



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 09:16 AM JST

PDB ID : 7W1V / pdb_00007w1v
EMDB ID : EMD-32257
Title : Active state CI from Rotenone-NADH dataset, Subclass 1
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-20
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

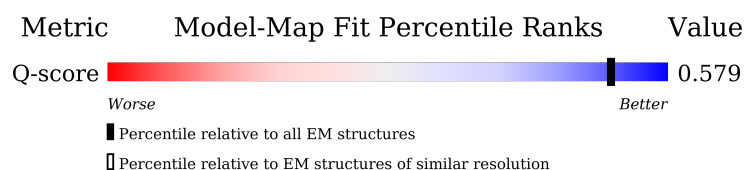
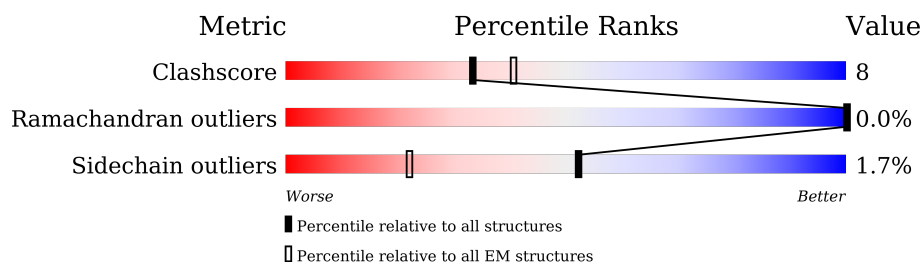
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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 $\leq 5\%$. 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	
2	B	176	
3	C	156	
4	E	115	

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

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Mol	Chain	Length	Quality of chain
29	f	49	
30	g	122	
31	h	105	
32	i	347	
33	j	115	
34	k	98	
35	l	606	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	124	
44	w	320	

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 68209 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
1	A	433	Total	C	N	O	S	0	0
			3330	2103	593	614	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	176	Total	C	N	O	S	0	0
			1411	887	243	268	13		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	86	Total	C	N	O	S	0	0
			684	431	129	122	2		

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			693	447	102	139	5		
6	X	88	Total	C	N	O	S	0	0
			693	448	103	137	5		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	690	Total	C	N	O	S	0	0
			5284	3314	923	1008	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	144	Total	C	N	O	S	0	0
			1200	767	217	212	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	217	Total	C	N	O	S	0	0
			1667	1062	280	315	10		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	104	Total	C	N	O	S	0	0
			856	548	142	162	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	49	Total	C	N	O	0	0
			377	246	65	66		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	606	Total	C	N	O	S	0	0
			4797	3181	743	822	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	175	Total	C	N	O	S	0	0
			1276	850	187	226	13		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	178	Total	C	N	O	S	0	0
			1530	979	278	265	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	459	Total	C	N	O	S	0	0
			3624	2406	572	608	38		

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

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

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

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

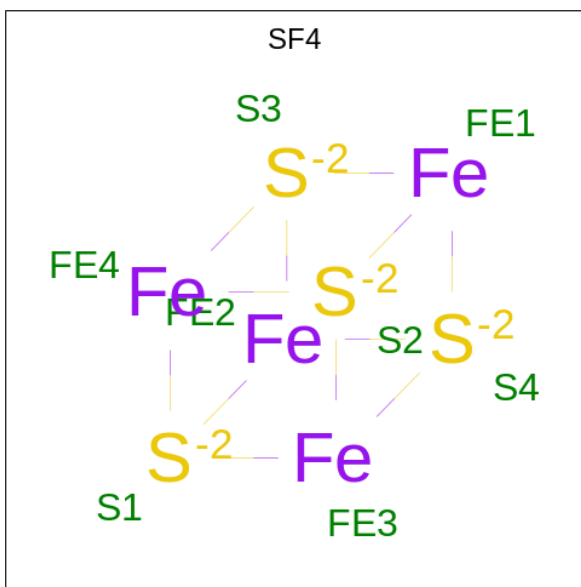
- Molecule 43 is a protein called Complex I-B18.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			1036	646	196	185	9		

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

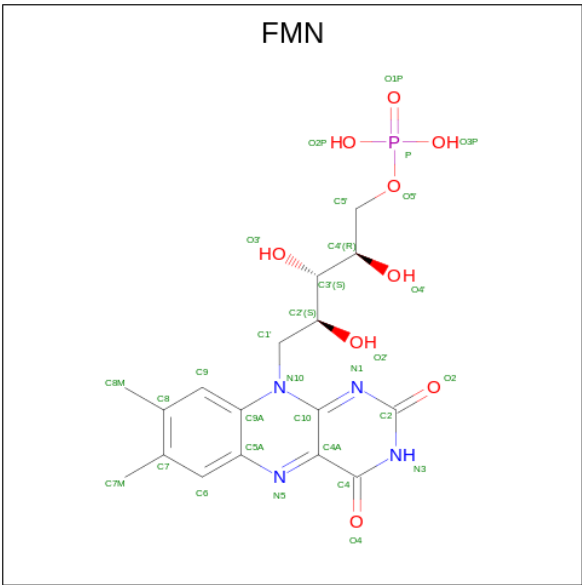
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2586	1646	439	491	10		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



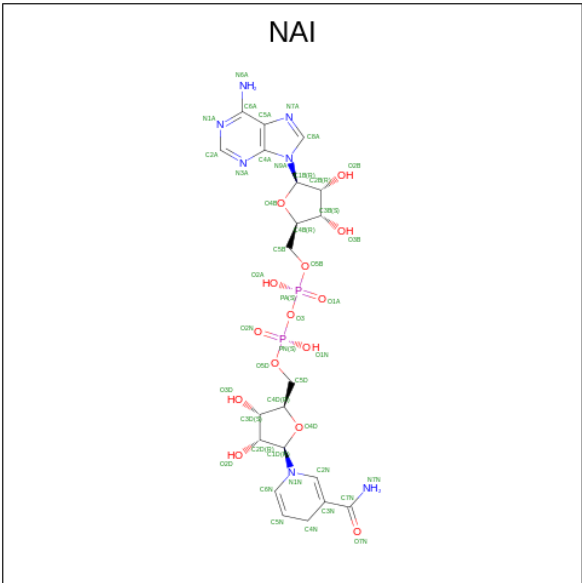
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



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

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



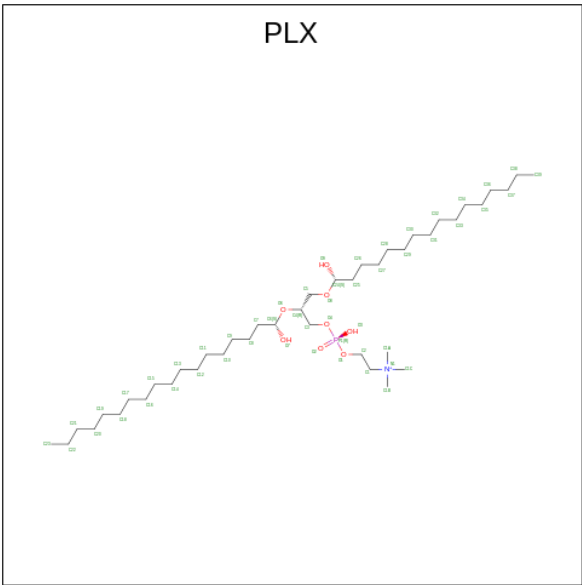
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

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



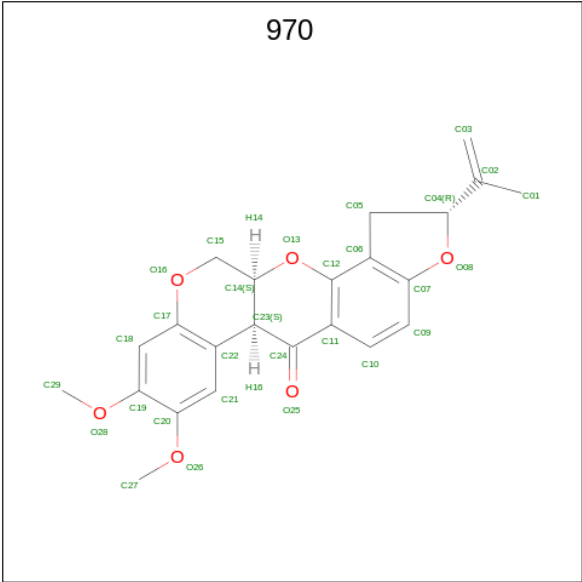
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	j	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	l	1	Total	C	N	O	P	0
			50	40	1	8	1	
48	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	r	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 49 is (9R,11S)-9-([[(1S)-1-HYDROXYHEXADECYL]OXY]METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



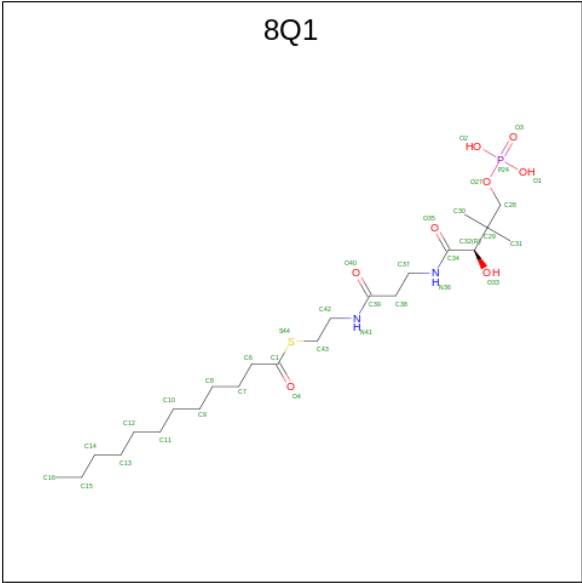
Mol	Chain	Residues	Atoms					AltConf
49	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	J	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42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

- Molecule 50 is (2R,6aS,12aS)-8,9-dimethoxy-2-(prop-1-en-2-yl)-1,2,12,12a-tetrahydrofuro[2',3':7,8][1]benzopyrano[2,3-c][1]benzopyran-6(6aH)-one (CCD ID: 970) (formula: C₂₃H₂₂O₆) (labeled as "Ligand of Interest" by depositor).



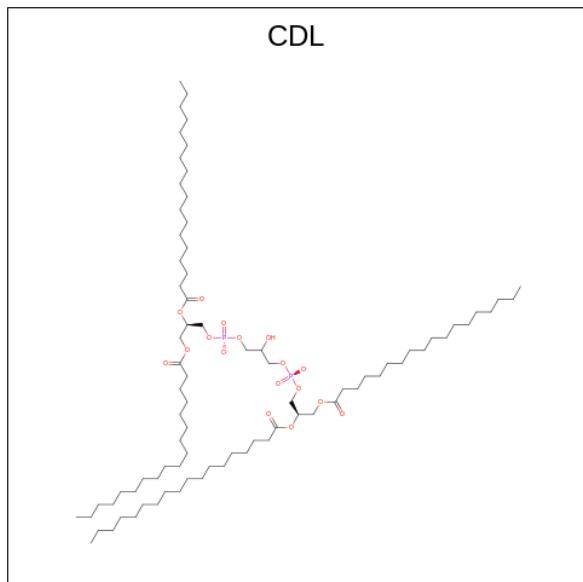
Mol	Chain	Residues	Atoms			AltConf
50	C	1	Total	C	O	0
			29	23	6	

- Molecule 51 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-a
lanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as
"Ligand of Interest" by depositor).



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

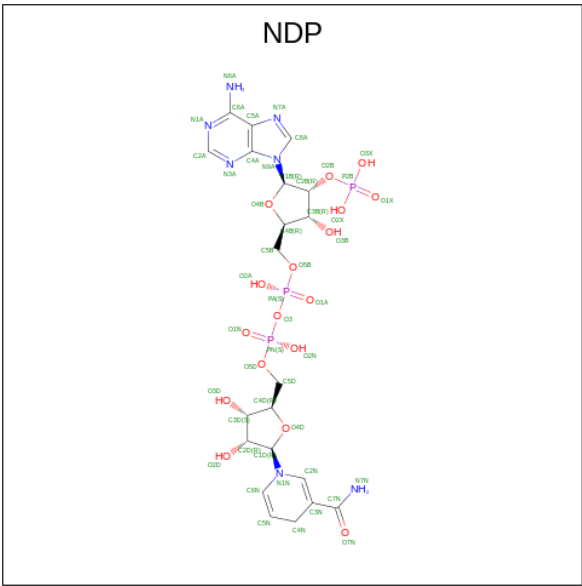
- Molecule 52 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
52	I	1	Total	C	O	P	0
			51	32	17	2	
52	V	1	Total	C	O	P	0
			94	75	17	2	
52	V	1	Total	C	O	P	0
			78	59	17	2	
52	a	1	Total	C	O	P	0
			100	81	17	2	
52	g	1	Total	C	O	P	0
			55	36	17	2	
52	i	1	Total	C	O	P	0
			100	81	17	2	
52	i	1	Total	C	O	P	0
			99	80	17	2	
52	l	1	Total	C	O	P	0
			99	80	17	2	
52	l	1	Total	C	O	P	0
			100	81	17	2	
52	o	1	Total	C	O	P	0
			100	81	17	2	
52	s	1	Total	C	O	P	0
			89	70	17	2	

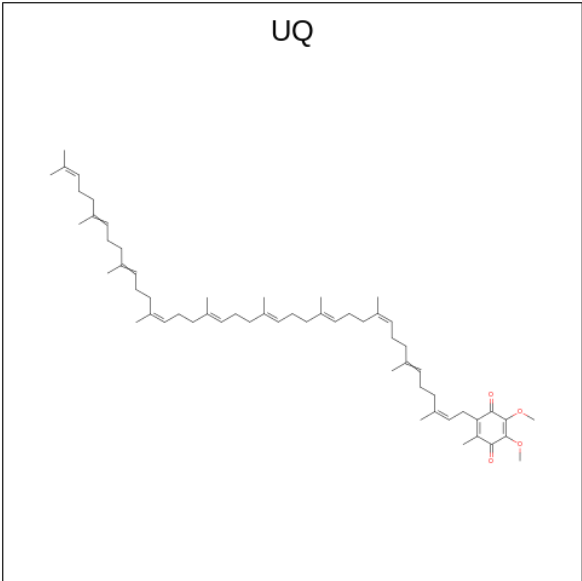
- Molecule 53 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest"

by depositor).



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

- Molecule 54 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



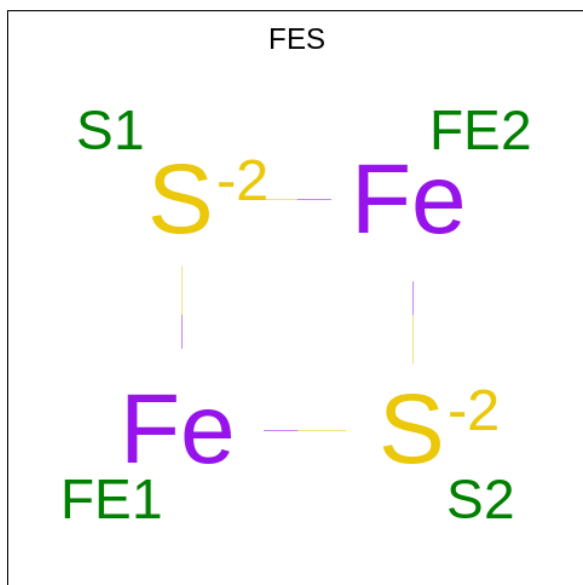
Mol	Chain	Residues	Atoms			AltConf
54	J	1	Total	C	O	0
			33	29	4	

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Mol	Chain	Residues	Atoms			AltConf
54	s	1	Total	C	O	0
			38	34	4	

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



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

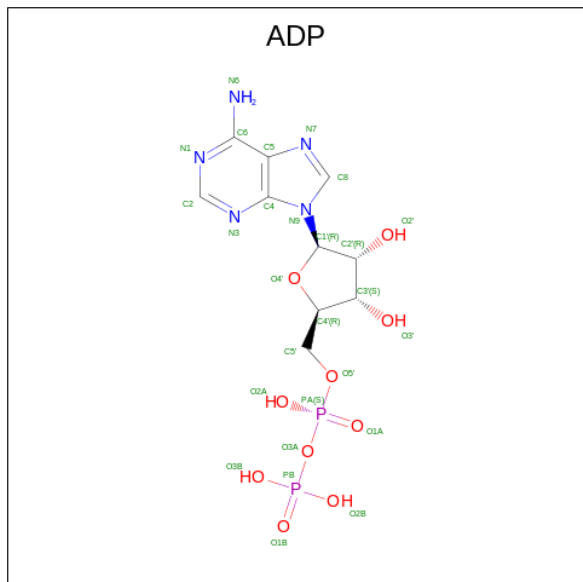
- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

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

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

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

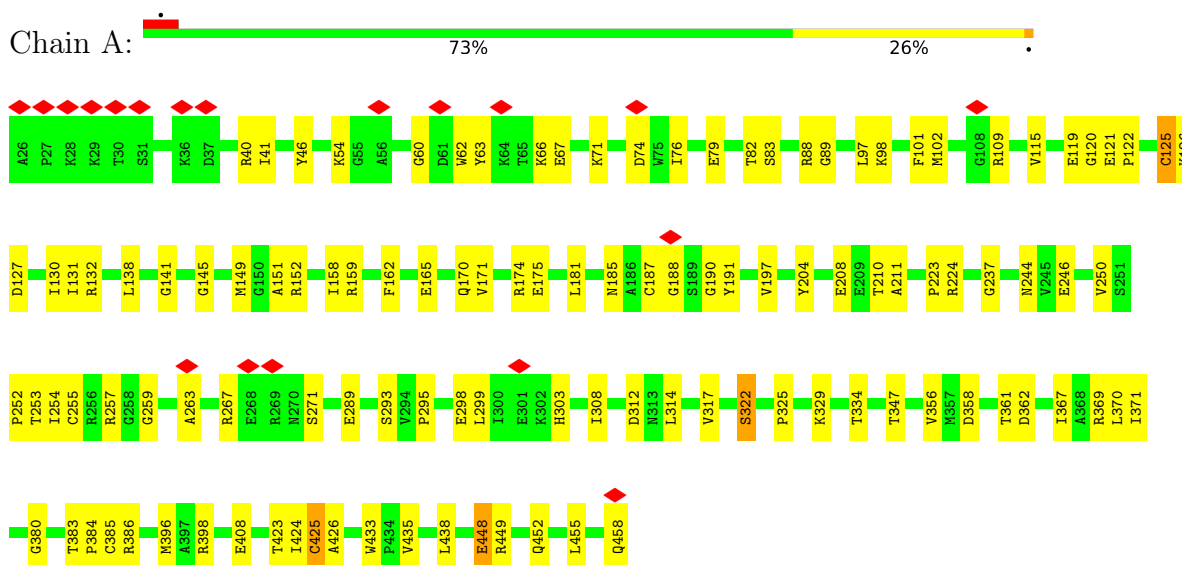


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	w	1	27	10	5	10	2	0

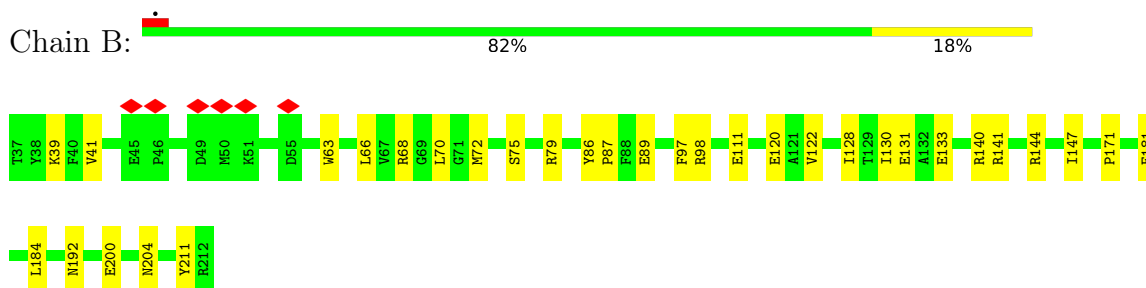
3 Residue-property plots

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.

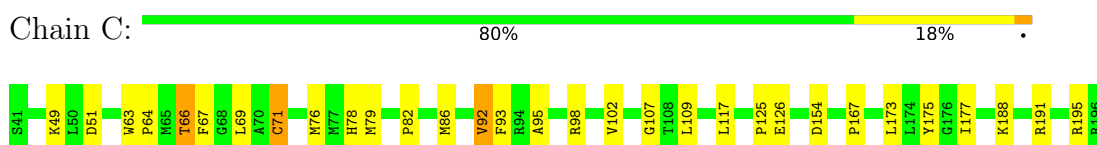
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



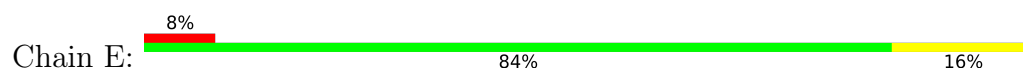
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



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



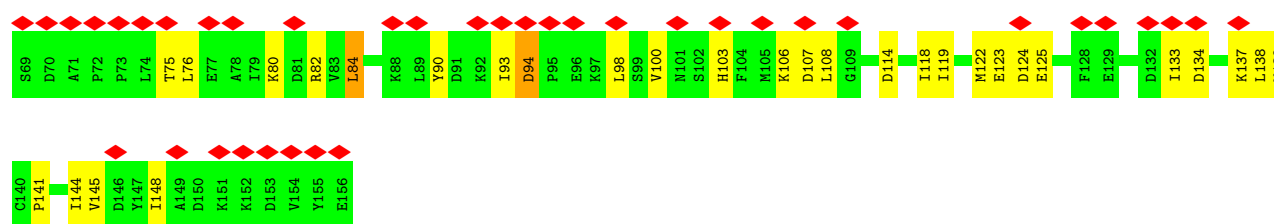
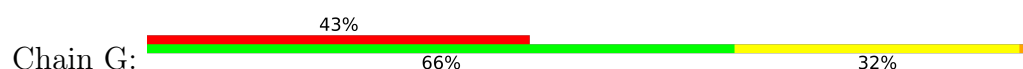
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



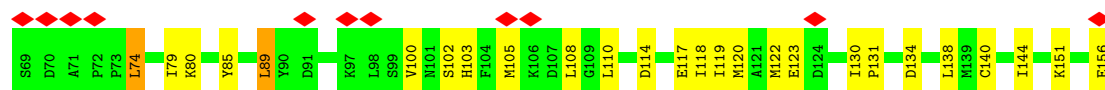
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



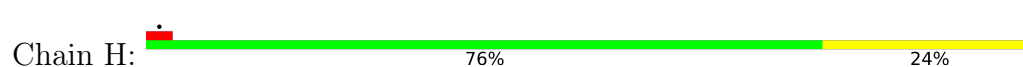
- Molecule 6: Acyl carrier protein



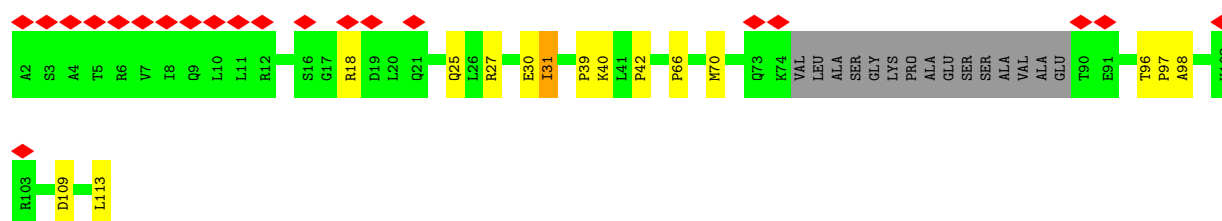
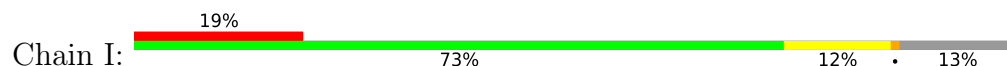
- Molecule 6: Acyl carrier protein



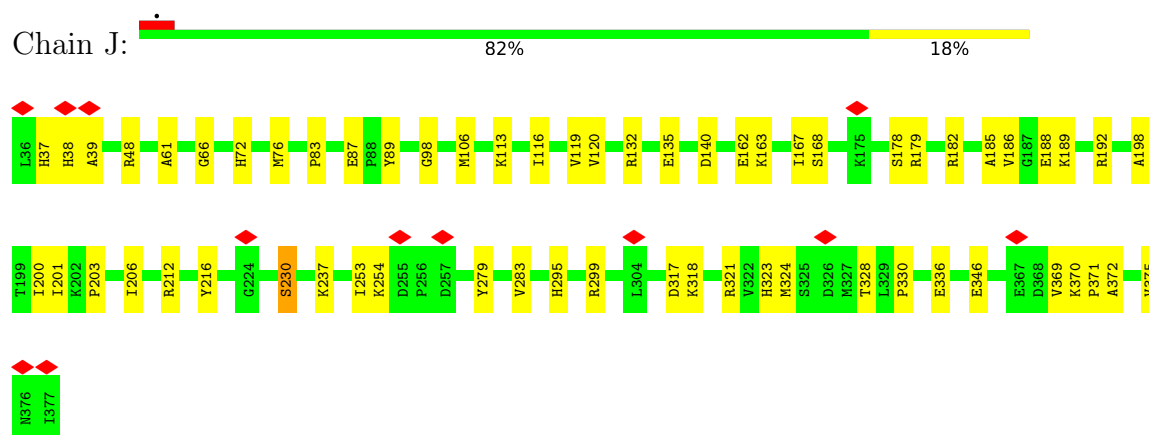
- Molecule 7: Complex I subunit B13



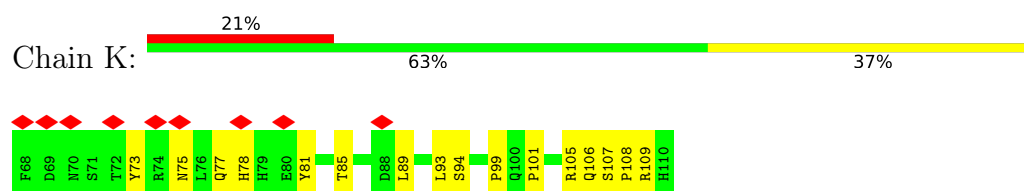
- Molecule 8: Complex I-B14.5a



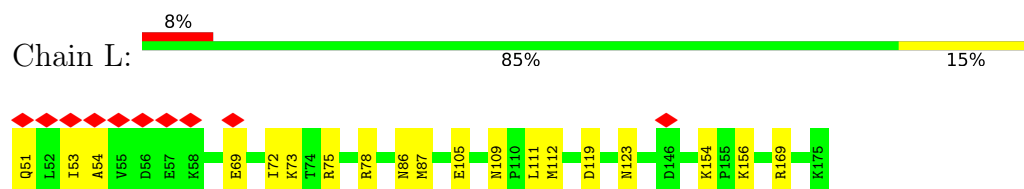
- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial



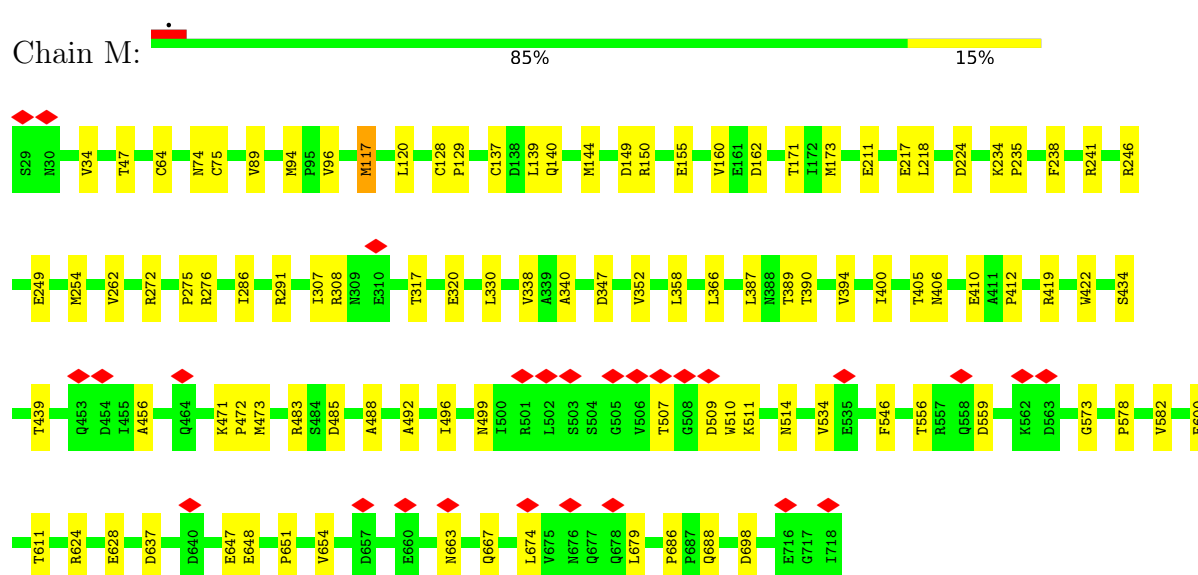
- Molecule 10: Complex I-9kD



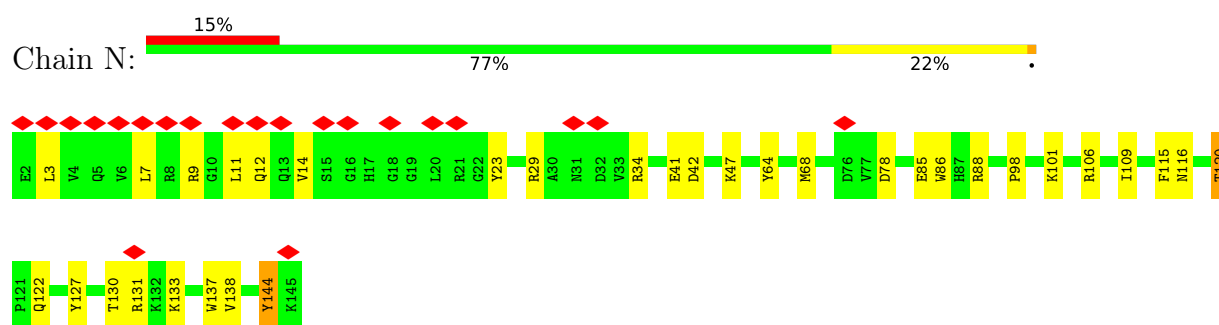
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



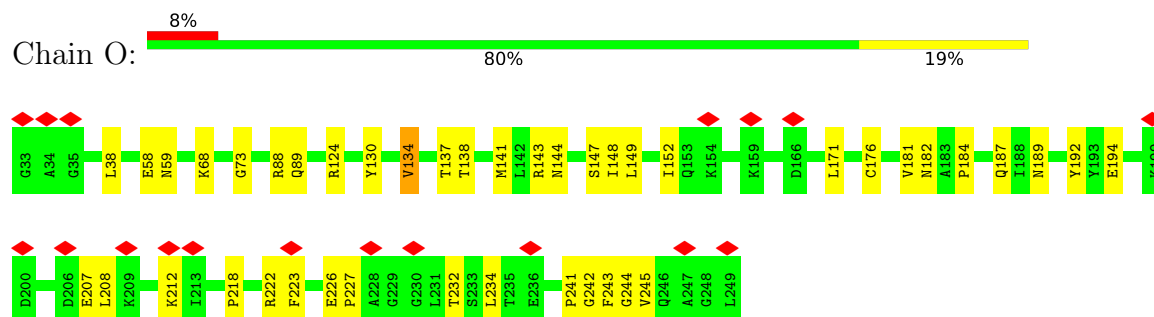
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



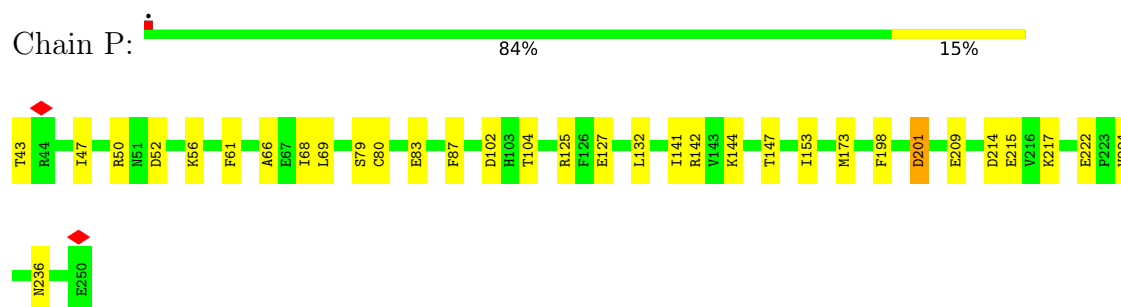
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



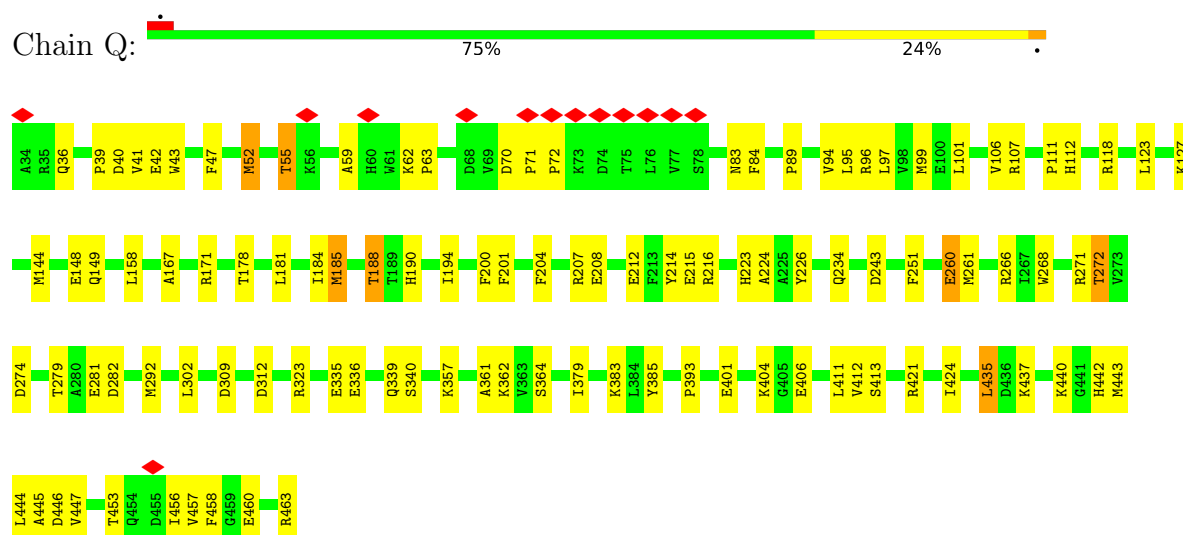
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



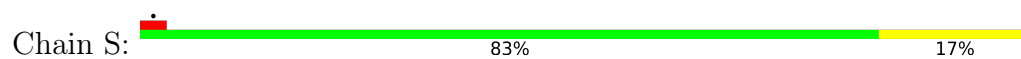
- Molecule 15: Complex I-30kD



- Molecule 16: Complex I-49kD



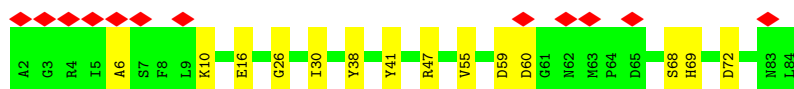
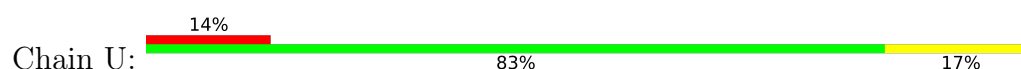
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



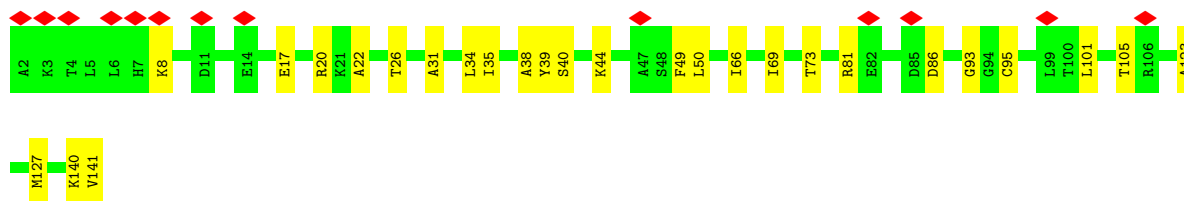
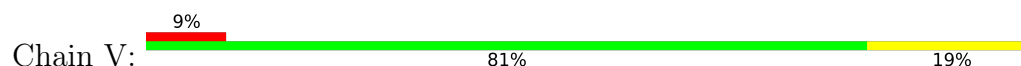
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



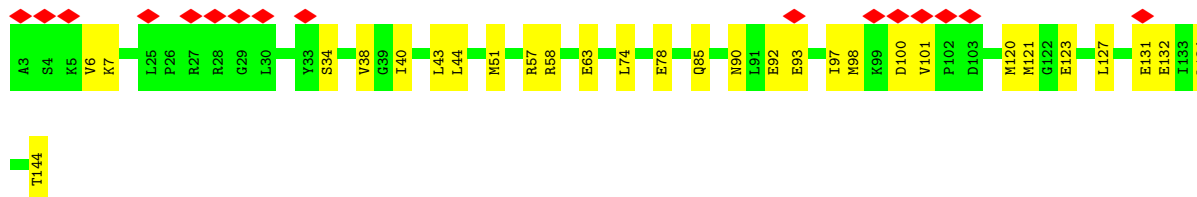
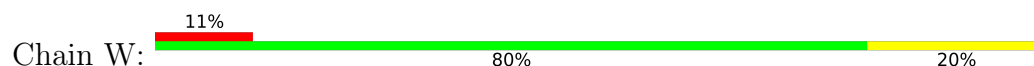
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



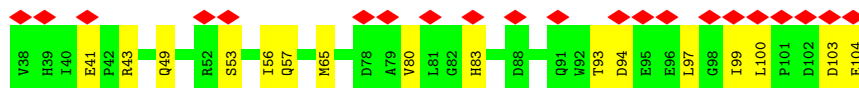
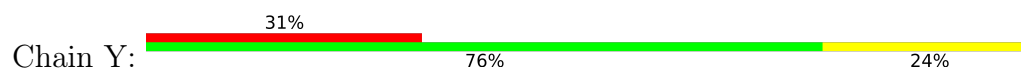
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



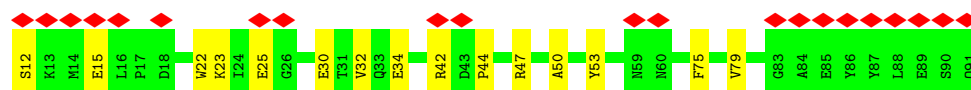
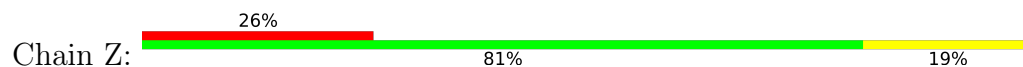
- Molecule 21: Complex I-B16.6



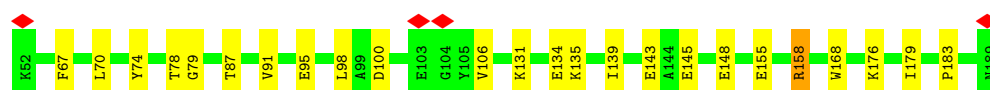
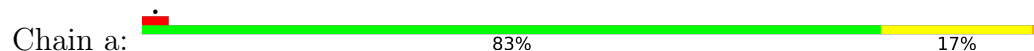
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



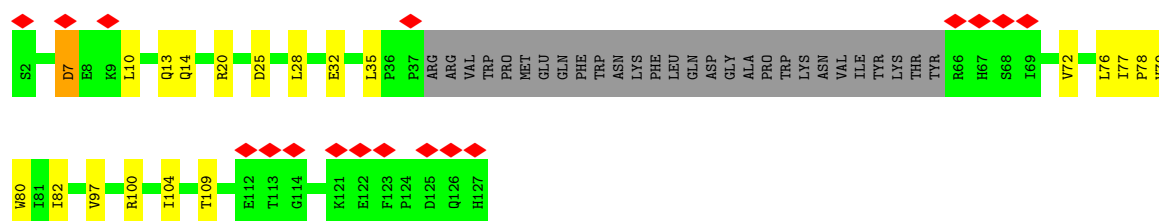
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



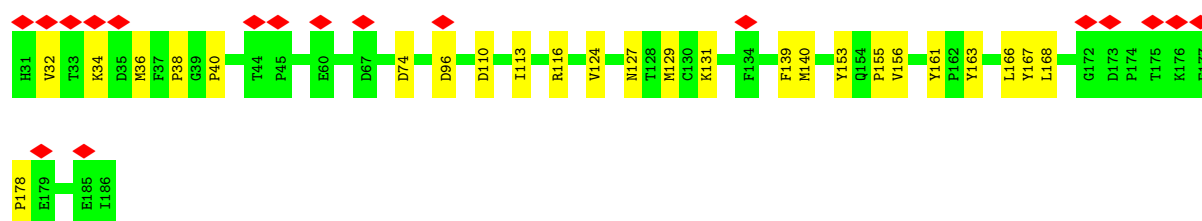
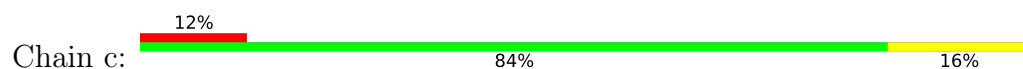
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



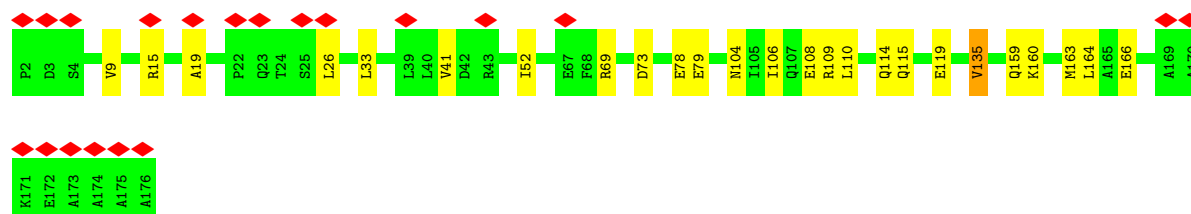
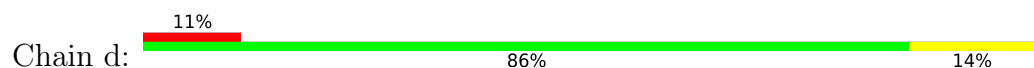
- Molecule 25: Complex I-B17



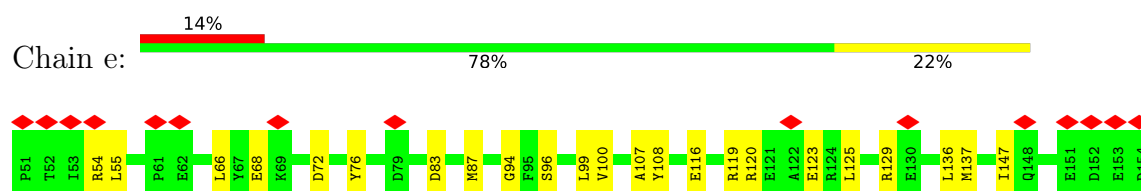
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



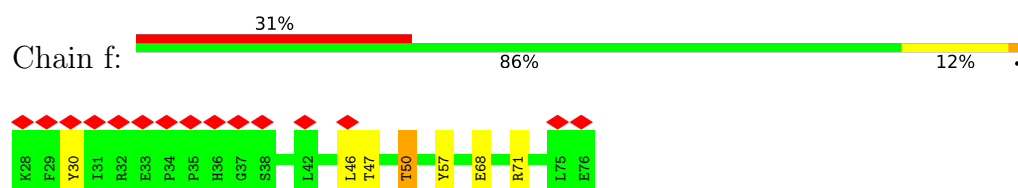
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



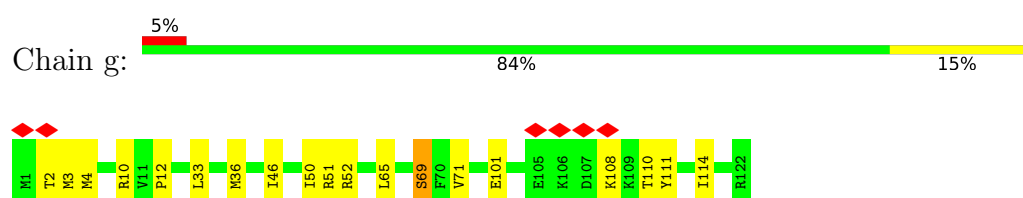
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



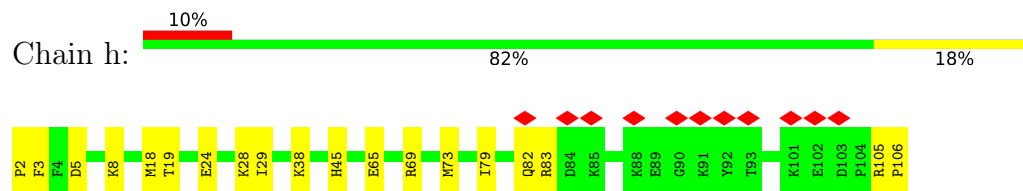
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



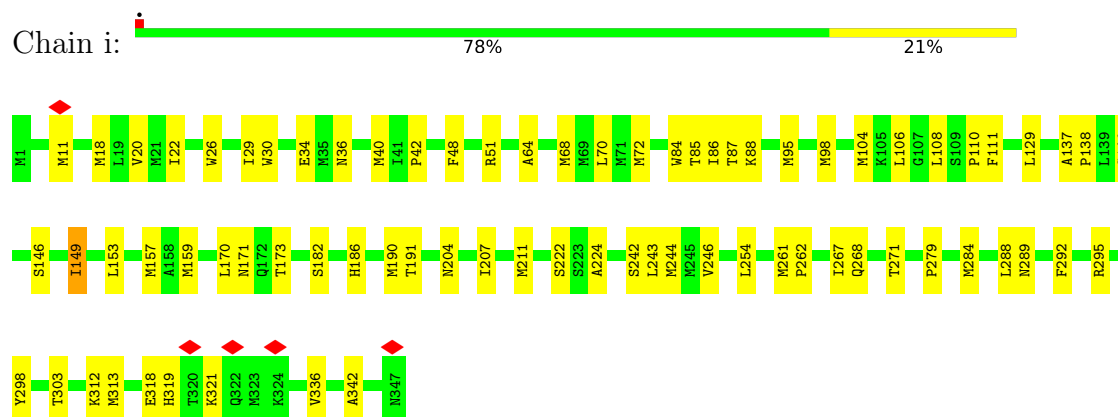
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



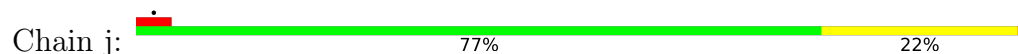
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

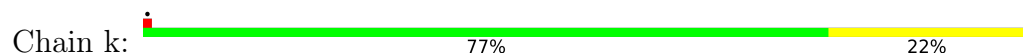


- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

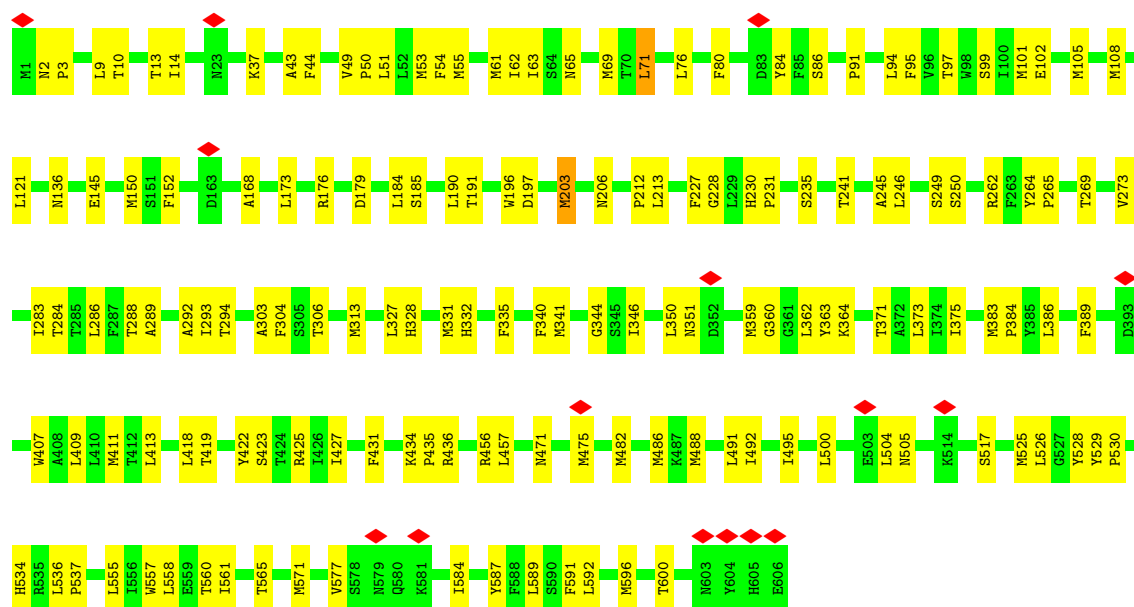




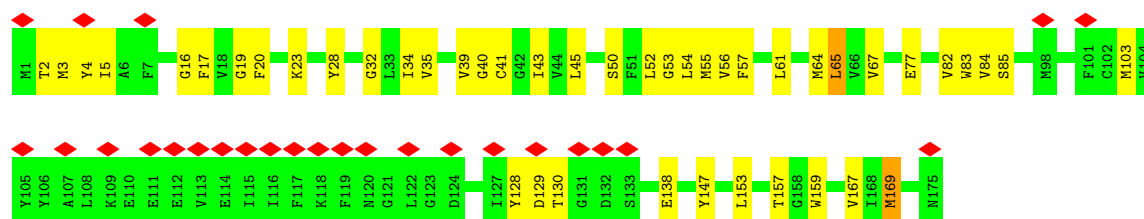
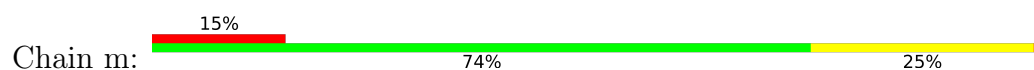
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L



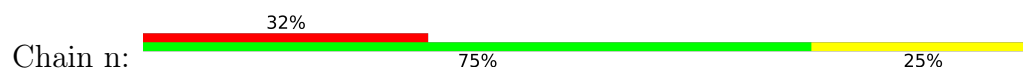
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

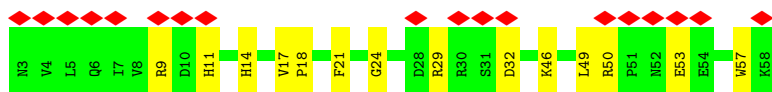


- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

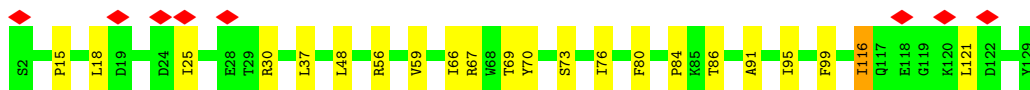
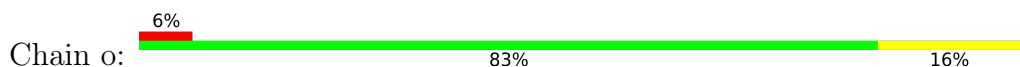


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

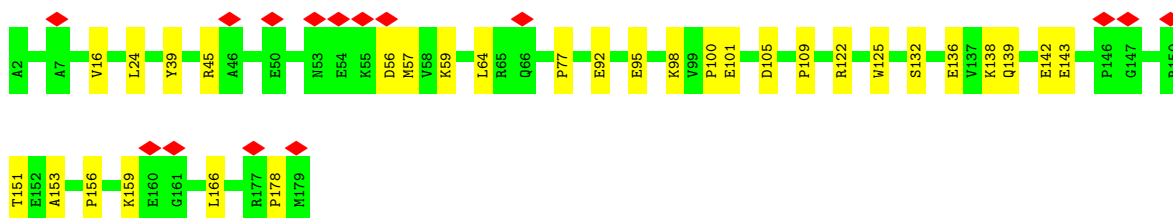
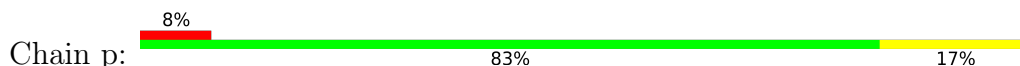




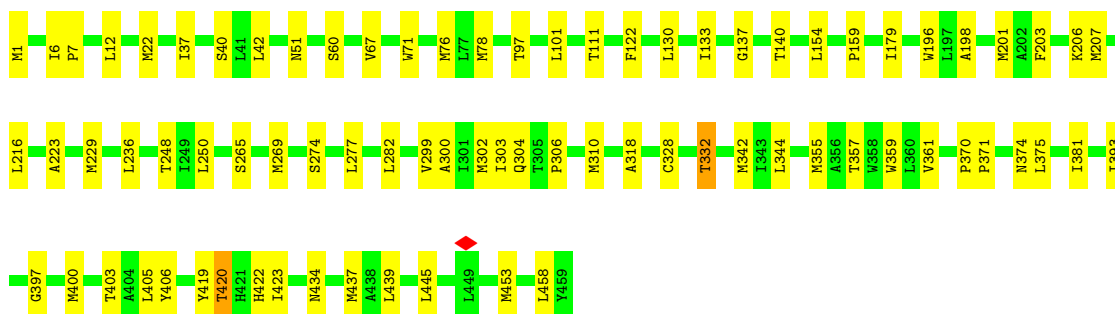
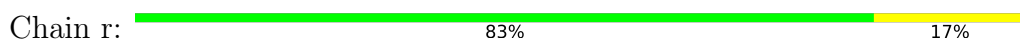
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



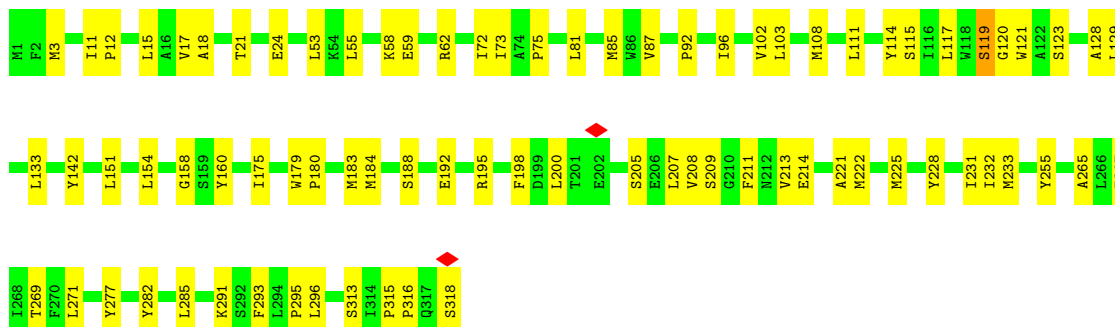
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



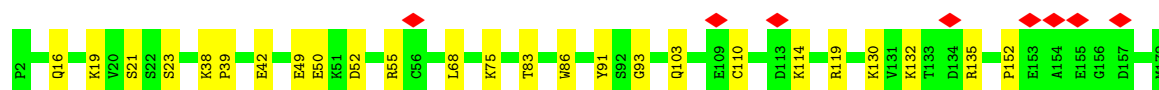
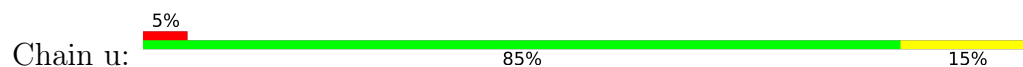
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4



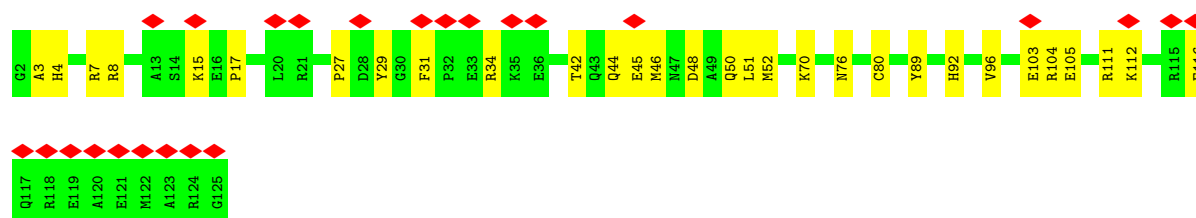
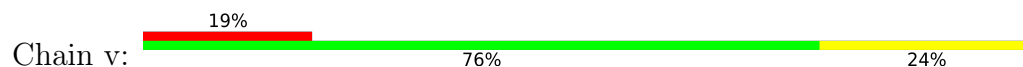
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1



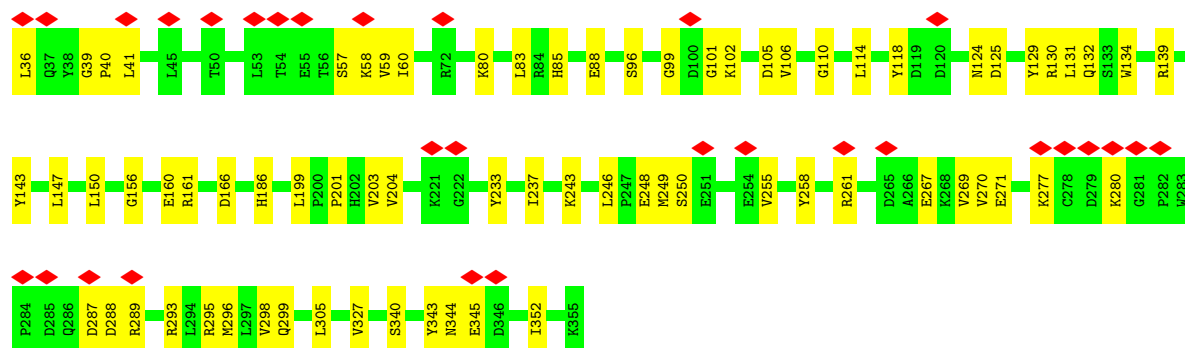
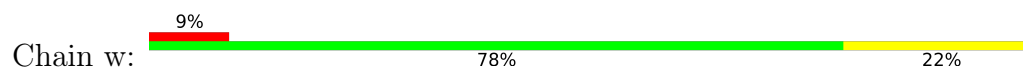
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 43: Complex I-B18



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63357	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 ($e^-/\text{\AA}^2$)	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	0.204	Depositor
Minimum map value	-0.134	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0336	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SF4, PEE, PLX, FMN, MG, 8Q1, 970, FES, NDP, UQ, ADP, 2MR, CDL, NAI

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.13	0/3406	0.34	0/4603
2	B	0.11	0/1442	0.29	0/1951
3	C	0.12	0/1279	0.32	0/1730
4	E	0.12	0/995	0.28	0/1340
5	F	0.16	0/695	0.44	0/936
6	G	0.14	0/705	0.38	0/956
6	X	0.14	0/705	0.39	0/955
7	H	0.12	0/929	0.33	0/1258
8	I	0.14	0/798	0.38	0/1079
9	J	0.11	0/2828	0.30	0/3834
10	K	0.18	0/377	0.42	0/509
11	L	0.11	0/1039	0.30	0/1403
12	M	0.11	0/5372	0.31	0/7279
13	N	0.14	0/1241	0.43	2/1690 (0.1%)
14	O	0.13	0/1707	0.35	0/2324
15	P	0.12	0/1789	0.31	0/2436
16	Q	0.15	0/3538	0.34	0/4796
17	S	0.13	0/581	0.35	0/781
18	T	0.10	0/755	0.28	0/1018
19	U	0.11	0/664	0.30	0/912
20	V	0.11	0/1042	0.26	0/1411
21	W	0.15	0/1192	0.35	0/1610
22	Y	0.12	0/610	0.31	0/836
23	Z	0.14	0/660	0.37	0/892
24	a	0.12	0/1184	0.29	0/1603
25	b	0.14	0/844	0.38	0/1149
26	c	0.15	0/1371	0.38	0/1875
27	d	0.11	0/1494	0.29	0/2015
28	e	0.14	0/880	0.38	0/1196
29	f	0.10	0/385	0.27	0/522
30	g	0.11	0/1036	0.26	0/1401
31	h	0.11	0/889	0.31	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.16	0/2773	0.39	1/3768 (0.0%)
33	j	0.12	0/938	0.31	0/1281
34	k	0.13	0/759	0.34	0/1029
35	l	0.14	0/4926	0.35	0/6700
36	m	0.21	0/1307	0.46	0/1777
37	n	0.13	0/491	0.29	0/663
38	o	0.12	0/1092	0.28	0/1481
39	p	0.12	0/1586	0.31	1/2151 (0.0%)
40	r	0.12	0/3715	0.29	0/5067
41	s	0.16	0/2581	0.37	0/3529
42	u	0.14	0/1436	0.35	0/1938
43	v	0.15	0/1060	0.35	0/1421
44	w	0.10	0/2646	0.30	0/3584
All	All	0.13	0/67742	0.34	4/91879 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N	138	VAL	CA-C-N	7.18	124.83	119.66
13	N	138	VAL	C-N-CA	7.18	124.83	119.66
39	p	109	PRO	CA-N-CD	-5.89	103.75	112.00
32	i	48	PHE	N-CA-C	5.02	116.91	108.73

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	87	0
2	B	1411	0	1360	25	0
3	C	1248	0	1254	25	0
4	E	971	0	975	14	0
5	F	684	0	698	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	693	0	671	20	0
6	X	693	0	678	19	0
7	H	910	0	950	17	0
8	I	780	0	808	15	0
9	J	2751	0	2773	40	0
10	K	366	0	338	12	0
11	L	1016	0	1016	16	0
12	M	5284	0	5311	68	0
13	N	1200	0	1151	24	0
14	O	1667	0	1662	33	0
15	P	1738	0	1693	23	0
16	Q	3459	0	3396	80	0
17	S	566	0	561	9	0
18	T	741	0	702	6	0
19	U	643	0	642	14	0
20	V	1021	0	1025	18	0
21	W	1161	0	1144	25	0
22	Y	584	0	529	11	0
23	Z	641	0	620	12	0
24	a	1151	0	1164	22	0
25	b	819	0	835	14	0
26	c	1315	0	1208	18	0
27	d	1461	0	1429	21	0
28	e	856	0	807	16	0
29	f	377	0	353	5	0
30	g	1005	0	999	15	0
31	h	867	0	871	17	0
32	i	2710	0	2874	62	0
33	j	914	0	951	27	0
34	k	748	0	799	20	0
35	l	4797	0	4935	113	0
36	m	1276	0	1243	47	0
37	n	479	0	486	13	0
38	o	1062	0	1072	14	0
39	p	1530	0	1459	21	0
40	r	3624	0	3832	56	0
41	s	2508	0	2607	64	0
42	u	1398	0	1374	20	0
43	v	1036	0	992	22	0
44	w	2586	0	2542	49	0
45	A	8	0	0	1	0
45	B	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	C	8	0	0	1	0
45	M	16	0	0	0	0
46	A	31	0	19	4	0
47	A	44	0	27	4	0
48	B	51	0	82	4	0
48	C	47	0	71	3	0
48	U	51	0	82	4	0
48	W	41	0	59	1	0
48	i	47	0	71	0	0
48	j	41	0	59	3	0
48	l	96	0	146	7	0
48	r	51	0	82	6	0
49	C	52	0	88	2	0
49	J	52	0	88	5	0
49	a	52	0	88	1	0
49	g	52	0	88	3	0
49	j	52	0	88	3	0
49	r	104	0	176	10	0
50	C	29	0	0	0	0
51	G	35	0	0	0	0
51	X	35	0	0	0	0
52	I	51	0	46	1	0
52	V	172	0	244	11	0
52	a	100	0	156	8	0
52	g	55	0	54	1	0
52	i	199	0	307	14	0
52	l	199	0	307	17	0
52	o	100	0	156	8	0
52	s	89	0	125	12	0
53	J	48	0	25	3	0
54	J	33	0	39	3	0
54	s	38	0	47	3	0
55	M	4	0	0	0	0
55	O	4	0	0	0	0
56	M	1	0	0	0	0
57	T	1	0	0	0	0
58	w	27	0	11	3	0
All	All	68209	0	68912	1138	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1138) 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)
53:J:401:NDP:O4D	53:J:401:NDP:C4D	1.68	1.20
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.17
1:A:89:GLY:HA2	1:A:244:ASN:HD22	1.02	1.14
36:m:64:MET:HE2	36:m:64:MET:HA	1.32	1.10
1:A:89:GLY:HA2	1:A:244:ASN:ND2	1.67	1.07
1:A:89:GLY:CA	1:A:244:ASN:HD22	1.72	1.01
36:m:65:LEU:HD12	41:s:117:LEU:HD11	1.63	0.80
1:A:63:TYR:HD2	14:O:241:PRO:HB2	1.47	0.79
41:s:24:GLU:HG3	41:s:271:LEU:HD22	1.63	0.79
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.64	0.79
33:j:67:LEU:HD11	34:k:68:ALA:HB3	1.65	0.79
16:Q:188:THR:OG1	16:Q:200:PHE:HA	1.83	0.79
33:j:105:GLU:HA	36:m:169:MET:HE1	1.65	0.78
30:g:51:ARG:HH22	32:i:319:HIS:HB3	1.48	0.78
34:k:28:SER:HB3	36:m:23:LYS:HG2	1.64	0.78
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.63	0.77
34:k:64:LEU:O	34:k:67:ALA:HB3	1.84	0.77
1:A:63:TYR:CD2	14:O:241:PRO:HB2	2.20	0.77
36:m:34:ILE:HG13	36:m:64:MET:HG3	1.67	0.76
36:m:64:MET:HA	36:m:64:MET:CE	2.15	0.75
41:s:184:MET:HE2	41:s:293:PHE:HA	1.69	0.75
21:W:121:MET:HB2	36:m:130:THR:HG23	1.69	0.74
27:d:163:MET:HA	27:d:166:GLU:HG2	1.68	0.74
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.70	0.74
16:Q:83:ASN:HB2	33:j:38:GLU:HG2	1.68	0.74
6:X:85:TYR:O	6:X:89:LEU:HD23	1.87	0.74
41:s:102:VAL:HG21	41:s:154:LEU:HD11	1.70	0.73
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.24	0.72
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.69	0.72
1:A:152:ARG:NH2	10:K:99:PRO:O	2.23	0.72
36:m:82:VAL:HG21	52:s:401:CDL:HB31	1.71	0.72
35:l:176:ARG:HA	35:l:179:ASP:HB2	1.72	0.72
52:V:201:CDL:H521	35:l:577:VAL:HA	1.72	0.71
16:Q:184:ILE:HD11	16:Q:251:PHE:HZ	1.55	0.71
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.72	0.71
36:m:64:MET:HE2	36:m:64:MET:CA	2.17	0.71
2:B:181:GLU:N	2:B:181:GLU:OE2	2.25	0.70
3:C:71:CYS:HB2	45:C:301:SF4:S4	2.32	0.70
21:W:85:GLN:OE1	31:h:105:ARG:NH1	2.24	0.70
14:O:38:LEU:O	14:O:124:ARG:NH2	2.25	0.70
1:A:308:ILE:HD12	1:A:308:ILE:H	1.57	0.69
36:m:82:VAL:HG12	36:m:85:SER:HB3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.72	0.69
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.74	0.69
28:e:68:GLU:N	28:e:68:GLU:OE1	2.25	0.69
4:E:41:ARG:NH1	6:G:124:ASP:OD1	2.26	0.69
1:A:396:MET:HE3	1:A:435:VAL:HG22	1.74	0.68
35:l:525:MET:HE2	39:p:77:PRO:HB3	1.75	0.68
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.26	0.68
44:w:139:ARG:HH12	58:w:401:ADP:HN61	1.41	0.68
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.26	0.68
1:A:385:CYS:HB3	45:A:501:SF4:S2	2.34	0.68
11:L:123:ASN:OD1	12:M:246:ARG:NH2	2.27	0.68
32:i:30:TRP:HD1	32:i:70:LEU:HD23	1.60	0.68
32:i:190:MET:HE2	32:i:204:ASN:HD22	1.59	0.67
35:l:351:ASN:O	35:l:351:ASN:ND2	2.26	0.67
26:c:116:ARG:HG2	48:l:703:PEE:H49	1.77	0.67
5:F:24:CYS:N	5:F:58:CYS:SG	2.67	0.67
27:d:79:GLU:HB2	30:g:108:LYS:HG2	1.77	0.67
21:W:57:ARG:HB3	41:s:316:PRO:HG3	1.77	0.67
40:r:370:PRO:HG3	40:r:375:LEU:HG	1.77	0.67
49:a:202:PLX:H92	40:r:40:SER:HB3	1.77	0.67
37:n:50:ARG:HB2	37:n:53:GLU:HG2	1.76	0.67
1:A:185:ASN:OD1	1:A:190:GLY:N	2.28	0.66
7:H:38:ILE:O	7:H:45:ARG:NH1	2.29	0.66
33:j:48:ARG:NH2	41:s:121:TRP:O	2.28	0.66
39:p:101:GLU:HG2	39:p:122:ARG:HH21	1.60	0.66
10:K:105:ARG:HH12	11:L:169:ARG:NE	1.93	0.66
35:l:3:PRO:HG2	35:l:53:MET:HE1	1.76	0.66
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.76	0.66
25:b:28:LEU:HD22	25:b:32:GLU:HG2	1.78	0.65
38:o:116:ILE:HG13	38:o:121:LEU:HD12	1.77	0.65
15:P:209:GLU:HG2	15:P:224:VAL:HA	1.78	0.65
52:l:701:CDL:H452	40:r:445:LEU:HB3	1.79	0.65
16:Q:52:MET:HE2	32:i:173:THR:HG22	1.78	0.65
44:w:345:GLU:HG3	44:w:352:ILE:HD12	1.77	0.65
12:M:89:VAL:HB	12:M:94:MET:HG3	1.79	0.65
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.79	0.64
25:b:7:ASP:OD1	25:b:7:ASP:N	2.28	0.64
24:a:179:ILE:HG21	31:h:38:LYS:HG3	1.79	0.64
27:d:33:LEU:HD13	35:l:49:VAL:HG13	1.80	0.64
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.31	0.64
44:w:132:GLN:NE2	44:w:166:ASP:OD1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:50:GLN:O	7:H:54:GLU:HG3	1.98	0.64
10:K:106:GLN:O	14:O:73:GLY:HA2	1.97	0.64
35:l:488:MET:HA	35:l:488:MET:HE3	1.79	0.64
24:a:135:LYS:NZ	40:r:51:ASN:O	2.31	0.64
27:d:110:LEU:HG	35:l:203:MET:HG3	1.80	0.64
41:s:75:PRO:HB2	41:s:222:MET:HE3	1.80	0.64
1:A:159:ARG:NH2	14:O:176:CYS:O	2.31	0.63
35:l:51:LEU:O	35:l:55:MET:HG3	1.97	0.63
1:A:40:ARG:NH1	1:A:289:GLU:O	2.31	0.63
1:A:299:LEU:HD12	1:A:303:HIS:HD2	1.63	0.63
16:Q:282:ASP:OD2	16:Q:437:LYS:NZ	2.32	0.63
1:A:109:ARG:NH1	1:A:237:GLY:O	2.30	0.63
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.80	0.63
2:B:111:GLU:O	2:B:141:ARG:NH1	2.31	0.63
4:E:23:ARG:HH12	11:L:51:GLN:HB3	1.64	0.62
6:G:144:ILE:O	6:G:148:ILE:HG13	1.99	0.62
38:o:91:ALA:O	38:o:95:ILE:HB	1.98	0.62
2:B:133:GLU:OE1	13:N:131:ARG:NH2	2.32	0.62
35:l:150:MET:HE3	35:l:150:MET:HA	1.80	0.62
36:m:129:ASP:O	36:m:130:THR:OG1	2.14	0.62
12:M:647:GLU:HB2	12:M:654:VAL:HG21	1.80	0.62
16:Q:52:MET:HE3	32:i:295:ARG:HD3	1.81	0.62
16:Q:62:LYS:HD3	16:Q:63:PRO:HD2	1.81	0.62
52:l:702:CDL:H142	52:l:702:CDL:H752	1.81	0.62
27:d:104:ASN:O	27:d:108:GLU:HG3	2.00	0.62
2:B:184:LEU:HB3	11:L:112:MET:HE2	1.82	0.62
13:N:144:TYR:HD1	13:N:144:TYR:H	1.48	0.62
40:r:76:MET:HG2	40:r:229:MET:HE2	1.81	0.62
9:J:135:GLU:HG2	9:J:140:ASP:HA	1.82	0.62
28:e:116:GLU:OE1	28:e:120:ARG:NH2	2.32	0.62
35:l:10:THR:HA	35:l:13:THR:HG22	1.81	0.62
6:G:90:TYR:HD2	6:G:93:ILE:HD12	1.64	0.61
31:h:18:MET:HE3	34:k:56:ALA:HA	1.82	0.61
17:S:66:LEU:HD13	42:u:75:LYS:HB2	1.82	0.61
35:l:592:LEU:HG	35:l:596:MET:HE2	1.81	0.61
33:j:27:LEU:HA	41:s:59:GLU:HG3	1.83	0.61
10:K:107:SER:OG	10:K:108:PRO:HD2	2.00	0.61
52:l:701:CDL:H822	52:l:701:CDL:H631	1.83	0.61
14:O:242:GLY:HA2	14:O:245:VAL:CG2	2.30	0.61
52:l:701:CDL:H411	40:r:371:PRO:HD2	1.83	0.61
14:O:134:VAL:HG11	14:O:149:LEU:HD13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:93:GLU:O	21:W:97:ILE:HD12	2.01	0.61
32:i:104:MET:HG3	32:i:111:PHE:HB3	1.83	0.61
36:m:16:GLY:HA2	52:s:401:CDL:H791	1.83	0.61
1:A:295:PRO:HG2	1:A:298:GLU:HB3	1.83	0.60
12:M:307:ILE:HG22	12:M:582:VAL:HG22	1.83	0.60
16:Q:99:MET:HE3	16:Q:101:LEU:HD21	1.83	0.60
20:V:17:GLU:OE2	20:V:20:ARG:NH1	2.34	0.60
35:l:228:GLY:HA3	48:l:703:PEE:H37	1.82	0.60
42:u:16:GLN:HG3	42:u:68:LEU:HD11	1.84	0.60
44:w:60:ILE:HG12	44:w:203:VAL:HB	1.83	0.60
32:i:87:THR:HG22	32:i:88:LYS:H	1.66	0.60
30:g:52:ARG:NH1	32:i:318:GLU:OE1	2.34	0.60
6:X:108:LEU:HB2	6:X:110:LEU:HD12	1.83	0.60
44:w:267:GLU:O	44:w:271:GLU:HG2	2.02	0.60
44:w:125:ASP:O	44:w:130:ARG:NH2	2.35	0.60
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.84	0.60
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.84	0.60
12:M:624:ARG:NH2	12:M:637:ASP:OD2	2.33	0.60
32:i:87:THR:CG2	32:i:88:LYS:H	2.15	0.60
34:k:23:ARG:HG3	36:m:23:LYS:HE2	1.84	0.60
44:w:39:GLY:HA2	44:w:296:MET:HE1	1.84	0.60
33:j:73:LEU:O	41:s:160:TYR:OH	2.20	0.60
39:p:138:LYS:O	39:p:142:GLU:HG2	2.02	0.60
44:w:250:SER:O	44:w:280:LYS:NZ	2.35	0.59
32:i:11:MET:HG2	52:i:401:CDL:H581	1.84	0.59
32:i:186:HIS:O	32:i:190:MET:HE3	2.02	0.59
41:s:222:MET:HG2	41:s:225:MET:HE3	1.83	0.59
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.35	0.59
11:L:105:GLU:HA	12:M:611:THR:HG21	1.84	0.59
11:L:109:ASN:ND2	11:L:111:LEU:O	2.35	0.59
20:V:123:ALA:O	20:V:127:MET:HG3	2.03	0.59
6:G:138:LEU:HD23	6:G:144:ILE:HG12	1.85	0.59
24:a:91:VAL:HG13	27:d:52:ILE:HG12	1.84	0.59
9:J:188:GLU:HG3	9:J:200:ILE:HD13	1.83	0.59
9:J:323:HIS:O	9:J:323:HIS:ND1	2.35	0.59
12:M:308:ARG:NH2	12:M:578:PRO:O	2.35	0.59
13:N:144:TYR:HD1	13:N:144:TYR:N	2.01	0.58
16:Q:185:MET:HE1	16:Q:204:PHE:HZ	1.67	0.58
32:i:207:ILE:HG22	32:i:211:MET:HE2	1.85	0.58
36:m:52:LEU:O	36:m:56:VAL:HG12	2.02	0.58
12:M:400:ILE:HG13	12:M:473:MET:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.85	0.58
12:M:224:ASP:OD2	12:M:291:ARG:NH2	2.31	0.58
1:A:79:GLU:O	1:A:83:SER:OG	2.21	0.58
23:Z:15:GLU:OE2	23:Z:15:GLU:N	2.37	0.58
43:v:70:LYS:HG2	43:v:80:CYS:SG	2.43	0.58
13:N:29:ARG:NH2	13:N:64:TYR:O	2.35	0.58
32:i:321:LYS:NZ	52:i:401:CDL:OA4	2.37	0.58
6:X:103:HIS:HE1	6:X:105:MET:HB2	1.69	0.58
32:i:246:VAL:HG21	52:i:403:CDL:H362	1.85	0.58
27:d:160:LYS:NZ	30:g:114:ILE:O	2.36	0.58
40:r:67:VAL:HG12	49:r:503:PLX:H362	1.85	0.58
8:I:70:MET:HG3	15:P:66:ALA:HB1	1.85	0.57
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.29	0.57
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.25	0.57
28:e:119:ARG:O	28:e:123:GLU:HG3	2.04	0.57
32:i:64:ALA:O	32:i:68:MET:HG2	2.03	0.57
3:C:78:HIS:HD1	16:Q:208:GLU:HG2	1.69	0.57
9:J:182:ARG:O	9:J:186:VAL:HG23	2.04	0.57
48:U:101:PEE:H26	41:s:295:PRO:HB3	1.85	0.57
9:J:212:ARG:O	9:J:216:TYR:HB2	2.03	0.57
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.85	0.57
11:L:69:GLU:H	11:L:69:GLU:CD	2.12	0.57
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.40	0.57
6:G:141:PRO:O	6:G:145:VAL:HG23	2.05	0.57
20:V:34:LEU:HD22	52:V:202:CDL:H261	1.87	0.57
28:e:129:ARG:NH1	28:e:136:LEU:O	2.34	0.57
6:G:133:ILE:HD12	6:G:134:ASP:H	1.70	0.57
8:I:40:LYS:HB3	21:W:7:LYS:H	1.70	0.57
6:X:89:LEU:O	23:Z:47:ARG:NH2	2.38	0.57
32:i:261:MET:HE1	32:i:336:VAL:HG12	1.85	0.57
34:k:65:VAL:HG11	36:m:157:THR:HG23	1.87	0.57
20:V:81:ARG:NH2	20:V:86:ASP:OD2	2.37	0.57
35:l:71:LEU:HD12	40:r:310:MET:HE1	1.87	0.57
41:s:265:ALA:O	41:s:269:THR:HG23	2.04	0.57
24:a:74:TYR:O	28:e:96:SER:OG	2.20	0.57
31:h:24:GLU:OE1	31:h:28:LYS:NZ	2.37	0.57
35:l:203:MET:HE2	35:l:203:MET:HA	1.85	0.57
1:A:425:CYS:SG	1:A:426:ALA:N	2.77	0.56
42:u:83:THR:HA	42:u:86:TRP:CD1	2.39	0.56
1:A:396:MET:HE1	1:A:438:LEU:HD23	1.87	0.56
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:218:PRO:HD2	14:O:223:PHE:HA	1.86	0.56
16:Q:302:LEU:HD11	16:Q:406:GLU:HG3	1.87	0.56
20:V:22:ALA:O	20:V:26:THR:OG1	2.23	0.56
32:i:312:LYS:HE3	44:w:327:VAL:HG11	1.87	0.56
40:r:306:PRO:O	40:r:310:MET:HG3	2.05	0.56
15:P:147:THR:HB	15:P:153:ILE:HD11	1.86	0.56
1:A:119:GLU:O	1:A:159:ARG:NH1	2.38	0.56
6:G:137:LYS:N	6:G:137:LYS:HD2	2.21	0.56
9:J:192:ARG:NH1	9:J:198:ALA:O	2.39	0.56
11:L:72:ILE:HG22	11:L:73:LYS:HD2	1.87	0.56
21:W:97:ILE:HD12	21:W:97:ILE:H	1.69	0.56
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.88	0.56
11:L:75:ARG:NH1	11:L:119:ASP:OD1	2.32	0.56
13:N:14:VAL:HG23	13:N:23:TYR:CG	2.41	0.56
41:s:119:SER:O	41:s:123:SER:OG	2.22	0.56
26:c:124:VAL:HG23	35:l:525:MET:HE1	1.87	0.56
37:n:24:GLY:HA2	40:r:6:ILE:HD12	1.88	0.56
1:A:448:GLU:O	1:A:452:GLN:HG3	2.05	0.56
32:i:95:MET:HE2	32:i:149:ILE:HG13	1.87	0.56
3:C:79:MET:HE2	3:C:86:MET:HB3	1.88	0.55
35:l:136:ASN:HA	35:l:197:ASP:HA	1.87	0.55
48:r:501:PEE:H81	49:r:502:PLX:H393	1.88	0.55
30:g:111:TYR:HA	30:g:114:ILE:HD12	1.88	0.55
27:d:159:GLN:O	27:d:163:MET:HG3	2.06	0.55
44:w:118:TYR:OH	58:w:401:ADP:O2'	2.24	0.55
27:d:15:ARG:HG3	27:d:15:ARG:O	2.05	0.55
1:A:60:GLY:HA2	14:O:241:PRO:HA	1.88	0.55
15:P:68:ILE:HG22	15:P:69:LEU:HG	1.88	0.55
26:c:167:TYR:HD2	26:c:168:LEU:HD22	1.71	0.55
32:i:146:SER:HA	32:i:149:ILE:HD12	1.88	0.55
12:M:394:VAL:HG22	12:M:473:MET:HE1	1.87	0.55
36:m:45:LEU:HG	36:m:50:SER:HA	1.87	0.55
5:F:25:GLN:NE2	5:F:57:GLU:OE1	2.38	0.55
15:P:173:MET:HB3	15:P:198:PHE:HB2	1.89	0.55
25:b:72:VAL:HA	25:b:76:LEU:HB2	1.87	0.55
25:b:100:ARG:NE	43:v:50:GLN:OE1	2.36	0.55
34:k:25:HIS:NE2	36:m:77:GLU:OE1	2.33	0.55
41:s:115:SER:O	41:s:119:SER:OG	2.20	0.55
41:s:228:TYR:HA	41:s:231:ILE:HD12	1.88	0.55
21:W:74:LEU:O	21:W:78:GLU:HG3	2.05	0.55
12:M:647:GLU:HA	12:M:651:PRO:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:130:TYR:HA	14:O:189:ASN:HD21	1.72	0.55
24:a:87:THR:O	24:a:91:VAL:HG23	2.07	0.55
11:L:78:ARG:NH2	12:M:249:GLU:OE1	2.39	0.54
14:O:207:GLU:HG3	14:O:212:LYS:HB2	1.89	0.54
35:l:419:THR:HA	35:l:422:TYR:CE2	2.42	0.54
1:A:171:VAL:O	1:A:175:GLU:HG2	2.08	0.54
13:N:144:TYR:N	13:N:144:TYR:CD1	2.73	0.54
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.89	0.54
21:W:90:ASN:ND2	21:W:123:GLU:O	2.40	0.54
6:X:117:GLU:OE1	39:p:45:ARG:NH1	2.40	0.54
35:l:558:LEU:HD21	52:o:201:CDL:H872	1.90	0.54
36:m:41:CYS:O	36:m:45:LEU:HD12	2.07	0.54
5:F:89:ARG:HE	5:F:89:ARG:HA	1.72	0.54
9:J:178:SER:OG	9:J:317:ASP:OD1	2.21	0.54
25:b:10:LEU:O	25:b:14:GLN:HG3	2.07	0.54
44:w:139:ARG:NH1	44:w:166:ASP:OD2	2.34	0.54
2:B:120:GLU:HB2	2:B:130:ILE:HD12	1.89	0.54
21:W:100:ASP:OD1	21:W:100:ASP:N	2.37	0.54
42:u:38:LYS:HB3	42:u:39:PRO:HD3	1.88	0.54
43:v:92:HIS:O	43:v:96:VAL:HG23	2.07	0.54
44:w:88:GLU:OE2	44:w:139:ARG:NH2	2.40	0.54
7:H:106:GLU:HG3	7:H:107:PRO:HD2	1.89	0.54
29:f:47:THR:HG23	30:g:65:LEU:HD22	1.89	0.54
35:l:99:SER:HB3	35:l:341:MET:HE1	1.88	0.54
35:l:423:SER:O	35:l:427:ILE:HG13	2.08	0.54
40:r:122:PHE:CE2	40:r:206:LYS:HD2	2.43	0.54
40:r:332:THR:HG21	40:r:355:MET:HE3	1.88	0.54
1:A:263:ALA:HA	1:A:271:SER:HB3	1.89	0.54
14:O:243:PHE:CD1	14:O:243:PHE:C	2.86	0.54
23:Z:75:PHE:O	23:Z:79:VAL:HG22	2.06	0.54
35:l:500:LEU:HD23	52:l:702:CDL:H562	1.89	0.54
37:n:29:ARG:O	37:n:32:ASP:HB2	2.06	0.54
48:B:303:PEE:H72	41:s:183:MET:HG2	1.90	0.54
21:W:51:MET:HA	41:s:313:SER:HB2	1.89	0.54
30:g:33:LEU:HD22	30:g:71:VAL:HG13	1.90	0.54
2:B:200:GLU:HG3	13:N:88:ARG:HB2	1.89	0.54
16:Q:261:MET:HE2	16:Q:261:MET:HA	1.90	0.54
40:r:265:SER:O	40:r:269:MET:HG3	2.07	0.54
7:H:58:MET:HE3	7:H:72:LEU:HD23	1.90	0.53
9:J:212:ARG:O	9:J:216:TYR:CB	2.56	0.53
12:M:144:MET:HG3	16:Q:383:LYS:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:28:LYS:NZ	42:u:91:TYR:OH	2.27	0.53
40:r:1:MET:HE3	40:r:111:THR:HG21	1.90	0.53
3:C:69:LEU:HB2	3:C:107:GLY:HA3	1.90	0.53
35:l:560:THR:O	35:l:565:THR:OG1	2.22	0.53
12:M:171:THR:HG23	12:M:173:MET:HE3	1.90	0.53
12:M:217:GLU:HG2	12:M:218:LEU:HG	1.89	0.53
16:Q:281:GLU:CD	16:Q:281:GLU:H	2.16	0.53
52:V:201:CDL:H581	32:i:110:PRO:HB3	1.89	0.53
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.42	0.53
16:Q:357:LYS:HD3	16:Q:364:SER:HB3	1.90	0.53
33:j:112:GLU:OE1	41:s:291:LYS:NZ	2.35	0.53
44:w:129:TYR:OH	44:w:186:HIS:ND1	2.31	0.53
32:i:30:TRP:O	32:i:34:GLU:HG2	2.09	0.53
6:G:119:ILE:O	6:G:123:GLU:HG3	2.09	0.53
40:r:122:PHE:HE2	40:r:206:LYS:HD2	1.72	0.53
44:w:246:LEU:HD22	44:w:255:VAL:HG11	1.90	0.53
20:V:69:ILE:O	20:V:73:THR:HG22	2.08	0.53
36:m:55:MET:HA	36:m:55:MET:HE2	1.91	0.53
6:G:122:MET:HE3	6:G:144:ILE:HG21	1.90	0.53
16:Q:268:TRP:O	16:Q:272:THR:OG1	2.21	0.53
15:P:50:ARG:NH1	15:P:80:CYS:SG	2.72	0.53
14:O:59:ASN:ND2	14:O:89:GLN:OE1	2.38	0.52
35:l:526:LEU:HD12	35:l:530:PRO:HG2	1.90	0.52
44:w:143:TYR:OH	44:w:199:LEU:O	2.23	0.52
12:M:330:LEU:HD21	12:M:546:PHE:CZ	2.44	0.52
19:U:16:GLU:HG3	48:U:101:PEE:H49	1.91	0.52
6:X:114:ASP:O	6:X:118:ILE:HG13	2.10	0.52
3:C:66:THR:HG22	3:C:95:ALA:HA	1.91	0.52
9:J:135:GLU:OE2	9:J:179:ARG:NH2	2.42	0.52
52:a:201:CDL:H592	48:l:704:PEE:H21	1.92	0.52
52:i:403:CDL:H332	52:i:403:CDL:H232	1.90	0.52
36:m:53:GLY:HA2	36:m:56:VAL:HG12	1.92	0.52
36:m:54:LEU:HD13	41:s:103:LEU:HB3	1.92	0.52
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.44	0.52
41:s:221:ALA:O	41:s:225:MET:HG2	2.09	0.52
3:C:175:TYR:HE1	13:N:78:ASP:HB2	1.75	0.52
6:X:85:TYR:O	6:X:89:LEU:CD2	2.54	0.52
6:G:114:ASP:O	6:G:118:ILE:HD12	2.10	0.52
19:U:59:ASP:OD1	42:u:130:LYS:HD3	2.10	0.52
6:X:103:HIS:CE1	6:X:105:MET:HB2	2.44	0.52
32:i:246:VAL:HG11	52:i:403:CDL:H392	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:o:56:ARG:NH2	40:r:422:HIS:O	2.43	0.52
41:s:62:ARG:NH2	52:s:401:CDL:OA3	2.43	0.52
12:M:389:THR:O	12:M:390:THR:OG1	2.25	0.52
24:a:70:LEU:HD13	28:e:87:MET:HE3	1.91	0.52
36:m:64:MET:HB2	41:s:114:TYR:OH	2.10	0.52
41:s:120:GLY:HA2	41:s:128:ALA:HB1	1.92	0.52
43:v:27:PRO:O	43:v:34:ARG:NH1	2.43	0.52
3:C:167:PRO:HD3	16:Q:223:HIS:CD2	2.45	0.52
12:M:307:ILE:HG23	12:M:317:THR:HG21	1.91	0.51
18:T:69:ASP:O	18:T:73:GLU:HG3	2.09	0.51
40:r:198:ALA:HB2	48:r:501:PEE:H22	1.91	0.51
1:A:185:ASN:ND2	1:A:187:CYS:O	2.42	0.51
2:B:131:GLU:HG3	2:B:144:ARG:HD2	1.92	0.51
14:O:182:ASN:OD1	14:O:222:ARG:NH2	2.44	0.51
32:i:20:VAL:HG11	32:i:137:ALA:HB1	1.92	0.51
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.90	0.51
17:S:53:ARG:NH1	31:h:106:PRO:O	2.43	0.51
22:Y:94:ASP:HB3	22:Y:99:ILE:HB	1.92	0.51
7:H:37:GLN:OE1	44:w:261:ARG:NH2	2.43	0.51
16:Q:188:THR:OG1	16:Q:200:PHE:CA	2.57	0.51
33:j:66:ASP:O	33:j:69:ILE:HG12	2.11	0.51
39:p:105:ASP:OD1	39:p:122:ARG:NH1	2.30	0.51
52:a:201:CDL:H521	48:l:704:PEE:H14	1.93	0.51
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.24	0.51
4:E:104:MET:HE3	4:E:104:MET:HA	1.92	0.51
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.46	0.51
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.91	0.51
35:l:245:ALA:O	35:l:249:SER:OG	2.26	0.51
12:M:330:LEU:HD21	12:M:546:PHE:HZ	1.75	0.51
26:c:153:TYR:OH	43:v:8:ARG:NH1	2.43	0.51
27:d:9:VAL:HA	27:d:109:ARG:HH21	1.76	0.51
32:i:204:ASN:OD1	32:i:262:PRO:HB2	2.11	0.51
41:s:179:TRP:CG	41:s:180:PRO:HD3	2.46	0.51
1:A:383:THR:HG21	12:M:120:LEU:HG	1.93	0.51
10:K:107:SER:OG	10:K:108:PRO:CD	2.58	0.51
27:d:73:ASP:OD1	27:d:73:ASP:N	2.35	0.51
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.46	0.51
1:A:141:GLY:HA2	1:A:252:PRO:HD3	1.92	0.50
1:A:423:THR:OG1	1:A:425:CYS:O	2.26	0.50
16:Q:40:ASP:OD1	16:Q:40:ASP:N	2.44	0.50
22:Y:103:ASP:OD1	22:Y:103:ASP:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:82:ILE:HD13	35:l:9:LEU:HB3	1.94	0.50
52:i:403:CDL:H821	40:r:101:LEU:HD21	1.93	0.50
35:l:227:PHE:O	35:l:230:HIS:ND1	2.41	0.50
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.93	0.50
1:A:210:THR:HB	1:A:224:ARG:H	1.77	0.50
7:H:58:MET:SD	7:H:71:GLN:HB3	2.51	0.50
15:P:125:ARG:NH2	15:P:201:ASP:OD1	2.38	0.50
17:S:54:ILE:HD11	42:u:19:LYS:HG2	1.92	0.50
35:l:102:GLU:HA	35:l:105:MET:HE3	1.93	0.50
12:M:472:PRO:O	12:M:510:TRP:NE1	2.38	0.50
13:N:9:ARG:O	13:N:12:GLN:HG3	2.12	0.50
21:W:98:MET:HE3	31:h:79:ILE:HD13	1.93	0.50
2:B:41:VAL:HA	8:I:113:LEU:HB2	1.93	0.50
8:I:30:GLU:OE2	8:I:30:GLU:N	2.33	0.50
9:J:167:ILE:HD13	9:J:201:ILE:HB	1.93	0.50
24:a:78:THR:HG22	28:e:100:VAL:HG11	1.94	0.50
36:m:55:MET:HE2	36:m:55:MET:CA	2.42	0.50
5:F:44:LEU:HD11	5:F:91:LEU:HD22	1.93	0.50
12:M:64:CYS:HB3	12:M:75:CYS:HB3	1.94	0.50
13:N:127:TYR:OH	18:T:61:GLU:O	2.23	0.50
30:g:46:ILE:O	30:g:50:ILE:HG13	2.11	0.50
34:k:41:PHE:HD1	34:k:42:ILE:HD12	1.77	0.50
39:p:92:GLU:HB3	39:p:95:GLU:HG3	1.94	0.50
7:H:55:LYS:HE3	15:P:104:THR:HG21	1.92	0.50
16:Q:111:PRO:HG3	16:Q:435:LEU:HD23	1.94	0.50
19:U:6:ALA:HB1	19:U:10:LYS:NZ	2.26	0.50
6:X:120:MET:HE1	39:p:24:LEU:HB3	1.94	0.50
48:B:303:PEE:O1P	16:Q:266:ARG:NH1	2.44	0.50
52:a:201:CDL:OB4	28:e:108:TYR:OH	2.24	0.50
5:F:21:ILE:HG12	5:F:65:LEU:HD12	1.92	0.50
9:J:185:ALA:O	9:J:189:LYS:HG3	2.12	0.50
19:U:68:SER:HA	42:u:130:LYS:HG2	1.93	0.50
35:l:241:THR:HG21	35:l:344:GLY:HA3	1.94	0.50
38:o:84:PRO:HG3	52:o:201:CDL:H522	1.93	0.50
17:S:7:PRO:O	17:S:11:VAL:HG23	2.12	0.50
32:i:298:TYR:O	32:i:303:THR:OG1	2.27	0.50
32:i:313:MET:HG2	44:w:305:LEU:HD13	1.94	0.50
1:A:131:ILE:HD13	1:A:158:ILE:HD12	1.94	0.49
8:I:27:ARG:HD2	8:I:31:ILE:HG21	1.94	0.49
12:M:117:MET:HE1	12:M:139:LEU:HD12	1.94	0.49
20:V:140:LYS:HE3	24:a:158:ARG:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:160:LYS:HE2	28:e:147:ILE:HG23	1.94	0.49
28:e:76:TYR:HB2	28:e:83:ASP:OD1	2.12	0.49
32:i:243:LEU:HD23	52:i:403:CDL:H361	1.94	0.49
35:l:332:HIS:HA	35:l:335:PHE:CZ	2.47	0.49
36:m:35:VAL:HG11	52:s:401:CDL:H792	1.94	0.49
3:C:66:THR:HG21	16:Q:89:PRO:HG3	1.94	0.49
8:I:42:PRO:HB3	21:W:6:VAL:HG21	1.94	0.49
14:O:137:THR:HG22	14:O:138:THR:H	1.77	0.49
52:V:202:CDL:H162	35:l:589:LEU:HD21	1.94	0.49
35:l:55:MET:HE2	35:l:471:ASN:HB2	1.93	0.49
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.94	0.49
37:n:18:PRO:O	37:n:21:PHE:HB3	2.12	0.49
5:F:27:SER:O	5:F:34:ARG:NH1	2.45	0.49
11:L:87:MET:HE2	12:M:272:ARG:HH12	1.77	0.49
13:N:85:GLU:HB2	13:N:98:PRO:HB3	1.94	0.49
31:h:69:ARG:O	31:h:73:MET:HG3	2.12	0.49
43:v:31:PHE:HD2	43:v:104:ARG:HH21	1.60	0.49
1:A:380:GLY:HA2	1:A:386:ARG:HB2	1.95	0.49
12:M:405:THR:OG1	12:M:410:GLU:OE1	2.31	0.49
23:Z:42:ARG:HH12	23:Z:44:PRO:HB3	1.77	0.49
35:l:54:PHE:CZ	35:l:84:TYR:HB2	2.47	0.49
1:A:151:ALA:O	1:A:191:TYR:OH	2.22	0.49
12:M:434:SER:HB2	12:M:686:PRO:HD2	1.94	0.49
35:l:346:ILE:HD12	35:l:362:LEU:HD13	1.95	0.49
1:A:185:ASN:O	1:A:187:CYS:N	2.45	0.49
1:A:204:TYR:OH	47:A:503:NAI:H5N	2.12	0.49
16:Q:52:MET:HB2	32:i:171:ASN:HA	1.94	0.49
22:Y:83:HIS:C	22:Y:83:HIS:CD2	2.90	0.49
46:A:502:FMN:O4'	46:A:502:FMN:O2'	2.26	0.49
18:T:105:GLU:OE2	18:T:122:HIS:HB3	2.13	0.49
31:h:2:PRO:HA	32:i:140:SER:HB2	1.94	0.49
44:w:114:LEU:HD12	44:w:131:LEU:HD21	1.93	0.49
1:A:299:LEU:HD12	1:A:303:HIS:CD2	2.47	0.49
1:A:312:ASP:HA	1:A:329:LYS:HE3	1.95	0.49
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.95	0.49
36:m:28:TYR:HB3	36:m:83:TRP:CH2	2.48	0.49
41:s:129:LEU:O	41:s:133:LEU:HD22	2.12	0.49
41:s:200:LEU:HG	41:s:282:TYR:HB3	1.95	0.49
1:A:46:TYR:CD1	14:O:234:LEU:HD12	2.47	0.49
12:M:406:ASN:ND2	12:M:688:GLN:O	2.41	0.49
24:a:145:GLU:O	24:a:148:GLU:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:596:MET:O	35:l:600:THR:HG23	2.12	0.49
1:A:89:GLY:O	47:A:503:NAI:H2N	2.13	0.49
1:A:126:LYS:O	1:A:130:ILE:HG13	2.12	0.49
3:C:188:LYS:HB3	3:C:191:ARG:HH11	1.77	0.49
25:b:109:THR:O	27:d:19:ALA:N	2.40	0.49
32:i:129:LEU:HD13	52:i:401:CDL:H311	1.94	0.49
35:l:293:ILE:HG13	35:l:294:THR:HG23	1.94	0.48
44:w:102:LYS:HE2	44:w:102:LYS:H	1.76	0.48
6:G:82:ARG:NE	6:G:125:GLU:OE1	2.47	0.48
12:M:509:ASP:OD1	12:M:509:ASP:N	2.46	0.48
35:l:359:MET:O	35:l:436:ARG:NH2	2.46	0.48
12:M:483:ARG:NH1	12:M:485:ASP:OD1	2.45	0.48
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.48	0.48
35:l:145:GLU:HA	35:l:145:GLU:OE1	2.13	0.48
40:r:328:CYS:HB3	40:r:437:MET:HE1	1.94	0.48
40:r:357:THR:O	40:r:361:VAL:HG23	2.12	0.48
44:w:204:VAL:HG21	44:w:249:MET:HG3	1.95	0.48
9:J:163:LYS:NZ	9:J:253:ILE:O	2.40	0.48
12:M:456:ALA:O	12:M:499:ASN:ND2	2.46	0.48
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.47	0.48
26:c:129:MET:HB3	35:l:528:TYR:CG	2.47	0.48
44:w:57:SER:HB3	44:w:150:LEU:HD21	1.94	0.48
44:w:80:LYS:HB2	44:w:270:VAL:HG21	1.95	0.48
44:w:340:SER:O	44:w:344:ASN:ND2	2.46	0.48
1:A:314:LEU:HD11	1:A:317:VAL:HG23	1.96	0.48
6:G:93:ILE:HG12	6:G:108:LEU:HD13	1.95	0.48
12:M:390:THR:HA	12:M:600:GLU:HG2	1.93	0.48
16:Q:107:ARG:O	16:Q:440:LYS:NZ	2.46	0.48
52:l:701:CDL:H572	52:l:701:CDL:H861	1.95	0.48
40:r:201:MET:HE1	49:r:502:PLX:H201	1.95	0.48
40:r:299:VAL:O	40:r:303:ILE:HG23	2.14	0.48
42:u:103:GLN:OE1	42:u:103:GLN:N	2.41	0.48
43:v:46:MET:HG2	43:v:51:LEU:HD12	1.96	0.48
2:B:98:ARG:NH2	16:Q:224:ALA:O	2.44	0.48
9:J:295:HIS:O	9:J:299:ARG:HG3	2.14	0.48
12:M:254:MET:HA	12:M:254:MET:HE2	1.96	0.48
16:Q:144:MET:O	16:Q:148:GLU:HG3	2.13	0.48
32:i:87:THR:HG22	32:i:88:LYS:N	2.28	0.48
35:l:292:ALA:HB2	35:l:304:PHE:HB3	1.96	0.48
40:r:203:PHE:O	40:r:207:MET:HG2	2.13	0.48
1:A:125:CYS:SG	14:O:181:VAL:HG13	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:ARG:HD3	16:Q:260:GLU:OE1	2.13	0.48
3:C:195:ARG:NE	3:C:195:ARG:HA	2.28	0.48
12:M:173:MET:HE2	12:M:173:MET:HA	1.95	0.48
14:O:88:ARG:HG2	14:O:88:ARG:HH11	1.79	0.48
15:P:52:ASP:O	15:P:56:LYS:HG3	2.14	0.48
19:U:30:ILE:HD12	48:U:101:PEE:H43	1.94	0.48
23:Z:53:TYR:CE2	35:l:434:LYS:HG3	2.49	0.48
24:a:134:GLU:OE1	37:n:57:TRP:NE1	2.33	0.48
38:o:25:ILE:HG12	38:o:30:ARG:NH2	2.29	0.48
39:p:151:THR:HG22	39:p:153:ALA:H	1.77	0.48
40:r:133:ILE:HG12	40:r:223:ALA:HB2	1.96	0.48
41:s:85:MET:SD	41:s:108:MET:HB2	2.53	0.48
4:E:120:SER:O	4:E:124:VAL:HG22	2.14	0.48
9:J:375:VAL:HG23	9:J:375:VAL:O	2.12	0.48
12:M:149:ASP:OD2	12:M:150:ARG:NH1	2.46	0.48
12:M:624:ARG:NH1	12:M:628:GLU:OE1	2.25	0.48
17:S:4:GLU:O	17:S:7:PRO:HD2	2.13	0.48
34:k:25:HIS:ND1	34:k:88:ASP:OD1	2.47	0.48
35:l:69:MET:HE3	35:l:76:LEU:HD12	1.96	0.48
2:B:97:PHE:HD2	2:B:171:PRO:HA	1.78	0.48
26:c:32:VAL:HG13	26:c:36:MET:HB2	1.95	0.48
35:l:373:LEU:HD23	35:l:431:PHE:CE1	2.49	0.48
49:r:502:PLX:H121	49:r:502:PLX:H92	1.53	0.48
5:F:62:GLN:HG3	5:F:63:PRO:HD2	1.94	0.48
20:V:39:TYR:HB3	52:V:201:CDL:H712	1.96	0.48
35:l:37:LYS:HE2	35:l:105:MET:HE1	1.95	0.48
32:i:40:MET:HE1	32:i:129:LEU:HD23	1.96	0.47
35:l:14:ILE:HD11	35:l:43:ALA:HA	1.95	0.47
40:r:282:LEU:HB2	40:r:342:MET:HG3	1.94	0.47
9:J:168:SER:O	9:J:203:PRO:HD2	2.14	0.47
27:d:115:GLN:HG2	35:l:62:ILE:HG12	1.96	0.47
12:M:47:THR:O	12:M:96:VAL:HG22	2.13	0.47
20:V:49:PHE:HA	52:V:202:CDL:HA62	1.96	0.47
30:g:101:GLU:CD	30:g:101:GLU:H	2.22	0.47
32:i:170:LEU:HD11	32:i:288:LEU:HD22	1.95	0.47
11:L:154:LYS:O	11:L:156:LYS:NZ	2.47	0.47
24:a:95:GLU:OE2	52:a:201:CDL:O1	2.23	0.47
33:j:97:LEU:HD11	49:j:202:PLX:H391	1.96	0.47
35:l:303:ALA:O	35:l:306:THR:HG22	2.14	0.47
35:l:491:LEU:O	35:l:495:ILE:HG22	2.15	0.47
40:r:78:MET:HE1	40:r:439:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:75:THR:OG1	6:G:76:LEU:N	2.46	0.47
6:G:94:ASP:OD1	6:G:94:ASP:N	2.34	0.47
9:J:230:SER:O	9:J:230:SER:OG	2.32	0.47
21:W:63:GLU:OE2	42:u:119:ARG:NH2	2.46	0.47
49:g:201:PLX:H332	32:i:342:ALA:HB3	1.97	0.47
33:j:73:LEU:HA	41:s:151:LEU:HD13	1.96	0.47
35:l:184:LEU:HD13	40:r:393:ILE:HG21	1.97	0.47
36:m:34:ILE:HD11	41:s:114:TYR:CE1	2.49	0.47
52:a:201:CDL:H512	48:l:704:PEE:H51	1.97	0.47
32:i:244:MET:HE2	32:i:244:MET:HB2	1.73	0.47
39:p:16:VAL:HG12	39:p:64:LEU:HD13	1.95	0.47
44:w:114:LEU:HD21	58:w:401:ADP:H1'	1.97	0.47
16:Q:123:LEU:O	16:Q:127:LYS:HG2	2.13	0.47
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	1.96	0.47
6:X:89:LEU:HD13	6:X:89:LEU:HA	1.77	0.47
27:d:114:GLN:HG2	35:l:203:MET:HE3	1.96	0.47
32:i:242:SER:O	32:i:246:VAL:HG23	2.14	0.47
32:i:254:LEU:HD21	40:r:154:LEU:HD11	1.96	0.47
37:n:9:ARG:HA	37:n:9:ARG:HD2	1.72	0.47
41:s:184:MET:HE1	41:s:296:LEU:HB3	1.96	0.47
4:E:47:VAL:HA	4:E:52:LEU:HD12	1.97	0.47
35:l:190:LEU:HB2	35:l:196:TRP:NE1	2.30	0.47
52:l:702:CDL:H201	52:l:702:CDL:H172	1.82	0.47
38:o:15:PRO:HG2	38:o:18:LEU:HD12	1.97	0.47
40:r:159:PRO:HG2	48:r:501:PEE:H35	1.96	0.47
41:s:267:THR:O	41:s:271:LEU:HG	2.15	0.47
43:v:29:TYR:OH	43:v:111:ARG:NH2	2.48	0.47
1:A:98:LYS:NZ	46:A:502:FMN:H5'2	2.30	0.47
1:A:102:MET:HE2	1:A:149:MET:HB3	1.96	0.47
48:C:302:PEE:H61	48:C:302:PEE:H55	1.67	0.47
4:E:42:GLU:OE1	4:E:46:THR:OG1	2.26	0.47
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.95	0.47
24:a:131:LYS:NZ	37:n:32:ASP:OD2	2.36	0.47
32:i:36:ASN:O	32:i:40:MET:HB2	2.15	0.47
34:k:10:MET:HE2	36:m:103:MET:SD	2.55	0.47
36:m:19:GLY:HA3	52:s:401:CDL:H772	1.97	0.47
43:v:15:LYS:HB3	43:v:15:LYS:HE3	1.60	0.47
1:A:119:GLU:OE1	1:A:127:ASP:HB2	2.15	0.47
5:F:68:ARG:HG3	5:F:74:GLU:HG3	1.96	0.47
9:J:206:ILE:HG13	53:J:401:NDP:H42N	1.97	0.47
6:X:122:MET:HG2	6:X:144:ILE:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:176:LYS:HB3	31:h:45:HIS:CG	2.50	0.47
29:f:46:LEU:O	29:f:50:THR:OG1	2.29	0.47
35:l:341:MET:HE3	35:l:457:LEU:HD12	1.97	0.47
48:B:303:PEE:H61	48:B:303:PEE:H55	1.68	0.46
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.97	0.46
21:W:134:LEU:HD21	36:m:2:THR:HB	1.96	0.46
24:a:79:GLY:HA3	52:a:201:CDL:H222	1.97	0.46
25:b:100:ARG:NH2	27:d:119:GLU:HG2	2.29	0.46
32:i:268:GLN:O	32:i:271:THR:OG1	2.31	0.46
40:r:306:PRO:HB3	40:r:458:LEU:HD12	1.97	0.46
12:M:667:GLN:N	12:M:667:GLN:OE1	2.48	0.46
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.80	0.46
29:f:30:TYR:N	44:w:99:GLY:O	2.38	0.46
32:i:222:SER:O	32:i:224:ALA:N	2.48	0.46
40:r:403:THR:HA	40:r:406:TYR:CE2	2.51	0.46
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.48	0.46
49:J:403:PLX:H101	33:j:24:LEU:HD13	1.96	0.46
35:l:409:LEU:O	35:l:413:LEU:HG	2.15	0.46
38:o:69:THR:O	38:o:73:SER:OG	2.29	0.46
41:s:55:LEU:HD13	41:s:221:ALA:HB2	1.97	0.46
41:s:213:VAL:HG13	41:s:214:GLU:HG2	1.97	0.46
52:s:401:CDL:H362	52:s:401:CDL:H391	1.71	0.46
1:A:317:VAL:HG22	1:A:356:VAL:HG22	1.96	0.46
12:M:144:MET:O	16:Q:362:LYS:NZ	2.45	0.46
19:U:38:TYR:HA	19:U:41:TYR:HD2	1.79	0.46
22:Y:65:MET:SD	35:l:375:ILE:HG12	2.55	0.46
31:h:65:GLU:OE2	31:h:69:ARG:HA	2.15	0.46
35:l:102:GLU:OE2	35:l:456:ARG:NH2	2.33	0.46
52:l:702:CDL:H362	52:l:702:CDL:H332	1.79	0.46
12:M:162:ASP:O	18:T:104:LYS:NZ	2.48	0.46
12:M:471:LYS:HB3	12:M:510:TRP:CZ2	2.51	0.46
12:M:559:ASP:N	12:M:559:ASP:OD1	2.49	0.46
48:l:704:PEE:N	49:r:503:PLX:O2	2.39	0.46
22:Y:100:LEU:HD13	22:Y:104:GLU:HB2	1.96	0.46
25:b:104:ILE:HB	43:v:48:ASP:HB3	1.97	0.46
27:d:69:ARG:NH2	37:n:46:LYS:O	2.40	0.46
14:O:152:ILE:HG21	14:O:171:LEU:HD13	1.97	0.46
39:p:132:SER:OG	39:p:136:GLU:OE2	2.30	0.46
42:u:38:LYS:HE2	42:u:38:LYS:HB2	1.69	0.46
1:A:67:GLU:O	1:A:71:LYS:HG2	2.16	0.46
3:C:125:PRO:HG2	41:s:58:LYS:NZ	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:97:PRO:HD3	15:P:61:PHE:CE1	2.51	0.46
52:V:202:CDL:HB62	34:k:23:ARG:HG2	1.97	0.46
49:j:202:PLX:H72	49:j:202:PLX:H4	1.68	0.46
35:l:327:LEU:O	35:l:331:MET:HG2	2.16	0.46
4:E:87:LYS:HB2	4:E:87:LYS:HE2	1.62	0.46
6:G:103:HIS:N	6:G:107:ASP:OD2	2.47	0.46
52:I:201:CDL:H111	52:I:201:CDL:H141	1.73	0.46
15:P:201:ASP:OD1	15:P:201:ASP:N	2.34	0.46
41:s:233:MET:HE3	41:s:233:MET:HB3	1.85	0.46
1:A:322:SER:HB3	1:A:370:LEU:HD22	1.97	0.46
5:F:61:VAL:HG13	5:F:62:GLN:N	2.30	0.46
9:J:119:VAL:HG23	9:J:120:VAL:HG13	1.98	0.46
9:J:328:THR:HG22	9:J:330:PRO:HD3	1.98	0.46
25:b:10:LEU:HA	25:b:13:GLN:HG3	1.98	0.46
32:i:207:ILE:O	32:i:211:MET:HG3	2.16	0.46
52:l:701:CDL:H321	52:l:701:CDL:H352	1.79	0.46
35:l:289:ALA:O	35:l:293:ILE:HG23	2.16	0.45
35:l:363:TYR:HD2	35:l:364:LYS:HG2	1.81	0.45
35:l:482:MET:HE2	35:l:482:MET:HB3	1.77	0.45
41:s:3:MET:HE3	41:s:3:MET:HB3	1.82	0.45
32:i:190:MET:HE2	32:i:204:ASN:ND2	2.27	0.45
32:i:284:MET:HE1	40:r:159:PRO:HG3	1.98	0.45
34:k:59:MET:HB3	34:k:60:PRO:HD3	1.99	0.45
35:l:49:VAL:HB	35:l:50:PRO:HD3	1.99	0.45
35:l:373:LEU:HD12	35:l:373:LEU:O	2.16	0.45
48:C:302:PEE:H62	33:j:24:LEU:HD21	1.99	0.45
5:F:69:TYR:HE2	5:F:75:LYS:HD2	1.82	0.45
9:J:317:ASP:OD2	9:J:321:ARG:NH1	2.46	0.45
26:c:34:LYS:HA	26:c:34:LYS:HD3	1.73	0.45
26:c:140:MET:HE3	35:l:283:ILE:HG13	1.97	0.45
32:i:20:VAL:HG13	32:i:29:ILE:HG23	1.98	0.45
32:i:26:TRP:CZ2	32:i:86:ILE:HG13	2.51	0.45
32:i:87:THR:CG2	32:i:88:LYS:N	2.80	0.45
35:l:313:MET:HG3	35:l:328:HIS:HD2	1.81	0.45
44:w:258:TYR:CE2	44:w:269:VAL:HG22	2.52	0.45
1:A:362:ASP:CG	1:A:449:ARG:HH12	2.23	0.45
16:Q:158:LEU:HD12	16:Q:411:LEU:HD23	1.96	0.45
21:W:121:MET:HE3	36:m:128:TYR:HB3	1.98	0.45
21:W:127:LEU:HA	31:h:83:ARG:HH22	1.82	0.45
33:j:71:LEU:HD21	36:m:157:THR:HG21	1.98	0.45
35:l:384:PRO:HA	35:l:389:PHE:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:277:LEU:HD21	40:r:405:LEU:HB3	1.98	0.45
43:v:3:ALA:O	43:v:7:ARG:HG3	2.17	0.45
1:A:367:ILE:O	1:A:371:ILE:HG12	2.17	0.45
16:Q:274:ASP:OD1	16:Q:323:ARG:NH2	2.50	0.45
26:c:127:ASN:O	26:c:131:LYS:HD2	2.17	0.45
35:l:51:LEU:HD22	35:l:91:PRO:HG3	1.99	0.45
41:s:81:LEU:HD11	41:s:111:LEU:HG	1.99	0.45
1:A:54:LYS:HE3	1:A:54:LYS:HB3	1.74	0.45
1:A:62:TRP:CE3	1:A:181:LEU:HD22	2.51	0.45
16:Q:443:MET:HE3	16:Q:443:MET:HB3	1.83	0.45
21:W:131:GLU:OE1	21:W:132:GLU:HG2	2.16	0.45
32:i:72:MET:HB2	34:k:40:LEU:HD21	1.97	0.45
32:i:111:PHE:HA	35:l:591:PHE:CE1	2.51	0.45
35:l:97:THR:O	35:l:101:MET:HG3	2.17	0.45
3:C:76:MET:HE3	3:C:93:PHE:CE1	2.52	0.45
15:P:236:ASN:OD1	15:P:236:ASN:N	2.49	0.45
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.99	0.45
16:Q:185:MET:HE1	16:Q:204:PHE:CZ	2.48	0.45
6:X:119:ILE:HD11	6:X:138:LEU:HD12	1.98	0.45
23:Z:22:TRP:HB3	23:Z:50:ALA:HB3	1.99	0.45
23:Z:32:VAL:HG13	39:p:39:TYR:HB2	1.98	0.45
28:e:137:MET:HE3	28:e:137:MET:HB2	1.86	0.45
35:l:37:LYS:HB3	35:l:37:LYS:HE3	1.72	0.45
35:l:407:TRP:O	35:l:411:MET:HG2	2.15	0.45
40:r:71:TRP:CD2	49:r:503:PLX:H341	2.52	0.45
41:s:195:ARG:HD3	41:s:231:ILE:HD11	1.99	0.45
42:u:83:THR:HA	42:u:86:TRP:NE1	2.32	0.45
2:B:39:LYS:HD2	16:Q:335:GLU:HG2	1.97	0.45
3:C:67:PHE:HE2	3:C:117:LEU:HD12	1.82	0.45
49:J:403:PLX:H121	49:J:403:PLX:H151	1.72	0.45
16:Q:41:VAL:HG23	28:e:55:LEU:HD23	1.99	0.45
16:Q:96:ARG:HB3	16:Q:112:HIS:HB2	1.99	0.45
35:l:213:LEU:HB3	35:l:273:VAL:HG11	1.99	0.45
52:s:401:CDL:H332	52:s:401:CDL:H182	1.98	0.45
43:v:17:PRO:HB3	43:v:105:GLU:CD	2.42	0.45
44:w:105:ASP:OD1	44:w:106:VAL:N	2.50	0.45
13:N:3:LEU:O	13:N:7:LEU:HG	2.16	0.45
16:Q:292:MET:HE3	16:Q:292:MET:HB3	1.80	0.45
22:Y:56:ILE:HG13	22:Y:57:GLN:N	2.31	0.45
24:a:176:LYS:HD2	31:h:45:HIS:CD2	2.52	0.45
35:l:293:ILE:HD13	35:l:418:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:243:LYS:HE2	44:w:243:LYS:HB2	1.85	0.45
44:w:287:ASP:CG	44:w:288:ASP:N	2.75	0.45
2:B:171:PRO:HG3	2:B:204:ASN:ND2	2.32	0.45
3:C:98:ARG:NH2	33:j:35:SER:O	2.45	0.45
5:F:43:GLU:OE1	5:F:43:GLU:HA	2.17	0.45
20:V:66:ILE:HD11	20:V:101:LEU:HD12	1.98	0.45
21:W:97:ILE:HG22	31:h:82:GLN:HG3	1.99	0.45
23:Z:23:LYS:HB3	23:Z:25:GLU:HG2	1.99	0.45
23:Z:25:GLU:HA	23:Z:30:GLU:OE1	2.17	0.45
25:b:80:TRP:HE1	27:d:41:VAL:HA	1.81	0.45
27:d:26:LEU:HD12	43:v:76:ASN:HB2	1.99	0.45
35:l:584:ILE:HG22	35:l:587:TYR:OH	2.16	0.45
1:A:185:ASN:C	1:A:187:CYS:H	2.24	0.44
1:A:455:LEU:O	1:A:458:GLN:NE2	2.50	0.44
2:B:79:ARG:NH1	8:I:25:GLN:OE1	2.47	0.44
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.53	0.44
7:H:7:LYS:HB3	7:H:7:LYS:HE3	1.66	0.44
54:J:402:UQ:H153	54:J:402:UQ:H121	1.84	0.44
21:W:92:GLU:OE2	21:W:92:GLU:HA	2.17	0.44
43:v:103:GLU:OE2	43:v:103:GLU:HA	2.16	0.44
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.52	0.44
8:I:18:ARG:NH2	16:Q:260:GLU:OE2	2.27	0.44
49:J:403:PLX:H201	33:j:20:ILE:HD11	1.99	0.44
16:Q:36:GLN:NE2	40:r:137:GLY:O	2.49	0.44
19:U:30:ILE:HD11	33:j:96:ILE:HD11	1.99	0.44
52:a:201:CDL:H392	52:a:201:CDL:H361	1.73	0.44
52:i:403:CDL:H832	52:i:403:CDL:H861	1.74	0.44
48:C:302:PEE:H29	48:C:302:PEE:H63	1.99	0.44
54:J:402:UQ:H121	54:J:402:UQ:H101	1.72	0.44
10:K:78:HIS:HA	10:K:81:TYR:CD2	2.52	0.44
19:U:69:HIS:HB3	19:U:72:ASP:OD1	2.17	0.44
35:l:184:LEU:HB2	40:r:393:ILE:HG12	1.99	0.44
39:p:139:GLN:NE2	39:p:156:PRO:O	2.50	0.44
6:X:80:LYS:HE3	6:X:80:LYS:HB3	1.72	0.44
5:F:36:PHE:HZ	5:F:44:LEU:HD13	1.82	0.44
8:I:66:PRO:HB3	15:P:79:SER:HA	1.99	0.44
9:J:37:HIS:O	9:J:39:ALA:N	2.50	0.44
9:J:162:GLU:HG3	9:J:163:LYS:HG3	1.99	0.44
12:M:275:PRO:HG3	12:M:286:ILE:HG12	1.99	0.44
16:Q:144:MET:HE2	16:Q:144:MET:HB2	1.77	0.44
17:S:40:HIS:N	17:S:44:GLN:OE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:40:ILE:O	21:W:44:LEU:HG	2.18	0.44
34:k:4:VAL:O	34:k:8:ILE:HG12	2.18	0.44
35:l:245:ALA:HB2	35:l:340:PHE:HB3	1.98	0.44
1:A:41:ILE:HG12	1:A:253:THR:HG21	1.98	0.44
2:B:128:ILE:HG12	2:B:147:ILE:HG12	2.00	0.44
12:M:347:ASP:OD1	12:M:347:ASP:N	2.47	0.44
14:O:242:GLY:HA2	14:O:245:VAL:HG23	1.99	0.44
16:Q:312:ASP:OD1	16:Q:312:ASP:N	2.45	0.44
16:Q:442:HIS:HB3	16:Q:446:ASP:HB2	2.00	0.44
20:V:40:SER:HA	52:V:201:CDL:HB61	2.00	0.44
21:W:120:MET:O	21:W:121:MET:HB3	2.16	0.44
35:l:486:MET:HE3	35:l:486:MET:HB3	1.74	0.44
35:l:529:TYR:HB3	35:l:530:PRO:HD3	1.99	0.44
52:o:201:CDL:H392	52:o:201:CDL:H361	1.62	0.44
43:v:112:LYS:O	43:v:116:GLU:HG3	2.17	0.44
1:A:250:VAL:O	1:A:254:ILE:HG12	2.17	0.44
49:C:303:PLX:H21	49:C:303:PLX:H1C3	1.84	0.44
5:F:18:GLU:O	5:F:19:ILE:HD13	2.18	0.44
32:i:284:MET:HE2	32:i:284:MET:HB2	1.88	0.44
33:j:1:MET:HA	33:j:4:MET:HE3	1.98	0.44
49:j:202:PLX:H22	49:j:202:PLX:H1C3	1.77	0.44
41:s:198:PHE:CD1	41:s:285:LEU:HD13	2.53	0.44
44:w:59:VAL:HG12	44:w:201:PRO:HB3	2.00	0.44
44:w:295:ARG:HA	44:w:298:VAL:HG22	1.99	0.44
9:J:283:VAL:HG22	9:J:369:VAL:HG11	1.98	0.44
14:O:130:TYR:CZ	14:O:208:LEU:HD22	2.53	0.44
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.52	0.44
16:Q:167:ALA:O	16:Q:171:ARG:HG3	2.17	0.44
16:Q:226:TYR:OH	16:Q:234:GLN:O	2.23	0.44
52:V:201:CDL:H611	52:V:201:CDL:H582	1.75	0.44
23:Z:42:ARG:HB3	23:Z:42:ARG:CZ	2.48	0.44
52:a:201:CDL:H342	52:a:201:CDL:H372	1.70	0.44
27:d:106:ILE:HG13	27:d:135:VAL:HG21	2.00	0.44
36:m:3:MET:HB3	36:m:5:ILE:HG12	1.99	0.44
52:o:201:CDL:H811	52:o:201:CDL:H842	1.88	0.44
41:s:207:LEU:O	41:s:209:SER:N	2.50	0.44
41:s:209:SER:HB3	41:s:213:VAL:HA	2.00	0.44
44:w:287:ASP:OD1	44:w:289:ARG:HG2	2.18	0.44
1:A:66:LYS:HE3	1:A:188:GLY:O	2.18	0.44
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.99	0.44
19:U:55:VAL:HG21	24:a:183:PRO:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:97:VAL:HG22	35:l:63:ILE:HG23	2.00	0.44
26:c:38:PRO:HG2	38:o:70:TYR:HD2	1.83	0.44
32:i:267:ILE:HG12	32:i:279:PRO:HB3	2.00	0.44
35:l:475:MET:HG3	43:v:52:MET:HE1	1.98	0.44
37:n:17:VAL:HG13	40:r:7:PRO:HB3	2.00	0.44
40:r:302:MET:HE2	40:r:302:MET:HA	2.00	0.44
52:s:401:CDL:H312	52:s:401:CDL:H342	1.45	0.44
1:A:115:VAL:HG11	1:A:138:LEU:HD11	1.99	0.43
17:S:35:GLU:OE1	42:u:93:GLY:N	2.48	0.43
52:V:202:CDL:H161	52:V:202:CDL:H191	1.85	0.43
24:a:106:VAL:O	37:n:50:ARG:NH2	2.51	0.43
31:h:29:ILE:HG21	36:m:138:GLU:HG3	2.00	0.43
2:B:144:ARG:HB2	13:N:130:THR:HG23	1.99	0.43
6:G:141:PRO:HA	6:G:144:ILE:HD12	2.00	0.43
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.99	0.43
12:M:573:GLY:HA3	13:N:137:TRP:CD1	2.53	0.43
16:Q:47:PHE:CD2	16:Q:52:MET:HE1	2.53	0.43
16:Q:457:VAL:HG13	16:Q:460:GLU:HG2	2.00	0.43
17:S:63:THR:HG23	42:u:21:SER:HB2	1.99	0.43
19:U:6:ALA:HB1	19:U:10:LYS:HZ1	1.81	0.43
22:Y:41:GLU:OE1	23:Z:12:SER:N	2.51	0.43
52:o:201:CDL:H142	52:o:201:CDL:H111	1.83	0.43
40:r:12:LEU:HD22	40:r:97:THR:HG23	1.99	0.43
44:w:124:ASN:OD1	44:w:124:ASN:N	2.45	0.43
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.53	0.43
3:C:49:LYS:HA	3:C:49:LYS:HD2	1.73	0.43
3:C:64:PRO:HA	3:C:102:VAL:O	2.17	0.43
4:E:110:THR:OG1	15:P:222:GLU:OE2	2.34	0.43
7:H:67:LYS:HE3	7:H:67:LYS:HB3	1.73	0.43
52:l:702:CDL:H371	52:l:702:CDL:H601	1.99	0.43
40:r:216:LEU:HD11	40:r:236:LEU:HD11	1.99	0.43
41:s:18:ALA:O	41:s:21:THR:OG1	2.29	0.43
9:J:87:GLU:HG3	9:J:89:TYR:H	1.82	0.43
12:M:492:ALA:O	12:M:496:ILE:HG13	2.18	0.43
15:P:87:PHE:CE2	15:P:144:LYS:HE3	2.54	0.43
16:Q:96:ARG:O	16:Q:112:HIS:HB2	2.18	0.43
19:U:60:ASP:OD1	19:U:60:ASP:N	2.49	0.43
26:c:161:TYR:HB3	26:c:166:LEU:HG	2.01	0.43
28:e:66:LEU:HA	28:e:66:LEU:HD23	1.78	0.43
32:i:106:LEU:HG	32:i:138:PRO:HB2	2.01	0.43
52:o:201:CDL:H721	52:o:201:CDL:H752	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:212:ARG:HG2	9:J:318:LYS:NZ	2.33	0.43
12:M:488:ALA:HB1	12:M:679:LEU:HD12	1.99	0.43
16:Q:335:GLU:O	16:Q:339:GLN:HG2	2.18	0.43
24:a:100:ASP:N	24:a:100:ASP:OD1	2.50	0.43
49:g:201:PLX:H122	49:g:201:PLX:H91	1.71	0.43
52:g:202:CDL:H771	52:i:403:CDL:H872	2.01	0.43
34:k:73:LEU:HD12	34:k:73:LEU:HA	1.85	0.43
35:l:383:MET:HB3	35:l:386:LEU:HD12	2.00	0.43
49:r:502:PLX:H101	49:r:502:PLX:H72	1.76	0.43
44:w:258:TYR:HE2	44:w:269:VAL:HG13	1.83	0.43
3:C:173:LEU:O	3:C:177:ILE:HG12	2.19	0.43
9:J:336:GLU:OE2	9:J:336:GLU:N	2.43	0.43
16:Q:271:ARG:NH2	16:Q:445:ALA:HB1	2.32	0.43
6:X:123:GLU:OE1	6:X:130:ILE:N	2.40	0.43
28:e:94:GLY:O	28:e:99:LEU:HB2	2.17	0.43
35:l:95:PHE:CZ	35:l:456:ARG:HG2	2.53	0.43
35:l:492:ILE:HA	35:l:495:ILE:HG22	2.01	0.43
36:m:82:VAL:HG13	36:m:84:VAL:H	1.82	0.43
44:w:58:LYS:O	44:w:60:ILE:HG13	2.18	0.43
1:A:88:ARG:HG3	1:A:246:GLU:OE2	2.18	0.43
6:G:84:LEU:HD13	6:G:84:LEU:HA	1.90	0.43
9:J:83:PRO:HA	9:J:106:MET:O	2.18	0.43
16:Q:215:GLU:C	16:Q:215:GLU:OE1	2.62	0.43
6:X:131:PRO:HG2	6:X:134:ASP:HB2	1.99	0.43
24:a:139:ILE:O	24:a:143:GLU:HG2	2.18	0.43
29:f:57:TYR:O	29:f:57:TYR:HD1	2.01	0.43
52:s:401:CDL:H141	52:s:401:CDL:H171	1.54	0.43
7:H:66:LYS:HB2	7:H:66:LYS:HE2	1.78	0.43
10:K:73:TYR:CZ	10:K:75:ASN:HB3	2.53	0.43
14:O:144:ASN:O	14:O:147:SER:OG	2.36	0.43
21:W:58:ARG:HD2	21:W:58:ARG:HA	1.78	0.43
30:g:12:PRO:HG3	31:h:8:LYS:HE3	1.99	0.43
35:l:136:ASN:OD1	35:l:136:ASN:N	2.51	0.43
38:o:80:PHE:HE1	38:o:86:THR:HG21	1.82	0.43
41:s:158:GLY:HA3	41:s:315:PRO:HB2	1.99	0.43
1:A:152:ARG:CZ	10:K:101:PRO:HD3	2.49	0.43
48:B:303:PEE:H59	41:s:277:TYR:CE2	2.53	0.43
49:C:303:PLX:H102	49:C:303:PLX:H261	2.01	0.43
5:F:30:SER:OG	5:F:63:PRO:HG3	2.19	0.43
12:M:129:PRO:O	12:M:241:ARG:NH2	2.52	0.43
20:V:66:ILE:CD1	20:V:101:LEU:HD12	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:67:PHE:CE2	40:r:434:ASN:HB3	2.53	0.43
30:g:65:LEU:O	30:g:69:SER:OG	2.34	0.43
31:h:19:THR:HA	32:i:84:TRP:HB2	2.01	0.43
35:l:95:PHE:HZ	35:l:456:ARG:HG2	1.83	0.43
36:m:53:GLY:HA2	36:m:56:VAL:CG1	2.49	0.43
39:p:138:LYS:HE3	39:p:138:LYS:HB3	1.68	0.43
1:A:145:GLY:O	1:A:149:MET:HG3	2.19	0.43
5:F:16:LEU:HD11	5:F:19:ILE:HD11	2.00	0.43
49:J:403:PLX:H272	49:J:403:PLX:H301	1.46	0.43
18:T:49:ASP:O	18:T:52:ARG:HD3	2.19	0.43
36:m:57:PHE:CZ	36:m:61:LEU:HD11	2.54	0.43
1:A:98:LYS:HA	1:A:101:PHE:HD2	1.84	0.42
1:A:211:ALA:HB2	1:A:223:PRO:HG3	1.99	0.42
8:I:109:ASP:OD1	8:I:109:ASP:C	2.62	0.42
10:K:109:ARG:O	12:M:422:TRP:CZ2	2.72	0.42
16:Q:71:PRO:HA	16:Q:72:PRO:HD3	1.93	0.42
35:l:332:HIS:HA	35:l:335:PHE:CE2	2.54	0.42
52:l:701:CDL:O1	40:r:357:THR:OG1	2.33	0.42
41:s:184:MET:O	41:s:188:SER:OG	2.33	0.42
42:u:52:ASP:HB3	42:u:55:ARG:HG3	2.00	0.42
1:A:76:ILE:HG23	1:A:255:CYS:SG	2.59	0.42
1:A:358:ASP:O	1:A:361:THR:HG22	2.20	0.42
26:c:40:PRO:O	26:c:74:ASP:HB3	2.20	0.42
40:r:344:LEU:O	40:r:420:THR:HG21	2.19	0.42
41:s:128:ALA:HA	41:s:211:PHE:HA	2.01	0.42
15:P:214:ASP:OD1	15:P:217:LYS:NZ	2.43	0.42
30:g:4:MET:O	30:g:10:ARG:NH1	2.52	0.42
52:i:401:CDL:H811	36:m:159:TRP:CH2	2.54	0.42
52:i:401:CDL:HB62	44:w:40:PRO:HB2	2.01	0.42
48:j:201:PEE:H13	41:s:72:ILE:HD13	2.00	0.42
44:w:96:SER:HA	44:w:101:GLY:HA2	2.01	0.42
1:A:325:PRO:O	1:A:347:THR:OG1	2.35	0.42
12:M:128:CYS:SG	12:M:140:GLN:NE2	2.86	0.42
15:P:43:THR:HG23	15:P:47:ILE:HD12	2.01	0.42
20:V:8:LYS:HB3	20:V:8:LYS:HE3	1.84	0.42
26:c:163:TYR:OH	43:v:42:THR:HA	2.19	0.42
32:i:72:MET:HE2	34:k:12:PHE:CD2	2.54	0.42
32:i:153:LEU:HG	32:i:157:MET:HE2	1.99	0.42
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.99	0.42
41:s:92:PRO:HB3	41:s:255:TYR:CD1	2.54	0.42
42:u:68:LEU:HD23	42:u:68:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:GLN:HE21	1:A:197:VAL:HB	1.85	0.42
1:A:244:ASN:CG	46:A:502:FMN:O2	2.63	0.42
4:E:23:ARG:NE	11:L:53:ILE:HG22	2.34	0.42
5:F:46:LYS:HZ3	12:M:674:LEU:HD21	1.84	0.42
7:H:12:VAL:HG12	16:Q:279:THR:HG22	2.00	0.42
9:J:323:HIS:O	9:J:323:HIS:CG	2.72	0.42
14:O:143:ARG:O	14:O:184:PRO:HG3	2.18	0.42
16:Q:443:MET:HE1	41:s:282:TYR:HE1	1.84	0.42
21:W:144:THR:HB	41:s:96:ILE:HG23	2.02	0.42
22:Y:43:ARG:HH11	22:Y:49:GLN:HB2	1.85	0.42
33:j:67:LEU:HD13	34:k:65:VAL:HA	2.00	0.42
33:j:77:TRP:HD1	41:s:318:SER:C	2.28	0.42
35:l:284:THR:O	35:l:288:THR:OG1	2.29	0.42
35:l:286:LEU:HD13	35:l:411:MET:SD	2.59	0.42
37:n:49:LEU:HD22	37:n:53:GLU:HG3	2.01	0.42
54:s:402:UQ:H202	54:s:402:UQ:H172	1.80	0.42
43:v:44:GLN:OE1	43:v:44:GLN:HA	2.19	0.42
43:v:89:TYR:HD1	43:v:89:TYR:O	2.02	0.42
44:w:83:LEU:HD22	44:w:156:GLY:HA3	2.02	0.42
4:E:68:MET:HE3	4:E:68:MET:HB3	1.92	0.42
10:K:77:GLN:H	10:K:77:GLN:HG2	1.60	0.42
12:M:211:GLU:OE1	12:M:211:GLU:HA	2.19	0.42
16:Q:404:LYS:HE2	16:Q:457:VAL:HG12	2.02	0.42
35:l:504:LEU:HD12	35:l:504:LEU:HA	1.86	0.42
39:p:139:GLN:O	39:p:143:GLU:HG3	2.20	0.42
41:s:73:ILE:HD11	52:s:401:CDL:H172	2.02	0.42
44:w:345:GLU:OE2	44:w:345:GLU:N	2.43	0.42
52:l:701:CDL:H202	52:l:701:CDL:H231	1.87	0.42
48:r:501:PEE:H62	48:r:501:PEE:H68	1.88	0.42
49:r:502:PLX:H22	49:r:502:PLX:H1C3	1.86	0.42
44:w:233:TYR:O	44:w:237:ILE:HG13	2.20	0.42
1:A:120:GLY:HA3	1:A:204:TYR:HD1	1.83	0.42
3:C:63:TRP:CD1	3:C:92:VAL:HG22	2.55	0.42
3:C:175:TYR:CE1	13:N:78:ASP:HB2	2.55	0.42
12:M:140:GLN:HG2	16:Q:379:ILE:HG23	2.02	0.42
21:W:34:SER:O	21:W:38:VAL:HG12	2.19	0.42
6:X:102:SER:HB3	6:X:108:LEU:HD21	2.02	0.42
35:l:121:LEU:HD22	35:l:246:LEU:HD23	2.01	0.42
36:m:2:THR:C	36:m:4:TYR:H	2.28	0.42
38:o:48:LEU:HB3	39:p:166:LEU:HD13	2.01	0.42
41:s:53:LEU:HD23	41:s:53:LEU:HA	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:82:PRO:HG3	16:Q:201:PHE:HB3	2.02	0.42
4:E:14:GLY:O	11:L:54:ALA:HA	2.20	0.42
6:G:103:HIS:CE1	6:G:139:MET:HG3	2.55	0.42
9:J:61:ALA:HA	9:J:66:GLY:HA3	2.01	0.42
9:J:76:MET:HE1	9:J:254:LYS:HE3	2.02	0.42
12:M:387:LEU:HD12	12:M:514:ASN:HB3	2.00	0.42
13:N:101:LYS:HE2	13:N:101:LYS:HB2	1.96	0.42
16:Q:336:GLU:O	16:Q:340:SER:OG	2.29	0.42
19:U:26:GLY:HA3	48:U:101:PEE:H38	2.02	0.42
25:b:25:ASP:OD2	39:p:125:TRP:NE1	2.53	0.42
30:g:36:MET:SD	49:g:201:PLX:H393	2.60	0.42
35:l:86:SER:OG	35:l:262:ARG:NH2	2.53	0.42
35:l:108:MET:HE3	35:l:108:MET:HB3	1.95	0.42
35:l:173:LEU:HD12	40:r:405:LEU:HD21	2.00	0.42
35:l:293:ILE:HG21	35:l:418:LEU:HD22	2.01	0.42
37:n:11:HIS:ND1	37:n:14:HIS:HE1	2.18	0.42
1:A:98:LYS:HA	1:A:101:PHE:CD2	2.55	0.42
9:J:116:ILE:HA	9:J:119:VAL:HG22	2.01	0.42
9:J:370:LYS:O	9:J:370:LYS:HD3	2.20	0.42
13:N:11:LEU:O	13:N:14:VAL:HG12	2.20	0.42
13:N:120:THR:HG22	13:N:122:GLN:H	1.85	0.42
25:b:77:ILE:HB	25:b:78:PRO:HD3	2.02	0.42
26:c:155:PRO:HD3	43:v:4:HIS:NE2	2.35	0.42
33:j:73:LEU:N	33:j:74:PRO:HD2	2.35	0.42
38:o:59:VAL:HG22	40:r:423:ILE:HG12	2.02	0.42
39:p:56:ASP:HB3	39:p:59:LYS:HD2	2.01	0.42
39:p:98:LYS:HG2	39:p:178:PRO:HG3	2.01	0.42
40:r:318:ALA:HB1	40:r:374:ASN:CG	2.45	0.42
40:r:397:GLY:HA2	40:r:400:MET:HE2	2.02	0.42
42:u:50:GLU:N	42:u:50:GLU:OE1	2.53	0.42
22:Y:53:SER:HA	22:Y:56:ILE:HG12	2.02	0.41
33:j:19:LEU:HD11	48:j:201:PEE:H48	2.02	0.41
35:l:206:ASN:OD1	35:l:206:ASN:N	2.43	0.41
38:o:95:ILE:HG23	38:o:99:PHE:CE2	2.55	0.41
44:w:110:GLY:HA2	44:w:134:TRP:CE2	2.55	0.41
3:C:51:ASP:OD2	3:C:188:LYS:HA	2.20	0.41
4:E:23:ARG:NH1	11:L:51:GLN:HB3	2.34	0.41
9:J:132:ARG:NH1	53:J:401:NDP:O3X	2.53	0.41
12:M:698:ASP:OD1	12:M:698:ASP:N	2.53	0.41
48:W:201:PEE:H45	52:s:401:CDL:H561	2.02	0.41
32:i:18:MET:O	32:i:22:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:71:LEU:HD23	33:j:94:LEU:HD21	2.02	0.41
35:l:230:HIS:N	35:l:231:PRO:HD3	2.35	0.41
44:w:293:ARG:HE	44:w:293:ARG:HB3	1.56	0.41
44:w:295:ARG:O	44:w:299:GLN:HG2	2.20	0.41
44:w:340:SER:HB2	44:w:343:TYR:HD1	1.85	0.41
9:J:116:ILE:O	9:J:120:VAL:HG22	2.21	0.41
12:M:511:LYS:HG2	12:M:663:ASN:HD22	1.85	0.41
14:O:187:GLN:HG3	14:O:192:TYR:CE1	2.55	0.41
20:V:101:LEU:O	20:V:105:THR:HG23	2.20	0.41
26:c:110:ASP:OD1	26:c:110:ASP:N	2.49	0.41
32:i:98:MET:HE2	32:i:98:MET:HB2	1.90	0.41
35:l:44:PHE:HB2	35:l:94:LEU:HB3	2.01	0.41
35:l:264:TYR:CG	35:l:265:PRO:HD3	2.55	0.41
35:l:517:SER:OG	52:l:702:CDL:OA3	2.37	0.41
35:l:555:LEU:HD13	38:o:76:ILE:HD12	2.01	0.41
35:l:571:MET:HE2	35:l:571:MET:HB3	1.76	0.41
40:r:37:ILE:HD13	40:r:37:ILE:HA	1.90	0.41
49:r:502:PLX:H51	49:r:502:PLX:H6	1.53	0.41
42:u:110:CYS:O	42:u:114:LYS:HB2	2.20	0.41
1:A:82:THR:HG23	1:A:259:GLY:HA3	2.01	0.41
3:C:92:VAL:HG21	54:s:402:UQ:H103	2.03	0.41
3:C:109:LEU:HD13	3:C:117:LEU:HD13	2.02	0.41
14:O:137:THR:O	14:O:141:MET:N	2.43	0.41
16:Q:55:THR:O	16:Q:59:ALA:N	2.52	0.41
16:Q:99:MET:HE1	16:Q:444:LEU:HD21	2.02	0.41
27:d:78:GLU:OE1	30:g:108:LYS:HB3	2.21	0.41
33:j:109:LYS:HA	33:j:109:LYS:HD3	1.92	0.41
52:l:701:CDL:H841	52:l:701:CDL:H811	1.67	0.41
52:o:201:CDL:H151	52:o:201:CDL:H362	2.03	0.41
48:r:501:PEE:H52	48:r:501:PEE:H59	1.91	0.41
41:s:81:LEU:HD21	41:s:111:LEU:HD23	2.01	0.41
41:s:142:TYR:CE1	41:s:192:GLU:HG2	2.55	0.41
54:s:402:UQ:H262	54:s:402:UQ:H221	1.80	0.41
6:G:103:HIS:CD2	6:G:106:LYS:HE2	2.56	0.41
12:M:234:LYS:HB3	12:M:235:PRO:HD3	2.02	0.41
16:Q:42:GLU:OE1	28:e:54:ARG:NH1	2.54	0.41
16:Q:178:THR:OG1	16:Q:214:TYR:OH	2.38	0.41
16:Q:440:LYS:HA	16:Q:440:LYS:HE2	2.02	0.41
26:c:38:PRO:HD3	38:o:67:ARG:HG2	2.03	0.41
48:j:201:PEE:H31	52:s:401:CDL:H222	2.01	0.41
35:l:350:LEU:HD23	35:l:350:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:342:MET:HE2	40:r:342:MET:HB3	1.97	0.41
1:A:267:ARG:HG3	1:A:293:SER:OG	2.20	0.41
16:Q:190:HIS:O	16:Q:194:ILE:HG12	2.19	0.41
19:U:72:ASP:OD1	19:U:72:ASP:N	2.53	0.41
6:X:74:LEU:HD21	6:X:79:ILE:HD11	2.01	0.41
31:h:2:PRO:HB2	31:h:3:PHE:H	1.60	0.41
33:j:71:LEU:O	36:m:147:TYR:OH	2.36	0.41
33:j:73:LEU:HD23	41:s:151:LEU:HD13	2.03	0.41
34:k:31:LEU:HD21	36:m:67:VAL:HG11	2.01	0.41
44:w:147:LEU:HD23	44:w:147:LEU:HA	1.88	0.41
1:A:97:LEU:HD23	1:A:97:LEU:HA	1.88	0.41
1:A:122:PRO:HA	14:O:176:CYS:SG	2.61	0.41
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.56	0.41
9:J:72:HIS:NE2	15:P:215:GLU:OE1	2.53	0.41
54:J:402:UQ:H71	54:J:402:UQ:HM53	1.77	0.41
13:N:68:MET:HE3	13:N:115:PHE:HD2	1.86	0.41
14:O:58:GLU:H	14:O:58:GLU:CD	2.29	0.41
24:a:155:GLU:OE2	24:a:158:ARG:NH1	2.53	0.41
1:A:46:TYR:HD1	14:O:234:LEU:HD12	1.83	0.41
2:B:70:LEU:HG	41:s:277:TYR:OH	2.20	0.41
7:H:40:LYS:HA	7:H:45:ARG:HD3	2.03	0.41
8:I:70:MET:O	8:I:70:MET:SD	2.78	0.41
12:M:358:LEU:HD11	12:M:546:PHE:CE1	2.55	0.41
14:O:148:ILE:O	14:O:152:ILE:HG13	2.20	0.41
14:O:222:ARG:NH1	14:O:226:GLU:O	2.42	0.41
19:U:47:ARG:HG3	33:j:82:ASN:OD1	2.20	0.41
22:Y:97:LEU:HB3	43:v:104:ARG:HB2	2.03	0.41
26:c:167:TYR:CG	26:c:178:PRO:HG3	2.56	0.41
28:e:107:ALA:HB2	49:r:503:PLX:H24	2.02	0.41
40:r:282:LEU:HD21	40:r:359:TRP:HH2	1.85	0.41
41:s:228:TYR:O	41:s:232:ILE:HG13	2.21	0.41
42:u:16:GLN:OE1	42:u:16:GLN:HA	2.21	0.41
44:w:85:HIS:NE2	44:w:160:GLU:OE2	2.40	0.41
7:H:48:THR:O	7:H:52:THR:OG1	2.29	0.41
7:H:62:GLU:HB3	7:H:68:LEU:HD13	2.03	0.41
8:I:96:THR:OG1	8:I:98:ALA:O	2.36	0.41
12:M:262:VAL:HG23	12:M:276:ARG:HB2	2.03	0.41
13:N:41:GLU:OE1	13:N:47:LYS:NZ	2.54	0.41
15:P:43:THR:HA	15:P:47:ILE:HD12	2.03	0.41
16:Q:393:PRO:HA	16:Q:413:SER:O	2.21	0.41
20:V:38:ALA:HA	52:V:202:CDL:H201	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:73:THR:HG23	20:V:93:GLY:HA2	2.02	0.41
22:Y:80:VAL:HG13	35:l:488:MET:HE1	2.03	0.41
24:a:168:TRP:HB3	30:g:3:MET:HG3	2.02	0.41
26:c:139:PHE:CD2	52:l:702:CDL:H851	2.56	0.41
52:i:403:CDL:H541	52:i:403:CDL:H511	1.81	0.41
35:l:425:ARG:HA	35:l:505:ASN:HD21	1.85	0.41
35:l:534:HIS:ND1	48:l:703:PEE:H13	2.36	0.41
52:l:701:CDL:H372	52:l:701:CDL:H341	1.84	0.41
36:m:32:GLY:O	36:m:35:VAL:HG12	2.21	0.41
36:m:153:LEU:HD23	36:m:153:LEU:HA	1.96	0.41
40:r:405:LEU:HD23	40:r:405:LEU:HA	1.91	0.41
4:E:108:HIS:HB3	4:E:111:GLU:HG3	2.03	0.41
10:K:105:ARG:HH12	11:L:169:ARG:HE	1.67	0.41
14:O:226:GLU:HG2	14:O:227:PRO:O	2.20	0.41
6:X:151:LYS:HA	6:X:151:LYS:HD2	1.82	0.41
34:k:59:MET:HE1	34:k:63:LEU:HD22	2.03	0.41
35:l:65:ASN:HD21	35:l:80:PHE:HE1	1.69	0.41
35:l:152:PHE:CD1	35:l:168:ALA:HB1	2.56	0.41
41:s:17:VAL:HG13	41:s:228:TYR:HB2	2.02	0.41
44:w:88:GLU:OE2	44:w:161:ARG:NH1	2.47	0.41
1:A:424:ILE:HD11	12:M:74:ASN:HA	2.03	0.40
3:C:126:GLU:OE2	9:J:89:TYR:OH	2.29	0.40
13:N:85:GLU:HG2	13:N:86:TRP:H	1.86	0.40
16:Q:70:ASP:OD1	32:i:51:ARG:HG3	2.21	0.40
35:l:304:PHE:CZ	35:l:526:LEU:HD22	2.55	0.40
35:l:557:TRP:O	35:l:561:ILE:HG23	2.21	0.40
52:l:701:CDL:H432	52:l:701:CDL:H602	2.03	0.40
40:r:42:LEU:HB3	40:r:453:MET:CE	2.51	0.40
41:s:11:ILE:HB	41:s:12:PRO:HD3	2.02	0.40
41:s:175:ILE:O	41:s:179:TRP:HB3	2.21	0.40
42:u:49:GLU:OE1	42:u:135:ARG:NH1	2.51	0.40
1:A:119:GLU:OE2	1:A:125:CYS:HA	2.19	0.40
6:G:80:LYS:HE3	6:G:100:VAL:HG11	2.03	0.40
7:H:18:GLU:O	7:H:19:THR:OG1	2.37	0.40
9:J:237:LYS:NZ	9:J:324:MET:O	2.48	0.40
12:M:34:VAL:HG11	12:M:96:VAL:HB	2.02	0.40
12:M:340:ALA:HB3	12:M:366:LEU:HD13	2.03	0.40
15:P:127:GLU:OE2	15:P:144:LYS:NZ	2.33	0.40
20:V:44:LYS:HB2	20:V:44:LYS:HE2	1.77	0.40
32:i:11:MET:HG2	52:i:401:CDL:H562	2.03	0.40
35:l:185:SER:OG	35:l:212:PRO:O	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:o:201:CDL:H512	52:o:201:CDL:H712	2.03	0.40
39:p:100:PRO:HD3	40:r:419:TYR:CZ	2.56	0.40
40:r:22:MET:HE3	40:r:22:MET:HB3	1.77	0.40
40:r:300:ALA:HB2	40:r:381:ILE:HG12	2.03	0.40
44:w:277:LYS:HA	44:w:277:LYS:HD3	1.86	0.40
1:A:257:ARG:HD3	14:O:244:GLY:HA3	2.03	0.40
8:I:27:ARG:NH1	16:Q:212:GLU:OE1	2.51	0.40
9:J:48:ARG:NH2	9:J:98:GLY:O	2.54	0.40
39:p:159:LYS:HE2	39:p:159:LYS:HB2	1.66	0.40
1:A:325:PRO:HG3	1:A:433:TRP:HB3	2.02	0.40
2:B:192:ASN:ND2	18:T:61:GLU:OE2	2.53	0.40
3:C:64:PRO:HD2	3:C:92:VAL:O	2.22	0.40
5:F:65:LEU:O	5:F:76:ASN:HA	2.20	0.40
12:M:419:ARG:NH1	12:M:439:THR:O	2.55	0.40
20:V:31:ALA:O	20:V:35:ILE:HG12	2.22	0.40
35:l:2:ASN:HD21	35:l:61:MET:HE1	1.85	0.40
35:l:9:LEU:HD23	35:l:9:LEU:HA	1.85	0.40
48:r:501:PEE:H59	48:r:501:PEE:H64	1.88	0.40
43:v:42:THR:N	43:v:45:GLU:OE2	2.54	0.40
1:A:369:ARG:HD2	1:A:369:ARG:HA	1.83	0.40
7:H:90:LEU:HB2	15:P:102:ASP:HB3	2.02	0.40
49:J:403:PLX:H251	49:J:403:PLX:H281	1.80	0.40
13:N:133:LYS:HA	13:N:133:LYS:HD3	1.74	0.40
16:Q:158:LEU:HD23	16:Q:158:LEU:HA	1.90	0.40
29:f:68:GLU:OE1	29:f:71:ARG:NH1	2.54	0.40
34:k:35:GLY:HA3	36:m:20:PHE:HZ	1.86	0.40
36:m:40:GLY:HA2	36:m:43:ILE:HD12	2.03	0.40
37:n:11:HIS:ND1	37:n:14:HIS:CE1	2.89	0.40
39:p:24:LEU:HD23	39:p:24:LEU:HA	1.95	0.40
44:w:36:LEU:HD11	44:w:41:LEU:HD23	2.02	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%)	418 (97%)	13 (3%)	0	100	100
2	B	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
3	C	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
4	E	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
5	F	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
6	G	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
6	X	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
7	H	110/112 (98%)	104 (94%)	5 (4%)	1 (1%)	14	48
8	I	93/112 (83%)	83 (89%)	10 (11%)	0	100	100
9	J	340/342 (99%)	330 (97%)	9 (3%)	1 (0%)	36	70
10	K	41/43 (95%)	41 (100%)	0	0	100	100
11	L	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
12	M	688/690 (100%)	672 (98%)	16 (2%)	0	100	100
13	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
14	O	215/217 (99%)	205 (95%)	10 (5%)	0	100	100
15	P	206/208 (99%)	199 (97%)	7 (3%)	0	100	100
16	Q	427/430 (99%)	411 (96%)	16 (4%)	0	100	100
17	S	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
18	T	94/96 (98%)	94 (100%)	0	0	100	100
19	U	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
20	V	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
21	W	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
22	Y	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
23	Z	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
24	a	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
25	b	94/126 (75%)	89 (95%)	5 (5%)	0	100	100
26	c	154/156 (99%)	142 (92%)	12 (8%)	0	100	100
27	d	173/175 (99%)	171 (99%)	2 (1%)	0	100	100
28	e	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
29	f	47/49 (96%)	43 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	g	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
31	h	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
32	i	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
33	j	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
34	k	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
35	l	604/606 (100%)	588 (97%)	16 (3%)	0	100	100
36	m	173/175 (99%)	162 (94%)	11 (6%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
39	p	176/178 (99%)	170 (97%)	6 (3%)	0	100	100
40	r	457/459 (100%)	454 (99%)	3 (1%)	0	100	100
41	s	316/318 (99%)	308 (98%)	7 (2%)	1 (0%)	36	70
42	u	169/171 (99%)	166 (98%)	2 (1%)	1 (1%)	21	56
43	v	122/124 (98%)	118 (97%)	4 (3%)	0	100	100
44	w	318/320 (99%)	307 (96%)	11 (4%)	0	100	100
All	All	8175/8313 (98%)	7919 (97%)	252 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	38	HIS
7	H	77	ILE
41	s	208	VAL
42	u	152	PRO

5.3.2 Protein sidechains ⓘ

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%)	340 (98%)	6 (2%)	53	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	150/151 (99%)	148 (99%)	2 (1%)	61	81
3	C	132/132 (100%)	128 (97%)	4 (3%)	36	69
4	E	107/107 (100%)	105 (98%)	2 (2%)	50	76
5	F	74/76 (97%)	74 (100%)	0	100	100
6	G	76/81 (94%)	73 (96%)	3 (4%)	28	62
6	X	76/81 (94%)	71 (93%)	5 (7%)	15	46
7	H	99/99 (100%)	98 (99%)	1 (1%)	68	84
8	I	87/97 (90%)	86 (99%)	1 (1%)	65	83
9	J	296/296 (100%)	294 (99%)	2 (1%)	76	86
10	K	42/42 (100%)	39 (93%)	3 (7%)	13	43
11	L	113/113 (100%)	112 (99%)	1 (1%)	70	85
12	M	576/580 (99%)	568 (99%)	8 (1%)	59	80
13	N	129/130 (99%)	125 (97%)	4 (3%)	35	68
14	O	182/183 (100%)	179 (98%)	3 (2%)	55	79
15	P	190/190 (100%)	189 (100%)	1 (0%)	81	89
16	Q	370/370 (100%)	360 (97%)	10 (3%)	39	71
17	S	57/58 (98%)	56 (98%)	1 (2%)	51	77
18	T	79/79 (100%)	78 (99%)	1 (1%)	61	81
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	98 (97%)	3 (3%)	36	69
21	W	121/123 (98%)	120 (99%)	1 (1%)	73	86
22	Y	62/62 (100%)	61 (98%)	1 (2%)	55	79
23	Z	62/62 (100%)	61 (98%)	1 (2%)	55	79
24	a	121/121 (100%)	119 (98%)	2 (2%)	53	78
25	b	90/119 (76%)	86 (96%)	4 (4%)	25	60
26	c	141/141 (100%)	138 (98%)	3 (2%)	47	75
27	d	155/155 (100%)	153 (99%)	2 (1%)	61	81
28	e	93/96 (97%)	91 (98%)	2 (2%)	45	74
29	f	35/45 (78%)	34 (97%)	1 (3%)	37	70
30	g	108/109 (99%)	105 (97%)	3 (3%)	38	70
31	h	93/93 (100%)	92 (99%)	1 (1%)	65	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	i	311/311 (100%)	307 (99%)	4 (1%)	61	81
33	j	100/100 (100%)	97 (97%)	3 (3%)	36	69
34	k	85/85 (100%)	83 (98%)	2 (2%)	43	73
35	l	536/540 (99%)	529 (99%)	7 (1%)	61	81
36	m	127/141 (90%)	124 (98%)	3 (2%)	43	73
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	113/113 (100%)	110 (97%)	3 (3%)	39	71
39	p	158/159 (99%)	157 (99%)	1 (1%)	78	88
40	r	409/410 (100%)	400 (98%)	9 (2%)	45	74
41	s	275/275 (100%)	272 (99%)	3 (1%)	65	83
42	u	153/153 (100%)	150 (98%)	3 (2%)	48	76
43	v	106/111 (96%)	106 (100%)	0	100	100
44	w	282/283 (100%)	281 (100%)	1 (0%)	84	90
All	All	7140/7241 (99%)	7019 (98%)	121 (2%)	52	78

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ASP
1	A	125	CYS
1	A	322	SER
1	A	334	THR
1	A	425	CYS
1	A	448	GLU
2	B	72	MET
2	B	75	SER
3	C	66	THR
3	C	71	CYS
3	C	92	VAL
3	C	154	ASP
4	E	15	THR
4	E	116	THR
6	G	84	LEU
6	G	94	ASP
6	G	98	LEU
7	H	49	GLU
8	I	31	ILE

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Mol	Chain	Res	Type
9	J	113	LYS
9	J	230	SER
10	K	85	THR
10	K	89	LEU
10	K	94	SER
11	L	86	ASN
12	M	117	MET
12	M	160	VAL
12	M	338	VAL
12	M	352	VAL
12	M	507	THR
12	M	534	VAL
12	M	556	THR
12	M	648	GLU
13	N	42	ASP
13	N	116	ASN
13	N	120	THR
13	N	144	TYR
14	O	68	LYS
14	O	134	VAL
14	O	232	THR
15	P	201	ASP
16	Q	52	MET
16	Q	55	THR
16	Q	94	VAL
16	Q	185	MET
16	Q	188	THR
16	Q	260	GLU
16	Q	272	THR
16	Q	435	LEU
16	Q	453	THR
16	Q	456	ILE
17	S	16	LEU
18	T	81	SER
20	V	50	LEU
20	V	95	CYS
20	V	141	VAL
21	W	101	VAL
6	X	74	LEU
6	X	89	LEU
6	X	100	VAL
6	X	140	CYS

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Mol	Chain	Res	Type
6	X	156	GLU
22	Y	93	THR
23	Z	34	GLU
24	a	98	LEU
24	a	158	ARG
25	b	7	ASP
25	b	20	ARG
25	b	35	LEU
25	b	79	VAL
26	c	96	ASP
26	c	113	ILE
26	c	156	VAL
27	d	135	VAL
27	d	164	LEU
28	e	72	ASP
28	e	125	LEU
29	f	50	THR
30	g	2	THR
30	g	69	SER
30	g	110	THR
31	h	5	ASP
32	i	85	THR
32	i	149	ILE
32	i	159	MET
32	i	182	SER
33	j	71	LEU
33	j	83	ASN
33	j	87	MET
34	k	24	SER
34	k	59	MET
35	l	71	LEU
35	l	191	THR
35	l	203	MET
35	l	235	SER
35	l	250	SER
35	l	269	THR
35	l	371	THR
36	m	39	VAL
36	m	65	LEU
36	m	169	MET
38	o	37	LEU
38	o	66	ILE

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Mol	Chain	Res	Type
38	o	116	ILE
39	p	57	MET
40	r	60	SER
40	r	130	LEU
40	r	140	THR
40	r	179	ILE
40	r	248	THR
40	r	274	SER
40	r	304	GLN
40	r	332	THR
40	r	420	THR
41	s	15	LEU
41	s	119	SER
41	s	205	SER
42	u	23	SER
42	u	42	GLU
42	u	132	LYS
44	w	248	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	170	GLN
1	A	277	ASN
3	C	111	ASN
4	E	26	ASN
5	F	93	ASN
9	J	102	GLN
9	J	122	HIS
9	J	128	ASN
12	M	278	HIS
12	M	388	ASN
12	M	604	GLN
13	N	31	ASN
13	N	112	ASN
13	N	123	GLN
15	P	55	HIS
15	P	82	ASN
15	P	228	GLN
16	Q	92	HIS
17	S	61	HIS

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Mol	Chain	Res	Type
18	T	123	HIS
19	U	71	GLN
20	V	129	GLN
22	Y	46	GLN
22	Y	83	HIS
22	Y	91	GLN
27	d	123	GLN
28	e	86	ASN
29	f	61	GLN
29	f	62	HIS
30	g	119	HIS
31	h	25	GLN
31	h	98	HIS
32	i	2	ASN
32	i	47	ASN
32	i	63	GLN
32	i	144	GLN
32	i	150	ASN
32	i	204	ASN
32	i	232	HIS
34	k	50	ASN
34	k	57	ASN
35	l	56	HIS
35	l	59	GLN
35	l	72	GLN
35	l	135	ASN
35	l	199	GLN
35	l	309	GLN
35	l	348	HIS
35	l	452	ASN
35	l	470	ASN
35	l	505	ASN
37	n	14	HIS
39	p	51	HIS
40	r	251	ASN
40	r	415	GLN
40	r	422	HIS
42	u	65	GLN
42	u	95	GLN
42	u	163	HIS
43	v	85	HIS
44	w	132	GLN

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Mol	Chain	Res	Type
44	w	286	GLN
44	w	299	GLN
44	w	322	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	2MR	Q	118	16	10,12,13	1.99	1 (10%)	5,13,15	5.82	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	5.75	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	11.89	130.38	119.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	CD-NE-CZ	4.07	131.03	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.20	130.94	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	s	401	-	88,88,99	1.14	9 (10%)	94,100,111	0.91	4 (4%)
52	CDL	o	201	-	99,99,99	1.09	9 (9%)	105,111,111	0.87	4 (3%)
47	NAI	A	503	-	45,48,48	3.91	20 (44%)	60,73,73	1.77	12 (20%)
53	NDP	J	401	-	49,52,52	4.39	23 (46%)	66,80,80	2.24	14 (21%)
48	PEE	l	704	-	45,45,50	1.22	6 (13%)	48,50,55	1.00	2 (4%)
55	FES	O	301	14	0,4,4	-	-	-	-	-
49	PLX	J	403	-	51,51,51	1.14	4 (7%)	55,59,59	0.61	1 (1%)
54	UQ	s	402	-	38,38,63	3.54	9 (23%)	46,49,79	2.85	16 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	PLX	a	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.61	1 (1%)
48	PEE	B	303	-	50,50,50	1.17	6 (12%)	53,55,55	0.97	2 (3%)
55	FES	M	803	12	0,4,4	-	-	-		
48	PEE	C	302	-	46,46,50	1.21	6 (13%)	49,51,55	0.97	2 (4%)
48	PEE	j	201	-	40,40,50	1.15	5 (12%)	43,45,55	1.01	2 (4%)
48	PEE	W	201	-	40,40,50	1.16	5 (12%)	43,45,55	0.97	2 (4%)
48	PEE	i	402	-	46,46,50	1.21	6 (13%)	49,51,55	0.97	2 (4%)
45	SF4	B	302	2	0,12,12	-	-	-		
45	SF4	B	301	2	0,12,12	-	-	-		
52	CDL	V	201	-	93,93,99	1.12	9 (9%)	99,105,111	0.85	4 (4%)
48	PEE	l	703	-	49,49,50	1.17	6 (12%)	52,54,55	0.95	2 (3%)
48	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	0.96	2 (3%)
52	CDL	i	401	-	99,99,99	1.10	9 (9%)	105,111,111	0.84	4 (3%)
52	CDL	I	201	-	50,50,99	1.41	8 (16%)	56,62,111	1.12	4 (7%)
58	ADP	w	401	-	27,29,29	2.97	8 (29%)	42,45,45	2.02	10 (23%)
46	FMN	A	502	-	33,33,33	1.07	2 (6%)	48,50,50	1.22	7 (14%)
54	UQ	J	402	-	33,33,63	3.47	8 (24%)	40,43,79	2.70	14 (35%)
52	CDL	V	202	-	77,77,99	1.20	7 (9%)	83,89,111	0.97	4 (4%)
48	PEE	U	101	-	50,50,50	1.16	6 (12%)	53,55,55	0.91	2 (3%)
45	SF4	A	501	1	0,12,12	-	-	-		
51	8Q1	X	201	-	31,34,34	1.70	6 (19%)	40,43,43	1.52	4 (10%)
49	PLX	r	502	-	51,51,51	1.16	5 (9%)	55,59,59	0.59	1 (1%)
52	CDL	i	403	-	98,98,99	1.10	9 (9%)	104,110,111	0.86	4 (3%)
52	CDL	l	702	-	99,99,99	1.09	9 (9%)	105,111,111	0.89	4 (3%)
45	SF4	M	802	12	0,12,12	-	-	-		
45	SF4	C	301	3	0,12,12	-	-	-		
45	SF4	M	801	12	0,12,12	-	-	-		
51	8Q1	G	201	6	31,34,34	1.70	6 (19%)	40,43,43	1.55	6 (15%)
52	CDL	a	201	-	99,99,99	1.09	8 (8%)	105,111,111	0.84	4 (3%)
52	CDL	g	202	-	54,54,99	1.37	8 (14%)	60,66,111	1.13	4 (6%)
52	CDL	l	701	-	98,98,99	1.09	8 (8%)	104,110,111	0.88	4 (3%)
49	PLX	j	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.60	1 (1%)
49	PLX	r	503	-	51,51,51	1.15	4 (7%)	55,59,59	0.55	1 (1%)
49	PLX	g	201	-	51,51,51	1.14	4 (7%)	55,59,59	0.62	1 (1%)
50	970	C	304	-	33,33,33	4.92	16 (48%)	48,50,50	2.53	18 (37%)
49	PLX	C	303	-	51,51,51	1.16	4 (7%)	55,59,59	0.60	1 (1%)

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	s	401	-	-	50/99/99/110	-
52	CDL	o	201	-	-	56/110/110/110	-
47	NAI	A	503	-	-	10/29/72/72	0/5/5/5
53	NDP	J	401	-	-	9/34/77/77	0/4/5/5
48	PEE	l	704	-	-	20/49/49/54	-
55	FES	O	301	14	-	-	0/1/1/1
49	PLX	J	403	-	-	29/55/55/55	-
54	UQ	s	402	-	-	12/33/57/87	0/1/1/1
49	PLX	a	202	-	-	32/55/55/55	-
48	PEE	B	303	-	-	26/54/54/54	-
55	FES	M	803	12	-	-	0/1/1/1
48	PEE	C	302	-	-	29/50/50/54	-
48	PEE	j	201	-	-	24/44/44/54	-
48	PEE	W	201	-	-	20/44/44/54	-
48	PEE	i	402	-	-	29/50/50/54	-
45	SF4	B	302	2	-	-	0/6/5/5
52	CDL	V	201	-	-	55/104/104/110	-
45	SF4	B	301	2	-	-	0/6/5/5
48	PEE	l	703	-	-	27/53/53/54	-
48	PEE	r	501	-	-	32/54/54/54	-
52	CDL	i	401	-	-	56/110/110/110	-
52	CDL	I	201	-	-	32/61/61/110	-
58	ADP	w	401	-	-	3/16/32/32	0/3/3/3
46	FMN	A	502	-	-	6/18/18/18	0/3/3/3
54	UQ	J	402	-	-	10/27/51/87	0/1/1/1
52	CDL	V	202	-	-	51/88/88/110	-
48	PEE	U	101	-	-	22/54/54/54	-
45	SF4	A	501	1	-	-	0/6/5/5
51	8Q1	X	201	-	-	16/41/41/41	-
49	PLX	r	502	-	-	32/55/55/55	-
52	CDL	i	403	-	-	62/109/109/110	-
52	CDL	l	702	-	-	54/110/110/110	-
45	SF4	M	802	12	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	C	301	3	-	-	0/6/5/5
51	8Q1	G	201	6	-	16/41/41/41	-
52	CDL	a	201	-	-	64/110/110/110	-
52	CDL	g	202	-	-	34/65/65/110	-
45	SF4	M	801	12	-	-	0/6/5/5
52	CDL	l	701	-	-	52/109/109/110	-
49	PLX	j	202	-	-	31/55/55/55	-
49	PLX	r	503	-	-	34/55/55/55	-
49	PLX	g	201	-	-	37/55/55/55	-
50	970	C	304	-	-	2/8/41/41	0/5/5/5
49	PLX	C	303	-	-	23/55/55/55	-

All (272) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	C	304	970	O16-C17	17.90	1.57	1.37
53	J	401	NDP	C3B-C2B	-12.77	1.24	1.52
53	J	401	NDP	C6N-C5N	12.48	1.55	1.33
50	C	304	970	O25-C24	11.10	1.37	1.22
53	J	401	NDP	O4D-C4D	10.66	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.27	1.26	1.53
50	C	304	970	C23-C24	10.19	1.63	1.52
53	J	401	NDP	C3D-C4D	-9.82	1.27	1.53
54	J	402	UQ	C18-C19	9.67	1.56	1.33
54	s	402	UQ	C18-C19	9.60	1.56	1.33
54	J	402	UQ	C13-C14	9.39	1.55	1.33
54	s	402	UQ	C13-C14	9.30	1.55	1.33
47	A	503	NAI	O4B-C1B	9.20	1.63	1.42
54	s	402	UQ	C23-C24	9.01	1.54	1.33
54	s	402	UQ	C8-C9	8.95	1.54	1.33
58	w	401	ADP	C3'-C4'	-8.90	1.30	1.53
54	J	402	UQ	C8-C9	8.90	1.54	1.33
47	A	503	NAI	O4B-C4B	-8.18	1.26	1.45
53	J	401	NDP	O4B-C4B	-7.93	1.27	1.45
54	J	402	UQ	C23-C24	7.80	1.54	1.32
58	w	401	ADP	O4'-C4'	7.75	1.62	1.45
54	s	402	UQ	C28-C29	7.69	1.54	1.32
47	A	503	NAI	C2D-C1D	-7.46	1.29	1.53
53	J	401	NDP	C2N-C3N	7.34	1.55	1.34
47	A	503	NAI	C2B-C1B	-7.21	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	C	304	970	C14-C23	-6.97	1.46	1.52
47	A	503	NAI	O4D-C4D	6.94	1.60	1.45
50	C	304	970	O08-C07	6.42	1.47	1.37
47	A	503	NAI	C2D-C3D	5.96	1.69	1.53
53	J	401	NDP	C6A-N6A	5.96	1.49	1.34
47	A	503	NAI	C7N-N7N	5.74	1.48	1.33
53	J	401	NDP	P2B-O2B	5.71	1.70	1.59
58	w	401	ADP	C6-N6	5.58	1.48	1.34
47	A	503	NAI	O4D-C1D	5.53	1.55	1.42
53	J	401	NDP	C3B-C4B	5.53	1.67	1.53
51	G	201	8Q1	C34-N36	5.48	1.45	1.33
51	X	201	8Q1	C34-N36	5.46	1.45	1.33
51	X	201	8Q1	C39-N41	5.38	1.45	1.33
51	G	201	8Q1	C39-N41	5.36	1.45	1.33
50	C	304	970	O13-C12	5.23	1.45	1.37
47	A	503	NAI	C6A-N6A	5.22	1.47	1.34
47	A	503	NAI	C4N-C3N	-5.03	1.40	1.49
50	C	304	970	C05-C04	-4.99	1.47	1.54
53	J	401	NDP	O4D-C1D	-4.94	1.30	1.42
53	J	401	NDP	C6N-N1N	4.86	1.49	1.37
50	C	304	970	C03-C02	4.72	1.53	1.34
47	A	503	NAI	O2B-C2B	4.57	1.53	1.43
53	J	401	NDP	O4B-C1B	4.53	1.52	1.42
53	J	401	NDP	C1B-N9A	-4.49	1.33	1.46
58	w	401	ADP	O4'-C1'	-4.44	1.31	1.42
53	J	401	NDP	C7N-N7N	4.22	1.44	1.33
53	J	401	NDP	O2D-C2D	-4.15	1.33	1.43
47	A	503	NAI	C6N-C5N	3.99	1.40	1.33
46	A	502	FMN	C4A-N5	3.86	1.38	1.30
48	B	303	PEE	C18-C19	3.74	1.53	1.31
48	l	703	PEE	C18-C19	3.74	1.53	1.31
48	W	201	PEE	C18-C19	3.74	1.53	1.31
48	j	201	PEE	C18-C19	3.74	1.53	1.31
48	r	501	PEE	C18-C19	3.74	1.53	1.31
48	C	302	PEE	C18-C19	3.74	1.53	1.31
48	i	402	PEE	C18-C19	3.74	1.53	1.31
48	U	101	PEE	C18-C19	3.73	1.53	1.31
48	l	704	PEE	C18-C19	3.72	1.53	1.31
48	U	101	PEE	C39-C38	3.67	1.53	1.31
48	r	501	PEE	C39-C38	3.67	1.53	1.31
48	B	303	PEE	C39-C38	3.65	1.53	1.31
48	l	704	PEE	C39-C38	3.65	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	C	302	PEE	C39-C38	3.65	1.52	1.31
48	l	703	PEE	C39-C38	3.65	1.52	1.31
48	i	402	PEE	C39-C38	3.64	1.52	1.31
47	A	503	NAI	C7N-C3N	3.61	1.56	1.48
52	V	202	CDL	OA8-CA7	3.50	1.43	1.33
52	I	201	CDL	OA8-CA7	3.49	1.43	1.33
52	i	401	CDL	OA8-CA7	3.49	1.43	1.33
52	g	202	CDL	OA8-CA7	3.47	1.43	1.33
52	V	201	CDL	OA8-CA7	3.46	1.43	1.33
52	a	201	CDL	OA8-CA7	3.44	1.43	1.33
52	o	201	CDL	OA8-CA7	3.44	1.43	1.33
52	i	403	CDL	OA8-CA7	3.42	1.43	1.33
52	l	701	CDL	OA8-CA7	3.42	1.43	1.33
52	s	401	CDL	OA8-CA7	3.42	1.43	1.33
52	l	702	CDL	OA8-CA7	3.39	1.43	1.33
50	C	304	970	C15-C14	3.38	1.57	1.51
50	C	304	970	C11-C24	3.33	1.54	1.48
47	A	503	NAI	C4N-C5N	-3.32	1.40	1.48
58	w	401	ADP	O2'-C2'	-3.30	1.35	1.43
52	V	202	CDL	OA6-CA5	3.27	1.43	1.34
58	w	401	ADP	C8-N9	-3.16	1.31	1.37
50	C	304	970	O16-C15	3.13	1.52	1.44
52	V	201	CDL	OA6-CA5	3.13	1.43	1.34
58	w	401	ADP	O3'-C3'	3.12	1.50	1.43
53	J	401	NDP	O3D-C3D	3.10	1.50	1.43
52	s	401	CDL	OB6-CB5	3.10	1.43	1.34
52	l	701	CDL	OB6-CB5	3.08	1.43	1.34
52	l	702	CDL	OB8-CB7	3.07	1.42	1.33
52	i	403	CDL	OB6-CB5	3.07	1.43	1.34
52	V	202	CDL	OB6-CB5	3.06	1.42	1.34
52	l	702	CDL	OB6-CB5	3.05	1.42	1.34
52	l	701	CDL	OB8-CB7	3.05	1.42	1.33
52	i	403	CDL	OB8-CB7	3.04	1.42	1.33
53	J	401	NDP	C7N-C3N	3.04	1.55	1.48
52	g	202	CDL	OB8-CB7	3.04	1.42	1.33
52	I	201	CDL	OB8-CB7	3.03	1.42	1.33
52	i	401	CDL	OB8-CB7	3.03	1.42	1.33
52	V	202	CDL	OB8-CB7	3.02	1.42	1.33
52	a	201	CDL	OB6-CB5	3.02	1.42	1.34
52	a	201	CDL	OB8-CB7	3.02	1.42	1.33
52	o	201	CDL	OB6-CB5	3.02	1.42	1.34
52	s	401	CDL	OB8-CB7	3.02	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	o	201	CDL	OB8-CB7	3.01	1.42	1.33
52	V	201	CDL	OB6-CB5	3.00	1.42	1.34
52	V	201	CDL	OB8-CB7	3.00	1.42	1.33
52	l	702	CDL	OA6-CA5	3.00	1.42	1.34
52	I	201	CDL	OB6-CB5	2.99	1.42	1.34
52	g	202	CDL	OB6-CB5	2.99	1.42	1.34
52	i	401	CDL	OB6-CB5	2.99	1.42	1.34
52	o	201	CDL	OA6-CA5	2.99	1.42	1.34
52	s	401	CDL	OA6-CA5	2.98	1.42	1.34
52	i	401	CDL	OA6-CA5	2.98	1.42	1.34
52	i	403	CDL	OA6-CA5	2.97	1.42	1.34
53	J	401	NDP	C8A-N9A	-2.96	1.32	1.37
52	a	201	CDL	OA6-CA5	2.95	1.42	1.34
52	g	202	CDL	OA6-CA5	2.94	1.42	1.34
52	I	201	CDL	OA6-CA5	2.92	1.42	1.34
52	l	701	CDL	OA6-CA5	2.88	1.42	1.34
53	J	401	NDP	C5A-N7A	-2.87	1.33	1.39
50	C	304	970	C12-C06	2.86	1.44	1.39
54	J	402	UQ	C6-C1	2.81	1.54	1.46
54	s	402	UQ	C6-C1	2.77	1.54	1.46
49	C	303	PLX	O6-C4	-2.73	1.41	1.44
49	g	201	PLX	O6-C4	-2.72	1.41	1.44
49	r	503	PLX	O6-C4	-2.69	1.41	1.44
49	a	202	PLX	O6-C4	-2.66	1.41	1.44
50	C	304	970	C09-C07	2.64	1.45	1.39
49	r	502	PLX	O6-C4	-2.54	1.41	1.44
46	A	502	FMN	C10-N1	2.54	1.38	1.33
48	B	303	PEE	O3-C30	2.52	1.40	1.33
48	U	101	PEE	O3-C30	2.51	1.40	1.33
47	A	503	NAI	C8A-N9A	-2.51	1.33	1.37
47	A	503	NAI	O3B-C3B	-2.50	1.37	1.43
49	j	202	PLX	O6-C4	-2.50	1.41	1.44
49	j	202	PLX	C7-C6	2.49	1.56	1.50
48	l	704	PEE	O3-C30	2.49	1.40	1.33
48	j	201	PEE	O3-C30	2.49	1.40	1.33
54	J	402	UQ	C7-C8	2.49	1.54	1.50
48	C	302	PEE	O3-C30	2.48	1.40	1.33
47	A	503	NAI	PN-O5D	2.47	1.69	1.59
48	l	703	PEE	O3-C30	2.47	1.40	1.33
54	s	402	UQ	C7-C8	2.47	1.54	1.50
49	J	403	PLX	O6-C4	-2.46	1.41	1.44
53	J	401	NDP	O2B-C2B	2.46	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	i	402	PEE	O3-C30	2.45	1.40	1.33
51	X	201	8Q1	C1-S44	2.45	1.82	1.76
48	W	201	PEE	O3-C30	2.44	1.40	1.33
48	r	501	PEE	O3-C30	2.44	1.40	1.33
48	C	302	PEE	O2-C2	-2.44	1.40	1.46
51	G	201	8Q1	C1-S44	2.42	1.82	1.76
52	l	701	CDL	OA6-CA4	-2.42	1.40	1.46
52	a	201	CDL	OA6-CA4	-2.42	1.40	1.46
48	j	201	PEE	O2-C2	-2.41	1.40	1.46
48	U	101	PEE	O2-C2	-2.40	1.40	1.46
48	i	402	PEE	O2-C2	-2.39	1.40	1.46
48	B	303	PEE	O2-C10	2.38	1.41	1.34
48	r	501	PEE	O2-C2	-2.37	1.40	1.46
52	i	401	CDL	OA6-CA4	-2.37	1.40	1.46
52	I	201	CDL	OA6-CA4	-2.37	1.40	1.46
52	g	202	CDL	OA6-CA4	-2.37	1.40	1.46
53	J	401	NDP	C2D-C3D	2.36	1.59	1.53
52	o	201	CDL	OA6-CA4	-2.36	1.40	1.46
48	l	704	PEE	O2-C2	-2.35	1.40	1.46
49	a	202	PLX	C7-C6	2.35	1.55	1.50
49	r	502	PLX	C7-C6	2.35	1.55	1.50
48	l	703	PEE	O2-C2	-2.34	1.40	1.46
48	W	201	PEE	O2-C2	-2.34	1.40	1.46
48	W	201	PEE	O2-C10	2.34	1.40	1.34
52	i	403	CDL	OA6-CA4	-2.34	1.40	1.46
52	l	702	CDL	OA6-CA4	-2.34	1.40	1.46
52	s	401	CDL	OA6-CA4	-2.32	1.40	1.46
49	r	503	PLX	C7-C6	2.32	1.55	1.50
49	C	303	PLX	C7-C6	2.32	1.55	1.50
48	B	303	PEE	O2-C2	-2.32	1.40	1.46
48	l	704	PEE	O2-C10	2.31	1.40	1.34
49	J	403	PLX	C7-C6	2.31	1.55	1.50
48	l	703	PEE	O2-C10	2.31	1.40	1.34
47	A	503	NAI	C5B-C4B	2.30	1.58	1.51
49	g	201	PLX	C7-C6	2.30	1.55	1.50
58	w	401	ADP	C5-N7	-2.28	1.34	1.39
48	r	501	PEE	O2-C10	2.28	1.40	1.34
48	i	402	PEE	O2-C10	2.27	1.40	1.34
51	G	201	8Q1	C6-C1	2.26	1.53	1.50
52	g	202	CDL	PB2-OB2	2.25	1.68	1.59
52	o	201	CDL	PB2-OB2	2.25	1.68	1.59
52	V	201	CDL	PB2-OB2	2.23	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	i	401	CDL	PB2-OB2	2.23	1.68	1.59
52	a	201	CDL	PB2-OB2	2.23	1.68	1.59
48	C	302	PEE	O2-C10	2.22	1.40	1.34
52	i	401	CDL	OB6-CB4	-2.22	1.41	1.46
51	G	201	8Q1	O35-C34	-2.22	1.19	1.23
48	U	101	PEE	O2-C10	2.22	1.40	1.34
52	i	403	CDL	PB2-OB2	2.22	1.68	1.59
52	V	201	CDL	OB6-CB4	-2.22	1.41	1.46
52	V	201	CDL	PB2-OB5	2.21	1.68	1.59
51	G	201	8Q1	O40-C39	-2.21	1.18	1.23
52	l	702	CDL	PB2-OB5	2.21	1.68	1.59
52	l	701	CDL	PB2-OB2	2.21	1.68	1.59
52	a	201	CDL	PB2-OB5	2.21	1.68	1.59
52	l	702	CDL	PB2-OB2	2.21	1.68	1.59
52	l	701	CDL	PB2-OB5	2.21	1.68	1.59
52	s	401	CDL	PB2-OB5	2.21	1.68	1.59
52	V	202	CDL	PB2-OB2	2.20	1.68	1.59
52	g	202	CDL	PB2-OB5	2.20	1.68	1.59
48	j	201	PEE	O2-C10	2.20	1.40	1.34
52	s	401	CDL	PB2-OB2	2.19	1.68	1.59
52	i	401	CDL	PB2-OB5	2.19	1.68	1.59
51	X	201	8Q1	O40-C39	-2.19	1.18	1.23
52	I	201	CDL	PB2-OB2	2.19	1.68	1.59
51	X	201	8Q1	O35-C34	-2.19	1.19	1.23
50	C	304	970	O28-C19	2.18	1.40	1.37
52	V	202	CDL	OB6-CB4	-2.18	1.41	1.46
53	J	401	NDP	PA-O5B	2.18	1.68	1.59
52	i	403	CDL	PB2-OB5	2.18	1.68	1.59
52	I	201	CDL	PB2-OB5	2.18	1.68	1.59
49	r	502	PLX	P1-O4	2.17	1.68	1.59
54	s	402	UQ	O4-C4	-2.17	1.18	1.23
52	o	201	CDL	PB2-OB5	2.17	1.68	1.59
52	V	202	CDL	PB2-OB5	2.16	1.68	1.59
52	g	202	CDL	OB6-CB4	-2.16	1.41	1.46
52	I	201	CDL	OB6-CB4	-2.16	1.41	1.46
52	o	201	CDL	OB6-CB4	-2.16	1.41	1.46
49	C	303	PLX	P1-O4	2.16	1.68	1.59
49	j	202	PLX	P1-O4	2.16	1.68	1.59
54	J	402	UQ	O4-C4	-2.15	1.18	1.23
51	X	201	8Q1	C6-C1	2.15	1.53	1.50
52	a	201	CDL	OB6-CB4	-2.15	1.41	1.46
50	C	304	970	C04-C02	2.15	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	l	702	CDL	OB6-CB4	-2.14	1.41	1.46
49	J	403	PLX	P1-O4	2.14	1.67	1.59
49	g	201	PLX	P1-O4	2.13	1.67	1.59
49	a	202	PLX	P1-O4	2.13	1.67	1.59
52	l	701	CDL	OB6-CB4	-2.13	1.41	1.46
49	r	503	PLX	P1-O4	2.13	1.67	1.59
52	i	403	CDL	OB6-CB4	-2.11	1.41	1.46
53	J	401	NDP	O7N-C7N	-2.11	1.19	1.24
50	C	304	970	O26-C20	2.10	1.40	1.37
52	V	201	CDL	OA6-CA4	-2.10	1.41	1.46
48	W	201	PEE	O3-C3	-2.10	1.40	1.45
48	l	703	PEE	O3-C3	-2.09	1.40	1.45
48	l	704	PEE	O3-C3	-2.08	1.40	1.45
48	i	402	PEE	O3-C3	-2.08	1.40	1.45
48	C	302	PEE	O3-C3	-2.07	1.40	1.45
52	s	401	CDL	OB6-CB4	-2.07	1.41	1.46
49	r	502	PLX	P1-O1	2.06	1.67	1.59
49	j	202	PLX	P1-O1	2.06	1.67	1.59
48	r	501	PEE	O3-C3	-2.06	1.40	1.45
48	B	303	PEE	O3-C3	-2.05	1.40	1.45
49	J	403	PLX	P1-O1	2.05	1.67	1.59
49	r	502	PLX	C25-C24	2.05	1.55	1.50
49	r	503	PLX	P1-O1	2.05	1.67	1.59
49	a	202	PLX	P1-O1	2.04	1.67	1.59
49	g	201	PLX	P1-O1	2.04	1.67	1.59
48	j	201	PEE	O3-C3	-2.03	1.40	1.45
52	V	201	CDL	C11-CA5	2.03	1.56	1.50
52	l	702	CDL	C11-CA5	2.03	1.56	1.50
54	s	402	UQ	O1-C1	-2.02	1.19	1.23
49	C	303	PLX	P1-O1	2.02	1.67	1.59
52	i	403	CDL	C11-CA5	2.02	1.56	1.50
48	U	101	PEE	O3-C3	-2.02	1.40	1.45
54	J	402	UQ	C21-C19	2.02	1.55	1.51
52	s	401	CDL	C11-CA5	2.01	1.56	1.50
52	o	201	CDL	C11-CA5	2.01	1.56	1.50
47	A	503	NAI	C2N-C3N	2.01	1.40	1.34
52	i	401	CDL	C11-CA5	2.01	1.56	1.50

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	J	401	NDP	C3N-C2N-N1N	-8.97	110.30	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	s	402	UQ	C7-C8-C9	-8.13	113.26	126.79
50	C	304	970	O25-C24-C11	-7.98	109.19	121.98
54	J	402	UQ	C7-C8-C9	-7.12	114.94	126.79
50	C	304	970	O08-C07-C06	-6.85	108.82	113.00
53	J	401	NDP	C1D-N1N-C2N	-6.75	109.87	121.11
54	s	402	UQ	C22-C23-C24	-6.08	113.01	127.66
54	J	402	UQ	C17-C18-C19	-5.96	113.32	127.66
54	s	402	UQ	C17-C18-C19	-5.91	113.44	127.66
53	J	401	NDP	C5A-C4A-N3A	-5.84	119.13	126.75
54	s	402	UQ	C12-C13-C14	-5.81	113.68	127.66
51	G	201	8Q1	C6-C1-S44	5.80	120.20	113.46
54	J	402	UQ	C12-C13-C14	-5.78	113.74	127.66
47	A	503	NAI	C5A-C4A-N3A	-5.73	119.28	126.75
58	w	401	ADP	C5-C4-N3	-5.69	119.33	126.75
51	X	201	8Q1	C6-C1-S44	5.53	119.89	113.46
50	C	304	970	C06-C05-C04	5.49	106.37	101.45
53	J	401	NDP	C1D-N1N-C6N	-4.97	110.12	120.83
54	J	402	UQ	C10-C9-C8	-4.86	111.20	123.68
54	s	402	UQ	C10-C9-C8	-4.50	112.13	123.68
58	w	401	ADP	N3-C2-N1	-4.48	121.59	128.60
54	J	402	UQ	C22-C23-C24	-4.45	112.52	127.75
58	w	401	ADP	N3-C4-N9	4.43	134.39	127.08
54	s	402	UQ	C27-C28-C29	-4.40	112.70	127.75
47	A	503	NAI	N3A-C2A-N1A	-4.30	121.88	128.60
50	C	304	970	C01-C02-C03	-4.24	111.18	121.38
52	l	702	CDL	OA6-CA5-C11	4.19	120.53	111.50
54	s	402	UQ	C26-C24-C23	-4.17	112.67	121.12
54	s	402	UQ	C25-C24-C23	-4.17	112.98	123.68
53	J	401	NDP	N3A-C4A-N9A	4.13	133.88	127.08
48	j	201	PEE	O2-C10-C11	4.12	120.38	111.50
52	g	202	CDL	OB6-CB5-C51	4.11	120.37	111.50
54	J	402	UQ	C21-C19-C18	-4.11	112.81	121.12
53	J	401	NDP	N3A-C2A-N1A	-4.09	122.20	128.60
52	l	702	CDL	OB6-CB5-C51	4.09	120.32	111.50
52	s	401	CDL	OA6-CA5-C11	4.07	120.27	111.50
48	l	704	PEE	O2-C10-C11	4.06	120.26	111.50
52	l	701	CDL	OB6-CB5-C51	4.06	120.25	111.50
54	J	402	UQ	C11-C9-C8	-4.05	112.92	121.12
48	B	303	PEE	O2-C10-C11	4.04	120.21	111.50
52	s	401	CDL	OB6-CB5-C51	4.04	120.21	111.50
54	s	402	UQ	C21-C19-C18	-4.02	112.98	121.12
47	A	503	NAI	N3A-C4A-N9A	4.02	133.70	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	r	501	PEE	O2-C10-C11	4.01	120.14	111.50
52	V	202	CDL	OB6-CB5-C51	3.99	120.11	111.50
52	g	202	CDL	OA6-CA5-C11	3.99	120.09	111.50
54	J	402	UQ	C20-C19-C18	-3.99	113.45	123.68
52	o	201	CDL	OA6-CA5-C11	3.98	120.08	111.50
52	l	701	CDL	OA6-CA5-C11	3.97	120.06	111.50
54	s	402	UQ	C20-C19-C18	-3.97	113.50	123.68
52	I	201	CDL	OB6-CB5-C51	3.96	120.04	111.50
52	i	401	CDL	OA6-CA5-C11	3.95	120.02	111.50
54	s	402	UQ	C16-C14-C13	-3.93	113.17	121.12
52	o	201	CDL	OB6-CB5-C51	3.92	119.95	111.50
52	i	403	CDL	OA6-CA5-C11	3.92	119.95	111.50
48	W	201	PEE	O2-C10-C11	3.92	119.94	111.50
48	C	302	PEE	O2-C10-C11	3.91	119.93	111.50
52	I	201	CDL	OA6-CA5-C11	3.90	119.90	111.50
52	i	403	CDL	OB6-CB5-C51	3.89	119.88	111.50
48	l	703	PEE	O2-C10-C11	3.88	119.86	111.50
52	a	201	CDL	OB6-CB5-C51	3.88	119.86	111.50
51	X	201	8Q1	C37-C38-C39	3.87	118.81	112.36
47	A	503	NAI	C2A-N3A-C4A	3.83	120.80	111.75
52	V	201	CDL	OB6-CB5-C51	3.82	119.73	111.50
48	i	402	PEE	O2-C10-C11	3.79	119.66	111.50
54	s	402	UQ	C15-C14-C13	-3.78	113.98	123.68
53	J	401	NDP	C2A-N3A-C4A	3.76	120.62	111.75
54	J	402	UQ	C15-C14-C13	-3.75	114.05	123.68
52	a	201	CDL	OA6-CA5-C11	3.75	119.58	111.50
50	C	304	970	O25-C24-C23	-3.74	115.62	121.00
52	V	201	CDL	OA6-CA5-C11	3.73	119.54	111.50
58	w	401	ADP	C2-N3-C4	3.72	120.53	111.75
50	C	304	970	O08-C07-C09	3.71	131.44	123.89
54	s	402	UQ	C11-C9-C8	-3.67	113.69	121.12
47	A	503	NAI	C5A-N7A-C8A	3.66	108.72	103.51
58	w	401	ADP	N9-C8-N7	-3.65	108.92	113.91
52	i	401	CDL	OB6-CB5-C51	3.64	119.34	111.50
48	U	101	PEE	O2-C10-C11	3.57	119.19	111.50
58	w	401	ADP	C5-N7-C8	3.50	108.49	103.51
52	V	202	CDL	OA6-CA5-C11	3.41	118.85	111.50
51	G	201	8Q1	O4-C1-C6	-3.40	119.98	123.99
47	A	503	NAI	N9A-C8A-N7A	-3.40	109.27	113.91
47	A	503	NAI	C3D-C2D-C1D	3.39	107.86	101.43
54	J	402	UQ	C25-C24-C23	-3.35	112.95	122.65
54	s	402	UQ	C30-C29-C28	-3.35	112.96	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	J	402	UQ	C16-C14-C13	-3.35	114.34	121.12
54	J	402	UQ	C26-C24-C23	-3.34	112.98	122.65
51	X	201	8Q1	O4-C1-C6	-3.31	120.08	123.99
53	J	401	NDP	C5A-N7A-C8A	3.29	108.19	103.51
51	G	201	8Q1	C37-C38-C39	3.28	117.83	112.36
52	g	202	CDL	OA8-CA7-C31	3.28	119.98	111.38
50	C	304	970	C04-C02-C03	-3.27	112.94	120.31
53	J	401	NDP	N9A-C8A-N7A	-3.25	109.47	113.91
50	C	304	970	C09-C07-C06	-3.23	119.74	123.20
54	s	402	UQ	C31-C29-C28	-3.22	113.34	122.65
47	A	503	NAI	C4A-C5A-N7A	-3.21	106.71	110.62
58	w	401	ADP	C4-N9-C8	3.13	109.12	105.73
50	C	304	970	O28-C19-C20	3.05	119.66	115.41
50	C	304	970	O26-C20-C19	3.04	119.64	115.41
46	A	502	FMN	C4-N3-C2	-3.01	120.07	125.64
53	J	401	NDP	C4A-C5A-N7A	-2.98	106.99	110.62
52	V	202	CDL	OB8-CB7-C71	2.89	120.98	111.91
50	C	304	970	O13-C14-C23	2.84	115.27	112.40
58	w	401	ADP	C4-C5-N7	-2.81	107.19	110.62
50	C	304	970	C22-C23-C14	2.75	113.41	109.56
47	A	503	NAI	C4D-O4D-C1D	-2.74	103.43	109.47
50	C	304	970	C05-C04-C02	-2.73	111.62	115.62
52	l	702	CDL	OB8-CB7-C71	2.72	120.43	111.91
48	B	303	PEE	O3-C30-C31	2.71	120.43	111.91
46	A	502	FMN	C4A-C4-N3	2.69	120.01	113.19
52	o	201	CDL	OB8-CB7-C71	2.68	120.32	111.91
52	V	202	CDL	OA8-CA7-C31	2.67	120.30	111.91
52	V	201	CDL	OB8-CB7-C71	2.67	120.28	111.91
52	I	201	CDL	OB8-CB7-C71	2.65	120.22	111.91
52	o	201	CDL	OA8-CA7-C31	2.65	120.22	111.91
48	r	501	PEE	O3-C30-C31	2.65	120.21	111.91
52	l	701	CDL	OA8-CA7-C31	2.65	120.21	111.91
53	J	401	NDP	PN-O3-PA	-2.64	123.78	132.83
48	l	703	PEE	O3-C30-C31	2.63	120.16	111.91
52	a	201	CDL	OB8-CB7-C71	2.63	120.15	111.91
52	I	201	CDL	OA8-CA7-C31	2.63	120.15	111.91
58	w	401	ADP	PA-O3A-PB	-2.61	123.86	132.83
52	s	401	CDL	OA8-CA7-C31	2.61	120.09	111.91
52	s	401	CDL	OB8-CB7-C71	2.61	120.09	111.91
48	U	101	PEE	O3-C30-C31	2.61	120.08	111.91
48	i	402	PEE	O3-C30-C31	2.60	120.06	111.91
52	i	401	CDL	OB8-CB7-C71	2.60	120.06	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	i	401	CDL	OA8-CA7-C31	2.60	120.05	111.91
52	i	403	CDL	OB8-CB7-C71	2.60	120.05	111.91
52	l	701	CDL	OB8-CB7-C71	2.58	120.01	111.91
48	l	704	PEE	O3-C30-C31	2.58	120.00	111.91
52	i	403	CDL	OA8-CA7-C31	2.58	120.00	111.91
52	l	702	CDL	OA8-CA7-C31	2.57	119.98	111.91
48	j	201	PEE	O3-C30-C31	2.57	119.98	111.91
48	C	302	PEE	O3-C30-C31	2.57	119.96	111.91
53	J	401	NDP	C2B-C3B-C4B	2.54	107.52	101.99
52	a	201	CDL	OA8-CA7-C31	2.53	119.86	111.91
46	A	502	FMN	O4-C4-C4A	-2.52	119.91	126.60
52	V	201	CDL	OA8-CA7-C31	2.52	119.83	111.91
54	J	402	UQ	CM5-C5-C6	-2.52	120.29	124.40
52	g	202	CDL	OB8-CB7-C71	2.49	119.73	111.91
48	W	201	PEE	O3-C30-C31	2.48	119.70	111.91
50	C	304	970	C11-C12-C06	-2.48	119.15	123.16
47	A	503	NAI	C2D-C3D-C4D	2.47	107.43	102.64
49	a	202	PLX	C1A-N1-C1	2.45	119.95	109.92
49	g	201	PLX	C1A-N1-C1	2.44	119.89	109.92
47	A	503	NAI	PN-O3-PA	-2.43	124.49	132.83
53	J	401	NDP	C4A-N9A-C8A	2.43	108.36	105.73
49	r	502	PLX	C1A-N1-C1	2.38	119.66	109.92
47	A	503	NAI	C4A-N9A-C8A	2.36	108.28	105.73
49	j	202	PLX	C1A-N1-C1	2.35	119.55	109.92
54	s	402	UQ	CM5-C5-C6	-2.34	120.58	124.40
46	A	502	FMN	C4A-C10-N10	2.33	119.88	116.48
49	J	403	PLX	C1A-N1-C1	2.31	119.36	109.92
46	A	502	FMN	C9A-C5A-N5	-2.30	119.93	122.43
49	C	303	PLX	C1A-N1-C1	2.24	119.07	109.92
46	A	502	FMN	C10-C4A-N5	-2.22	120.14	124.86
46	A	502	FMN	C4A-C10-N1	-2.22	119.58	124.73
51	X	201	8Q1	C43-S44-C1	2.22	108.77	101.87
50	C	304	970	C15-C14-C23	2.16	112.37	110.62
49	r	503	PLX	C1A-N1-C1	2.16	118.74	109.92
51	G	201	8Q1	C38-C39-N41	2.15	120.05	116.42
51	G	201	8Q1	O4-C1-S44	-2.15	119.82	122.61
58	w	401	ADP	C4'-O4'-C1'	-2.13	104.76	109.47
53	J	401	NDP	C2B-C1B-N9A	-2.13	109.94	113.53
51	G	201	8Q1	C43-S44-C1	2.10	108.42	101.87
50	C	304	970	C07-C06-C12	2.08	120.78	118.74
50	C	304	970	C01-C02-C04	-2.07	111.67	116.47
50	C	304	970	O26-C20-C21	-2.06	120.57	124.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	J	402	UQ	C10-C9-C11	-2.03	111.85	115.27

There are no chirality outliers.

All (1097) 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'
47	A	503	NAI	C5B-O5B-PA-O3
48	B	303	PEE	C11-C10-O2-C2
48	B	303	PEE	O4-C10-O2-C2
48	C	302	PEE	C17-C18-C19-C20
48	C	302	PEE	C1-O3P-P-O1P
48	C	302	PEE	O4P-C4-C5-N
48	U	101	PEE	C1-O3P-P-O1P
48	W	201	PEE	C1-O3P-P-O2P
48	W	201	PEE	C1-O3P-P-O1P
48	W	201	PEE	C4-O4P-P-O2P
48	W	201	PEE	O4P-C4-C5-N
48	i	402	PEE	C11-C10-O2-C2
48	i	402	PEE	C1-O3P-P-O2P
48	i	402	PEE	C1-O3P-P-O1P
48	i	402	PEE	C1-O3P-P-O4P
48	i	402	PEE	C4-O4P-P-O3P
48	i	402	PEE	C4-O4P-P-O2P
48	i	402	PEE	C4-O4P-P-O1P
48	j	201	PEE	C1-O3P-P-O2P
48	j	201	PEE	C4-O4P-P-O2P
48	j	201	PEE	C4-O4P-P-O1P
48	j	201	PEE	O4P-C4-C5-N
48	l	703	PEE	O3P-C1-C2-O2
48	r	501	PEE	C1-O3P-P-O1P
48	r	501	PEE	C1-O3P-P-O4P
48	r	501	PEE	C4-O4P-P-O1P
49	C	303	PLX	O6-C4-C5-O8
49	C	303	PLX	N1-C1-C2-O1
49	J	403	PLX	O7-C6-O6-C4
49	J	403	PLX	N1-C1-C2-O1
49	a	202	PLX	O7-C6-O6-C4
49	a	202	PLX	C2-O1-P1-O2
49	a	202	PLX	C2-O1-P1-O3
49	a	202	PLX	O9-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
49	g	201	PLX	O7-C6-C7-C8
49	g	201	PLX	O7-C6-O6-C4
49	g	201	PLX	C3-O4-P1-O2
49	g	201	PLX	C3-O4-P1-O3
49	g	201	PLX	C2-O1-P1-O4
49	g	201	PLX	C2-O1-P1-O2
49	g	201	PLX	C2-O1-P1-O3
49	g	201	PLX	O9-C24-O8-C5
49	g	201	PLX	O9-C24-C25-C26
49	j	202	PLX	O7-C6-C7-C8
49	j	202	PLX	C7-C6-O6-C4
49	j	202	PLX	C3-O4-P1-O1
49	j	202	PLX	C3-O4-P1-O2
49	j	202	PLX	C3-O4-P1-O3
49	j	202	PLX	O9-C24-O8-C5
49	r	502	PLX	O7-C6-C7-C8
49	r	502	PLX	O7-C6-O6-C4
49	r	502	PLX	C5-C4-O6-C6
49	r	502	PLX	O9-C24-C25-C26
49	r	503	PLX	C3-O4-P1-O2
49	r	503	PLX	C2-O1-P1-O4
49	r	503	PLX	O9-C24-C25-C26
50	C	304	970	C03-C02-C04-C05
50	C	304	970	C03-C02-C04-O08
51	G	201	8Q1	C28-C29-C32-C34
51	G	201	8Q1	C28-C29-C32-O33
51	G	201	8Q1	C30-C29-C32-C34
51	G	201	8Q1	C30-C29-C32-O33
51	G	201	8Q1	C31-C29-C32-C34
51	G	201	8Q1	C31-C29-C32-O33
51	G	201	8Q1	C42-C43-S44-C1
51	G	201	8Q1	C28-O27-P24-O2
51	G	201	8Q1	C28-O27-P24-O1
51	X	201	8Q1	O4-C1-S44-C43
51	X	201	8Q1	C6-C1-S44-C43
51	X	201	8Q1	C28-C29-C32-C34
51	X	201	8Q1	C28-C29-C32-O33
51	X	201	8Q1	C30-C29-C32-C34
51	X	201	8Q1	C30-C29-C32-O33
51	X	201	8Q1	C31-C29-C32-C34
51	X	201	8Q1	C31-C29-C32-O33
51	X	201	8Q1	N41-C42-C43-S44

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Mol	Chain	Res	Type	Atoms
51	X	201	8Q1	C28-O27-P24-O2
51	X	201	8Q1	C28-O27-P24-O1
52	I	201	CDL	CA2-OA2-PA1-OA3
52	I	201	CDL	CA2-OA2-PA1-OA4
52	I	201	CDL	CA2-OA2-PA1-OA5
52	I	201	CDL	CA3-OA5-PA1-OA3
52	I	201	CDL	CB2-OB2-PB2-OB3
52	I	201	CDL	CB2-OB2-PB2-OB4
52	I	201	CDL	CB2-OB2-PB2-OB5
52	I	201	CDL	CB3-OB5-PB2-OB3
52	V	201	CDL	CB2-OB2-PB2-OB3
52	V	201	CDL	CB3-OB5-PB2-OB4
52	V	202	CDL	CA2-OA2-PA1-OA3
52	V	202	CDL	CA2-OA2-PA1-OA4
52	V	202	CDL	CA2-OA2-PA1-OA5
52	V	202	CDL	CA3-OA5-PA1-OA3
52	V	202	CDL	OA6-CA4-CA6-OA8
52	V	202	CDL	CB2-OB2-PB2-OB3
52	V	202	CDL	CB3-OB5-PB2-OB2
52	V	202	CDL	CB3-OB5-PB2-OB3
52	V	202	CDL	CB3-OB5-PB2-OB4
52	a	201	CDL	O1-C1-CA2-OA2
52	a	201	CDL	CA2-OA2-PA1-OA3
52	a	201	CDL	CA2-OA2-PA1-OA4
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	g	202	CDL	O1-C1-CB2-OB2
52	g	202	CDL	CA3-OA5-PA1-OA3
52	g	202	CDL	CA3-OA5-PA1-OA4
52	g	202	CDL	CB3-OB5-PB2-OB2
52	g	202	CDL	CB3-OB5-PB2-OB3
52	g	202	CDL	CB3-OB5-PB2-OB4
52	i	401	CDL	CB3-OB5-PB2-OB3
52	i	403	CDL	CA3-OA5-PA1-OA2
52	i	403	CDL	CA3-OA5-PA1-OA3
52	i	403	CDL	CB3-OB5-PB2-OB3
52	i	403	CDL	CB3-OB5-PB2-OB4
52	l	701	CDL	O1-C1-CA2-OA2
52	l	701	CDL	CA2-OA2-PA1-OA3
52	l	701	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
52	l	701	CDL	CB2-OB2-PB2-OB3
52	l	701	CDL	CB2-OB2-PB2-OB4
52	l	701	CDL	CB3-OB5-PB2-OB3
52	l	702	CDL	O1-C1-CB2-OB2
52	l	702	CDL	CA3-OA5-PA1-OA3
52	l	702	CDL	CB2-OB2-PB2-OB4
52	l	702	CDL	C51-CB5-OB6-CB4
52	o	201	CDL	CA2-OA2-PA1-OA3
52	o	201	CDL	CA2-OA2-PA1-OA4
52	o	201	CDL	CA3-OA5-PA1-OA3
52	o	201	CDL	OA6-CA4-CA6-OA8
52	o	201	CDL	CB3-OB5-PB2-OB3
52	o	201	CDL	CB3-OB5-PB2-OB4
52	s	401	CDL	O1-C1-CA2-OA2
52	s	401	CDL	CB2-C1-CA2-OA2
52	s	401	CDL	CA2-OA2-PA1-OA3
52	s	401	CDL	CA2-OA2-PA1-OA4
52	s	401	CDL	CA3-OA5-PA1-OA2
52	s	401	CDL	CA3-OA5-PA1-OA3
52	s	401	CDL	CA3-OA5-PA1-OA4
52	s	401	CDL	CB2-OB2-PB2-OB3
52	s	401	CDL	CB2-OB2-PB2-OB4
52	s	401	CDL	C51-CB5-OB6-CB4
53	J	401	NDP	C5B-O5B-PA-O1A
53	J	401	NDP	O4B-C4B-C5B-O5B
54	J	402	UQ	C7-C8-C9-C11
54	J	402	UQ	C17-C18-C19-C21
54	s	402	UQ	C7-C8-C9-C10
54	s	402	UQ	C7-C8-C9-C11
54	s	402	UQ	C22-C23-C24-C26
58	w	401	ADP	PA-O3A-PB-O2B
48	U	101	PEE	O5-C30-O3-C3
52	i	401	CDL	OA9-CA7-OA8-CA6
52	l	701	CDL	OA9-CA7-OA8-CA6
52	l	702	CDL	OB9-CB7-OB8-CB6
48	C	302	PEE	O4-C10-O2-C2
48	i	402	PEE	O4-C10-O2-C2
48	l	704	PEE	O4-C10-O2-C2
52	i	403	CDL	OB7-CB5-OB6-CB4
52	l	702	CDL	OB7-CB5-OB6-CB4
52	s	401	CDL	OB7-CB5-OB6-CB4
48	U	101	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
52	l	701	CDL	C31-CA7-OA8-CA6
48	C	302	PEE	C11-C10-O2-C2
48	l	704	PEE	C11-C10-O2-C2
52	a	201	CDL	C51-CB5-OB6-CB4
52	i	403	CDL	C51-CB5-OB6-CB4
54	s	402	UQ	C12-C11-C9-C10
54	s	402	UQ	C23-C24-C26-C27
52	i	401	CDL	C31-CA7-OA8-CA6
52	i	403	CDL	C71-CB7-OB8-CB6
52	l	702	CDL	C71-CB7-OB8-CB6
48	U	101	PEE	C17-C18-C19-C20
48	W	201	PEE	C17-C18-C19-C20
48	l	704	PEE	C37-C38-C39-C40
54	J	402	UQ	C22-C23-C24-C26
54	J	402	UQ	C7-C8-C9-C10
49	J	403	PLX	C27-C28-C29-C30
54	J	402	UQ	C12-C13-C14-C16
54	s	402	UQ	C17-C18-C19-C21
52	l	701	CDL	C32-C33-C34-C35
52	g	202	CDL	O1-C1-CA2-OA2
52	i	403	CDL	O1-C1-CA2-OA2
52	l	701	CDL	O1-C1-CB2-OB2
52	l	702	CDL	O1-C1-CA2-OA2
48	l	703	PEE	C11-C10-O2-C2
52	V	201	CDL	C11-CA5-OA6-CA4
52	o	201	CDL	C51-CB5-OB6-CB4
52	V	201	CDL	C11-C12-C13-C14
52	l	701	CDL	C55-C56-C57-C58
52	l	702	CDL	C35-C36-C37-C38
49	r	502	PLX	C9-C10-C11-C12
52	V	202	CDL	C73-C74-C75-C76
52	l	702	CDL	C75-C76-C77-C78
49	C	303	PLX	C25-C26-C27-C28
58	w	401	ADP	O4'-C4'-C5'-O5'
58	w	401	ADP	C3'-C4'-C5'-O5'
52	o	201	CDL	OB7-CB5-OB6-CB4
49	J	403	PLX	C25-C26-C27-C28
52	i	403	CDL	OB9-CB7-OB8-CB6
49	g	201	PLX	C9-C10-C11-C12
49	r	502	PLX	C11-C12-C13-C14
54	J	402	UQ	C12-C11-C9-C8
49	g	201	PLX	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
48	W	201	PEE	C31-C30-O3-C3
52	l	702	CDL	C33-C34-C35-C36
52	s	401	CDL	C14-C15-C16-C17
49	C	303	PLX	C27-C28-C29-C30
52	I	201	CDL	C51-C52-C53-C54
52	V	202	CDL	CB2-C1-CA2-OA2
52	a	201	CDL	CB2-C1-CA2-OA2
52	g	202	CDL	CA2-C1-CB2-OB2
52	l	701	CDL	CB2-C1-CA2-OA2
52	l	701	CDL	CA2-C1-CB2-OB2
52	l	702	CDL	CB2-C1-CA2-OA2
52	l	702	CDL	CA2-C1-CB2-OB2
48	l	703	PEE	O4-C10-O2-C2
49	j	202	PLX	C13-C14-C15-C16
49	r	502	PLX	C7-C8-C9-C10
48	i	402	PEE	C31-C30-O3-C3
48	l	703	PEE	C31-C30-O3-C3
52	V	201	CDL	C31-CA7-OA8-CA6
52	a	201	CDL	C71-CB7-OB8-CB6
52	l	701	CDL	C71-CB7-OB8-CB6
52	s	401	CDL	C31-C32-C33-C34
49	j	202	PLX	O4-C3-C4-O6
52	V	201	CDL	OB5-CB3-CB4-OB6
52	V	201	CDL	OB6-CB4-CB6-OB8
48	l	703	PEE	O5-C30-O3-C3
49	J	403	PLX	C12-C13-C14-C15
48	j	201	PEE	C11-C10-O2-C2
48	i	402	PEE	C11-C12-C13-C14
53	J	401	NDP	C2D-C1D-N1N-C6N
52	a	201	CDL	CB7-C71-C72-C73
52	i	401	CDL	CB5-C51-C52-C53
52	i	401	CDL	CB7-C71-C72-C73
52	l	702	CDL	CB5-C51-C52-C53
48	r	501	PEE	C17-C18-C19-C20
54	s	402	UQ	C27-C28-C29-C30
54	J	402	UQ	C17-C18-C19-C20
48	i	402	PEE	O5-C30-O3-C3
48	C	302	PEE	C30-C31-C32-C33
52	I	201	CDL	CB5-C51-C52-C53
52	i	401	CDL	CA7-C31-C32-C33
52	i	403	CDL	CB7-C71-C72-C73
52	l	701	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
52	l	702	CDL	CB7-C71-C72-C73
52	s	401	CDL	CA7-C31-C32-C33
52	V	201	CDL	OA7-CA5-OA6-CA4
49	g	201	PLX	C2-C1-N1-C1A
52	l	701	CDL	CB5-C51-C52-C53
52	s	401	CDL	CB7-C71-C72-C73
48	B	303	PEE	C34-C35-C36-C37
48	r	501	PEE	C11-C10-O2-C2
52	l	701	CDL	OB9-CB7-OB8-CB6
52	o	201	CDL	C36-C37-C38-C39
52	V	201	CDL	C62-C63-C64-C65
52	a	201	CDL	OB9-CB7-OB8-CB6
52	a	201	CDL	CA5-C11-C12-C13
52	V	202	CDL	O1-C1-CA2-OA2
52	a	201	CDL	O1-C1-CB2-OB2
52	i	401	CDL	O1-C1-CA2-OA2
52	o	201	CDL	O1-C1-CA2-OA2
48	W	201	PEE	O5-C30-O3-C3
52	V	201	CDL	OA9-CA7-OA8-CA6
48	l	704	PEE	C21-C22-C23-C24
48	B	303	PEE	C17-C18-C19-C20
48	i	402	PEE	C37-C38-C39-C40
48	r	501	PEE	C41-C42-C43-C44
52	l	701	CDL	C81-C82-C83-C84
52	V	201	CDL	C58-C59-C60-C61
48	C	302	PEE	C1-O3P-P-O4P
48	C	302	PEE	C4-O4P-P-O3P
48	U	101	PEE	C1-O3P-P-O4P
48	W	201	PEE	C1-O3P-P-O4P
48	W	201	PEE	C4-O4P-P-O3P
48	j	201	PEE	C1-O3P-P-O4P
48	r	501	PEE	C4-O4P-P-O3P
49	a	202	PLX	C2-O1-P1-O4
49	g	201	PLX	C3-O4-P1-O1
49	r	502	PLX	C3-O4-P1-O1
52	I	201	CDL	CB3-OB5-PB2-OB2
52	V	201	CDL	CB2-OB2-PB2-OB5
52	V	202	CDL	CA3-OA5-PA1-OA2
52	a	201	CDL	CA2-OA2-PA1-OA5
52	a	201	CDL	CA3-OA5-PA1-OA2
52	a	201	CDL	CB2-OB2-PB2-OB5
52	a	201	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
52	g	202	CDL	CA3-OA5-PA1-OA2
52	g	202	CDL	CB2-OB2-PB2-OB5
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	i	403	CDL	CB2-OB2-PB2-OB5
52	i	403	CDL	CB3-OB5-PB2-OB2
52	l	701	CDL	CB2-OB2-PB2-OB5
52	o	201	CDL	CB3-OB5-PB2-OB2
52	s	401	CDL	CA2-OA2-PA1-OA5
52	s	401	CDL	CB2-OB2-PB2-OB5
52	a	201	CDL	C31-CA7-OA8-CA6
52	I	201	CDL	C11-C12-C13-C14
52	g	202	CDL	CB2-C1-CA2-OA2
52	i	403	CDL	CB2-C1-CA2-OA2
52	o	201	CDL	CB2-C1-CA2-OA2
48	j	201	PEE	O4-C10-O2-C2
48	r	501	PEE	O4-C10-O2-C2
49	g	201	PLX	C2-C1-N1-C1B
49	a	202	PLX	O6-C6-C7-C8
49	r	502	PLX	O6-C6-C7-C8
49	j	202	PLX	C16-C17-C18-C19
49	r	502	PLX	C27-C28-C29-C30
52	V	202	CDL	C76-C77-C78-C79
48	i	402	PEE	C21-C22-C23-C24
48	r	501	PEE	C21-C22-C23-C24
49	C	303	PLX	C10-C11-C12-C13
49	C	303	PLX	C35-C36-C37-C38
49	a	202	PLX	C17-C18-C19-C20
49	g	201	PLX	C28-C29-C30-C31
49	j	202	PLX	C27-C28-C29-C30
52	V	201	CDL	C31-C32-C33-C34
52	i	401	CDL	C59-C60-C61-C62
52	l	701	CDL	C11-C12-C13-C14
52	l	701	CDL	C59-C60-C61-C62
52	l	702	CDL	C55-C56-C57-C58
52	o	201	CDL	C17-C18-C19-C20
52	o	201	CDL	C54-C55-C56-C57
52	o	201	CDL	C60-C61-C62-C63
52	s	401	CDL	C73-C74-C75-C76
49	J	403	PLX	C33-C34-C35-C36
49	r	502	PLX	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
49	r	503	PLX	C25-C26-C27-C28
52	V	201	CDL	C35-C36-C37-C38
52	V	201	CDL	C71-C72-C73-C74
52	V	201	CDL	C78-C79-C80-C81
52	g	202	CDL	C75-C76-C77-C78
52	o	201	CDL	C14-C15-C16-C17
52	o	201	CDL	C82-C83-C84-C85
48	W	201	PEE	C12-C13-C14-C15
49	a	202	PLX	C10-C11-C12-C13
49	a	202	PLX	C9-C10-C11-C12
49	j	202	PLX	C14-C15-C16-C17
52	g	202	CDL	C55-C56-C57-C58
52	l	702	CDL	C37-C38-C39-C40
48	j	201	PEE	C23-C24-C25-C26
48	j	201	PEE	C13-C14-C15-C16
49	C	303	PLX	C9-C10-C11-C12
49	J	403	PLX	C30-C31-C32-C33
49	r	502	PLX	C12-C13-C14-C15
52	V	202	CDL	C71-C72-C73-C74
52	i	401	CDL	C18-C19-C20-C21
52	i	403	CDL	C32-C33-C34-C35
52	l	701	CDL	C52-C53-C54-C55
48	r	501	PEE	C20-C21-C22-C23
49	C	303	PLX	C11-C12-C13-C14
49	j	202	PLX	C33-C34-C35-C36
49	r	503	PLX	C10-C11-C12-C13
52	g	202	CDL	C73-C74-C75-C76
52	i	401	CDL	C55-C56-C57-C58
52	o	201	CDL	C37-C38-C39-C40
52	I	201	CDL	CA7-C31-C32-C33
52	l	702	CDL	C31-CA7-OA8-CA6
48	W	201	PEE	C21-C22-C23-C24
49	g	201	PLX	C13-C14-C15-C16
49	g	201	PLX	C30-C31-C32-C33
49	j	202	PLX	C11-C12-C13-C14
49	j	202	PLX	C25-C26-C27-C28
52	V	202	CDL	C75-C76-C77-C78
52	a	201	CDL	C37-C38-C39-C40
52	i	401	CDL	C76-C77-C78-C79
52	l	701	CDL	C37-C38-C39-C40
52	l	701	CDL	C75-C76-C77-C78
52	l	702	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
52	l	702	CDL	C32-C33-C34-C35
52	s	401	CDL	C59-C60-C61-C62
52	s	401	CDL	C71-C72-C73-C74
52	a	201	CDL	OA9-CA7-OA8-CA6
49	C	303	PLX	C15-C16-C17-C18
49	j	202	PLX	C10-C11-C12-C13
52	a	201	CDL	C17-C18-C19-C20
52	l	702	CDL	C82-C83-C84-C85
52	o	201	CDL	C12-C13-C14-C15
48	j	201	PEE	C12-C13-C14-C15
49	J	403	PLX	C9-C10-C11-C12
49	g	201	PLX	C14-C15-C16-C17
49	r	502	PLX	C33-C34-C35-C36
52	V	201	CDL	C75-C76-C77-C78
52	g	202	CDL	C52-C53-C54-C55
52	i	403	CDL	C31-C32-C33-C34
52	i	403	CDL	C80-C81-C82-C83
52	l	701	CDL	C71-C72-C73-C74
52	l	701	CDL	C73-C74-C75-C76
52	l	701	CDL	C82-C83-C84-C85
52	l	702	CDL	C62-C63-C64-C65
52	l	702	CDL	C71-C72-C73-C74
52	o	201	CDL	C83-C84-C85-C86
48	r	501	PEE	C14-C15-C16-C17
49	g	201	PLX	C32-C33-C34-C35
49	r	503	PLX	C16-C17-C18-C19
52	V	201	CDL	C15-C16-C17-C18
52	i	401	CDL	C38-C39-C40-C41
52	l	701	CDL	C62-C63-C64-C65
49	J	403	PLX	C7-C8-C9-C10
52	a	201	CDL	C62-C63-C64-C65
52	i	401	CDL	C82-C83-C84-C85
52	l	702	CDL	C80-C81-C82-C83
52	s	401	CDL	C35-C36-C37-C38
48	B	303	PEE	C35-C36-C37-C38
48	r	501	PEE	C15-C16-C17-C18
48	W	201	PEE	C13-C14-C15-C16
49	a	202	PLX	C27-C28-C29-C30
49	g	201	PLX	C10-C11-C12-C13
52	V	201	CDL	C17-C18-C19-C20
52	V	201	CDL	C56-C57-C58-C59
52	a	201	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
52	s	401	CDL	C36-C37-C38-C39
48	l	703	PEE	C11-C12-C13-C14
51	X	201	8Q1	C6-C7-C8-C9
52	V	201	CDL	C40-C41-C42-C43
52	V	201	CDL	C55-C56-C57-C58
52	V	202	CDL	C11-C12-C13-C14
52	V	202	CDL	C17-C18-C19-C20
52	a	201	CDL	C52-C53-C54-C55
52	a	201	CDL	C82-C83-C84-C85
52	i	403	CDL	C19-C20-C21-C22
52	s	401	CDL	C52-C53-C54-C55
49	C	303	PLX	C30-C31-C32-C33
49	J	403	PLX	C28-C29-C30-C31
49	r	502	PLX	C28-C29-C30-C31
52	V	201	CDL	C72-C73-C74-C75
52	a	201	CDL	C60-C61-C62-C63
52	s	401	CDL	C17-C18-C19-C20
49	g	201	PLX	C11-C10-C9-C8
49	r	503	PLX	C28-C29-C30-C31
52	a	201	CDL	C75-C76-C77-C78
52	i	403	CDL	C52-C53-C54-C55
48	r	501	PEE	C12-C13-C14-C15
49	g	201	PLX	C33-C34-C35-C36
52	V	201	CDL	C73-C74-C75-C76
52	i	401	CDL	C75-C76-C77-C78
52	l	701	CDL	C33-C34-C35-C36
48	l	704	PEE	C34-C35-C36-C37
49	C	303	PLX	C14-C15-C16-C17
49	C	303	PLX	C33-C34-C35-C36
49	g	201	PLX	C27-C28-C29-C30
52	V	201	CDL	C59-C60-C61-C62
49	J	403	PLX	C14-C15-C16-C17
52	l	701	CDL	C14-C15-C16-C17
49	J	403	PLX	C31-C32-C33-C34
52	i	403	CDL	C59-C60-C61-C62
52	o	201	CDL	C32-C33-C34-C35
52	I	201	CDL	C51-CB5-OB6-CB4
52	V	201	CDL	C51-CB5-OB6-CB4
49	a	202	PLX	C34-C35-C36-C37
52	V	202	CDL	C81-C82-C83-C84
52	i	403	CDL	C55-C56-C57-C58
54	s	402	UQ	C27-C28-C29-C31

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Mol	Chain	Res	Type	Atoms
49	C	303	PLX	O9-C24-C25-C26
49	a	202	PLX	O9-C24-C25-C26
48	l	704	PEE	C11-C12-C13-C14
49	r	502	PLX	C25-C26-C27-C28
49	r	502	PLX	C30-C31-C32-C33
52	V	201	CDL	C57-C58-C59-C60
52	l	701	CDL	C36-C37-C38-C39
52	o	201	CDL	C59-C60-C61-C62
48	U	101	PEE	C35-C36-C37-C38
48	W	201	PEE	C19-C20-C21-C22
48	i	402	PEE	C19-C20-C21-C22
49	a	202	PLX	C33-C34-C35-C36
49	g	201	PLX	C25-C26-C27-C28
52	g	202	CDL	CB7-C71-C72-C73
52	a	201	CDL	CA2-C1-CB2-OB2
52	I	201	CDL	OB7-CB5-OB6-CB4
52	V	201	CDL	OB7-CB5-OB6-CB4
49	J	403	PLX	C26-C27-C28-C29
52	V	201	CDL	C52-C53-C54-C55
52	l	701	CDL	C34-C35-C36-C37
52	s	401	CDL	C75-C76-C77-C78
48	j	201	PEE	C11-C12-C13-C14
52	i	403	CDL	C43-C44-C45-C46
52	i	403	CDL	C73-C74-C75-C76
52	s	401	CDL	C32-C33-C34-C35
49	a	202	PLX	C7-C8-C9-C10
52	o	201	CDL	C57-C58-C59-C60
52	V	201	CDL	C71-CB7-OB8-CB6
48	B	303	PEE	C40-C41-C42-C43
52	o	201	CDL	C74-C75-C76-C77
49	a	202	PLX	C13-C14-C15-C16
52	V	201	CDL	OB9-CB7-OB8-CB6
52	l	702	CDL	OA9-CA7-OA8-CA6
52	i	401	CDL	C14-C15-C16-C17
48	j	201	PEE	C19-C20-C21-C22
52	l	702	CDL	OA7-CA5-OA6-CA4
52	l	701	CDL	CA7-C31-C32-C33
52	i	401	CDL	C71-CB7-OB8-CB6
52	a	201	CDL	C36-C37-C38-C39
52	i	401	CDL	C77-C78-C79-C80
52	o	201	CDL	C35-C36-C37-C38
52	l	702	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
49	g	201	PLX	C16-C17-C18-C19
52	i	403	CDL	C41-C42-C43-C44
52	s	401	CDL	C78-C79-C80-C81
52	l	702	CDL	C81-C82-C83-C84
52	o	201	CDL	C55-C56-C57-C58
52	a	201	CDL	C11-C12-C13-C14
52	i	401	CDL	C73-C74-C75-C76
52	i	403	CDL	C51-C52-C53-C54
52	l	701	CDL	C51-CB5-OB6-CB4
52	l	702	CDL	C11-CA5-OA6-CA4
52	I	201	CDL	OA5-CA3-CA4-OA6
52	V	202	CDL	OA5-CA3-CA4-OA6
52	i	401	CDL	OA5-CA3-CA4-OA6
52	o	201	CDL	OB5-CB3-CB4-OB6
48	r	501	PEE	C31-C32-C33-C34
52	l	702	CDL	C39-C40-C41-C42
52	V	202	CDL	OB6-CB4-CB6-OB8
52	i	403	CDL	OB6-CB4-CB6-OB8
48	B	303	PEE	C12-C13-C14-C15
49	a	202	PLX	C30-C31-C32-C33
52	g	202	CDL	C54-C55-C56-C57
49	g	201	PLX	C2-C1-N1-C1C
49	J	403	PLX	C16-C17-C18-C19
52	a	201	CDL	C22-C23-C24-C25
48	l	703	PEE	C23-C24-C25-C26
49	r	503	PLX	C11-C12-C13-C14
52	s	401	CDL	C11-C12-C13-C14
48	l	703	PEE	C31-C32-C33-C34
52	I	201	CDL	C71-C72-C73-C74
49	j	202	PLX	C7-C8-C9-C10
49	r	502	PLX	C16-C17-C18-C19
49	r	503	PLX	C7-C8-C9-C10
52	i	401	CDL	OB9-CB7-OB8-CB6
52	l	701	CDL	OB7-CB5-OB6-CB4
49	g	201	PLX	C12-C13-C14-C15
49	r	503	PLX	C14-C15-C16-C17
49	r	503	PLX	C30-C31-C32-C33
52	V	201	CDL	C14-C15-C16-C17
52	l	702	CDL	C59-C60-C61-C62
48	U	101	PEE	C36-C37-C38-C39
46	A	502	FMN	O2'-C2'-C3'-C4'
48	j	201	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
49	a	202	PLX	C3-O4-P1-O1
49	r	503	PLX	C3-O4-P1-O1
52	V	201	CDL	CB3-OB5-PB2-OB2
52	V	202	CDL	CB2-OB2-PB2-OB5
52	l	701	CDL	CB3-OB5-PB2-OB2
52	l	702	CDL	CA3-OA5-PA1-OA2
52	l	702	CDL	CB2-OB2-PB2-OB5
52	o	201	CDL	CA2-OA2-PA1-OA5
52	i	403	CDL	C72-C73-C74-C75
46	A	502	FMN	C3'-C4'-C5'-O5'
48	l	703	PEE	O3P-C1-C2-C3
52	V	201	CDL	OB5-CB3-CB4-CB6
52	i	401	CDL	OA5-CA3-CA4-CA6
52	i	401	CDL	OB5-CB3-CB4-CB6
52	a	201	CDL	C39-C40-C41-C42
48	U	101	PEE	C12-C13-C14-C15
49	r	502	PLX	C34-C35-C36-C37
52	V	201	CDL	C37-C38-C39-C40
52	i	403	CDL	C11-C12-C13-C14
52	i	403	CDL	C62-C63-C64-C65
48	l	703	PEE	C19-C20-C21-C22
52	o	201	CDL	CA7-C31-C32-C33
52	i	403	CDL	C21-C22-C23-C24
52	s	401	CDL	C54-C55-C56-C57
52	l	701	CDL	C74-C75-C76-C77
48	U	101	PEE	C11-C12-C13-C14
48	W	201	PEE	C24-C25-C26-C27
52	a	201	CDL	C35-C36-C37-C38
52	i	403	CDL	CA5-C11-C12-C13
48	l	703	PEE	C40-C41-C42-C43
52	V	202	CDL	C14-C15-C16-C17
52	i	403	CDL	C17-C18-C19-C20
52	i	403	CDL	C76-C77-C78-C79
48	C	302	PEE	C1-C2-C3-O3
48	W	201	PEE	C1-C2-C3-O3
48	i	402	PEE	C1-C2-C3-O3
48	j	201	PEE	C1-C2-C3-O3
48	j	201	PEE	C32-C33-C34-C35
49	C	303	PLX	C3-C4-C5-O8
49	J	403	PLX	C3-C4-C5-O8
49	r	503	PLX	C13-C14-C15-C16
52	V	201	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
52	V	201	CDL	CB3-CB4-CB6-OB8
52	V	202	CDL	CA3-CA4-CA6-OA8
52	V	202	CDL	C32-C33-C34-C35
52	i	403	CDL	CA3-CA4-CA6-OA8
52	o	201	CDL	CA3-CA4-CA6-OA8
52	o	201	CDL	CB3-CB4-CB6-OB8
48	l	704	PEE	C13-C14-C15-C16
49	C	303	PLX	C19-C20-C21-C22
49	C	303	PLX	C28-C29-C30-C31
49	J	403	PLX	C4-C5-O8-C24
48	B	303	PEE	C23-C24-C25-C26
49	r	503	PLX	C36-C37-C38-C39
52	s	401	CDL	C12-C11-CA5-OA6
52	i	403	CDL	C42-C43-C44-C45
52	l	702	CDL	C17-C18-C19-C20
49	J	403	PLX	O8-C24-C25-C26
49	j	202	PLX	O6-C6-C7-C8
49	j	202	PLX	O8-C24-C25-C26
49	r	502	PLX	O8-C24-C25-C26
49	r	503	PLX	C29-C30-C31-C32
52	g	202	CDL	C74-C75-C76-C77
48	B	303	PEE	C38-C39-C40-C41
48	W	201	PEE	C15-C16-C17-C18
52	a	201	CDL	C32-C33-C34-C35
47	A	503	NAI	C3D-C4D-C5D-O5D
52	i	403	CDL	C15-C16-C17-C18
52	s	401	CDL	C33-C34-C35-C36
52	V	201	CDL	C32-C33-C34-C35
52	i	401	CDL	C40-C41-C42-C43
48	C	302	PEE	C42-C43-C44-C45
49	a	202	PLX	C11-C12-C13-C14
52	I	201	CDL	C12-C13-C14-C15
52	l	702	CDL	C44-C45-C46-C47
48	r	501	PEE	C44-C45-C46-C47
51	G	201	8Q1	C28-O27-P24-O3
51	X	201	8Q1	C28-O27-P24-O3
49	C	303	PLX	C17-C18-C19-C20
52	i	403	CDL	C22-C23-C24-C25
48	B	303	PEE	C31-C30-O3-C3
48	l	704	PEE	C31-C30-O3-C3
49	J	403	PLX	O4-C3-C4-O6
49	g	201	PLX	O4-C3-C4-O6

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Mol	Chain	Res	Type	Atoms
52	V	202	CDL	OB5-CB3-CB4-OB6
52	l	701	CDL	OB5-CB3-CB4-OB6
52	i	401	CDL	C35-C36-C37-C38
49	j	202	PLX	C19-C20-C21-C22
48	l	703	PEE	C15-C16-C17-C18
52	l	702	CDL	C16-C17-C18-C19
48	l	703	PEE	O2-C2-C3-O3
49	j	202	PLX	O6-C4-C5-O8
52	i	401	CDL	OB6-CB4-CB6-OB8
52	i	403	CDL	OA6-CA4-CA6-OA8
52	o	201	CDL	OB6-CB4-CB6-OB8
52	o	201	CDL	C72-C73-C74-C75
52	a	201	CDL	C64-C65-C66-C67
52	l	701	CDL	C35-C36-C37-C38
48	l	704	PEE	C10-C11-C12-C13
49	j	202	PLX	C18-C19-C20-C21
52	V	202	CDL	C12-C13-C14-C15
48	C	302	PEE	C12-C13-C14-C15
52	i	401	CDL	C31-C32-C33-C34
52	i	401	CDL	C71-C72-C73-C74
53	J	401	NDP	PN-O3-PA-O1A
48	j	201	PEE	C22-C23-C24-C25
49	j	202	PLX	C15-C16-C17-C18
48	r	501	PEE	C36-C37-C38-C39
48	r	501	PEE	C38-C39-C40-C41
48	i	402	PEE	O3P-C1-C2-C3
49	J	403	PLX	O4-C3-C4-C5
49	j	202	PLX	O4-C3-C4-C5
52	I	201	CDL	OA5-CA3-CA4-CA6
52	I	201	CDL	OB5-CB3-CB4-CB6
52	V	202	CDL	OA5-CA3-CA4-CA6
48	l	703	PEE	C30-C31-C32-C33
49	a	202	PLX	C25-C26-C27-C28
52	i	403	CDL	C14-C15-C16-C17
52	V	202	CDL	C31-CA7-OA8-CA6
52	i	403	CDL	C31-CA7-OA8-CA6
49	r	503	PLX	C17-C18-C19-C20
49	r	503	PLX	C27-C28-C29-C30
48	j	201	PEE	C31-C30-O3-C3
52	i	403	CDL	CB5-C51-C52-C53
48	r	501	PEE	C43-C44-C45-C46
52	i	401	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
52	i	403	CDL	C36-C37-C38-C39
48	i	402	PEE	C2-C1-O3P-P
48	l	704	PEE	C18-C19-C20-C21
48	C	302	PEE	C11-C12-C13-C14
49	r	502	PLX	C31-C32-C33-C34
52	a	201	CDL	C34-C35-C36-C37
52	a	201	CDL	C20-C21-C22-C23
48	B	303	PEE	C13-C14-C15-C16
52	V	202	CDL	C19-C20-C21-C22
52	s	401	CDL	C15-C16-C17-C18
48	l	704	PEE	C1-C2-C3-O3
49	r	503	PLX	C3-C4-C5-O8
52	V	202	CDL	CB3-CB4-CB6-OB8
52	i	403	CDL	CB3-CB4-CB6-OB8
49	r	502	PLX	C14-C15-C16-C17
52	V	202	CDL	C52-C53-C54-C55
52	a	201	CDL	C74-C75-C76-C77
52	i	401	CDL	C11-C12-C13-C14
48	l	704	PEE	O5-C30-O3-C3
52	V	201	CDL	C54-C55-C56-C57
49	J	403	PLX	C5-C4-O6-C6
49	a	202	PLX	C5-C4-O6-C6
49	r	502	PLX	C3-C4-O6-C6
49	r	503	PLX	C5-C4-O6-C6
48	i	402	PEE	C10-C11-C12-C13
49	J	403	PLX	C34-C35-C36-C37
52	I	201	CDL	C52-C53-C54-C55
52	V	201	CDL	OA5-CA3-CA4-OA6
52	l	702	CDL	OB5-CB3-CB4-OB6
52	V	202	CDL	C71-CB7-OB8-CB6
48	B	303	PEE	O5-C30-O3-C3
48	r	501	PEE	C10-C11-C12-C13
52	i	403	CDL	C82-C83-C84-C85
49	g	201	PLX	C19-C20-C21-C22
52	a	201	CDL	C21-C22-C23-C24
48	i	402	PEE	O2-C2-C3-O3
48	j	201	PEE	O2-C2-C3-O3
48	l	704	PEE	O2-C2-C3-O3
49	J	403	PLX	O6-C4-C5-O8
52	s	401	CDL	OB6-CB4-CB6-OB8
48	C	302	PEE	C44-C45-C46-C47
48	r	501	PEE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
52	o	201	CDL	C11-C12-C13-C14
48	C	302	PEE	C13-C14-C15-C16
51	X	201	8Q1	C11-C10-C9-C8
52	o	201	CDL	CA2-C1-CB2-OB2
52	s	401	CDL	C55-C56-C57-C58
52	i	401	CDL	CA5-C11-C12-C13
49	J	403	PLX	C15-C16-C17-C18
49	r	502	PLX	C13-C14-C15-C16
52	i	401	CDL	C44-C45-C46-C47
48	C	302	PEE	C34-C35-C36-C37
52	s	401	CDL	C40-C41-C42-C43
49	g	201	PLX	C36-C37-C38-C39
48	r	501	PEE	C30-C31-C32-C33
52	V	202	CDL	C84-C85-C86-C87
49	a	202	PLX	C12-C13-C14-C15
49	r	503	PLX	C12-C13-C14-C15
52	l	702	CDL	C12-C13-C14-C15
49	r	503	PLX	O8-C24-C25-C26
52	V	202	CDL	C82-C83-C84-C85
48	C	302	PEE	O3P-C1-C2-C3
49	g	201	PLX	O4-C3-C4-C5
52	V	201	CDL	OA5-CA3-CA4-CA6
52	l	701	CDL	OB5-CB3-CB4-CB6
52	l	702	CDL	OB5-CB3-CB4-CB6
52	o	201	CDL	OB5-CB3-CB4-CB6
48	B	303	PEE	C11-C12-C13-C14
48	r	501	PEE	C34-C35-C36-C37
52	a	201	CDL	C14-C15-C16-C17
48	U	101	PEE	C15-C16-C17-C18
49	J	403	PLX	C13-C14-C15-C16
52	V	202	CDL	CA5-C11-C12-C13
49	j	202	PLX	C11-C10-C9-C8
52	o	201	CDL	C75-C76-C77-C78
52	o	201	CDL	C73-C74-C75-C76
52	V	201	CDL	CA6-CA4-OA6-CA5
48	i	402	PEE	C24-C25-C26-C27
52	V	202	CDL	C53-C54-C55-C56
52	I	201	CDL	C71-CB7-OB8-CB6
52	o	201	CDL	OA5-CA3-CA4-OA6
52	i	401	CDL	C64-C65-C66-C67
52	o	201	CDL	C53-C54-C55-C56
47	A	503	NAI	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
48	j	201	PEE	O5-C30-O3-C3
52	V	202	CDL	OA9-CA7-OA8-CA6
52	i	403	CDL	OA9-CA7-OA8-CA6
49	r	503	PLX	C35-C36-C37-C38
52	g	202	CDL	C56-C57-C58-C59
48	W	201	PEE	O2-C2-C3-O3
49	r	503	PLX	O6-C4-C5-O8
52	g	202	CDL	C71-C72-C73-C74
53	J	401	NDP	C5B-O5B-PA-O3
52	V	202	CDL	OB9-CB7-OB8-CB6
52	i	403	CDL	C71-C72-C73-C74
52	I	201	CDL	OB9-CB7-OB8-CB6
51	G	201	8Q1	C12-C13-C14-C15
52	i	403	CDL	C83-C84-C85-C86
52	s	401	CDL	C56-C57-C58-C59
49	a	202	PLX	C24-C25-C26-C27
48	l	704	PEE	C4-O4P-P-O3P
49	J	403	PLX	C2-O1-P1-O4
49	r	502	PLX	C2-O1-P1-O4
52	V	201	CDL	CA3-OA5-PA1-OA2
52	i	403	CDL	CA2-OA2-PA1-OA5
52	i	401	CDL	C39-C40-C41-C42
52	i	401	CDL	O1-C1-CB2-OB2
54	J	402	UQ	C15-C14-C16-C17
48	l	704	PEE	C2-C1-O3P-P
52	i	401	CDL	C1-CB2-OB2-PB2
52	i	403	CDL	C1-CB2-OB2-PB2
52	o	201	CDL	C1-CB2-OB2-PB2
47	A	503	NAI	C5B-O5B-PA-O1A
48	C	302	PEE	C1-O3P-P-O2P
48	C	302	PEE	C4-O4P-P-O2P
48	C	302	PEE	C4-O4P-P-O1P
48	W	201	PEE	C4-O4P-P-O1P
48	j	201	PEE	C1-O3P-P-O1P
48	r	501	PEE	C1-O3P-P-O2P
48	r	501	PEE	C4-O4P-P-O2P
49	C	303	PLX	C2-O1-P1-O3
49	J	403	PLX	C2-O1-P1-O2
49	J	403	PLX	C2-O1-P1-O3
49	a	202	PLX	C3-O4-P1-O3
49	r	502	PLX	C3-O4-P1-O2
49	r	502	PLX	C3-O4-P1-O3

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Mol	Chain	Res	Type	Atoms
49	r	502	PLX	C2-O1-P1-O3
49	r	503	PLX	C2-O1-P1-O3
52	I	201	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	CA3-OA5-PA1-OA4
52	V	202	CDL	CB2-OB2-PB2-OB4
52	a	201	CDL	CA3-OA5-PA1-OA3
52	a	201	CDL	CA3-OA5-PA1-OA4
52	a	201	CDL	CB2-OB2-PB2-OB4
52	g	202	CDL	CB2-OB2-PB2-OB3
52	i	401	CDL	CA2-OA2-PA1-OA4
52	i	401	CDL	CA3-OA5-PA1-OA3
52	i	401	CDL	CA3-OA5-PA1-OA4
52	i	401	CDL	CB3-OB5-PB2-OB4
52	i	403	CDL	CA2-OA2-PA1-OA4
52	i	403	CDL	CB2-OB2-PB2-OB3
52	i	403	CDL	CB2-OB2-PB2-OB4
52	l	701	CDL	CB3-OB5-PB2-OB4
52	l	702	CDL	CA3-OA5-PA1-OA4
52	l	702	CDL	CB2-OB2-PB2-OB3
52	o	201	CDL	CB2-OB2-PB2-OB4
52	g	202	CDL	C53-C54-C55-C56
52	o	201	CDL	C64-C65-C66-C67
48	B	303	PEE	O3P-C1-C2-C3
52	o	201	CDL	OA5-CA3-CA4-CA6
52	s	401	CDL	OA5-CA3-CA4-CA6
52	s	401	CDL	CB5-C51-C52-C53
52	g	202	CDL	C57-C58-C59-C60
52	l	702	CDL	C73-C74-C75-C76
52	V	201	CDL	C12-C13-C14-C15
52	i	401	CDL	C74-C75-C76-C77
52	i	403	CDL	C39-C40-C41-C42
52	s	401	CDL	C39-C40-C41-C42
46	A	502	FMN	C1'-C2'-C3'-O3'
49	C	303	PLX	C25-C24-O8-C5
49	J	403	PLX	C1-C2-O1-P1
49	J	403	PLX	C25-C24-O8-C5
49	a	202	PLX	C25-C24-O8-C5
49	j	202	PLX	C25-C24-O8-C5
48	l	704	PEE	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
48	B	303	PEE	O3P-C1-C2-O2
48	C	302	PEE	O3P-C1-C2-O2
48	i	402	PEE	O3P-C1-C2-O2
52	I	201	CDL	OB5-CB3-CB4-OB6
52	s	401	CDL	OA5-CA3-CA4-OA6
48	C	302	PEE	C41-C42-C43-C44
48	U	101	PEE	C22-C23-C24-C25
52	i	403	CDL	C74-C75-C76-C77
52	l	701	CDL	C38-C39-C40-C41
48	l	704	PEE	C33-C34-C35-C36
52	i	403	CDL	C44-C45-C46-C47
52	o	201	CDL	O1-C1-CB2-OB2
48	B	303	PEE	C20-C21-C22-C23
48	l	703	PEE	C1-C2-C3-O3
48	r	501	PEE	C1-C2-C3-O3
51	G	201	8Q1	O27-C28-C29-C32
48	C	302	PEE	O2-C2-C3-O3
48	r	501	PEE	O2-C2-C3-O3
49	r	502	PLX	O6-C4-C5-O8
52	V	201	CDL	OA6-CA4-CA6-OA8
48	U	101	PEE	C24-C25-C26-C27
52	V	201	CDL	C64-C65-C66-C67
48	r	501	PEE	C31-C30-O3-C3
52	l	702	CDL	C13-C14-C15-C16
52	o	201	CDL	C32-C31-CA7-OA8
52	a	201	CDL	C71-C72-C73-C74
48	l	703	PEE	C10-C11-C12-C13
49	r	503	PLX	C31-C32-C33-C34
49	g	201	PLX	O8-C24-C25-C26
52	o	201	CDL	C84-C85-C86-C87
52	V	201	CDL	CA7-C31-C32-C33
48	l	703	PEE	C37-C38-C39-C40
52	s	401	CDL	C16-C17-C18-C19
49	j	202	PLX	C12-C13-C14-C15
49	r	503	PLX	C33-C34-C35-C36
51	G	201	8Q1	O27-C28-C29-C30
48	r	501	PEE	O5-C30-O3-C3
48	l	703	PEE	C3-C2-O2-C10
52	V	202	CDL	OB5-CB3-CB4-CB6
52	i	401	CDL	CB2-C1-CA2-OA2
52	o	201	CDL	C62-C63-C64-C65
48	i	402	PEE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
52	i	401	CDL	OB5-CB3-CB4-OB6
49	j	202	PLX	C30-C31-C32-C33
52	i	401	CDL	C15-C16-C17-C18
52	s	401	CDL	C37-C38-C39-C40
49	a	202	PLX	C2-C1-N1-C1A
47	A	503	NAI	O4D-C1D-N1N-C2N
48	l	703	PEE	C32-C33-C34-C35
52	o	201	CDL	C81-C82-C83-C84
52	g	202	CDL	C51-CB5-OB6-CB4
52	i	403	CDL	C33-C34-C35-C36
48	U	101	PEE	C4-O4P-P-O3P
49	C	303	PLX	C3-O4-P1-O1
52	I	201	CDL	CA3-OA5-PA1-OA2
52	V	201	CDL	CA2-OA2-PA1-OA5
52	l	702	CDL	CA2-OA2-PA1-OA5
52	s	401	CDL	CB3-OB5-PB2-OB2
48	B	303	PEE	C44-C45-C46-C47
52	o	201	CDL	C77-C78-C79-C80
49	j	202	PLX	C3-C4-C5-O8
52	i	401	CDL	CB3-CB4-CB6-OB8
52	a	201	CDL	C56-C57-C58-C59
52	g	202	CDL	C32-C31-CA7-OA8
48	U	101	PEE	C31-C32-C33-C34
48	r	501	PEE	C24-C25-C26-C27
52	l	702	CDL	C38-C39-C40-C41
48	C	302	PEE	C31-C32-C33-C34
52	a	201	CDL	C84-C85-C86-C87
52	g	202	CDL	C1-CB2-OB2-PB2
52	a	201	CDL	C12-C13-C14-C15
52	s	401	CDL	C13-C14-C15-C16
52	i	403	CDL	C79-C80-C81-C82
52	s	401	CDL	C60-C61-C62-C63
49	a	202	PLX	C6-C7-C8-C9
52	a	201	CDL	CA7-C31-C32-C33
52	g	202	CDL	C31-CA7-OA8-CA6
46	A	502	FMN	O2'-C2'-C3'-O3'
52	g	202	CDL	OA9-CA7-OA8-CA6
52	i	401	CDL	C61-C62-C63-C64
52	l	702	CDL	C31-C32-C33-C34
52	a	201	CDL	C38-C39-C40-C41
48	C	302	PEE	C16-C17-C18-C19
48	i	402	PEE	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
54	J	402	UQ	C9-C11-C12-C13
52	i	401	CDL	C33-C34-C35-C36
52	V	201	CDL	C51-C52-C53-C54
52	o	201	CDL	C44-C45-C46-C47
48	C	302	PEE	C38-C39-C40-C41
48	l	703	PEE	C16-C17-C18-C19
52	g	202	CDL	OB7-CB5-OB6-CB4
52	l	701	CDL	C16-C17-C18-C19
52	l	702	CDL	C56-C57-C58-C59
52	s	401	CDL	C76-C77-C78-C79
49	g	201	PLX	O6-C6-C7-C8
52	g	202	CDL	C32-C31-CA7-OA9
52	l	701	CDL	OB6-CB4-CB6-OB8
48	l	703	PEE	C33-C34-C35-C36
48	j	201	PEE	C31-C32-C33-C34
48	l	704	PEE	C23-C24-C25-C26
49	j	202	PLX	C29-C30-C31-C32
49	C	303	PLX	C11-C10-C9-C8
49	r	503	PLX	C24-C25-C26-C27
52	l	701	CDL	C17-C18-C19-C20
52	i	401	CDL	C37-C38-C39-C40
52	s	401	CDL	CB3-CB4-CB6-OB8
52	s	401	CDL	C12-C11-CA5-OA7
51	G	201	8Q1	O27-C28-C29-C31
48	U	101	PEE	C20-C21-C22-C23
52	i	403	CDL	C13-C14-C15-C16
52	o	201	CDL	CB2-OB2-PB2-OB5
49	a	202	PLX	C14-C15-C16-C17
47	A	503	NAI	C2D-C1D-N1N-C6N
52	V	201	CDL	C36-C37-C38-C39
48	r	501	PEE	O3P-C1-C2-O2
48	B	303	PEE	C18-C19-C20-C21
49	r	502	PLX	C18-C19-C20-C21
52	i	401	CDL	C62-C63-C64-C65
52	i	401	CDL	C32-C33-C34-C35
48	i	402	PEE	C32-C33-C34-C35
51	G	201	8Q1	C13-C14-C15-C16
49	g	201	PLX	C17-C18-C19-C20
52	g	202	CDL	C72-C73-C74-C75
52	l	702	CDL	C53-C54-C55-C56
48	C	302	PEE	C35-C36-C37-C38
48	l	704	PEE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
53	J	401	NDP	O4D-C1D-N1N-C6N
48	B	303	PEE	C37-C38-C39-C40
54	s	402	UQ	C24-C26-C27-C28
48	W	201	PEE	C16-C17-C18-C19
52	o	201	CDL	C16-C17-C18-C19
48	B	303	PEE	C24-C25-C26-C27
49	r	503	PLX	C26-C27-C28-C29
49	r	503	PLX	C2-C1-N1-C1C
49	g	201	PLX	C11-C12-C13-C14
48	U	101	PEE	C38-C39-C40-C41
48	l	703	PEE	C42-C43-C44-C45
49	a	202	PLX	C3-C4-C5-O8
49	r	502	PLX	C3-C4-C5-O8
54	J	402	UQ	C20-C19-C21-C22
52	i	403	CDL	C12-C13-C14-C15
48	U	101	PEE	C43-C44-C45-C46
52	a	201	CDL	C43-C44-C45-C46
52	a	201	CDL	C61-C62-C63-C64
48	C	302	PEE	C18-C19-C20-C21
48	W	201	PEE	C18-C19-C20-C21
52	a	201	CDL	OB5-CB3-CB4-OB6
52	a	201	CDL	C15-C16-C17-C18
49	j	202	PLX	C34-C35-C36-C37
49	g	201	PLX	C31-C32-C33-C34
52	a	201	CDL	OB5-CB3-CB4-CB6
48	l	703	PEE	C13-C14-C15-C16
49	r	502	PLX	C4-C3-O4-P1
49	r	503	PLX	C19-C20-C21-C22
47	A	503	NAI	O4D-C4D-C5D-O5D
53	J	401	NDP	O4D-C4D-C5D-O5D
49	a	202	PLX	C16-C17-C18-C19
53	J	401	NDP	C2B-O2B-P2B-O1X
52	l	701	CDL	C63-C64-C65-C66
52	o	201	CDL	CA3-OA5-PA1-OA2
49	r	502	PLX	C19-C20-C21-C22
52	V	202	CDL	C16-C17-C18-C19
52	I	201	CDL	C12-C11-CA5-OA6
52	V	202	CDL	C12-C11-CA5-OA6
52	I	201	CDL	C52-C51-CB5-OB6
52	V	201	CDL	C32-C31-CA7-OA8
52	l	702	CDL	C12-C11-CA5-OA6
48	U	101	PEE	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
48	i	402	PEE	C38-C39-C40-C41
48	j	201	PEE	C18-C19-C20-C21
48	l	704	PEE	C38-C39-C40-C41
52	V	202	CDL	CA6-CA4-OA6-CA5
49	g	201	PLX	C26-C27-C28-C29
52	a	201	CDL	OA7-CA5-OA6-CA4
47	A	503	NAI	O4D-C1D-N1N-C6N
52	a	201	CDL	C12-C11-CA5-OA6
48	B	303	PEE	O2-C10-C11-C12
48	C	302	PEE	O3-C30-C31-C32
48	U	101	PEE	O3-C30-C31-C32
52	l	702	CDL	C32-C31-CA7-OA8
48	B	303	PEE	C41-C42-C43-C44
52	l	701	CDL	C72-C71-CB7-OB8
49	a	202	PLX	C2-C1-N1-C1C
52	l	701	CDL	C21-C22-C23-C24
51	X	201	8Q1	C13-C14-C15-C16
48	B	303	PEE	C16-C17-C18-C19
48	i	402	PEE	C16-C17-C18-C19
48	i	402	PEE	C36-C37-C38-C39
48	i	402	PEE	C13-C14-C15-C16
49	r	503	PLX	C2-C1-N1-C1B
49	r	503	PLX	C2-C1-N1-C1A
49	C	303	PLX	O7-C6-C7-C8
53	J	401	NDP	C2B-O2B-P2B-O2X
48	j	201	PEE	C24-C25-C26-C27
52	a	201	CDL	C11-CA5-OA6-CA4
52	l	702	CDL	C72-C71-CB7-OB8
52	i	403	CDL	C64-C65-C66-C67
49	r	503	PLX	C11-C10-C9-C8
48	j	201	PEE	C16-C17-C18-C19
52	i	401	CDL	C12-C11-CA5-OA6
48	B	303	PEE	C22-C23-C24-C25
52	I	201	CDL	C72-C71-CB7-OB8
48	C	302	PEE	O5-C30-C31-C32
52	g	202	CDL	C52-C51-CB5-OB6
48	l	703	PEE	C38-C39-C40-C41
48	U	101	PEE	C34-C35-C36-C37
52	V	202	CDL	C77-C78-C79-C80
52	a	201	CDL	C53-C54-C55-C56
52	I	201	CDL	C12-C11-CA5-OA7
52	V	202	CDL	C12-C11-CA5-OA7

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Mol	Chain	Res	Type	Atoms
52	s	401	CDL	C31-CA7-OA8-CA6
52	a	201	CDL	C76-C77-C78-C79
52	I	201	CDL	C72-C71-CB7-OB9
52	l	702	CDL	C32-C31-CA7-OA9
52	V	202	CDL	CA7-C31-C32-C33
48	B	303	PEE	O4-C10-C11-C12
49	C	303	PLX	C2-O1-P1-O4
48	U	101	PEE	C21-C22-C23-C24
48	r	501	PEE	C40-C41-C42-C43
52	a	201	CDL	C12-C11-CA5-OA7
52	i	401	CDL	C12-C11-CA5-OA7
52	l	701	CDL	OA7-CA5-OA6-CA4
48	l	703	PEE	C36-C37-C38-C39
47	A	503	NAI	C5B-O5B-PA-O2A
47	A	503	NAI	C2N-C3N-C7N-N7N
48	B	303	PEE	C1-O3P-P-O1P
48	l	703	PEE	C1-O3P-P-O1P
49	a	202	PLX	C3-O4-P1-O2
49	a	202	PLX	C2-C1-N1-C1B
49	j	202	PLX	C2-O1-P1-O2
54	s	402	UQ	C6-C7-C8-C9
52	l	701	CDL	C24-C25-C26-C27
48	U	101	PEE	O5-C30-C31-C32
52	i	403	CDL	OB5-CB3-CB4-CB6
52	a	201	CDL	C44-C45-C46-C47
52	l	702	CDL	C60-C61-C62-C63
52	i	403	CDL	C57-C58-C59-C60
52	I	201	CDL	C52-C51-CB5-OB7
52	l	701	CDL	C72-C71-CB7-OB9
54	s	402	UQ	C12-C13-C14-C16
52	a	201	CDL	C72-C73-C74-C75
52	g	202	CDL	C52-C51-CB5-OB7
54	s	402	UQ	C1-C2-O2-CM2
48	l	703	PEE	C1-C2-O2-C10
48	r	501	PEE	C5-C4-O4P-P
52	V	202	CDL	CA3-CA4-OA6-CA5
52	s	401	CDL	OA9-CA7-OA8-CA6
51	X	201	8Q1	C12-C13-C14-C15
52	g	202	CDL	C12-C11-CA5-OA6
48	i	402	PEE	C39-C40-C41-C42
52	V	202	CDL	C32-C31-CA7-OA8
52	V	201	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
52	l	701	CDL	C20-C21-C22-C23
52	l	702	CDL	C72-C71-CB7-OB9
52	i	401	CDL	C32-C31-CA7-OA8
52	o	201	CDL	C52-C51-CB5-OB6
52	o	201	CDL	C52-C51-CB5-OB7
49	r	503	PLX	C9-C10-C11-C12
52	a	201	CDL	C33-C34-C35-C36
52	i	403	CDL	C72-C71-CB7-OB8
52	V	202	CDL	C32-C31-CA7-OA9
51	G	201	8Q1	C11-C10-C9-C8
52	i	401	CDL	C32-C31-CA7-OA9

There are no ring outliers.

34 monomers are involved in 138 short contacts:

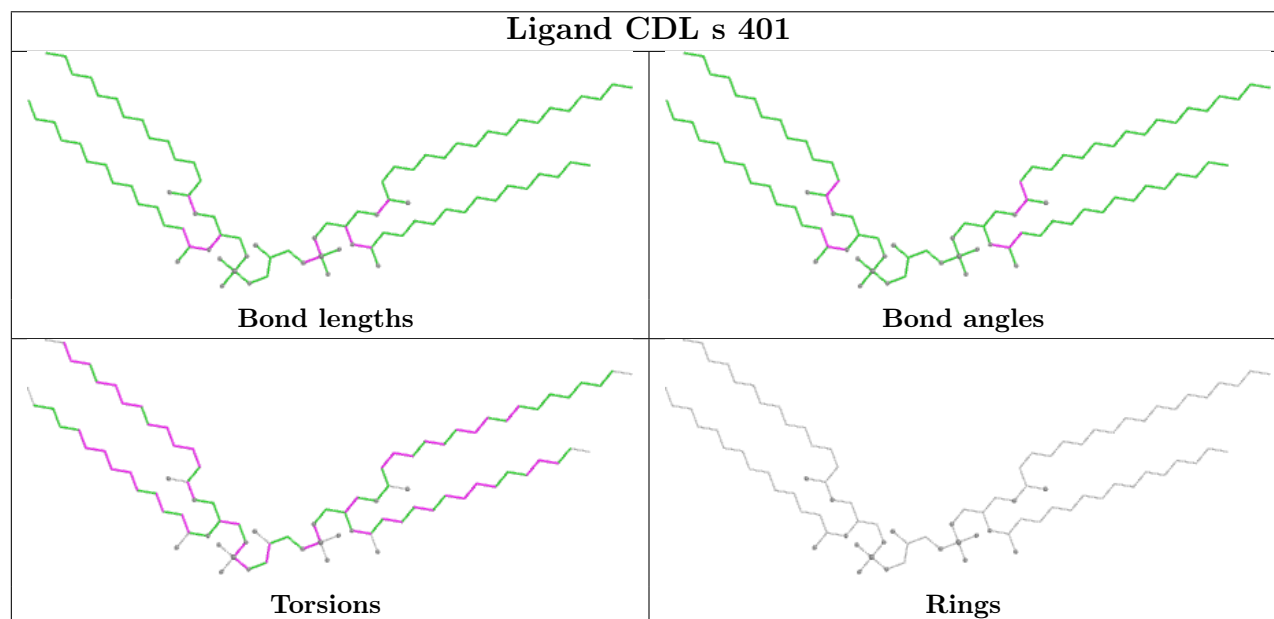
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	s	401	CDL	12	0
52	o	201	CDL	8	0
47	A	503	NAI	4	0
53	J	401	NDP	3	0
48	l	704	PEE	4	0
49	J	403	PLX	5	0
54	s	402	UQ	3	0
49	a	202	PLX	1	0
48	B	303	PEE	4	0
48	C	302	PEE	3	0
48	j	201	PEE	3	0
48	W	201	PEE	1	0
52	V	201	CDL	5	0
48	l	703	PEE	3	0
48	r	501	PEE	6	0
52	i	401	CDL	6	0
52	I	201	CDL	1	0
58	w	401	ADP	3	0
46	A	502	FMN	4	0
54	J	402	UQ	3	0
52	V	202	CDL	6	0
48	U	101	PEE	4	0
45	A	501	SF4	1	0
49	r	502	PLX	6	0
52	i	403	CDL	8	0
52	l	702	CDL	7	0

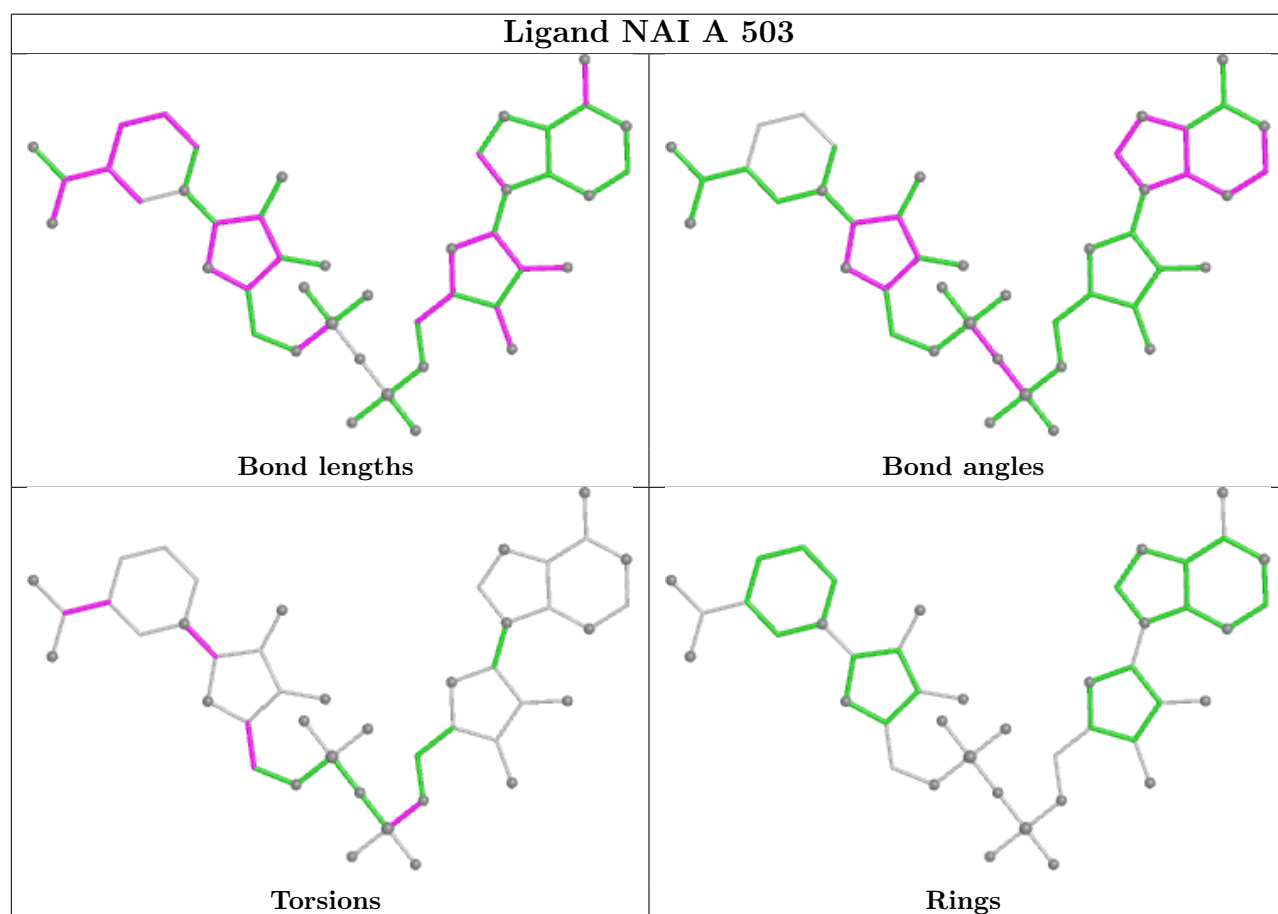
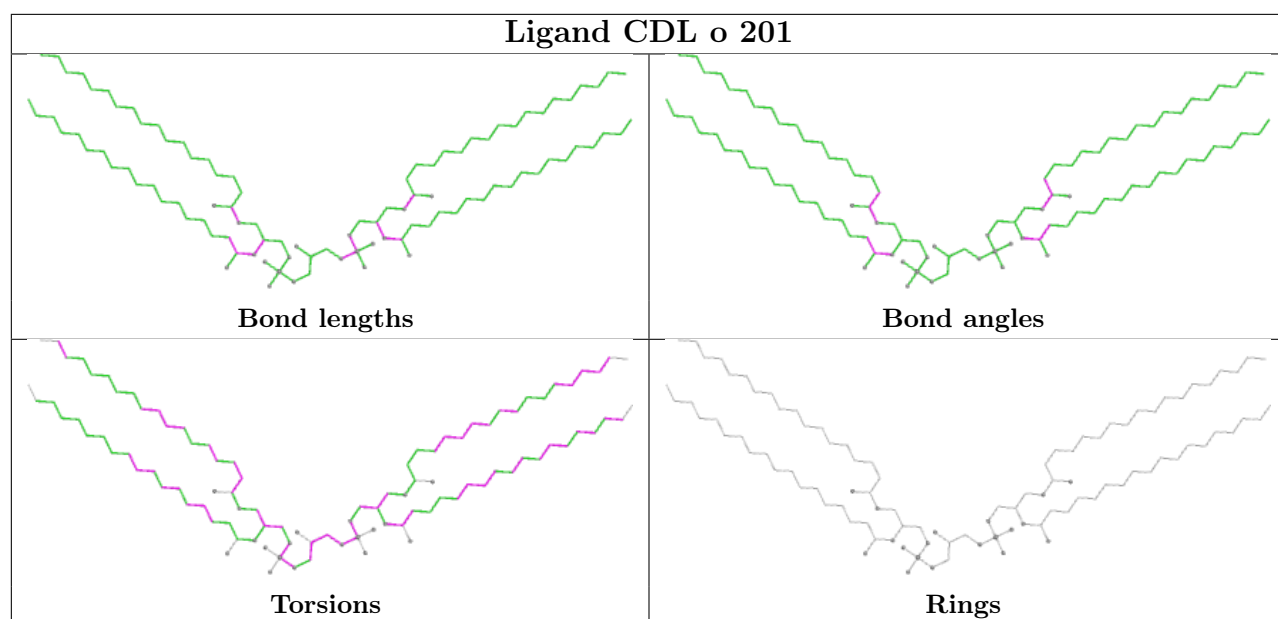
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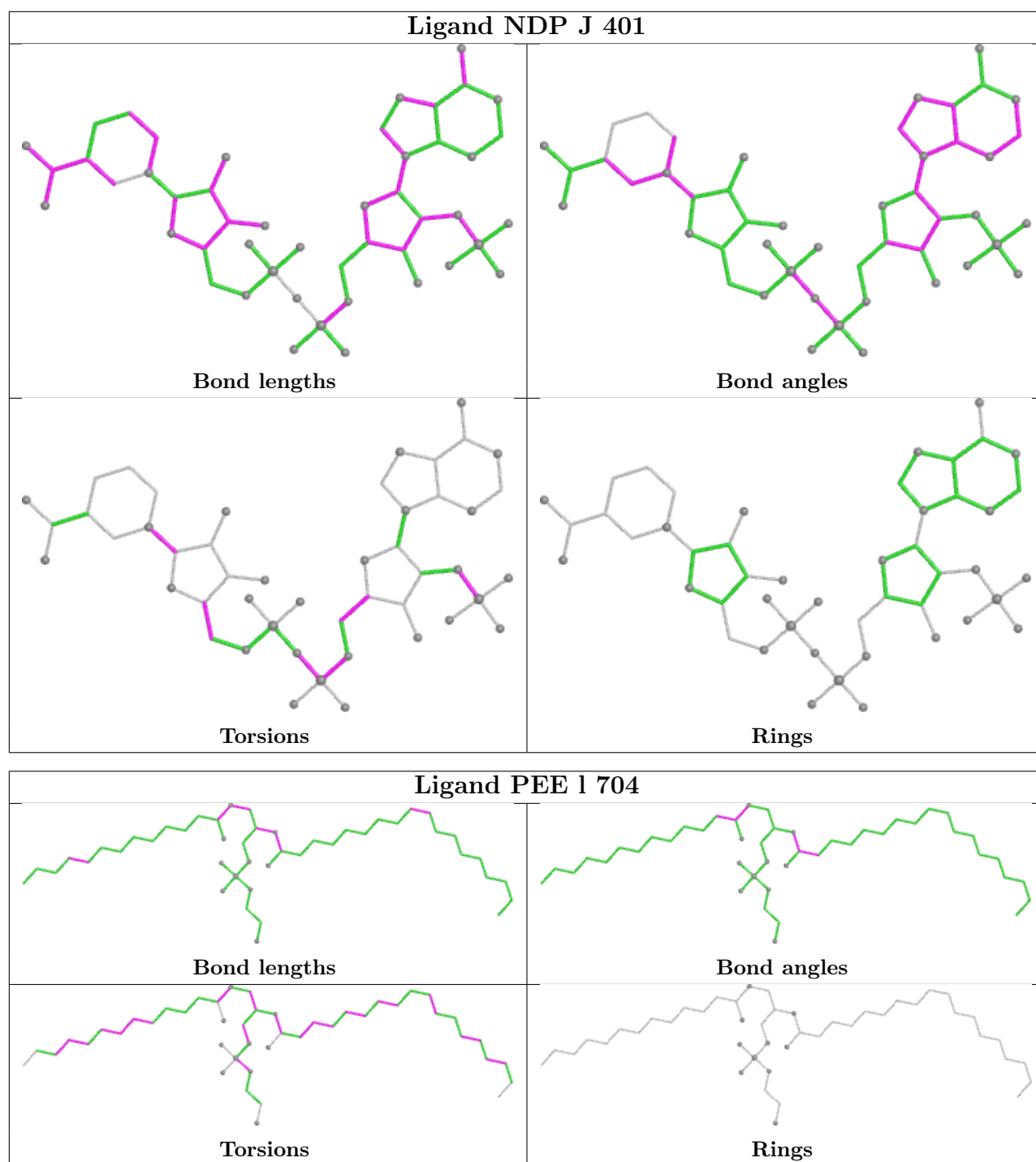
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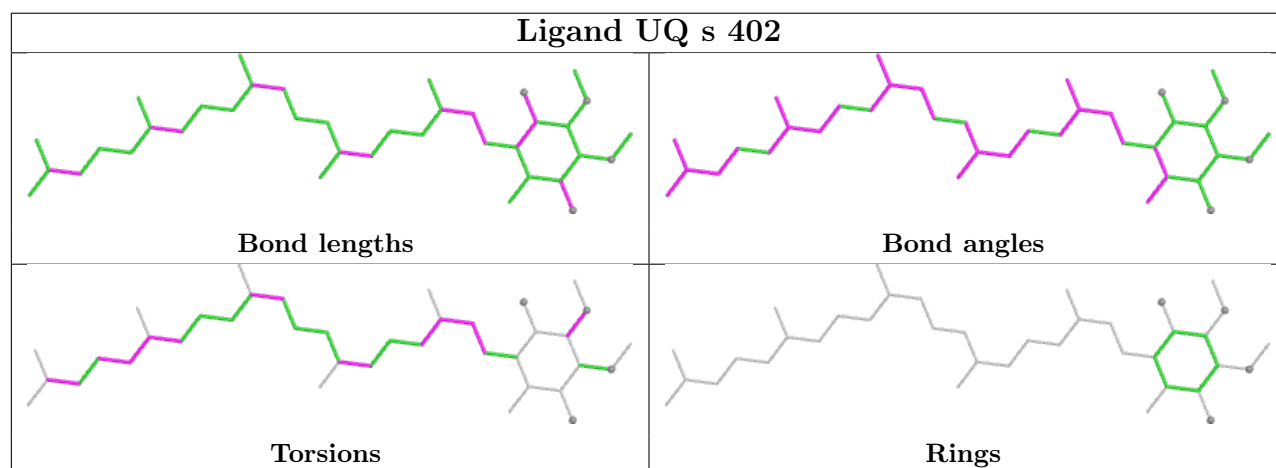
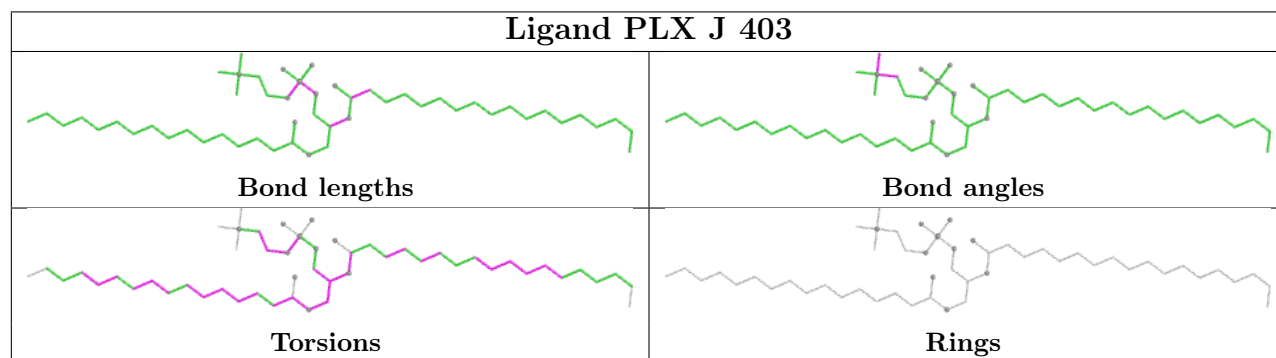
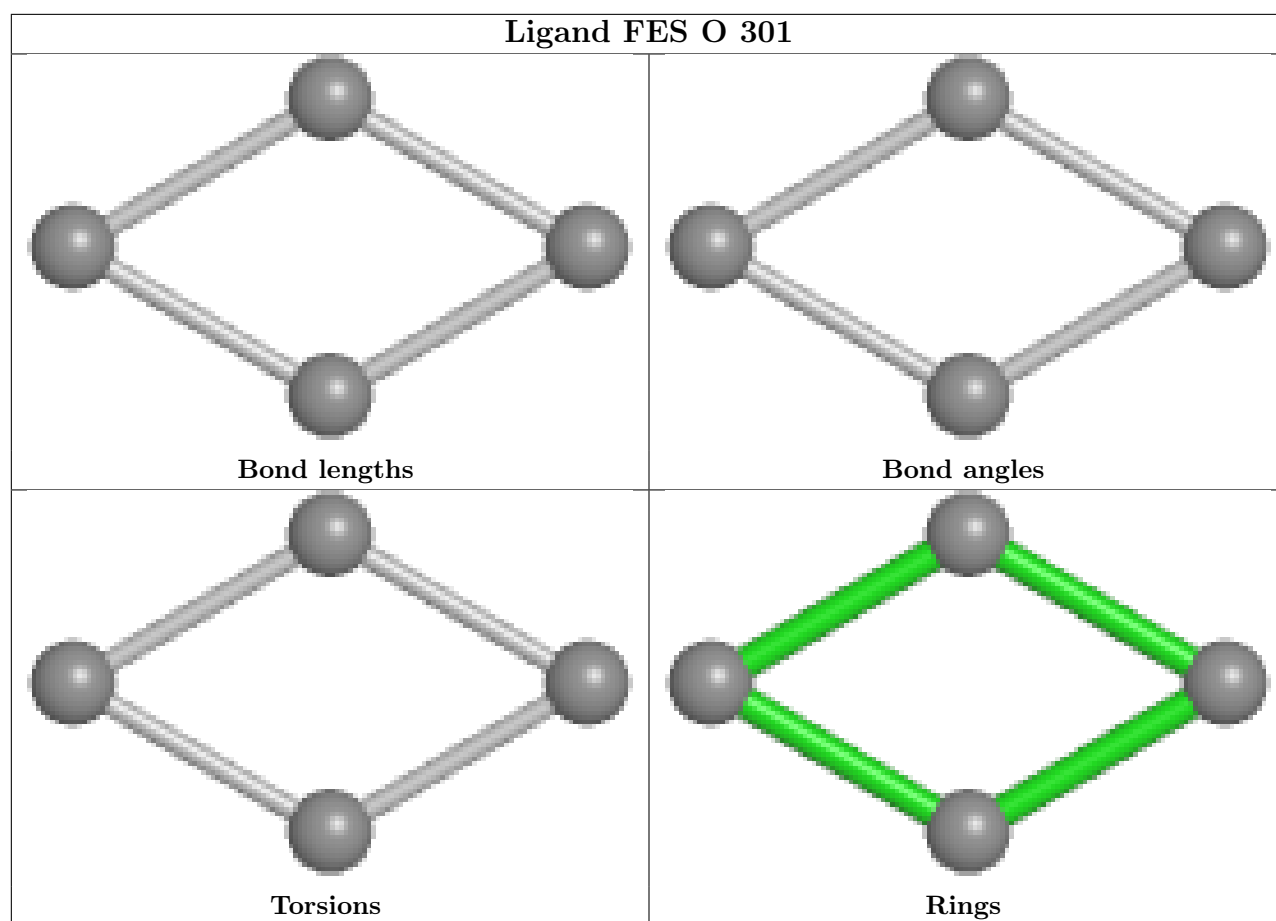
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	C	301	SF4	1	0
52	a	201	CDL	8	0
52	g	202	CDL	1	0
52	l	701	CDL	10	0
49	j	202	PLX	3	0
49	r	503	PLX	4	0
49	g	201	PLX	3	0
49	C	303	PLX	2	0

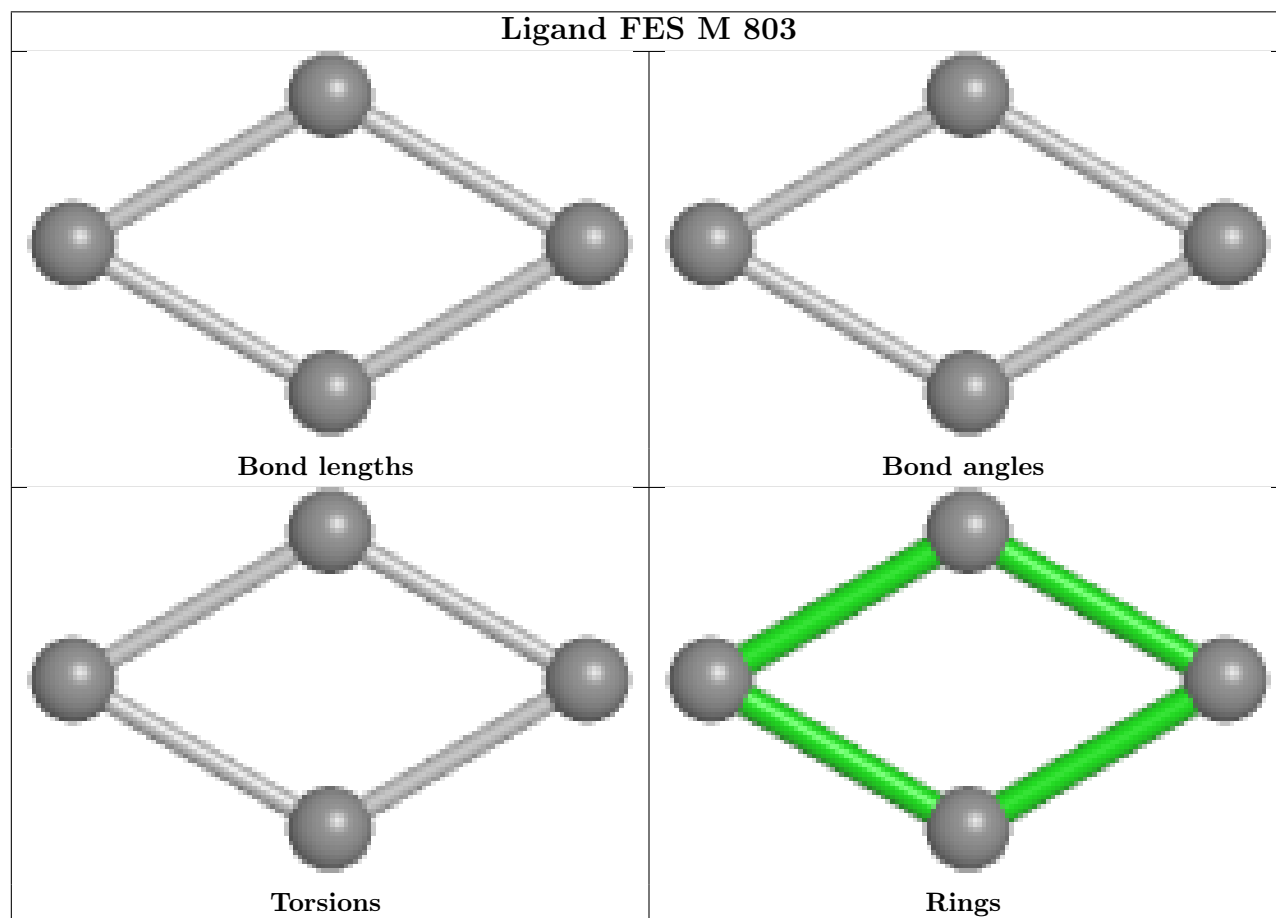
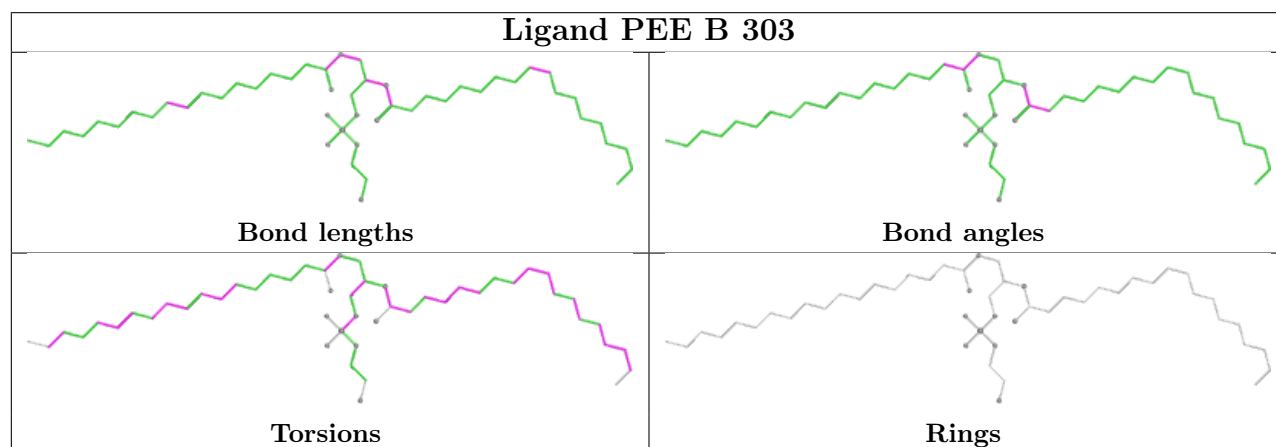
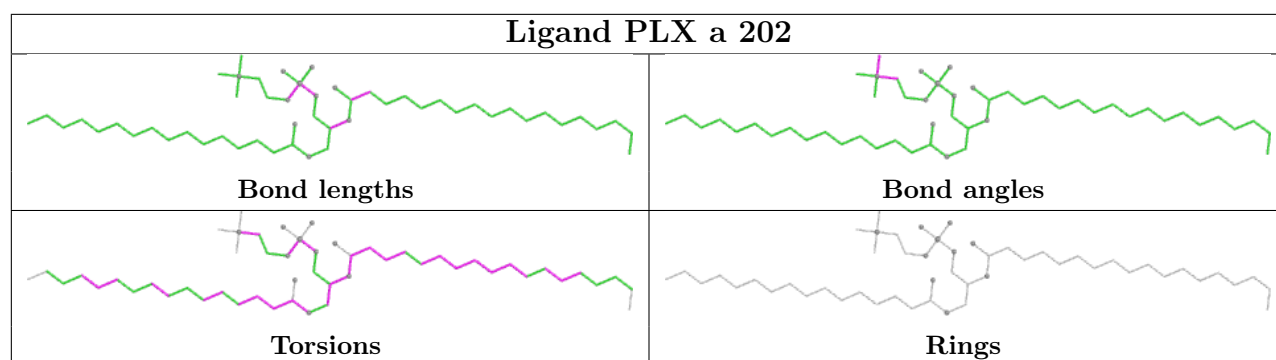
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

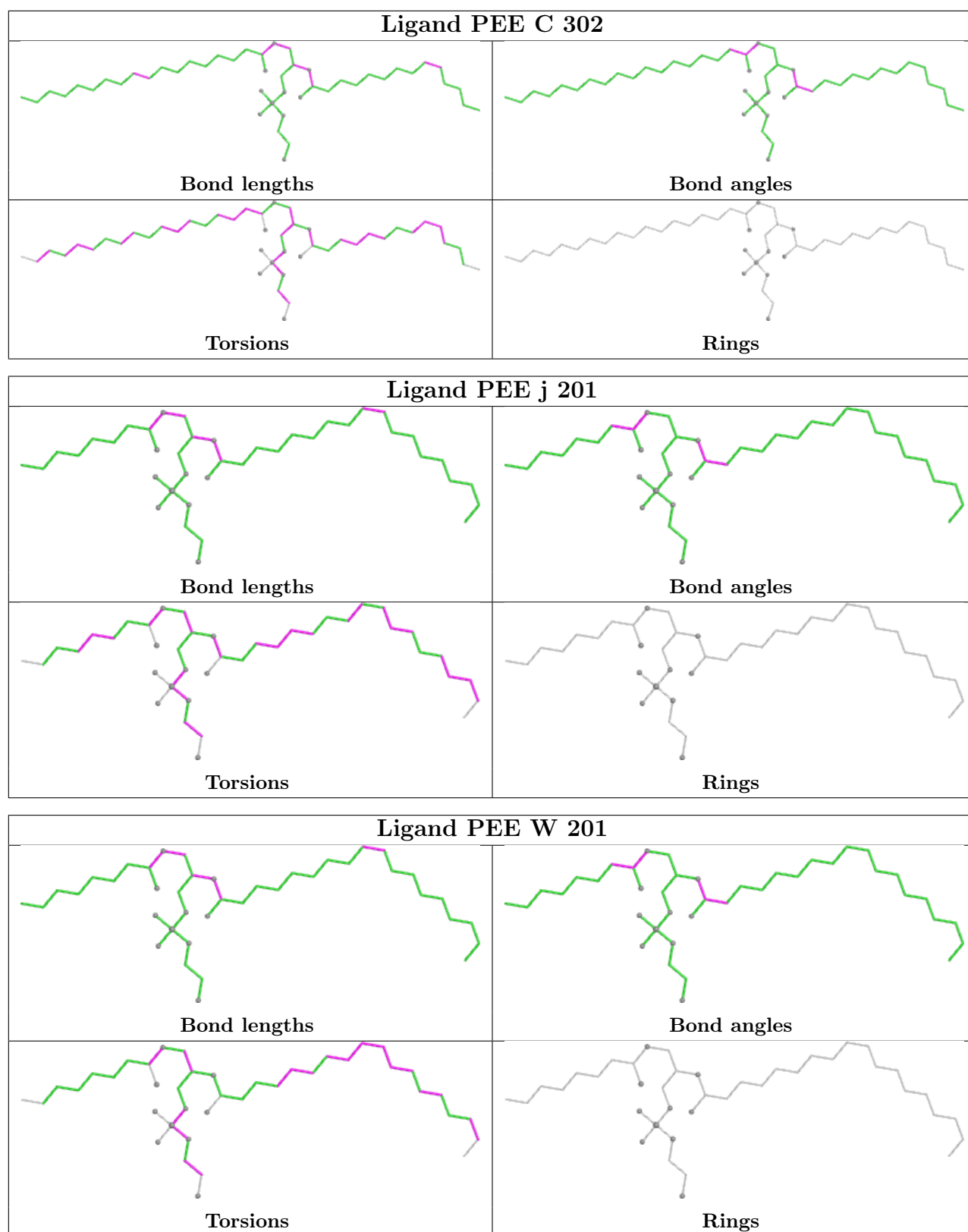


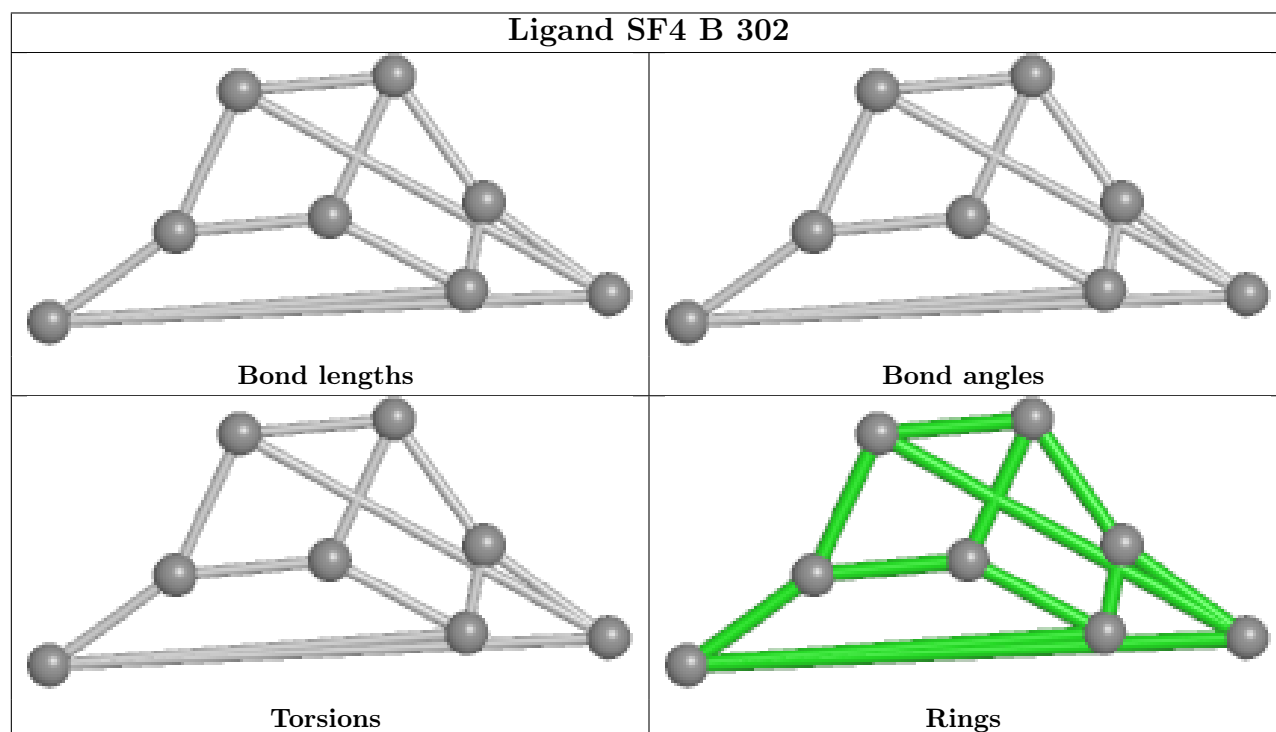
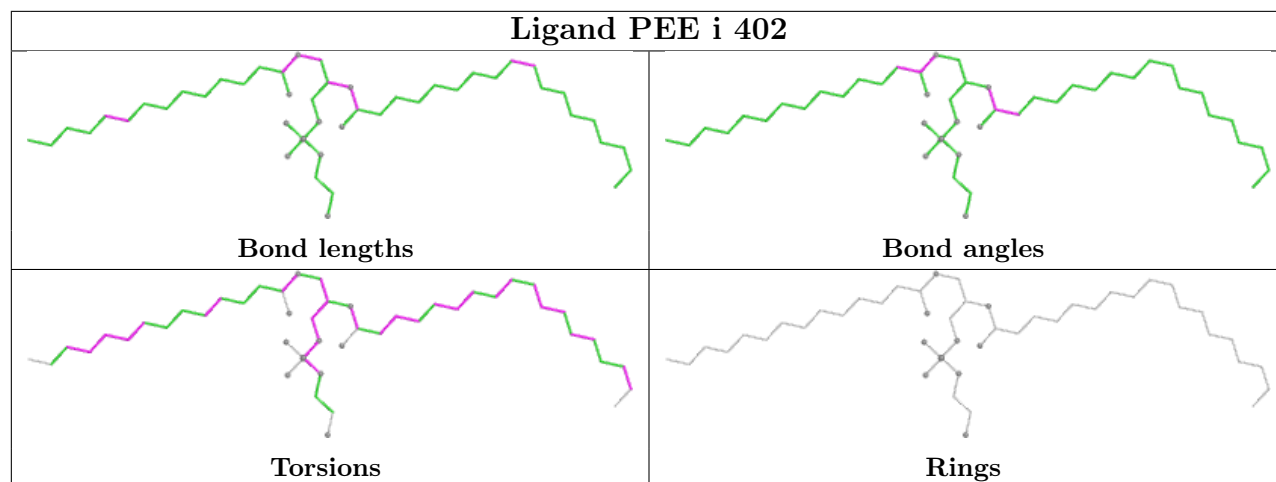


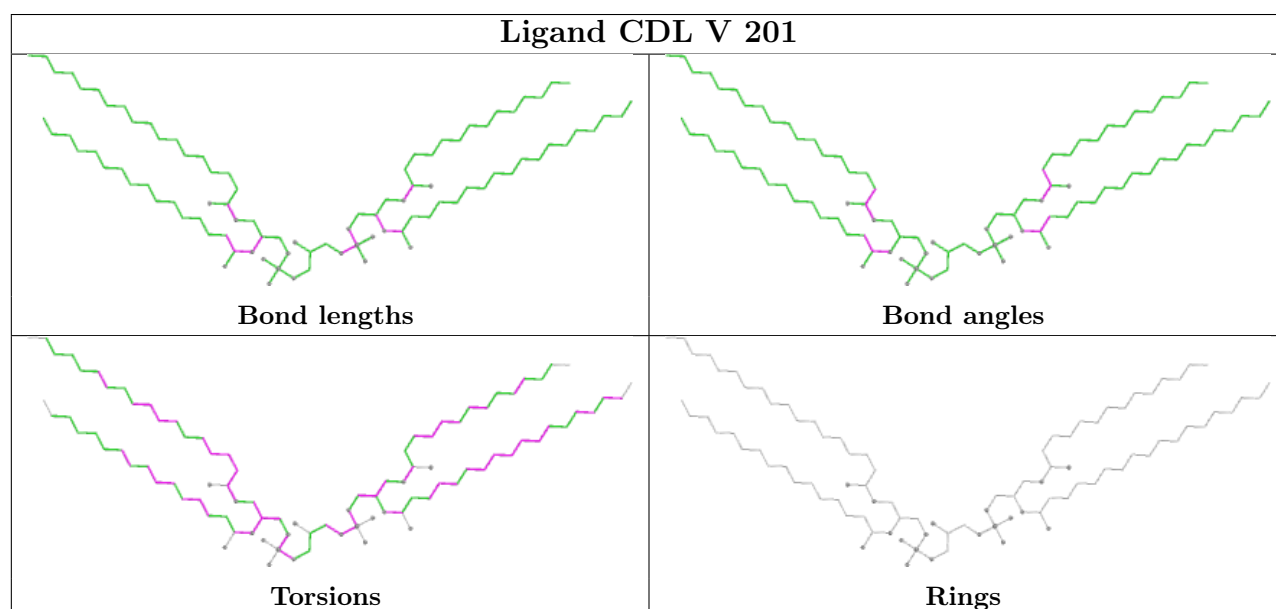
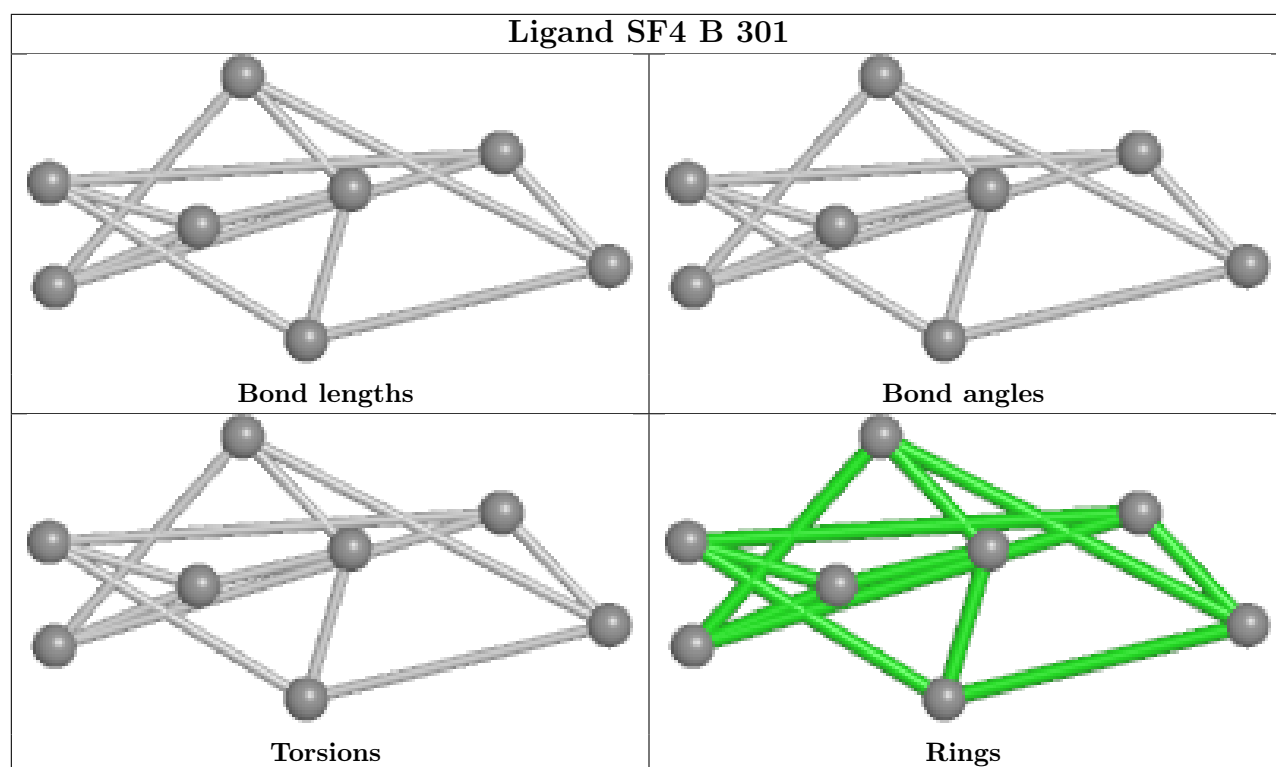


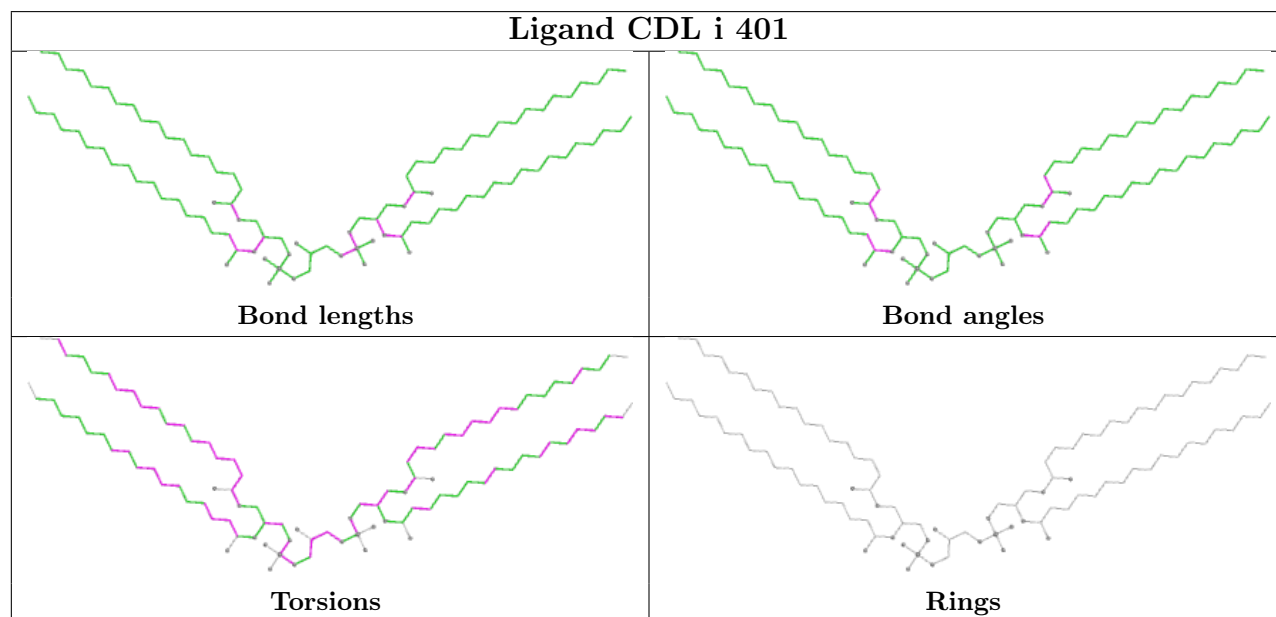
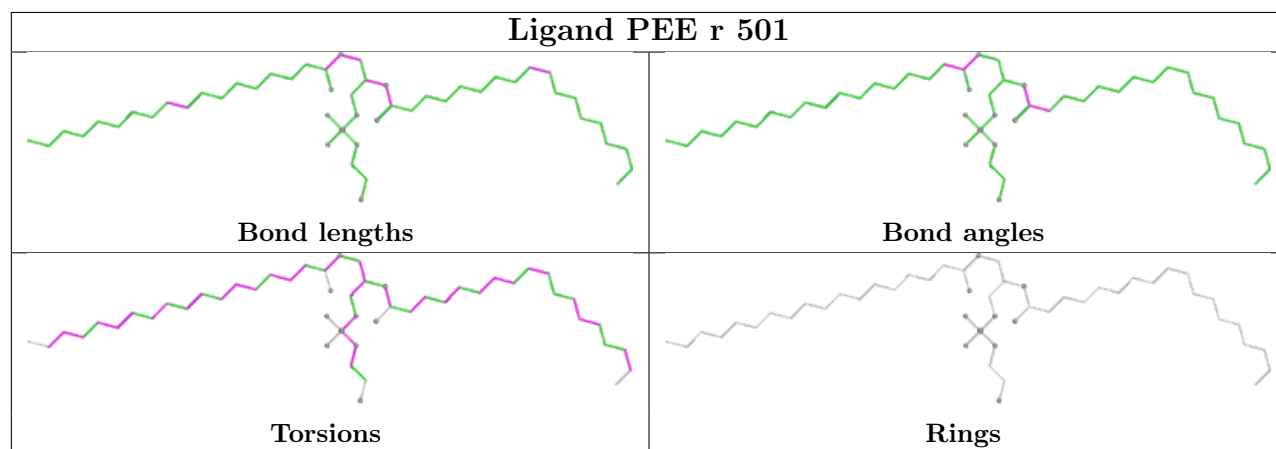
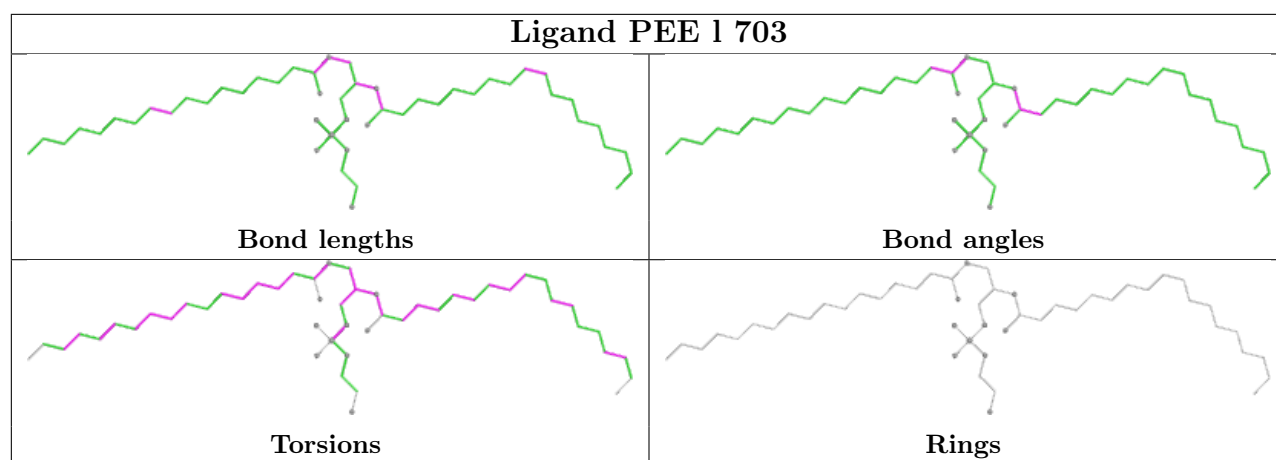


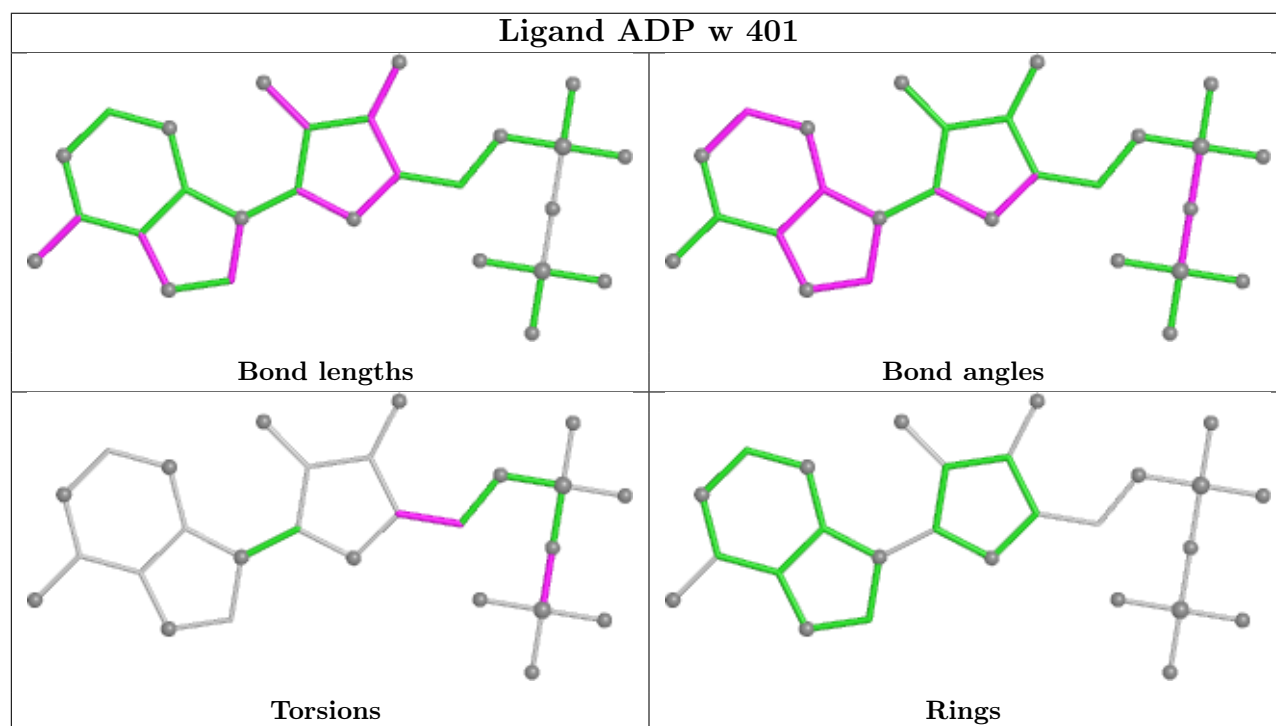
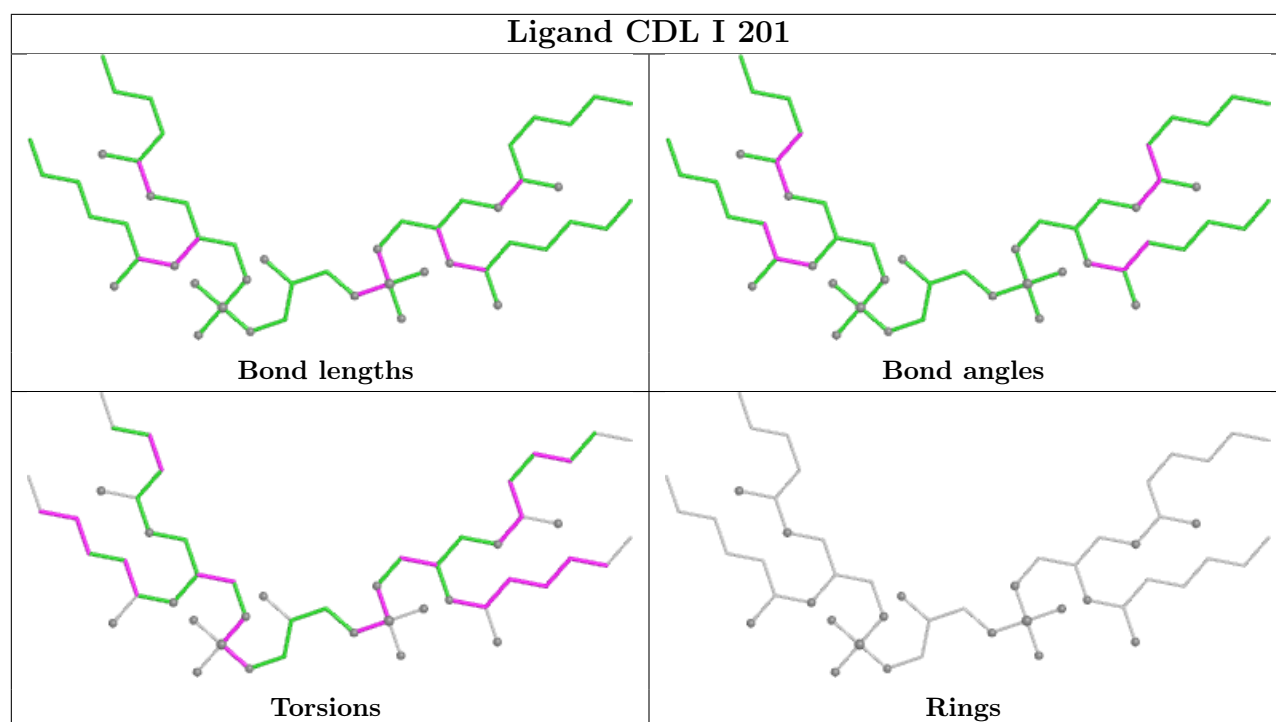


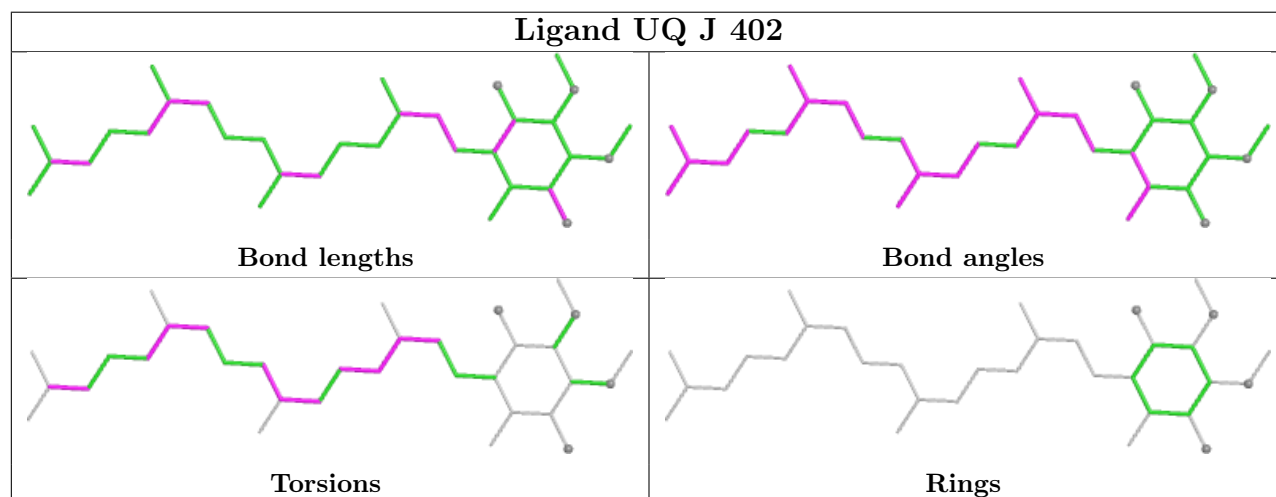
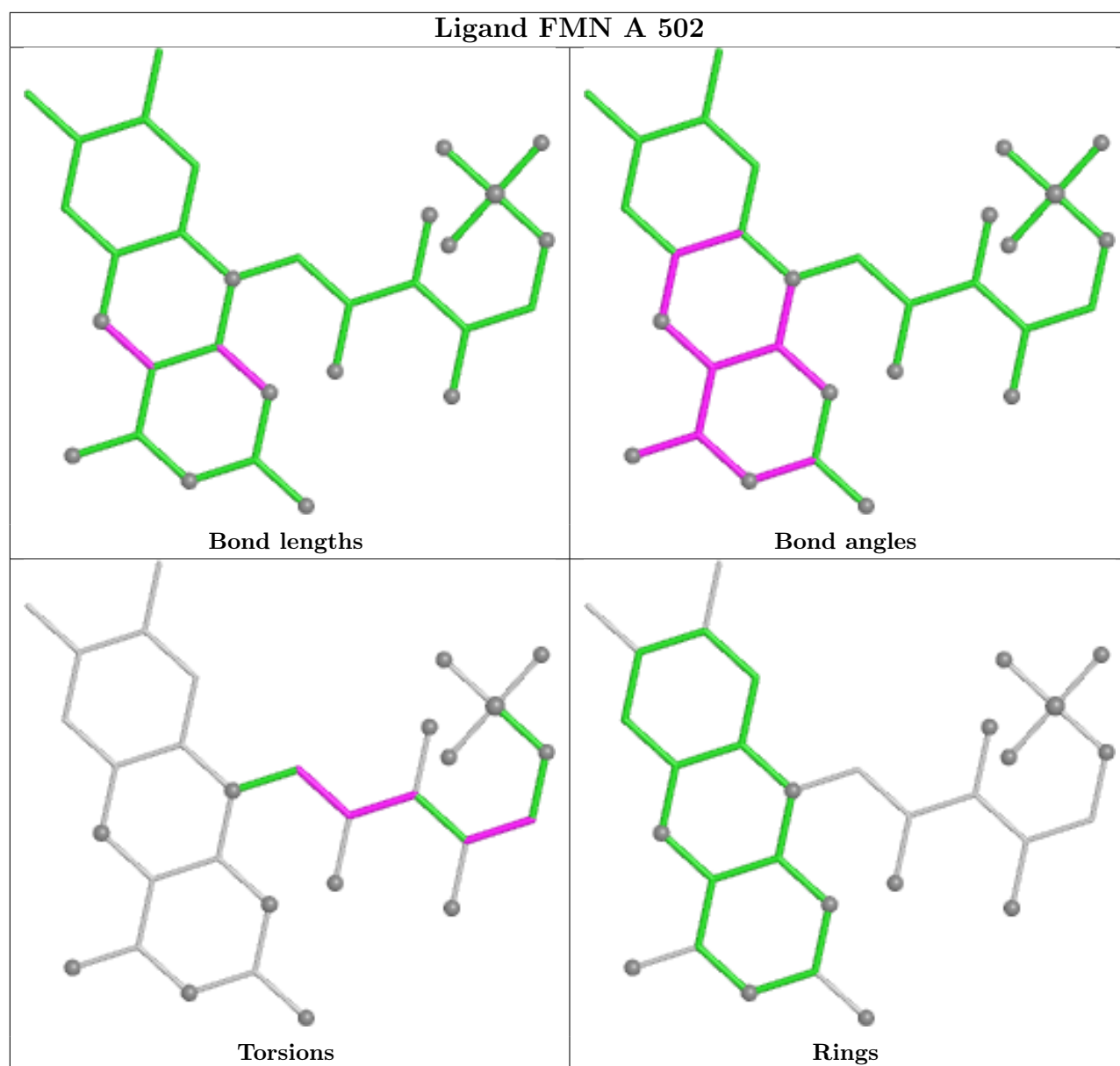


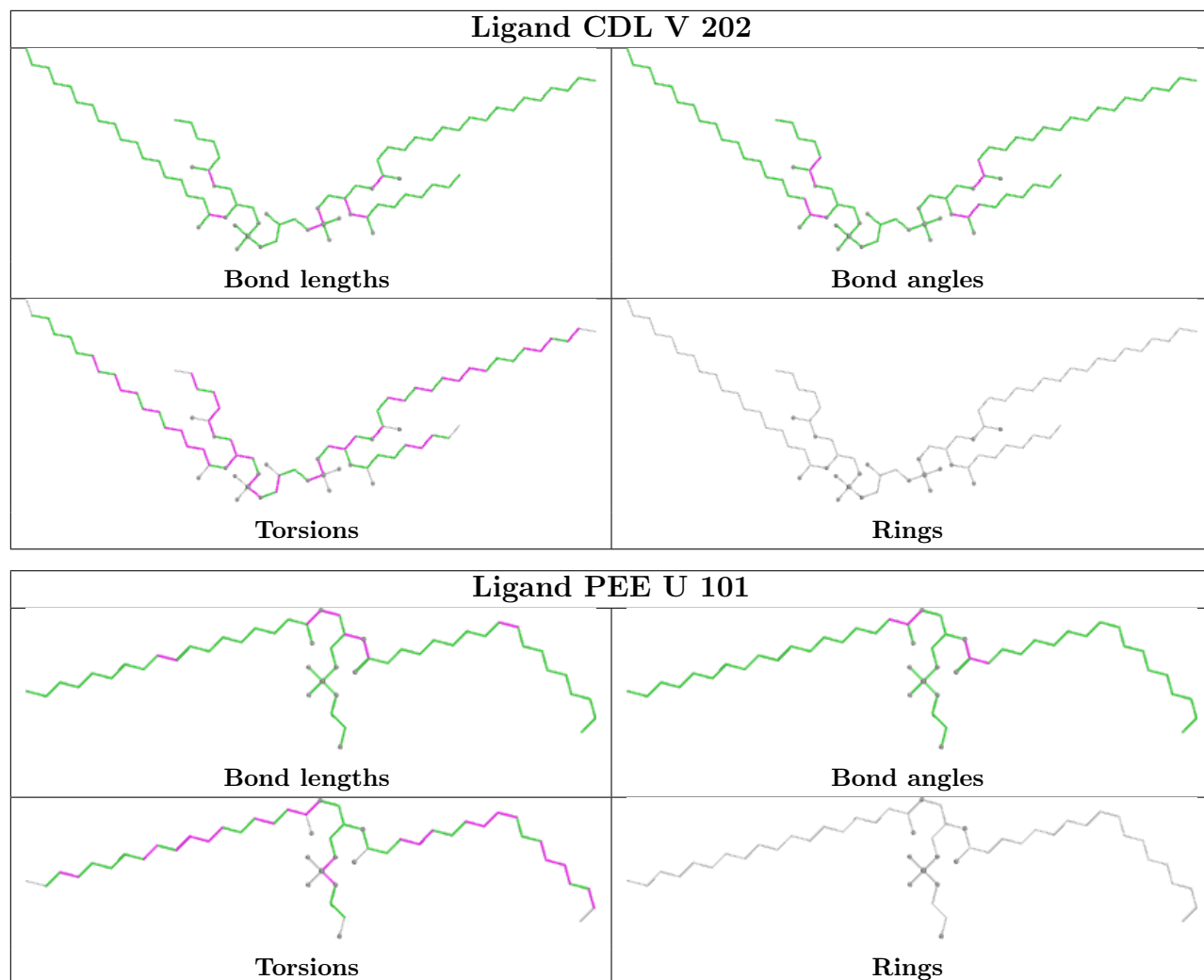


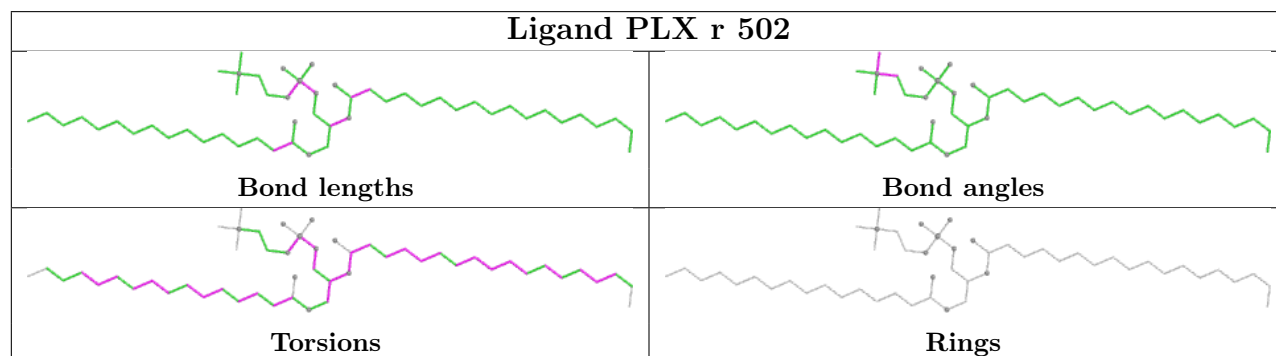
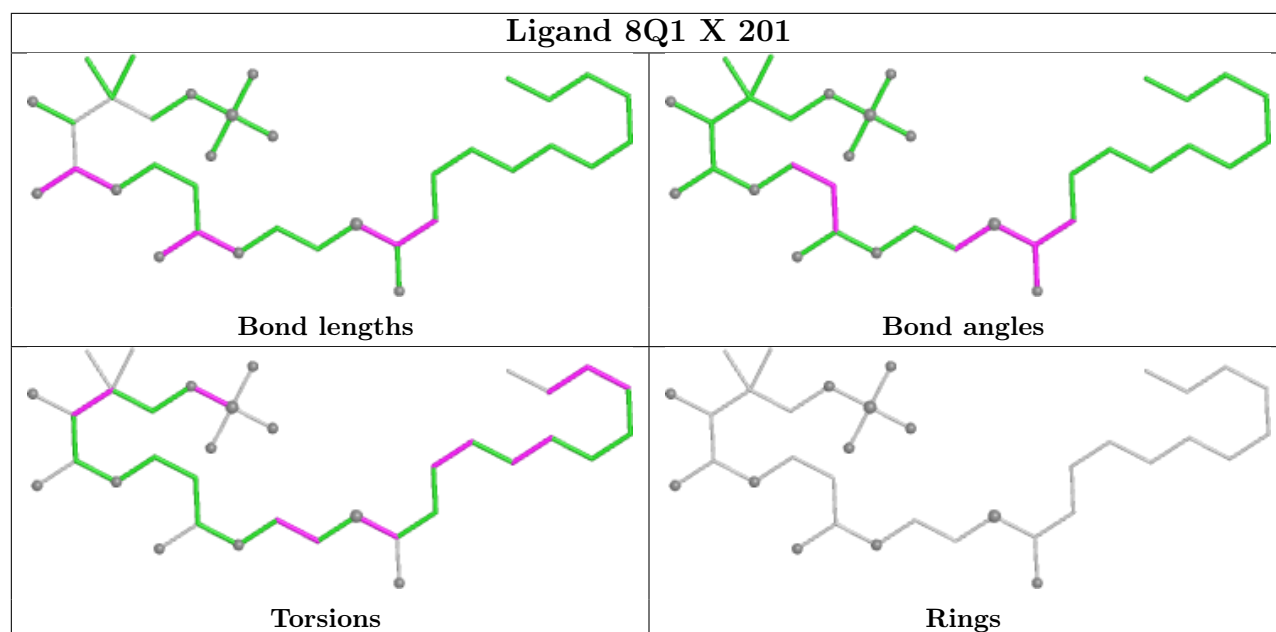
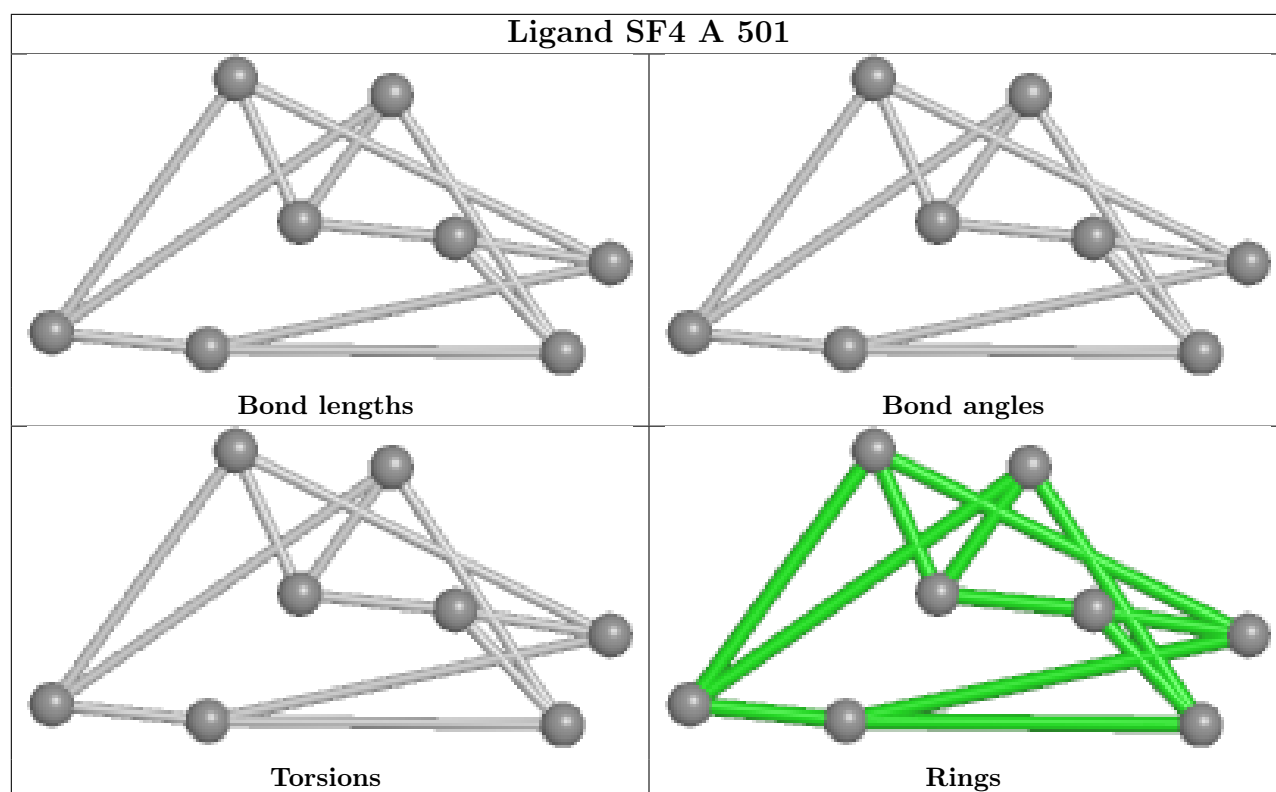


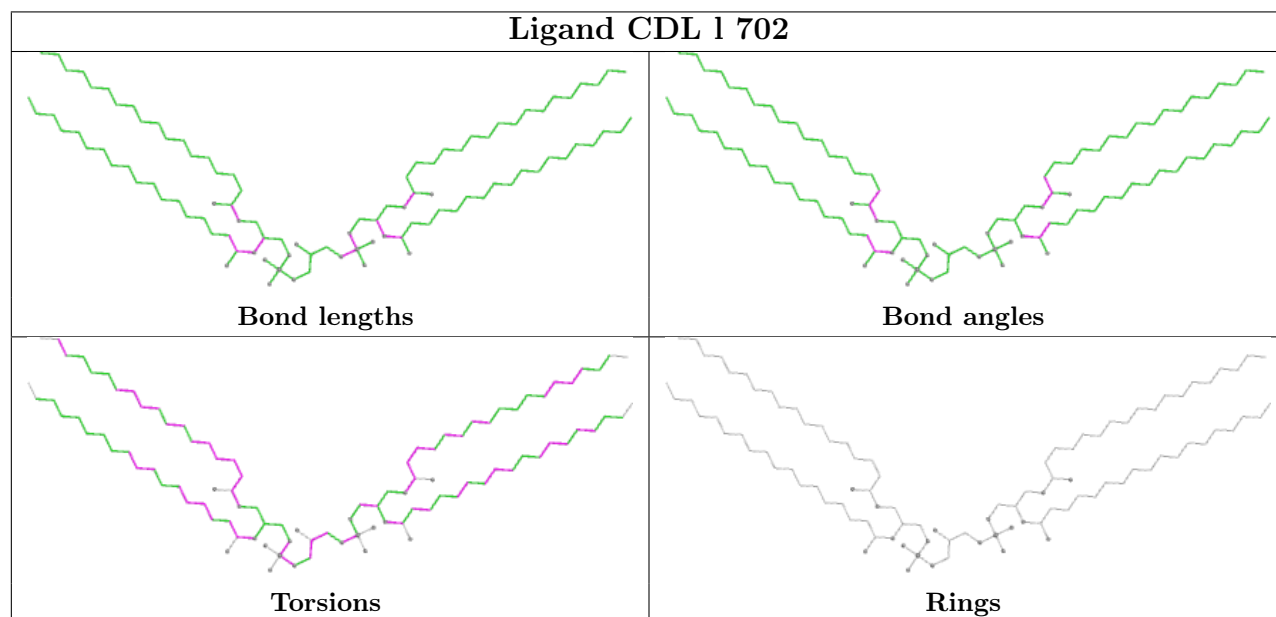
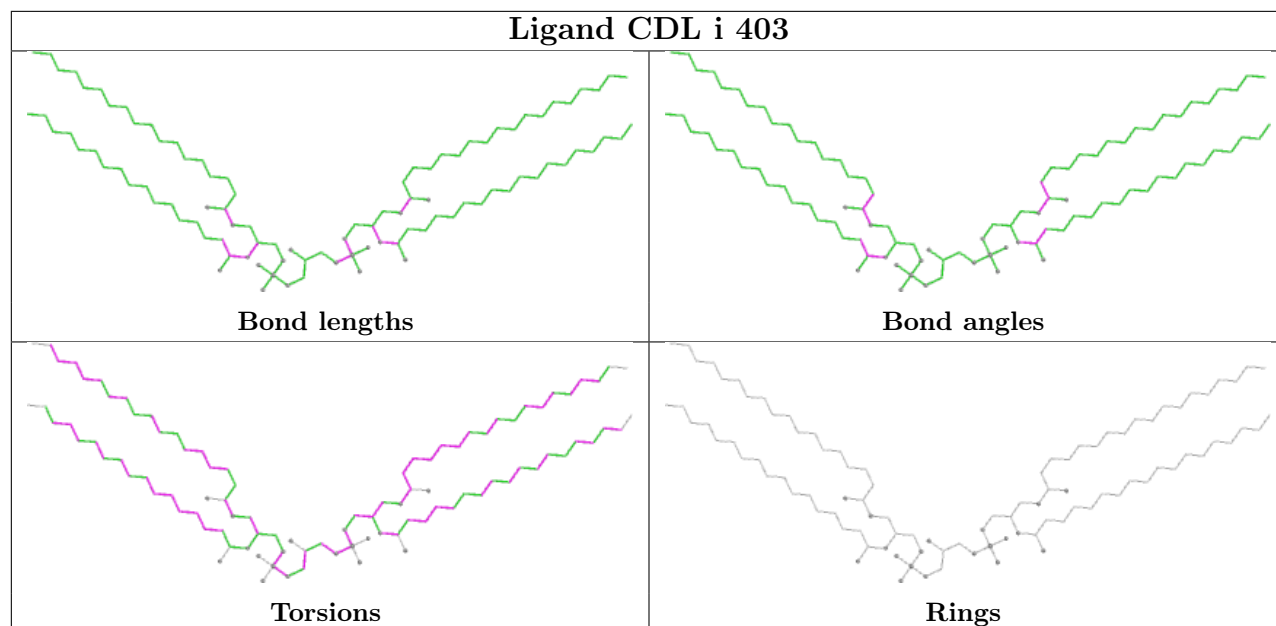




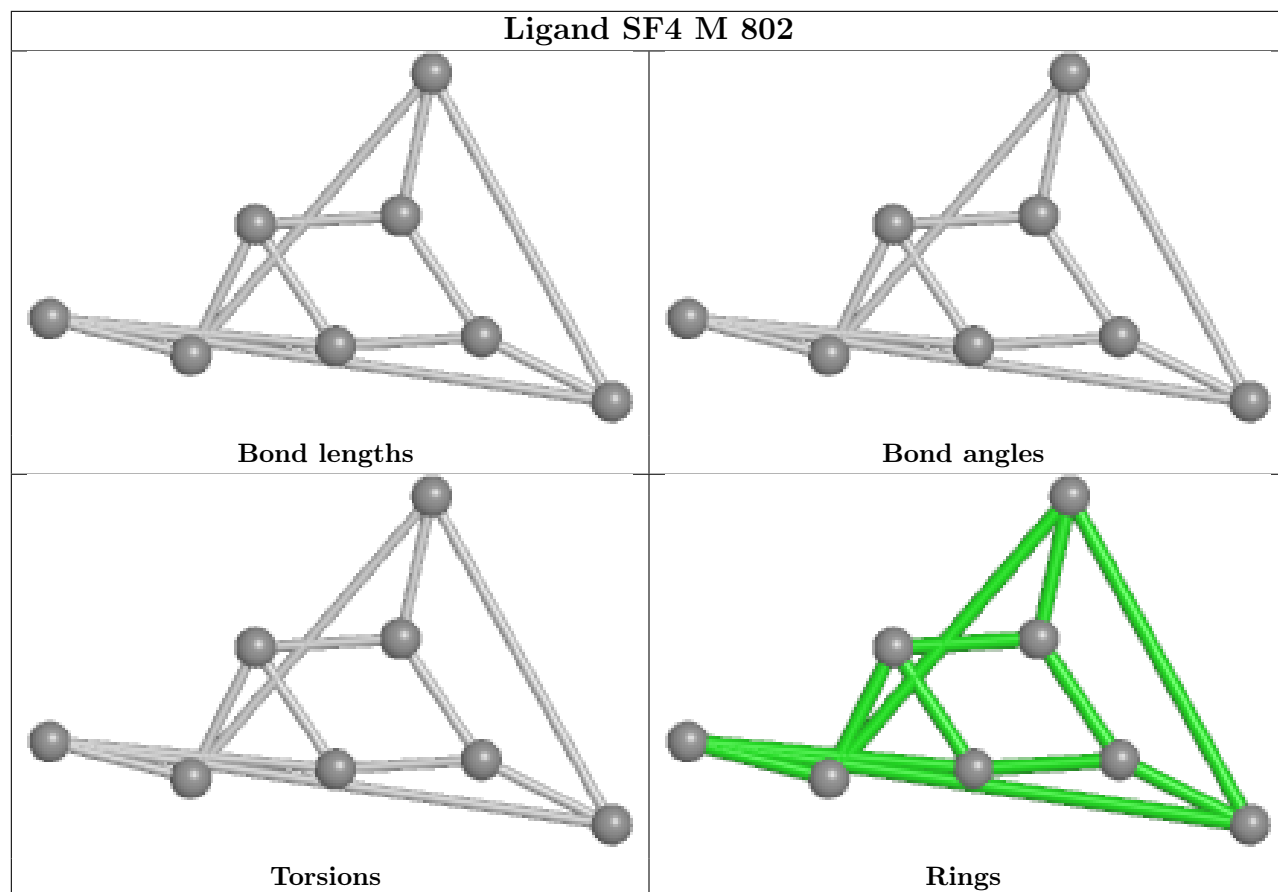




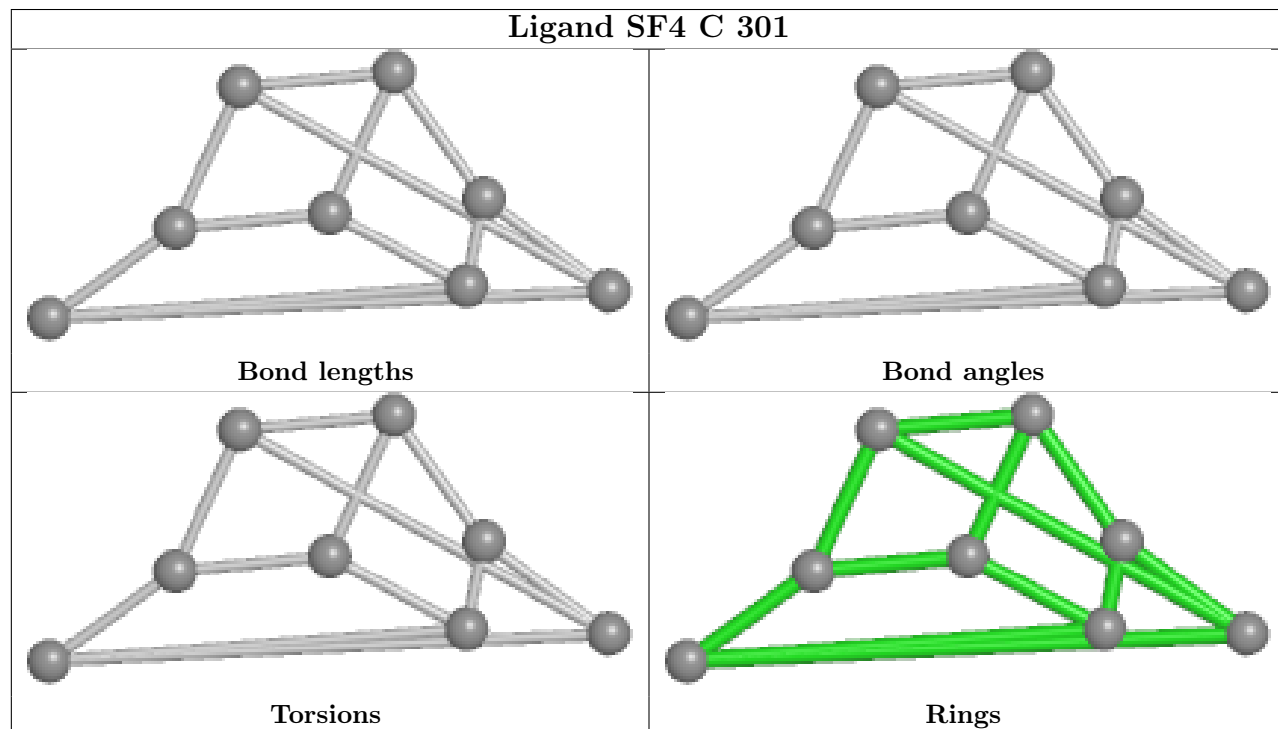


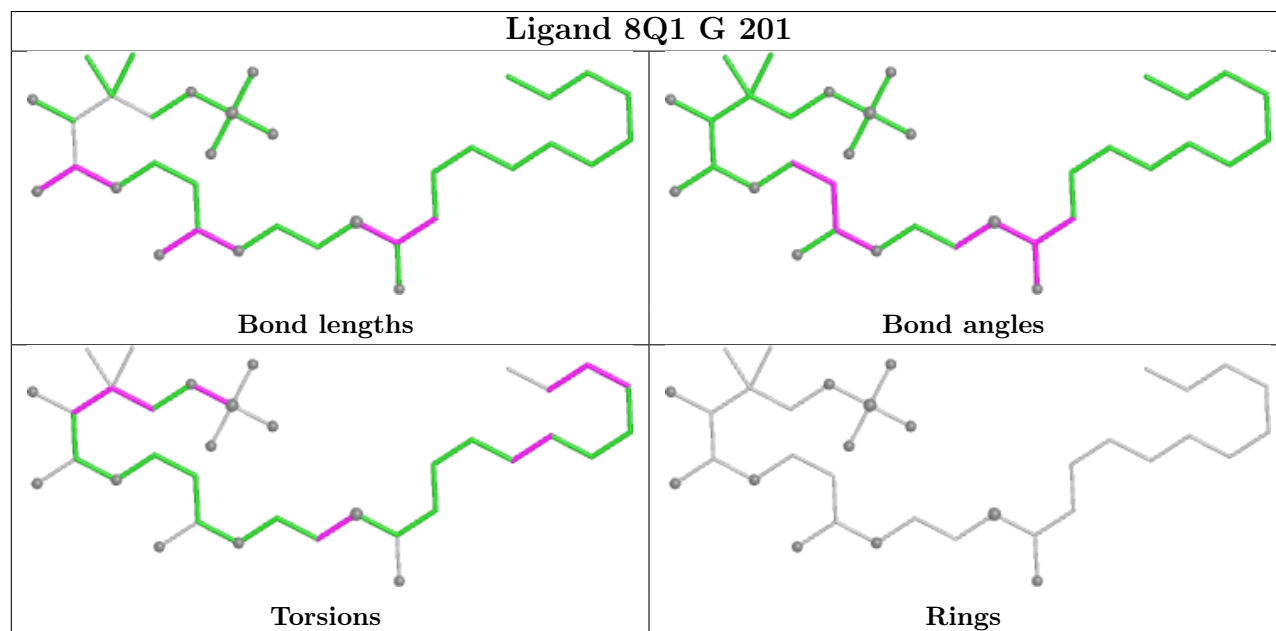
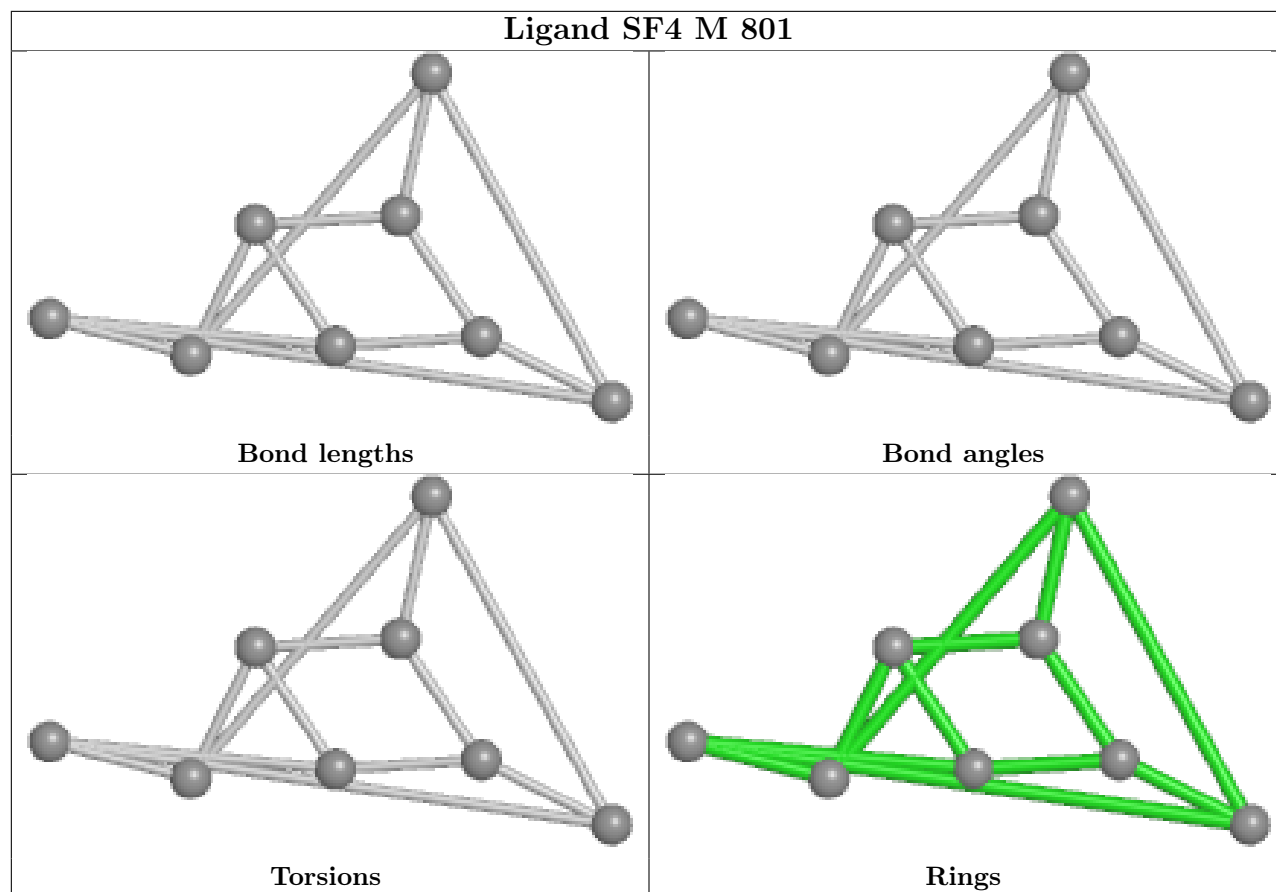


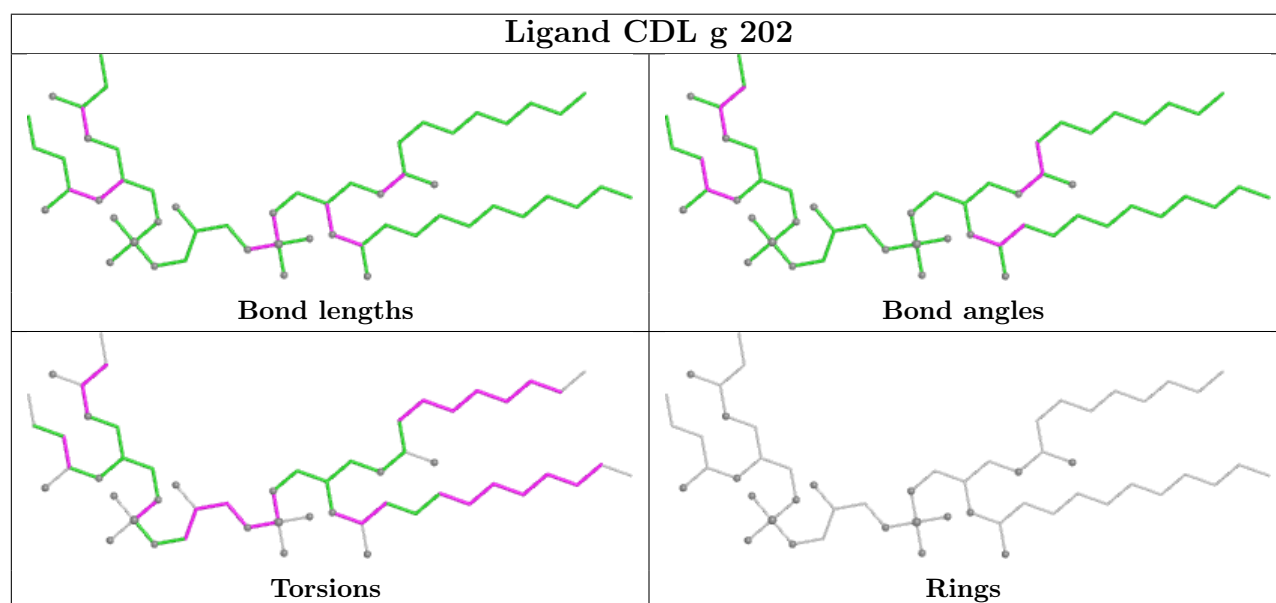
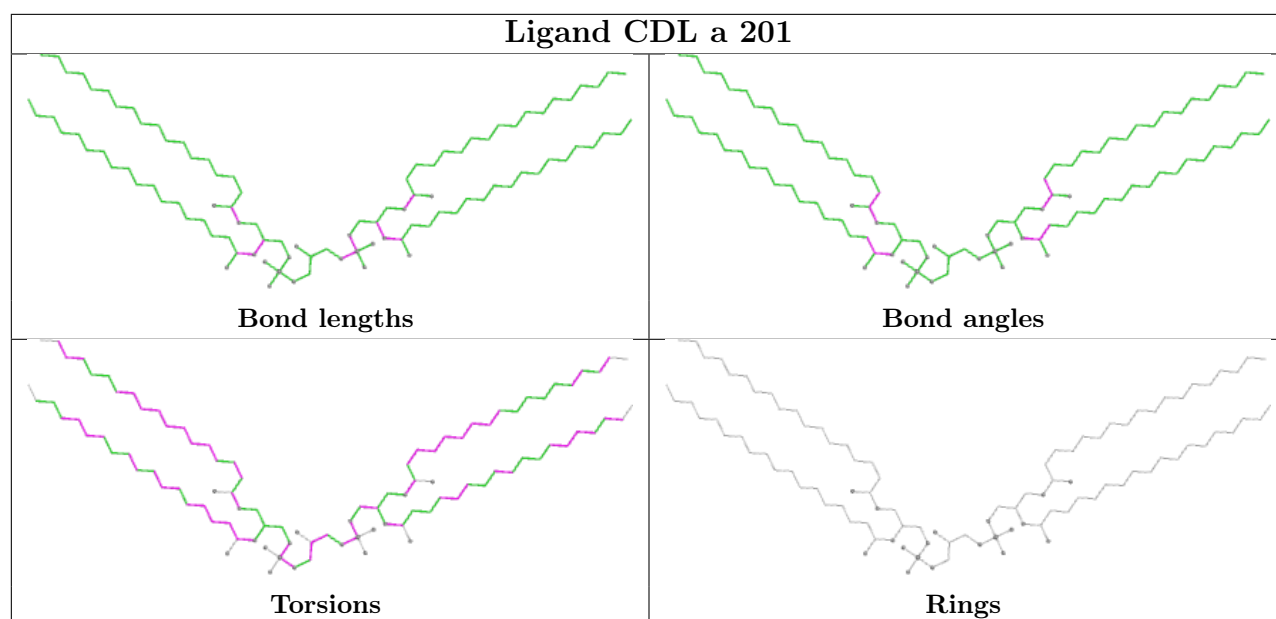
Ligand SF4 M 802

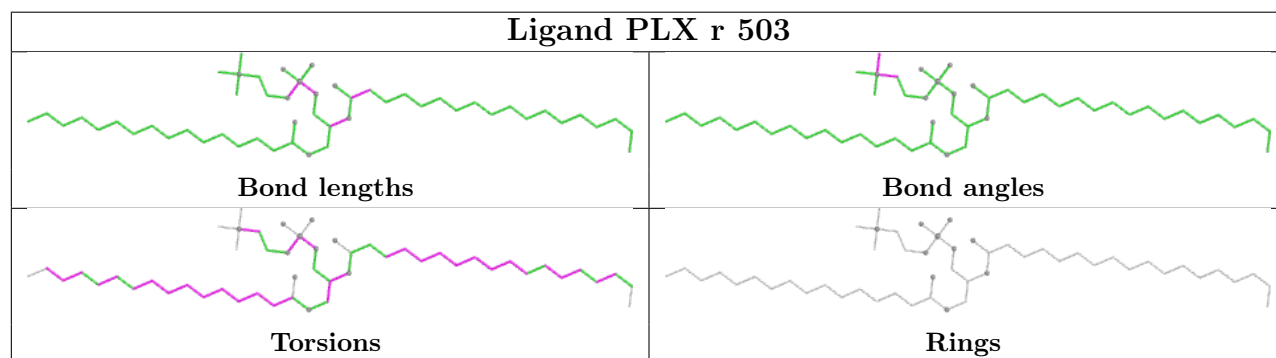
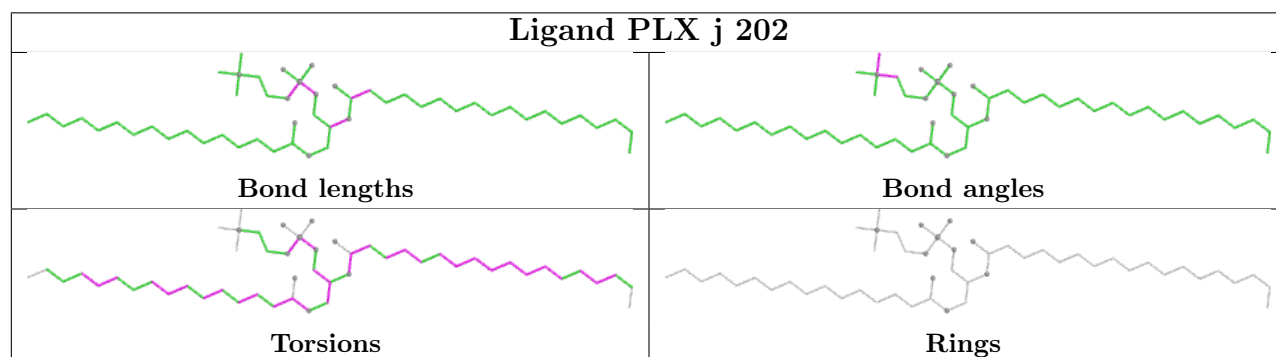
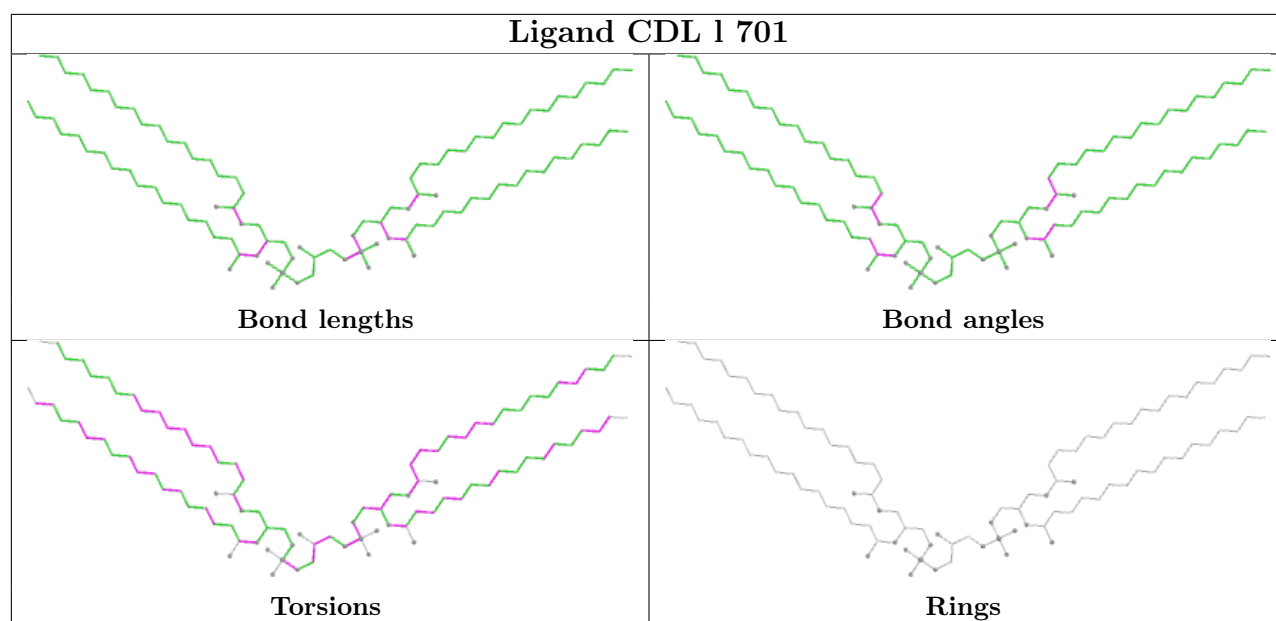


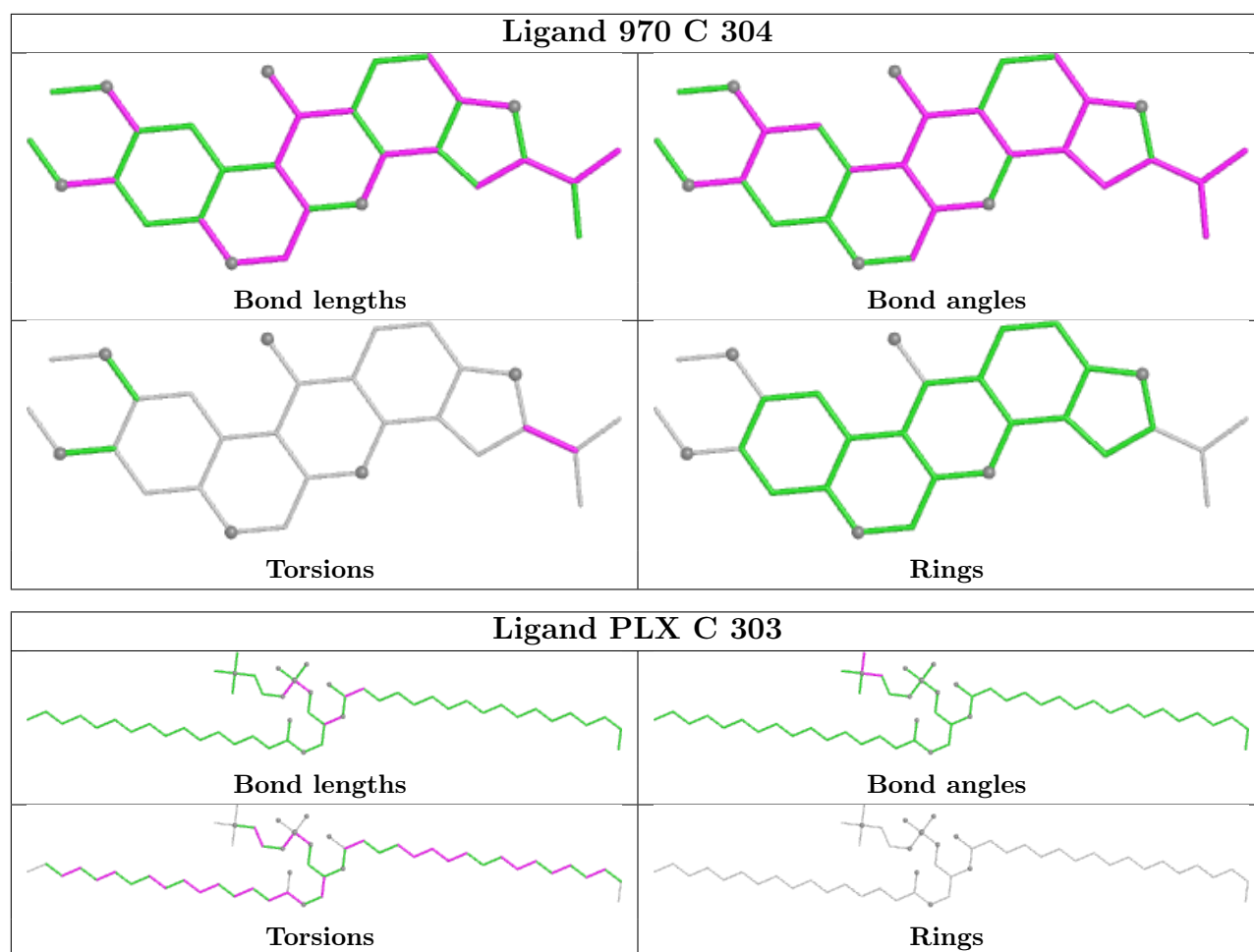
Ligand SF4 C 301











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.

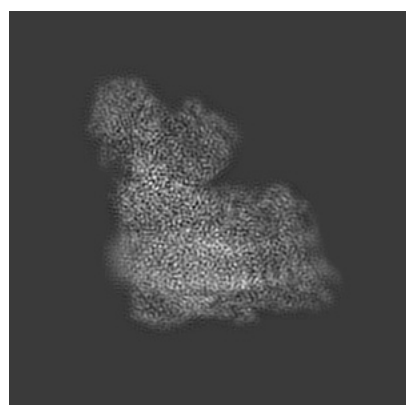
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32257. These allow visual inspection of the internal detail of the map and identification of artifacts.

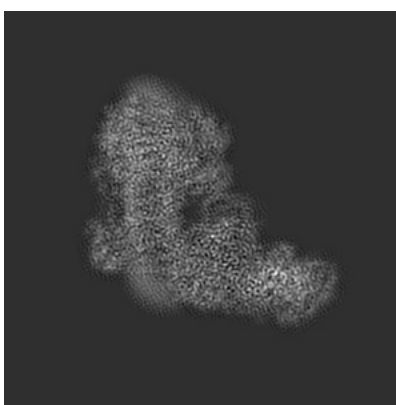
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

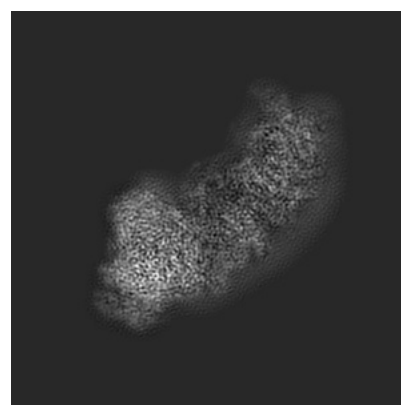
6.1.1 Primary map



X



Y

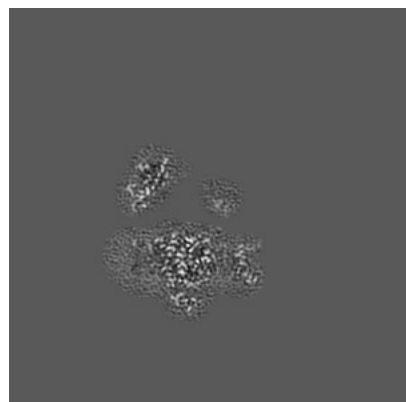


Z

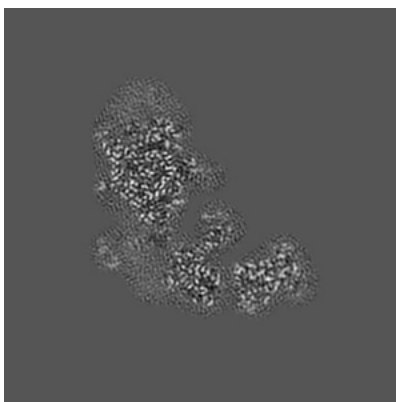
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

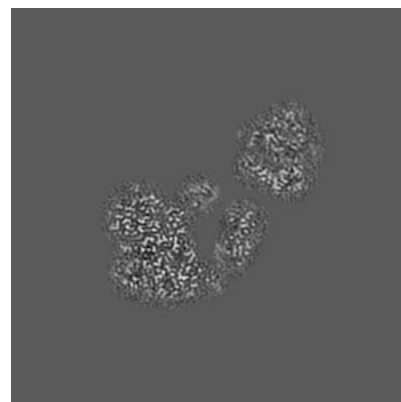
6.2.1 Primary map



X Index: 155



Y Index: 155

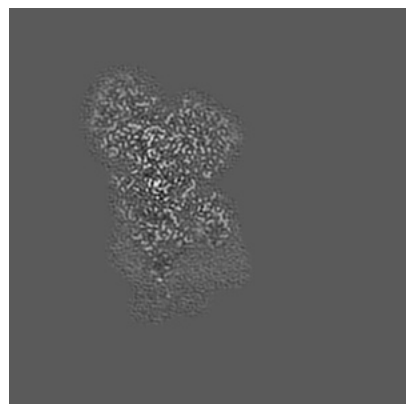


Z Index: 155

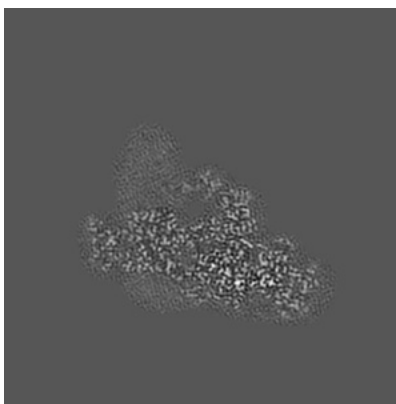
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

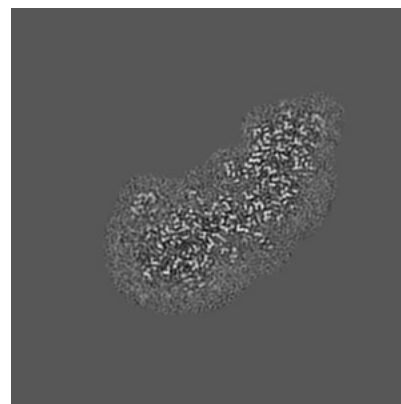
6.3.1 Primary map



X Index: 105



Y Index: 112

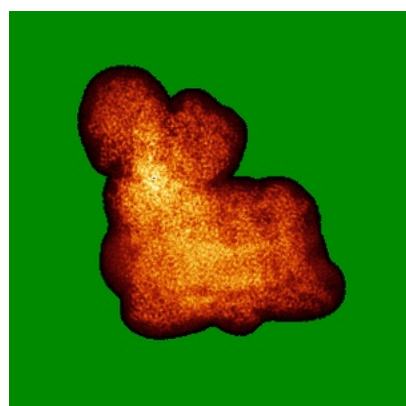


Z Index: 128

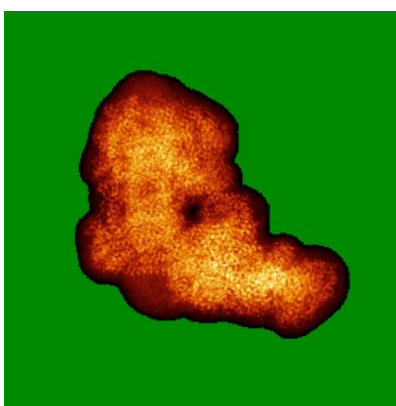
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

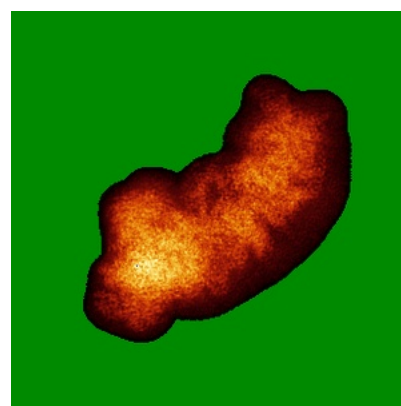
6.4.1 Primary map



X



Y

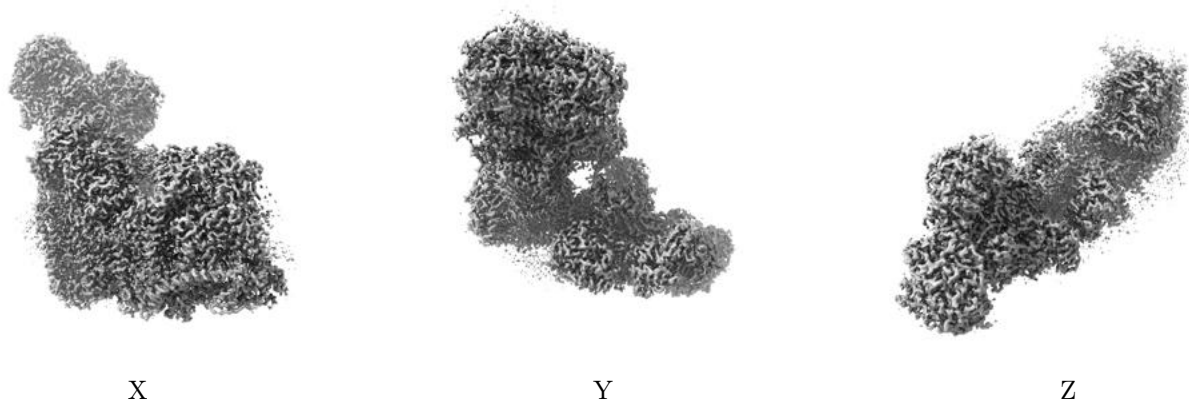


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.0336. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

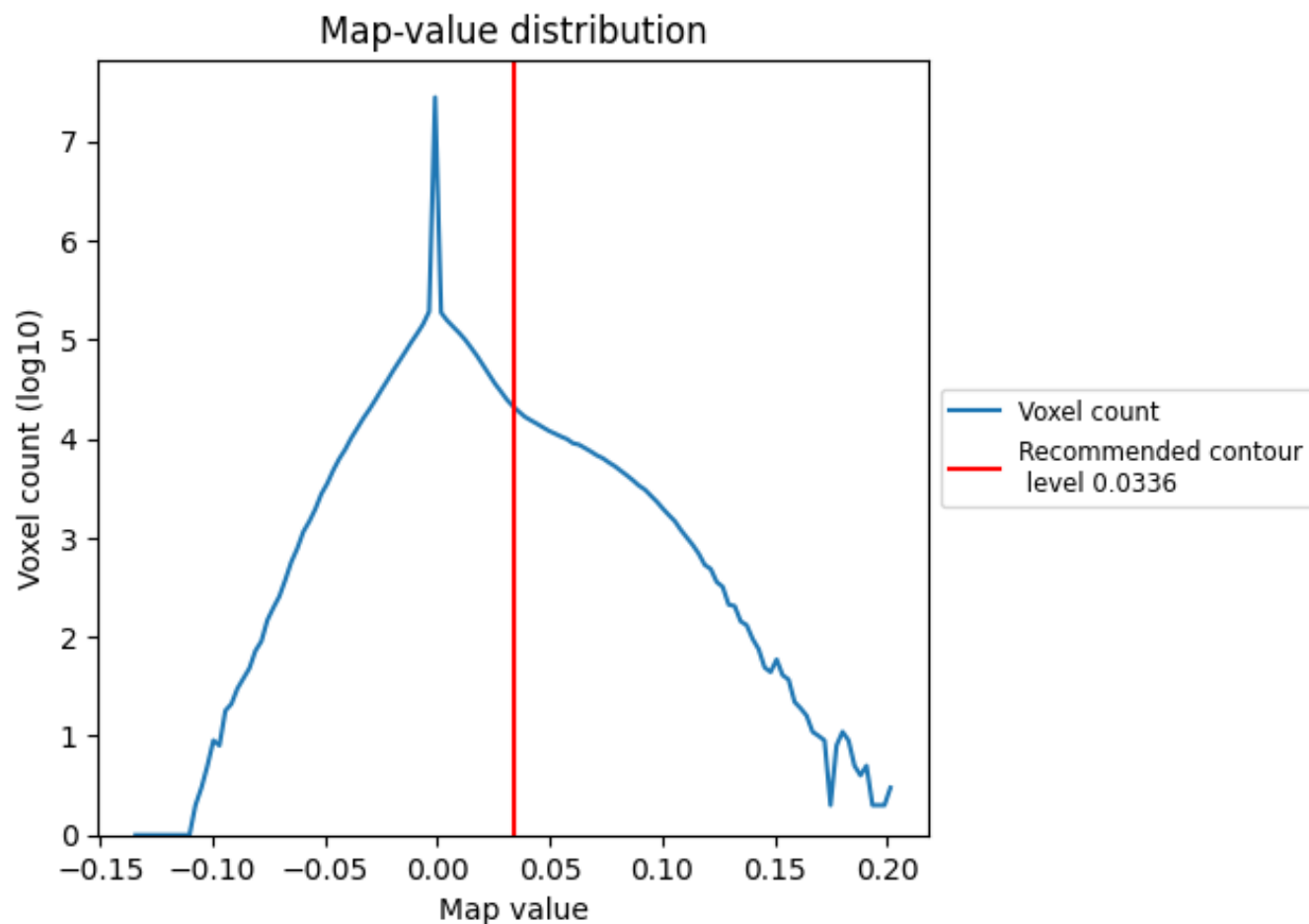
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

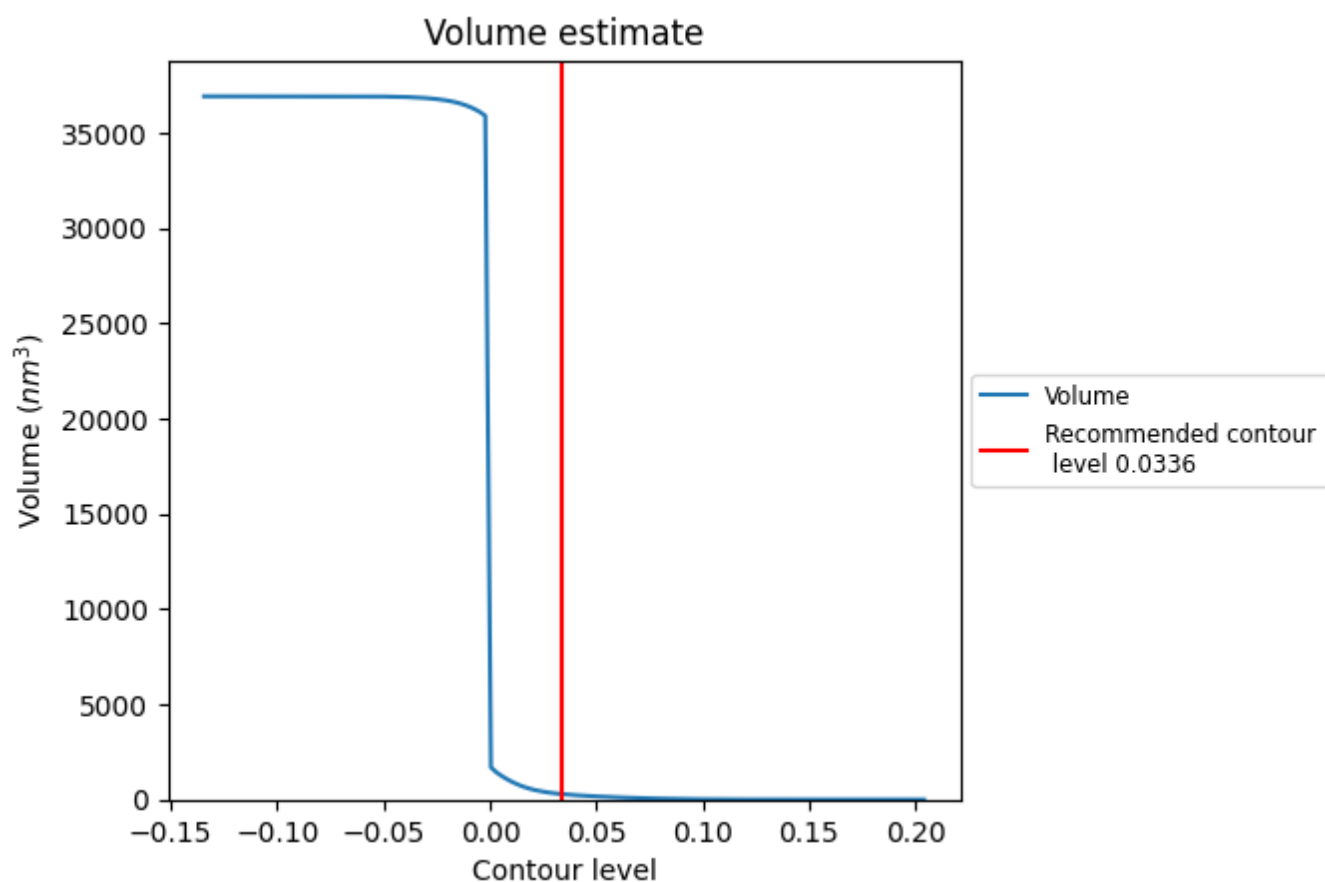
This section contains the results of statistical analysis of the map.

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.

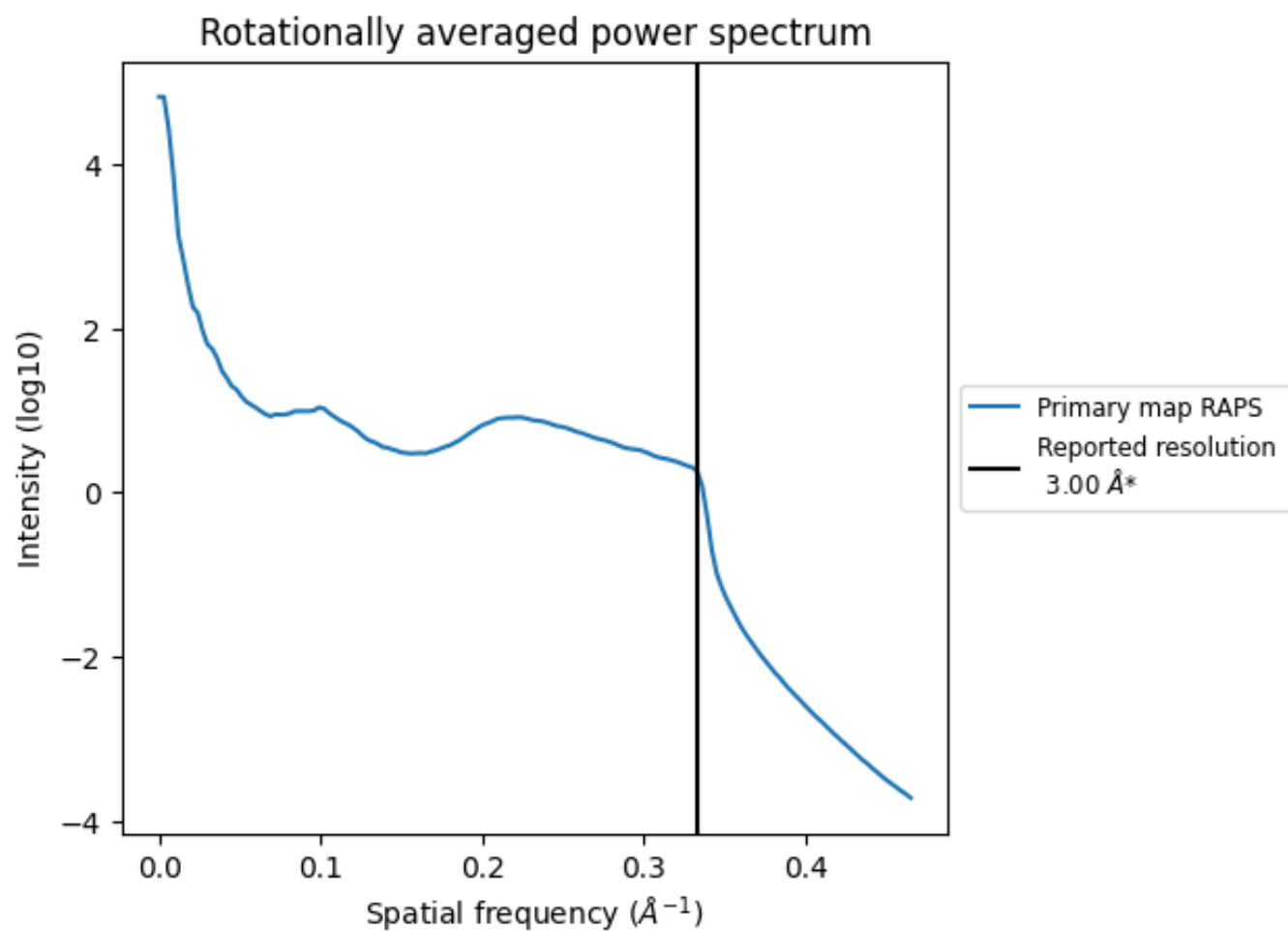
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 291 nm³; this corresponds to an approximate mass of 263 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

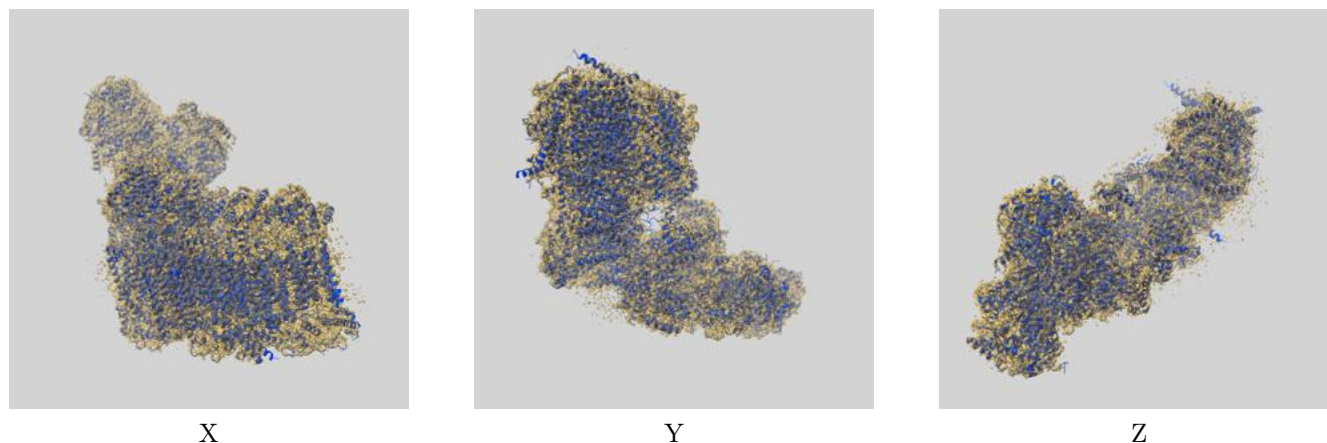
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

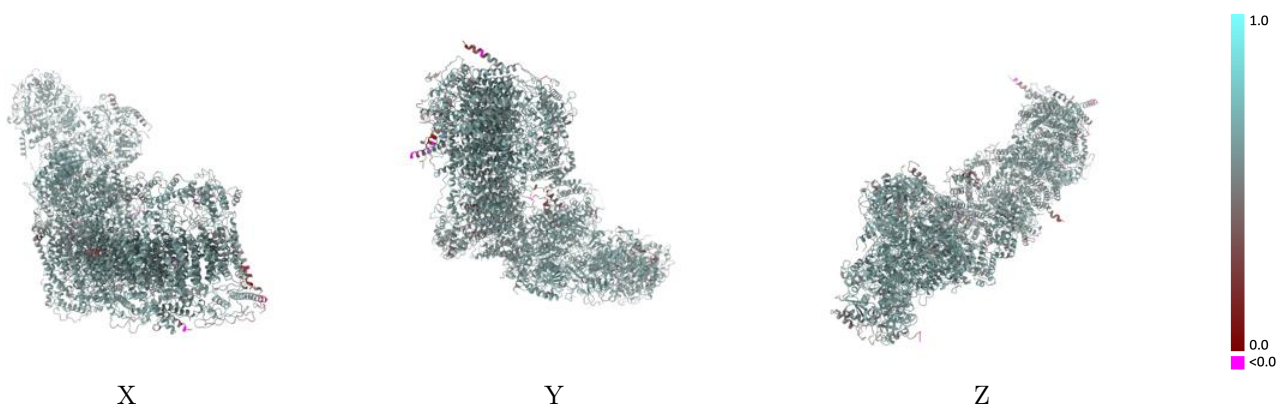
This section contains information regarding the fit between EMDB map EMD-32257 and PDB model 7W1V. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



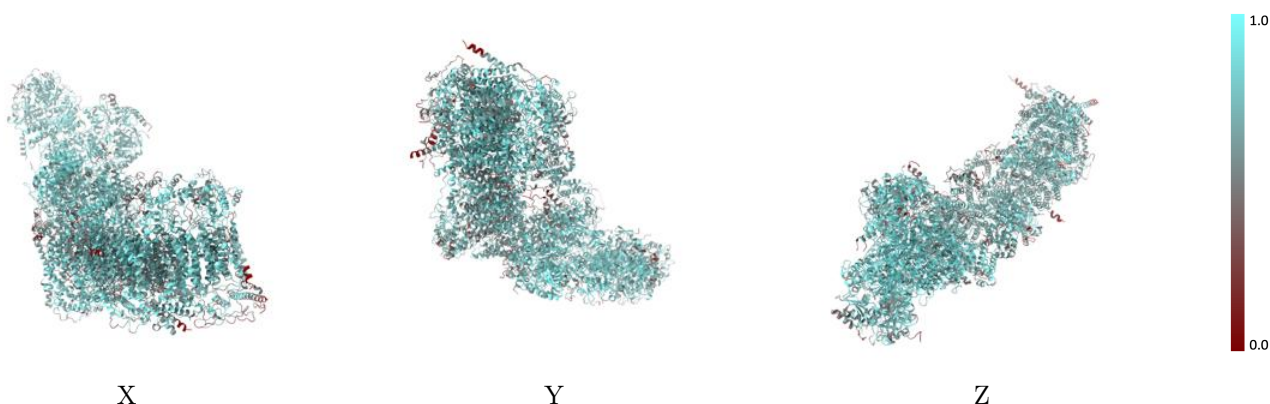
The images above show the 3D surface view of the map at the recommended contour level 0.0336 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



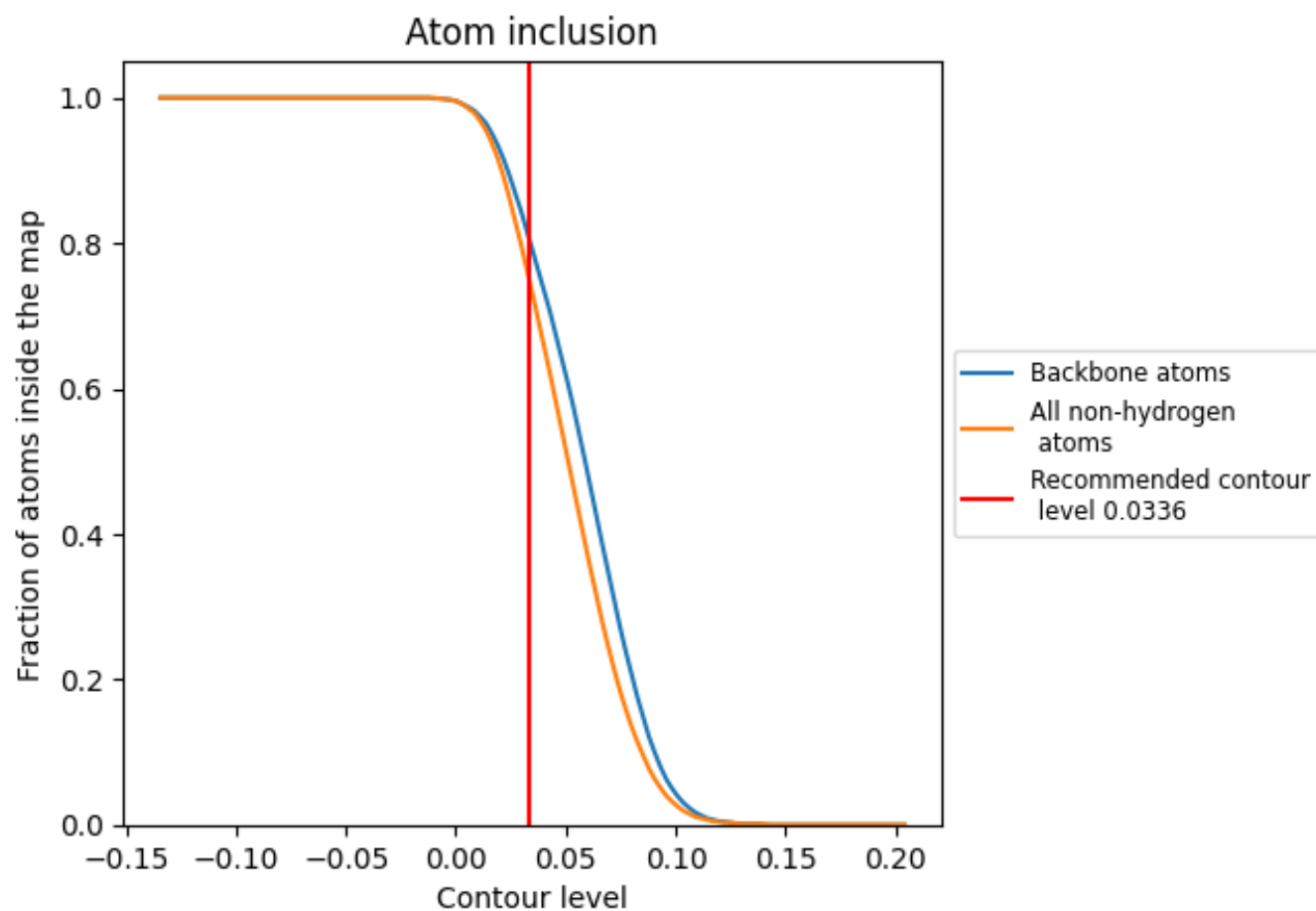
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.0336).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0336) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7470	 0.5790
A	 0.7400	 0.5720
B	 0.8570	 0.6170
C	 0.8590	 0.6170
E	 0.7860	 0.5940
F	 0.6410	 0.5260
G	 0.4720	 0.4590
H	 0.7530	 0.5850
I	 0.6170	 0.5480
J	 0.7820	 0.5930
K	 0.6390	 0.5370
L	 0.7900	 0.5950
M	 0.7980	 0.5910
N	 0.6980	 0.5790
O	 0.7230	 0.5570
P	 0.8710	 0.6220
Q	 0.8480	 0.6150
S	 0.7930	 0.5980
T	 0.7420	 0.5850
U	 0.6680	 0.5410
V	 0.6160	 0.5560
W	 0.7110	 0.5670
X	 0.6580	 0.5520
Y	 0.6130	 0.5150
Z	 0.5650	 0.4840
a	 0.7240	 0.5920
b	 0.6670	 0.5420
c	 0.7220	 0.5760
d	 0.6820	 0.5500
e	 0.6730	 0.5570
f	 0.5370	 0.4900
g	 0.7290	 0.5780
h	 0.7150	 0.5650
i	 0.7950	 0.5970
j	 0.7190	 0.5810



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Chain	Atom inclusion	Q-score
k	 0.8280	 0.6060
l	 0.7590	 0.5880
m	 0.6870	 0.5510
n	 0.5500	 0.5050
o	 0.6760	 0.5720
p	 0.7230	 0.5730
r	 0.8080	 0.6010
s	 0.8010	 0.5970
u	 0.7350	 0.5760
v	 0.6000	 0.5160
w	 0.7230	 0.5710