Full wwPDB EM Validation Report (i)

Aug 5, 2026 – 10:19 PM JST

PDB ID	:	7V2C / pdb_00007v2c
EMDB ID	:	EMD-31640
Title	:	Active state complex I from Q10 dataset
Authors	:	Gu, J.K.; Yang, M.J.
Deposited on	:	2021-08-08
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:

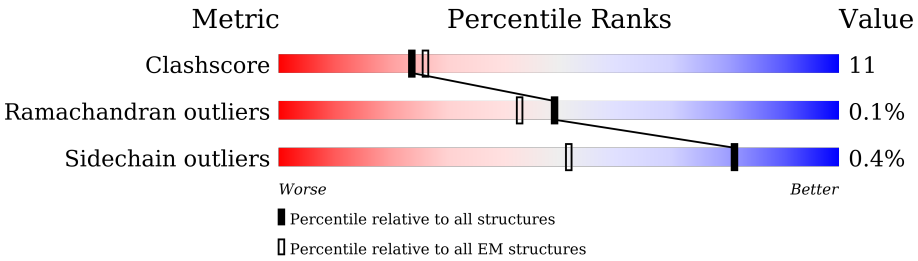
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

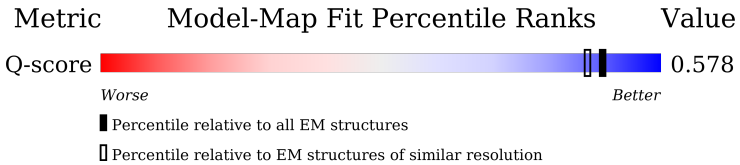
1 Overall quality at a glance (i)

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	433	75% 25%
2	B	176	84% 16%
3	C	156	84% 16%
4	E	115	72% 27%

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Mol	Chain	Length	Quality of chain
5	F	86	5% 73% 27%
6	G	88	8% 70% 24%
6	X	88	84% 16%
7	H	112	81% 16%
8	I	112	68% 18% 13%
9	J	342	84% 16%
10	K	43	77% 21%
11	L	125	5% 84% 16%
12	M	690	77% 23%
13	N	144	85% 15%
14	O	217	81% 19%
15	P	208	78% 21%
16	Q	430	78% 22%
17	S	70	80% 19%
18	T	96	85% 15%
19	U	83	88% 12%
20	V	140	86% 14%
21	W	142	82% 18%
22	Y	67	90% 10%
23	Z	80	9% 90% 10%
24	a	138	86% 13%
25	b	126	63% 14% 22%
26	c	156	78% 22%
27	d	175	74% 26%
28	e	104	68% 32%

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Mol	Chain	Length	Quality of chain
29	f	49	16% 100%
30	g	121	87% 12%
31	h	105	82% 16%
32	i	347	73% 26%
33	j	115	79% 21%
34	k	98	76% 24%
35	l	606	73% 26%
36	m	175	79% 21%
37	n	56	11% 71% 27%
38	o	128	84% 15%
39	p	178	88% 12%
40	r	459	82% 17%
41	s	318	74% 24%
42	u	171	80% 19%
43	v	125	79% 20%
44	w	320	82% 18%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	A	501	-	-	X	-
45	SF4	M	802	-	-	X	-
46	FMN	A	502	-	-	X	-
51	UQ	s	501	-	-	X	-

2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 68315 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	88	690	446	102	137	5	0	0
6	X	88	694	447	103	139	5	0	0

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

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 NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	43	366	228	68	69	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	5296	3320	923	1014	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	1671	1065	281	315	10	0	0

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

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 NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	430	3459	2212	594	629	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	566	364	103	94	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	53	ARG	CYS	conflict	UNP K7GR43

- 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 NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

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 NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	b	98	819	537	144	137	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	104	867	553	142	168	4	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	f	49	378	246	65	67	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	2710	1782	420	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	115	914	615	134	158	7	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	606	4816	3193	746	826	51	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	175	1291	861	188	229	13	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	479	311	88	79	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	1062	691	182	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	318	2508	1678	385	424	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	1028	642	195	182	9	0	0

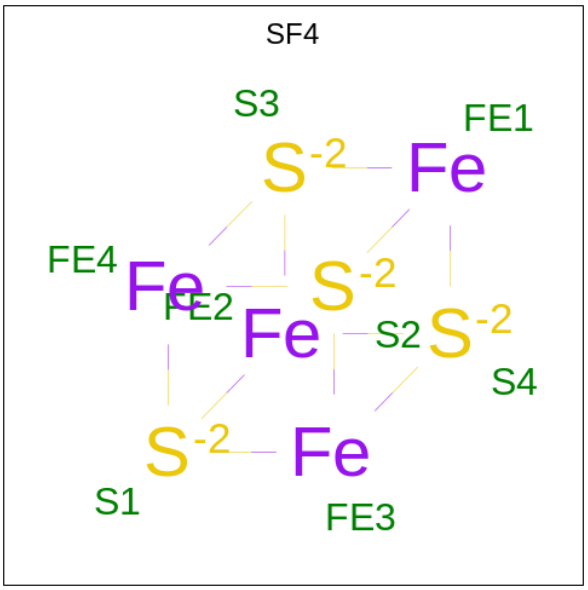
There is a discrepancy between the modelled and reference sequences:

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

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

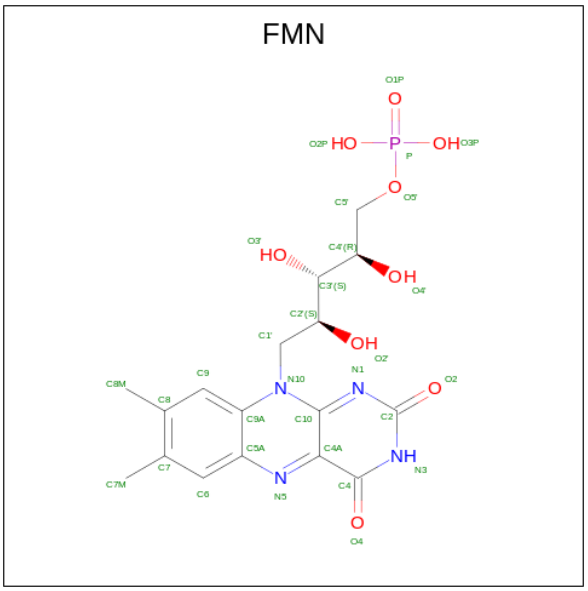
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	w	320	2590	1649	440	491	10	0	0

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



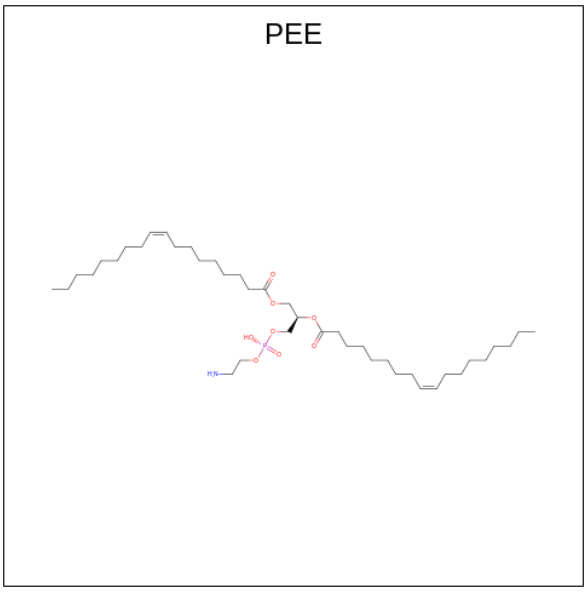
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	A	1	8	4	4	0
45	B	1	8	4	4	0
45	B	1	8	4	4	0
45	C	1	8	4	4	0
45	M	1	8	4	4	0
45	M	1	8	4	4	0

- 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 1,2-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	
47	B	1	51	41	1	8	1	0
			Total	C	N	O	P	
47	C	1	47	37	1	8	1	0

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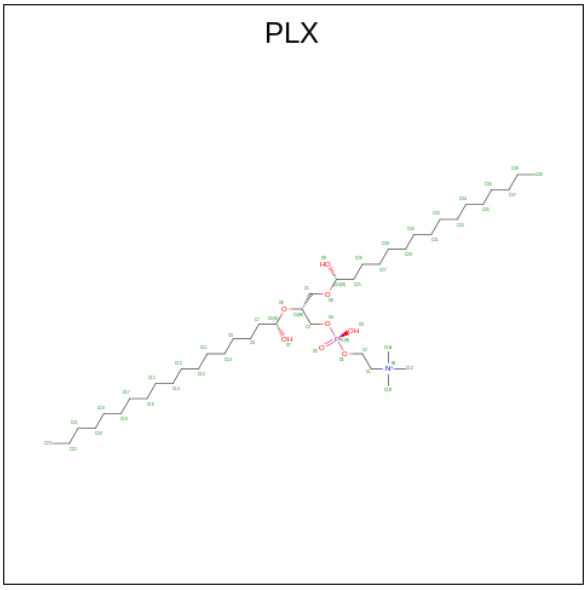
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	Q	1	47	37	1	8	1	0
47	W	1	41	31	1	8	1	0
47	b	1	46	36	1	8	1	0
47	j	1	51	41	1	8	1	0
47	j	1	41	31	1	8	1	0
47	l	1	40	30	1	8	1	0
47	l	1	51	41	1	8	1	0
47	r	1	51	41	1	8	1	0

- Molecule 48 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).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	C	1	52	42	1	8	1	0
48	J	1	52	42	1	8	1	0

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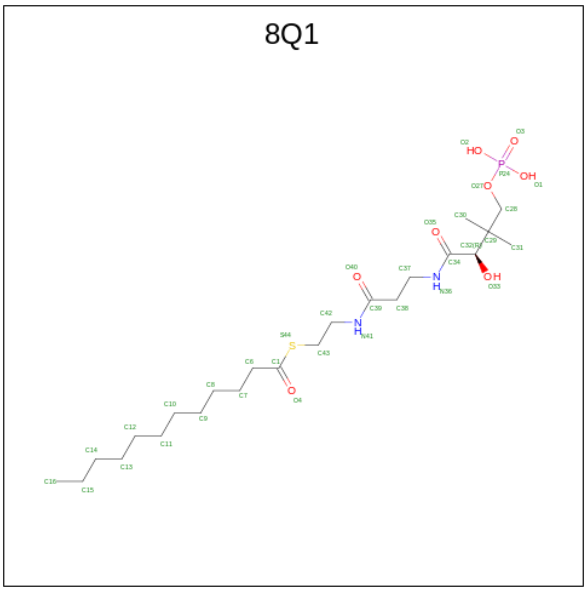
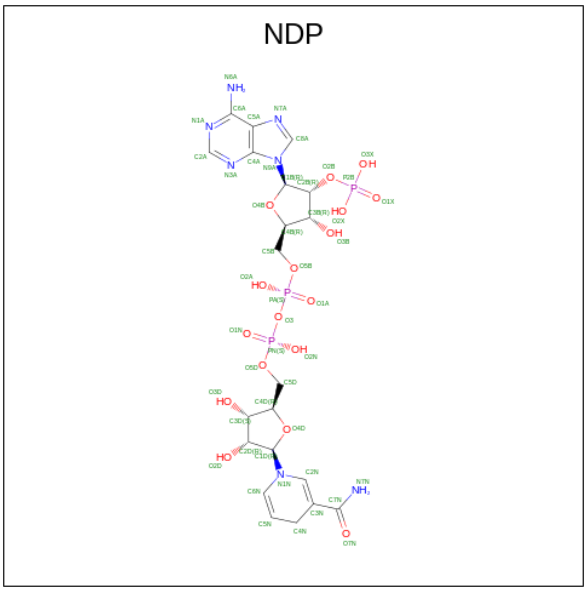
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	N	1	52	42	1	8	1	0
			Total	C	N	O	P	
48	g	1	52	42	1	8	1	0
			Total	C	N	O	P	
48	j	1	52	42	1	8	1	0
			Total	C	N	O	P	
48	n	1	52	42	1	8	1	0
			Total	C	N	O	P	
48	r	1	52	42	1	8	1	0
			Total	C	N	O	P	
48	r	1	52	42	1	8	1	0

- Molecule 49 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).



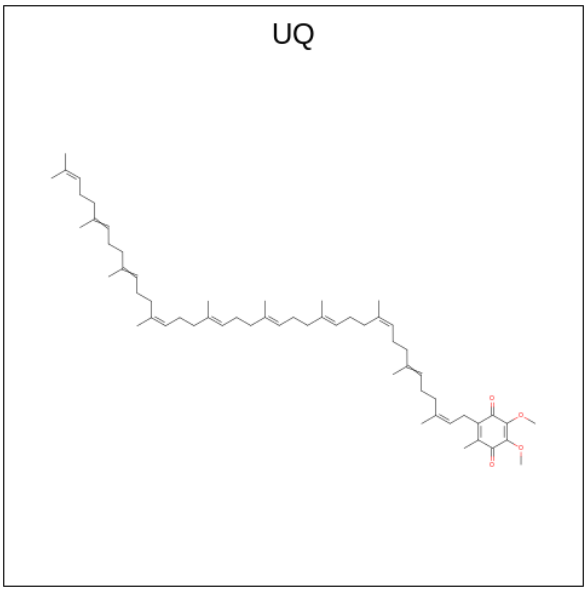
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
49	E	1	35	23	2	8	1	1	0
			Total	C	N	O	P	S	
49	X	1	35	23	2	8	1	1	0

- Molecule 50 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).



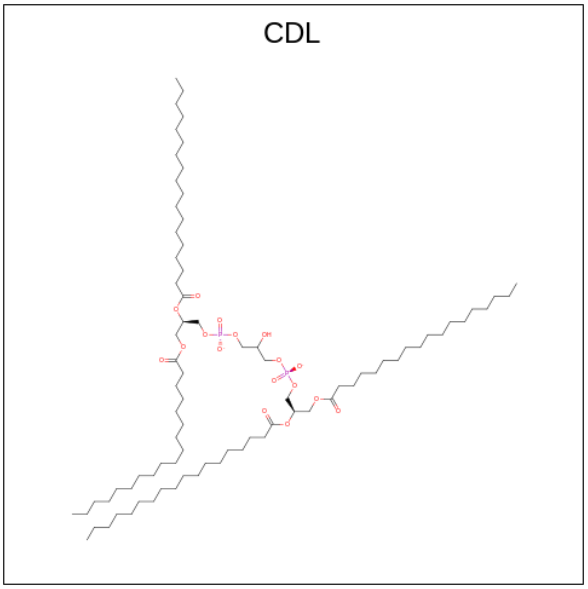
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
50	J	1	48	21	7	17	3	0

- Molecule 51 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).



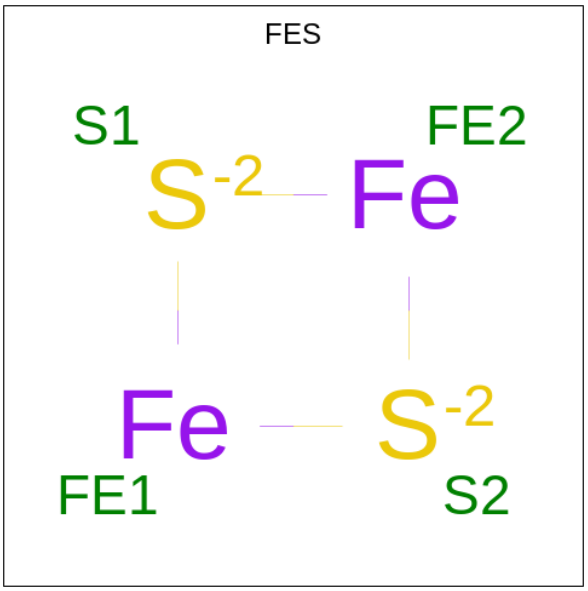
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
51	J	1	33	29	4	0
51	s	1	63	59	4	0

- Molecule 52 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
			Total	C	O	P	
52	J	1	89	70	17	2	0
52	N	1	51	32	17	2	0
52	V	1	94	75	17	2	0
52	V	1	100	81	17	2	0
52	a	1	100	81	17	2	0
52	i	1	68	49	17	2	0
52	l	1	99	80	17	2	0
52	l	1	100	81	17	2	0
52	m	1	100	81	17	2	0
52	r	1	100	81	17	2	0
52	u	1	55	36	17	2	0

- Molecule 53 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	
53	M	1	4	2	2	0
53	O	1	4	2	2	0

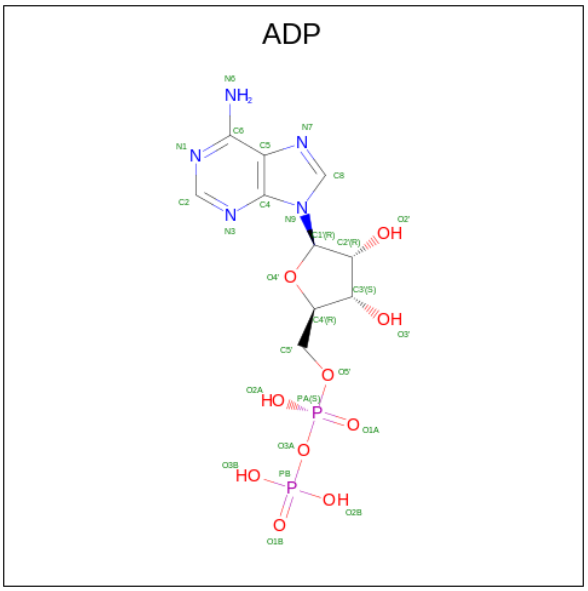
- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 56 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	
56	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: 75% 25%

A26 P27 K28 K29 R48 H49 D50 L53 K54 G55 A56 R59 G60 D61 W62 Y63 E67 K71 I76 K81 G87 R88 G96 L97 K98 M102 P110 N116 E119 D127 R128 I131 R132 H136 G141 G146 M149 R152 I158

R159 G160 E161 E165 R174 Y177 F193 D194 A201 Y204 K222 P227 A231 C238 P239 T240 T241 V242 A243 N244 V245 V248 A249 V250 S251 P252 T253 T254 C255 R256 F262 A263 N270 S271 G272 T273 H281 P285 V288 M292 P295 L296

K297 E298 H303 V317 P325 L326 D338 D358 D362 I363 A366 E377 S378 C379 G380 C385 R386 E387 G388 V389 D390 W391 M392 R398 D403 E408 S411 E414 T415 S416 E420 G421 H422 T423 T424 C425 A426 D429 W433 Q436 E448

R449 Q452 Q458

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

Chain B: 84% 16%

T37 Y38 K39 M43 S47 R56 W63 L66 L74 S75 Y76 R79 E80 I84 E89 S94 R98 G99 E100 H101 E111 R141 R144 Y145 D146 M149 E160 D165 E169 L184 Y185 N192 E200 Y211 R212

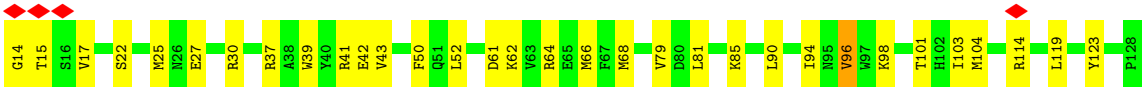
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7,mitochondrial

Chain C: 84% 16%

S41 R42 V46 L50 D51 D52 L53 V54 N55 W56 A73 Y74 E75 M76 W77 R83 R88 A95 S96 Q99 M103 L109 L117 R118 K119 V120 Y121 P125 Y147 P167 K188 R189 L190 R196

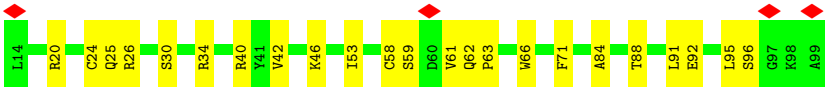
• Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain E: 72% 27%



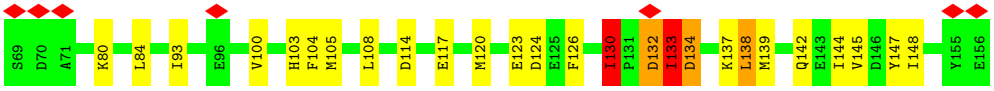
• Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain F:



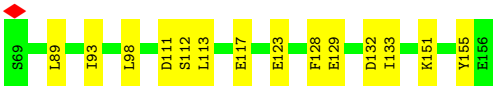
• Molecule 6: Acyl carrier protein, mitochondrial

Chain G:



• Molecule 6: Acyl carrier protein, mitochondrial

Chain X:

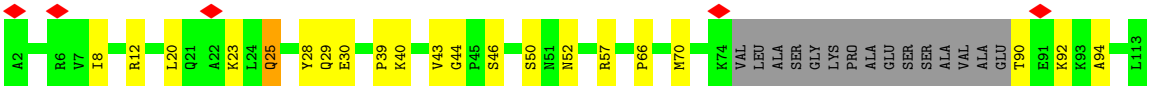


• Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain H:

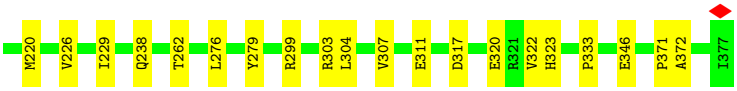
• Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain I:



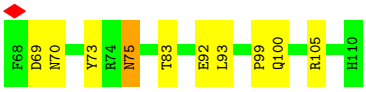
• Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain J:



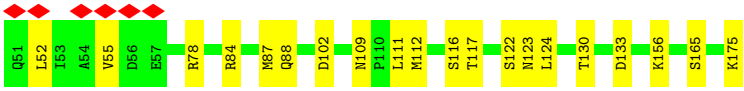
• Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain K:



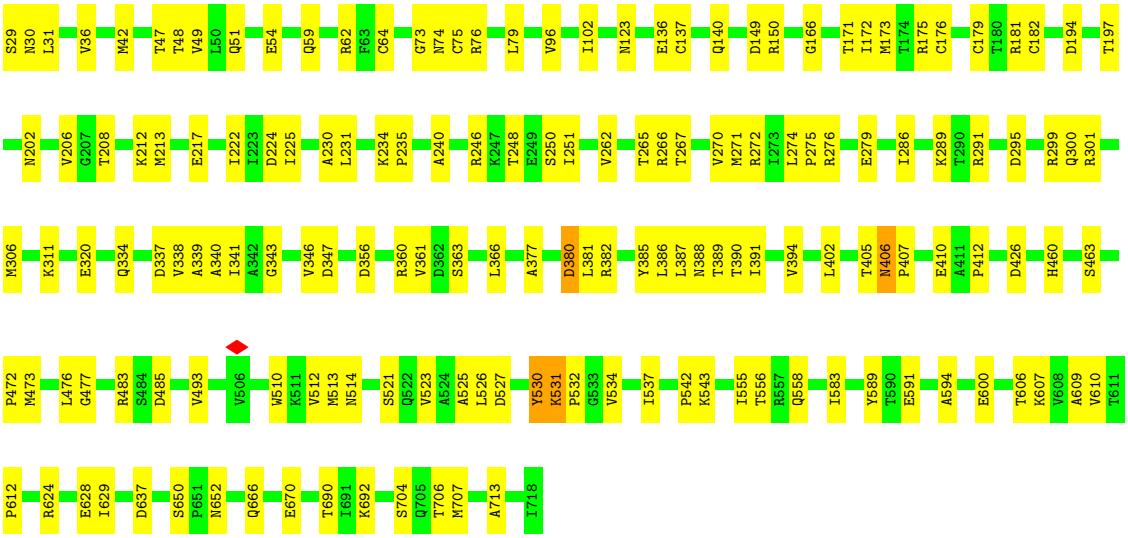
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain L:



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

Chain M:

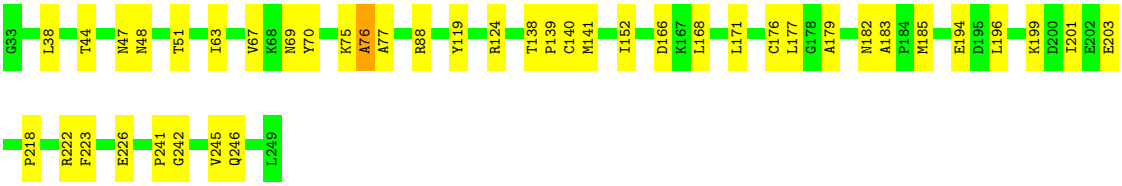


• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain N:

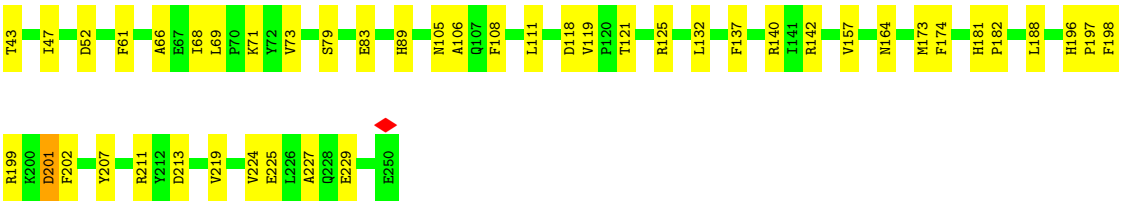
• Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain O:



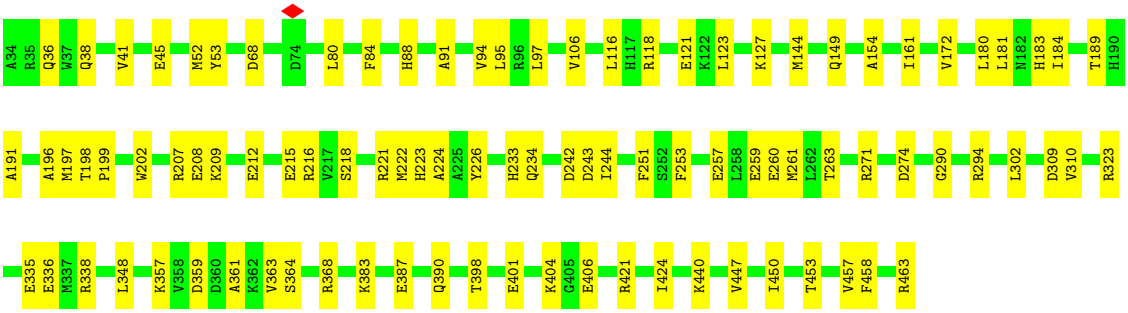
• Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain P: 78% 21%



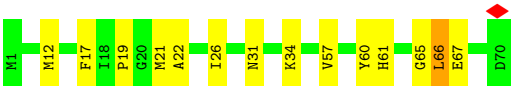
• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain Q: 78% 22%



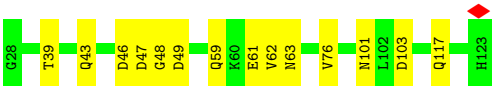
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S: 80% 19%



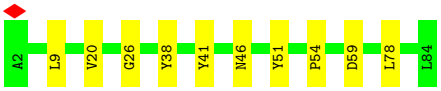
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T: 85% 15%



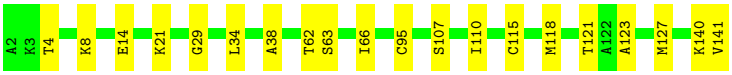
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U: 88% 12%



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

Chain V:

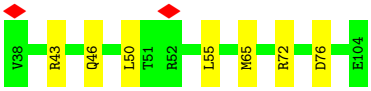


• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:

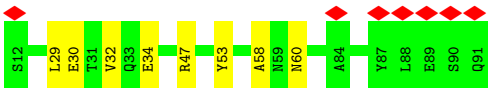
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y:



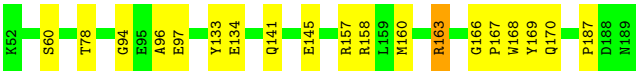
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z:



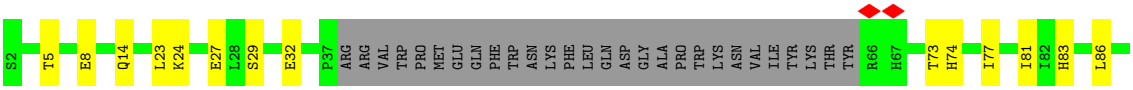
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

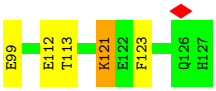
Chain a:



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

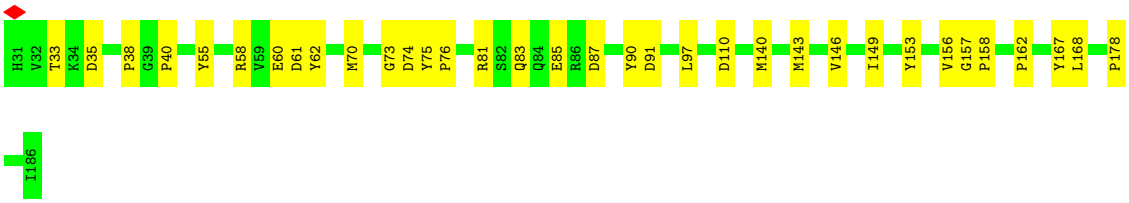
Chain b:





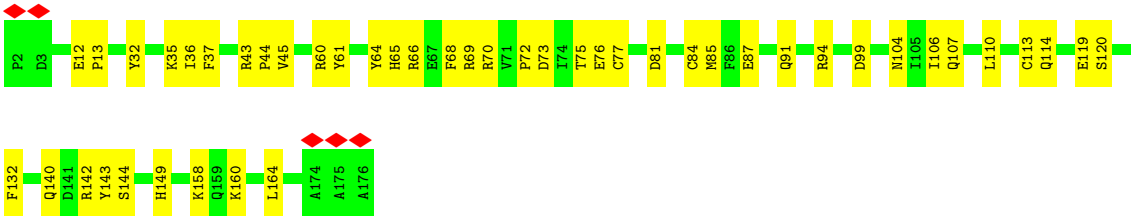
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c:



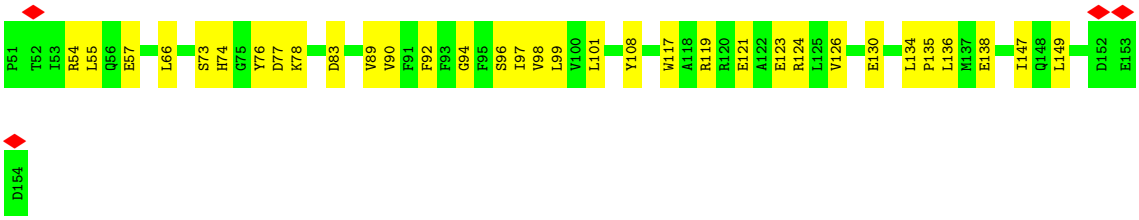
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d:



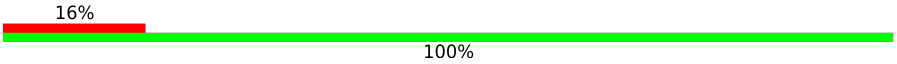
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

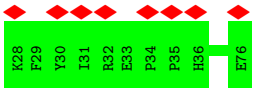
Chain e:



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

Chain f:



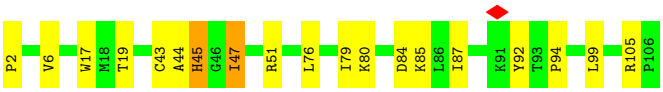


• Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g:

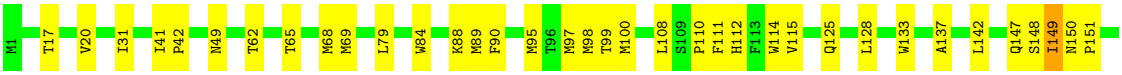
• Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

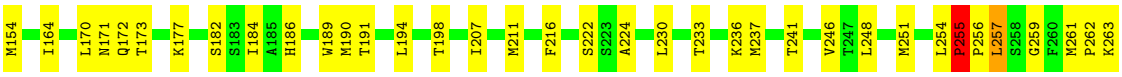
Chain h:

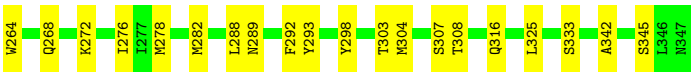


• Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain i:







• Molecule 33: NADH-ubiquinone oxidoreductase chain 3

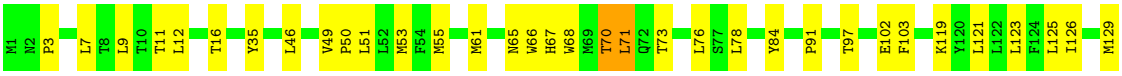
Chain j:

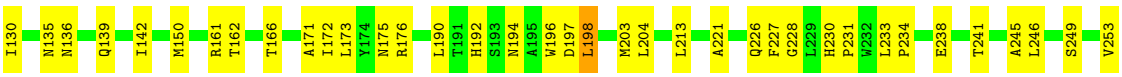
• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

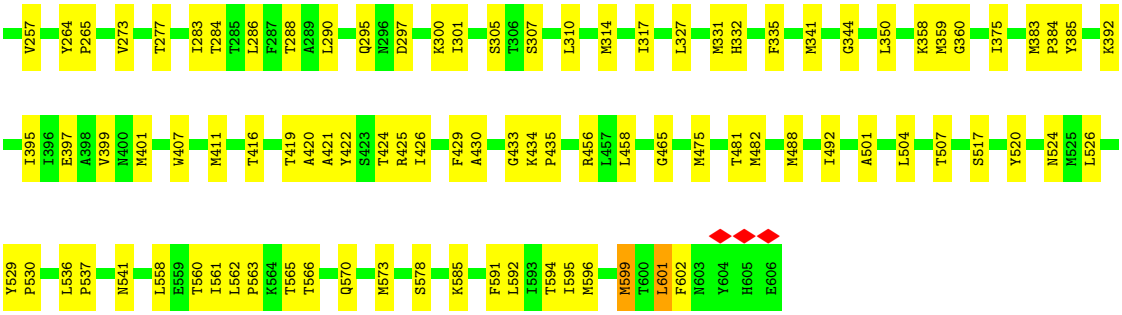
Chain k:

• Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l:

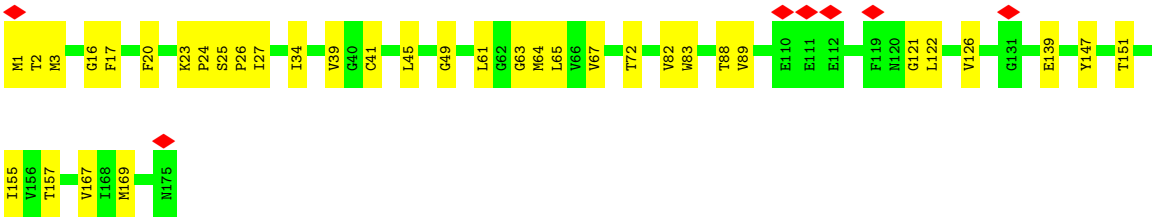






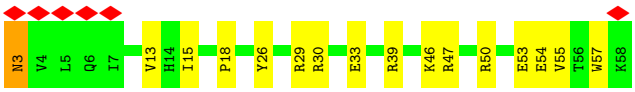
• Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain m:



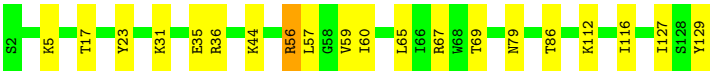
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n:



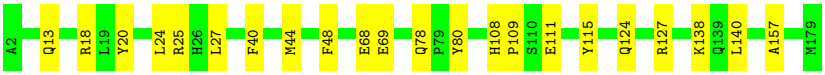
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o:



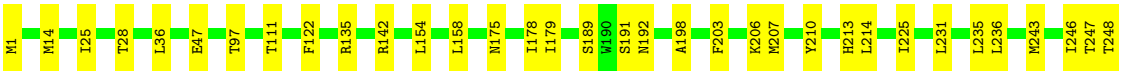
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p:



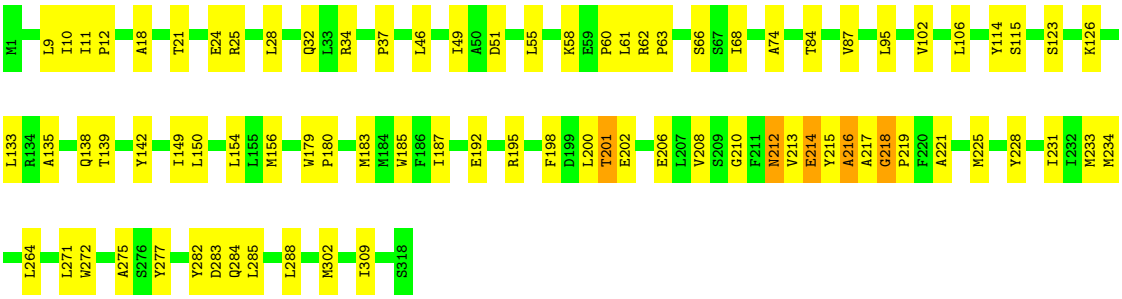
• Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r:



• Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s:

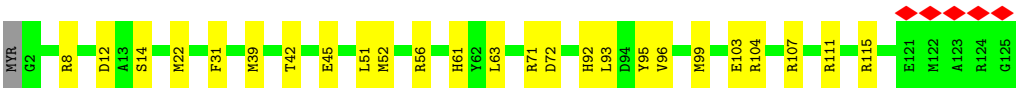


• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:

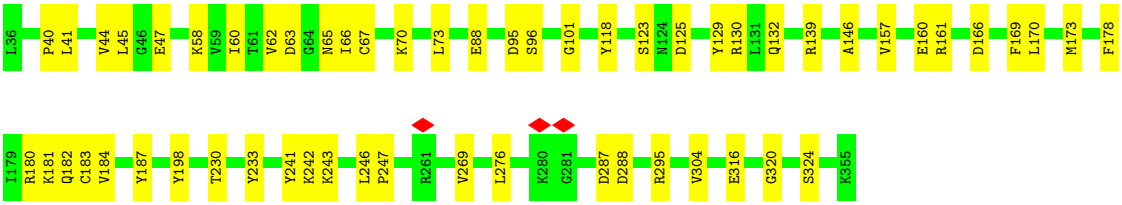
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v:



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

Chain w:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	252573	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	0.211	Depositor
Minimum map value	-0.081	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	354.48602, 354.48602, 354.48602	wwPDB
Map dimensions	330, 330, 330	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: PEE, FMN, ADP, SF4, FES, 2MR, ZN, CDL, 8Q1, NDP, MG, UQ, PLX

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	0.19	0/3406	0.41	0/4603
2	B	0.19	0/1443	0.32	0/1952
3	C	0.22	0/1279	0.38	0/1730
4	E	0.18	0/995	0.42	0/1340
5	F	0.18	0/698	0.47	0/940
6	G	0.27	0/702	0.81	7/952 (0.7%)
6	X	0.15	0/705	0.36	0/954
7	H	0.17	0/929	0.46	1/1258 (0.1%)
8	I	0.20	0/798	0.50	0/1079
9	J	0.19	0/2828	0.39	1/3834 (0.0%)
10	K	0.10	0/377	0.23	0/509
11	L	0.17	0/1039	0.41	0/1403
12	M	0.22	0/5384	0.55	9/7295 (0.1%)
13	N	0.12	0/1245	0.30	0/1694
14	O	0.18	0/1711	0.48	2/2328 (0.1%)
15	P	0.25	0/1789	0.56	3/2436 (0.1%)
16	Q	0.21	0/3538	0.39	0/4796
17	S	0.22	0/581	0.55	0/781
18	T	0.17	0/755	0.35	0/1018
19	U	0.13	0/664	0.28	0/912
20	V	0.16	0/1042	0.33	0/1411
21	W	0.17	0/1192	0.36	0/1610
22	Y	0.13	0/610	0.34	0/836
23	Z	0.15	0/660	0.37	0/892
24	a	0.18	0/1184	0.44	1/1603 (0.1%)
25	b	0.17	0/844	0.41	0/1149
26	c	0.16	0/1371	0.37	0/1875
27	d	0.15	0/1494	0.36	0/2015
28	e	0.16	0/891	0.40	0/1210
29	f	0.15	0/386	0.35	0/523
30	g	0.16	0/1031	0.38	1/1394 (0.1%)
31	h	0.19	0/889	0.52	2/1190 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	i	0.22	0/2773	0.51	1/3768 (0.0%)
33	j	0.18	0/938	0.41	0/1281
34	k	0.21	0/759	0.48	1/1029 (0.1%)
35	l	0.19	0/4947	0.44	3/6728 (0.0%)
36	m	0.17	0/1323	0.42	0/1797
37	n	0.13	0/491	0.32	0/663
38	o	0.17	0/1092	0.44	0/1481
39	p	0.13	0/1590	0.29	0/2155
40	r	0.19	0/3723	0.41	1/5078 (0.0%)
41	s	0.22	0/2581	0.54	5/3529 (0.1%)
42	u	0.17	0/1436	0.40	0/1938
43	v	0.13	0/1052	0.36	0/1411
44	w	0.15	0/2650	0.37	1/3588 (0.0%)
All	All	0.19	0/67815	0.44	39/91968 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
25	b	0	1
32	i	0	1
All	All	0	3

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	s	216	ALA	N-CA-C	10.79	123.12	111.36
40	r	250	LEU	N-CA-C	8.70	120.76	111.28
41	s	206	GLU	N-CA-C	8.52	120.34	111.14
35	l	192	HIS	N-CA-C	8.11	120.20	111.36
12	M	74	ASN	N-CA-C	8.09	120.17	111.36
32	i	115	VAL	CB-CA-C	-7.10	106.83	114.35
35	l	68	TRP	N-CA-C	6.85	118.63	111.03
15	P	52	ASP	N-CA-C	6.35	118.28	111.36
41	s	210	GLY	N-CA-C	5.98	122.14	111.02
30	g	3	MET	N-CA-C	5.86	117.67	111.28
44	w	243	LYS	N-CA-C	5.79	117.67	111.36
6	G	133	ILE	CA-C-N	5.76	132.54	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	133	ILE	C-N-CA	5.76	132.54	121.54
9	J	213	PHE	N-CA-C	5.67	117.14	111.07
31	h	47	ILE	N-CA-C	5.63	116.36	110.62
12	M	531	LYS	CA-C-N	5.61	125.54	119.76
12	M	531	LYS	C-N-CA	5.61	125.54	119.76
24	a	163	ARG	N-CA-C	5.60	117.46	111.36
15	P	202	PHE	CA-C-N	5.58	125.48	119.85
15	P	202	PHE	C-N-CA	5.58	125.48	119.85
12	M	612	PRO	CA-C-N	5.55	125.46	119.85
12	M	612	PRO	C-N-CA	5.55	125.46	119.85
12	M	173	MET	N-CA-C	5.54	119.30	112.54
7	H	104	VAL	N-CA-C	5.53	116.26	110.62
12	M	406	ASN	CA-C-N	5.53	125.18	119.05
12	M	406	ASN	C-N-CA	5.53	125.18	119.05
6	G	130	ILE	CA-C-N	5.51	125.48	120.03
6	G	130	ILE	C-N-CA	5.51	125.48	120.03
35	l	198	LEU	N-CA-C	5.35	117.11	111.28
34	k	55	LEU	N-CA-C	5.33	117.09	111.28
6	G	132	ASP	CA-C-N	5.19	131.31	121.97
6	G	132	ASP	C-N-CA	5.19	131.31	121.97
31	h	44	ALA	N-CA-C	5.17	117.00	111.36
41	s	214	GLU	N-CA-C	5.14	116.97	111.36
14	O	70	TYR	CA-C-N	5.10	125.04	119.78
14	O	70	TYR	C-N-CA	5.10	125.04	119.78
6	G	133	ILE	N-CA-CB	5.08	119.61	111.23
41	s	218	GLY	O-C-N	5.06	122.89	121.07
12	M	300	GLN	N-CA-C	5.05	118.56	111.74

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	227	PRO	Peptide
25	b	121	LYS	Peptide
32	i	255	PRO	Peptide

5.2 Too-close contacts (i)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3330	0	3292	94	0
2	B	1412	0	1363	35	0
3	C	1248	0	1254	33	0
4	E	971	0	975	29	0
5	F	687	0	700	17	0
6	G	690	0	669	37	0
6	X	694	0	674	16	0
7	H	910	0	950	15	0
8	I	780	0	808	28	0
9	J	2751	0	2773	47	0
10	K	366	0	338	13	0
11	L	1016	0	1016	23	0
12	M	5296	0	5328	122	0
13	N	1204	0	1162	23	0
14	O	1671	0	1673	39	0
15	P	1738	0	1693	47	0
16	Q	3459	0	3396	89	0
17	S	566	0	561	12	0
18	T	741	0	702	12	0
19	U	643	0	642	10	0
20	V	1021	0	1025	21	0
21	W	1161	0	1144	24	0
22	Y	584	0	529	5	0
23	Z	641	0	620	6	0
24	a	1151	0	1164	36	0
25	b	819	0	835	19	0
26	c	1315	0	1208	27	0
27	d	1461	0	1429	46	0
28	e	867	0	817	29	0
29	f	378	0	356	0	0
30	g	1000	0	994	22	0
31	h	867	0	871	17	0
32	i	2710	0	2874	106	0
33	j	914	0	951	21	0
34	k	748	0	799	25	0
35	l	4816	0	4955	146	0
36	m	1291	0	1265	34	0
37	n	479	0	486	13	0
38	o	1062	0	1072	27	0
39	p	1534	0	1470	23	0
40	r	3631	0	3839	80	0
41	s	2508	0	2607	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	u	1398	0	1374	40	0
43	v	1028	0	982	20	0
44	w	2590	0	2553	49	0
45	A	8	0	0	2	0
45	B	16	0	0	0	0
45	C	8	0	0	0	0
45	M	16	0	0	5	0
46	A	31	0	19	14	0
47	B	51	0	82	7	0
47	C	47	0	71	3	0
47	Q	47	0	71	18	0
47	W	41	0	59	6	0
47	b	46	0	69	19	0
47	j	92	0	141	14	0
47	l	91	0	136	14	0
47	r	51	0	82	8	0
48	C	52	0	88	19	0
48	J	52	0	88	0	0
48	N	52	0	88	0	0
48	g	52	0	88	5	0
48	j	52	0	88	2	0
48	n	52	0	88	1	0
48	r	104	0	176	10	0
49	E	35	0	0	1	0
49	X	35	0	0	12	0
50	J	48	0	26	0	0
51	J	33	0	39	10	0
51	s	63	0	90	36	0
52	J	89	0	125	11	0
52	N	51	0	46	11	0
52	V	194	0	294	7	0
52	a	100	0	156	18	0
52	i	68	0	80	17	0
52	l	199	0	307	31	0
52	m	100	0	156	11	0
52	r	100	0	156	7	0
52	u	55	0	54	14	0
53	M	4	0	0	1	0
53	O	4	0	0	0	0
54	M	1	0	0	0	0
55	T	1	0	0	0	0
56	w	27	0	11	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	68315	0	69162	1493	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 11.

All (1493) 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)
32:i:207:ILE:HD11	32:i:261:MET:CE	1.39	1.52
32:i:95:MET:HE3	32:i:149:ILE:CD1	1.39	1.50
16:Q:197:MET:CE	51:s:501:UQ:H23	1.43	1.46
6:X:112:SER:CB	49:X:201:8Q1:O1	1.66	1.42
32:i:95:MET:CE	32:i:149:ILE:CD1	2.09	1.31
32:i:95:MET:CE	32:i:149:ILE:HD12	1.61	1.29
24:a:97:GLU:OE1	27:d:60:ARG:NH2	1.63	1.27
32:i:99:THR:OG1	32:i:149:ILE:HD11	1.35	1.27
32:i:207:ILE:CD1	32:i:261:MET:CE	2.16	1.23
32:i:97:MET:SD	35:l:599:MET:HE1	1.81	1.21
16:Q:197:MET:HE2	51:s:501:UQ:H23	1.22	1.17
1:A:149:MET:HE1	1:A:241:THR:HB	1.26	1.14
4:E:30:ARG:HH21	6:G:133:ILE:HD13	1.12	1.13
42:u:169:PHE:HE1	52:u:201:CDL:H551	0.95	1.11
52:i:401:CDL:HB31	44:w:40:PRO:CB	1.80	1.11
32:i:88:LYS:O	32:i:148:SER:HB3	1.50	1.10
42:u:169:PHE:CE1	52:u:201:CDL:H551	1.87	1.09
32:i:88:LYS:O	32:i:148:SER:CB	2.00	1.08
1:A:149:MET:HE1	1:A:241:THR:CB	1.84	1.08
17:S:31:ASN:ND2	17:S:60:TYR:OH	1.88	1.07
32:i:154:MET:HE3	32:i:154:MET:HA	1.35	1.07
32:i:207:ILE:HD11	32:i:261:MET:HE1	1.34	1.07
48:C:303:PLX:H212	48:C:303:PLX:H172	1.36	1.06
52:a:201:CDL:H521	47:b:201:PEE:C11	1.86	1.06
16:Q:197:MET:CE	51:s:501:UQ:C23	2.33	1.06
52:a:201:CDL:H512	47:b:201:PEE:H13	1.31	1.06
2:B:98:ARG:HB3	2:B:169:GLU:OE1	1.53	1.05
32:i:207:ILE:HD11	32:i:261:MET:HE3	1.34	1.05
38:o:59:VAL:HG22	40:r:423:ILE:HG12	1.35	1.05
14:O:182:ASN:ND2	14:O:194:GLU:OE1	1.87	1.04
32:i:95:MET:CE	32:i:149:ILE:HD13	1.85	1.04
16:Q:197:MET:HE1	51:s:501:UQ:H23	1.39	1.03
15:P:105:ASN:O	15:P:137:PHE:CE2	2.12	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:207:ILE:CD1	32:i:261:MET:HE3	1.82	1.03
52:a:201:CDL:H521	47:b:201:PEE:C12	1.89	1.02
16:Q:197:MET:HE2	51:s:501:UQ:C23	1.88	1.01
12:M:182:CYS:SG	45:M:802:SF4:FE3	1.53	1.00
47:Q:501:PEE:H37	47:Q:501:PEE:C37	1.91	1.00
51:J:402:UQ:H152	51:J:402:UQ:H112	1.38	0.99
27:d:104:ASN:OD1	35:l:73:THR:O	1.81	0.99
6:X:112:SER:CB	49:X:201:8Q1:P24	2.50	0.99
3:C:119:LYS:NZ	33:j:32:GLU:OE1	1.94	0.98
6:G:137:LYS:O	6:G:139:MET:N	1.97	0.98
52:u:201:CDL:H581	52:u:201:CDL:H541	1.44	0.97
10:K:100:GLN:NE2	14:O:69:ASN:O	1.97	0.97
52:i:401:CDL:HB31	44:w:40:PRO:HB3	1.42	0.97
8:I:23:LYS:HD2	16:Q:253:PHE:CD2	2.00	0.96
15:P:125:ARG:NH2	15:P:201:ASP:OD1	1.98	0.96
52:a:201:CDL:H521	47:b:201:PEE:H16	1.47	0.96
47:Q:501:PEE:H37	47:Q:501:PEE:H61	1.45	0.95
32:i:97:MET:SD	35:l:599:MET:CE	2.54	0.95
47:j:202:PEE:O1P	41:s:62:ARG:NH2	1.99	0.95
1:A:56:ALA:O	1:A:61:ASP:HB2	1.66	0.95
40:r:256:TYR:OH	48:r:502:PLX:C9	2.14	0.95
32:i:125:GLN:NE2	52:i:401:CDL:OA3	2.00	0.95
42:u:169:PHE:HE1	52:u:201:CDL:C55	1.81	0.94
52:N:202:CDL:C55	52:N:202:CDL:H322	1.97	0.93
27:d:106:ILE:HD11	28:e:136:LEU:HD21	1.51	0.93
32:i:95:MET:HE3	32:i:149:ILE:HD12	0.94	0.92
41:s:25:ARG:HD2	51:s:501:UQ:C35	1.99	0.92
35:l:305:SER:HB2	35:l:422:TYR:OH	1.69	0.92
9:J:208:GLY:H	9:J:211:ASP:CG	1.76	0.92
6:G:105:MET:HG3	6:G:139:MET:HE3	1.48	0.92
52:a:201:CDL:C51	47:b:201:PEE:H13	1.99	0.91
35:l:73:THR:HG21	38:o:127:ILE:HG21	1.51	0.91
20:V:140:LYS:HE2	24:a:158:ARG:HD3	1.53	0.91
20:V:140:LYS:HE2	24:a:158:ARG:CD	2.00	0.91
40:r:251:ASN:HD21	40:r:304:GLN:HE22	1.14	0.91
35:l:601:LEU:HD23	35:l:602:PHE:CD2	2.05	0.90
32:i:207:ILE:HD11	32:i:261:MET:HE2	1.53	0.90
20:V:140:LYS:HD3	20:V:141:VAL:HG23	1.54	0.90
15:P:174:PHE:O	15:P:199:ARG:NH2	2.05	0.89
47:j:202:PEE:H10	47:j:202:PEE:H3	1.52	0.89
32:i:100:MET:HE1	35:l:595:ILE:HA	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:30:ARG:NH2	6:G:133:ILE:HD13	1.86	0.89
49:X:201:8Q1:C10	39:p:44:MET:CE	2.51	0.88
52:a:201:CDL:H512	47:b:201:PEE:C11	2.03	0.88
35:l:119:LYS:NZ	52:l:702:CDL:OA3	2.06	0.88
12:M:213:MET:HE1	12:M:713:ALA:HB1	1.56	0.87
46:A:502:FMN:N1	46:A:502:FMN:O3'	2.08	0.87
32:i:95:MET:SD	32:i:149:ILE:HD12	2.15	0.87
40:r:256:TYR:OH	48:r:502:PLX:C8	2.22	0.87
12:M:176:CYS:HG	45:M:802:SF4:FE4	0.89	0.86
48:C:303:PLX:H352	48:C:303:PLX:H393	1.57	0.86
27:d:107:GLN:HE22	35:l:194:ASN:ND2	1.73	0.86
16:Q:226:TYR:OH	16:Q:234:GLN:O	1.92	0.85
2:B:79:ARG:NH2	8:I:20:LEU:HD22	1.90	0.85
4:E:42:GLU:CD	4:E:94:ILE:HD13	2.01	0.85
52:a:201:CDL:C52	47:b:201:PEE:C11	2.55	0.85
35:l:541:ASN:HD22	47:l:704:PEE:H60	1.41	0.84
9:J:208:GLY:O	9:J:211:ASP:OD1	1.95	0.84
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.59	0.84
32:i:207:ILE:CD1	32:i:261:MET:HE2	2.05	0.84
35:l:601:LEU:CD2	35:l:602:PHE:CE2	2.60	0.84
47:Q:501:PEE:H28	47:Q:501:PEE:H36	1.59	0.84
27:d:107:GLN:HE22	35:l:194:ASN:HD22	1.25	0.84
31:h:47:ILE:HG22	31:h:51:ARG:NH1	1.93	0.84
24:a:170:GLN:HE22	42:u:151:ASN:HD21	1.26	0.84
24:a:94:GLY:O	27:d:61:TYR:OH	1.96	0.83
30:g:7:ARG:HH21	30:g:91:ASP:CG	1.85	0.83
47:Q:501:PEE:H28	47:Q:501:PEE:C22	2.05	0.83
12:M:385:TYR:OH	12:M:527:ASP:OD1	1.97	0.83
16:Q:218:SER:CB	16:Q:224:ALA:HB1	2.08	0.83
32:i:95:MET:HE1	32:i:149:ILE:HD13	1.61	0.83
12:M:337:ASP:O	12:M:542:PRO:CB	2.27	0.83
8:I:23:LYS:HD2	16:Q:253:PHE:CE2	2.12	0.83
37:n:30:ARG:NE	52:u:201:CDL:OA4	2.12	0.82
8:I:25:GLN:O	16:Q:209:LYS:NZ	2.12	0.82
24:a:160:MET:HE3	24:a:167:PRO:HD2	1.62	0.82
12:M:382:ARG:NH2	12:M:527:ASP:OD2	2.11	0.82
40:r:191:SER:HB3	47:r:501:PEE:H3	1.61	0.82
24:a:170:GLN:HE22	42:u:151:ASN:ND2	1.77	0.82
24:a:170:GLN:NE2	42:u:151:ASN:ND2	2.28	0.81
35:l:3:PRO:HG2	35:l:53:MET:HE1	1.63	0.81
24:a:160:MET:HE3	24:a:166:GLY:HA3	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:s:501:UQ:C33	51:s:501:UQ:H301	2.11	0.81
30:g:89:ASP:OD2	42:u:161:ALA:HB1	1.80	0.80
9:J:136:THR:HG23	9:J:139:PHE:H	1.44	0.80
41:s:200:LEU:HD13	41:s:282:TYR:CB	2.12	0.80
9:J:299:ARG:NH2	9:J:320:GLU:OE2	2.15	0.80
47:Q:501:PEE:H42	47:Q:501:PEE:H34	1.62	0.80
13:N:3:LEU:HD13	52:N:202:CDL:OA7	1.83	0.79
47:Q:501:PEE:H37	47:Q:501:PEE:H60	1.64	0.78
47:j:202:PEE:H10	47:j:202:PEE:C1	2.13	0.78
5:F:71:PHE:HE1	12:M:334:GLN:HE21	1.31	0.78
1:A:87:GLY:HA3	46:A:502:FMN:O2P	1.84	0.78
47:Q:501:PEE:H34	47:Q:501:PEE:C25	2.13	0.78
2:B:79:ARG:NH1	8:I:25:GLN:OE1	2.17	0.78
35:l:517:SER:HB3	52:l:703:CDL:HA32	1.65	0.77
32:i:207:ILE:HD12	32:i:261:MET:HE3	1.65	0.77
37:n:3:ASN:N	37:n:3:ASN:HD22	1.81	0.77
17:S:65:GLY:O	17:S:67:GLU:N	2.18	0.77
38:o:59:VAL:CG2	40:r:423:ILE:HG12	2.14	0.77
30:g:7:ARG:NH2	30:g:91:ASP:OD1	2.17	0.77
49:X:201:8Q1:C10	39:p:44:MET:HE1	2.15	0.77
52:u:201:CDL:H581	52:u:201:CDL:C54	2.14	0.77
41:s:200:LEU:HD13	41:s:282:TYR:HB3	1.67	0.76
4:E:42:GLU:CD	4:E:94:ILE:CD1	2.59	0.76
27:d:107:GLN:NE2	35:l:194:ASN:HD22	1.83	0.76
5:F:25:GLN:HG3	5:F:26:ARG:HD3	1.66	0.76
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.68	0.76
9:J:207:PHE:HA	9:J:211:ASP:OD2	1.86	0.76
1:A:149:MET:CE	1:A:241:THR:CB	2.63	0.76
12:M:171:THR:HG22	12:M:231:LEU:CD2	2.16	0.76
12:M:182:CYS:HG	45:M:802:SF4:FE3	0.46	0.76
48:C:303:PLX:C21	51:s:501:UQ:H551	2.15	0.76
9:J:50:SER:OG	15:P:225:GLU:OE2	2.04	0.75
20:V:141:VAL:O	24:a:169:TYR:OH	2.01	0.75
32:i:133:TRP:HE3	52:i:401:CDL:H362	1.51	0.75
26:c:40:PRO:O	26:c:74:ASP:HB2	1.87	0.75
21:W:81:ARG:NH2	42:u:64:ASN:OD1	2.20	0.75
19:U:9:LEU:HD11	47:j:201:PEE:H68	1.69	0.75
35:l:286:LEU:HD13	35:l:411:MET:SD	2.27	0.75
49:X:201:8Q1:C10	39:p:44:MET:HE2	2.15	0.74
16:Q:53:TYR:OH	47:Q:501:PEE:H2	1.87	0.74
51:J:402:UQ:O1	51:J:402:UQ:H102	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:e:121:GLU:OE2	28:e:124:ARG:NH2	2.20	0.74
11:L:112:MET:HE3	13:N:126:PRO:HB2	1.69	0.74
35:l:573:MET:HE3	47:l:701:PEE:H18	1.69	0.74
3:C:53:LEU:HD22	48:C:303:PLX:H322	1.68	0.74
3:C:125:PRO:HG2	41:s:58:LYS:HE3	1.69	0.74
52:N:202:CDL:H532	52:N:202:CDL:OA9	1.88	0.74
22:Y:72:ARG:NH1	22:Y:76:ASP:OD2	2.21	0.74
31:h:45:HIS:O	31:h:45:HIS:ND1	2.21	0.74
3:C:77:MET:HE2	51:s:501:UQ:H8	1.69	0.73
6:G:130:ILE:HD12	6:G:130:ILE:N	2.02	0.73
52:a:201:CDL:C51	47:b:201:PEE:C11	2.65	0.73
32:i:259:GLY:O	32:i:262:PRO:HD2	1.88	0.73
6:G:103:HIS:NE2	6:G:139:MET:HG2	2.04	0.73
47:b:201:PEE:H10	48:r:503:PLX:O2	1.87	0.73
32:i:99:THR:OG1	32:i:149:ILE:CD1	2.26	0.73
3:C:73:ALA:CB	51:s:501:UQ:HM53	2.19	0.73
41:s:25:ARG:HD2	51:s:501:UQ:H352	1.71	0.73
32:i:95:MET:HE3	32:i:149:ILE:CG1	2.16	0.73
52:i:401:CDL:CB3	44:w:40:PRO:HB3	2.19	0.73
51:J:402:UQ:H152	51:J:402:UQ:C11	2.18	0.72
15:P:43:THR:HA	15:P:47:ILE:HD13	1.71	0.72
40:r:256:TYR:OH	48:r:502:PLX:H91	1.88	0.72
41:s:51:ASP:HB3	51:s:501:UQ:H412	1.70	0.72
15:P:125:ARG:HH22	15:P:201:ASP:CG	1.96	0.72
6:X:112:SER:CA	49:X:201:8Q1:O1	2.37	0.72
28:e:126:VAL:O	28:e:130:GLU:HG2	1.89	0.72
30:g:36:MET:HE1	48:g:201:PLX:H393	1.70	0.72
32:i:268:GLN:HE22	32:i:272:LYS:HE3	1.52	0.72
35:l:601:LEU:HD23	35:l:602:PHE:CE2	2.25	0.72
13:N:68:MET:HG3	13:N:69:ASN:H	1.54	0.72
20:V:110:ILE:HG12	47:l:701:PEE:H48	1.71	0.72
48:C:303:PLX:H172	48:C:303:PLX:C21	2.18	0.72
32:i:112:HIS:HB2	32:i:184:ILE:HD13	1.71	0.72
40:r:243:MET:O	40:r:247:THR:HG23	1.89	0.72
12:M:295:ASP:OD2	12:M:706:THR:OG1	2.02	0.72
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.23	0.71
4:E:52:LEU:HD22	4:E:104:MET:HE3	1.71	0.71
35:l:190:LEU:C	35:l:190:LEU:HD23	2.14	0.71
12:M:337:ASP:O	12:M:542:PRO:HB2	1.89	0.71
3:C:77:MET:CE	51:s:501:UQ:H8	2.19	0.71
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:419:THR:HA	35:l:422:TYR:CE2	2.26	0.71
6:G:137:LYS:O	6:G:139:MET:HB2	1.90	0.71
13:N:73:THR:HG21	13:N:81:MET:HE1	1.73	0.70
9:J:304:LEU:C	9:J:304:LEU:HD23	2.15	0.70
1:A:262:PHE:CE2	1:A:272:GLY:HA3	2.26	0.70
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.70	0.70
34:k:37:MET:HG2	34:k:67:ALA:HB2	1.72	0.70
40:r:256:TYR:OH	48:r:502:PLX:H82	1.89	0.70
6:G:137:LYS:O	6:G:139:MET:CB	2.39	0.70
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.21	0.70
1:A:110:PRO:O	1:A:238:CYS:HB3	1.91	0.69
6:G:104:PHE:HA	6:G:108:LEU:HB2	1.72	0.69
52:a:201:CDL:H521	47:b:201:PEE:H14	1.72	0.69
10:K:105:ARG:NH2	12:M:426:ASP:OD2	2.25	0.69
20:V:110:ILE:HG12	47:l:701:PEE:C31	2.22	0.69
3:C:190:LEU:CD2	47:C:302:PEE:H13	2.22	0.69
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.25	0.69
38:o:59:VAL:HG22	40:r:423:ILE:CG1	2.17	0.69
52:a:201:CDL:C52	47:b:201:PEE:H13	2.20	0.69
34:k:21:MET:HB3	52:m:201:CDL:HB61	1.74	0.69
5:F:24:CYS:N	5:F:58:CYS:SG	2.66	0.69
40:r:210:TYR:O	40:r:213:HIS:ND1	2.22	0.69
30:g:2:THR:HB	32:i:198:THR:OG1	1.92	0.68
42:u:169:PHE:CE1	52:u:201:CDL:C55	2.66	0.68
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.27	0.68
19:U:20:VAL:HG13	47:j:201:PEE:H67	1.74	0.68
47:Q:501:PEE:H42	47:Q:501:PEE:C21	2.23	0.68
38:o:23:TYR:OH	39:p:68:GLU:OE1	2.11	0.68
38:o:59:VAL:HG22	40:r:423:ILE:HG23	1.76	0.68
1:A:49:HIS:O	1:A:59:ARG:NH1	2.25	0.68
1:A:414:GLU:OE2	8:I:50:SER:O	2.11	0.68
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.26	0.68
35:l:102:GLU:OE1	35:l:456:ARG:NH2	2.26	0.68
6:G:134:ASP:OD1	6:G:147:TYR:CE2	2.47	0.68
12:M:171:THR:HG22	12:M:231:LEU:HD22	1.75	0.68
40:r:251:ASN:ND2	40:r:304:GLN:HE22	1.89	0.68
32:i:142:LEU:HB3	32:i:194:LEU:HD21	1.76	0.68
19:U:46:ASN:OD1	21:W:58:ARG:NH2	2.27	0.68
11:L:124:LEU:HD21	15:P:201:ASP:O	1.93	0.67
44:w:125:ASP:O	44:w:130:ARG:NH2	2.28	0.67
1:A:390:ASP:OD2	12:M:202:ASN:ND2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:190:LEU:HD22	47:C:302:PEE:H13	1.75	0.67
7:H:101:GLU:HB3	7:H:102:PRO:HD2	1.75	0.67
4:E:64:ARG:NH1	6:G:117:GLU:OE2	2.27	0.67
6:G:80:LYS:HE2	6:G:100:VAL:HG21	1.76	0.67
15:P:61:PHE:CZ	15:P:106:ALA:HB2	2.30	0.67
16:Q:197:MET:HE1	51:s:501:UQ:C23	2.14	0.67
47:W:201:PEE:C1	47:W:201:PEE:H10	2.25	0.67
27:d:149:HIS:HE1	40:r:247:THR:OG1	1.76	0.67
52:l:703:CDL:H121	52:l:703:CDL:H321	1.77	0.67
32:i:133:TRP:CE3	52:i:401:CDL:H362	2.29	0.67
12:M:248:THR:HG21	12:M:609:ALA:HA	1.77	0.67
26:c:38:PRO:HD3	38:o:67:ARG:HG3	1.77	0.67
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.25	0.67
27:d:69:ARG:NH2	37:n:46:LYS:O	2.28	0.67
47:W:201:PEE:H10	47:W:201:PEE:H2	1.77	0.66
14:O:140:CYS:SG	14:O:183:ALA:CB	2.83	0.66
17:S:12:MET:HE3	41:s:264:LEU:HD22	1.76	0.66
6:X:112:SER:CB	49:X:201:8Q1:O2	2.43	0.66
1:A:50:ASP:HB3	1:A:55:GLY:HA3	1.76	0.66
32:i:154:MET:HA	32:i:154:MET:CE	2.19	0.66
11:L:123:ASN:OD1	12:M:246:ARG:NH2	2.29	0.66
12:M:208:THR:HG21	12:M:212:LYS:HB3	1.78	0.66
6:X:155:TYR:CE1	25:b:23:LEU:HB3	2.30	0.66
2:B:79:ARG:NH2	8:I:20:LEU:CD2	2.59	0.66
6:X:155:TYR:HE1	25:b:23:LEU:HB3	1.61	0.66
35:l:73:THR:HG21	38:o:127:ILE:CG2	2.23	0.66
41:s:25:ARG:HD2	51:s:501:UQ:H353	1.77	0.66
12:M:299:ARG:HG3	12:M:299:ARG:HH11	1.60	0.66
12:M:526:LEU:HD21	12:M:532:PRO:HB3	1.78	0.66
48:C:303:PLX:H211	51:s:501:UQ:H551	1.77	0.66
8:I:8:ILE:HD11	52:N:202:CDL:H142	1.76	0.66
3:C:73:ALA:CB	51:s:501:UQ:CM5	2.74	0.65
52:i:401:CDL:CB3	44:w:40:PRO:CB	2.67	0.65
6:G:130:ILE:HD12	6:G:130:ILE:H	1.61	0.65
52:J:404:CDL:H162	47:j:202:PEE:H26	1.77	0.65
15:P:164:ASN:OD1	15:P:181:HIS:HE1	1.79	0.65
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.29	0.65
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.77	0.65
35:l:419:THR:HA	35:l:422:TYR:CD2	2.32	0.65
7:H:105:GLU:HA	7:H:105:GLU:OE1	1.97	0.65
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:139:ARG:NH1	44:w:166:ASP:OD2	2.28	0.65
2:B:79:ARG:HH21	8:I:20:LEU:CD2	2.09	0.65
6:G:93:ILE:HG12	6:G:108:LEU:HD13	1.79	0.65
12:M:650:SER:OG	12:M:652:ASN:ND2	2.29	0.65
15:P:164:ASN:OD1	15:P:181:HIS:CE1	2.50	0.65
36:m:49:GLY:HA2	36:m:139:GLU:OE1	1.97	0.65
35:l:119:LYS:CE	52:l:702:CDL:OA3	2.45	0.65
6:G:104:PHE:HD1	6:G:108:LEU:HD12	1.62	0.65
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.78	0.65
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	1.79	0.65
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.79	0.65
1:A:422:HIS:O	12:M:76:ARG:HD2	1.97	0.64
46:A:502:FMN:HO3'	46:A:502:FMN:C2	2.05	0.64
44:w:118:TYR:OH	56:w:401:ADP:O2'	2.14	0.64
14:O:38:LEU:O	14:O:124:ARG:NH2	2.31	0.64
28:e:98:VAL:HG22	40:r:36:LEU:HB2	1.80	0.64
33:j:71:LEU:O	36:m:147:TYR:OH	2.12	0.64
32:i:95:MET:SD	32:i:149:ILE:CD1	2.83	0.64
1:A:244:ASN:HB2	46:A:502:FMN:O1P	1.97	0.64
3:C:167:PRO:HD3	16:Q:223:HIS:CD2	2.32	0.64
3:C:167:PRO:HD3	16:Q:223:HIS:HD2	1.62	0.64
7:H:105:GLU:HB3	15:P:89:HIS:CD2	2.32	0.64
14:O:140:CYS:SG	14:O:183:ALA:HB2	2.38	0.64
27:d:65:HIS:HE2	28:e:124:ARG:NH2	1.96	0.64
3:C:73:ALA:HB3	51:s:501:UQ:HM53	1.79	0.64
35:l:290:LEU:HD11	52:l:703:CDL:H731	1.77	0.64
35:l:573:MET:CE	47:l:701:PEE:H18	2.28	0.64
31:h:47:ILE:HG22	31:h:51:ARG:CZ	2.28	0.64
4:E:68:MET:SD	49:E:201:8Q1:C30	2.86	0.64
13:N:3:LEU:HD11	52:N:202:CDL:C31	2.28	0.64
33:j:79:SER:HA	33:j:87:MET:HE2	1.80	0.64
3:C:56:TRP:CZ2	48:C:303:PLX:H112	2.33	0.64
24:a:163:ARG:HH22	30:g:102:ASP:CG	2.06	0.64
52:i:401:CDL:HB31	44:w:40:PRO:CG	2.28	0.64
38:o:5:LYS:NZ	39:p:69:GLU:OE2	2.31	0.63
32:i:236:LYS:HG3	32:i:237:MET:HG3	1.80	0.63
52:J:404:CDL:H221	52:J:404:CDL:H552	1.78	0.63
24:a:160:MET:CE	24:a:167:PRO:HD2	2.27	0.63
44:w:88:GLU:OE2	44:w:161:ARG:NH1	2.31	0.63
4:E:37:ARG:NH1	6:G:132:ASP:OD1	2.31	0.63
3:C:96:SER:HB2	41:s:213:VAL:HG23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:103:MET:HE1	3:C:121:TYR:HB2	1.81	0.63
16:Q:387:GLU:OE2	16:Q:390:GLN:NE2	2.32	0.63
52:i:401:CDL:HB62	44:w:40:PRO:HB2	1.79	0.63
1:A:149:MET:CE	1:A:241:THR:HB	2.15	0.63
1:A:159:ARG:NH2	14:O:176:CYS:O	2.31	0.63
16:Q:218:SER:OG	16:Q:224:ALA:HB1	1.97	0.63
35:l:425:ARG:NH2	52:l:703:CDL:OB3	2.32	0.63
47:B:303:PEE:H59	41:s:277:TYR:HE2	1.64	0.63
17:S:65:GLY:C	17:S:67:GLU:H	2.07	0.63
26:c:55:TYR:OH	26:c:74:ASP:O	2.13	0.63
1:A:262:PHE:CZ	1:A:272:GLY:HA3	2.33	0.62
26:c:140:MET:HE1	35:l:411:MET:HE3	1.81	0.62
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.81	0.62
15:P:61:PHE:CE1	15:P:106:ALA:HB2	2.34	0.62
28:e:126:VAL:HG13	28:e:136:LEU:HD11	1.82	0.62
35:l:257:VAL:HG13	35:l:317:ILE:HD11	1.81	0.62
52:r:504:CDL:H401	52:r:504:CDL:H221	1.82	0.62
12:M:390:THR:HB	12:M:600:GLU:OE2	2.00	0.62
25:b:81:ILE:HG23	47:b:201:PEE:H58	1.81	0.62
16:Q:197:MET:HE3	51:s:501:UQ:H23	1.69	0.62
17:S:57:VAL:O	17:S:57:VAL:HG22	2.00	0.62
48:g:201:PLX:H361	48:g:201:PLX:H311	1.80	0.62
52:N:202:CDL:H532	52:N:202:CDL:CA7	2.30	0.62
30:g:7:ARG:CZ	30:g:87:LEU:HD11	2.29	0.62
1:A:127:ASP:HB3	1:A:245:VAL:HG11	1.82	0.62
51:J:402:UQ:H112	51:J:402:UQ:C15	2.18	0.62
9:J:192:ARG:NH1	9:J:198:ALA:O	2.33	0.62
1:A:98:LYS:NZ	46:A:502:FMN:O3P	2.33	0.61
12:M:460:HIS:O	12:M:463:SER:OG	2.18	0.61
18:T:39:THR:HG22	18:T:62:VAL:HG22	1.80	0.61
21:W:63:GLU:OE2	42:u:119:ARG:NH2	2.33	0.61
31:h:84:ASP:HA	31:h:87:ILE:HG12	1.80	0.61
6:G:134:ASP:HB2	6:G:137:LYS:HE2	1.81	0.61
24:a:78:THR:HG21	28:e:96:SER:HA	1.81	0.61
41:s:233:MET:HE1	41:s:234:MET:HE2	1.81	0.61
1:A:285:PRO:O	14:O:222:ARG:NH2	2.33	0.61
16:Q:260:GLU:OE2	21:W:25:LEU:HD22	2.00	0.61
28:e:77:ASP:OD1	28:e:78:LYS:N	2.31	0.61
35:l:426:ILE:O	35:l:430:ALA:HB3	2.00	0.61
16:Q:80:LEU:HD21	41:s:126:LYS:HD3	1.82	0.61
48:C:303:PLX:H212	48:C:303:PLX:C17	2.20	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:96:VAL:HG12	4:E:96:VAL:O	2.00	0.61
27:d:144:SER:OG	27:d:158:LYS:NZ	2.28	0.61
32:i:95:MET:HE3	32:i:149:ILE:CA	2.31	0.61
1:A:88:ARG:NH2	1:A:273:THR:O	2.34	0.61
16:Q:36:GLN:HE21	40:r:142:ARG:NH2	1.98	0.61
16:Q:294:ARG:NH2	16:Q:401:GLU:OE2	2.34	0.61
7:H:38:ILE:O	7:H:45:ARG:NH1	2.33	0.61
30:g:7:ARG:HG2	30:g:8:PRO:HD2	1.83	0.61
38:o:59:VAL:CG2	40:r:423:ILE:HG23	2.31	0.61
51:J:402:UQ:HM33	51:J:402:UQ:O2	2.01	0.60
12:M:534:VAL:HG22	12:M:534:VAL:O	2.00	0.60
16:Q:68:ASP:O	32:i:49:ASN:ND2	2.34	0.60
26:c:110:ASP:OD2	40:r:278:ARG:NE	2.29	0.60
1:A:116:ASN:ND2	46:A:502:FMN:C2	2.64	0.60
12:M:405:THR:HB	12:M:477:GLY:HA3	1.82	0.60
16:Q:144:MET:HG2	16:Q:222:MET:O	2.00	0.60
23:Z:60:ASN:ND2	35:l:433:GLY:O	2.31	0.60
25:b:74:HIS:NE2	35:l:35:TYR:OH	2.29	0.60
1:A:251:SER:N	1:A:252:PRO:HD2	2.16	0.60
2:B:192:ASN:ND2	18:T:61:GLU:OE2	2.32	0.60
41:s:214:GLU:OE1	41:s:214:GLU:HA	2.00	0.60
1:A:149:MET:HE1	1:A:241:THR:CG2	2.30	0.60
12:M:136:GLU:OE2	12:M:272:ARG:NH2	2.30	0.60
52:i:401:CDL:OB4	44:w:40:PRO:HG3	2.01	0.60
36:m:1:MET:HG3	36:m:2:THR:HG23	1.83	0.60
41:s:208:VAL:HG13	41:s:208:VAL:O	2.01	0.60
9:J:136:THR:HG22	9:J:139:PHE:O	2.01	0.60
22:Y:76:ASP:O	35:l:385:TYR:OH	2.19	0.60
40:r:251:ASN:HD21	40:r:304:GLN:NE2	1.92	0.60
1:A:48:ARG:NH2	14:O:226:GLU:OE1	2.34	0.60
2:B:47:SER:O	2:B:56:ARG:NH2	2.34	0.60
27:d:119:GLU:HG2	43:v:52:MET:HA	1.84	0.60
52:i:401:CDL:HB31	44:w:40:PRO:HB2	1.80	0.60
12:M:472:PRO:O	12:M:510:TRP:NE1	2.31	0.60
37:n:47:ARG:NH2	37:n:53:GLU:OE2	2.34	0.60
9:J:311:GLU:HG3	9:J:311:GLU:O	2.02	0.60
30:g:2:THR:HG23	30:g:2:THR:O	2.00	0.60
47:C:302:PEE:O5	47:C:302:PEE:H52	2.00	0.60
30:g:7:ARG:CG	30:g:8:PRO:HD2	2.32	0.60
37:n:3:ASN:N	37:n:3:ASN:ND2	2.49	0.60
9:J:135:GLU:HG3	9:J:140:ASP:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:110:ILE:HD11	47:l:701:PEE:H1	1.83	0.60
36:m:25:SER:O	36:m:27:ILE:N	2.34	0.60
1:A:152:ARG:NH2	10:K:99:PRO:O	2.35	0.59
6:G:105:MET:CG	6:G:139:MET:HE3	2.27	0.59
14:O:177:LEU:HD12	14:O:185:MET:HE2	1.84	0.59
36:m:61:LEU:O	41:s:114:TYR:OH	2.16	0.59
51:s:501:UQ:H301	51:s:501:UQ:H33	1.82	0.59
9:J:173:ASP:HB3	9:J:176:SER:HB2	1.85	0.59
32:i:268:GLN:NE2	32:i:272:LYS:HE3	2.17	0.59
36:m:72:THR:HG21	41:s:133:LEU:HD21	1.84	0.59
12:M:531:LYS:O	12:M:531:LYS:HG2	2.00	0.59
44:w:169:PHE:O	44:w:173:MET:HG3	2.02	0.59
3:C:56:TRP:CE2	48:C:303:PLX:H112	2.38	0.59
11:L:109:ASN:ND2	11:L:111:LEU:O	2.34	0.59
26:c:58:ARG:NH1	26:c:61:ASP:OD2	2.35	0.59
35:l:481:THR:HG1	43:v:92:HIS:HD1	1.51	0.59
36:m:65:LEU:HD11	41:s:139:THR:HG21	1.83	0.59
4:E:17:VAL:HG21	11:L:55:VAL:HG12	1.84	0.59
26:c:143:MET:HA	26:c:146:VAL:HG12	1.85	0.59
47:B:303:PEE:H36	21:W:43:LEU:CD1	2.32	0.59
15:P:207:TYR:C	15:P:224:VAL:HG23	2.27	0.59
42:u:169:PHE:CZ	52:u:201:CDL:C56	2.86	0.59
12:M:166:GLY:HA2	12:M:213:MET:HE3	1.84	0.59
17:S:65:GLY:C	17:S:67:GLU:N	2.60	0.59
32:i:186:HIS:O	32:i:190:MET:HG3	2.03	0.59
15:P:211:ARG:NH2	15:P:213:ASP:OD2	2.35	0.59
20:V:123:ALA:O	20:V:127:MET:HG3	2.02	0.59
35:l:520:TYR:HE1	52:l:703:CDL:OB4	1.85	0.59
34:k:17:ALA:O	34:k:21:MET:HG2	2.03	0.59
9:J:303:ARG:O	9:J:303:ARG:HD3	2.03	0.58
16:Q:38:GLN:OE1	16:Q:38:GLN:HA	2.03	0.58
40:r:231:LEU:HD23	40:r:235:LEU:HD12	1.85	0.58
24:a:163:ARG:NH1	30:g:102:ASP:OD2	2.33	0.58
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.85	0.58
51:J:402:UQ:O1	51:J:402:UQ:HM23	2.03	0.58
12:M:337:ASP:O	12:M:542:PRO:HB3	2.02	0.58
32:i:84:TRP:HH2	34:k:59:MET:HE2	1.68	0.58
13:N:129:THR:HA	18:T:43:GLN:HG2	1.85	0.58
8:I:70:MET:HE2	15:P:66:ALA:HB1	1.85	0.58
32:i:95:MET:HE3	32:i:149:ILE:CB	2.32	0.58
12:M:690:THR:HG21	12:M:692:LYS:HE3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:95:MET:HE3	32:i:149:ILE:HA	1.85	0.58
42:u:83:THR:HA	42:u:86:TRP:CD1	2.38	0.58
12:M:224:ASP:OD2	12:M:291:ARG:NH2	2.27	0.58
32:i:304:MET:HE3	40:r:135:ARG:HH22	1.68	0.58
36:m:82:VAL:HG22	36:m:83:TRP:H	1.67	0.58
2:B:160:GLU:OE2	16:Q:233:HIS:NE2	2.37	0.58
48:C:303:PLX:H352	48:C:303:PLX:C39	2.32	0.58
14:O:140:CYS:SG	14:O:183:ALA:HB1	2.44	0.58
49:X:201:8Q1:O2	39:p:13:GLN:NE2	2.37	0.58
25:b:86:LEU:HD11	35:l:9:LEU:HD12	1.86	0.58
2:B:76:TYR:OH	16:Q:257:GLU:OE1	2.22	0.58
34:k:23:ARG:HG3	36:m:23:LYS:HE2	1.85	0.58
49:X:201:8Q1:C8	39:p:48:PHE:CE1	2.87	0.57
34:k:31:LEU:HD21	36:m:67:VAL:HG11	1.86	0.57
40:r:247:THR:HA	40:r:250:LEU:HD23	1.84	0.57
24:a:96:ALA:HB2	27:d:61:TYR:CE1	2.39	0.57
32:i:147:GLN:OE1	32:i:147:GLN:N	2.26	0.57
47:l:704:PEE:C11	47:l:704:PEE:H7	2.33	0.57
3:C:95:ALA:HB1	41:s:208:VAL:HG23	1.86	0.57
12:M:182:CYS:SG	45:M:802:SF4:S2	3.02	0.57
18:T:76:VAL:HG12	18:T:117:GLN:HB2	1.86	0.57
52:a:201:CDL:C52	47:b:201:PEE:C12	2.75	0.57
27:d:110:LEU:HD11	35:l:203:MET:HE2	1.87	0.57
35:l:190:LEU:HD23	35:l:190:LEU:O	2.03	0.57
52:l:702:CDL:H521	48:r:503:PLX:H211	1.85	0.57
24:a:134:GLU:OE1	37:n:57:TRP:NE1	2.29	0.57
27:d:114:GLN:CG	35:l:203:MET:HG2	2.34	0.57
27:d:132:PHE:CE2	35:l:204:LEU:HD11	2.40	0.57
51:s:501:UQ:HM22	51:s:501:UQ:O1	2.02	0.57
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.45	0.57
9:J:64:PHE:CZ	9:J:211:ASP:HB3	2.39	0.57
24:a:170:GLN:OE1	24:a:170:GLN:HA	2.04	0.57
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.86	0.57
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.86	0.57
25:b:24:LYS:NZ	25:b:27:GLU:OE1	2.33	0.57
25:b:83:HIS:HD2	27:d:45:VAL:HG21	1.68	0.57
42:u:169:PHE:CE1	52:u:201:CDL:C56	2.87	0.57
9:J:201:ILE:HG22	9:J:203:PRO:HD3	1.86	0.57
32:i:79:LEU:HB2	34:k:47:ILE:CD1	2.33	0.57
43:v:51:LEU:O	43:v:52:MET:HG3	2.05	0.57
5:F:91:LEU:O	5:F:95:LEU:HD12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:20:VAL:HG11	32:i:137:ALA:HB1	1.87	0.57
52:l:703:CDL:OA7	52:l:703:CDL:HA61	2.04	0.57
44:w:73:LEU:HD11	44:w:269:VAL:HG21	1.86	0.57
14:O:242:GLY:HA2	14:O:245:VAL:HG23	1.87	0.57
15:P:111:LEU:HD12	15:P:132:LEU:HD23	1.85	0.57
34:k:65:VAL:HG11	36:m:157:THR:HG23	1.87	0.57
35:l:123:LEU:HB2	35:l:150:MET:HE2	1.86	0.57
12:M:382:ARG:HE	12:M:527:ASP:CG	2.13	0.56
16:Q:294:ARG:NH1	16:Q:336:GLU:OE2	2.38	0.56
20:V:62:THR:O	20:V:66:ILE:HG12	2.04	0.56
40:r:443:PRO:HB3	48:r:503:PLX:H352	1.87	0.56
8:I:40:LYS:HB3	21:W:7:LYS:H	1.71	0.56
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.86	0.56
1:A:250:VAL:C	1:A:252:PRO:HD2	2.29	0.56
48:C:303:PLX:C22	51:s:501:UQ:H551	2.35	0.56
8:I:12:ARG:HB3	8:I:20:LEU:HD12	1.87	0.56
21:W:85:GLN:OE1	31:h:105:ARG:NH1	2.38	0.56
26:c:58:ARG:NH2	26:c:60:GLU:OE2	2.39	0.56
5:F:61:VAL:HG13	5:F:62:GLN:H	1.71	0.56
9:J:220:MET:HE3	9:J:226:VAL:HG13	1.88	0.56
25:b:99:GLU:HG3	35:l:61:MET:HG2	1.86	0.56
47:b:201:PEE:C4	48:r:503:PLX:O2	2.54	0.56
35:l:7:LEU:HD22	35:l:46:LEU:HD11	1.87	0.56
6:G:134:ASP:O	6:G:138:LEU:HG	2.06	0.56
37:n:50:ARG:HB2	37:n:53:GLU:HG2	1.86	0.56
1:A:60:GLY:HA2	14:O:241:PRO:HB3	1.88	0.56
5:F:71:PHE:CE1	12:M:334:GLN:NE2	2.73	0.56
26:c:158:PRO:HD3	43:v:22:MET:HE3	1.88	0.56
31:h:94:PRO:HG2	31:h:99:LEU:HD21	1.88	0.56
35:l:119:LYS:HE2	52:l:702:CDL:OA3	2.06	0.56
35:l:190:LEU:HD11	40:r:307:TRP:CH2	2.41	0.56
40:r:122:PHE:HZ	40:r:206:LYS:HG3	1.70	0.56
41:s:74:ALA:O	41:s:115:SER:OG	2.24	0.56
6:X:93:ILE:HG21	6:X:98:LEU:HD12	1.87	0.56
32:i:248:LEU:HD23	32:i:251:MET:HE2	1.87	0.56
34:k:37:MET:HG2	34:k:67:ALA:CB	2.36	0.56
40:r:191:SER:HB3	47:r:501:PEE:C1	2.33	0.56
21:W:68:ARG:O	21:W:72:MET:HG3	2.06	0.56
6:X:112:SER:N	49:X:201:8Q1:O1	2.39	0.56
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.87	0.55
5:F:24:CYS:O	5:F:34:ARG:NH1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:l:702:CDL:H452	40:r:445:LEU:HB3	1.87	0.55
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.41	0.55
40:r:403:THR:HA	40:r:406:TYR:CE2	2.42	0.55
3:C:147:TYR:CZ	15:P:197:PRO:HB3	2.40	0.55
12:M:171:THR:HG22	12:M:231:LEU:HD23	1.87	0.55
19:U:38:TYR:HD1	19:U:41:TYR:HD2	1.54	0.55
6:G:144:ILE:O	6:G:148:ILE:HG13	2.06	0.55
15:P:105:ASN:O	15:P:137:PHE:CZ	2.59	0.55
21:W:70:ALA:HB2	42:u:125:LEU:HD13	1.89	0.55
40:r:203:PHE:O	40:r:207:MET:HG2	2.06	0.55
44:w:70:LYS:NZ	44:w:160:GLU:OE1	2.39	0.55
44:w:242:LYS:O	44:w:247:PRO:HD3	2.06	0.55
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.88	0.55
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.87	0.55
41:s:62:ARG:HD2	41:s:68:ILE:HD12	1.89	0.55
2:B:76:TYR:HE2	16:Q:202:TRP:CD2	2.24	0.55
1:A:426:ALA:HB3	46:A:502:FMN:HM82	1.89	0.55
15:P:61:PHE:CZ	15:P:106:ALA:CB	2.89	0.55
16:Q:218:SER:HB3	16:Q:224:ALA:HB1	1.88	0.55
35:l:173:LEU:HD12	40:r:405:LEU:HD21	1.87	0.55
40:r:189:SER:OG	40:r:192:ASN:OD1	2.25	0.55
27:d:120:SER:HB3	43:v:56:ARG:HH22	1.71	0.55
27:d:160:LYS:HE2	28:e:147:ILE:HG23	1.89	0.55
32:i:62:THR:HG21	32:i:114:TRP:CD1	2.42	0.55
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.89	0.55
52:i:401:CDL:OB9	44:w:44:VAL:HG21	2.06	0.55
40:r:259:TYR:O	40:r:263:MET:HG2	2.06	0.55
9:J:188:GLU:HG3	9:J:200:ILE:HD13	1.89	0.54
12:M:340:ALA:HB3	12:M:366:LEU:HD23	1.89	0.54
35:l:171:ALA:O	35:l:175:ASN:ND2	2.40	0.54
1:A:388:GLY:O	1:A:392:MET:HG3	2.07	0.54
52:J:404:CDL:HB31	36:m:82:VAL:HG21	1.89	0.54
16:Q:202:TRP:CZ3	16:Q:261:MET:HG3	2.43	0.54
21:W:50:MET:HG2	41:s:156:MET:SD	2.47	0.54
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.40	0.54
1:A:295:PRO:HG2	1:A:298:GLU:HB3	1.88	0.54
3:C:50:LEU:O	3:C:54:VAL:HG23	2.07	0.54
15:P:173:MET:HB3	15:P:198:PHE:HB2	1.88	0.54
16:Q:208:GLU:OE2	16:Q:221:ARG:NH2	2.40	0.54
6:X:123:GLU:HG2	6:X:129:GLU:HA	1.90	0.54
1:A:98:LYS:NZ	1:A:242:VAL:O	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:53:LEU:HD22	48:C:303:PLX:C32	2.37	0.54
9:J:174:ILE:HG23	9:J:175:LYS:HD2	1.89	0.54
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.88	0.54
30:g:89:ASP:OD2	42:u:161:ALA:CB	2.54	0.54
12:M:36:VAL:HG22	12:M:102:ILE:HD12	1.89	0.54
16:Q:259:GLU:OE2	21:W:23:ARG:NE	2.39	0.54
6:X:132:ASP:OD2	39:p:18:ARG:NH1	2.40	0.54
21:W:134:LEU:HD21	36:m:2:THR:HB	1.89	0.54
52:V:201:CDL:H751	52:V:201:CDL:H381	1.89	0.54
27:d:140:GLN:O	27:d:144:SER:HB3	2.07	0.54
32:i:147:GLN:H	32:i:147:GLN:CD	2.14	0.54
1:A:378:SER:OG	1:A:385:CYS:SG	2.64	0.54
48:C:303:PLX:O4	48:C:303:PLX:O7	2.18	0.54
12:M:262:VAL:HG23	12:M:276:ARG:HB2	1.89	0.54
35:l:504:LEU:O	35:l:507:THR:OG1	2.26	0.54
35:l:558:LEU:HB3	40:r:214:LEU:HD21	1.89	0.54
2:B:39:LYS:NZ	16:Q:335:GLU:OE2	2.41	0.54
7:H:107:PRO:O	7:H:108:PRO:O	2.26	0.54
9:J:87:GLU:HG3	9:J:89:TYR:H	1.72	0.54
33:j:23:TRP:CZ3	47:j:202:PEE:H11	2.43	0.54
10:K:100:GLN:NE2	14:O:69:ASN:C	2.65	0.54
12:M:394:VAL:HA	12:M:473:MET:HE1	1.89	0.54
21:W:103:ASP:OD1	21:W:103:ASP:N	2.41	0.54
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.90	0.54
38:o:56:ARG:NH2	40:r:424:ASN:HD21	2.06	0.54
12:M:250:SER:OG	12:M:251:ILE:N	2.40	0.53
41:s:46:LEU:HD23	41:s:49:ILE:HD12	1.90	0.53
1:A:249:ALA:O	1:A:252:PRO:HD2	2.07	0.53
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.44	0.53
14:O:75:LYS:O	14:O:77:ALA:N	2.40	0.53
23:Z:58:ALA:O	35:l:434:LYS:NZ	2.40	0.53
38:o:59:VAL:HG22	40:r:423:ILE:CG2	2.37	0.53
16:Q:144:MET:HE3	16:Q:222:MET:O	2.08	0.53
20:V:140:LYS:CE	24:a:158:ARG:HD3	2.31	0.53
12:M:51:GLN:HA	12:M:54:GLU:HG2	1.91	0.53
12:M:339:ALA:HB1	12:M:537:ILE:HD12	1.91	0.53
52:V:202:CDL:H852	35:l:558:LEU:HD21	1.90	0.53
27:d:32:TYR:CZ	27:d:36:ILE:HD11	2.43	0.53
14:O:218:PRO:HD2	14:O:223:PHE:HA	1.91	0.53
6:X:132:ASP:OD1	6:X:133:ILE:N	2.39	0.53
24:a:160:MET:HE3	24:a:166:GLY:CA	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:44:TYR:O	7:H:48:THR:HG22	2.08	0.53
12:M:556:THR:HG23	12:M:558:GLN:H	1.73	0.53
47:W:201:PEE:H42	47:W:201:PEE:H33	1.90	0.53
35:l:51:LEU:O	35:l:55:MET:HG3	2.09	0.53
35:l:520:TYR:HB2	52:l:703:CDL:OA3	2.09	0.53
44:w:146:ALA:HB1	44:w:157:VAL:HG21	1.90	0.53
1:A:263:ALA:HA	1:A:271:SER:HB3	1.90	0.53
11:L:116:SER:OG	15:P:227:ALA:O	2.24	0.53
52:a:201:CDL:H712	52:a:201:CDL:H172	1.89	0.53
35:l:397:GLU:HG2	35:l:482:MET:HE1	1.90	0.53
52:l:702:CDL:H591	52:l:702:CDL:H332	1.90	0.53
2:B:144:ARG:NH1	11:L:112:MET:O	2.40	0.53
52:N:202:CDL:CA7	52:N:202:CDL:C34	2.86	0.53
28:e:119:ARG:O	28:e:123:GLU:HG3	2.08	0.53
35:l:585:LYS:NZ	52:m:201:CDL:OB3	2.35	0.53
47:l:704:PEE:O5	47:l:704:PEE:H1	2.09	0.53
40:r:243:MET:HA	40:r:246:ILE:HG22	1.91	0.53
41:s:106:LEU:HD21	41:s:150:LEU:HD12	1.90	0.53
1:A:48:ARG:NH1	10:K:70:ASN:O	2.42	0.53
2:B:100:GLU:OE2	2:B:185:TYR:OH	2.21	0.52
27:d:73:ASP:OD1	27:d:75:THR:OG1	2.27	0.52
35:l:245:ALA:O	35:l:249:SER:OG	2.26	0.52
35:l:401:MET:SD	35:l:482:MET:HG2	2.50	0.52
1:A:414:GLU:CD	8:I:50:SER:O	2.51	0.52
10:K:83:THR:HG23	14:O:88:ARG:HH11	1.75	0.52
12:M:240:ALA:HB2	12:M:271:MET:HE2	1.91	0.52
22:Y:43:ARG:HB3	22:Y:46:GLN:HB2	1.92	0.52
22:Y:50:LEU:HD13	22:Y:55:LEU:HD21	1.91	0.52
26:c:153:TYR:OH	43:v:8:ARG:NH1	2.40	0.52
35:l:227:PHE:O	35:l:230:HIS:ND1	2.43	0.52
5:F:92:GLU:O	5:F:96:SER:OG	2.24	0.52
11:L:122:SER:HB2	15:P:229:GLU:OE2	2.10	0.52
16:Q:94:VAL:HG21	16:Q:116:LEU:HB2	1.91	0.52
32:i:278:MET:O	32:i:282:MET:HG3	2.09	0.52
52:l:702:CDL:H621	52:l:702:CDL:H432	1.90	0.52
8:I:52:ASN:OD1	8:I:57:ARG:NE	2.41	0.52
32:i:84:TRP:CH2	34:k:59:MET:HE2	2.44	0.52
35:l:562:LEU:HB3	35:l:563:PRO:HD3	1.90	0.52
41:s:200:LEU:HD13	41:s:282:TYR:CA	2.39	0.52
48:C:303:PLX:H221	51:s:501:UQ:H551	1.90	0.52
15:P:140:ARG:NH2	16:Q:406:GLU:OE2	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:350:LEU:HD12	35:l:359:MET:HG2	1.91	0.52
35:l:375:ILE:HD12	35:l:458:LEU:HD11	1.91	0.52
52:l:702:CDL:H651	52:l:702:CDL:H832	1.91	0.52
1:A:116:ASN:ND2	46:A:502:FMN:O3'	2.43	0.52
6:G:123:GLU:HB3	6:G:130:ILE:HD13	1.90	0.52
12:M:591:GLU:HA	12:M:610:VAL:O	2.09	0.52
12:M:650:SER:HG	12:M:652:ASN:ND2	2.07	0.52
16:Q:274:ASP:OD1	16:Q:323:ARG:NH2	2.42	0.52
19:U:78:LEU:HD13	42:u:123:GLY:HA3	1.90	0.52
35:l:228:GLY:HA3	47:l:704:PEE:H38	1.92	0.52
4:E:114:ARG:HH12	9:J:45:LYS:HD2	1.73	0.52
8:I:29:GLN:O	8:I:29:GLN:HG3	2.08	0.52
8:I:90:THR:HG22	8:I:92:LYS:HG2	1.92	0.52
12:M:380:ASP:OD1	12:M:380:ASP:N	2.42	0.52
12:M:666:GLN:NE2	12:M:670:GLU:OE2	2.42	0.52
26:c:70:MET:SD	38:o:86:THR:HG22	2.50	0.52
32:i:125:GLN:CG	52:i:401:CDL:OA3	2.58	0.52
25:b:14:GLN:HE22	39:p:157:ALA:HB3	1.74	0.52
27:d:110:LEU:O	27:d:113:CYS:HB3	2.10	0.52
31:h:47:ILE:CG2	31:h:51:ARG:CZ	2.87	0.52
5:F:20:ARG:HB2	5:F:66:TRP:HB2	1.92	0.52
47:Q:501:PEE:C22	47:Q:501:PEE:C18	2.86	0.52
52:V:202:CDL:H591	52:V:202:CDL:H192	1.92	0.52
2:B:79:ARG:HE	8:I:20:LEU:HD13	1.75	0.52
16:Q:52:MET:HG3	32:i:173:THR:HG22	1.91	0.52
32:i:233:THR:HG23	32:i:241:THR:HG22	1.92	0.52
2:B:200:GLU:HG3	13:N:88:ARG:HD3	1.91	0.51
4:E:39:TRP:O	4:E:43:VAL:HG23	2.10	0.51
6:G:130:ILE:N	6:G:130:ILE:CD1	2.73	0.51
9:J:208:GLY:N	9:J:211:ASP:HB3	2.25	0.51
17:S:19:PRO:HB3	41:s:9:LEU:HD12	1.92	0.51
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.91	0.51
40:r:420:THR:HB	40:r:423:ILE:HD12	1.92	0.51
44:w:180:ARG:NH2	44:w:182:GLN:OE1	2.43	0.51
5:F:59:SER:O	5:F:61:VAL:N	2.43	0.51
9:J:229:ILE:HB	9:J:323:HIS:CD2	2.45	0.51
9:J:304:LEU:O	9:J:307:VAL:HG22	2.10	0.51
11:L:111:LEU:HD11	13:N:126:PRO:HG2	1.92	0.51
13:N:6:VAL:HG22	13:N:9:ARG:NH2	2.26	0.51
16:Q:259:GLU:OE1	16:Q:338:ARG:NH2	2.34	0.51
40:r:191:SER:CB	47:r:501:PEE:H3	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:61:LEU:H	41:s:216:ALA:HB3	1.75	0.51
6:G:117:GLU:HA	6:G:120:MET:HE3	1.92	0.51
38:o:57:LEU:O	38:o:57:LEU:HG	2.11	0.51
42:u:162:LYS:HG3	42:u:163:HIS:CD2	2.45	0.51
12:M:512:VAL:O	12:M:514:ASN:ND2	2.44	0.51
35:l:407:TRP:CZ2	35:l:411:MET:HE2	2.45	0.51
9:J:37:HIS:O	9:J:40:LEU:N	2.40	0.51
21:W:90:ASN:ND2	21:W:123:GLU:O	2.43	0.51
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.92	0.51
41:s:28:LEU:HD22	41:s:275:ALA:HB2	1.92	0.51
44:w:62:VAL:O	44:w:160:GLU:O	2.29	0.51
12:M:299:ARG:HH11	12:M:299:ARG:CG	2.22	0.51
12:M:341:ILE:HD11	12:M:555:ILE:HD12	1.91	0.51
27:d:142:ARG:NE	28:e:138:GLU:O	2.44	0.51
1:A:67:GLU:O	1:A:71:LYS:HG2	2.11	0.51
40:r:441:ILE:HD12	40:r:444:LEU:HD12	1.93	0.51
40:r:336:ARG:NH1	40:r:433:GLU:OE2	2.32	0.51
44:w:63:ASP:HB3	44:w:241:TYR:CE1	2.46	0.51
1:A:426:ALA:HB3	46:A:502:FMN:C8M	2.41	0.51
9:J:207:PHE:HB2	9:J:214:LEU:HG	1.93	0.51
12:M:48:THR:OG1	12:M:51:GLN:HG3	2.11	0.51
12:M:266:ARG:HG2	12:M:267:THR:HG23	1.93	0.51
12:M:690:THR:HG23	12:M:692:LYS:HG2	1.92	0.51
19:U:54:PRO:HD3	21:W:69:ILE:HD13	1.92	0.51
27:d:81:ASP:O	27:d:85:MET:HG3	2.11	0.51
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.46	0.51
8:I:46:SER:O	8:I:52:ASN:ND2	2.41	0.50
40:r:175:ASN:O	40:r:179:ILE:HG12	2.11	0.50
41:s:24:GLU:OE1	41:s:228:TYR:OH	2.19	0.50
5:F:61:VAL:HG13	5:F:62:GLN:N	2.26	0.50
51:J:402:UQ:C11	51:J:402:UQ:C15	2.86	0.50
16:Q:36:GLN:HE21	40:r:142:ARG:CZ	2.25	0.50
35:l:76:LEU:HD21	35:l:196:TRP:HE3	1.75	0.50
52:l:702:CDL:H611	52:l:702:CDL:H811	1.93	0.50
2:B:111:GLU:O	2:B:141:ARG:NH1	2.44	0.50
9:J:180:TYR:HB2	9:J:317:ASP:OD2	2.12	0.50
12:M:29:SER:OG	12:M:30:ASN:N	2.43	0.50
32:i:182:SER:HB2	32:i:293:TYR:OH	2.11	0.50
41:s:215:TYR:HD2	41:s:219:PRO:HB2	1.76	0.50
33:j:10:ASN:ND2	41:s:10:ILE:HD11	2.26	0.50
52:J:404:CDL:H791	36:m:16:GLY:HA2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:124:LEU:CD2	15:P:201:ASP:O	2.60	0.50
12:M:194:ASP:OD2	12:M:212:LYS:NZ	2.44	0.50
19:U:51:TYR:O	21:W:68:ARG:NH1	2.44	0.50
25:b:29:SER:H	25:b:32:GLU:HG3	1.76	0.50
30:g:15:PHE:HB2	48:g:201:PLX:H6	1.93	0.50
32:i:88:LYS:O	32:i:148:SER:HB2	2.05	0.50
35:l:420:ALA:O	35:l:424:THR:HG22	2.12	0.50
52:u:201:CDL:C54	52:u:201:CDL:C58	2.86	0.50
2:B:192:ASN:OD1	18:T:63:ASN:ND2	2.41	0.50
48:C:303:PLX:C21	48:C:303:PLX:C17	2.86	0.50
8:I:43:VAL:HG23	8:I:44:GLY:H	1.76	0.50
40:r:371:PRO:O	40:r:448:THR:OG1	2.26	0.50
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.94	0.50
12:M:73:GLY:HA2	53:M:803:FES:S2	2.52	0.50
32:i:31:ILE:HD11	34:k:62:ILE:HG21	1.94	0.50
32:i:68:MET:HE1	34:k:37:MET:HE2	1.94	0.50
6:G:134:ASP:OD1	6:G:147:TYR:HE2	1.93	0.50
11:L:112:MET:HA	11:L:112:MET:HE2	1.94	0.50
14:O:166:ASP:OD2	14:O:168:LEU:HD13	2.12	0.50
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.47	0.50
32:i:268:GLN:HG3	42:u:168:PHE:HZ	1.77	0.50
52:i:401:CDL:OB4	44:w:40:PRO:CG	2.60	0.50
40:r:246:ILE:O	40:r:249:ILE:HG12	2.12	0.50
52:r:504:CDL:H782	52:r:504:CDL:H232	1.94	0.50
44:w:230:THR:HG23	44:w:233:TYR:H	1.75	0.50
2:B:84:ILE:HA	13:N:58:ARG:HD3	1.94	0.49
12:M:525:ALA:O	12:M:530:TYR:HB2	2.12	0.49
35:l:136:ASN:HA	35:l:197:ASP:HA	1.94	0.49
38:o:59:VAL:HG21	40:r:337:VAL:HG13	1.93	0.49
41:s:225:MET:HG3	51:s:501:UQ:H452	1.93	0.49
44:w:67:CYS:N	56:w:401:ADP:O2A	2.35	0.49
6:G:137:LYS:O	6:G:138:LEU:C	2.55	0.49
32:i:150:ASN:OD1	32:i:151:PRO:HD2	2.12	0.49
35:l:253:VAL:HB	35:l:310:LEU:HD11	1.92	0.49
1:A:387:GLU:OE1	12:M:123:ASN:ND2	2.39	0.49
33:j:105:GLU:HG3	36:m:169:MET:HE1	1.93	0.49
27:d:132:PHE:HE2	35:l:204:LEU:HD11	1.76	0.49
35:l:71:LEU:N	35:l:71:LEU:HD22	2.27	0.49
9:J:213:PHE:HZ	9:J:276:LEU:HD21	1.78	0.49
12:M:275:PRO:HG3	12:M:286:ILE:HG12	1.93	0.49
16:Q:357:LYS:HD3	16:Q:364:SER:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:o:56:ARG:HH11	38:o:60:ILE:HG13	1.76	0.49
1:A:48:ARG:HH11	10:K:70:ASN:HB3	1.77	0.49
1:A:174:ARG:NH1	10:K:92:GLU:OE1	2.46	0.49
1:A:231:ALA:O	1:A:239:PRO:HB3	2.13	0.49
49:X:201:8Q1:N36	49:X:201:8Q1:O40	2.45	0.49
24:a:168:TRP:HB3	30:g:3:MET:HB2	1.93	0.49
26:c:146:VAL:HA	26:c:149:ILE:HG12	1.94	0.49
35:l:135:ASN:O	35:l:198:LEU:HG	2.12	0.49
42:u:169:PHE:HZ	52:u:201:CDL:H562	1.78	0.49
44:w:132:GLN:NE2	44:w:166:ASP:OD1	2.45	0.49
26:c:162:PRO:HG3	43:v:39:MET:HE2	1.93	0.49
28:e:97:ILE:O	28:e:101:LEU:HB2	2.12	0.49
35:l:561:ILE:HG13	35:l:562:LEU:H	1.77	0.49
3:C:96:SER:CB	41:s:213:VAL:HG23	2.42	0.49
4:E:42:GLU:OE1	4:E:94:ILE:CD1	2.60	0.49
5:F:53:ILE:O	12:M:380:ASP:HB3	2.11	0.49
9:J:304:LEU:HD23	9:J:304:LEU:O	2.12	0.49
25:b:99:GLU:OE1	25:b:99:GLU:N	2.45	0.49
32:i:41:ILE:HG13	34:k:73:LEU:HD21	1.94	0.49
33:j:53:MET:HE3	33:j:55:PHE:CE2	2.47	0.49
9:J:208:GLY:H	9:J:211:ASP:CB	2.26	0.49
44:w:66:ILE:HA	56:w:401:ADP:O2A	2.12	0.49
47:W:201:PEE:H38	36:m:39:VAL:HG22	1.95	0.49
52:r:504:CDL:H271	52:r:504:CDL:H721	1.95	0.49
11:L:109:ASN:HB2	11:L:116:SER:OG	2.13	0.48
12:M:406:ASN:O	12:M:410:GLU:HG3	2.13	0.48
28:e:76:TYR:HB2	28:e:83:ASP:OD1	2.13	0.48
32:i:256:PRO:HD2	32:i:257:LEU:HD22	1.94	0.48
33:j:22:PHE:HA	41:s:60:PRO:HG3	1.95	0.48
40:r:306:PRO:HB3	40:r:458:LEU:HD12	1.95	0.48
41:s:179:TRP:O	41:s:183:MET:HG3	2.12	0.48
3:C:99:GLN:HE22	41:s:212:ASN:HD22	1.60	0.48
12:M:197:THR:HG22	12:M:206:VAL:HG22	1.95	0.48
13:N:73:THR:HG22	13:N:77:VAL:HG12	1.94	0.48
17:S:34:LYS:NZ	17:S:61:HIS:O	2.37	0.48
18:T:101:ASN:ND2	18:T:103:ASP:OD2	2.43	0.48
27:d:70:ARG:NH1	27:d:91:GLN:OE1	2.45	0.48
32:i:171:ASN:O	32:i:171:ASN:ND2	2.46	0.48
1:A:272:GLY:O	1:A:292:MET:HB2	2.12	0.48
7:H:48:THR:HA	7:H:51:ILE:HG12	1.95	0.48
12:M:172:ILE:HD12	12:M:175:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:26:GLY:HA3	47:j:201:PEE:H37	1.95	0.48
30:g:7:ARG:NH1	30:g:87:LEU:HD11	2.28	0.48
32:i:264:TRP:CZ2	42:u:168:PHE:CD2	3.01	0.48
32:i:276:ILE:HG21	47:r:501:PEE:H14	1.95	0.48
35:l:7:LEU:O	35:l:11:THR:HG23	2.13	0.48
52:l:703:CDL:H412	52:l:703:CDL:H621	1.93	0.48
40:r:370:PRO:HG3	40:r:375:LEU:HD22	1.94	0.48
25:b:29:SER:HB2	25:b:32:GLU:HG2	1.95	0.48
33:j:68:GLU:HG3	33:j:98:LEU:HD13	1.94	0.48
35:l:12:LEU:HD22	35:l:129:MET:HB3	1.96	0.48
35:l:596:MET:HE1	52:m:201:CDL:H622	1.95	0.48
16:Q:52:MET:CE	47:Q:501:PEE:H9	2.44	0.48
24:a:133:TYR:OH	27:d:87:GLU:OE1	2.28	0.48
25:b:121:LYS:HD3	25:b:121:LYS:O	2.14	0.48
27:d:106:ILE:HD11	28:e:136:LEU:CD2	2.33	0.48
32:i:17:THR:HG21	32:i:133:TRP:NE1	2.29	0.48
38:o:31:LYS:O	38:o:35:GLU:HG3	2.13	0.48
36:m:24:PRO:HG3	36:m:83:TRP:NE1	2.29	0.48
41:s:139:THR:HA	41:s:142:TYR:CE2	2.48	0.48
7:H:44:TYR:HB2	15:P:68:ILE:HG23	1.95	0.48
15:P:61:PHE:HZ	15:P:106:ALA:CB	2.26	0.48
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	1.95	0.48
25:b:5:THR:OG1	25:b:8:GLU:HG3	2.14	0.48
35:l:358:LYS:HG3	39:p:80:TYR:CE1	2.48	0.48
52:l:702:CDL:O1	40:r:357:THR:OG1	2.24	0.48
38:o:112:LYS:O	38:o:116:ILE:HG12	2.13	0.48
1:A:102:MET:HE2	1:A:149:MET:HE2	1.95	0.48
4:E:62:LYS:O	4:E:66:MET:HG2	2.13	0.48
9:J:167:ILE:HD13	9:J:201:ILE:HB	1.95	0.48
9:J:303:ARG:HD3	9:J:303:ARG:C	2.38	0.48
13:N:55:PHE:CZ	13:N:58:ARG:HG3	2.49	0.48
14:O:182:ASN:CG	14:O:194:GLU:OE1	2.54	0.48
27:d:106:ILE:CD1	28:e:136:LEU:HD21	2.34	0.48
38:o:65:LEU:O	38:o:69:THR:HG23	2.12	0.48
1:A:149:MET:CE	1:A:241:THR:OG1	2.62	0.48
32:i:230:LEU:O	32:i:233:THR:HG22	2.14	0.48
35:l:119:LYS:HZ1	52:l:702:CDL:H512	1.79	0.48
35:l:421:ALA:O	35:l:424:THR:CG2	2.62	0.48
42:u:34:ALA:HB2	42:u:120:PRO:HG3	1.95	0.48
12:M:343:GLY:O	12:M:521:SER:OG	2.30	0.48
39:p:108:HIS:HB3	39:p:111:GLU:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:119:VAL:HG12	15:P:121:THR:HG22	1.96	0.47
52:a:201:CDL:H511	47:b:201:PEE:H52	1.95	0.47
26:c:156:VAL:HG11	43:v:95:TYR:CZ	2.49	0.47
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.96	0.47
1:A:67:GLU:OE1	1:A:67:GLU:N	2.44	0.47
2:B:98:ARG:NH2	16:Q:224:ALA:O	2.41	0.47
48:C:303:PLX:H341	48:C:303:PLX:H191	1.96	0.47
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.49	0.47
12:M:382:ARG:NE	12:M:527:ASP:OD2	2.47	0.47
47:Q:501:PEE:H47	47:r:501:PEE:C24	2.45	0.47
40:r:269:MET:SD	40:r:399:ASN:ND2	2.88	0.47
1:A:398:ARG:HG2	1:A:403:ASP:HB3	1.97	0.47
8:I:70:MET:HE1	15:P:73:VAL:HG12	1.94	0.47
12:M:295:ASP:OD1	12:M:704:SER:OG	2.31	0.47
17:S:34:LYS:NZ	17:S:61:HIS:HB2	2.30	0.47
26:c:91:ASP:O	38:o:44:LYS:NZ	2.40	0.47
31:h:84:ASP:OD1	31:h:85:LYS:N	2.47	0.47
32:i:65:THR:O	32:i:69:MET:HG3	2.15	0.47
32:i:222:SER:O	32:i:224:ALA:N	2.47	0.47
35:l:65:ASN:OD1	35:l:66:TRP:N	2.48	0.47
44:w:65:ASN:O	44:w:66:ILE:C	2.57	0.47
8:I:66:PRO:HB3	15:P:79:SER:HA	1.96	0.47
42:u:169:PHE:CZ	52:u:201:CDL:H562	2.48	0.47
44:w:96:SER:HA	44:w:101:GLY:HA2	1.95	0.47
15:P:105:ASN:O	15:P:137:PHE:HE2	1.87	0.47
21:W:23:ARG:HD3	21:W:25:LEU:HG	1.96	0.47
32:i:189:TRP:CH2	32:i:263:LYS:HG3	2.49	0.47
35:l:560:THR:O	35:l:565:THR:OG1	2.29	0.47
1:A:281:HIS:ND1	1:A:358:ASP:OD1	2.48	0.47
33:j:95:LEU:HD13	41:s:302:MET:HG3	1.96	0.47
34:k:23:ARG:HG2	52:m:201:CDL:HB62	1.96	0.47
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.49	0.47
41:s:24:GLU:HG3	41:s:271:LEU:HD22	1.97	0.47
4:E:14:GLY:O	11:L:52:LEU:HD11	2.14	0.47
6:G:126:PHE:CD2	6:G:148:ILE:HG21	2.49	0.47
9:J:304:LEU:C	9:J:304:LEU:CD2	2.85	0.47
51:J:402:UQ:H201	51:J:402:UQ:H221	1.56	0.47
52:J:404:CDL:H171	52:J:404:CDL:H141	1.67	0.47
14:O:75:LYS:C	14:O:77:ALA:N	2.70	0.47
19:U:59:ASP:CG	42:u:130:LYS:HD3	2.39	0.47
32:i:79:LEU:HB2	34:k:47:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:63:LEU:HD21	36:m:63:GLY:HA2	1.97	0.47
35:l:84:TYR:CE2	35:l:475:MET:HE1	2.49	0.47
35:l:227:PHE:N	35:l:284:THR:OG1	2.48	0.47
35:l:233:LEU:HB3	35:l:234:PRO:HD3	1.96	0.47
52:J:404:CDL:H372	52:J:404:CDL:H401	1.57	0.47
11:L:84:ARG:NH1	11:L:88:GLN:O	2.48	0.47
47:Q:501:PEE:H61	47:Q:501:PEE:C23	2.31	0.47
32:i:110:PRO:HG2	35:l:594:THR:HG21	1.97	0.47
40:r:97:THR:HG21	52:r:504:CDL:H242	1.97	0.47
9:J:208:GLY:N	9:J:211:ASP:CG	2.59	0.47
12:M:171:THR:CG2	12:M:231:LEU:CD2	2.92	0.47
12:M:289:LYS:HA	12:M:707:MET:HE1	1.96	0.47
14:O:48:ASN:OD1	14:O:51:THR:OG1	2.25	0.47
24:a:160:MET:HE3	24:a:167:PRO:CD	2.40	0.47
52:a:201:CDL:C52	47:b:201:PEE:H16	2.34	0.47
26:c:58:ARG:NH1	38:o:36:ARG:HE	2.13	0.47
47:j:202:PEE:C1	47:j:202:PEE:C4	2.86	0.47
3:C:83:ARG:NH1	16:Q:212:GLU:OE2	2.34	0.47
11:L:78:ARG:HD2	12:M:607:LYS:HE2	1.96	0.47
12:M:299:ARG:CZ	12:M:299:ARG:HB3	2.45	0.47
12:M:377:ALA:CB	12:M:381:LEU:HD12	2.45	0.47
12:M:382:ARG:NH2	12:M:652:ASN:OD1	2.48	0.47
14:O:179:ALA:HB3	14:O:185:MET:SD	2.56	0.47
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.50	0.47
35:l:481:THR:OG1	43:v:92:HIS:ND1	2.39	0.47
4:E:103:ILE:HG22	4:E:104:MET:HE2	1.97	0.46
6:G:133:ILE:HD12	6:G:133:ILE:HA	1.74	0.46
38:o:56:ARG:O	38:o:56:ARG:HD3	2.15	0.46
44:w:62:VAL:HG12	44:w:70:LYS:HB2	1.97	0.46
9:J:49:SER:HB2	15:P:225:GLU:HG2	1.97	0.46
17:S:17:PHE:HB3	17:S:21:MET:HE3	1.97	0.46
26:c:167:TYR:HD2	26:c:168:LEU:HD12	1.80	0.46
37:n:54:GLU:HG2	37:n:55:VAL:HG13	1.98	0.46
5:F:42:VAL:HG12	5:F:46:LYS:HE3	1.96	0.46
10:K:73:TYR:CZ	10:K:75:ASN:HB3	2.51	0.46
13:N:3:LEU:HD11	52:N:202:CDL:H312	1.96	0.46
47:Q:501:PEE:H47	47:r:501:PEE:H40	1.96	0.46
35:l:67:HIS:HE1	35:l:70:THR:HG22	1.80	0.46
35:l:78:LEU:HD12	35:l:139:GLN:NE2	2.30	0.46
35:l:221:ALA:HA	35:l:226:GLN:HG2	1.98	0.46
41:s:55:LEU:HD13	41:s:221:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:LEU:HD23	11:L:112:MET:HG3	1.97	0.46
24:a:96:ALA:HB2	27:d:61:TYR:CD1	2.50	0.46
27:d:142:ARG:HB3	27:d:143:TYR:CD1	2.51	0.46
31:h:80:LYS:NZ	36:m:1:MET:HE1	2.31	0.46
32:i:207:ILE:HG22	32:i:211:MET:HE2	1.97	0.46
52:l:702:CDL:H611	52:l:702:CDL:H581	1.73	0.46
40:r:122:PHE:CZ	40:r:206:LYS:HG3	2.48	0.46
52:J:404:CDL:H341	52:J:404:CDL:H312	1.73	0.46
12:M:389:THR:HG21	12:M:473:MET:HE2	1.98	0.46
41:s:198:PHE:CD1	41:s:285:LEU:HD13	2.50	0.46
44:w:132:GLN:HE22	56:w:401:ADP:HN62	1.62	0.46
12:M:483:ARG:NH1	12:M:485:ASP:OD1	2.49	0.46
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.97	0.46
16:Q:242:ASP:OD1	21:W:16:TYR:OH	2.34	0.46
24:a:160:MET:CE	24:a:168:TRP:H	2.29	0.46
26:c:62:TYR:OH	26:c:74:ASP:OD1	2.32	0.46
28:e:90:VAL:HG22	40:r:28:THR:HG21	1.97	0.46
31:h:19:THR:HA	32:i:84:TRP:HB2	1.97	0.46
32:i:111:PHE:HA	35:l:591:PHE:CE1	2.50	0.46
41:s:215:TYR:HD2	41:s:219:PRO:CB	2.29	0.46
3:C:109:LEU:HD13	3:C:117:LEU:HD13	1.97	0.46
16:Q:53:TYR:CE1	47:Q:501:PEE:O4P	2.69	0.46
20:V:107:SER:HB3	20:V:110:ILE:HB	1.98	0.46
24:a:170:GLN:NE2	42:u:151:ASN:HD22	2.11	0.46
35:l:121:LEU:HD22	35:l:246:LEU:HD23	1.98	0.46
35:l:517:SER:CB	52:l:703:CDL:HA32	2.39	0.46
41:s:283:ASP:OD1	41:s:284:GLN:N	2.49	0.46
1:A:204:TYR:HB3	1:A:377:GLU:HB3	1.98	0.46
6:G:123:GLU:HB3	6:G:130:ILE:CD1	2.45	0.46
12:M:476:LEU:HD22	12:M:493:VAL:HG21	1.98	0.46
16:Q:172:VAL:HG21	16:Q:310:VAL:HG22	1.98	0.46
35:l:305:SER:HB2	35:l:422:TYR:CZ	2.50	0.46
35:l:327:LEU:O	35:l:331:MET:HG2	2.16	0.46
43:v:95:TYR:HD2	43:v:99:MET:HE2	1.81	0.46
1:A:270:ASN:O	1:A:292:MET:HG2	2.16	0.46
3:C:73:ALA:HB1	51:s:501:UQ:HM51	1.97	0.46
9:J:168:SER:O	9:J:203:PRO:HD2	2.16	0.46
15:P:118:ASP:OD1	15:P:125:ARG:HG2	2.16	0.46
20:V:141:VAL:HG12	24:a:157:ARG:NH2	2.31	0.46
27:d:114:GLN:HG3	35:l:203:MET:HG2	1.98	0.46
28:e:92:PHE:O	28:e:96:SER:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:g:201:PLX:H102	48:g:201:PLX:H71	1.58	0.46
31:h:45:HIS:ND1	31:h:45:HIS:C	2.73	0.46
35:l:573:MET:HE3	47:l:701:PEE:C13	2.40	0.46
41:s:32:GLN:OE1	41:s:34:ARG:NH2	2.49	0.46
41:s:135:ALA:HB2	41:s:201:THR:CG2	2.45	0.46
1:A:448:GLU:O	1:A:452:GLN:HG2	2.16	0.46
2:B:94:SER:OG	16:Q:215:GLU:OE2	2.23	0.46
7:H:103:LEU:HD12	15:P:71:LYS:O	2.16	0.46
12:M:382:ARG:HG2	12:M:386:LEU:CD1	2.46	0.46
47:b:201:PEE:H34	52:l:702:CDL:H242	1.97	0.46
32:i:207:ILE:HD12	32:i:262:PRO:HG3	1.98	0.46
32:i:276:ILE:HG21	47:r:501:PEE:H7	1.98	0.46
35:l:426:ILE:O	35:l:430:ALA:CB	2.64	0.46
52:r:504:CDL:H772	52:r:504:CDL:H741	1.43	0.46
41:s:87:VAL:HG12	41:s:95:LEU:HD23	1.96	0.46
32:i:125:GLN:HG2	52:i:401:CDL:OA3	2.16	0.45
48:r:502:PLX:H72	48:r:502:PLX:H101	1.70	0.45
43:v:31:PHE:HE2	43:v:104:ARG:HE	1.64	0.45
1:A:81:LYS:HG2	1:A:96:GLY:HA3	1.98	0.45
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.67	0.45
47:B:303:PEE:H71	47:B:303:PEE:H77	1.61	0.45
32:i:211:MET:HG2	32:i:333:SER:OG	2.16	0.45
41:s:102:VAL:HG21	41:s:154:LEU:HD11	1.97	0.45
10:K:69:ASP:N	10:K:69:ASP:OD1	2.50	0.45
12:M:171:THR:HA	12:M:230:ALA:O	2.17	0.45
19:U:20:VAL:HA	47:j:201:PEE:H64	1.98	0.45
20:V:118:MET:HA	20:V:121:THR:HG22	1.97	0.45
31:h:87:ILE:HG22	31:h:92:TYR:HB3	1.97	0.45
35:l:529:TYR:HB3	35:l:530:PRO:HD3	1.98	0.45
41:s:11:ILE:HB	41:s:12:PRO:HD3	1.98	0.45
24:a:160:MET:CE	24:a:166:GLY:HA3	2.42	0.45
47:B:303:PEE:H56	41:s:187:ILE:CD1	2.47	0.45
9:J:37:HIS:NE2	18:T:48:GLY:O	2.49	0.45
11:L:117:THR:HG21	15:P:229:GLU:HG3	1.98	0.45
14:O:138:THR:HG22	14:O:139:PRO:HD3	1.97	0.45
24:a:163:ARG:NH2	30:g:102:ASP:OD2	2.49	0.45
27:d:66:ARG:HD3	27:d:68:PHE:CE1	2.51	0.45
35:l:526:LEU:HD12	35:l:530:PRO:HG2	1.98	0.45
1:A:255:CYS:O	14:O:246:GLN:NE2	2.50	0.45
2:B:101:HIS:ND1	2:B:149:MET:HE1	2.32	0.45
35:l:230:HIS:N	35:l:231:PRO:HD3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:524:ASN:HD21	39:p:78:GLN:HB2	1.82	0.45
36:m:121:GLY:C	36:m:122:LEU:HD23	2.41	0.45
52:r:504:CDL:H872	52:r:504:CDL:H841	1.77	0.45
1:A:292:MET:HE3	1:A:338:ASP:HA	1.99	0.45
1:A:296:LEU:HD11	1:A:317:VAL:HG11	1.97	0.45
4:E:81:LEU:O	4:E:85:LYS:HG3	2.17	0.45
6:G:117:GLU:HA	6:G:120:MET:CE	2.46	0.45
12:M:391:ILE:HG13	12:M:600:GLU:OE2	2.17	0.45
15:P:157:VAL:HG21	15:P:182:PRO:HD3	1.99	0.45
49:X:201:8Q1:C8	39:p:48:PHE:CZ	3.00	0.45
28:e:57:GLU:OE1	44:w:320:GLY:HA3	2.17	0.45
28:e:73:SER:O	28:e:74:HIS:HB2	2.15	0.45
52:m:201:CDL:H361	52:m:201:CDL:H272	1.99	0.45
1:A:177:TYR:OH	1:A:194:ASP:OD1	2.22	0.45
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.52	0.45
9:J:322:VAL:HG13	9:J:323:HIS:ND1	2.32	0.45
20:V:34:LEU:HD22	52:m:201:CDL:H261	1.97	0.45
33:j:38:GLU:HB2	33:j:41:PHE:O	2.17	0.45
44:w:320:GLY:O	44:w:324:SER:OG	2.32	0.45
3:C:73:ALA:CB	51:s:501:UQ:HM51	2.45	0.45
5:F:88:THR:O	5:F:92:GLU:OE1	2.35	0.45
16:Q:259:GLU:HG3	16:Q:263:THR:OG1	2.17	0.45
16:Q:440:LYS:HD3	16:Q:440:LYS:HA	1.69	0.45
26:c:33:THR:HG23	26:c:35:ASP:H	1.81	0.45
30:g:93:PHE:HA	30:g:96:VAL:HG12	1.99	0.45
32:i:172:GLN:OE1	35:l:578:SER:OG	2.28	0.45
33:j:1:MET:HE1	36:m:3:MET:HE1	1.99	0.45
35:l:561:ILE:HG13	35:l:562:LEU:N	2.32	0.45
52:l:702:CDL:H861	52:l:702:CDL:H572	1.99	0.45
51:s:501:UQ:C33	51:s:501:UQ:C30	2.86	0.45
42:u:40:ASN:O	42:u:44:MET:HG2	2.17	0.45
3:C:75:GLU:HG3	3:C:167:PRO:HB2	1.98	0.45
10:K:75:ASN:C	10:K:75:ASN:HD22	2.25	0.45
16:Q:88:HIS:HB3	16:Q:91:ALA:HB2	1.99	0.45
21:W:133:ILE:O	21:W:137:THR:HG22	2.17	0.45
6:X:111:ASP:OD1	6:X:111:ASP:N	2.43	0.45
35:l:277:THR:HG23	35:l:314:MET:HG3	1.98	0.45
8:I:8:ILE:HD11	52:N:202:CDL:H111	1.99	0.44
8:I:30:GLU:CD	8:I:30:GLU:H	2.24	0.44
14:O:152:ILE:HG21	14:O:171:LEU:HD13	1.99	0.44
31:h:17:TRP:H	31:h:17:TRP:CD1	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:o:129:TYR:CD1	38:o:129:TYR:N	2.84	0.44
22:Y:65:MET:SD	35:l:375:ILE:HG12	2.58	0.44
24:a:60:SER:OG	39:p:111:GLU:OE2	2.33	0.44
47:j:201:PEE:H55	47:j:201:PEE:H60	1.77	0.44
48:j:203:PLX:H352	36:m:155:ILE:HG23	1.98	0.44
52:J:404:CDL:HB61	52:J:404:CDL:H321	1.99	0.44
12:M:391:ILE:N	12:M:600:GLU:OE2	2.31	0.44
13:N:127:TYR:OH	18:T:61:GLU:O	2.30	0.44
26:c:87:ASP:OD2	26:c:90:TYR:N	2.51	0.44
28:e:94:GLY:O	28:e:99:LEU:HB2	2.17	0.44
35:l:392:LYS:HE2	35:l:416:THR:HG23	1.99	0.44
36:m:41:CYS:O	36:m:45:LEU:HD23	2.18	0.44
44:w:181:LYS:O	44:w:184:VAL:HG22	2.18	0.44
2:B:43:MET:HE1	7:H:8:THR:HG21	1.99	0.44
12:M:382:ARG:CZ	12:M:527:ASP:OD2	2.64	0.44
16:Q:95:LEU:HD22	16:Q:458:PHE:HZ	1.82	0.44
52:V:202:CDL:H752	52:V:202:CDL:H721	1.55	0.44
25:b:123:PHE:CZ	43:v:61:HIS:HB2	2.53	0.44
32:i:79:LEU:HB2	34:k:47:ILE:HD11	1.98	0.44
35:l:49:VAL:HB	35:l:50:PRO:HD3	1.99	0.44
44:w:287:ASP:OD1	44:w:288:ASP:N	2.48	0.44
3:C:75:GLU:OE1	16:Q:221:ARG:NH1	2.51	0.44
21:W:120:MET:HG2	36:m:126:VAL:O	2.18	0.44
24:a:96:ALA:HB2	27:d:61:TYR:HE1	1.82	0.44
35:l:395:ILE:O	35:l:399:VAL:HG23	2.18	0.44
41:s:195:ARG:HD3	41:s:231:ILE:HD11	1.99	0.44
1:A:411:SER:O	1:A:415:ILE:HG13	2.17	0.44
47:B:303:PEE:H7	41:s:288:LEU:HD11	2.00	0.44
9:J:217:PHE:HD1	9:J:220:MET:HE2	1.82	0.44
34:k:26:LEU:HB3	34:k:78:LEU:HD12	2.00	0.44
35:l:16:THR:HG22	35:l:126:ILE:HD13	2.00	0.44
41:s:212:ASN:HD22	41:s:212:ASN:C	2.26	0.44
51:s:501:UQ:H261	51:s:501:UQ:H222	1.62	0.44
42:u:44:MET:HE3	42:u:48:TRP:CZ3	2.52	0.44
1:A:119:GLU:O	1:A:159:ARG:NH1	2.50	0.44
3:C:51:ASP:OD2	3:C:188:LYS:HA	2.18	0.44
4:E:14:GLY:O	4:E:15:THR:OG1	2.31	0.44
16:Q:41:VAL:O	16:Q:45:GLU:HG3	2.18	0.44
6:X:89:LEU:HD21	23:Z:47:ARG:C	2.43	0.44
24:a:160:MET:HE1	24:a:168:TRP:H	1.83	0.44
32:i:268:GLN:HG3	42:u:168:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:3:LEU:HD23	36:m:121:GLY:HA2	2.00	0.44
35:l:383:MET:SD	35:l:384:PRO:HD2	2.58	0.44
40:r:357:THR:O	40:r:361:VAL:HG23	2.17	0.44
43:v:71:ARG:NH2	43:v:72:ASP:OD1	2.39	0.44
9:J:119:VAL:HG23	9:J:120:VAL:HG13	2.00	0.44
12:M:47:THR:O	12:M:96:VAL:HG22	2.17	0.44
12:M:76:ARG:HD3	12:M:79:LEU:HD21	1.99	0.44
12:M:301:ARG:HD2	12:M:301:ARG:HA	1.69	0.44
15:P:106:ALA:HB1	15:P:108:PHE:HE2	1.82	0.44
52:V:201:CDL:H322	52:V:201:CDL:H352	1.58	0.44
52:V:201:CDL:H402	52:V:201:CDL:H762	2.00	0.44
26:c:75:TYR:CG	26:c:76:PRO:HD2	2.53	0.44
32:i:112:HIS:CE1	32:i:164:ILE:HG21	2.53	0.44
32:i:307:SER:OG	32:i:308:THR:N	2.51	0.44
35:l:51:LEU:HD22	35:l:91:PRO:HG3	2.00	0.44
37:n:29:ARG:O	37:n:33:GLU:HG3	2.18	0.44
12:M:299:ARG:CG	12:M:299:ARG:NH1	2.79	0.44
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.48	0.44
12:M:624:ARG:NH1	12:M:628:GLU:OE1	2.33	0.44
13:N:73:THR:HG23	13:N:76:ASP:O	2.18	0.44
14:O:138:THR:HA	14:O:141:MET:HB3	1.99	0.44
27:d:65:HIS:NE2	28:e:124:ARG:NH2	2.64	0.44
33:j:22:PHE:CG	47:j:202:PEE:O4	2.71	0.44
1:A:201:ALA:O	14:O:119:TYR:HB3	2.18	0.43
2:B:76:TYR:CD2	16:Q:202:TRP:CE2	3.06	0.43
12:M:338:VAL:HG23	12:M:363:SER:CB	2.48	0.43
35:l:425:ARG:O	35:l:429:PHE:HB2	2.18	0.43
1:A:424:ILE:HG12	12:M:76:ARG:NH2	2.34	0.43
8:I:20:LEU:O	8:I:23:LYS:O	2.35	0.43
15:P:173:MET:HE2	15:P:188:LEU:HB2	2.00	0.43
27:d:94:ARG:NE	40:r:47:GLU:OE2	2.38	0.43
30:g:13:LEU:HD11	31:h:6:VAL:HG12	2.01	0.43
32:i:298:TYR:O	32:i:303:THR:OG1	2.32	0.43
32:i:316:GLN:NE2	44:w:95:ASP:OD1	2.46	0.43
35:l:142:ILE:HG12	40:r:370:PRO:HB2	2.00	0.43
35:l:172:ILE:HG21	40:r:408:LEU:HD12	2.00	0.43
35:l:241:THR:HG21	35:l:344:GLY:HA3	1.99	0.43
42:u:169:PHE:CZ	52:u:201:CDL:H561	2.53	0.43
1:A:60:GLY:HA2	14:O:241:PRO:HA	2.01	0.43
4:E:90:LEU:O	4:E:94:ILE:HG12	2.18	0.43
52:V:202:CDL:H441	52:V:202:CDL:H242	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:167:TYR:CG	26:c:178:PRO:HG3	2.53	0.43
27:d:65:HIS:CE1	28:e:117:TRP:CD1	3.07	0.43
31:h:76:LEU:O	31:h:80:LYS:HG3	2.18	0.43
32:i:177:LYS:NZ	34:k:98:CYS:O	2.38	0.43
35:l:520:TYR:CE1	52:l:703:CDL:OB4	2.69	0.43
39:p:124:GLN:HG3	39:p:127:ARG:HH12	1.82	0.43
40:r:267:TRP:O	40:r:271:MET:HG2	2.18	0.43
41:s:149:ILE:HG21	41:s:185:TRP:HB2	2.00	0.43
44:w:276:LEU:HD23	44:w:276:LEU:HA	1.84	0.43
2:B:144:ARG:NH1	2:B:146:ASP:OD2	2.43	0.43
47:B:303:PEE:H52	41:s:187:ILE:HD12	2.00	0.43
20:V:140:LYS:HE2	24:a:158:ARG:HD2	1.97	0.43
47:W:201:PEE:H14	47:W:201:PEE:H20	1.65	0.43
23:Z:53:TYR:CE2	35:l:434:LYS:HG3	2.53	0.43
35:l:596:MET:HE1	52:m:201:CDL:H652	2.00	0.43
36:m:34:ILE:HG13	36:m:64:MET:HG3	1.99	0.43
40:r:231:LEU:HA	40:r:235:LEU:HB2	2.00	0.43
6:G:103:HIS:NE2	6:G:139:MET:HE2	2.33	0.43
21:W:120:MET:C	21:W:122:GLY:H	2.25	0.43
47:l:704:PEE:H7	47:l:704:PEE:H13	2.01	0.43
38:o:56:ARG:HH21	40:r:424:ASN:HD21	1.67	0.43
3:C:77:MET:HE3	51:s:501:UQ:H8	1.97	0.43
4:E:119:LEU:HD21	12:M:629:ILE:HD11	1.99	0.43
52:J:404:CDL:H331	52:J:404:CDL:H362	1.81	0.43
12:M:31:LEU:HB2	12:M:42:MET:HE3	1.99	0.43
12:M:265:THR:HG22	12:M:270:VAL:HA	2.01	0.43
14:O:75:LYS:C	14:O:77:ALA:H	2.25	0.43
21:W:125:TYR:HA	21:W:128:ARG:HD2	2.01	0.43
25:b:112:GLU:HG2	25:b:113:THR:N	2.34	0.43
26:c:73:GLY:HA3	38:o:79:ASN:ND2	2.34	0.43
26:c:157:GLY:HA2	43:v:22:MET:HE3	2.00	0.43
40:r:225:ILE:HD13	40:r:331:ASN:HB2	2.01	0.43
40:r:281:ASP:OD1	40:r:282:LEU:N	2.49	0.43
44:w:58:LYS:O	44:w:60:ILE:HG13	2.17	0.43
48:C:303:PLX:H362	48:C:303:PLX:H331	1.73	0.43
7:H:18:GLU:O	7:H:19:THR:OG1	2.36	0.43
11:L:122:SER:CB	15:P:229:GLU:OE2	2.67	0.43
12:M:388:ASN:ND2	12:M:513:MET:O	2.49	0.43
13:N:122:GLN:HA	18:T:59:GLN:HG2	2.01	0.43
14:O:44:THR:HG23	14:O:47:ASN:H	1.83	0.43
26:c:81:ARG:HB3	26:c:85:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:37:PHE:CE1	35:l:3:PRO:HB3	2.53	0.43
33:j:88:LEU:HD13	41:s:309:ILE:HD12	2.00	0.43
34:k:45:THR:O	34:k:49:LEU:HG	2.18	0.43
37:n:26:TYR:CE1	37:n:30:ARG:HD2	2.53	0.43
40:r:154:LEU:HD23	40:r:154:LEU:HA	1.84	0.43
40:r:198:ALA:HB2	47:r:501:PEE:H17	2.01	0.43
1:A:87:GLY:CA	46:A:502:FMN:O2P	2.60	0.43
9:J:204:SER:OG	9:J:238:GLN:O	2.37	0.43
12:M:137:CYS:HB3	12:M:140:GLN:HB2	2.01	0.43
13:N:85:GLU:CD	13:N:85:GLU:H	2.26	0.43
15:P:198:PHE:N	15:P:198:PHE:CD1	2.87	0.43
16:Q:450:ILE:HA	16:Q:453:THR:HG22	2.00	0.43
52:a:201:CDL:OB4	28:e:108:TYR:OH	2.31	0.43
27:d:72:PRO:HB3	27:d:76:GLU:OE2	2.18	0.43
38:o:56:ARG:NH2	40:r:424:ASN:ND2	2.67	0.43
39:p:108:HIS:CD2	39:p:109:PRO:HD2	2.54	0.43
40:r:249:ILE:HG13	40:r:250:LEU:HD22	1.99	0.43
43:v:103:GLU:O	43:v:107:ARG:HG2	2.18	0.43
1:A:53:LEU:HB2	1:A:136:HIS:CE1	2.54	0.43
1:A:116:ASN:HD21	46:A:502:FMN:C2	2.32	0.43
3:C:73:ALA:HB1	51:s:501:UQ:CM5	2.49	0.43
6:G:126:PHE:CE2	6:G:148:ILE:HG21	2.54	0.43
9:J:208:GLY:N	9:J:211:ASP:CB	2.82	0.43
12:M:624:ARG:NH2	12:M:637:ASP:OD1	2.42	0.43
21:W:98:MET:CE	31:h:79:ILE:HA	2.49	0.43
21:W:144:THR:CG2	47:W:201:PEE:H2	2.49	0.43
35:l:162:THR:O	35:l:166:THR:HG23	2.18	0.43
37:n:15:ILE:C	37:n:18:PRO:HD2	2.44	0.43
44:w:198:TYR:OH	44:w:304:VAL:HG13	2.19	0.43
1:A:76:ILE:HG23	1:A:255:CYS:SG	2.59	0.43
17:S:65:GLY:O	17:S:66:LEU:C	2.61	0.43
23:Z:30:GLU:O	23:Z:34:GLU:OE1	2.37	0.43
35:l:295:GLN:HB2	35:l:301:ILE:HG12	2.01	0.43
37:n:13:VAL:HB	40:r:14:MET:HG2	1.99	0.43
41:s:55:LEU:O	41:s:217:ALA:HB1	2.19	0.43
1:A:420:GLU:HG3	1:A:429:ASP:OD1	2.19	0.42
4:E:25:MET:HE1	4:E:79:VAL:HG21	2.01	0.42
6:G:137:LYS:O	6:G:139:MET:CA	2.66	0.42
11:L:102:ASP:N	11:L:102:ASP:OD1	2.50	0.42
12:M:311:LYS:HB2	12:M:311:LYS:HE3	1.77	0.42
16:Q:290:GLY:HA2	16:Q:294:ARG:HH21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:187:PRO:CB	42:u:47:ARG:HG3	2.49	0.42
52:a:201:CDL:H191	52:a:201:CDL:H732	2.01	0.42
28:e:66:LEU:HD23	28:e:66:LEU:HA	1.89	0.42
34:k:30:LEU:O	34:k:34:GLU:HG3	2.18	0.42
35:l:332:HIS:HA	35:l:335:PHE:CZ	2.54	0.42
36:m:23:LYS:N	36:m:24:PRO:HD3	2.34	0.42
40:r:285:LEU:HD13	40:r:342:MET:HE1	2.01	0.42
44:w:47:GLU:OE2	44:w:295:ARG:NH1	2.52	0.42
44:w:246:LEU:HB2	44:w:247:PRO:HD3	2.01	0.42
1:A:131:ILE:HD13	1:A:158:ILE:HD13	2.01	0.42
1:A:326:LEU:HD22	1:A:363:ILE:HD11	2.01	0.42
3:C:88:ARG:HA	41:s:37:PRO:HA	2.01	0.42
12:M:346:VAL:H	12:M:521:SER:HB3	1.84	0.42
14:O:199:LYS:O	14:O:203:GLU:HG3	2.18	0.42
35:l:601:LEU:O	35:l:601:LEU:HG	2.18	0.42
39:p:138:LYS:HE2	39:p:138:LYS:HB3	1.84	0.42
40:r:445:LEU:HA	40:r:448:THR:HG22	2.01	0.42
40:r:455:LEU:HD23	40:r:455:LEU:HA	1.87	0.42
43:v:93:LEU:HA	43:v:96:VAL:HG22	2.01	0.42
47:B:303:PEE:H56	41:s:187:ILE:HD11	2.00	0.42
51:J:402:UQ:HM53	51:J:402:UQ:H71	1.80	0.42
16:Q:161:ILE:HD13	16:Q:363:VAL:HG11	2.01	0.42
6:X:93:ILE:HD13	6:X:98:LEU:HD12	2.01	0.42
39:p:25:ARG:HD3	39:p:25:ARG:HA	1.83	0.42
40:r:266:MET:HA	40:r:269:MET:HE2	2.01	0.42
40:r:398:MET:O	40:r:402:ILE:HG13	2.19	0.42
51:s:501:UQ:H13	51:s:501:UQ:H171	1.95	0.42
43:v:12:ASP:OD1	43:v:14:SER:OG	2.35	0.42
1:A:416:SER:OG	1:A:436:GLN:NE2	2.52	0.42
12:M:589:TYR:O	12:M:606:THR:HG21	2.19	0.42
14:O:242:GLY:HA2	14:O:245:VAL:CG2	2.49	0.42
16:Q:154:ALA:HA	16:Q:398:THR:HG21	2.00	0.42
16:Q:404:LYS:HE2	16:Q:457:VAL:HG23	2.02	0.42
32:i:254:LEU:HA	32:i:255:PRO:HD3	1.85	0.42
52:l:702:CDL:H1O1	40:r:357:THR:HG1	1.51	0.42
41:s:63:PRO:HB2	41:s:66:SER:HB3	2.01	0.42
2:B:74:LEU:HB2	41:s:272:TRP:CZ2	2.54	0.42
8:I:94:ALA:HB1	15:P:105:ASN:HD21	1.84	0.42
51:J:402:UQ:H101	51:J:402:UQ:H121	1.83	0.42
14:O:196:LEU:HD13	14:O:201:ILE:HD13	2.02	0.42
27:d:99:ASP:OD2	27:d:142:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:73:LEU:HD23	33:j:73:LEU:HA	1.89	0.42
47:l:704:PEE:H81	47:l:704:PEE:H74	1.89	0.42
44:w:129:TYR:CG	44:w:183:CYS:HB3	2.55	0.42
4:E:64:ARG:HH22	6:G:114:ASP:CG	2.27	0.42
11:L:130:THR:OG1	11:L:133:ASP:OD2	2.38	0.42
47:Q:501:PEE:H34	47:Q:501:PEE:H41	2.00	0.42
32:i:170:LEU:HD11	32:i:288:LEU:HD22	2.02	0.42
33:j:73:LEU:N	33:j:74:PRO:HD2	2.34	0.42
35:l:601:LEU:CD2	35:l:602:PHE:CD2	2.82	0.42
41:s:84:THR:O	41:s:87:VAL:HG22	2.19	0.42
12:M:49:VAL:HG13	12:M:102:ILE:HD13	2.01	0.42
16:Q:123:LEU:O	16:Q:127:LYS:HG2	2.19	0.42
35:l:297:ASP:HB3	35:l:300:LYS:HG3	2.02	0.42
52:l:703:CDL:H361	52:l:703:CDL:H332	1.80	0.42
36:m:88:THR:HG23	52:m:201:CDL:H521	2.02	0.42
43:v:51:LEU:HD13	43:v:63:LEU:HD23	2.01	0.42
1:A:29:LYS:H	1:A:29:LYS:HG3	1.70	0.42
3:C:42:ARG:O	3:C:46:VAL:HG23	2.20	0.42
9:J:135:GLU:OE2	9:J:140:ASP:HB2	2.20	0.42
12:M:64:CYS:HB3	12:M:75:CYS:HB3	2.01	0.42
13:N:5:GLN:HG2	13:N:9:ARG:NH1	2.35	0.42
35:l:601:LEU:HD22	35:l:602:PHE:CE2	2.52	0.42
40:r:420:THR:O	40:r:421:HIS:HB2	2.20	0.42
42:u:85:TYR:CE1	42:u:104:GLN:HB2	2.54	0.42
42:u:152:PRO:O	42:u:153:GLU:HB2	2.20	0.42
44:w:170:LEU:HD22	44:w:187:TYR:CD1	2.53	0.42
1:A:141:GLY:HA3	1:A:248:VAL:O	2.19	0.42
1:A:423:THR:HB	45:A:501:SF4:S4	2.59	0.42
48:C:303:PLX:O2	13:N:75:TRP:HB3	2.20	0.42
4:E:101:THR:OG1	15:P:219:VAL:O	2.26	0.42
9:J:37:HIS:NE2	18:T:49:ASP:HA	2.35	0.42
12:M:59:GLN:HG2	12:M:62:ARG:NH2	2.35	0.42
12:M:182:CYS:SG	45:M:802:SF4:S4	3.18	0.42
52:N:202:CDL:C55	52:N:202:CDL:C32	2.86	0.42
14:O:75:LYS:O	14:O:76:ALA:C	2.62	0.42
14:O:245:VAL:HG12	14:O:246:GLN:O	2.20	0.42
18:T:46:ASP:O	18:T:47:ASP:C	2.60	0.42
20:V:4:THR:O	20:V:8:LYS:HG2	2.20	0.42
6:X:113:LEU:O	6:X:117:GLU:HG3	2.19	0.42
26:c:83:GLN:NE2	26:c:97:LEU:O	2.49	0.42
28:e:134:LEU:HB3	28:e:135:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:27:LEU:HD21	39:p:40:PHE:HB3	2.00	0.42
39:p:140:LEU:HD23	39:p:140:LEU:HA	1.87	0.42
43:v:111:ARG:CZ	43:v:115:ARG:HH21	2.33	0.42
6:X:128:PHE:CE2	6:X:151:LYS:HD3	2.55	0.42
23:Z:29:LEU:HA	23:Z:32:VAL:HG12	2.01	0.42
25:b:73:THR:HA	25:b:77:ILE:HD12	2.01	0.42
48:g:201:PLX:H1C2	31:h:2:PRO:HD2	2.01	0.42
52:i:401:CDL:CB3	44:w:40:PRO:HB2	2.46	0.42
35:l:78:LEU:HD12	35:l:139:GLN:HE21	1.84	0.42
42:u:38:LYS:HB3	42:u:39:PRO:HD3	2.01	0.42
16:Q:180:LEU:HD23	16:Q:180:LEU:HA	1.92	0.41
16:Q:383:LYS:HA	16:Q:383:LYS:HD2	1.89	0.41
52:a:201:CDL:H201	52:a:201:CDL:H772	2.02	0.41
30:g:39:LEU:HD23	30:g:39:LEU:HA	1.85	0.41
52:l:702:CDL:H541	52:l:702:CDL:HA61	2.01	0.41
51:s:501:UQ:H251	51:s:501:UQ:H272	1.83	0.41
12:M:338:VAL:CG2	12:M:363:SER:HB2	2.49	0.41
20:V:95:CYS:HA	20:V:115:CYS:HA	2.01	0.41
27:d:12:GLU:HA	27:d:13:PRO:HD3	1.89	0.41
47:j:201:PEE:H35	47:j:201:PEE:H30	1.59	0.41
34:k:4:VAL:O	34:k:8:ILE:HG12	2.19	0.41
35:l:424:THR:HG21	35:l:501:ALA:HB3	2.02	0.41
37:n:39:ARG:NH1	37:n:57:TRP:O	2.39	0.41
40:r:154:LEU:O	40:r:158:LEU:HD23	2.19	0.41
52:J:404:CDL:H831	52:J:404:CDL:H411	2.01	0.41
12:M:179:CYS:SG	12:M:181:ARG:HB2	2.61	0.41
12:M:338:VAL:HG21	12:M:361:VAL:HG21	2.02	0.41
12:M:386:LEU:HD21	12:M:523:VAL:HG13	2.01	0.41
16:Q:121:GLU:OE1	16:Q:421:ARG:NH1	2.41	0.41
20:V:29:GLY:O	20:V:63:SER:HB3	2.20	0.41
32:i:79:LEU:HD21	34:k:1:MET:SD	2.61	0.41
34:k:26:LEU:O	34:k:30:LEU:HG	2.20	0.41
35:l:331:MET:SD	35:l:465:GLY:HA2	2.60	0.41
52:m:201:CDL:H622	52:m:201:CDL:H652	1.69	0.41
48:r:502:PLX:H121	48:r:502:PLX:H92	1.75	0.41
44:w:41:LEU:O	44:w:45:LEU:HD23	2.21	0.41
1:A:250:VAL:O	1:A:251:SER:C	2.63	0.41
2:B:79:ARG:HH21	8:I:20:LEU:HD22	1.67	0.41
4:E:42:GLU:OE2	4:E:94:ILE:HD13	2.18	0.41
12:M:250:SER:OG	12:M:606:THR:HG23	2.20	0.41
12:M:347:ASP:OD1	12:M:347:ASP:N	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:106:ALA:HB1	15:P:108:PHE:CE2	2.54	0.41
16:Q:53:TYR:HE1	47:Q:501:PEE:H12	1.86	0.41
32:i:17:THR:HG21	32:i:133:TRP:HE1	1.85	0.41
41:s:123:SER:HB3	41:s:214:GLU:HG3	2.01	0.41
11:L:87:MET:HE2	12:M:274:LEU:HD21	2.02	0.41
13:N:3:LEU:HD11	52:N:202:CDL:H311	2.02	0.41
15:P:174:PHE:CE1	15:P:198:PHE:O	2.73	0.41
16:Q:189:THR:HB	51:s:501:UQ:HM21	2.02	0.41
16:Q:202:TRP:CH2	16:Q:261:MET:HG3	2.55	0.41
32:i:171:ASN:C	32:i:171:ASN:HD22	2.24	0.41
48:j:203:PLX:H132	48:j:203:PLX:H161	1.58	0.41
35:l:71:LEU:HD22	35:l:71:LEU:H	1.85	0.41
35:l:78:LEU:HA	35:l:139:GLN:HE21	1.85	0.41
41:s:51:ASP:CB	51:s:501:UQ:H412	2.44	0.41
41:s:212:ASN:C	41:s:212:ASN:ND2	2.79	0.41
42:u:84:GLU:OE1	42:u:106:LYS:NZ	2.37	0.41
52:J:404:CDL:H382	52:J:404:CDL:H212	2.03	0.41
12:M:356:ASP:O	12:M:360:ARG:HG2	2.21	0.41
12:M:543:LYS:HE3	12:M:543:LYS:HB3	1.88	0.41
15:P:196:HIS:HA	15:P:197:PRO:HD3	1.89	0.41
16:Q:183:HIS:NE2	16:Q:336:GLU:OE1	2.53	0.41
30:g:35:TYR:HE1	52:u:201:CDL:H771	1.84	0.41
33:j:90:MET:SD	36:m:151:THR:HG23	2.61	0.41
35:l:190:LEU:C	35:l:190:LEU:CD2	2.85	0.41
38:o:17:THR:O	38:o:23:TYR:OH	2.38	0.41
51:s:501:UQ:H353	51:s:501:UQ:H371	1.93	0.41
44:w:173:MET:HB3	44:w:178:PHE:HB2	2.03	0.41
1:A:161:GLU:HG2	14:O:177:LEU:HD22	2.03	0.41
1:A:222:LYS:O	11:L:175:LYS:NZ	2.42	0.41
1:A:250:VAL:O	1:A:253:THR:N	2.54	0.41
2:B:80:GLU:OE1	8:I:28:TYR:OH	2.39	0.41
4:E:41:ARG:HH12	6:G:124:ASP:CG	2.27	0.41
16:Q:144:MET:SD	16:Q:144:MET:N	2.94	0.41
16:Q:198:THR:OG1	16:Q:202:TRP:NE1	2.54	0.41
20:V:38:ALA:HA	52:m:201:CDL:H232	2.03	0.41
32:i:251:MET:HE3	32:i:293:TYR:CE1	2.55	0.41
35:l:161:ARG:NH2	35:l:238:GLU:OE1	2.49	0.41
35:l:573:MET:HE3	47:l:701:PEE:C14	2.51	0.41
47:l:704:PEE:H58	47:l:704:PEE:H53	1.47	0.41
40:r:1:MET:SD	40:r:111:THR:HG21	2.61	0.41
43:v:42:THR:HG22	43:v:45:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:40:ARG:NH2	5:F:84:ALA:HB1	2.36	0.41
15:P:68:ILE:HG22	15:P:69:LEU:HG	2.02	0.41
20:V:14:GLU:HA	20:V:21:LYS:HE3	2.03	0.41
25:b:14:GLN:NE2	39:p:157:ALA:HB3	2.35	0.41
26:c:140:MET:HE2	35:l:283:ILE:HG13	2.02	0.41
32:i:95:MET:CE	32:i:149:ILE:CA	2.97	0.41
32:i:325:LEU:HD12	52:i:401:CDL:H151	2.02	0.41
52:l:702:CDL:H342	52:l:702:CDL:H372	1.61	0.41
42:u:80:GLU:HB3	42:u:81:PRO:HD3	2.03	0.41
1:A:141:GLY:HA2	1:A:252:PRO:HD3	2.03	0.41
1:A:146:GLY:HA3	1:A:193:PHE:CE1	2.56	0.41
1:A:366:ALA:HA	14:O:141:MET:HE1	2.03	0.41
1:A:380:GLY:O	1:A:386:ARG:HD3	2.21	0.41
46:A:502:FMN:O4'	46:A:502:FMN:O2'	2.36	0.41
2:B:39:LYS:HD2	16:Q:335:GLU:HG2	2.01	0.41
4:E:50:PHE:HE2	4:E:98:LYS:O	2.03	0.41
4:E:61:ASP:OD1	4:E:62:LYS:N	2.53	0.41
5:F:30:SER:OG	5:F:63:PRO:HG3	2.21	0.41
6:G:84:LEU:HD21	6:G:100:VAL:HG22	2.03	0.41
6:G:142:GLN:O	6:G:145:VAL:HG22	2.20	0.41
7:H:77:ILE:HA	7:H:80:VAL:HG23	2.03	0.41
9:J:100:LEU:HD23	9:J:100:LEU:HA	1.89	0.41
9:J:262:THR:O	9:J:333:PRO:HD2	2.21	0.41
11:L:156:LYS:NZ	12:M:279:GLU:OE2	2.49	0.41
16:Q:189:THR:HG21	51:s:501:UQ:HM23	2.03	0.41
16:Q:198:THR:HG23	16:Q:199:PRO:HD3	2.02	0.41
17:S:22:ALA:O	17:S:26:ILE:HG12	2.20	0.41
20:V:140:LYS:HE2	24:a:158:ARG:CG	2.50	0.41
24:a:141:GLN:O	24:a:145:GLU:HG3	2.21	0.41
24:a:169:TYR:CZ	30:g:3:MET:HB3	2.55	0.41
52:a:201:CDL:C51	47:b:201:PEE:H14	2.48	0.41
25:b:32:GLU:HB3	39:p:115:TYR:HD1	1.86	0.41
47:b:201:PEE:H60	47:b:201:PEE:H55	1.90	0.41
27:d:43:ARG:HB3	27:d:44:PRO:HD3	2.02	0.41
33:j:103:ALA:HB2	47:j:201:PEE:H19	2.02	0.41
34:k:28:SER:HB3	36:m:23:LYS:HG2	2.02	0.41
52:l:702:CDL:H222	52:l:702:CDL:H251	1.87	0.41
41:s:18:ALA:O	41:s:21:THR:OG1	2.29	0.41
41:s:200:LEU:HD13	41:s:282:TYR:HA	2.03	0.41
41:s:218:GLY:N	41:s:219:PRO:CD	2.84	0.41
44:w:180:ARG:NH1	44:w:316:GLU:OE2	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:SER:N	1:A:252:PRO:CD	2.84	0.41
1:A:325:PRO:HG3	1:A:433:TRP:HB3	2.03	0.41
12:M:234:LYS:HB3	12:M:235:PRO:HD3	2.03	0.41
14:O:63:ILE:O	14:O:67:VAL:HG23	2.21	0.41
28:e:54:ARG:C	28:e:55:LEU:HD12	2.46	0.41
30:g:30:ASP:OD1	42:u:172:MET:HE1	2.21	0.41
32:i:246:VAL:HG11	52:r:504:CDL:H392	2.03	0.41
48:n:101:PLX:H1C3	48:n:101:PLX:H22	1.79	0.41
39:p:20:TYR:CZ	39:p:24:LEU:HD11	2.56	0.41
40:r:236:LEU:HB3	40:r:294:MET:HE2	2.03	0.41
41:s:24:GLU:HA	41:s:271:LEU:HD13	2.02	0.41
1:A:288:VAL:HG21	1:A:303:HIS:CD2	2.56	0.40
12:M:402:LEU:HD13	12:M:407:PRO:HG2	2.03	0.40
16:Q:53:TYR:HE1	47:Q:501:PEE:O4P	2.02	0.40
28:e:136:LEU:HD12	28:e:136:LEU:HA	1.85	0.40
32:i:88:LYS:HE2	32:i:90:PHE:CD1	2.56	0.40
32:i:264:TRP:HZ2	42:u:168:PHE:CD2	2.39	0.40
35:l:103:PHE:HB2	35:l:341:MET:HE3	2.03	0.40
42:u:44:MET:HE3	42:u:48:TRP:HZ3	1.86	0.40
48:C:303:PLX:C39	48:C:303:PLX:C35	2.97	0.40
4:E:22:SER:HB2	4:E:27:GLU:HB2	2.02	0.40
10:K:100:GLN:CD	14:O:69:ASN:O	2.62	0.40
18:T:43:GLN:CD	18:T:43:GLN:C	2.89	0.40
27:d:35:LYS:HE3	27:d:35:LYS:HB3	1.95	0.40
27:d:164:LEU:HD23	28:e:149:LEU:HD13	2.03	0.40
32:i:95:MET:CE	32:i:149:ILE:HA	2.50	0.40
35:l:297:ASP:O	35:l:301:ILE:HG13	2.21	0.40
35:l:566:THR:O	35:l:570:GLN:HG2	2.20	0.40
40:r:336:ARG:NH2	40:r:429:SER:HA	2.36	0.40
41:s:179:TRP:CG	41:s:180:PRO:HD3	2.56	0.40
44:w:62:VAL:CG1	44:w:70:LYS:HB2	2.51	0.40
44:w:123:SER:OG	44:w:125:ASP:OD1	2.19	0.40
1:A:128:ARG:O	1:A:132:ARG:HG2	2.22	0.40
1:A:362:ASP:OD1	1:A:449:ARG:NH2	2.41	0.40
1:A:398:ARG:CG	1:A:403:ASP:HB3	2.51	0.40
16:Q:244:ILE:HG22	16:Q:348:LEU:HD11	2.04	0.40
27:d:77:CYS:SG	27:d:84:CYS:HB3	2.62	0.40
35:l:130:ILE:HD13	52:l:702:CDL:H252	2.03	0.40
35:l:213:LEU:HB3	35:l:273:VAL:HG11	2.02	0.40
35:l:288:THR:HG21	35:l:307:SER:OG	2.21	0.40
35:l:488:MET:O	35:l:492:ILE:HG13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:l:703:CDL:H712	52:l:703:CDL:H312	2.03	0.40
36:m:24:PRO:HB3	36:m:89:VAL:HG11	2.03	0.40
1:A:358:ASP:OD1	1:A:358:ASP:N	2.50	0.40
6:G:134:ASP:CG	6:G:147:TYR:HE2	2.29	0.40
12:M:306:MET:HE3	12:M:583:ILE:HD12	2.03	0.40
16:Q:271:ARG:HD2	16:Q:271:ARG:HA	1.91	0.40
32:i:89:MET:HE1	32:i:98:MET:HE2	2.03	0.40
32:i:128:LEU:HD12	32:i:216:PHE:HB3	2.03	0.40
33:j:34:THR:HG22	41:s:61:LEU:HD11	2.02	0.40
41:s:138:GLN:HG3	41:s:285:LEU:HD21	2.03	0.40
42:u:83:THR:HA	42:u:86:TRP:NE1	2.35	0.40
44:w:242:LYS:HA	44:w:246:LEU:HD12	2.03	0.40
1:A:63:TYR:O	1:A:256:ARG:HD3	2.22	0.40
2:B:98:ARG:CB	2:B:169:GLU:OE1	2.45	0.40
2:B:200:GLU:HG3	13:N:88:ARG:HB2	2.03	0.40
5:F:25:GLN:HG3	5:F:26:ARG:CD	2.44	0.40
7:H:30:LYS:O	7:H:34:VAL:HG23	2.21	0.40
7:H:105:GLU:HB3	15:P:89:HIS:NE2	2.36	0.40
13:N:144:TYR:CE2	13:N:145:LYS:HD2	2.57	0.40
32:i:342:ALA:O	32:i:345:SER:OG	2.38	0.40
35:l:176:ARG:HH22	40:r:367:LEU:HD13	1.86	0.40
35:l:592:LEU:O	35:l:596:MET:HG3	2.22	0.40
52:m:201:CDL:H222	52:m:201:CDL:H331	2.03	0.40
40:r:178:ILE:HD13	40:r:178:ILE:HA	1.89	0.40
41:s:192:GLU:OE1	41:s:234:MET:HE3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	431/433 (100%)	410 (95%)	21 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
3	C	154/156 (99%)	147 (96%)	7 (4%)	0	100	100
4	E	113/115 (98%)	110 (97%)	2 (2%)	1 (1%)	14	41
5	F	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
6	G	86/88 (98%)	78 (91%)	6 (7%)	2 (2%)	5	19
6	X	86/88 (98%)	80 (93%)	6 (7%)	0	100	100
7	H	110/112 (98%)	103 (94%)	5 (4%)	2 (2%)	6	25
8	I	93/112 (83%)	80 (86%)	13 (14%)	0	100	100
9	J	340/342 (99%)	327 (96%)	13 (4%)	0	100	100
10	K	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	664 (96%)	24 (4%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	204 (95%)	10 (5%)	1 (0%)	24	54
15	P	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
16	Q	427/430 (99%)	413 (97%)	14 (3%)	0	100	100
17	S	68/70 (97%)	63 (93%)	4 (6%)	1 (2%)	8	28
18	T	94/96 (98%)	94 (100%)	0	0	100	100
19	U	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
20	V	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
21	W	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
22	Y	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
23	Z	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
24	a	136/138 (99%)	132 (97%)	4 (3%)	0	100	100
25	b	94/126 (75%)	91 (97%)	3 (3%)	0	100	100
26	c	154/156 (99%)	141 (92%)	13 (8%)	0	100	100
27	d	173/175 (99%)	165 (95%)	8 (5%)	0	100	100
28	e	102/104 (98%)	94 (92%)	8 (8%)	0	100	100
29	f	47/49 (96%)	41 (87%)	6 (13%)	0	100	100
30	g	119/121 (98%)	112 (94%)	7 (6%)	0	100	100
31	h	103/105 (98%)	100 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	i	345/347 (99%)	330 (96%)	14 (4%)	1 (0%)	36	65
33	j	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
34	k	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
35	l	604/606 (100%)	574 (95%)	30 (5%)	0	100	100
36	m	173/175 (99%)	164 (95%)	8 (5%)	1 (1%)	21	51
37	n	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
38	o	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
39	p	176/178 (99%)	170 (97%)	6 (3%)	0	100	100
40	r	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
41	s	316/318 (99%)	305 (96%)	11 (4%)	0	100	100
42	u	169/171 (99%)	164 (97%)	4 (2%)	1 (1%)	21	51
43	v	122/125 (98%)	118 (97%)	4 (3%)	0	100	100
44	w	318/320 (99%)	304 (96%)	14 (4%)	0	100	100
All	All	8174/8313 (98%)	7839 (96%)	325 (4%)	10 (0%)	49	77

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	138	LEU
7	H	108	PRO
17	S	66	LEU
6	G	133	ILE
14	O	76	ALA
32	i	255	PRO
36	m	26	PRO
4	E	96	VAL
7	H	77	ILE
42	u	152	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	346/346 (100%)	345 (100%)	1 (0%)	86	96
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	75/76 (99%)	75 (100%)	0	100	100
6	G	75/81 (93%)	72 (96%)	3 (4%)	28	62
6	X	76/81 (94%)	76 (100%)	0	100	100
7	H	99/99 (100%)	98 (99%)	1 (1%)	68	89
8	I	87/97 (90%)	86 (99%)	1 (1%)	65	88
9	J	296/296 (100%)	295 (100%)	1 (0%)	86	96
10	K	42/42 (100%)	41 (98%)	1 (2%)	43	75
11	L	113/113 (100%)	112 (99%)	1 (1%)	70	90
12	M	580/580 (100%)	578 (100%)	2 (0%)	86	96
13	N	130/130 (100%)	130 (100%)	0	100	100
14	O	183/183 (100%)	183 (100%)	0	100	100
15	P	190/190 (100%)	189 (100%)	1 (0%)	81	93
16	Q	370/370 (100%)	370 (100%)	0	100	100
17	S	57/58 (98%)	57 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	101 (100%)	0	100	100
21	W	121/123 (98%)	121 (100%)	0	100	100
22	Y	62/62 (100%)	62 (100%)	0	100	100
23	Z	62/62 (100%)	62 (100%)	0	100	100
24	a	121/121 (100%)	121 (100%)	0	100	100
25	b	90/119 (76%)	90 (100%)	0	100	100
26	c	141/141 (100%)	141 (100%)	0	100	100
27	d	155/155 (100%)	154 (99%)	1 (1%)	78	93
28	e	96/96 (100%)	96 (100%)	0	100	100
29	f	36/45 (80%)	36 (100%)	0	100	100
30	g	108/108 (100%)	108 (100%)	0	100	100
31	h	93/93 (100%)	91 (98%)	2 (2%)	45	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	i	311/311 (100%)	309 (99%)	2 (1%)	78	93
33	j	100/100 (100%)	100 (100%)	0	100	100
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	540/540 (100%)	536 (99%)	4 (1%)	76	92
36	m	130/141 (92%)	130 (100%)	0	100	100
37	n	53/53 (100%)	52 (98%)	1 (2%)	50	79
38	o	113/113 (100%)	112 (99%)	1 (1%)	70	90
39	p	159/159 (100%)	159 (100%)	0	100	100
40	r	410/410 (100%)	408 (100%)	2 (0%)	81	93
41	s	275/275 (100%)	272 (99%)	3 (1%)	65	88
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	104/111 (94%)	104 (100%)	0	100	100
44	w	283/283 (100%)	283 (100%)	0	100	100
All	All	7159/7240 (99%)	7131 (100%)	28 (0%)	81	94

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	VAL
6	G	130	ILE
6	G	133	ILE
6	G	134	ASP
7	H	104	VAL
8	I	25	GLN
9	J	132	ARG
10	K	75	ASN
11	L	165	SER
12	M	380	ASP
12	M	530	TYR
15	P	201	ASP
27	d	64	TYR
31	h	43	CYS
31	h	45	HIS
32	i	149	ILE
32	i	257	LEU
35	l	70	THR
35	l	71	LEU

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Mol	Chain	Res	Type
35	l	599	MET
35	l	601	LEU
37	n	3	ASN
38	o	56	ARG
40	r	248	THR
40	r	251	ASN
41	s	201	THR
41	s	202	GLU
41	s	212	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	244	ASN
1	A	436	GLN
1	A	457	HIS
7	H	83	GLN
7	H	86	ASN
8	I	47	HIS
9	J	128	ASN
9	J	356	HIS
10	K	75	ASN
10	K	79	HIS
12	M	39	GLN
12	M	331	GLN
12	M	406	ASN
12	M	652	ASN
13	N	31	ASN
14	O	74	HIS
14	O	90	ASN
14	O	131	HIS
14	O	153	GLN
15	P	77	GLN
15	P	181	HIS
15	P	196	HIS
15	P	228	GLN
16	Q	36	GLN
16	Q	60	HIS
16	Q	160	ASN
16	Q	223	HIS
17	S	25	HIS

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Mol	Chain	Res	Type
17	S	31	ASN
19	U	74	GLN
20	V	89	ASN
6	X	142	GLN
22	Y	39	HIS
22	Y	49	GLN
23	Z	21	GLN
23	Z	91	GLN
26	c	127	ASN
26	c	154	GLN
27	d	107	GLN
27	d	149	HIS
28	e	86	ASN
31	h	97	HIS
31	h	98	HIS
32	i	268	GLN
32	i	289	ASN
33	j	10	ASN
34	k	50	ASN
34	k	57	ASN
35	l	67	HIS
35	l	139	GLN
35	l	541	ASN
38	o	50	GLN
38	o	79	ASN
39	p	33	HIS
40	r	30	HIS
40	r	138	ASN
40	r	168	GLN
40	r	175	ASN
40	r	251	ASN
40	r	415	GLN
40	r	424	ASN
41	s	212	ASN
42	u	65	GLN
42	u	151	ASN
42	u	163	HIS
43	v	50	GLN
43	v	55	GLN

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	1.97	1 (10%)	5,13,15	5.97	3 (60%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.58	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	12.23	130.69	119.48
16	Q	118	2MR	CD-NE-CZ	4.08	131.05	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.14	130.81	123.86

There are no chirality outliers.

All (2) 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

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 46 ligands modelled in this entry, 2 are monoatomic - leaving 44 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	$\#\|Z\| > 2$
52	CDL	J	404	-	88,88,99	1.13	8 (9%)	94,100,111	0.92	4 (4%)
52	CDL	l	703	-	99,99,99	0.91	4 (4%)	105,111,111	1.08	7 (6%)
47	PEE	b	201	-	45,45,50	1.22	6 (13%)	48,50,55	0.99	2 (4%)
52	CDL	l	702	-	98,98,99	1.09	8 (8%)	104,110,111	0.90	4 (3%)
56	ADP	w	401	-	27,29,29	2.97	8 (29%)	42,45,45	2.01	10 (23%)
52	CDL	a	201	-	99,99,99	1.09	8 (8%)	105,111,111	0.87	4 (3%)
48	PLX	C	303	-	51,51,51	0.62	0	55,59,59	0.67	0
47	PEE	r	501	-	50,50,50	1.16	5 (10%)	53,55,55	0.96	2 (3%)
47	PEE	Q	501	-	46,46,50	1.20	6 (13%)	49,51,55	1.01	2 (4%)
52	CDL	i	401	-	67,67,99	1.12	4 (5%)	73,79,111	1.22	6 (8%)
51	UQ	s	501	-	63,63,63	3.63	15 (23%)	76,79,79	3.21	31 (40%)
49	8Q1	X	201	-	31,34,34	1.70	6 (19%)	40,43,43	1.57	6 (15%)
53	FES	M	803	12	0,4,4	-	-	-		
45	SF4	M	802	12	0,12,12	-	-	-		
45	SF4	B	301	2	0,12,12	-	-	-		
47	PEE	B	303	-	50,50,50	1.16	6 (12%)	53,55,55	0.98	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
51	UQ	J	402	-	33,33,63	3.44	9 (27%)	40,43,79	2.80	13 (32%)
48	PLX	N	201	-	51,51,51	1.14	4 (7%)	55,59,59	0.60	1 (1%)
48	PLX	r	502	-	51,51,51	1.14	4 (7%)	55,59,59	0.58	1 (1%)
48	PLX	J	403	-	51,51,51	1.14	3 (5%)	55,59,59	0.59	1 (1%)
45	SF4	B	302	2	0,12,12	-	-	-		
47	PEE	W	201	-	40,40,50	1.13	5 (12%)	43,45,55	1.01	2 (4%)
47	PEE	C	302	-	46,46,50	1.21	6 (13%)	49,51,55	0.99	2 (4%)
47	PEE	l	704	-	50,50,50	1.16	6 (12%)	53,55,55	0.98	2 (3%)
45	SF4	A	501	1	0,12,12	-	-	-		
48	PLX	n	101	-	51,51,51	1.15	4 (7%)	55,59,59	0.59	1 (1%)
52	CDL	r	504	-	99,99,99	1.08	8 (8%)	105,111,111	0.87	4 (3%)
52	CDL	u	201	-	54,54,99	1.23	4 (7%)	60,66,111	1.24	5 (8%)
46	FMN	A	502	-	33,33,33	1.40	5 (15%)	48,50,50	1.28	7 (14%)
52	CDL	V	201	-	93,93,99	1.11	8 (8%)	99,105,111	0.87	4 (4%)
48	PLX	j	203	-	51,51,51	1.15	4 (7%)	55,59,59	0.59	1 (1%)
49	8Q1	E	201	-	31,34,34	2.06	6 (19%)	40,43,43	1.70	11 (27%)
47	PEE	j	201	-	50,50,50	1.15	6 (12%)	53,55,55	0.98	2 (3%)
47	PEE	j	202	-	40,40,50	1.15	5 (12%)	43,45,55	1.02	2 (4%)
52	CDL	N	202	-	50,50,99	1.28	4 (8%)	56,62,111	1.29	5 (8%)
48	PLX	g	201	-	51,51,51	1.13	3 (5%)	55,59,59	0.65	1 (1%)
48	PLX	r	503	-	51,51,51	1.14	4 (7%)	55,59,59	0.59	1 (1%)
45	SF4	M	801	12	0,12,12	-	-	-		
45	SF4	C	301	3	0,12,12	-	-	-		
50	NDP	J	401	-	49,52,52	2.18	5 (10%)	66,80,80	1.66	14 (21%)
52	CDL	V	202	-	99,99,99	1.08	8 (8%)	105,111,111	0.88	4 (3%)
53	FES	O	301	14	0,4,4	-	-	-		
52	CDL	m	201	-	99,99,99	1.08	8 (8%)	105,111,111	0.85	4 (3%)
47	PEE	l	701	-	39,39,50	1.31	6 (15%)	41,44,55	1.04	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	CDL	J	404	-	-	48/99/99/110	-
52	CDL	l	703	-	-	38/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	PEE	b	201	-	-	24/49/49/54	-
52	CDL	l	702	-	-	57/109/109/110	-
56	ADP	w	401	-	-	4/16/32/32	0/3/3/3
52	CDL	a	201	-	-	56/110/110/110	-
48	PLX	C	303	-	-	16/55/55/55	-
47	PEE	r	501	-	-	23/54/54/54	-
47	PEE	Q	501	-	-	27/50/50/54	-
52	CDL	i	401	-	-	33/78/78/110	-
51	UQ	s	501	-	-	32/63/87/87	0/1/1/1
49	8Q1	X	201	-	-	14/41/41/41	-
53	FES	M	803	12	-	-	0/1/1/1
45	SF4	M	802	12	-	-	0/6/5/5
45	SF4	B	301	2	-	-	0/6/5/5
47	PEE	B	303	-	-	28/54/54/54	-
51	UQ	J	402	-	-	17/27/51/87	0/1/1/1
48	PLX	N	201	-	-	28/55/55/55	-
48	PLX	r	502	-	-	24/55/55/55	-
48	PLX	J	403	-	-	35/55/55/55	-
47	PEE	W	201	-	-	24/44/44/54	-
48	PLX	n	101	-	-	26/55/55/55	-
47	PEE	C	302	-	-	25/50/50/54	-
47	PEE	l	704	-	-	29/54/54/54	-
52	CDL	r	504	-	-	59/110/110/110	-
52	CDL	u	201	-	-	23/65/65/110	-
45	SF4	A	501	1	-	-	0/6/5/5
45	SF4	B	302	2	-	-	0/6/5/5
46	FMN	A	502	-	-	7/18/18/18	0/3/3/3
52	CDL	V	201	-	-	53/104/104/110	-
48	PLX	j	203	-	-	30/55/55/55	-
49	8Q1	E	201	-	-	23/41/41/41	-
47	PEE	j	201	-	-	27/54/54/54	-
47	PEE	j	202	-	-	25/44/44/54	-
52	CDL	N	202	-	-	21/61/61/110	-
48	PLX	g	201	-	-	29/55/55/55	-
48	PLX	r	503	-	-	26/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	C	301	3	-	-	0/6/5/5
45	SF4	M	801	12	-	-	0/6/5/5
50	NDP	J	401	-	-	10/34/77/77	0/5/5/5
52	CDL	V	202	-	-	61/110/110/110	-
53	FES	O	301	14	-	-	0/1/1/1
52	CDL	m	201	-	-	61/110/110/110	-
47	PEE	l	701	-	-	25/43/43/54	-

All (209) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	J	401	NDP	P2B-O2B	12.43	1.82	1.59
51	s	501	UQ	C18-C19	9.56	1.55	1.33
51	J	402	UQ	C18-C19	9.55	1.55	1.33
51	s	501	UQ	C13-C14	9.24	1.55	1.33
51	J	402	UQ	C13-C14	9.21	1.55	1.33
51	s	501	UQ	C23-C24	9.10	1.54	1.33
51	J	402	UQ	C8-C9	8.99	1.54	1.33
56	w	401	ADP	C3'-C4'	-8.95	1.30	1.53
51	s	501	UQ	C28-C29	8.90	1.54	1.33
51	s	501	UQ	C8-C9	8.89	1.54	1.33
51	s	501	UQ	C33-C34	8.50	1.53	1.33
51	s	501	UQ	C43-C44	8.25	1.52	1.33
51	s	501	UQ	C38-C39	8.22	1.52	1.33
51	s	501	UQ	C48-C49	7.92	1.52	1.33
51	J	402	UQ	C23-C24	7.80	1.54	1.32
49	E	201	8Q1	P24-O27	7.69	1.85	1.60
56	w	401	ADP	O4'-C4'	7.62	1.62	1.45
51	s	501	UQ	C53-C54	7.36	1.53	1.32
56	w	401	ADP	C6-N6	5.57	1.48	1.34
49	X	201	8Q1	C34-N36	5.43	1.45	1.33
49	X	201	8Q1	C39-N41	5.35	1.45	1.33
46	A	502	FMN	C9A-C5A	4.71	1.49	1.41
56	w	401	ADP	O4'-C1'	-4.46	1.31	1.42
52	i	401	CDL	OB8-CB7	4.30	1.45	1.33
52	i	401	CDL	OA8-CA7	4.28	1.45	1.33
52	u	201	CDL	OA8-CA7	4.26	1.45	1.33
52	N	202	CDL	OB8-CB7	4.25	1.45	1.33
52	l	703	CDL	OA8-CA7	4.25	1.45	1.33
52	u	201	CDL	OB8-CB7	4.23	1.45	1.33
52	N	202	CDL	OA8-CA7	4.23	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	u	201	CDL	OB6-CB5	4.18	1.46	1.34
52	i	401	CDL	OB6-CB5	4.17	1.46	1.34
52	l	703	CDL	OB8-CB7	4.16	1.45	1.33
52	N	202	CDL	OB6-CB5	4.12	1.45	1.34
52	N	202	CDL	OA6-CA5	4.11	1.45	1.34
52	l	703	CDL	OA6-CA5	4.09	1.45	1.34
52	i	401	CDL	OA6-CA5	4.04	1.45	1.34
52	l	703	CDL	OB6-CB5	4.02	1.45	1.34
52	u	201	CDL	OA6-CA5	4.01	1.45	1.34
50	J	401	NDP	PN-O5D	3.83	1.74	1.59
49	E	201	8Q1	C1-S44	3.76	1.85	1.76
47	r	501	PEE	C18-C19	3.75	1.53	1.31
47	j	202	PEE	C18-C19	3.74	1.53	1.31
47	l	704	PEE	C18-C19	3.74	1.53	1.31
47	C	302	PEE	C18-C19	3.73	1.53	1.31
47	l	701	PEE	C18-C19	3.73	1.53	1.31
47	B	303	PEE	C18-C19	3.72	1.53	1.31
47	b	201	PEE	C18-C19	3.72	1.53	1.31
47	j	201	PEE	C18-C19	3.71	1.53	1.31
47	W	201	PEE	C18-C19	3.69	1.53	1.31
47	Q	501	PEE	C18-C19	3.68	1.53	1.31
47	l	701	PEE	C39-C38	3.66	1.53	1.31
47	C	302	PEE	C39-C38	3.65	1.52	1.31
47	r	501	PEE	C39-C38	3.64	1.52	1.31
47	b	201	PEE	C39-C38	3.63	1.52	1.31
47	B	303	PEE	C39-C38	3.63	1.52	1.31
47	j	201	PEE	C39-C38	3.62	1.52	1.31
47	l	704	PEE	C39-C38	3.62	1.52	1.31
47	Q	501	PEE	C39-C38	3.62	1.52	1.31
49	E	201	8Q1	C34-N36	3.58	1.41	1.33
52	V	201	CDL	OA8-CA7	3.45	1.43	1.33
52	J	404	CDL	OA8-CA7	3.42	1.43	1.33
52	V	202	CDL	OA8-CA7	3.42	1.43	1.33
52	l	702	CDL	OA8-CA7	3.41	1.43	1.33
52	a	201	CDL	OA8-CA7	3.38	1.43	1.33
52	r	504	CDL	OA8-CA7	3.38	1.43	1.33
49	E	201	8Q1	O27-C28	-3.36	1.33	1.43
52	m	201	CDL	OA8-CA7	3.36	1.43	1.33
56	w	401	ADP	O2'-C2'	-3.23	1.35	1.43
56	w	401	ADP	O3'-C3'	3.16	1.50	1.43
56	w	401	ADP	C8-N9	-3.14	1.31	1.37
52	m	201	CDL	OA6-CA5	3.11	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	V	201	CDL	OA6-CA5	3.11	1.43	1.34
46	A	502	FMN	C8-C7	3.09	1.48	1.40
52	a	201	CDL	OB6-CB5	3.06	1.42	1.34
50	J	401	NDP	O2B-C2B	-3.05	1.33	1.44
49	E	201	8Q1	C6-C1	3.03	1.53	1.50
52	r	504	CDL	OB6-CB5	3.03	1.42	1.34
52	V	202	CDL	OB6-CB5	3.01	1.42	1.34
52	m	201	CDL	OB8-CB7	3.00	1.42	1.33
52	l	702	CDL	OB6-CB5	2.99	1.42	1.34
52	J	404	CDL	OA6-CA5	2.98	1.42	1.34
52	J	404	CDL	OB6-CB5	2.98	1.42	1.34
52	a	201	CDL	OB8-CB7	2.97	1.42	1.33
52	r	504	CDL	OB8-CB7	2.97	1.42	1.33
52	l	702	CDL	OB8-CB7	2.97	1.42	1.33
49	E	201	8Q1	C39-N41	2.96	1.40	1.33
52	V	201	CDL	OB6-CB5	2.95	1.42	1.34
52	m	201	CDL	OB6-CB5	2.95	1.42	1.34
52	a	201	CDL	OA6-CA5	2.95	1.42	1.34
52	J	404	CDL	OB8-CB7	2.92	1.41	1.33
52	V	201	CDL	OB8-CB7	2.91	1.41	1.33
52	V	202	CDL	OB8-CB7	2.91	1.41	1.33
52	V	202	CDL	OA6-CA5	2.90	1.42	1.34
52	l	702	CDL	OA6-CA5	2.90	1.42	1.34
52	r	504	CDL	OA6-CA5	2.86	1.42	1.34
46	A	502	FMN	C4-N3	-2.83	1.33	1.38
48	n	101	PLX	O6-C4	-2.75	1.40	1.44
48	r	502	PLX	O6-C4	-2.69	1.41	1.44
48	g	201	PLX	O6-C4	-2.68	1.41	1.44
51	s	501	UQ	C6-C1	2.65	1.54	1.46
51	J	402	UQ	C6-C1	2.63	1.54	1.46
48	N	201	PLX	O6-C4	-2.63	1.41	1.44
47	B	303	PEE	O2-C2	-2.63	1.40	1.46
48	j	203	PLX	O6-C4	-2.61	1.41	1.44
48	r	503	PLX	O6-C4	-2.58	1.41	1.44
47	C	302	PEE	O3-C30	2.56	1.40	1.33
47	r	501	PEE	O3-C30	2.54	1.40	1.33
47	Q	501	PEE	O2-C2	-2.52	1.40	1.46
47	l	704	PEE	O2-C2	-2.50	1.40	1.46
48	j	203	PLX	C7-C6	2.49	1.56	1.50
52	a	201	CDL	OA6-CA4	-2.49	1.40	1.46
47	C	302	PEE	O2-C2	-2.49	1.40	1.46
52	r	504	CDL	OA6-CA4	-2.49	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	l	701	PEE	O3-C30	2.46	1.40	1.33
47	r	501	PEE	O2-C2	-2.44	1.40	1.46
47	b	201	PEE	O3-C30	2.44	1.40	1.33
51	J	402	UQ	C7-C8	2.43	1.54	1.50
47	B	303	PEE	O3-C30	2.43	1.40	1.33
52	V	202	CDL	OA6-CA4	-2.43	1.40	1.46
47	j	202	PEE	O3-C30	2.42	1.40	1.33
47	W	201	PEE	O3-C30	2.42	1.40	1.33
48	J	403	PLX	O6-C4	-2.42	1.41	1.44
47	j	202	PEE	O2-C2	-2.40	1.40	1.46
47	W	201	PEE	O2-C2	-2.39	1.40	1.46
47	j	201	PEE	O2-C2	-2.39	1.40	1.46
47	l	701	PEE	O2-C2	-2.39	1.40	1.46
52	J	404	CDL	OA6-CA4	-2.39	1.40	1.46
51	s	501	UQ	C7-C8	2.38	1.54	1.50
52	l	702	CDL	OA6-CA4	-2.38	1.40	1.46
47	j	201	PEE	O3-C30	2.38	1.40	1.33
48	r	503	PLX	C7-C6	2.37	1.55	1.50
47	b	201	PEE	O2-C2	-2.35	1.40	1.46
49	X	201	8Q1	C1-S44	2.35	1.81	1.76
47	Q	501	PEE	O3-C30	2.35	1.40	1.33
48	J	403	PLX	C7-C6	2.35	1.55	1.50
48	r	502	PLX	C7-C6	2.32	1.55	1.50
47	l	704	PEE	O3-C30	2.32	1.40	1.33
48	g	201	PLX	C7-C6	2.30	1.55	1.50
48	N	201	PLX	C7-C6	2.29	1.55	1.50
51	s	501	UQ	O4-C4	-2.29	1.18	1.23
52	V	201	CDL	OB6-CB4	-2.29	1.40	1.46
49	X	201	8Q1	C6-C1	2.28	1.53	1.50
48	n	101	PLX	C7-C6	2.27	1.55	1.50
49	X	201	8Q1	O35-C34	-2.27	1.18	1.23
56	w	401	ADP	C5-N7	-2.26	1.34	1.39
47	l	701	PEE	O2-C10	2.26	1.40	1.34
47	j	201	PEE	O2-C10	2.25	1.40	1.34
47	b	201	PEE	O2-C10	2.25	1.40	1.34
52	V	201	CDL	PB2-OB2	2.24	1.68	1.59
47	l	704	PEE	O2-C10	2.24	1.40	1.34
49	X	201	8Q1	O40-C39	-2.23	1.18	1.23
52	m	201	CDL	OB6-CB4	-2.23	1.41	1.46
47	C	302	PEE	O2-C10	2.22	1.40	1.34
46	A	502	FMN	C4A-N5	2.22	1.35	1.30
47	j	202	PEE	O2-C10	2.22	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	V	202	CDL	PB2-OB2	2.22	1.68	1.59
51	J	402	UQ	O4-C4	-2.21	1.18	1.23
47	W	201	PEE	O2-C10	2.20	1.40	1.34
52	l	702	CDL	OB6-CB4	-2.20	1.41	1.46
47	r	501	PEE	O2-C10	2.20	1.40	1.34
52	V	202	CDL	PB2-OB5	2.20	1.68	1.59
52	J	404	CDL	OB6-CB4	-2.19	1.41	1.46
46	A	502	FMN	C5A-N5	-2.18	1.35	1.39
52	r	504	CDL	PB2-OB2	2.18	1.68	1.59
47	j	201	PEE	O3-C3	-2.18	1.40	1.45
52	V	202	CDL	OB6-CB4	-2.18	1.41	1.46
52	J	404	CDL	PB2-OB2	2.17	1.68	1.59
52	m	201	CDL	PB2-OB2	2.16	1.68	1.59
52	m	201	CDL	OA6-CA4	-2.16	1.41	1.46
52	V	201	CDL	PB2-OB5	2.16	1.68	1.59
48	N	201	PLX	P1-O4	2.16	1.68	1.59
52	a	201	CDL	PB2-OB2	2.16	1.68	1.59
47	Q	501	PEE	O3-C3	-2.16	1.40	1.45
52	l	702	CDL	PB2-OB2	2.15	1.68	1.59
47	l	704	PEE	O3-C3	-2.15	1.40	1.45
47	Q	501	PEE	O2-C10	2.15	1.40	1.34
52	a	201	CDL	PB2-OB5	2.15	1.68	1.59
47	b	201	PEE	O3-C3	-2.14	1.40	1.45
52	r	504	CDL	OB6-CB4	-2.14	1.41	1.46
48	r	502	PLX	P1-O4	2.14	1.68	1.59
50	J	401	NDP	C5A-C4A	2.14	1.43	1.39
52	l	702	CDL	PB2-OB5	2.13	1.67	1.59
52	m	201	CDL	PB2-OB5	2.13	1.67	1.59
47	j	202	PEE	O3-C3	-2.13	1.40	1.45
48	n	101	PLX	P1-O4	2.13	1.67	1.59
51	J	402	UQ	O1-C1	-2.12	1.18	1.23
48	J	403	PLX	P1-O4	2.12	1.67	1.59
48	j	203	PLX	P1-O4	2.12	1.67	1.59
47	W	201	PEE	O3-C3	-2.11	1.40	1.45
47	B	303	PEE	O2-C10	2.11	1.40	1.34
48	g	201	PLX	P1-O4	2.10	1.67	1.59
52	r	504	CDL	PB2-OB5	2.09	1.67	1.59
52	J	404	CDL	PB2-OB5	2.09	1.67	1.59
52	a	201	CDL	OB6-CB4	-2.08	1.41	1.46
52	V	201	CDL	OA6-CA4	-2.08	1.41	1.46
47	l	701	PEE	O3-C3	-2.07	1.40	1.45
50	J	401	NDP	O5D-C5D	-2.07	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	r	503	PLX	P1-O4	2.06	1.67	1.59
51	s	501	UQ	O1-C1	-2.06	1.18	1.23
48	N	201	PLX	P1-O1	2.06	1.67	1.59
48	r	502	PLX	P1-O1	2.05	1.67	1.59
48	j	203	PLX	P1-O1	2.05	1.67	1.59
47	B	303	PEE	O3-C3	-2.04	1.40	1.45
51	J	402	UQ	C21-C19	2.02	1.55	1.51
48	n	101	PLX	P1-O1	2.02	1.67	1.59
51	s	501	UQ	O3-CM3	-2.02	1.40	1.45
47	C	302	PEE	O3-C3	-2.01	1.40	1.45
48	r	503	PLX	P1-O1	2.01	1.67	1.59

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	J	402	UQ	C7-C8-C9	-8.04	113.41	126.79
51	s	501	UQ	C7-C8-C9	-7.84	113.75	126.79
50	J	401	NDP	PN-O3-PA	-7.11	108.43	132.83
51	s	501	UQ	C42-C43-C44	-6.49	112.04	127.66
51	s	501	UQ	C12-C13-C14	-6.39	112.27	127.66
51	s	501	UQ	C47-C48-C49	-6.19	112.77	127.66
51	s	501	UQ	C32-C33-C34	-6.19	112.77	127.66
51	J	402	UQ	C17-C18-C19	-6.14	112.88	127.66
51	s	501	UQ	C37-C38-C39	-6.11	112.94	127.66
51	s	501	UQ	C17-C18-C19	-6.06	113.07	127.66
51	J	402	UQ	C12-C13-C14	-6.06	113.08	127.66
51	s	501	UQ	C22-C23-C24	-6.02	113.16	127.66
51	s	501	UQ	C27-C28-C29	-5.99	113.25	127.66
49	X	201	8Q1	C6-C1-S44	5.86	120.28	113.46
56	w	401	ADP	C5-C4-N3	-5.79	119.20	126.75
49	E	201	8Q1	C6-C1-S44	4.62	118.84	113.46
52	i	401	CDL	OA6-CA5-C11	4.52	121.25	111.50
51	s	501	UQ	C30-C29-C28	-4.47	112.21	123.68
56	w	401	ADP	N3-C4-N9	4.46	134.44	127.08
56	w	401	ADP	N3-C2-N1	-4.43	121.68	128.60
51	s	501	UQ	C45-C44-C43	-4.37	112.46	123.68
51	s	501	UQ	C15-C14-C13	-4.37	112.47	123.68
51	J	402	UQ	C22-C23-C24	-4.36	112.85	127.75
51	s	501	UQ	C52-C53-C54	-4.35	112.89	127.75
51	s	501	UQ	C11-C9-C8	-4.34	112.34	121.12
51	s	501	UQ	C20-C19-C18	-4.33	112.58	123.68
52	a	201	CDL	OB6-CB5-C51	4.30	120.78	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	s	501	UQ	C35-C34-C33	-4.29	112.67	123.68
51	s	501	UQ	C31-C29-C28	-4.26	112.50	121.12
51	s	501	UQ	C10-C9-C8	-4.24	112.80	123.68
51	s	501	UQ	C21-C19-C18	-4.24	112.53	121.12
51	J	402	UQ	C20-C19-C18	-4.24	112.80	123.68
51	s	501	UQ	C50-C49-C48	-4.22	112.85	123.68
51	s	501	UQ	C51-C49-C48	-4.21	112.59	121.12
51	s	501	UQ	C25-C24-C23	-4.19	112.92	123.68
51	J	402	UQ	C10-C9-C8	-4.19	112.94	123.68
52	l	703	CDL	OB6-CB5-C51	4.18	120.50	111.50
51	J	402	UQ	C11-C9-C8	-4.18	112.67	121.12
51	J	402	UQ	C15-C14-C13	-4.17	112.97	123.68
47	l	704	PEE	O2-C10-C11	4.17	120.48	111.50
47	j	202	PEE	O2-C10-C11	4.15	120.45	111.50
47	j	201	PEE	O2-C10-C11	4.13	120.40	111.50
51	s	501	UQ	C46-C44-C43	-4.12	112.77	121.12
52	l	702	CDL	OA6-CA5-C11	4.12	120.39	111.50
52	l	703	CDL	OA6-CA5-C11	4.10	120.34	111.50
51	J	402	UQ	C16-C14-C13	-4.10	112.82	121.12
47	C	302	PEE	O2-C10-C11	4.08	120.29	111.50
52	J	404	CDL	OB6-CB5-C51	4.08	120.29	111.50
52	V	201	CDL	OA6-CA5-C11	4.08	120.28	111.50
52	N	202	CDL	OA6-CA5-C11	4.06	120.26	111.50
52	N	202	CDL	OB6-CB5-C51	4.06	120.26	111.50
47	B	303	PEE	O2-C10-C11	4.06	120.25	111.50
51	s	501	UQ	C40-C39-C38	-4.06	113.27	123.68
47	l	701	PEE	O2-C10-C11	4.05	120.22	111.50
52	i	401	CDL	OB6-CB5-C51	4.04	120.22	111.50
52	J	404	CDL	OA6-CA5-C11	4.04	120.20	111.50
51	J	402	UQ	C21-C19-C18	-4.03	112.96	121.12
47	r	501	PEE	O2-C10-C11	4.03	120.18	111.50
51	s	501	UQ	C41-C39-C38	-4.01	113.01	121.12
47	b	201	PEE	O2-C10-C11	4.00	120.12	111.50
52	l	702	CDL	OB6-CB5-C51	3.98	120.08	111.50
52	r	504	CDL	OA6-CA5-C11	3.98	120.08	111.50
52	V	202	CDL	OB6-CB5-C51	3.97	120.06	111.50
51	s	501	UQ	C36-C34-C33	-3.96	113.11	121.12
52	u	201	CDL	OB6-CB5-C51	3.95	120.01	111.50
52	m	201	CDL	OB6-CB5-C51	3.95	120.01	111.50
47	Q	501	PEE	O2-C10-C11	3.94	120.00	111.50
47	W	201	PEE	O2-C10-C11	3.93	119.97	111.50
52	V	202	CDL	OA6-CA5-C11	3.92	119.95	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	V	201	CDL	OB6-CB5-C51	3.90	119.91	111.50
51	s	501	UQ	C16-C14-C13	-3.90	113.22	121.12
52	u	201	CDL	OA6-CA5-C11	3.87	119.85	111.50
49	E	201	8Q1	C43-S44-C1	3.81	113.74	101.87
52	a	201	CDL	OA6-CA5-C11	3.77	119.62	111.50
52	r	504	CDL	OB6-CB5-C51	3.76	119.61	111.50
51	s	501	UQ	C26-C24-C23	-3.73	113.57	121.12
56	w	401	ADP	C2-N3-C4	3.72	120.53	111.75
52	m	201	CDL	OA6-CA5-C11	3.66	119.38	111.50
56	w	401	ADP	N9-C8-N7	-3.64	108.94	113.91
56	w	401	ADP	C5-N7-C8	3.51	108.49	103.51
49	X	201	8Q1	O4-C1-C6	-3.50	119.86	123.99
51	s	501	UQ	C56-C54-C53	-3.40	112.83	122.65
51	J	402	UQ	C26-C24-C23	-3.39	112.84	122.65
51	s	501	UQ	C55-C54-C53	-3.39	112.85	122.65
51	J	402	UQ	C25-C24-C23	-3.31	113.07	122.65
52	u	201	CDL	OA8-CA7-C31	3.30	120.04	111.38
50	J	401	NDP	O2B-P2B-O1X	-3.26	96.81	109.39
49	E	201	8Q1	O35-C34-N36	-3.16	116.21	122.99
49	X	201	8Q1	C37-C38-C39	3.13	117.58	112.36
52	i	401	CDL	CA4-OA6-CA5	-3.09	110.17	117.79
56	w	401	ADP	C4-N9-C8	3.08	109.07	105.73
50	J	401	NDP	PA-O5B-C5B	-3.00	104.09	121.68
52	u	201	CDL	OB8-CB7-C71	2.98	121.24	111.91
46	A	502	FMN	C4A-C10-N1	-2.92	117.95	124.73
50	J	401	NDP	PN-O5D-C5D	-2.87	104.87	121.68
56	w	401	ADP	C4-C5-N7	-2.86	107.13	110.62
56	w	401	ADP	PA-O3A-PB	-2.85	123.05	132.83
49	E	201	8Q1	O2-P24-O27	-2.82	99.23	106.73
47	B	303	PEE	O3-C30-C31	2.79	120.66	111.91
52	a	201	CDL	OB8-CB7-C71	2.78	120.63	111.91
52	l	703	CDL	OB8-CB7-C71	2.77	120.62	111.91
52	m	201	CDL	OB8-CB7-C71	2.77	120.59	111.91
47	l	704	PEE	O3-C30-C31	2.77	120.59	111.91
52	l	703	CDL	CB4-OB6-CB5	-2.75	111.02	117.79
52	V	202	CDL	OB8-CB7-C71	2.74	120.52	111.91
52	m	201	CDL	OA8-CA7-C31	2.74	120.51	111.91
52	N	202	CDL	OB8-CB7-C71	2.73	120.47	111.91
47	r	501	PEE	O3-C30-C31	2.73	120.47	111.91
52	r	504	CDL	OB8-CB7-C71	2.72	120.46	111.91
52	l	702	CDL	OA8-CA7-C31	2.72	120.45	111.91
49	E	201	8Q1	C32-C34-N36	2.72	121.99	116.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	N	202	CDL	OA8-CA7-C31	2.70	120.38	111.91
51	s	501	UQ	CM5-C5-C6	-2.69	120.01	124.40
47	Q	501	PEE	O3-C30-C31	2.68	120.32	111.91
52	l	703	CDL	OA8-CA7-C31	2.68	120.31	111.91
52	J	404	CDL	OA8-CA7-C31	2.67	120.28	111.91
52	l	702	CDL	OB8-CB7-C71	2.65	120.22	111.91
47	W	201	PEE	O3-C30-C31	2.63	120.17	111.91
48	g	201	PLX	C1A-N1-C1	2.63	120.68	109.92
47	j	201	PEE	O3-C30-C31	2.63	120.16	111.91
52	V	201	CDL	OB8-CB7-C71	2.62	120.14	111.91
52	V	202	CDL	OA8-CA7-C31	2.60	120.08	111.91
52	i	401	CDL	OB8-CB7-C71	2.59	120.05	111.91
52	a	201	CDL	OA8-CA7-C31	2.58	120.00	111.91
47	b	201	PEE	O3-C30-C31	2.58	120.00	111.91
47	l	701	PEE	O3-C30-C31	2.57	119.99	111.91
49	E	201	8Q1	O40-C39-N41	-2.56	118.19	123.01
52	i	401	CDL	OA8-CA7-C31	2.55	119.92	111.91
50	J	401	NDP	O3X-P2B-O2X	2.55	117.37	107.64
51	J	402	UQ	CM5-C5-C6	-2.54	120.26	124.40
47	j	202	PEE	O3-C30-C31	2.53	119.85	111.91
52	r	504	CDL	OA8-CA7-C31	2.53	119.84	111.91
50	J	401	NDP	N3A-C4A-N9A	2.52	131.23	127.08
47	C	302	PEE	O3-C30-C31	2.50	119.77	111.91
49	X	201	8Q1	C43-S44-C1	2.50	109.65	101.87
50	J	401	NDP	O5D-PN-O1N	-2.49	99.32	109.07
52	V	201	CDL	OA8-CA7-C31	2.47	119.67	111.91
50	J	401	NDP	O4B-C4B-C3B	2.45	109.96	105.11
48	j	203	PLX	C1A-N1-C1	2.42	119.82	109.92
50	J	401	NDP	C2A-N1A-C6A	-2.40	114.66	118.77
49	E	201	8Q1	O1-P24-O2	2.39	116.78	107.64
52	N	202	CDL	CB4-OB6-CB5	-2.39	111.91	117.79
48	n	101	PLX	C1A-N1-C1	2.38	119.66	109.92
48	r	503	PLX	C1A-N1-C1	2.36	119.56	109.92
52	J	404	CDL	OB8-CB7-C71	2.35	119.29	111.91
50	J	401	NDP	C5A-C4A-N3A	-2.35	123.68	126.75
50	J	401	NDP	O2N-PN-O1N	2.35	123.86	112.24
48	N	201	PLX	C1A-N1-C1	2.35	119.52	109.92
48	J	403	PLX	C1A-N1-C1	2.34	119.48	109.92
48	r	502	PLX	C1A-N1-C1	2.33	119.45	109.92
46	A	502	FMN	O4-C4-C4A	-2.28	120.54	126.60
50	J	401	NDP	C5B-C4B-C3B	-2.25	106.76	115.18
49	X	201	8Q1	C38-C39-N41	2.24	120.20	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	E	201	8Q1	O4-C1-C6	-2.23	121.35	123.99
46	A	502	FMN	C10-N1-C2	2.19	121.28	116.90
46	A	502	FMN	C4A-C4-N3	2.16	118.68	113.19
49	E	201	8Q1	O4-C1-S44	-2.16	119.81	122.61
49	E	201	8Q1	C38-C39-N41	2.16	120.06	116.42
46	A	502	FMN	C4-N3-C2	-2.12	121.73	125.64
49	X	201	8Q1	O4-C1-S44	-2.11	119.87	122.61
46	A	502	FMN	C4-C4A-N5	2.11	121.24	118.23
46	A	502	FMN	O2-C2-N1	-2.10	118.34	121.83
52	i	401	CDL	OA6-CA5-OA7	-2.10	118.63	123.70
56	w	401	ADP	C4'-O4'-C1'	-2.08	104.89	109.47
49	E	201	8Q1	C37-C38-C39	2.04	115.75	112.36
50	J	401	NDP	O7N-C7N-C3N	2.02	124.69	120.90
52	l	703	CDL	CA4-OA6-CA5	-2.01	112.84	117.79
52	u	201	CDL	OB8-CB7-OB9	-2.01	118.52	123.59
50	J	401	NDP	C5A-C6A-N1A	2.01	121.70	117.39
52	l	703	CDL	OB6-CB5-OB7	-2.00	118.87	123.70

There are no chirality outliers.

All (1088) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C1'-C2'-C3'-O3'
46	A	502	FMN	C1'-C2'-C3'-C4'
47	B	303	PEE	C11-C10-O2-C2
47	C	302	PEE	C4-O4P-P-O1P
47	Q	501	PEE	C11-C10-O2-C2
47	Q	501	PEE	C4-O4P-P-O1P
47	Q	501	PEE	O4P-C4-C5-N
47	W	201	PEE	O4P-C4-C5-N
47	b	201	PEE	C37-C38-C39-C40
47	j	201	PEE	C17-C18-C19-C20
47	j	201	PEE	C1-O3P-P-O1P
47	j	202	PEE	C11-C10-O2-C2
47	j	202	PEE	C1-O3P-P-O2P
47	j	202	PEE	C1-O3P-P-O1P
47	j	202	PEE	C1-O3P-P-O4P
47	l	701	PEE	C11-C10-O2-C2
47	l	701	PEE	C1-O3P-P-O2P
47	l	701	PEE	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
47	l	701	PEE	C1-O3P-P-O4P
47	l	701	PEE	C4-O4P-P-O2P
47	l	701	PEE	C4-O4P-P-O1P
47	l	704	PEE	C11-C10-O2-C2
47	l	704	PEE	C4-O4P-P-O2P
47	r	501	PEE	C11-C10-O2-C2
48	C	303	PLX	C2-O1-P1-O2
48	C	303	PLX	C2-O1-P1-O3
48	J	403	PLX	O7-C6-O6-C4
48	J	403	PLX	C2-O1-P1-O2
48	N	201	PLX	O7-C6-O6-C4
48	N	201	PLX	C2-O1-P1-O2
48	N	201	PLX	C2-O1-P1-O3
48	N	201	PLX	O9-C24-O8-C5
48	g	201	PLX	C2-O1-P1-O4
48	j	203	PLX	O7-C6-C7-C8
48	j	203	PLX	C2-O1-P1-O2
48	n	101	PLX	O7-C6-C7-C8
48	n	101	PLX	O7-C6-O6-C4
48	n	101	PLX	C3-O4-P1-O3
48	n	101	PLX	C2-O1-P1-O2
48	r	502	PLX	O6-C6-C7-C8
48	r	502	PLX	O9-C24-C25-C26
49	E	201	8Q1	C1-C6-C7-C8
49	E	201	8Q1	O27-C28-C29-C32
49	E	201	8Q1	C28-C29-C32-C34
49	E	201	8Q1	C28-C29-C32-O33
49	E	201	8Q1	C30-C29-C32-C34
49	E	201	8Q1	C30-C29-C32-O33
49	E	201	8Q1	C31-C29-C32-C34
49	E	201	8Q1	C31-C29-C32-O33
49	E	201	8Q1	C42-C43-S44-C1
49	E	201	8Q1	C28-O27-P24-O3
49	E	201	8Q1	C28-O27-P24-O2
49	E	201	8Q1	C28-O27-P24-O1
49	X	201	8Q1	O4-C1-S44-C43
49	X	201	8Q1	C6-C1-S44-C43
49	X	201	8Q1	N36-C37-C38-C39
49	X	201	8Q1	N41-C42-C43-S44
49	X	201	8Q1	C42-C43-S44-C1
49	X	201	8Q1	C28-O27-P24-O2
49	X	201	8Q1	C28-O27-P24-O1

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Mol	Chain	Res	Type	Atoms
50	J	401	NDP	C5B-O5B-PA-O1A
50	J	401	NDP	C5B-O5B-PA-O2A
50	J	401	NDP	O4B-C4B-C5B-O5B
50	J	401	NDP	C3B-C4B-C5B-O5B
50	J	401	NDP	C2B-O2B-P2B-O3X
50	J	401	NDP	O4D-C4D-C5D-O5D
51	J	402	UQ	C7-C8-C9-C10
51	J	402	UQ	C7-C8-C9-C11
51	J	402	UQ	C12-C11-C9-C10
51	J	402	UQ	C11-C12-C13-C14
51	J	402	UQ	C12-C13-C14-C15
51	J	402	UQ	C15-C14-C16-C17
51	J	402	UQ	C14-C16-C17-C18
51	J	402	UQ	C17-C18-C19-C20
51	J	402	UQ	C17-C18-C19-C21
51	J	402	UQ	C18-C19-C21-C22
51	J	402	UQ	C19-C21-C22-C23
51	s	501	UQ	C7-C8-C9-C10
51	s	501	UQ	C16-C17-C18-C19
51	s	501	UQ	C17-C18-C19-C20
51	s	501	UQ	C20-C19-C21-C22
51	s	501	UQ	C25-C24-C26-C27
51	s	501	UQ	C27-C28-C29-C31
51	s	501	UQ	C28-C29-C31-C32
51	s	501	UQ	C32-C33-C34-C36
51	s	501	UQ	C42-C43-C44-C45
51	s	501	UQ	C42-C43-C44-C46
51	s	501	UQ	C47-C48-C49-C51
52	J	404	CDL	O1-C1-CA2-OA2
52	J	404	CDL	CB2-C1-CA2-OA2
52	J	404	CDL	CA2-OA2-PA1-OA3
52	J	404	CDL	CA2-OA2-PA1-OA4
52	J	404	CDL	CB3-OB5-PB2-OB2
52	J	404	CDL	OB6-CB4-CB6-OB8
52	N	202	CDL	CA2-OA2-PA1-OA4
52	N	202	CDL	CA3-OA5-PA1-OA4
52	N	202	CDL	CB2-OB2-PB2-OB4
52	N	202	CDL	CB3-OB5-PB2-OB2
52	V	201	CDL	CA2-OA2-PA1-OA5
52	V	201	CDL	C11-CA5-OA6-CA4
52	V	201	CDL	CB2-OB2-PB2-OB3
52	V	201	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
52	V	202	CDL	CA3-OA5-PA1-OA3
52	V	202	CDL	C51-CB5-OB6-CB4
52	a	201	CDL	CB2-C1-CA2-OA2
52	a	201	CDL	CA2-OA2-PA1-OA3
52	a	201	CDL	CB2-OB2-PB2-OB3
52	a	201	CDL	CB3-OB5-PB2-OB3
52	a	201	CDL	CB3-OB5-PB2-OB4
52	a	201	CDL	OB7-CB5-OB6-CB4
52	i	401	CDL	CA2-OA2-PA1-OA4
52	i	401	CDL	CB2-OB2-PB2-OB3
52	i	401	CDL	CB2-OB2-PB2-OB4
52	i	401	CDL	CB2-OB2-PB2-OB5
52	i	401	CDL	CB3-OB5-PB2-OB3
52	l	702	CDL	O1-C1-CB2-OB2
52	l	702	CDL	CA2-OA2-PA1-OA4
52	l	702	CDL	CA3-OA5-PA1-OA3
52	l	702	CDL	CB2-OB2-PB2-OB4
52	l	702	CDL	CB3-OB5-PB2-OB3
52	l	703	CDL	CA2-OA2-PA1-OA4
52	l	703	CDL	CA3-OA5-PA1-OA4
52	l	703	CDL	CB2-OB2-PB2-OB3
52	l	703	CDL	CB2-OB2-PB2-OB4
52	m	201	CDL	CA2-OA2-PA1-OA3
52	m	201	CDL	CA2-OA2-PA1-OA4
52	m	201	CDL	CA2-OA2-PA1-OA5
52	m	201	CDL	CA3-OA5-PA1-OA3
52	m	201	CDL	CB3-OB5-PB2-OB2
52	m	201	CDL	CB3-OB5-PB2-OB3
52	m	201	CDL	CB3-OB5-PB2-OB4
52	r	504	CDL	CA2-OA2-PA1-OA3
52	r	504	CDL	CA3-OA5-PA1-OA2
52	r	504	CDL	CA3-OA5-PA1-OA3
52	r	504	CDL	CB2-OB2-PB2-OB3
52	r	504	CDL	CB2-OB2-PB2-OB4
52	r	504	CDL	CB2-OB2-PB2-OB5
52	r	504	CDL	CB3-OB5-PB2-OB3
52	r	504	CDL	C51-CB5-OB6-CB4
52	u	201	CDL	CA2-OA2-PA1-OA3
52	u	201	CDL	CA2-OA2-PA1-OA4
52	u	201	CDL	CA2-OA2-PA1-OA5
52	u	201	CDL	CA3-OA5-PA1-OA3
52	u	201	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
52	u	201	CDL	CB3-OB5-PB2-OB2
52	u	201	CDL	CB3-OB5-PB2-OB3
52	u	201	CDL	CB3-OB5-PB2-OB4
56	w	401	ADP	C5'-O5'-PA-O1A
56	w	401	ADP	C5'-O5'-PA-O2A
56	w	401	ADP	C5'-O5'-PA-O3A
52	J	404	CDL	OA9-CA7-OA8-CA6
52	J	404	CDL	C31-CA7-OA8-CA6
52	i	401	CDL	OA9-CA7-OA8-CA6
52	l	702	CDL	OA9-CA7-OA8-CA6
47	B	303	PEE	O4-C10-O2-C2
47	j	202	PEE	O4-C10-O2-C2
47	l	701	PEE	O4-C10-O2-C2
47	l	704	PEE	O4-C10-O2-C2
47	r	501	PEE	O4-C10-O2-C2
52	V	201	CDL	OA7-CA5-OA6-CA4
52	V	202	CDL	OB7-CB5-OB6-CB4
52	r	504	CDL	OB7-CB5-OB6-CB4
52	l	702	CDL	C31-CA7-OA8-CA6
52	a	201	CDL	C51-CB5-OB6-CB4
51	s	501	UQ	C52-C53-C54-C55
51	s	501	UQ	C43-C44-C46-C47
47	Q	501	PEE	O5-C30-O3-C3
48	r	502	PLX	C11-C12-C13-C14
47	Q	501	PEE	C31-C30-O3-C3
47	j	201	PEE	C31-C30-O3-C3
52	i	401	CDL	C31-CA7-OA8-CA6
47	B	303	PEE	C17-C18-C19-C20
47	l	704	PEE	C37-C38-C39-C40
51	s	501	UQ	C27-C28-C29-C30
51	s	501	UQ	C37-C38-C39-C40
51	s	501	UQ	C47-C48-C49-C50
47	Q	501	PEE	O4-C10-O2-C2
51	s	501	UQ	C12-C13-C14-C16
51	s	501	UQ	C17-C18-C19-C21
51	s	501	UQ	C22-C23-C24-C26
48	g	201	PLX	C2-C1-N1-C1A
52	a	201	CDL	O1-C1-CA2-OA2
52	a	201	CDL	O1-C1-CB2-OB2
52	l	702	CDL	O1-C1-CA2-OA2
52	r	504	CDL	O1-C1-CA2-OA2
52	V	201	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
47	C	302	PEE	C11-C10-O2-C2
52	N	202	CDL	C11-CA5-OA6-CA4
51	J	402	UQ	C22-C23-C24-C26
52	r	504	CDL	C74-C75-C76-C77
47	l	704	PEE	C33-C34-C35-C36
48	g	201	PLX	C9-C10-C11-C12
48	g	201	PLX	C7-C8-C9-C10
52	J	404	CDL	C37-C38-C39-C40
52	V	201	CDL	C62-C63-C64-C65
52	V	202	CDL	C11-C12-C13-C14
52	m	201	CDL	C73-C74-C75-C76
47	B	303	PEE	C42-C43-C44-C45
48	r	502	PLX	C9-C10-C11-C12
48	j	203	PLX	C13-C14-C15-C16
52	V	202	CDL	C32-C33-C34-C35
52	l	702	CDL	C81-C82-C83-C84
47	j	201	PEE	O5-C30-O3-C3
52	V	201	CDL	OB9-CB7-OB8-CB6
51	s	501	UQ	C48-C49-C51-C52
47	j	201	PEE	C30-C31-C32-C33
52	m	201	CDL	C62-C63-C64-C65
51	s	501	UQ	C14-C16-C17-C18
51	s	501	UQ	C34-C36-C37-C38
48	r	502	PLX	C7-C8-C9-C10
52	V	201	CDL	C32-C33-C34-C35
52	l	702	CDL	C32-C33-C34-C35
51	s	501	UQ	C22-C23-C24-C25
47	b	201	PEE	C10-C11-C12-C13
52	a	201	CDL	CA2-C1-CB2-OB2
52	l	702	CDL	CA2-C1-CB2-OB2
47	C	302	PEE	O4-C10-O2-C2
52	l	702	CDL	CB5-C51-C52-C53
52	m	201	CDL	C36-C37-C38-C39
52	V	201	CDL	C59-C60-C61-C62
52	l	702	CDL	C58-C59-C60-C61
52	r	504	CDL	C60-C61-C62-C63
52	N	202	CDL	O1-C1-CB2-OB2
52	i	401	CDL	O1-C1-CB2-OB2
52	l	703	CDL	O1-C1-CA2-OA2
52	u	201	CDL	O1-C1-CB2-OB2
52	a	201	CDL	CA7-C31-C32-C33
48	g	201	PLX	O6-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
52	J	404	CDL	C31-C32-C33-C34
47	r	501	PEE	C41-C42-C43-C44
52	l	702	CDL	C34-C35-C36-C37
47	l	701	PEE	C31-C30-O3-C3
52	V	201	CDL	C31-CA7-OA8-CA6
52	J	404	CDL	CA7-C31-C32-C33
52	J	404	CDL	CB5-C51-C52-C53
52	V	202	CDL	C72-C73-C74-C75
46	A	502	FMN	O2'-C2'-C3'-O3'
47	Q	501	PEE	C30-C31-C32-C33
52	J	404	CDL	CB7-C71-C72-C73
52	V	202	CDL	CB7-C71-C72-C73
52	i	401	CDL	CA7-C31-C32-C33
52	m	201	CDL	CA5-C11-C12-C13
52	r	504	CDL	CA5-C11-C12-C13
50	J	401	NDP	C3D-C4D-C5D-O5D
52	N	202	CDL	OA7-CA5-OA6-CA4
47	l	704	PEE	C30-C31-C32-C33
52	a	201	CDL	CA5-C11-C12-C13
52	l	702	CDL	CA7-C31-C32-C33
52	J	404	CDL	C14-C15-C16-C17
52	l	703	CDL	C51-C52-C53-C54
52	m	201	CDL	C13-C14-C15-C16
52	a	201	CDL	CB5-C51-C52-C53
47	l	701	PEE	O5-C30-O3-C3
47	l	701	PEE	C17-C18-C19-C20
47	b	201	PEE	C11-C10-O2-C2
47	j	201	PEE	C11-C10-O2-C2
52	m	201	CDL	C11-CA5-OA6-CA4
47	C	302	PEE	C4-O4P-P-O3P
47	Q	501	PEE	C4-O4P-P-O3P
47	W	201	PEE	C4-O4P-P-O3P
47	l	701	PEE	C4-O4P-P-O3P
47	l	704	PEE	C4-O4P-P-O3P
48	C	303	PLX	C2-O1-P1-O4
48	J	403	PLX	C3-O4-P1-O1
48	J	403	PLX	C2-O1-P1-O4
48	N	201	PLX	C2-O1-P1-O4
48	n	101	PLX	C3-O4-P1-O1
52	J	404	CDL	CA2-OA2-PA1-OA5
52	J	404	CDL	CA3-OA5-PA1-OA2
52	N	202	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
52	N	202	CDL	CA3-OA5-PA1-OA2
52	N	202	CDL	CB2-OB2-PB2-OB5
52	V	201	CDL	CB2-OB2-PB2-OB5
52	V	202	CDL	CB3-OB5-PB2-OB2
52	a	201	CDL	CB2-OB2-PB2-OB5
52	a	201	CDL	CB3-OB5-PB2-OB2
52	i	401	CDL	CA2-OA2-PA1-OA5
52	i	401	CDL	CA3-OA5-PA1-OA2
52	i	401	CDL	CB3-OB5-PB2-OB2
52	l	702	CDL	CA2-OA2-PA1-OA5
52	l	702	CDL	CB2-OB2-PB2-OB5
52	l	702	CDL	CB3-OB5-PB2-OB2
52	l	703	CDL	CA2-OA2-PA1-OA5
52	l	703	CDL	CA3-OA5-PA1-OA2
52	l	703	CDL	CB2-OB2-PB2-OB5
52	m	201	CDL	CA3-OA5-PA1-OA2
52	r	504	CDL	CA2-OA2-PA1-OA5
52	r	504	CDL	CB3-OB5-PB2-OB2
52	u	201	CDL	CA3-OA5-PA1-OA2
52	u	201	CDL	CB2-OB2-PB2-OB5
47	W	201	PEE	C10-C11-C12-C13
48	J	403	PLX	C11-C10-C9-C8
52	r	504	CDL	CB2-C1-CA2-OA2
47	b	201	PEE	O4-C10-O2-C2
47	j	201	PEE	O4-C10-O2-C2
52	m	201	CDL	OA7-CA5-OA6-CA4
47	j	201	PEE	C32-C33-C34-C35
48	g	201	PLX	C2-C1-N1-C1C
47	b	201	PEE	C31-C30-O3-C3
47	j	201	PEE	C19-C20-C21-C22
48	J	403	PLX	C7-C8-C9-C10
48	N	201	PLX	C14-C15-C16-C17
48	r	502	PLX	C11-C10-C9-C8
52	V	201	CDL	C37-C38-C39-C40
52	l	702	CDL	C56-C57-C58-C59
52	J	404	CDL	C51-CB5-OB6-CB4
52	V	201	CDL	C51-CB5-OB6-CB4
52	l	702	CDL	C51-CB5-OB6-CB4
47	r	501	PEE	C12-C13-C14-C15
48	N	201	PLX	C29-C30-C31-C32
48	g	201	PLX	C25-C26-C27-C28
48	g	201	PLX	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
48	j	203	PLX	C31-C32-C33-C34
48	n	101	PLX	C25-C26-C27-C28
48	n	101	PLX	C31-C32-C33-C34
48	r	502	PLX	C30-C31-C32-C33
52	J	404	CDL	C71-C72-C73-C74
52	V	201	CDL	C74-C75-C76-C77
52	V	202	CDL	C59-C60-C61-C62
52	a	201	CDL	C75-C76-C77-C78
52	l	702	CDL	C75-C76-C77-C78
49	E	201	8Q1	O27-C28-C29-C30
49	E	201	8Q1	O27-C28-C29-C31
52	l	702	CDL	C71-CB7-OB8-CB6
52	l	703	CDL	C71-CB7-OB8-CB6
47	W	201	PEE	C11-C12-C13-C14
47	b	201	PEE	C31-C32-C33-C34
47	j	202	PEE	C11-C12-C13-C14
48	j	203	PLX	C14-C15-C16-C17
48	r	503	PLX	C13-C14-C15-C16
48	r	503	PLX	C10-C11-C12-C13
49	E	201	8Q1	C10-C11-C12-C13
52	V	201	CDL	C52-C53-C54-C55
52	a	201	CDL	C37-C38-C39-C40
52	m	201	CDL	C59-C60-C61-C62
52	N	202	CDL	CA6-CA4-OA6-CA5
52	J	404	CDL	OB7-CB5-OB6-CB4
52	V	201	CDL	OB7-CB5-OB6-CB4
46	A	502	FMN	O2'-C2'-C3'-C4'
48	J	403	PLX	C31-C32-C33-C34
48	N	201	PLX	C33-C34-C35-C36
52	V	201	CDL	C58-C59-C60-C61
52	V	202	CDL	C33-C34-C35-C36
52	a	201	CDL	C17-C18-C19-C20
52	a	201	CDL	C62-C63-C64-C65
52	r	504	CDL	C32-C33-C34-C35
48	N	201	PLX	C12-C13-C14-C15
48	j	203	PLX	C16-C17-C18-C19
52	V	201	CDL	C33-C34-C35-C36
52	a	201	CDL	C73-C74-C75-C76
52	m	201	CDL	C32-C33-C34-C35
52	r	504	CDL	C35-C36-C37-C38
52	l	703	CDL	O1-C1-CB2-OB2
52	J	404	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
52	V	202	CDL	C17-C18-C19-C20
52	V	202	CDL	C37-C38-C39-C40
52	l	702	CDL	CB7-C71-C72-C73
47	W	201	PEE	C31-C30-O3-C3
52	a	201	CDL	C71-CB7-OB8-CB6
48	g	201	PLX	C11-C12-C13-C14
48	g	201	PLX	C27-C28-C29-C30
52	m	201	CDL	C55-C56-C57-C58
52	r	504	CDL	C14-C15-C16-C17
47	j	202	PEE	C33-C34-C35-C36
47	l	704	PEE	C40-C41-C42-C43
52	V	201	CDL	C31-C32-C33-C34
52	a	201	CDL	C60-C61-C62-C63
52	l	702	CDL	C14-C15-C16-C17
52	m	201	CDL	C75-C76-C77-C78
47	l	704	PEE	C22-C23-C24-C25
48	N	201	PLX	C27-C28-C29-C30
48	g	201	PLX	C14-C15-C16-C17
48	j	203	PLX	C9-C10-C11-C12
48	j	203	PLX	C7-C8-C9-C10
48	n	101	PLX	C27-C28-C29-C30
48	r	503	PLX	C35-C36-C37-C38
49	X	201	8Q1	C11-C12-C13-C14
52	J	404	CDL	C59-C60-C61-C62
52	J	404	CDL	C73-C74-C75-C76
52	V	201	CDL	C11-C12-C13-C14
52	V	202	CDL	C13-C14-C15-C16
52	V	202	CDL	C42-C43-C44-C45
52	m	201	CDL	C71-C72-C73-C74
52	V	201	CDL	OA9-CA7-OA8-CA6
47	C	302	PEE	C42-C43-C44-C45
47	W	201	PEE	C12-C13-C14-C15
48	J	403	PLX	C9-C10-C11-C12
48	n	101	PLX	C10-C11-C12-C13
52	J	404	CDL	C75-C76-C77-C78
52	V	202	CDL	C74-C75-C76-C77
52	l	702	CDL	C11-C12-C13-C14
52	l	702	CDL	C36-C37-C38-C39
52	l	702	CDL	C39-C40-C41-C42
52	l	702	CDL	C74-C75-C76-C77
52	r	504	CDL	C57-C58-C59-C60
52	l	702	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
48	J	403	PLX	C28-C29-C30-C31
48	r	502	PLX	C28-C29-C30-C31
48	r	503	PLX	C25-C26-C27-C28
52	J	404	CDL	C36-C37-C38-C39
47	l	704	PEE	C19-C20-C21-C22
47	l	701	PEE	C10-C11-C12-C13
47	B	303	PEE	C12-C13-C14-C15
47	b	201	PEE	C33-C34-C35-C36
47	l	704	PEE	C21-C22-C23-C24
47	r	501	PEE	C40-C41-C42-C43
48	J	403	PLX	C14-C15-C16-C17
48	j	203	PLX	C12-C13-C14-C15
48	j	203	PLX	C28-C29-C30-C31
48	j	203	PLX	C33-C34-C35-C36
48	r	502	PLX	C25-C26-C27-C28
52	J	404	CDL	C55-C56-C57-C58
52	V	202	CDL	C34-C35-C36-C37
52	a	201	CDL	C33-C34-C35-C36
52	l	702	CDL	C71-C72-C73-C74
52	r	504	CDL	C37-C38-C39-C40
48	g	201	PLX	C2-C1-N1-C1B
48	N	201	PLX	C25-C26-C27-C28
52	J	404	CDL	C52-C53-C54-C55
52	m	201	CDL	C79-C80-C81-C82
47	B	303	PEE	O4P-C4-C5-N
48	g	201	PLX	C13-C14-C15-C16
52	V	201	CDL	C71-C72-C73-C74
52	V	202	CDL	C14-C15-C16-C17
52	V	202	CDL	C75-C76-C77-C78
47	Q	501	PEE	C33-C34-C35-C36
48	g	201	PLX	C12-C13-C14-C15
48	r	502	PLX	C13-C14-C15-C16
48	r	502	PLX	C27-C28-C29-C30
49	E	201	8Q1	C11-C10-C9-C8
52	r	504	CDL	C73-C74-C75-C76
48	J	403	PLX	C13-C14-C15-C16
48	n	101	PLX	C14-C15-C16-C17
52	V	202	CDL	C82-C83-C84-C85
52	r	504	CDL	C11-C12-C13-C14
48	J	403	PLX	C30-C31-C32-C33
48	r	503	PLX	C29-C30-C31-C32
52	V	201	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
52	r	504	CDL	C31-C32-C33-C34
48	J	403	PLX	C33-C34-C35-C36
48	n	101	PLX	C13-C14-C15-C16
52	V	202	CDL	C15-C16-C17-C18
52	l	702	CDL	C52-C53-C54-C55
52	r	504	CDL	C62-C63-C64-C65
47	W	201	PEE	C17-C18-C19-C20
47	l	701	PEE	C37-C38-C39-C40
48	r	503	PLX	C14-C15-C16-C17
52	r	504	CDL	C75-C76-C77-C78
52	r	504	CDL	C77-C78-C79-C80
52	r	504	CDL	CB7-C71-C72-C73
52	V	202	CDL	C52-C53-C54-C55
52	l	702	CDL	C55-C56-C57-C58
52	l	702	CDL	C62-C63-C64-C65
47	l	704	PEE	C31-C30-O3-C3
47	l	704	PEE	C32-C33-C34-C35
48	C	303	PLX	O7-C6-C7-C8
48	J	403	PLX	O9-C24-C25-C26
48	r	502	PLX	O7-C6-C7-C8
47	l	704	PEE	C20-C21-C22-C23
48	g	201	PLX	C28-C29-C30-C31
48	r	503	PLX	C11-C10-C9-C8
52	J	404	CDL	C35-C36-C37-C38
52	r	504	CDL	C83-C84-C85-C86
52	u	201	CDL	C73-C74-C75-C76
47	b	201	PEE	O5-C30-O3-C3
47	l	704	PEE	C44-C45-C46-C47
48	C	303	PLX	C10-C11-C12-C13
48	N	201	PLX	C10-C11-C12-C13
52	J	404	CDL	C34-C35-C36-C37
52	a	201	CDL	C11-C12-C13-C14
52	m	201	CDL	C61-C62-C63-C64
52	l	702	CDL	OB9-CB7-OB8-CB6
52	J	404	CDL	CA2-C1-CB2-OB2
52	l	702	CDL	CB2-C1-CA2-OA2
47	B	303	PEE	C13-C14-C15-C16
52	V	202	CDL	C73-C74-C75-C76
52	m	201	CDL	C18-C19-C20-C21
52	m	201	CDL	C41-C42-C43-C44
52	r	504	CDL	C41-C42-C43-C44
52	r	504	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
47	W	201	PEE	C21-C22-C23-C24
47	W	201	PEE	C13-C14-C15-C16
47	j	201	PEE	C23-C24-C25-C26
47	j	202	PEE	C22-C23-C24-C25
47	r	501	PEE	C13-C14-C15-C16
48	g	201	PLX	C30-C31-C32-C33
52	J	404	CDL	C82-C83-C84-C85
52	a	201	CDL	C15-C16-C17-C18
47	W	201	PEE	O5-C30-O3-C3
47	Q	501	PEE	C31-C32-C33-C34
47	B	303	PEE	C23-C24-C25-C26
52	J	404	CDL	C17-C18-C19-C20
52	l	703	CDL	C15-C16-C17-C18
52	l	703	CDL	C73-C74-C75-C76
52	m	201	CDL	C20-C21-C22-C23
52	i	401	CDL	C11-CA5-OA6-CA4
47	l	704	PEE	C34-C35-C36-C37
48	j	203	PLX	C29-C30-C31-C32
52	J	404	CDL	C51-C52-C53-C54
52	V	201	CDL	C55-C56-C57-C58
52	l	702	CDL	C16-C17-C18-C19
52	m	201	CDL	C11-C12-C13-C14
52	r	504	CDL	C43-C44-C45-C46
52	a	201	CDL	OB9-CB7-OB8-CB6
52	l	703	CDL	OB9-CB7-OB8-CB6
47	W	201	PEE	C24-C25-C26-C27
49	E	201	8Q1	C12-C13-C14-C15
51	J	402	UQ	C20-C19-C21-C22
47	l	704	PEE	O5-C30-O3-C3
47	r	501	PEE	C20-C21-C22-C23
52	V	202	CDL	C35-C36-C37-C38
52	a	201	CDL	C71-C72-C73-C74
47	Q	501	PEE	C35-C36-C37-C38
52	u	201	CDL	CB7-C71-C72-C73
52	V	202	CDL	C71-CB7-OB8-CB6
52	r	504	CDL	C71-CB7-OB8-CB6
47	l	704	PEE	C13-C14-C15-C16
48	N	201	PLX	C7-C8-C9-C10
48	r	503	PLX	C30-C31-C32-C33
48	r	503	PLX	C31-C32-C33-C34
52	m	201	CDL	C16-C17-C18-C19
48	J	403	PLX	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
52	a	201	CDL	C32-C33-C34-C35
47	B	303	PEE	C31-C32-C33-C34
47	l	701	PEE	C11-C12-C13-C14
47	l	701	PEE	C32-C33-C34-C35
48	r	503	PLX	C11-C12-C13-C14
49	E	201	8Q1	N36-C37-C38-C39
48	g	201	PLX	C10-C11-C12-C13
48	r	502	PLX	C33-C34-C35-C36
52	V	201	CDL	C14-C15-C16-C17
52	a	201	CDL	C31-C32-C33-C34
52	m	201	CDL	C60-C61-C62-C63
52	V	201	CDL	OB5-CB3-CB4-OB6
52	m	201	CDL	OA5-CA3-CA4-OA6
48	J	403	PLX	C11-C12-C13-C14
48	r	503	PLX	C18-C19-C20-C21
48	r	503	PLX	C28-C29-C30-C31
48	r	503	PLX	C26-C27-C28-C29
52	u	201	CDL	O1-C1-CA2-OA2
52	i	401	CDL	OA7-CA5-OA6-CA4
52	i	401	CDL	OB6-CB4-CB6-OB8
48	r	503	PLX	C27-C28-C29-C30
47	C	302	PEE	C13-C14-C15-C16
52	a	201	CDL	C21-C22-C23-C24
52	m	201	CDL	C34-C35-C36-C37
47	B	303	PEE	C35-C36-C37-C38
47	j	202	PEE	C15-C16-C17-C18
47	r	501	PEE	C39-C40-C41-C42
48	j	203	PLX	C11-C12-C13-C14
47	b	201	PEE	C13-C14-C15-C16
47	r	501	PEE	C37-C38-C39-C40
52	l	702	CDL	C35-C36-C37-C38
52	V	202	CDL	CA7-C31-C32-C33
47	j	201	PEE	C34-C35-C36-C37
47	Q	501	PEE	C18-C19-C20-C21
48	j	203	PLX	C2-O1-P1-O4
48	n	101	PLX	C2-O1-P1-O4
47	C	302	PEE	C11-C12-C13-C14
47	Q	501	PEE	C34-C35-C36-C37
48	n	101	PLX	C28-C29-C30-C31
52	u	201	CDL	CB5-C51-C52-C53
52	r	504	CDL	OB9-CB7-OB8-CB6
52	V	201	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
52	a	201	CDL	OB5-CB3-CB4-CB6
52	l	703	CDL	OB5-CB3-CB4-CB6
47	b	201	PEE	C22-C23-C24-C25
52	l	702	CDL	C59-C60-C61-C62
47	j	202	PEE	C12-C13-C14-C15
48	j	203	PLX	C25-C26-C27-C28
48	n	101	PLX	C16-C17-C18-C19
52	V	201	CDL	C54-C55-C56-C57
48	J	403	PLX	C34-C35-C36-C37
48	r	502	PLX	C14-C15-C16-C17
48	n	101	PLX	C15-C16-C17-C18
52	V	202	CDL	C60-C61-C62-C63
52	V	202	CDL	C62-C63-C64-C65
52	a	201	CDL	C52-C53-C54-C55
52	i	401	CDL	C37-C38-C39-C40
47	C	302	PEE	C15-C16-C17-C18
48	J	403	PLX	C25-C26-C27-C28
52	a	201	CDL	C35-C36-C37-C38
52	V	202	CDL	CA2-C1-CB2-OB2
48	n	101	PLX	C30-C31-C32-C33
52	m	201	CDL	C33-C34-C35-C36
47	r	501	PEE	C36-C37-C38-C39
52	V	202	CDL	C84-C85-C86-C87
52	V	202	CDL	O1-C1-CB2-OB2
52	m	201	CDL	O1-C1-CA2-OA2
47	Q	501	PEE	C20-C21-C22-C23
49	X	201	8Q1	C6-C7-C8-C9
52	V	202	CDL	C40-C41-C42-C43
47	C	302	PEE	C1-C2-C3-O3
47	b	201	PEE	C1-C2-C3-O3
48	g	201	PLX	C3-C4-C5-O8
48	j	203	PLX	C3-C4-C5-O8
49	X	201	8Q1	C10-C11-C12-C13
52	m	201	CDL	CA3-CA4-CA6-OA8
52	m	201	CDL	CB3-CB4-CB6-OB8
47	Q	501	PEE	C24-C25-C26-C27
47	j	202	PEE	C24-C25-C26-C27
52	m	201	CDL	C84-C85-C86-C87
47	B	303	PEE	C36-C37-C38-C39
52	V	202	CDL	C64-C65-C66-C67
47	W	201	PEE	C15-C16-C17-C18
47	l	701	PEE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
47	l	704	PEE	C15-C16-C17-C18
52	V	202	CDL	OB9-CB7-OB8-CB6
52	l	702	CDL	C21-C22-C23-C24
52	l	703	CDL	C51-CB5-OB6-CB4
47	l	701	PEE	C33-C34-C35-C36
47	j	201	PEE	C40-C41-C42-C43
52	V	202	CDL	C12-C13-C14-C15
52	l	702	CDL	C63-C64-C65-C66
52	V	202	CDL	CB5-C51-C52-C53
52	r	504	CDL	CA7-C31-C32-C33
49	X	201	8Q1	C13-C14-C15-C16
48	N	201	PLX	C31-C32-C33-C34
52	V	202	CDL	C41-C42-C43-C44
52	r	504	CDL	C42-C43-C44-C45
52	r	504	CDL	C59-C60-C61-C62
47	j	201	PEE	C38-C39-C40-C41
49	X	201	8Q1	C28-O27-P24-O3
52	l	703	CDL	C21-C22-C23-C24
47	j	202	PEE	C31-C30-O3-C3
52	J	404	CDL	C71-CB7-OB8-CB6
52	l	702	CDL	OB5-CB3-CB4-OB6
48	g	201	PLX	C11-C10-C9-C8
52	J	404	CDL	C54-C55-C56-C57
52	r	504	CDL	C64-C65-C66-C67
47	l	704	PEE	O2-C2-C3-O3
52	V	202	CDL	OA6-CA4-CA6-OA8
48	J	403	PLX	C27-C28-C29-C30
48	n	101	PLX	C29-C30-C31-C32
52	m	201	CDL	C14-C15-C16-C17
49	X	201	8Q1	C12-C13-C14-C15
52	r	504	CDL	C33-C34-C35-C36
52	r	504	CDL	C56-C57-C58-C59
51	J	402	UQ	C3-C2-O2-CM2
51	s	501	UQ	C3-C2-O2-CM2
52	V	201	CDL	CA7-C31-C32-C33
47	j	202	PEE	C23-C24-C25-C26
48	r	502	PLX	C12-C13-C14-C15
52	N	202	CDL	C31-CA7-OA8-CA6
52	r	504	CDL	C84-C85-C86-C87
47	l	704	PEE	C17-C18-C19-C20
47	C	302	PEE	C44-C45-C46-C47
48	g	201	PLX	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
52	a	201	CDL	C38-C39-C40-C41
47	Q	501	PEE	O3P-C1-C2-C3
52	m	201	CDL	OA5-CA3-CA4-CA6
52	m	201	CDL	C19-C20-C21-C22
47	l	701	PEE	O4P-C4-C5-N
47	l	704	PEE	C14-C15-C16-C17
47	r	501	PEE	C14-C15-C16-C17
51	s	501	UQ	C45-C44-C46-C47
51	s	501	UQ	C13-C14-C16-C17
52	l	703	CDL	CB7-C71-C72-C73
52	V	201	CDL	C75-C76-C77-C78
52	J	404	CDL	OB9-CB7-OB8-CB6
47	B	303	PEE	C41-C42-C43-C44
47	r	501	PEE	C21-C22-C23-C24
49	E	201	8Q1	C6-C7-C8-C9
52	m	201	CDL	C71-CB7-OB8-CB6
52	V	201	CDL	C1-CB2-OB2-PB2
52	r	504	CDL	C1-CB2-OB2-PB2
47	B	303	PEE	C44-C45-C46-C47
48	N	201	PLX	C28-C29-C30-C31
52	a	201	CDL	C36-C37-C38-C39
46	A	502	FMN	C2'-C1'-N10-C10
48	n	101	PLX	C26-C27-C28-C29
52	m	201	CDL	C58-C59-C60-C61
52	r	504	CDL	C39-C40-C41-C42
47	Q	501	PEE	C1-C2-C3-O3
47	W	201	PEE	C1-C2-C3-O3
47	r	501	PEE	C1-C2-C3-O3
48	N	201	PLX	C3-C4-C5-O8
48	r	502	PLX	C3-C4-C5-O8
52	J	404	CDL	CB3-CB4-CB6-OB8
52	N	202	CDL	CA3-CA4-CA6-OA8
52	i	401	CDL	CB3-CB4-CB6-OB8
47	r	501	PEE	C17-C18-C19-C20
52	l	702	CDL	C73-C74-C75-C76
52	m	201	CDL	C31-C32-C33-C34
49	E	201	8Q1	C29-C32-C34-N36
52	l	702	CDL	C31-C32-C33-C34
48	n	101	PLX	C9-C10-C11-C12
52	m	201	CDL	C82-C83-C84-C85
47	j	201	PEE	C1-O3P-P-O4P
48	J	403	PLX	C5-C4-O6-C6

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Mol	Chain	Res	Type	Atoms
48	r	502	PLX	C3-C4-O6-C6
52	V	201	CDL	CB3-OB5-PB2-OB2
52	V	202	CDL	CA3-OA5-PA1-OA2
52	a	201	CDL	CA2-OA2-PA1-OA5
48	n	101	PLX	C11-C12-C13-C14
52	J	404	CDL	C40-C41-C42-C43
48	N	201	PLX	O9-C24-C25-C26
48	r	503	PLX	O7-C6-C7-C8
48	r	503	PLX	O9-C24-C25-C26
47	Q	501	PEE	O3P-C1-C2-O2
47	b	201	PEE	O3P-C1-C2-O2
48	N	201	PLX	O4-C3-C4-O6
48	r	502	PLX	O4-C3-C4-O6
52	V	201	CDL	OA5-CA3-CA4-OA6
52	u	201	CDL	OB5-CB3-CB4-OB6
47	j	202	PEE	O5-C30-O3-C3
47	C	302	PEE	O2-C2-C3-O3
47	W	201	PEE	O2-C2-C3-O3
47	r	501	PEE	O2-C2-C3-O3
48	N	201	PLX	O6-C4-C5-O8
48	n	101	PLX	O6-C4-C5-O8
52	m	201	CDL	OB6-CB4-CB6-OB8
48	r	503	PLX	C36-C37-C38-C39
51	J	402	UQ	C9-C11-C12-C13
48	r	502	PLX	C16-C17-C18-C19
52	V	202	CDL	C31-C32-C33-C34
52	u	201	CDL	C72-C73-C74-C75
52	l	703	CDL	OB7-CB5-OB6-CB4
52	r	504	CDL	C13-C14-C15-C16
52	N	202	CDL	OA9-CA7-OA8-CA6
47	B	303	PEE	C21-C22-C23-C24
52	J	404	CDL	C84-C85-C86-C87
52	m	201	CDL	C64-C65-C66-C67
47	W	201	PEE	C11-C10-O2-C2
52	l	703	CDL	C56-C57-C58-C59
47	j	202	PEE	C10-C11-C12-C13
47	r	501	PEE	C10-C11-C12-C13
47	W	201	PEE	C20-C21-C22-C23
52	l	702	CDL	C54-C55-C56-C57
48	j	203	PLX	O6-C6-C7-C8
48	r	502	PLX	O4-C3-C4-C5
47	C	302	PEE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
48	C	303	PLX	C9-C10-C11-C12
47	B	303	PEE	C11-C12-C13-C14
52	l	702	CDL	C18-C19-C20-C21
52	l	703	CDL	CA6-CA4-OA6-CA5
52	m	201	CDL	CA6-CA4-OA6-CA5
47	W	201	PEE	O4-C10-O2-C2
47	j	202	PEE	C13-C14-C15-C16
47	l	704	PEE	C41-C42-C43-C44
48	n	101	PLX	C12-C13-C14-C15
47	B	303	PEE	C32-C33-C34-C35
52	V	202	CDL	C54-C55-C56-C57
52	l	703	CDL	C79-C80-C81-C82
52	i	401	CDL	C71-C72-C73-C74
52	l	703	CDL	C71-C72-C73-C74
47	W	201	PEE	C19-C20-C21-C22
47	l	704	PEE	C1-C2-C3-O3
48	J	403	PLX	C3-C4-C5-O8
48	r	503	PLX	C3-C4-C5-O8
52	r	504	CDL	C15-C16-C17-C18
52	r	504	CDL	C51-C52-C53-C54
48	r	503	PLX	O4-C3-C4-O6
52	V	202	CDL	C32-C31-CA7-OA8
52	V	201	CDL	C21-C22-C23-C24
52	l	703	CDL	C31-CA7-OA8-CA6
47	r	501	PEE	C38-C39-C40-C41
52	V	202	CDL	CB2-C1-CA2-OA2
52	m	201	CDL	OB9-CB7-OB8-CB6
52	l	702	CDL	C84-C85-C86-C87
47	Q	501	PEE	O2-C2-C3-O3
47	b	201	PEE	O2-C2-C3-O3
48	r	502	PLX	O6-C4-C5-O8
52	V	201	CDL	OB6-CB4-CB6-OB8
52	m	201	CDL	OA6-CA4-CA6-OA8
48	r	503	PLX	C7-C8-C9-C10
48	j	203	PLX	C32-C33-C34-C35
52	V	202	CDL	C71-C72-C73-C74
52	m	201	CDL	C52-C53-C54-C55
52	a	201	CDL	C13-C14-C15-C16
47	Q	501	PEE	C11-C12-C13-C14
52	m	201	CDL	C15-C16-C17-C18
47	Q	501	PEE	C39-C40-C41-C42
47	j	202	PEE	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
47	C	302	PEE	C1-O3P-P-O4P
48	r	503	PLX	C3-O4-P1-O1
50	J	401	NDP	O4D-C1D-N1N-C6N
52	V	202	CDL	CB2-OB2-PB2-OB5
52	a	201	CDL	C22-C23-C24-C25
52	m	201	CDL	C17-C18-C19-C20
52	u	201	CDL	C71-C72-C73-C74
47	B	303	PEE	C4-O4P-P-O1P
47	C	302	PEE	C1-O3P-P-O2P
47	C	302	PEE	C4-O4P-P-O2P
47	Q	501	PEE	C4-O4P-P-O2P
47	W	201	PEE	C4-O4P-P-O2P
47	W	201	PEE	C4-O4P-P-O1P
47	j	201	PEE	C1-O3P-P-O2P
47	r	501	PEE	C1-O3P-P-O2P
48	J	403	PLX	C3-O4-P1-O2
48	J	403	PLX	C3-O4-P1-O3
48	J	403	PLX	C2-O1-P1-O3
48	N	201	PLX	C3-O4-P1-O3
48	j	203	PLX	C2-O1-P1-O3
48	n	101	PLX	C3-O4-P1-O2
48	n	101	PLX	C2-O1-P1-O3
48	r	503	PLX	C3-O4-P1-O2
48	r	503	PLX	C3-O4-P1-O3
52	J	404	CDL	CA3-OA5-PA1-OA3
52	J	404	CDL	CA3-OA5-PA1-OA4
52	N	202	CDL	CB3-OB5-PB2-OB4
52	V	201	CDL	CA3-OA5-PA1-OA3
52	V	201	CDL	CB2-OB2-PB2-OB4
52	V	201	CDL	CB3-OB5-PB2-OB3
52	V	202	CDL	CB2-OB2-PB2-OB3
52	V	202	CDL	CB2-OB2-PB2-OB4
52	V	202	CDL	CB3-OB5-PB2-OB3
52	V	202	CDL	CB3-OB5-PB2-OB4
52	a	201	CDL	CB2-OB2-PB2-OB4
52	i	401	CDL	CA3-OA5-PA1-OA3
52	l	702	CDL	CA2-OA2-PA1-OA3
52	l	702	CDL	CB3-OB5-PB2-OB4
52	m	201	CDL	CA3-OA5-PA1-OA4
52	r	504	CDL	CA2-OA2-PA1-OA4
52	r	504	CDL	CB3-OB5-PB2-OB4
52	u	201	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
47	b	201	PEE	O3P-C1-C2-C3
48	N	201	PLX	O4-C3-C4-C5
48	r	503	PLX	O4-C3-C4-C5
52	V	201	CDL	OA5-CA3-CA4-CA6
52	l	702	CDL	OB5-CB3-CB4-CB6
52	u	201	CDL	OB5-CB3-CB4-CB6
48	g	201	PLX	C33-C34-C35-C36
52	r	504	CDL	C54-C55-C56-C57
52	a	201	CDL	C43-C44-C45-C46
47	B	303	PEE	C5-C4-O4P-P
47	W	201	PEE	C5-C4-O4P-P
48	g	201	PLX	C25-C24-O8-C5
48	j	203	PLX	C25-C24-O8-C5
48	N	201	PLX	C13-C14-C15-C16
52	l	703	CDL	OA9-CA7-OA8-CA6
48	J	403	PLX	C26-C27-C28-C29
47	l	704	PEE	C39-C40-C41-C42
48	C	303	PLX	C33-C34-C35-C36
48	N	201	PLX	C26-C27-C28-C29
52	i	401	CDL	C35-C36-C37-C38
52	V	201	CDL	CB2-C1-CA2-OA2
47	b	201	PEE	C34-C35-C36-C37
47	l	701	PEE	O3P-C1-C2-O2
52	a	201	CDL	OA5-CA3-CA4-OA6
52	l	703	CDL	OB5-CB3-CB4-OB6
52	l	703	CDL	CB5-C51-C52-C53
47	B	303	PEE	C38-C39-C40-C41
52	J	404	CDL	O1-C1-CB2-OB2
52	V	201	CDL	O1-C1-CA2-OA2
52	V	201	CDL	C40-C41-C42-C43
52	r	504	CDL	CB5-C51-C52-C53
48	C	303	PLX	N1-C1-C2-O1
48	J	403	PLX	N1-C1-C2-O1
48	r	503	PLX	O6-C4-C5-O8
52	N	202	CDL	OA6-CA4-CA6-OA8
47	C	302	PEE	C12-C13-C14-C15
52	i	401	CDL	C75-C76-C77-C78
52	l	703	CDL	C77-C78-C79-C80
48	J	403	PLX	C12-C13-C14-C15
48	J	403	PLX	C10-C11-C12-C13
52	V	201	CDL	CA4-CA3-OA5-PA1
52	m	201	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
52	V	201	CDL	C34-C35-C36-C37
47	B	303	PEE	C31-C30-O3-C3
47	W	201	PEE	C23-C24-C25-C26
48	g	201	PLX	O6-C6-C7-C8
52	V	202	CDL	C63-C64-C65-C66
51	s	501	UQ	C9-C11-C12-C13
47	B	303	PEE	O5-C30-O3-C3
48	g	201	PLX	O7-C6-C7-C8
47	b	201	PEE	C14-C15-C16-C17
47	b	201	PEE	C30-C31-C32-C33
47	W	201	PEE	C22-C23-C24-C25
47	Q	501	PEE	C17-C18-C19-C20
52	V	202	CDL	C57-C58-C59-C60
52	a	201	CDL	C84-C85-C86-C87
52	i	401	CDL	C73-C74-C75-C76
52	m	201	CDL	C42-C43-C44-C45
48	g	201	PLX	C36-C37-C38-C39
52	l	702	CDL	C22-C23-C24-C25
47	r	501	PEE	C33-C34-C35-C36
48	j	203	PLX	C30-C31-C32-C33
52	V	201	CDL	CA6-CA4-OA6-CA5
47	l	701	PEE	O3P-C1-C2-C3
52	a	201	CDL	OA5-CA3-CA4-CA6
52	l	703	CDL	OA7-CA5-OA6-CA4
52	V	202	CDL	C58-C59-C60-C61
47	C	302	PEE	C34-C35-C36-C37
47	l	701	PEE	C2-C1-O3P-P
47	B	303	PEE	C22-C23-C24-C25
47	j	201	PEE	O3P-C1-C2-O2
52	V	202	CDL	OB5-CB3-CB4-OB6
52	a	201	CDL	OB5-CB3-CB4-OB6
51	s	501	UQ	C52-C53-C54-C56
48	C	303	PLX	C11-C12-C13-C14
52	a	201	CDL	C12-C13-C14-C15
52	u	201	CDL	C57-C58-C59-C60
47	j	201	PEE	C12-C13-C14-C15
52	r	504	CDL	C20-C21-C22-C23
52	l	703	CDL	C11-CA5-OA6-CA4
47	b	201	PEE	C16-C17-C18-C19
48	J	403	PLX	O6-C4-C5-O8
48	j	203	PLX	O6-C4-C5-O8
48	C	303	PLX	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
52	V	201	CDL	C22-C23-C24-C25
47	b	201	PEE	C4-O4P-P-O3P
47	r	501	PEE	C1-O3P-P-O4P
48	C	303	PLX	C3-O4-P1-O1
52	V	202	CDL	CA2-OA2-PA1-OA5
48	n	101	PLX	C3-C4-C5-O8
52	V	202	CDL	CA3-CA4-CA6-OA8
48	g	201	PLX	C15-C16-C17-C18
52	a	201	CDL	C18-C19-C20-C21
51	J	402	UQ	C4-C3-O3-CM3
48	j	203	PLX	C27-C28-C29-C30
47	l	704	PEE	C42-C43-C44-C45
52	l	703	CDL	C82-C83-C84-C85
48	N	201	PLX	C4-C3-O4-P1
48	J	403	PLX	C35-C36-C37-C38
47	b	201	PEE	C18-C19-C20-C21
47	j	201	PEE	C36-C37-C38-C39
48	j	203	PLX	C24-C25-C26-C27
52	m	201	CDL	CB2-C1-CA2-OA2
52	u	201	CDL	CA2-C1-CB2-OB2
47	B	303	PEE	C39-C40-C41-C42
47	Q	501	PEE	C15-C16-C17-C18
52	J	404	CDL	C72-C71-CB7-OB8
52	m	201	CDL	OB5-CB3-CB4-OB6
52	a	201	CDL	C74-C75-C76-C77
52	l	702	CDL	C42-C43-C44-C45
47	C	302	PEE	C41-C42-C43-C44
49	E	201	8Q1	C9-C10-C11-C12
52	N	202	CDL	O1-C1-CA2-OA2
47	l	701	PEE	C39-C40-C41-C42
48	N	201	PLX	O8-C24-C25-C26
51	s	501	UQ	C4-C3-O3-CM3
48	j	203	PLX	C15-C16-C17-C18
52	l	703	CDL	C17-C18-C19-C20
52	N	202	CDL	CA2-C1-CB2-OB2
52	V	201	CDL	CA3-CA4-CA6-OA8
52	a	201	CDL	C64-C65-C66-C67
48	r	503	PLX	C16-C17-C18-C19
52	a	201	CDL	C55-C56-C57-C58
52	i	401	CDL	CA6-CA4-OA6-CA5
47	Q	501	PEE	C10-C11-C12-C13
47	C	302	PEE	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
47	j	201	PEE	C44-C45-C46-C47
48	j	203	PLX	C3-C4-O6-C6
48	C	303	PLX	O4-C3-C4-O6
48	r	502	PLX	C18-C19-C20-C21
52	V	202	CDL	OB5-CB3-CB4-CB6
47	C	302	PEE	C18-C19-C20-C21
48	J	403	PLX	C29-C30-C31-C32
48	g	201	PLX	C18-C19-C20-C21
52	J	404	CDL	C15-C16-C17-C18
47	j	202	PEE	C32-C33-C34-C35
52	l	703	CDL	OB6-CB4-CB6-OB8
52	r	504	CDL	OA6-CA4-CA6-OA8
52	l	702	CDL	C76-C77-C78-C79
52	u	201	CDL	C75-C76-C77-C78
52	V	202	CDL	C23-C24-C25-C26
47	B	303	PEE	C37-C38-C39-C40
47	j	201	PEE	C41-C42-C43-C44
52	l	703	CDL	CB2-C1-CA2-OA2
48	N	201	PLX	C16-C17-C18-C19
52	l	702	CDL	C51-C52-C53-C54
51	s	501	UQ	C12-C11-C9-C8
52	V	201	CDL	C64-C65-C66-C67
47	j	201	PEE	C16-C17-C18-C19
51	s	501	UQ	C40-C39-C41-C42
47	l	704	PEE	C12-C13-C14-C15
47	C	302	PEE	C36-C37-C38-C39
47	W	201	PEE	C16-C17-C18-C19
47	B	303	PEE	O3P-C1-C2-O2
47	j	202	PEE	O3P-C1-C2-O2
47	C	302	PEE	C30-C31-C32-C33
52	V	201	CDL	C60-C61-C62-C63
52	l	702	CDL	C12-C11-CA5-OA6
52	V	202	CDL	C44-C45-C46-C47
52	i	401	CDL	OB9-CB7-OB8-CB6
48	r	502	PLX	O8-C24-C25-C26
49	X	201	8Q1	C1-C6-C7-C8
52	J	404	CDL	C74-C75-C76-C77
52	r	504	CDL	C17-C18-C19-C20
52	a	201	CDL	C12-C11-CA5-OA6
52	l	702	CDL	C72-C71-CB7-OB8
52	m	201	CDL	C77-C78-C79-C80
47	B	303	PEE	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
47	r	501	PEE	C16-C17-C18-C19
52	r	504	CDL	C21-C22-C23-C24
47	j	202	PEE	O3-C30-C31-C32
47	b	201	PEE	C2-C3-O3-C30
48	r	502	PLX	C26-C27-C28-C29
47	B	303	PEE	C34-C35-C36-C37
47	j	202	PEE	C14-C15-C16-C17
48	J	403	PLX	C36-C37-C38-C39
52	m	201	CDL	C12-C11-CA5-OA6
52	i	401	CDL	C15-C16-C17-C18
52	J	404	CDL	C12-C11-CA5-OA6
52	a	201	CDL	C32-C31-CA7-OA8
52	a	201	CDL	C39-C40-C41-C42
48	j	203	PLX	C7-C6-O6-C4
47	Q	501	PEE	C37-C38-C39-C40
48	j	203	PLX	C18-C19-C20-C21
52	V	202	CDL	C22-C23-C24-C25
48	C	303	PLX	C6-C7-C8-C9
52	l	703	CDL	C58-C59-C60-C61
47	b	201	PEE	C38-C39-C40-C41
51	J	402	UQ	C12-C13-C14-C16
52	N	202	CDL	C51-C52-C53-C54
52	l	703	CDL	C55-C56-C57-C58
47	B	303	PEE	O3P-C1-C2-C3
47	j	201	PEE	O3P-C1-C2-C3
52	i	401	CDL	OA5-CA3-CA4-CA6
47	j	201	PEE	C24-C25-C26-C27
47	j	201	PEE	O2-C10-C11-C12
47	l	701	PEE	O2-C10-C11-C12
52	i	401	CDL	C12-C11-CA5-OA6
52	r	504	CDL	C12-C13-C14-C15
48	C	303	PLX	O6-C4-C5-O8
52	N	202	CDL	OB6-CB4-CB6-OB8
48	g	201	PLX	C6-C7-C8-C9
48	g	201	PLX	O9-C24-C25-C26
50	J	401	NDP	C5B-O5B-PA-O3
52	i	401	CDL	C71-CB7-OB8-CB6
52	a	201	CDL	C16-C17-C18-C19
52	l	703	CDL	C59-C60-C61-C62
47	C	302	PEE	C38-C39-C40-C41
47	j	202	PEE	C16-C17-C18-C19
47	j	201	PEE	O3-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
52	V	201	CDL	C52-C51-CB5-OB6
52	r	504	CDL	C72-C71-CB7-OB8
47	j	202	PEE	O5-C30-C31-C32
48	C	303	PLX	C35-C36-C37-C38
51	s	501	UQ	C2-C3-O3-CM3
56	w	401	ADP	PB-O3A-PA-O2A
47	C	302	PEE	C16-C17-C18-C19
47	j	202	PEE	C30-C31-C32-C33
52	a	201	CDL	C12-C11-CA5-OA7
47	Q	501	PEE	C40-C41-C42-C43
52	r	504	CDL	C44-C45-C46-C47
52	a	201	CDL	C32-C31-CA7-OA9
52	J	404	CDL	C12-C11-CA5-OA7
52	l	702	CDL	C72-C71-CB7-OB9
48	j	203	PLX	C10-C11-C12-C13
52	V	201	CDL	CB3-CB4-CB6-OB8
52	V	201	CDL	CA3-OA5-PA1-OA2
52	V	202	CDL	O1-C1-CA2-OA2
52	m	201	CDL	C12-C11-CA5-OA7
49	E	201	8Q1	C11-C12-C13-C14
47	b	201	PEE	C24-C25-C26-C27
47	C	302	PEE	C1-O3P-P-O1P
47	b	201	PEE	C1-O3P-P-O1P
50	J	401	NDP	C2N-C3N-C7N-N7N
52	i	401	CDL	CB3-OB5-PB2-OB4
52	m	201	CDL	CB2-OB2-PB2-OB4
47	l	701	PEE	O4-C10-C11-C12
48	n	101	PLX	O4-C3-C4-C5
47	r	501	PEE	C31-C32-C33-C34
48	j	203	PLX	C35-C36-C37-C38
48	C	303	PLX	C25-C26-C27-C28
52	r	504	CDL	C82-C83-C84-C85
47	j	201	PEE	O4-C10-C11-C12
52	m	201	CDL	C74-C75-C76-C77
52	V	202	CDL	C32-C31-CA7-OA9
47	r	501	PEE	C42-C43-C44-C45
48	N	201	PLX	C1-C2-O1-P1
48	N	201	PLX	C25-C24-O8-C5
49	E	201	8Q1	C29-C32-C34-O35
52	i	401	CDL	CA3-CA4-OA6-CA5
47	j	202	PEE	C20-C21-C22-C23
52	l	703	CDL	C57-C58-C59-C60

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Mol	Chain	Res	Type	Atoms
52	J	404	CDL	C38-C39-C40-C41
47	l	704	PEE	C31-C32-C33-C34
52	i	401	CDL	CA5-C11-C12-C13
52	i	401	CDL	C12-C11-CA5-OA7
47	l	704	PEE	C24-C25-C26-C27
52	N	202	CDL	C52-C51-CB5-OB6
52	a	201	CDL	C82-C83-C84-C85
48	J	403	PLX	C6-C7-C8-C9
48	J	403	PLX	O4-C3-C4-O6
52	i	401	CDL	OA5-CA3-CA4-OA6
47	j	201	PEE	O5-C30-C31-C32
47	l	701	PEE	O3-C30-C31-C32
52	J	404	CDL	C57-C58-C59-C60
52	l	702	CDL	C44-C45-C46-C47
52	V	202	CDL	C55-C56-C57-C58
48	J	403	PLX	C17-C18-C19-C20
52	m	201	CDL	C43-C44-C45-C46
52	r	504	CDL	C32-C31-CA7-OA8

There are no ring outliers.

36 monomers are involved in 313 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	J	404	CDL	11	0
52	l	703	CDL	12	0
47	b	201	PEE	19	0
52	l	702	CDL	19	0
56	w	401	ADP	4	0
52	a	201	CDL	18	0
48	C	303	PLX	19	0
47	r	501	PEE	8	0
47	Q	501	PEE	18	0
52	i	401	CDL	17	0
51	s	501	UQ	36	0
49	X	201	8Q1	12	0
53	M	803	FES	1	0
45	M	802	SF4	5	0
47	B	303	PEE	7	0
51	J	402	UQ	10	0
48	r	502	PLX	6	0
47	W	201	PEE	6	0
47	C	302	PEE	3	0

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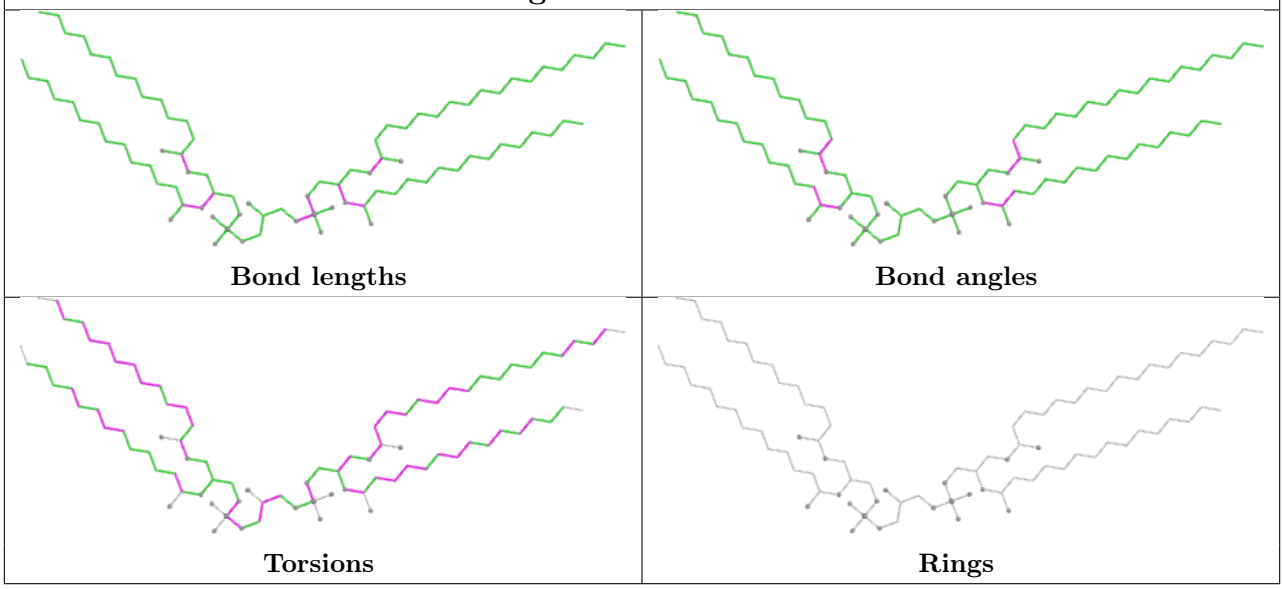
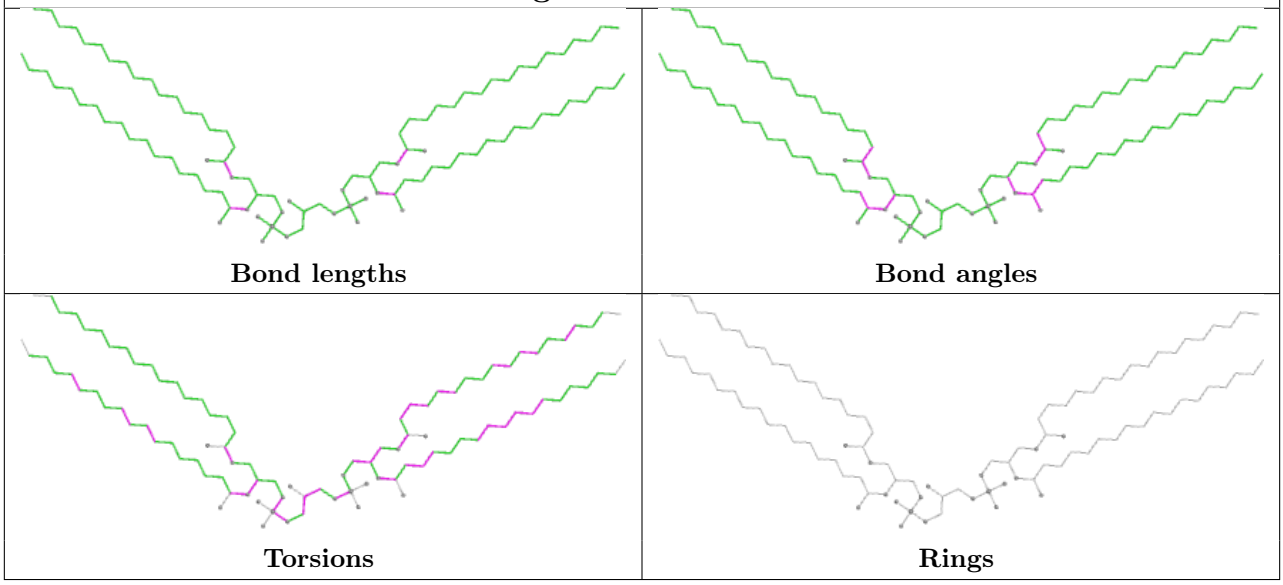
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	l	704	PEE	7	0
45	A	501	SF4	2	0
48	n	101	PLX	1	0
52	r	504	CDL	7	0
52	u	201	CDL	14	0
46	A	502	FMN	14	0
52	V	201	CDL	3	0
48	j	203	PLX	2	0
49	E	201	8Q1	1	0
47	j	201	PEE	7	0
47	j	202	PEE	7	0
52	N	202	CDL	11	0
48	g	201	PLX	5	0
48	r	503	PLX	4	0
52	V	202	CDL	4	0
52	m	201	CDL	11	0
47	l	701	PEE	7	0

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

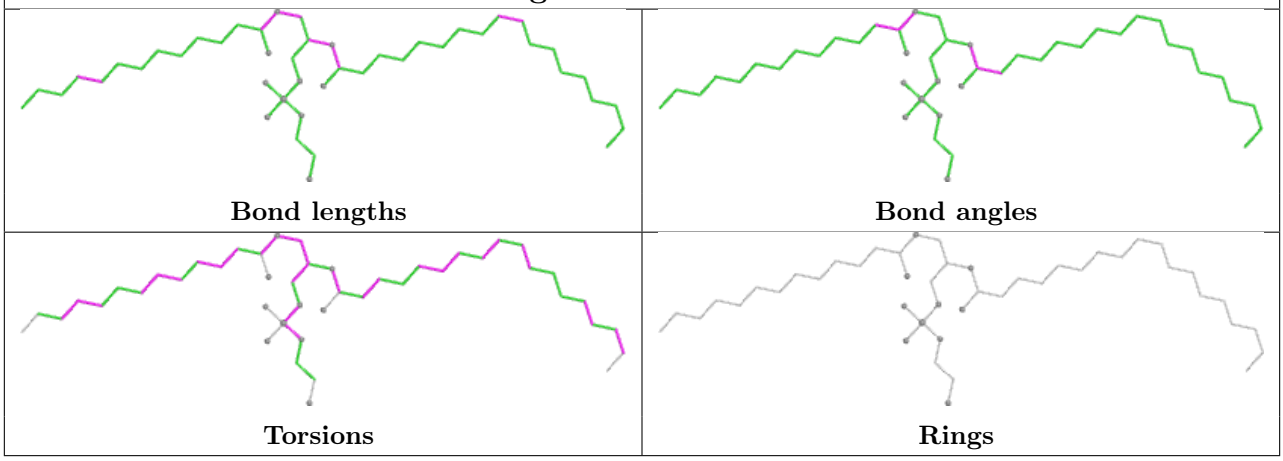
Ligand CDL J 404



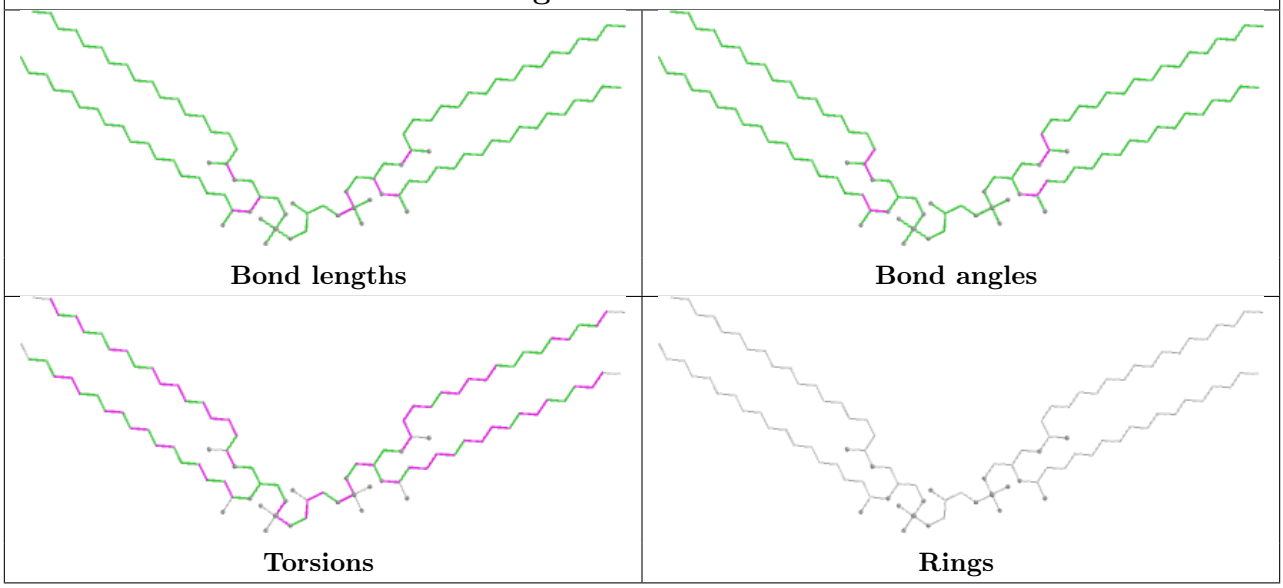
Ligand CDL l 703



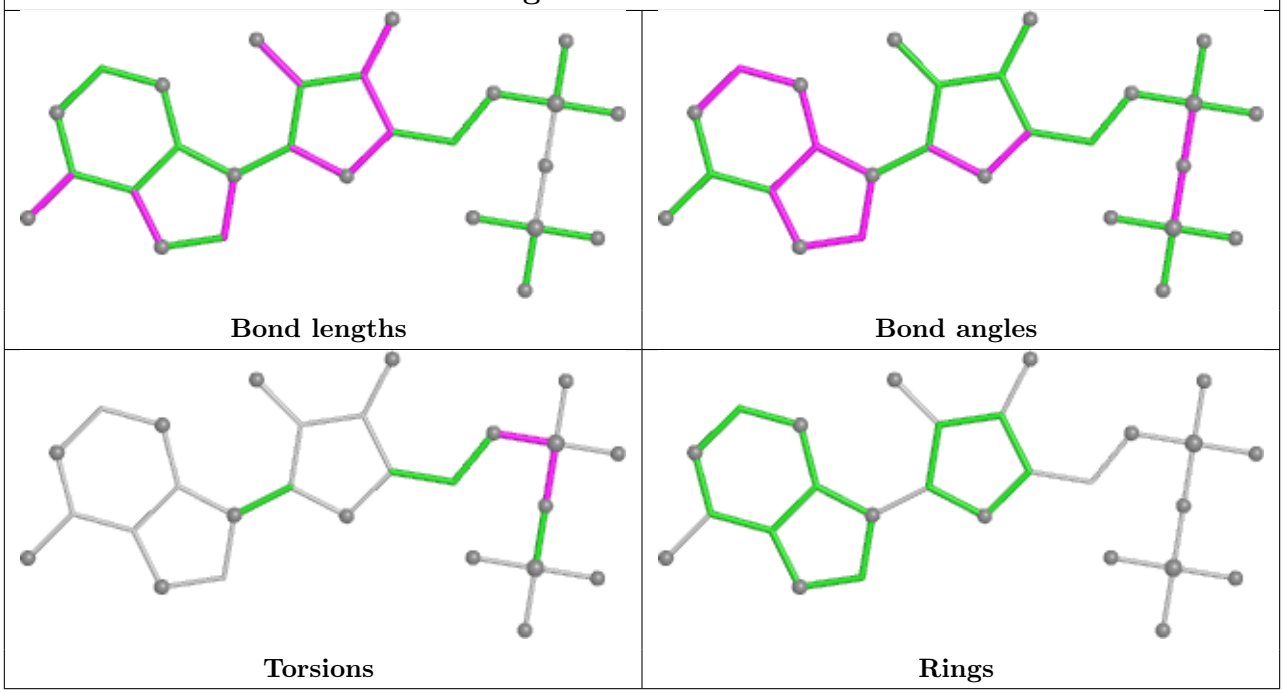
Ligand PEE b 201



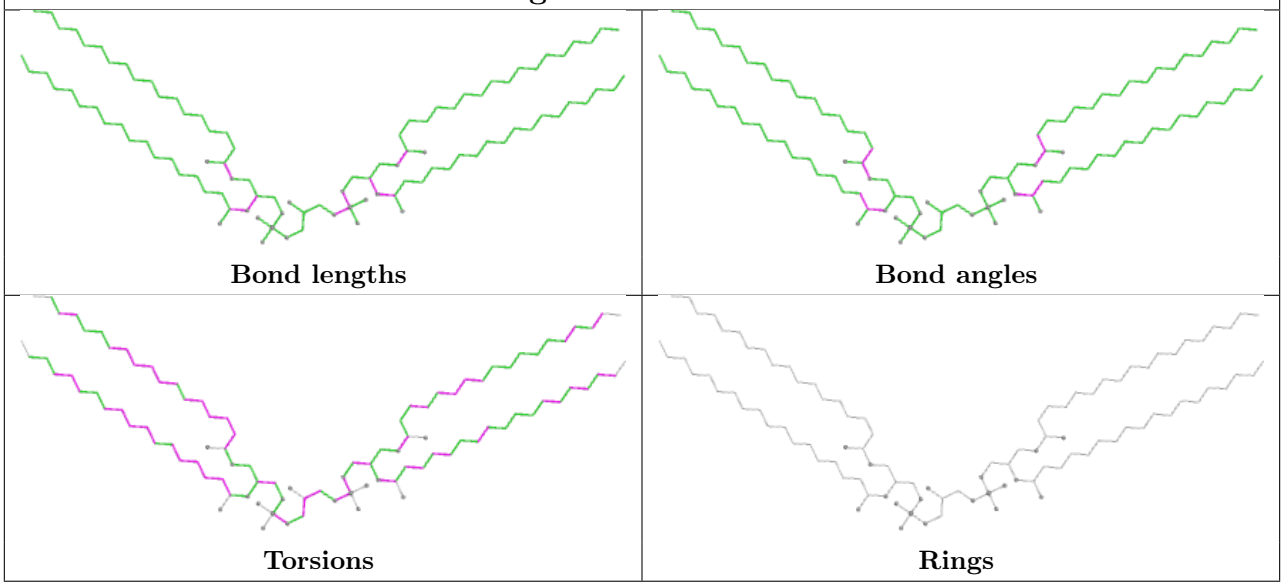
Ligand CDL l 702



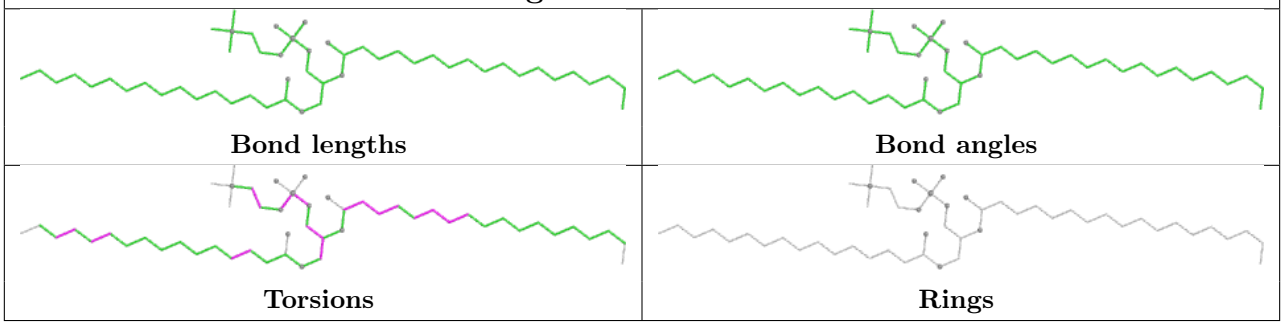
Ligand ADP w 401



Ligand CDL a 201



Ligand PLX C 303



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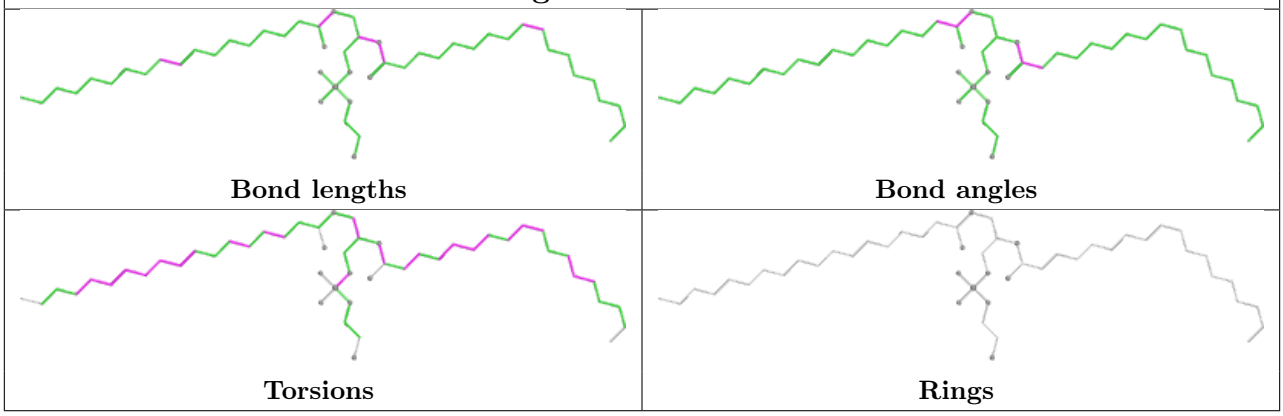

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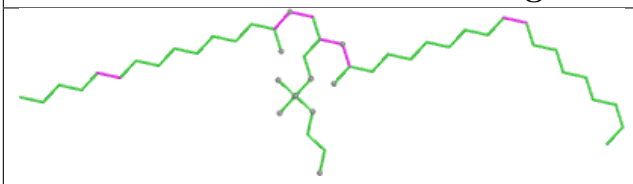
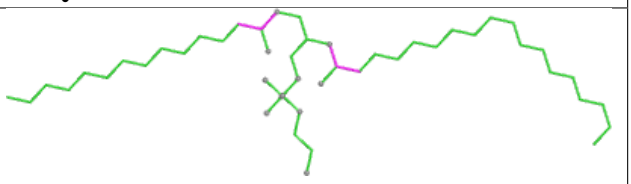
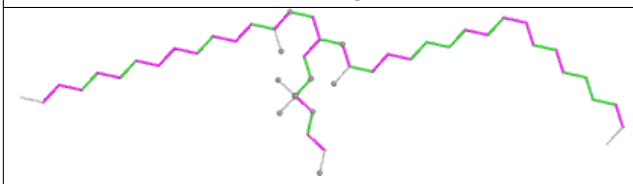


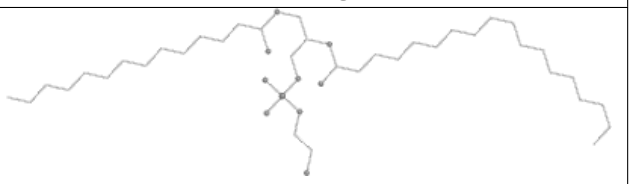
Bond lengths



Bond angles

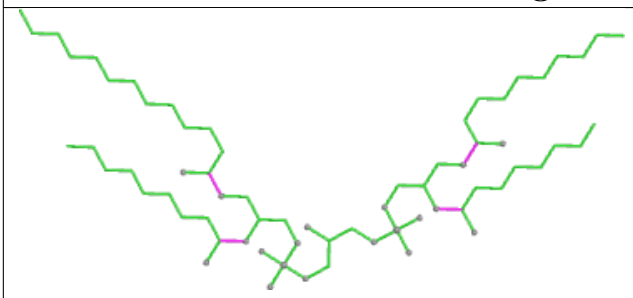


Torsions



Rings

Ligand CDL i 401



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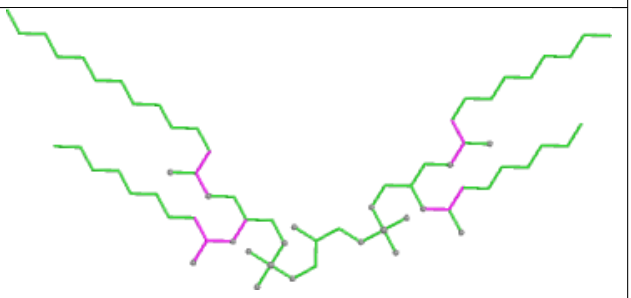
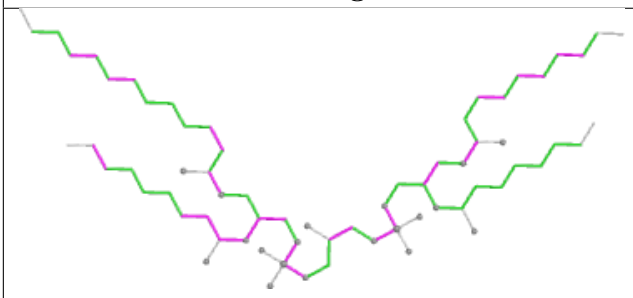
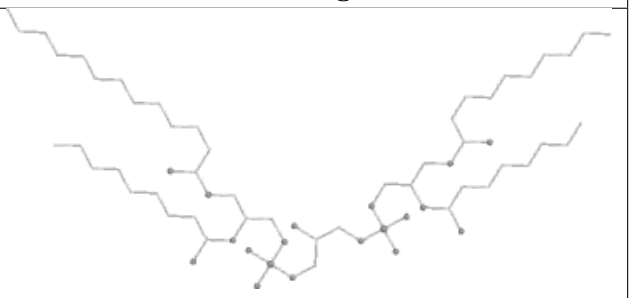


Bond angles

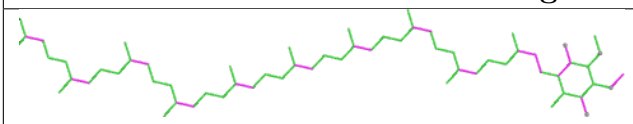


Torsions



Rings

Ligand UQ s 501



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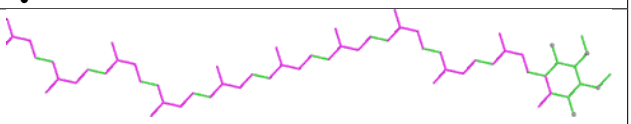
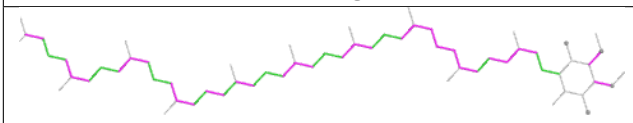
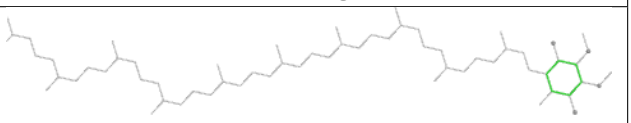


Bond angles

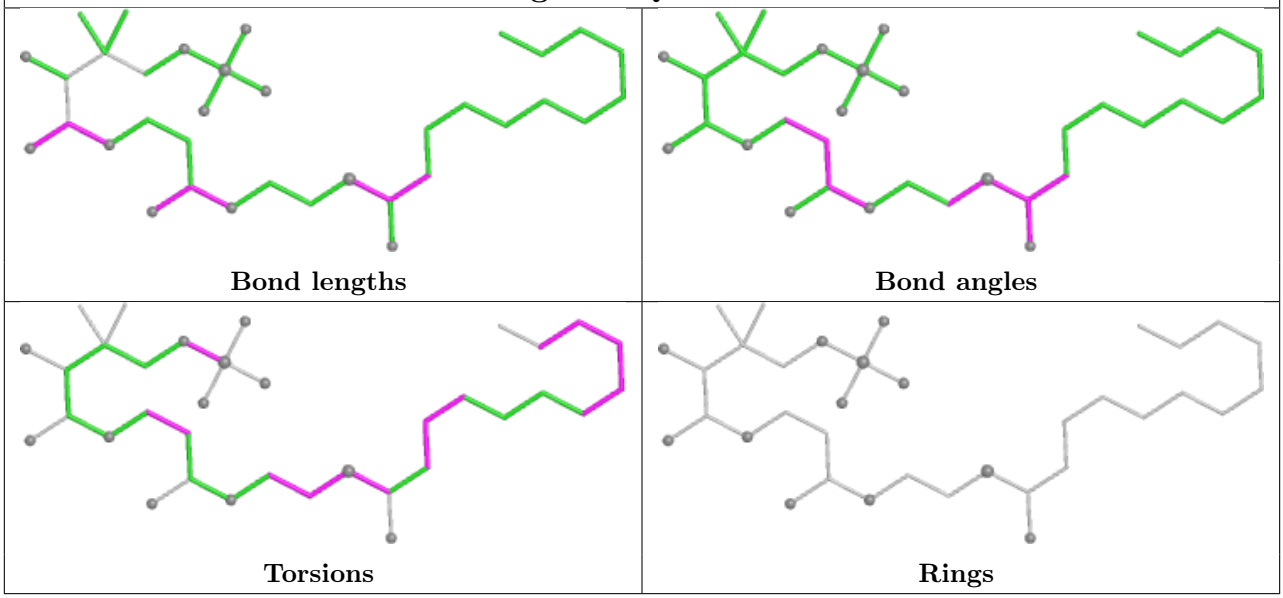


Torsions

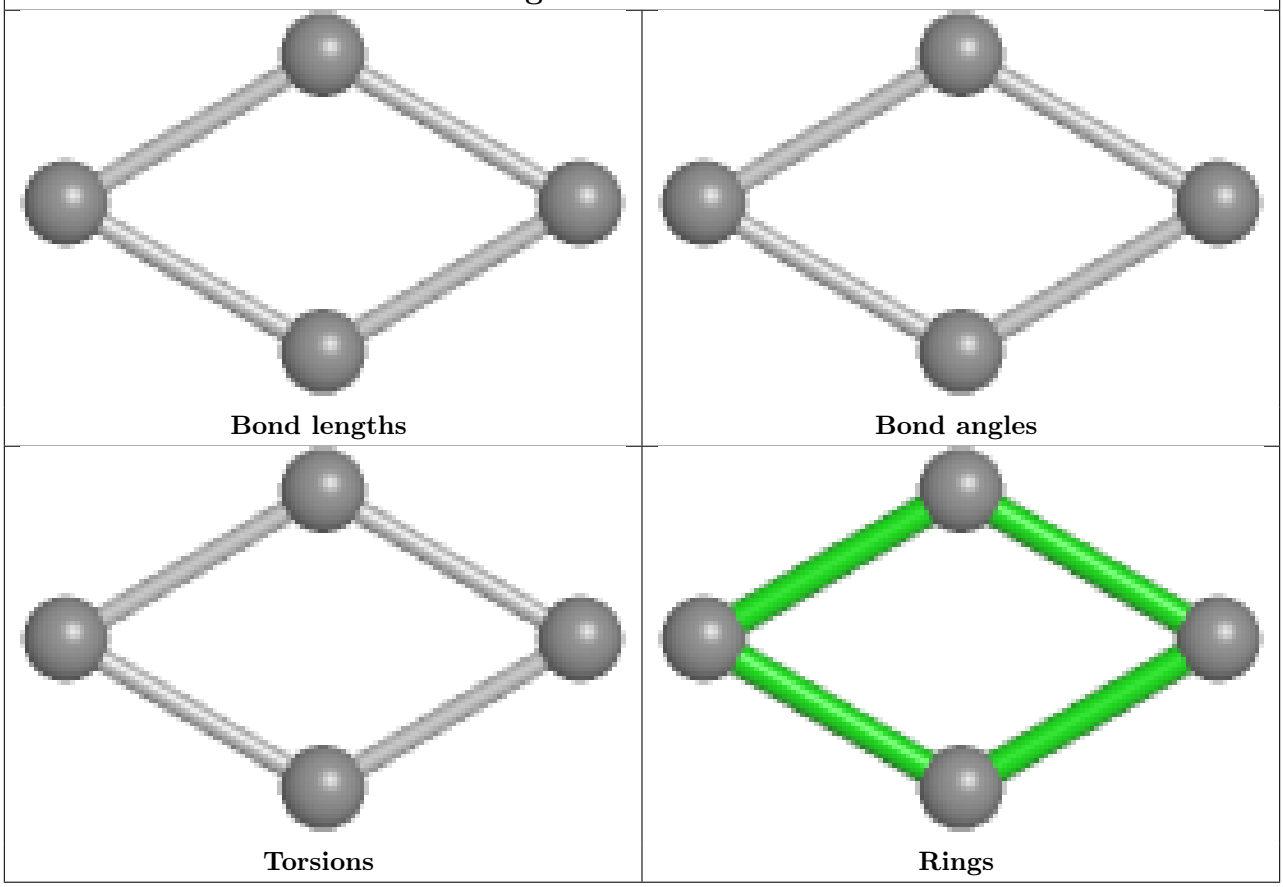


Rings

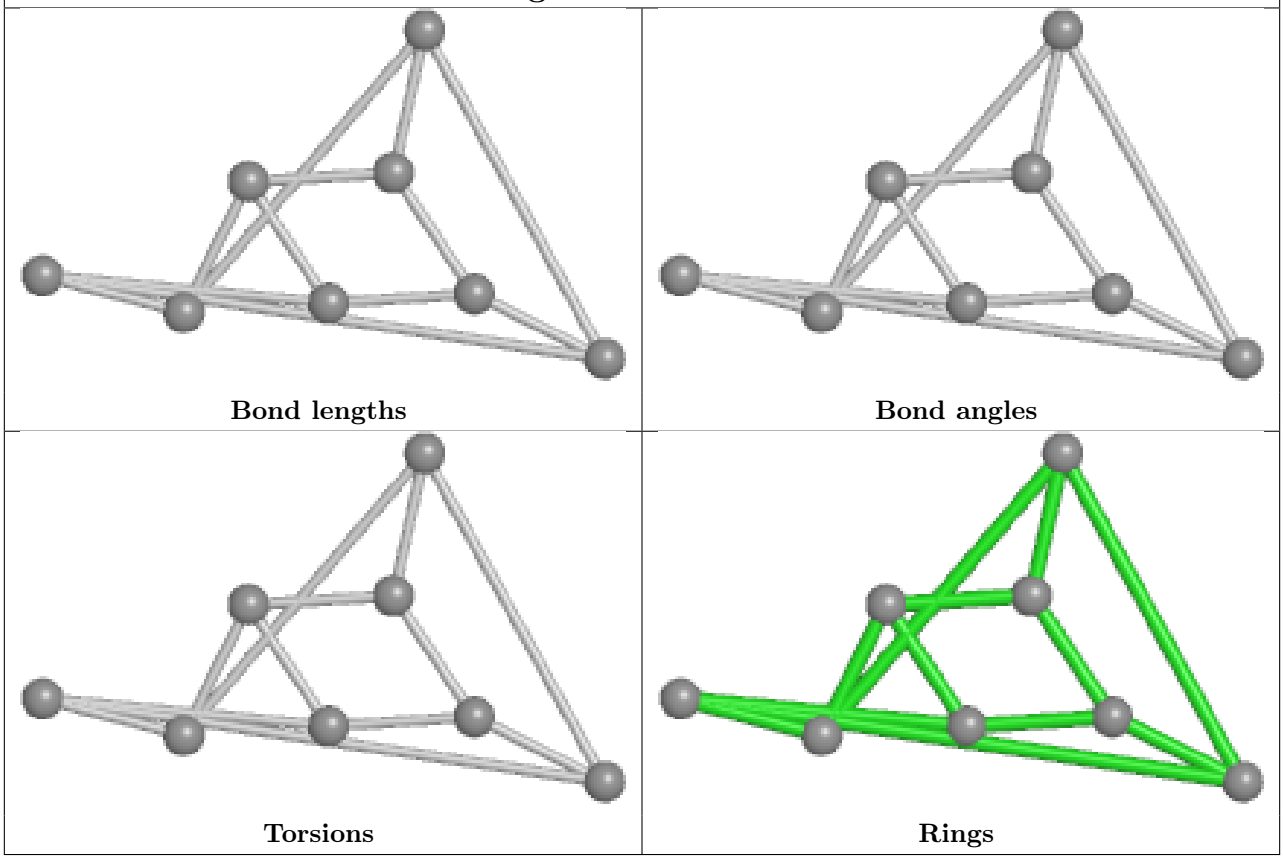
Ligand 8Q1 X 201



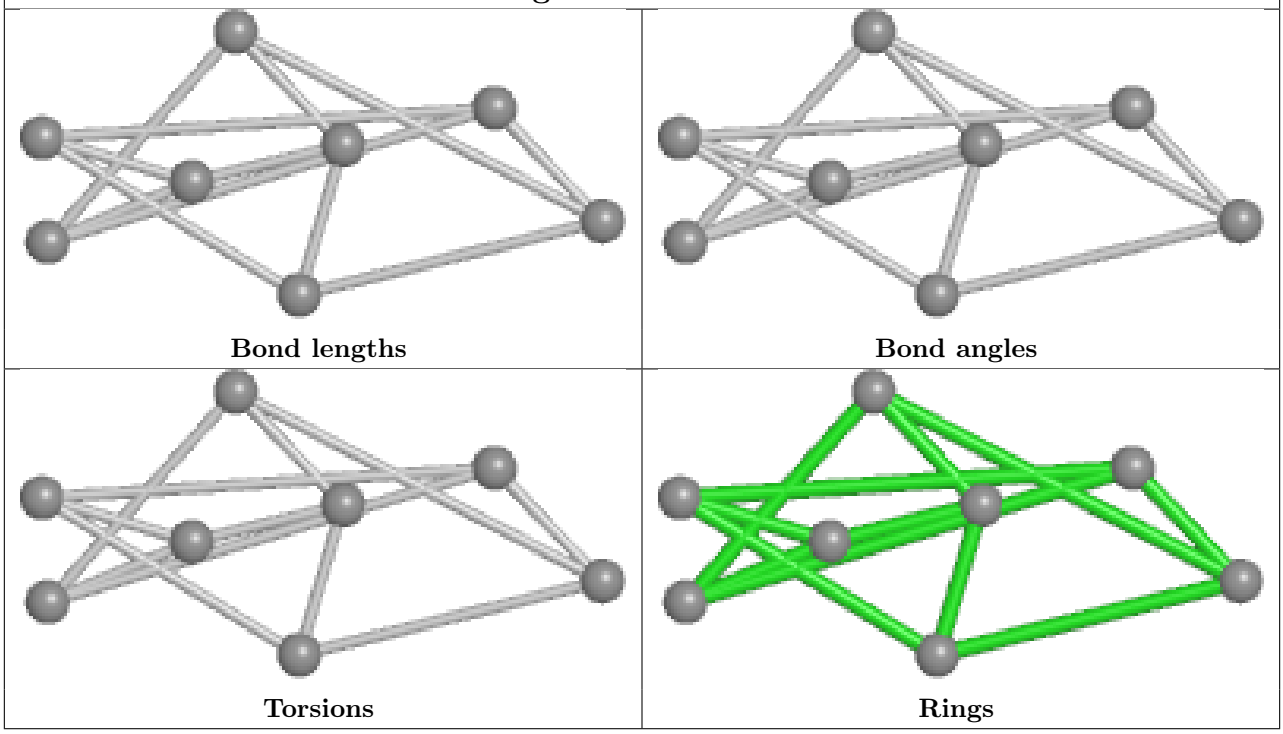
Ligand FES M 803



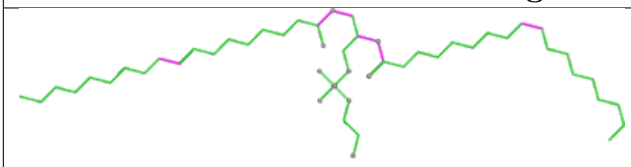
Ligand SF4 M 802



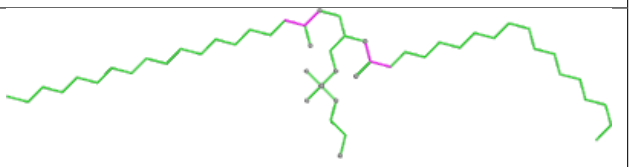
Ligand SF4 B 301



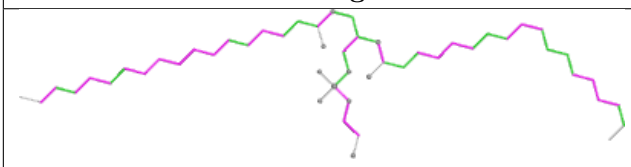
Ligand PEE B 303



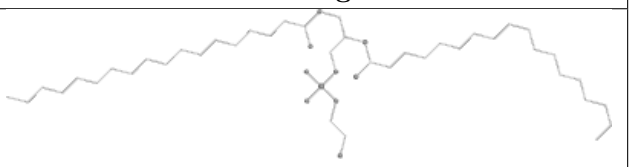
Bond lengths



Bond angles

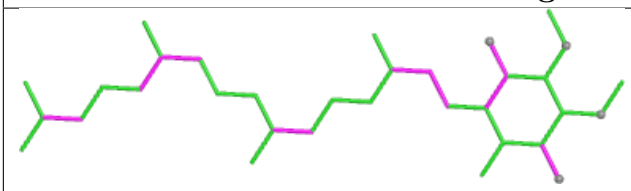


Torsions

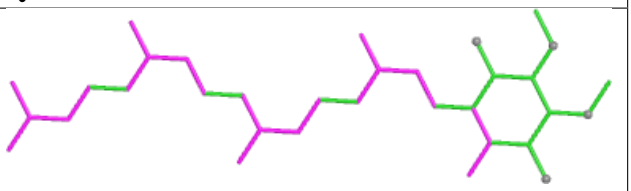


Rings

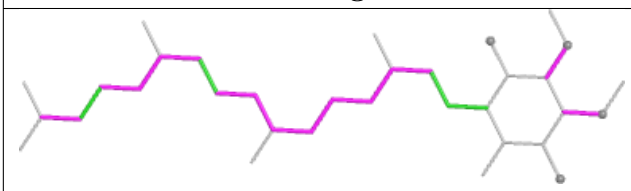
Ligand UQ J 402



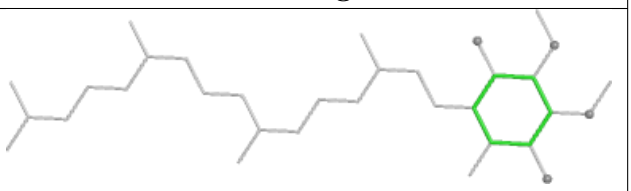
Bond lengths



Bond angles

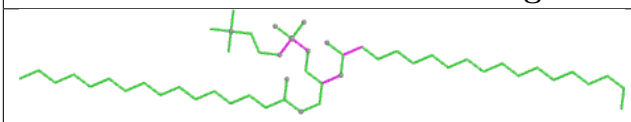


Torsions



Rings

Ligand PLX N 201



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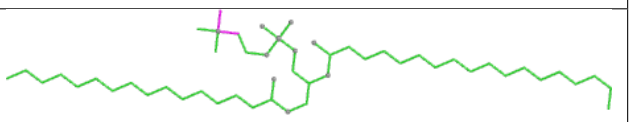
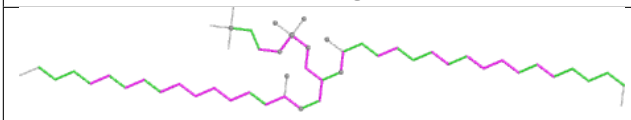
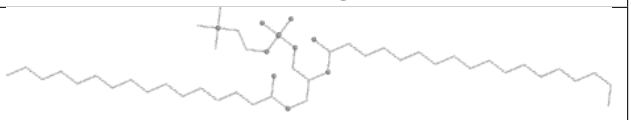


Bond angles

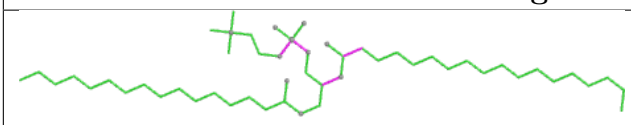


Torsions

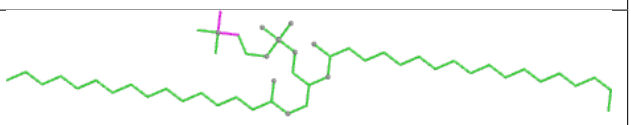


Rings

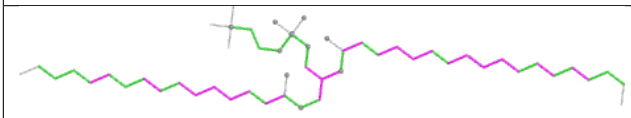
Ligand PLX r 502



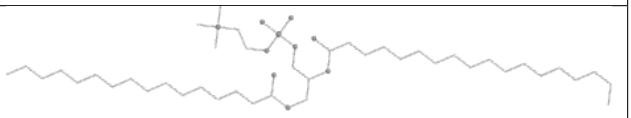
Bond lengths



Bond angles

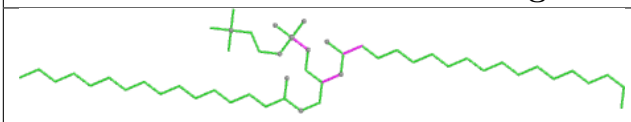


Torsions

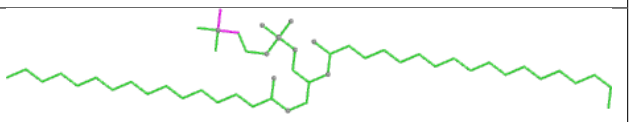


Rings

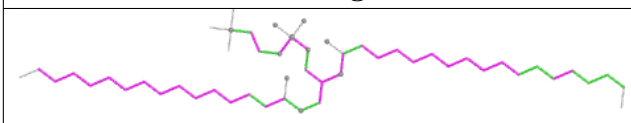
Ligand PLX J 403



Bond lengths



Bond angles



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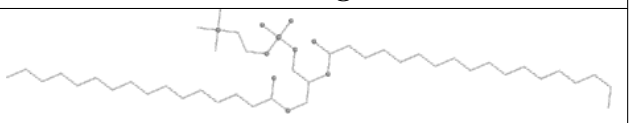
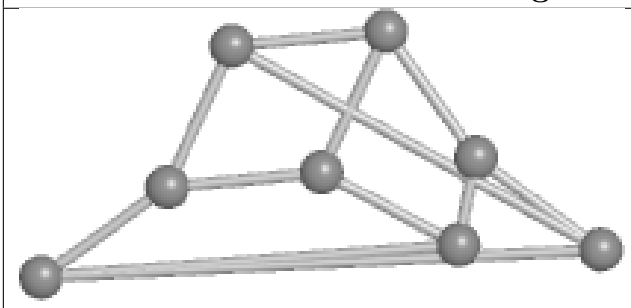


Rings

Ligand SF4 B 302



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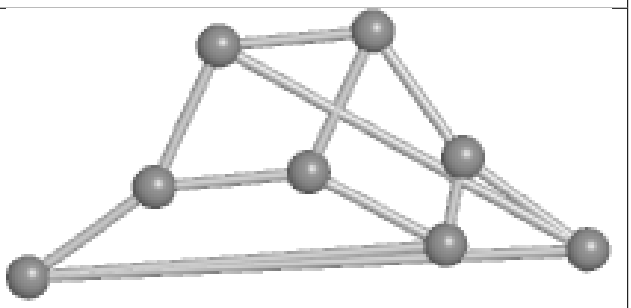

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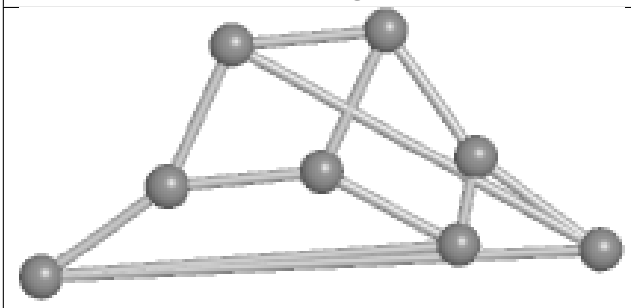

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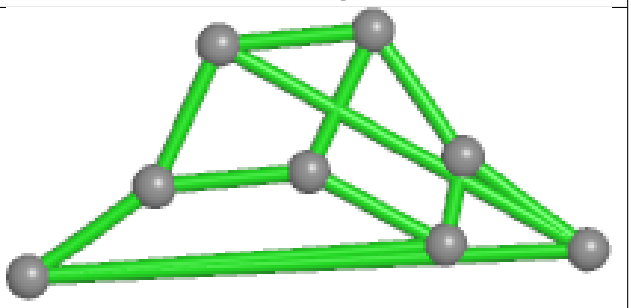
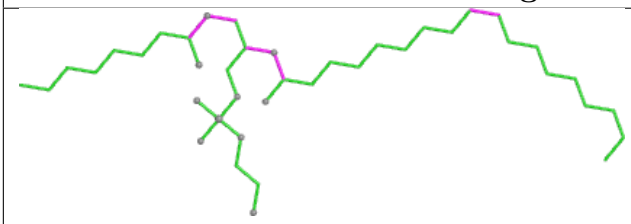


Rings

Ligand PEE W 201



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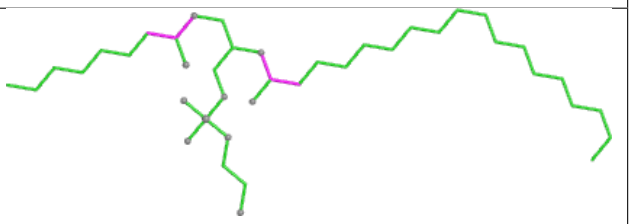
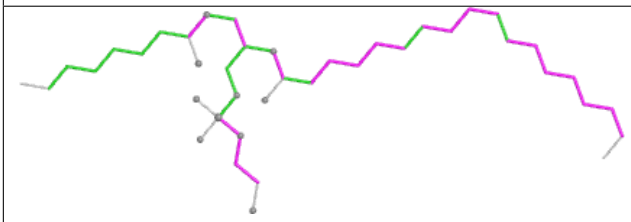


Bond angles



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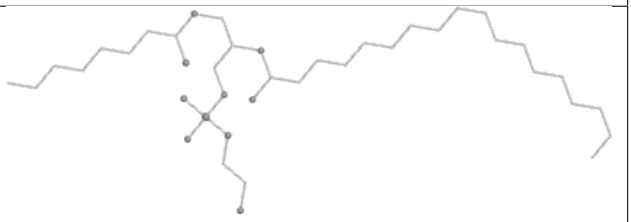
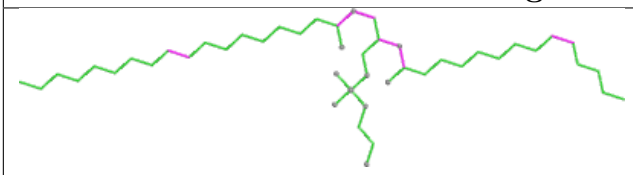


Rings

Ligand PEE C 302



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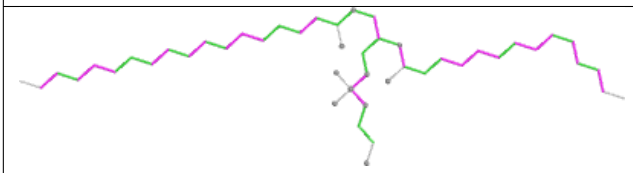

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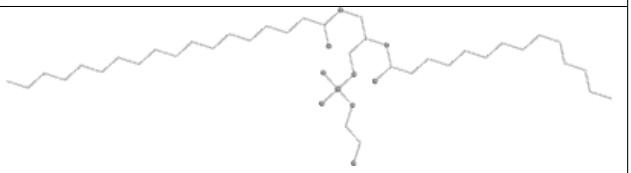
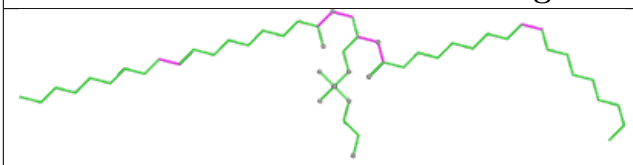


Rings

Ligand PEE l 704



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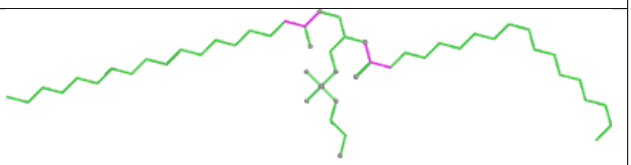

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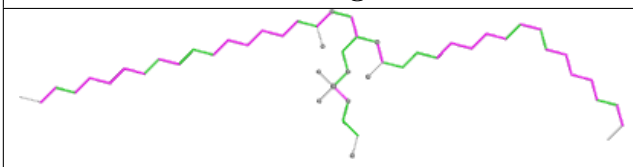

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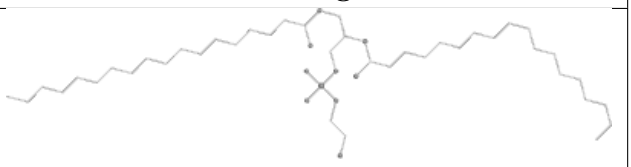
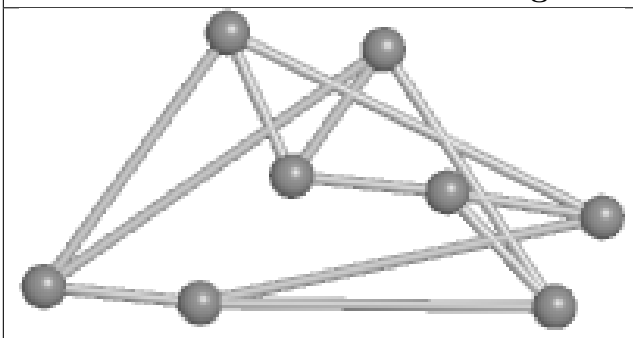


Rings

Ligand SF4 A 501



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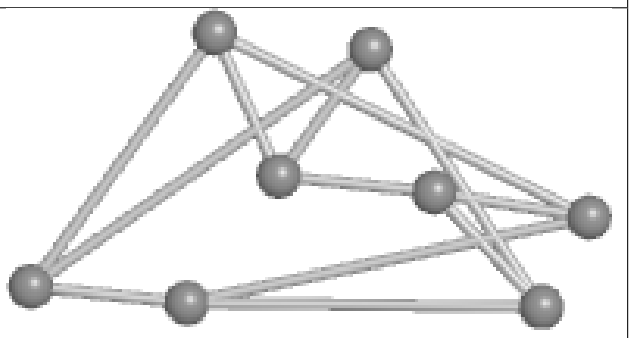
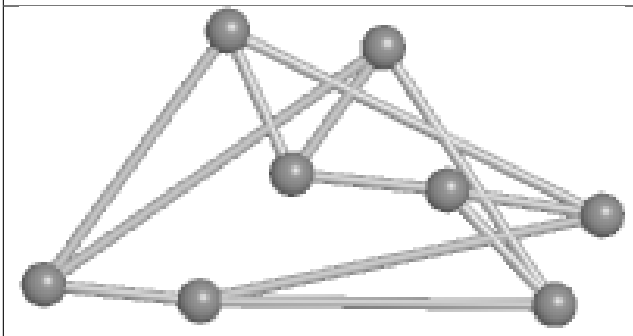


Bond angles



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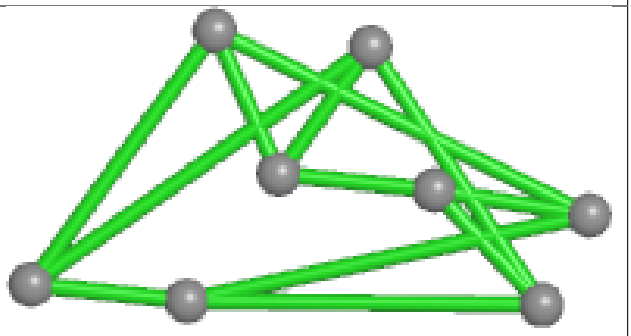
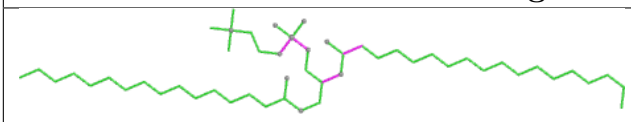


Rings

Ligand PLX n 101



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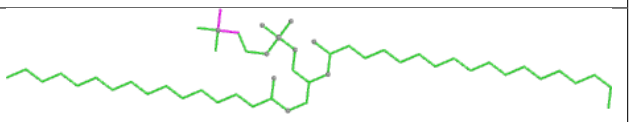

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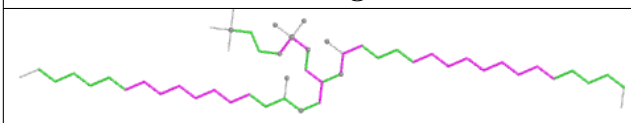

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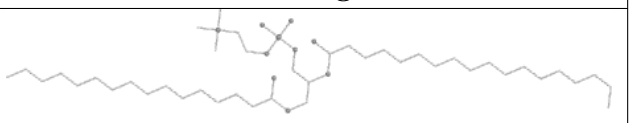
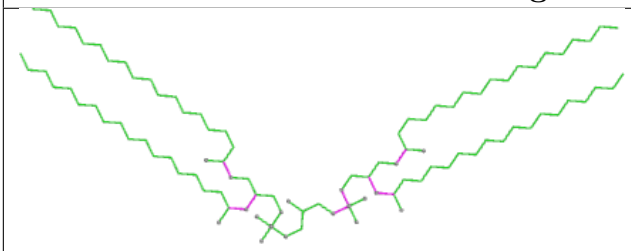


Rings

Ligand CDL r 504



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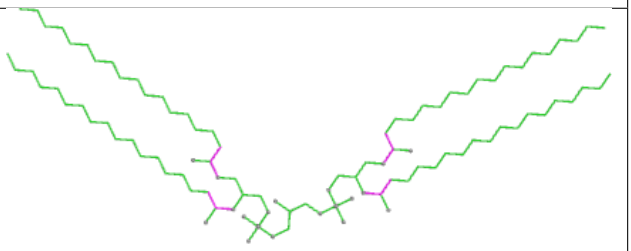
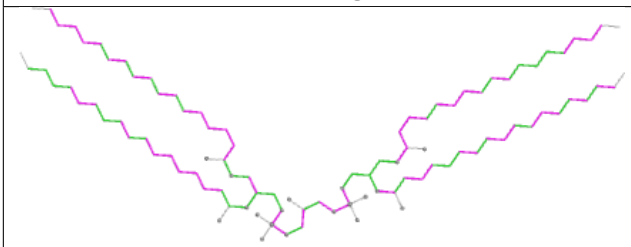


Bond angles



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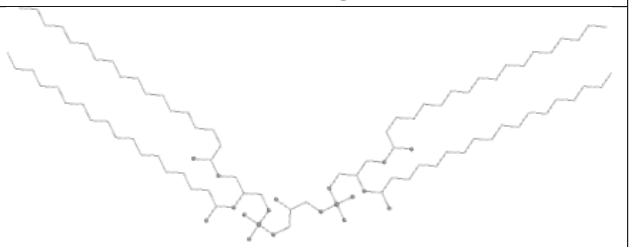
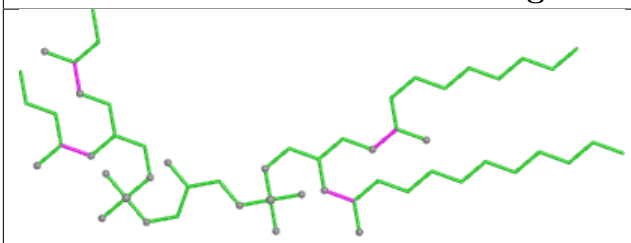


Rings

Ligand CDL u 201



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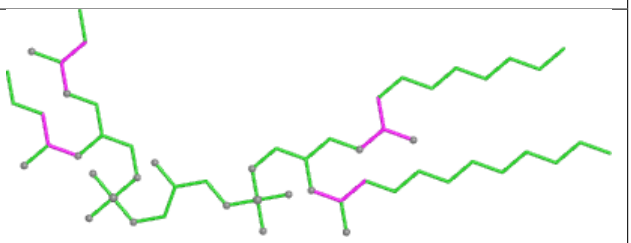

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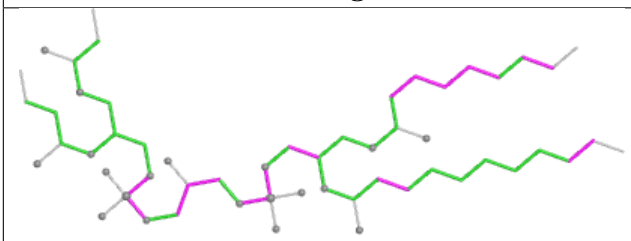

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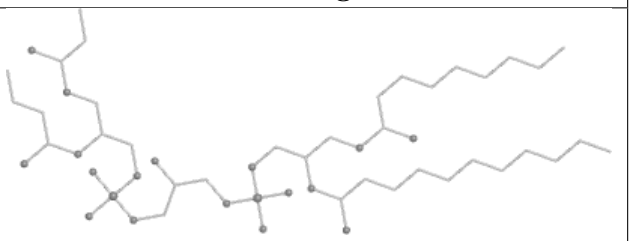
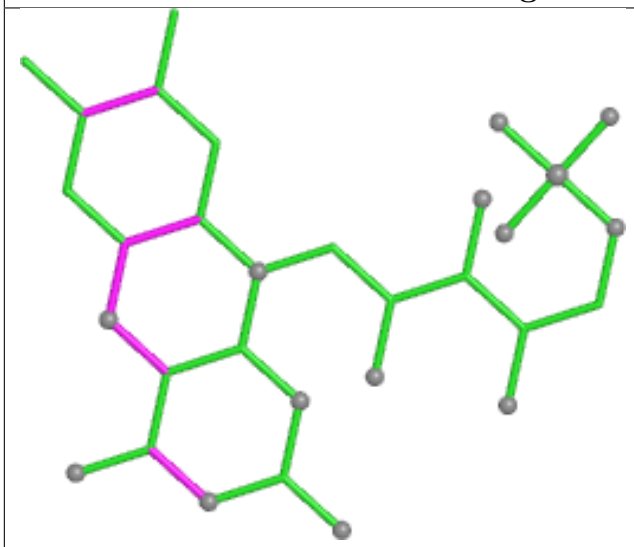


Rings

Ligand FMN A 502



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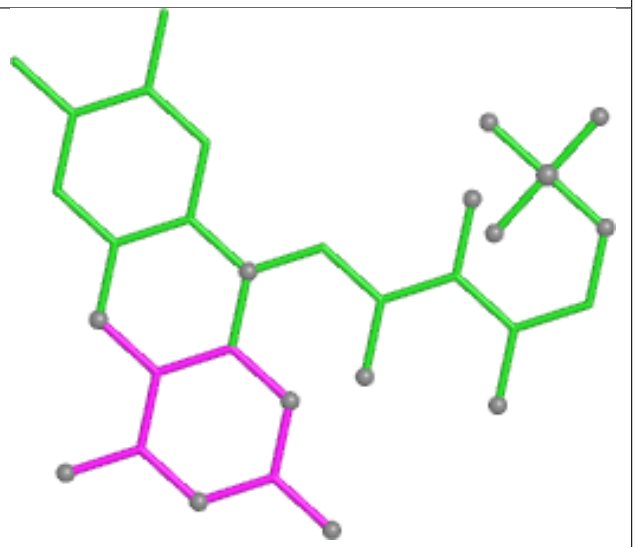

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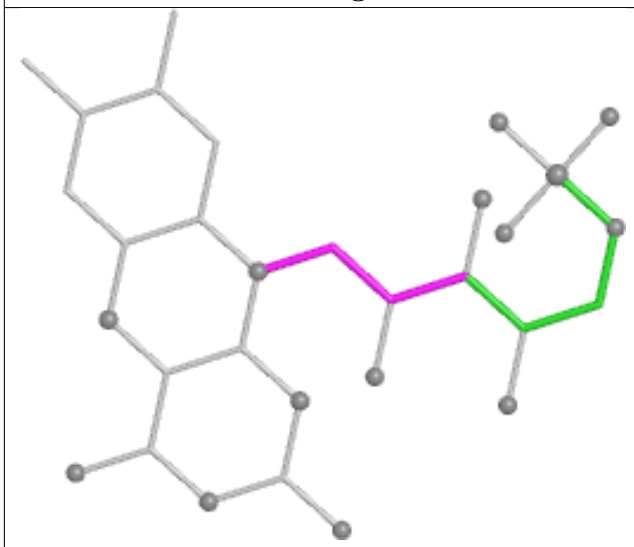

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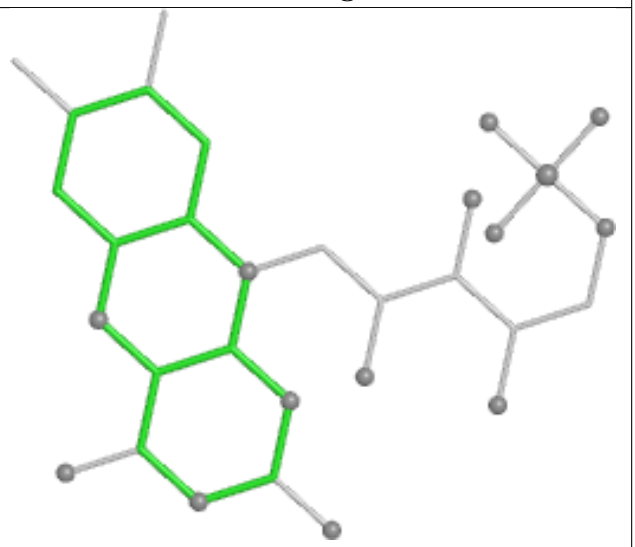
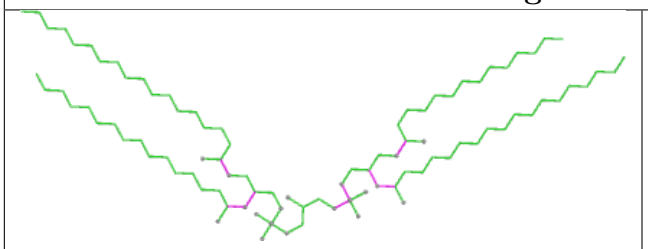


Rings

Ligand CDL V 201



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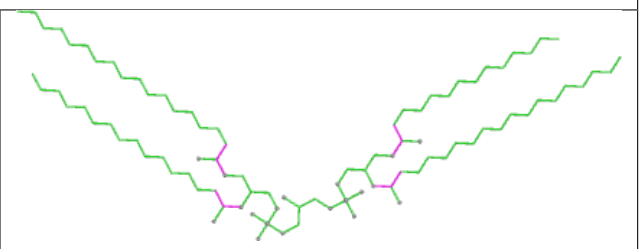

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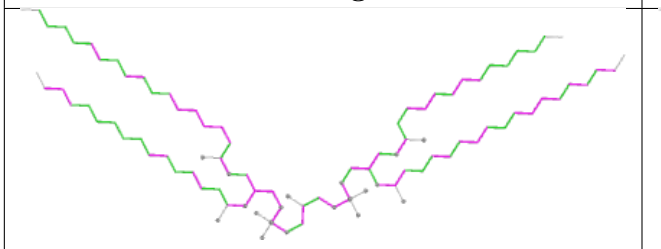

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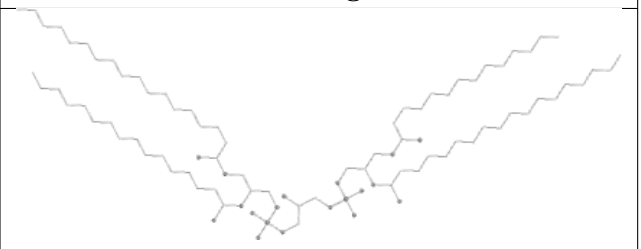
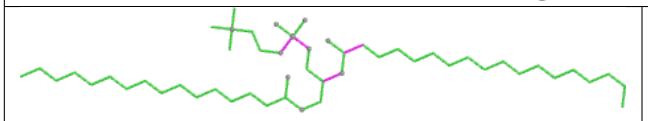


Rings

Ligand PLX j 203



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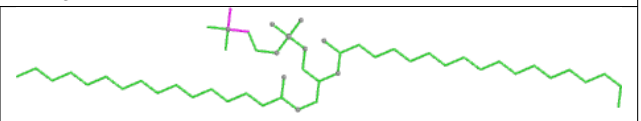

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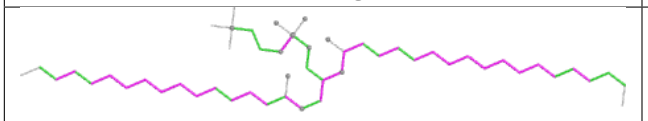

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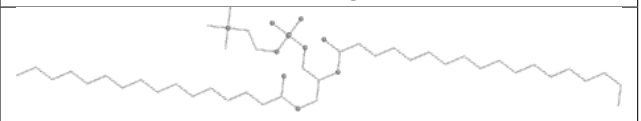
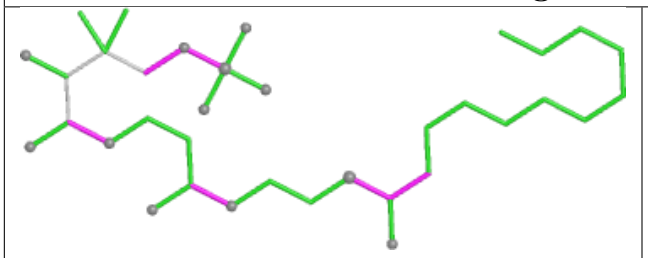


Rings

Ligand 8Q1 E 201



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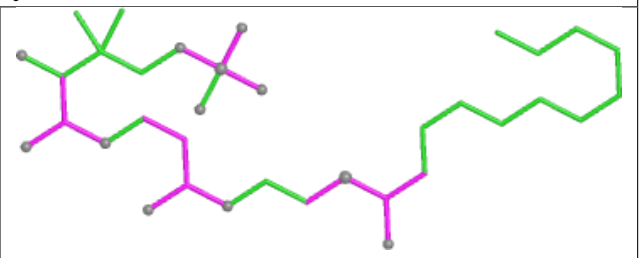
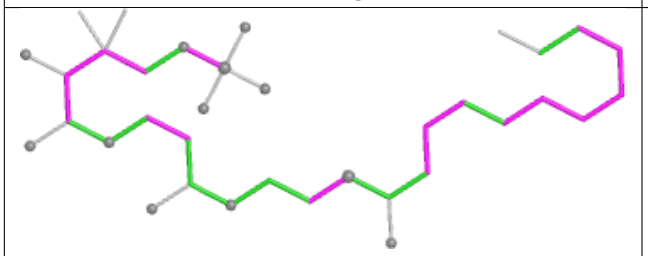


Bond angles



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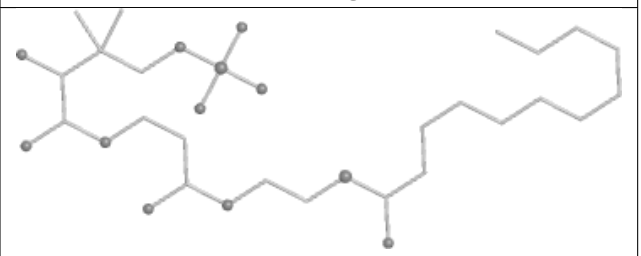
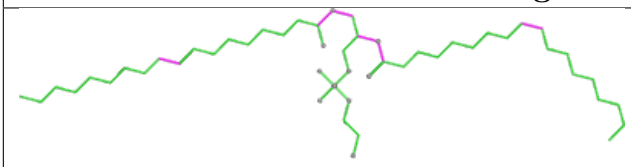


Rings

Ligand PEE j 201



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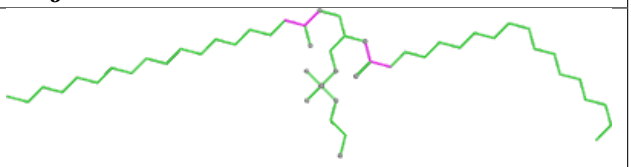
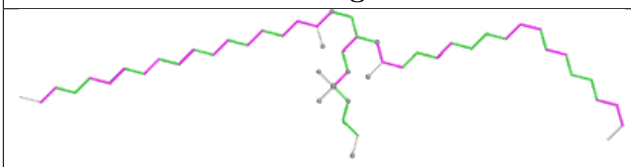
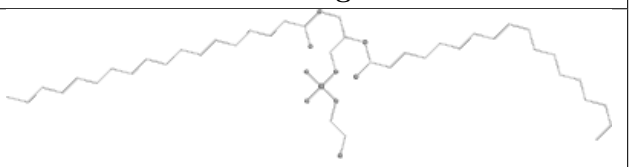


Bond angles

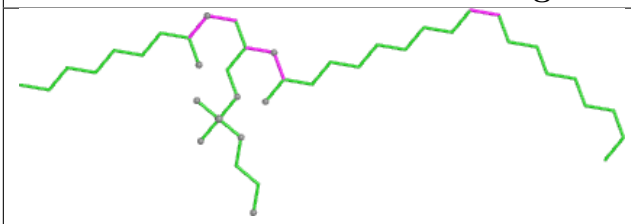


Torsions

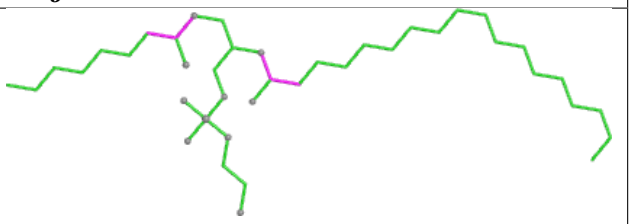


Rings

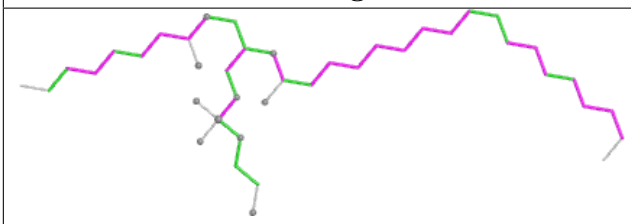
Ligand PEE j 202



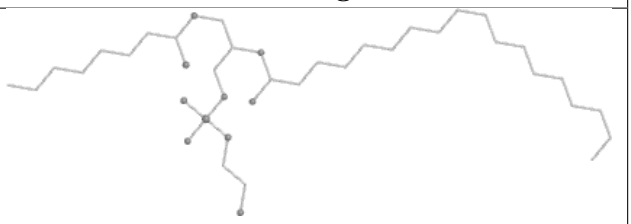
Bond lengths



Bond angles

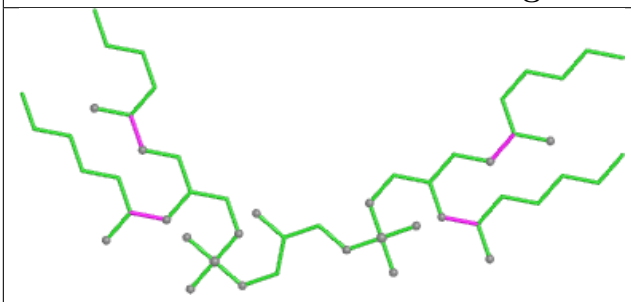


Torsions

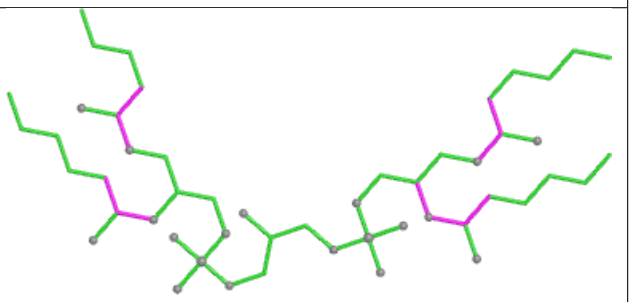


Rings

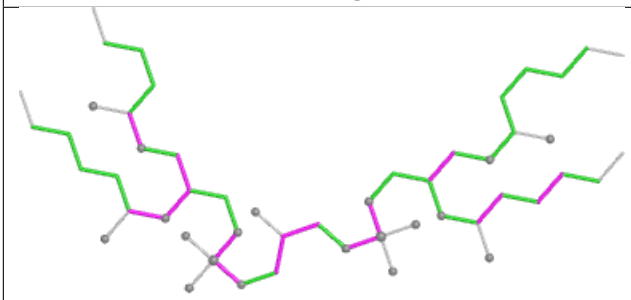
Ligand CDL N 202



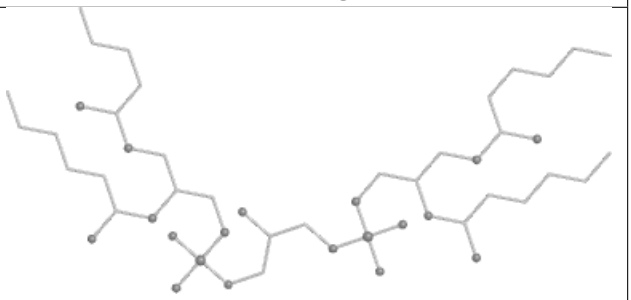
Bond lengths



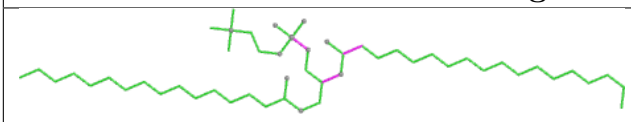
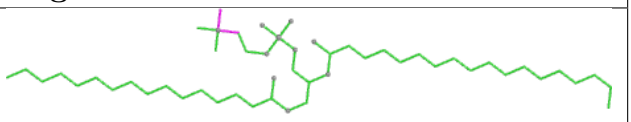
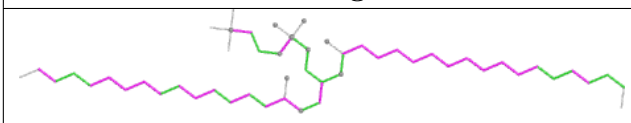
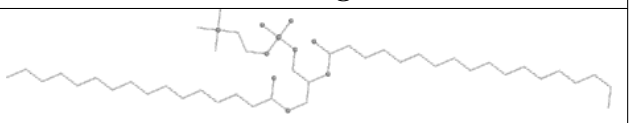
Bond angles

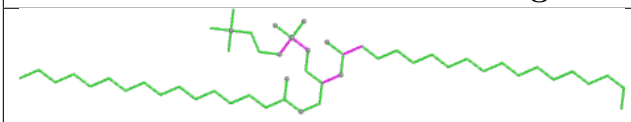
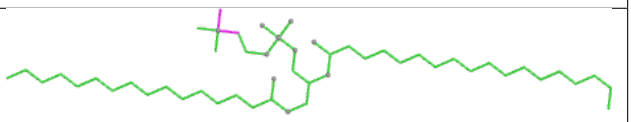
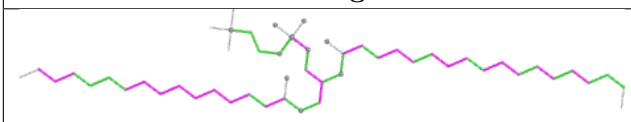
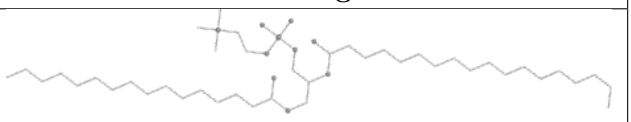


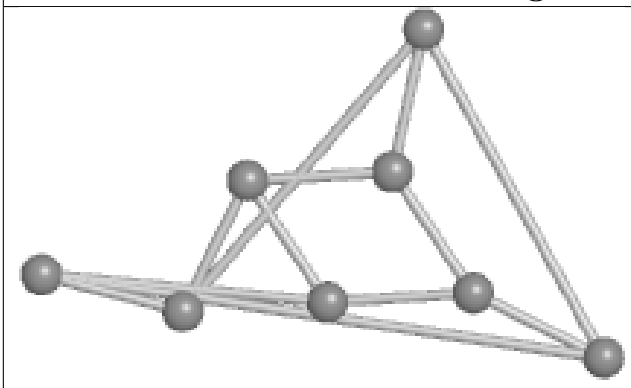
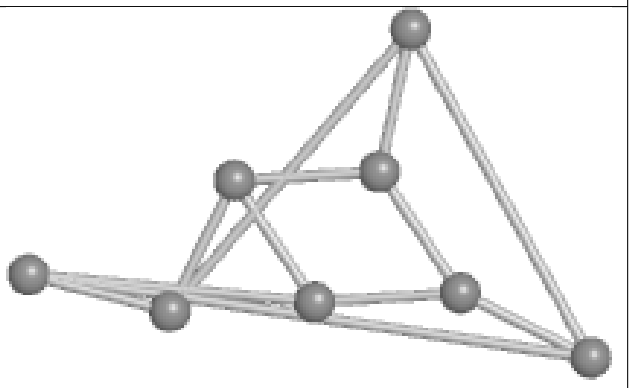
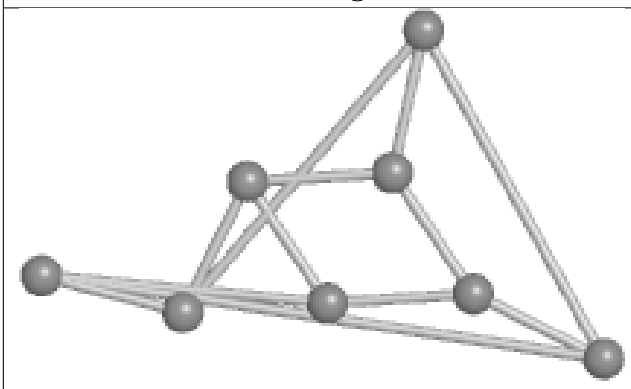
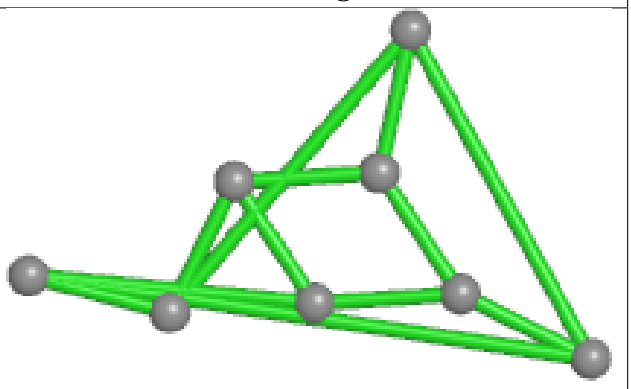
Torsions



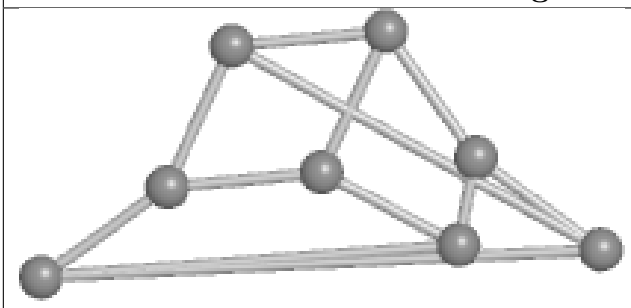
Rings

Ligand PLX g 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

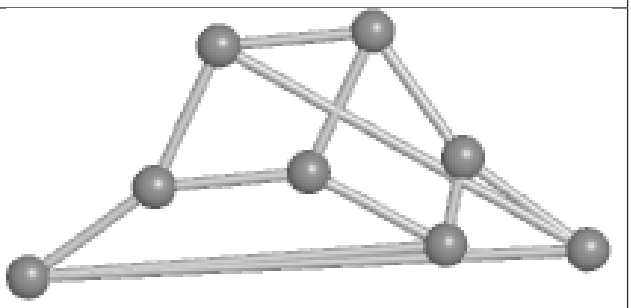
Ligand PLX r 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SF4 M 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

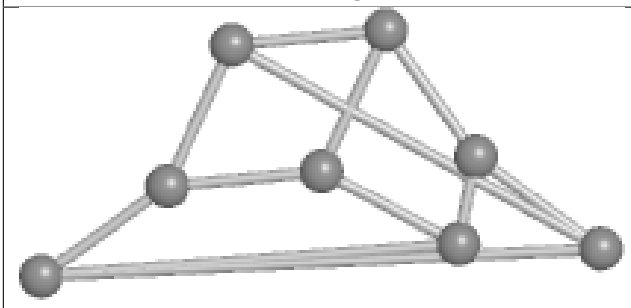
Ligand SF4 C 301



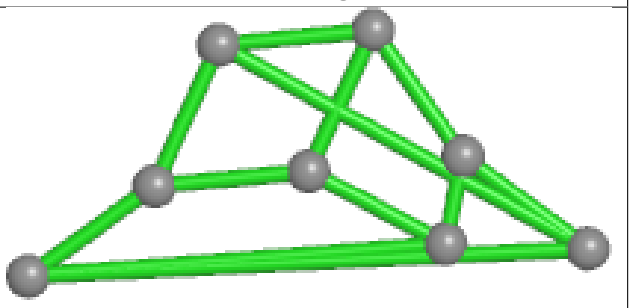
Bond lengths



Bond angles

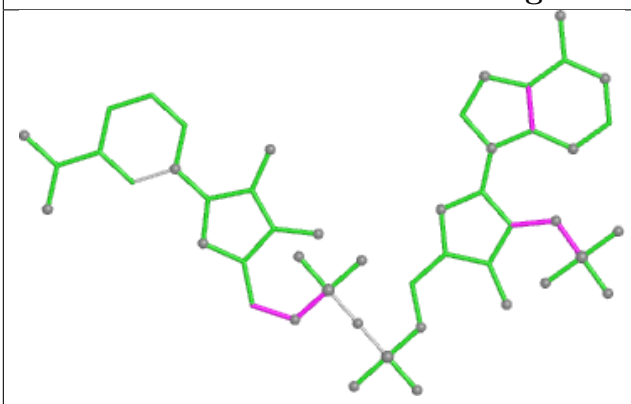


Torsions

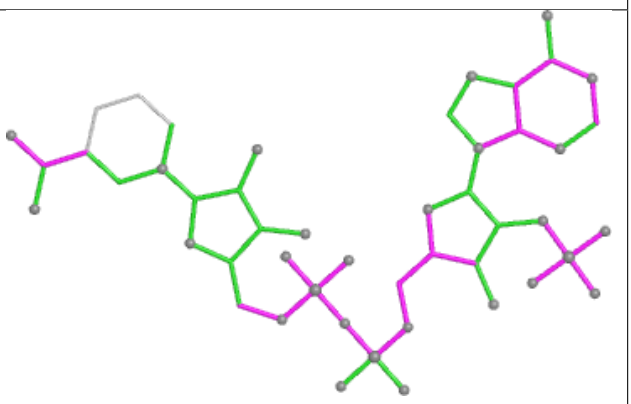


Rings

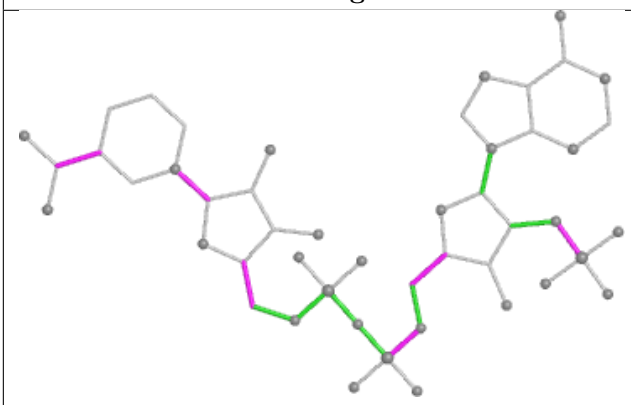
Ligand NDP J 401



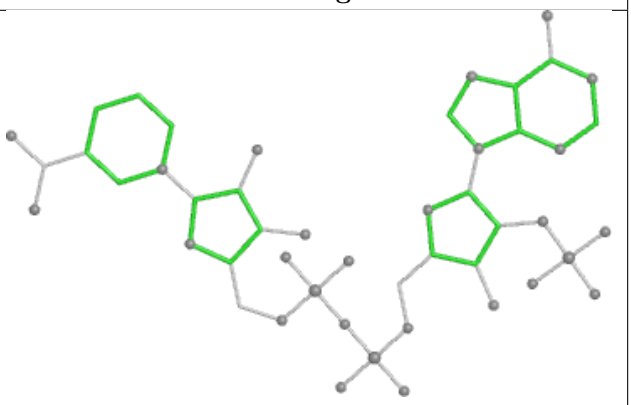
Bond lengths



Bond angles

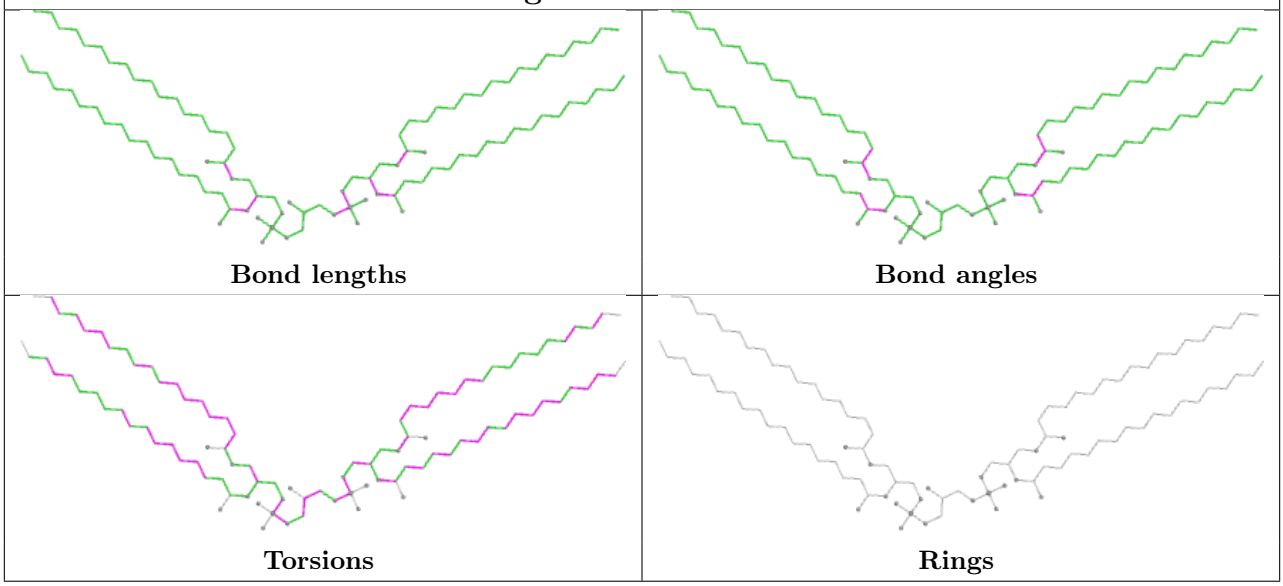


Torsions

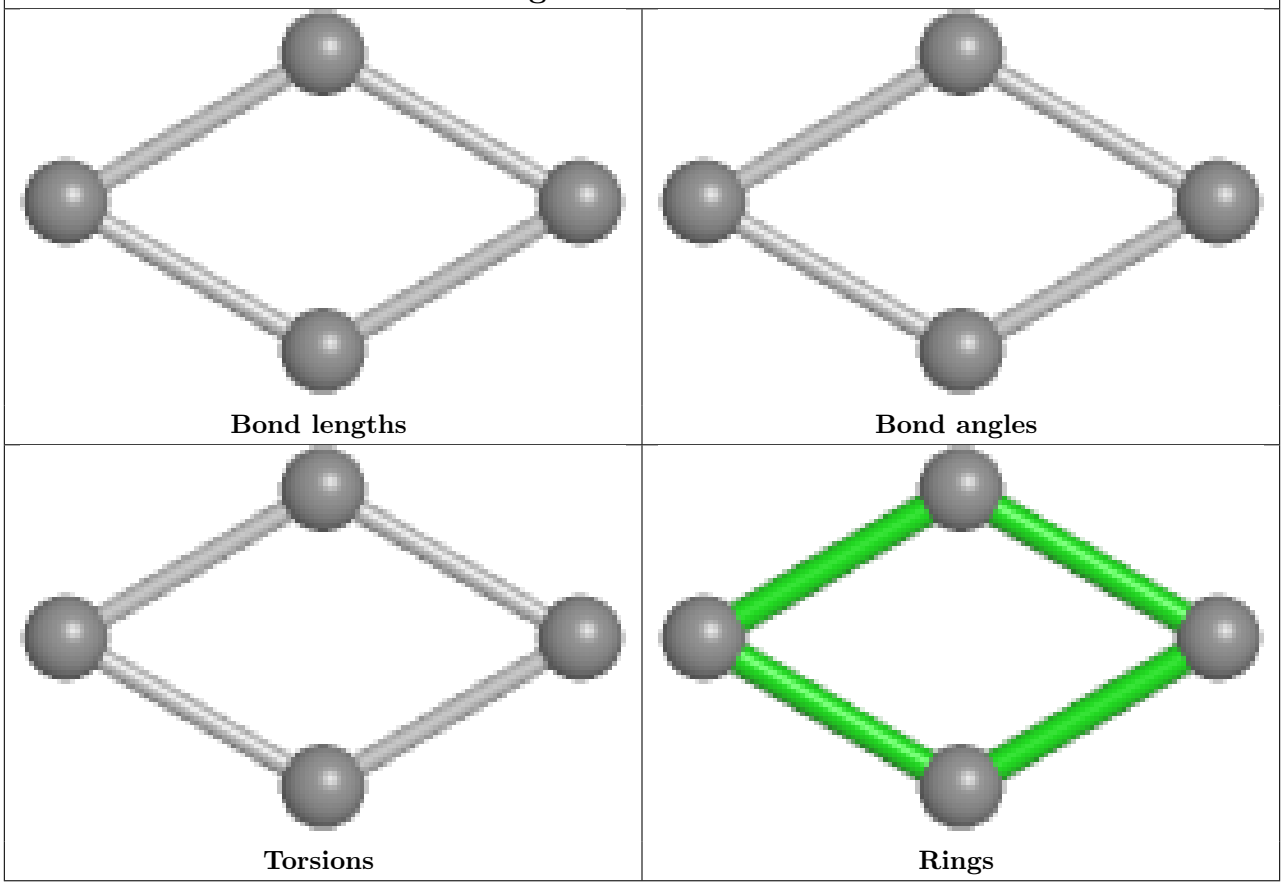


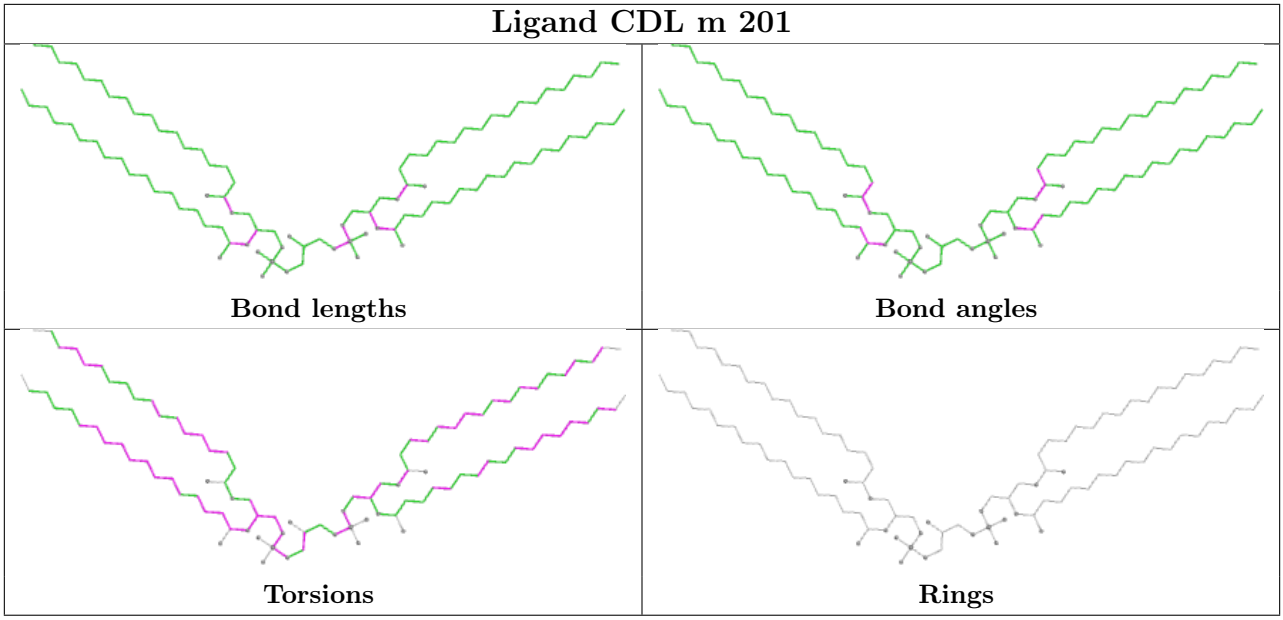
Rings

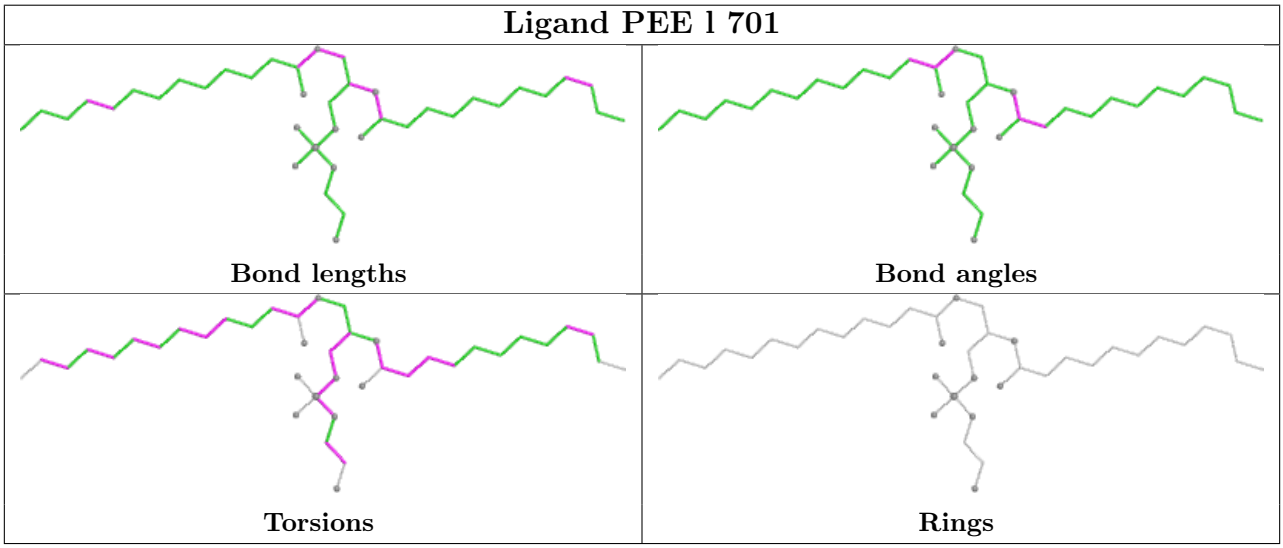
Ligand CDL V 202



Ligand FES O 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.

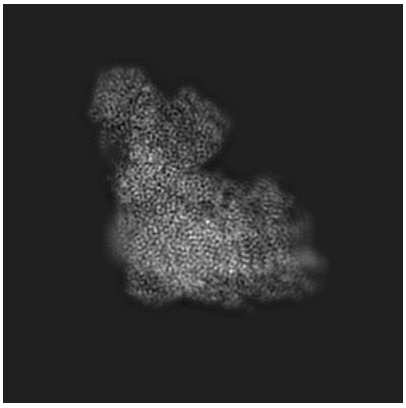
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-31640. These allow visual inspection of the internal detail of the map and identification of artifacts.

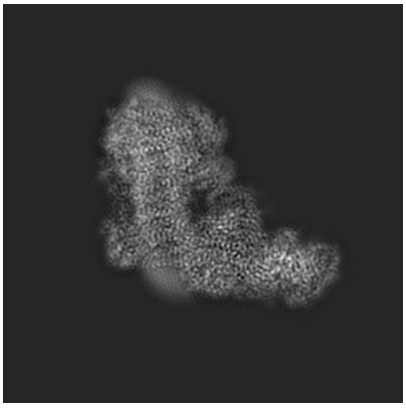
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

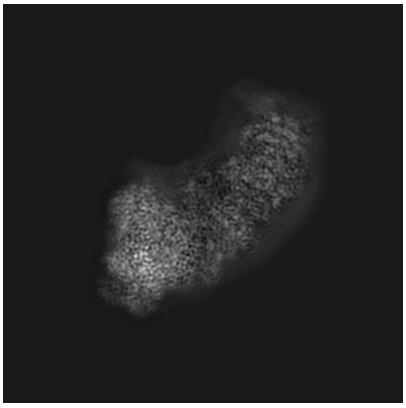
6.1.1 Primary map



X



Y

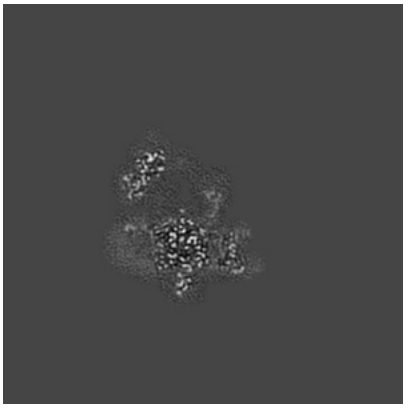


Z

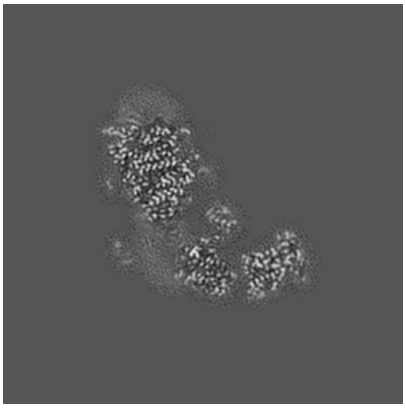
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

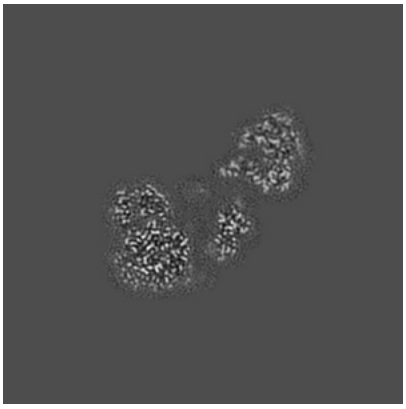
6.2.1 Primary map



X Index: 165



Y Index: 165

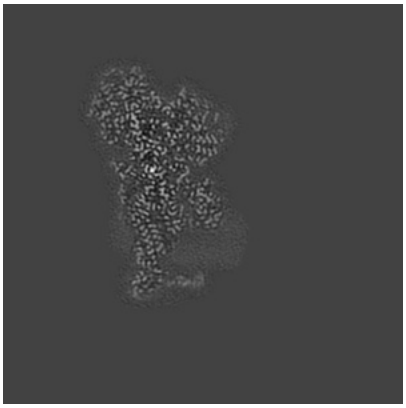


Z Index: 165

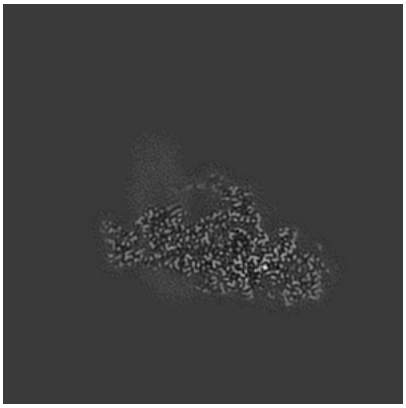
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

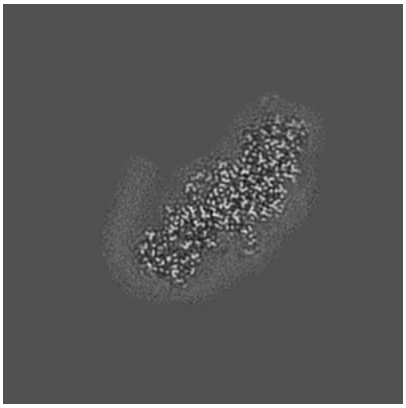
6.3.1 Primary map



X Index: 116



Y Index: 118

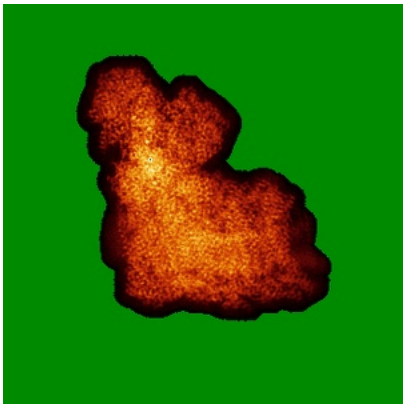


Z Index: 136

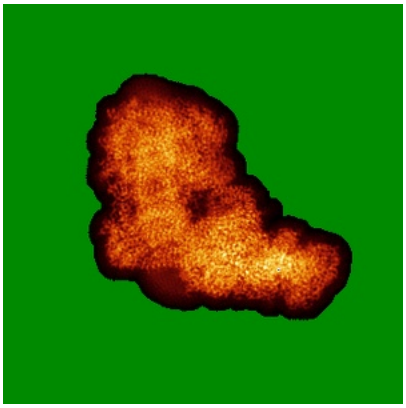
The images above show the largest variance slices of the map in three orthogonal directions.

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

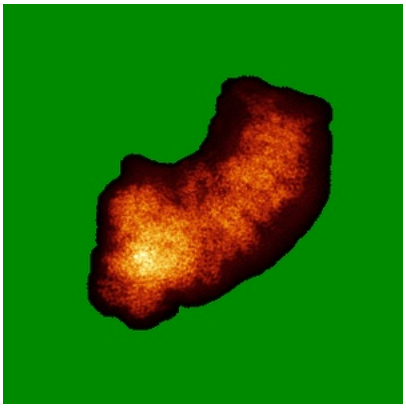
6.4.1 Primary map



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

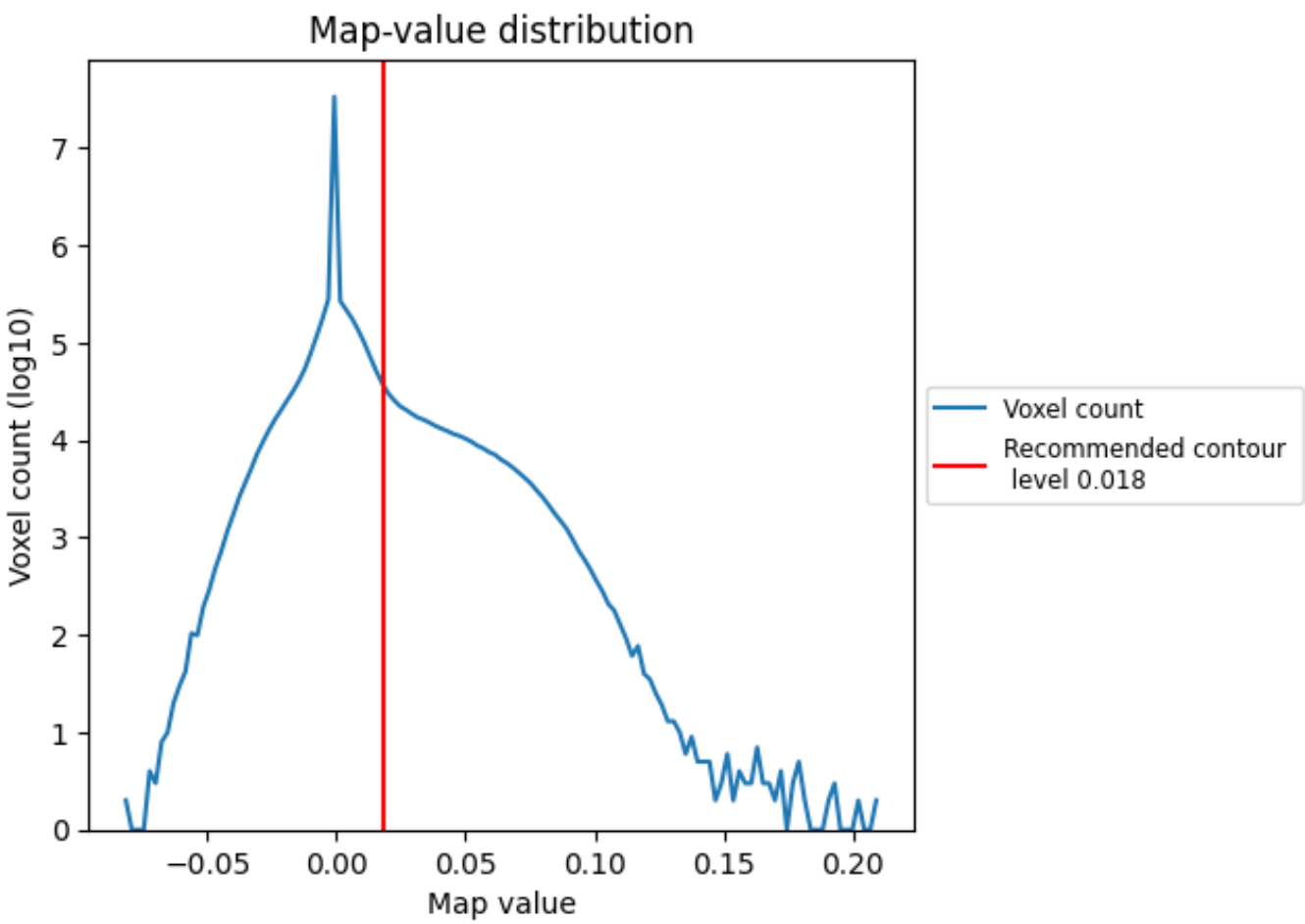
6.6 Mask visualisation (i)

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

7 Map analysis (i)

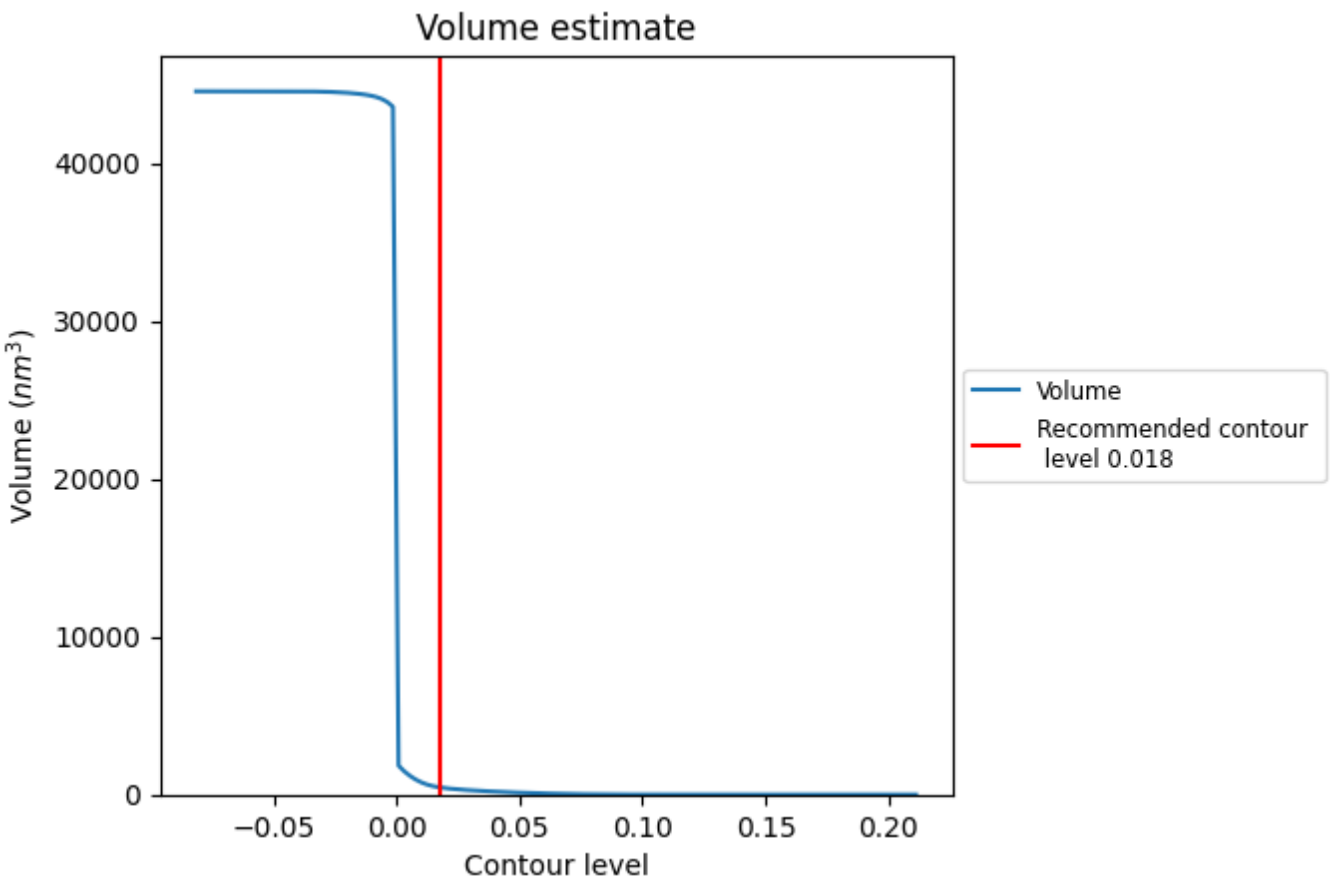
This section contains the results of statistical analysis of the map.

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.

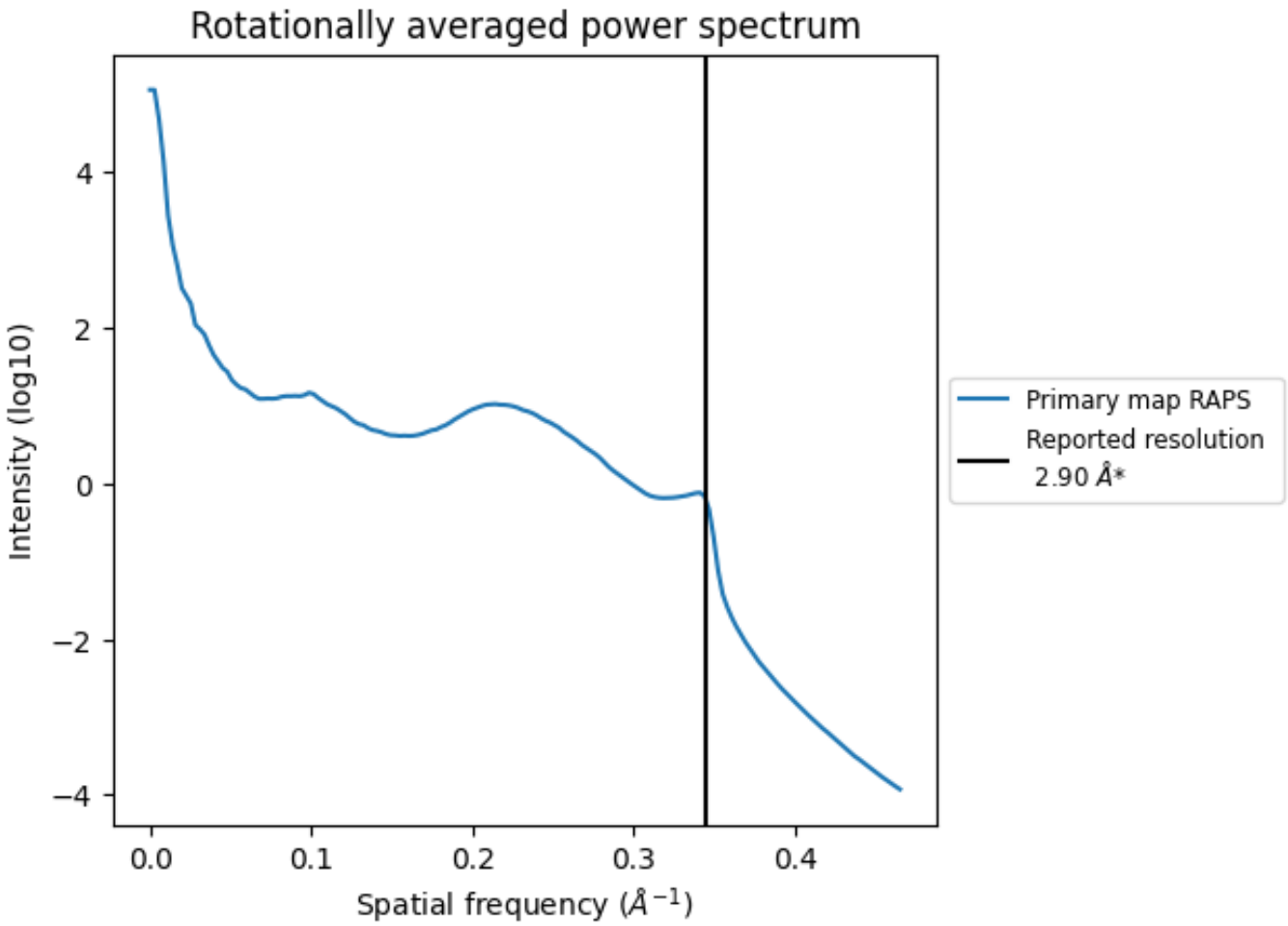
7.2 Volume estimate (i)



The volume at the recommended contour level is 447 nm^3; this corresponds to an approximate mass of 404 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}

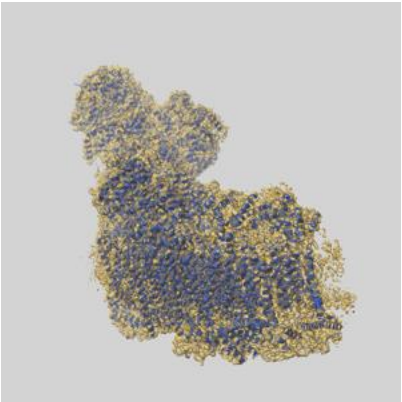
8 Fourier-Shell correlation (i)

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

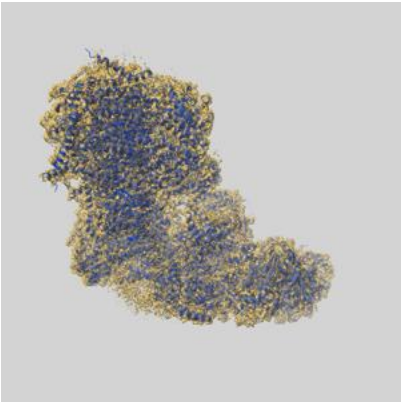
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-31640 and PDB model 7V2C. Per-residue inclusion information can be found in section 3 on page 20.

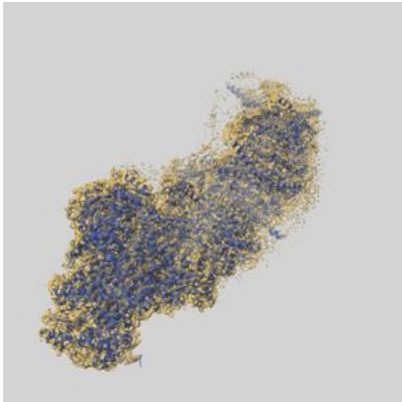
9.1 Map-model overlay (i)



X



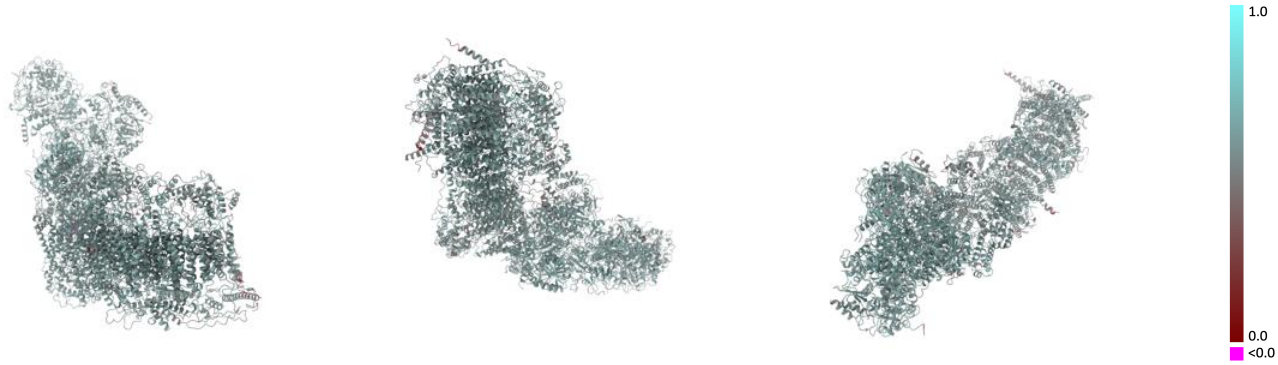
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 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.

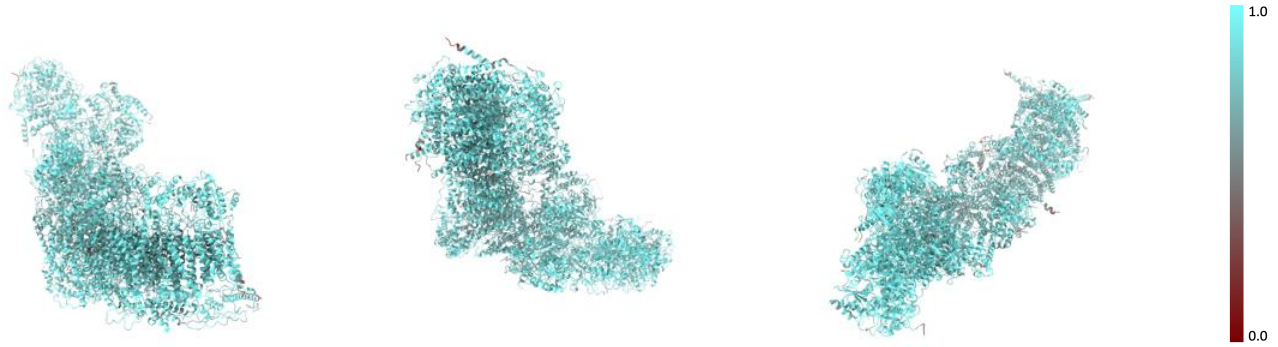
9.2 Q-score mapped to coordinate model (i)



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.

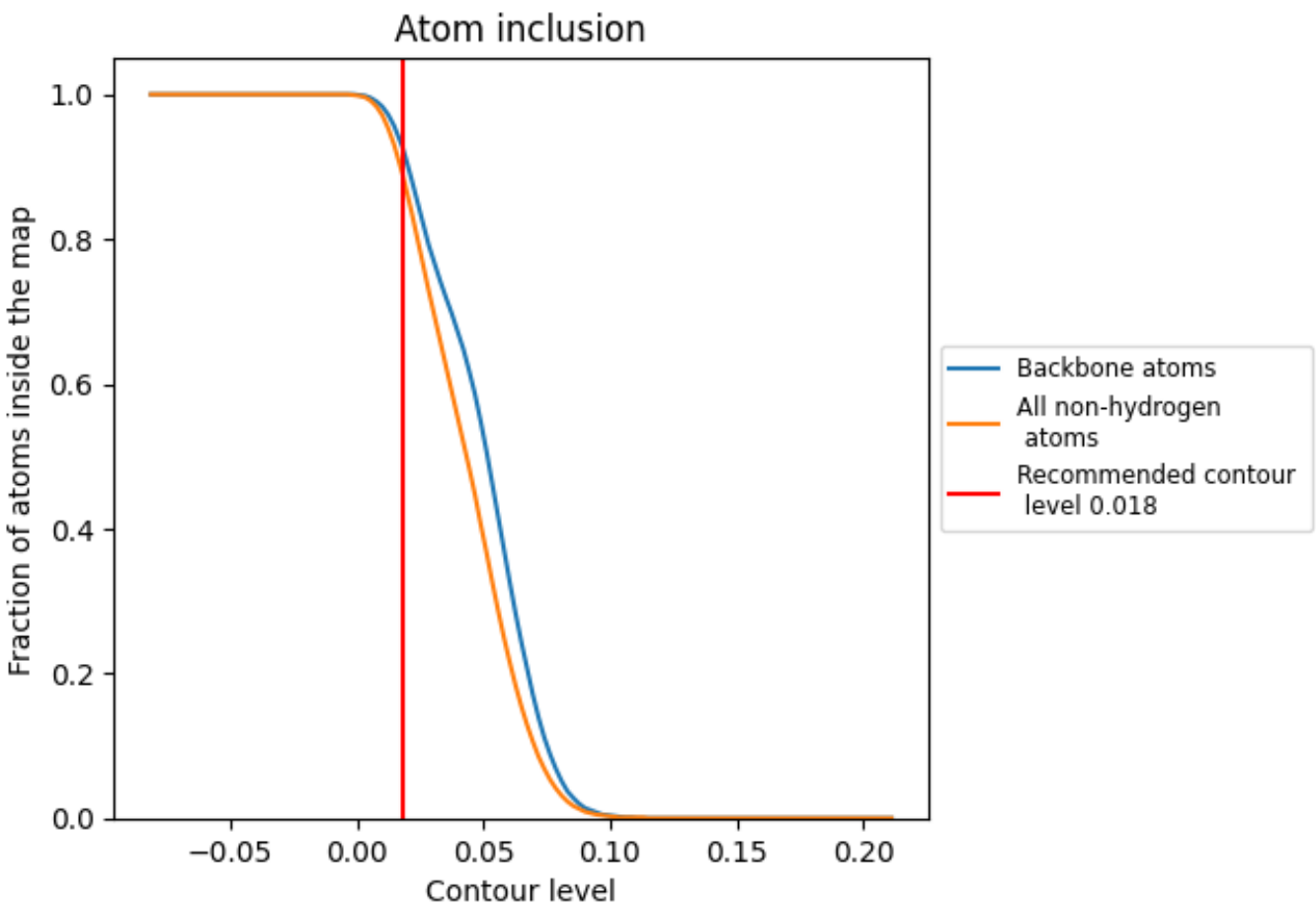
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.018).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 89% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8900	0.5780
A	0.9130	0.5780
B	0.9530	0.6110
C	0.9440	0.6120
E	0.8940	0.5840
F	0.8580	0.5310
G	0.7430	0.4670
H	0.8980	0.5710
I	0.8290	0.5600
J	0.9060	0.5930
K	0.8870	0.5600
L	0.9030	0.5970
M	0.9220	0.5900
N	0.8240	0.5740
O	0.8940	0.5680
P	0.9450	0.6160
Q	0.9390	0.6080
S	0.9310	0.5880
T	0.8950	0.5910
U	0.9000	0.5730
V	0.8050	0.5580
W	0.8960	0.5690
X	0.8380	0.5260
Y	0.8400	0.5310
Z	0.7790	0.5190
a	0.8870	0.5860
b	0.8480	0.5440
c	0.8730	0.5660
d	0.8480	0.5480
e	0.8320	0.5510
f	0.7840	0.5260
g	0.8950	0.5820
h	0.8760	0.5610
i	0.9210	0.5940
j	0.8770	0.5950

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Chain	Atom inclusion	Q-score
k	0.9160	0.5940
l	0.8800	0.5790
m	0.8400	0.5590
n	0.7870	0.5380
o	0.8680	0.5650
p	0.8830	0.5660
r	0.9050	0.5940
s	0.9190	0.5960
u	0.9010	0.5790
v	0.8340	0.5210
w	0.8770	0.5640