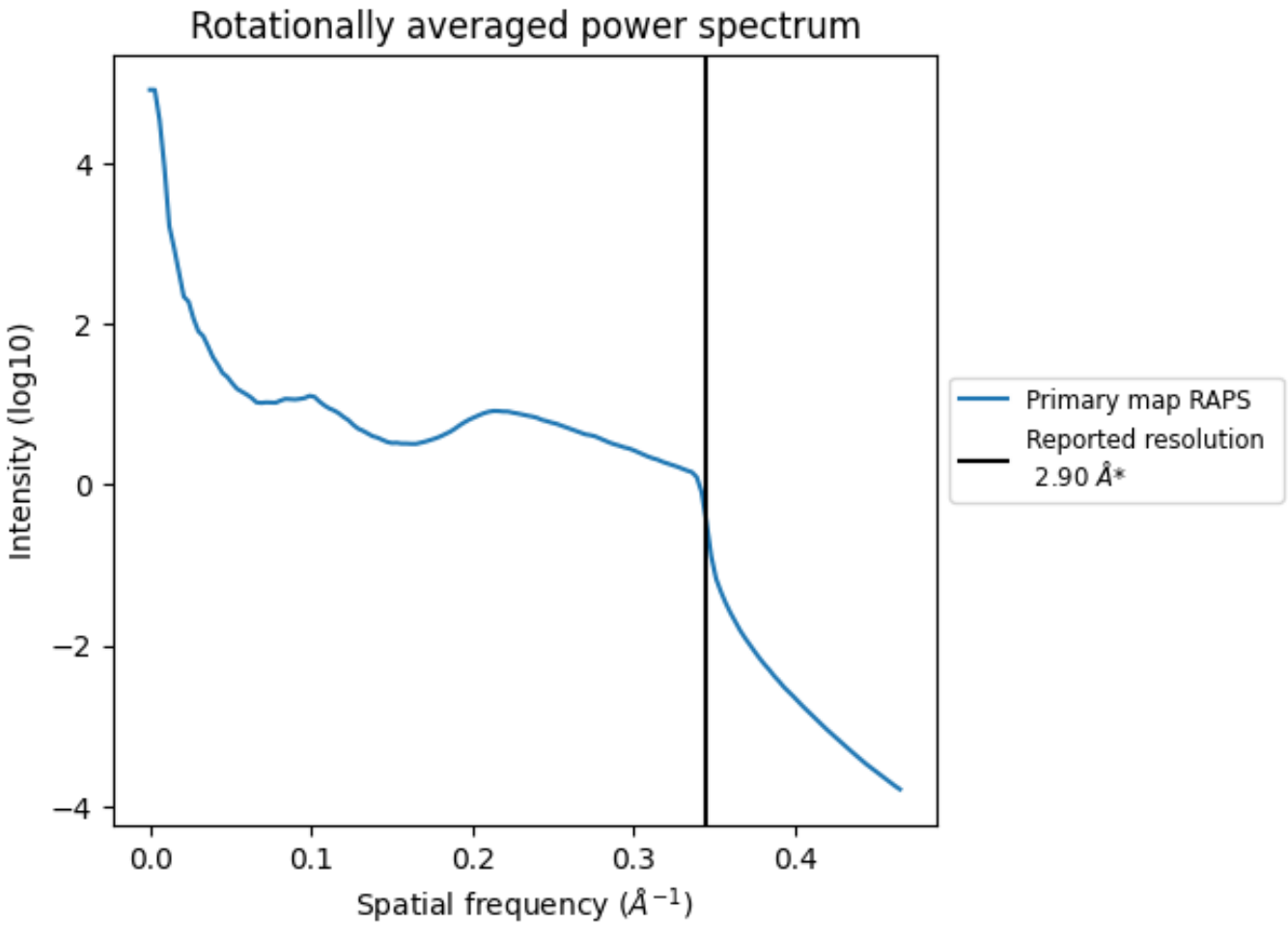
7.2 Volume estimate (i)



The volume at the recommended contour level is 312 nm^3; this corresponds to an approximate mass of 282 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 0.345 Å^{-1}

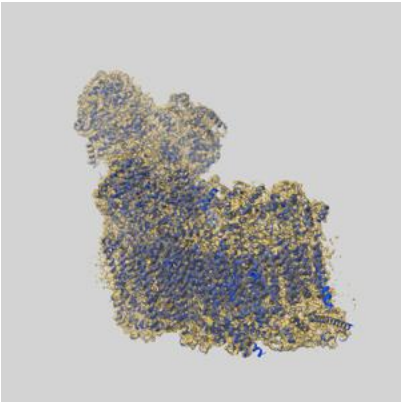
8 Fourier-Shell correlation (i)

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

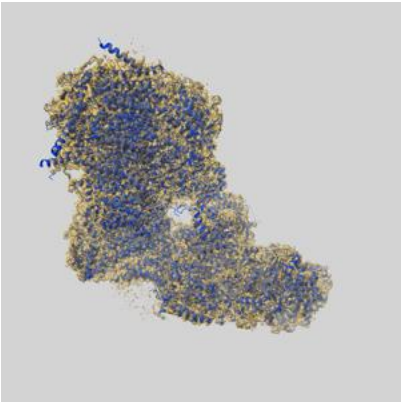
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-32263 and PDB model 7W2K. Per-residue inclusion information can be found in section 3 on page 20.

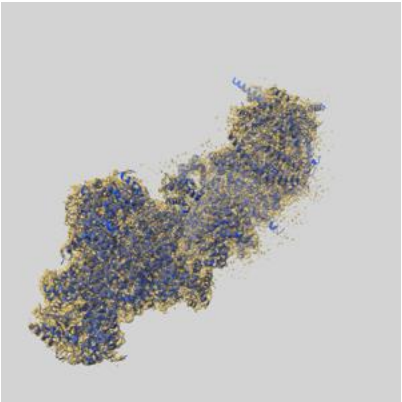
9.1 Map-model overlay (i)



X



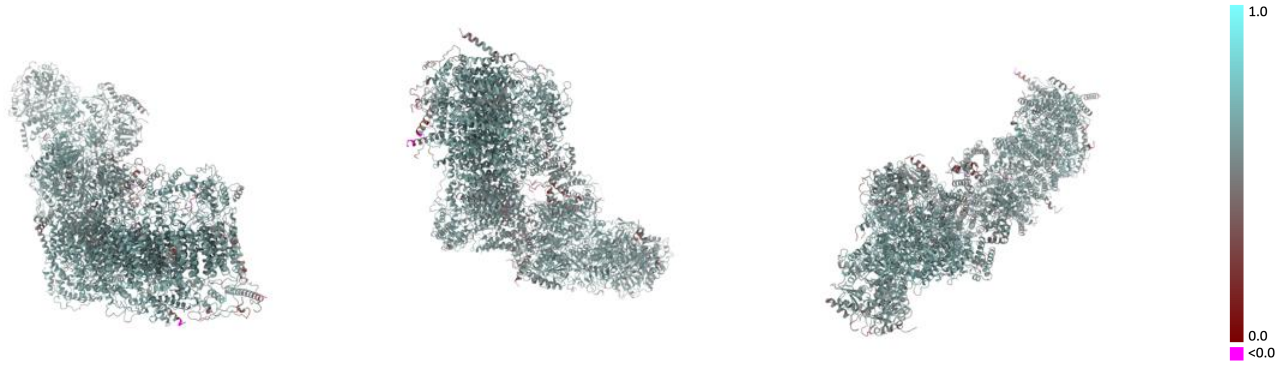
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0279 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

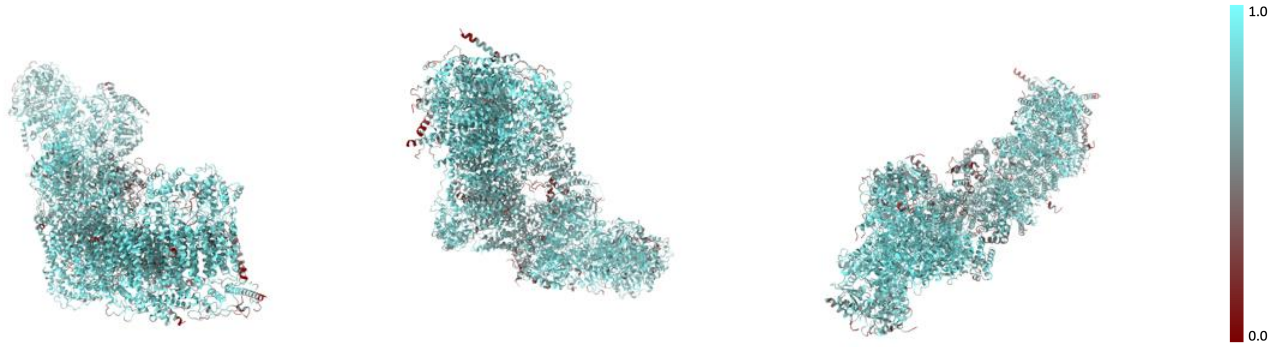
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

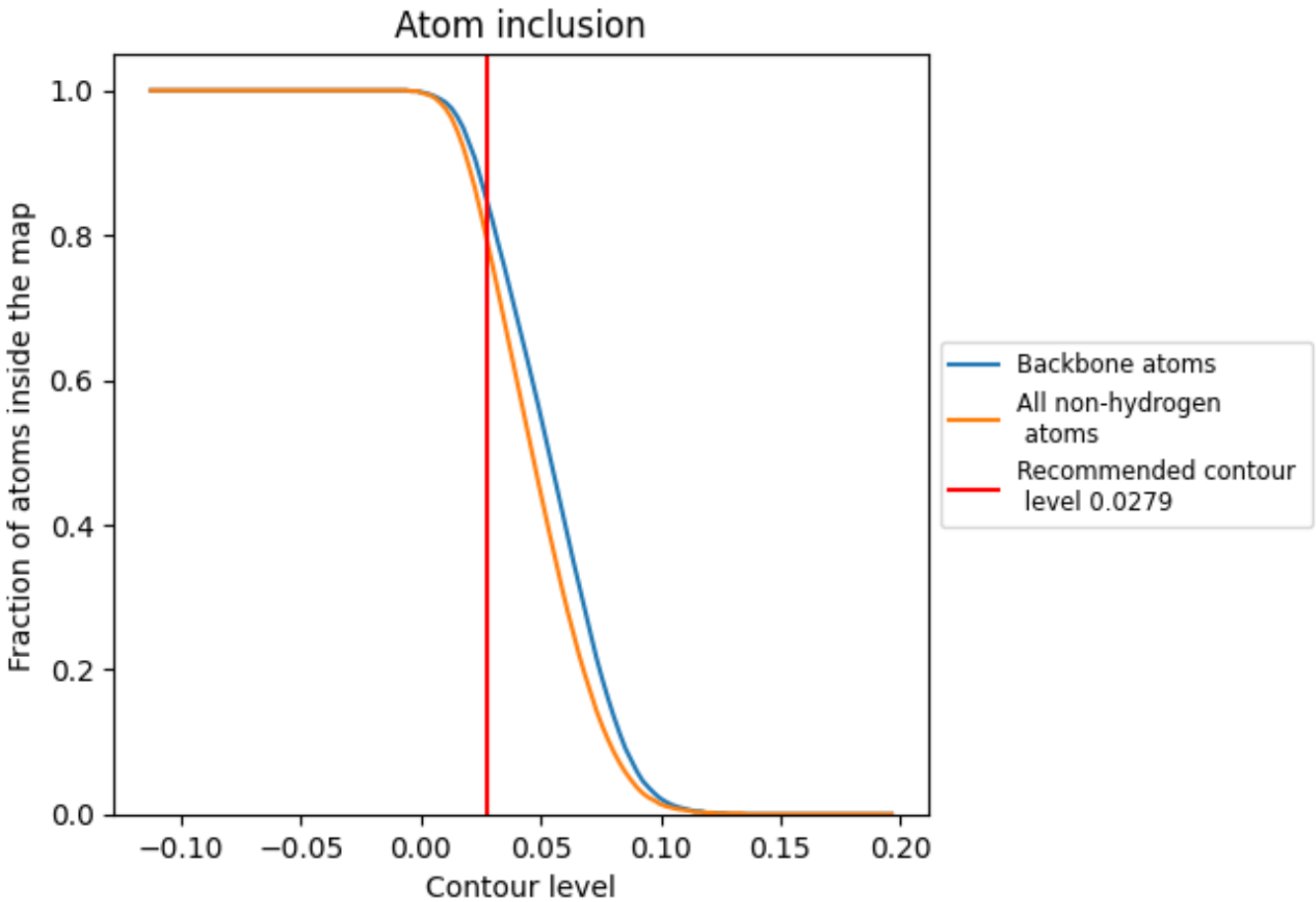
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0279).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0279) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7890	0.5830
A	0.7720	0.5670
B	0.9180	0.6290
C	0.8490	0.6110
E	0.7430	0.5680
F	0.6400	0.5080
G	0.4400	0.4210
H	0.7530	0.5670
I	0.7470	0.5830
J	0.7200	0.5600
K	0.6890	0.5540
L	0.8300	0.6020
M	0.8200	0.5880
N	0.7650	0.5930
O	0.7330	0.5490
P	0.8990	0.6210
Q	0.8790	0.6190
S	0.8790	0.6060
T	0.8010	0.5970
U	0.7890	0.5740
V	0.5860	0.5290
W	0.8150	0.5890
X	0.7450	0.5670
Y	0.7030	0.5440
Z	0.5870	0.4990
a	0.8110	0.6030
b	0.6740	0.5370
c	0.7720	0.5710
d	0.7650	0.5680
e	0.7190	0.5630
f	0.6920	0.5520
g	0.8330	0.6010
h	0.8110	0.5930
i	0.8660	0.6180
j	0.6570	0.5630

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Chain	Atom inclusion	Q-score
k	0.7560	0.5920
l	0.8270	0.6020
m	0.7320	0.5680
n	0.6840	0.5620
o	0.7800	0.5840
p	0.7850	0.5700
r	0.8740	0.6180
s	0.8280	0.5970
u	0.8140	0.5980
v	0.6880	0.5220
w	0.7360	0.5630