



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 06:18 AM UTC

PDB ID : 7W1U / pdb_00007w1u
EMDB ID : EMD-32256
Title : Active state CI from Rotenone dataset, Subclass 2
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-20
Resolution : 3.20 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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 EMD 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) : 2.49

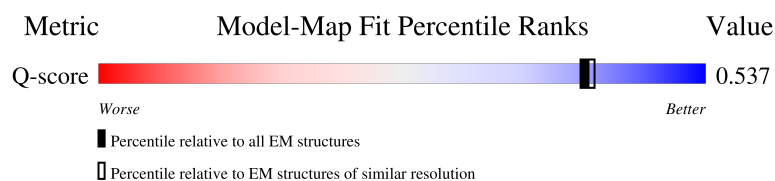
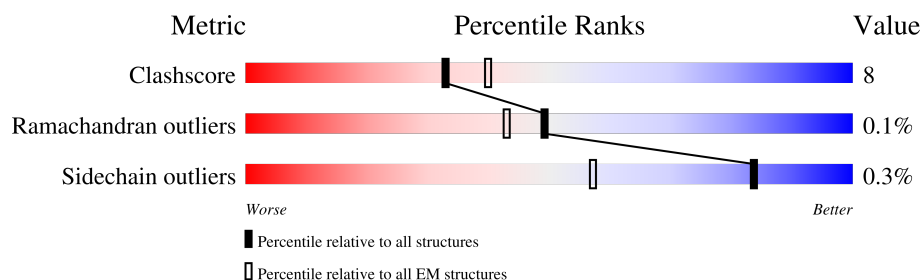
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	6% 81% 19%
2	B	176	82% 18%
3	C	156	75% 25%
4	E	115	10% 83% 17%

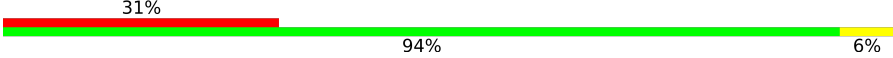
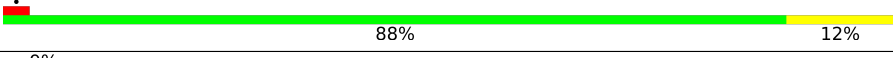
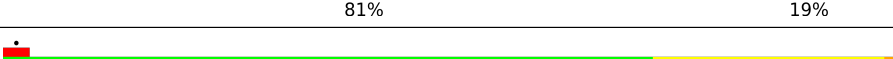
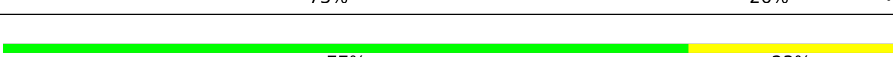
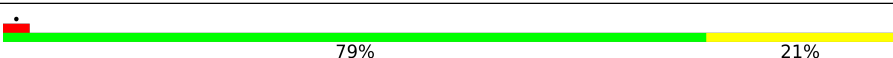
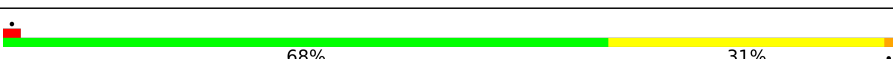
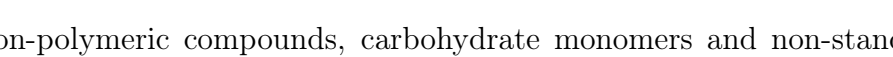
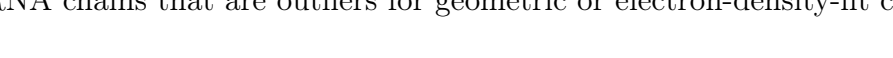
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Mol	Chain	Length	Quality of chain
5	F	86	
6	G	88	
6	X	88	
7	H	112	
8	I	112	
9	J	342	
10	K	43	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	67	
23	Z	80	
24	a	138	
25	b	126	
26	c	156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

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Mol	Chain	Length	Quality of chain
29	f	49	
30	g	121	
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	125	
44	w	320	

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

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

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 67815 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
			3324	2100	590	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
			1392	875	239	267	11		

- 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
			1247	794	227	212	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
			687	432	129	124	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
			690	446	102	137	5		
6	X	88	Total	C	N	O	S	0	0
			699	450	103	141	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
			5292	3318	923	1012	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
			1204	770	218	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
			1671	1065	281	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
			3450	2206	591	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
			639	414	109	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
			1167	752	200	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
			867	553	142	168	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	121	Total	C	N	O	S	0	0
			1000	650	173	171	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
			4816	3193	746	826	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
			1290	862	188	227	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
			1534	982	279	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
			3631	2412	572	609	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
			2498	1673	382	422	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 NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			1028	642	195	182	9		

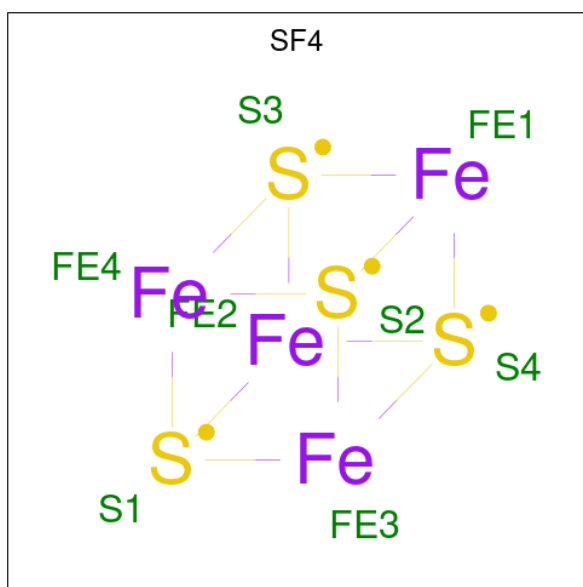
There is a discrepancy between the modelled and reference sequences:

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

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

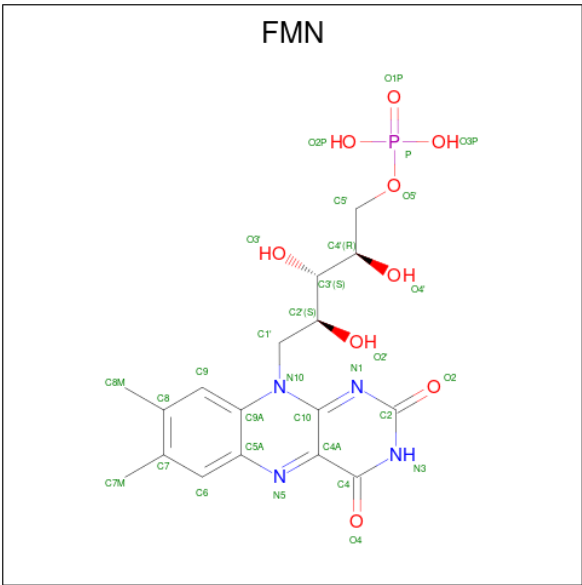
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2582	1644	438	490	10		

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



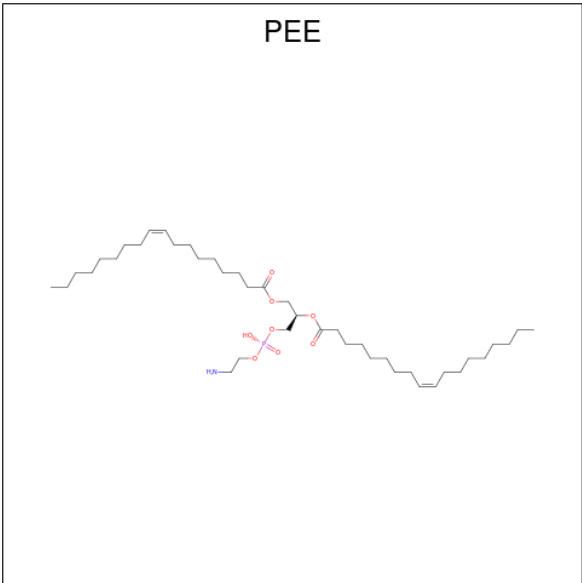
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (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 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



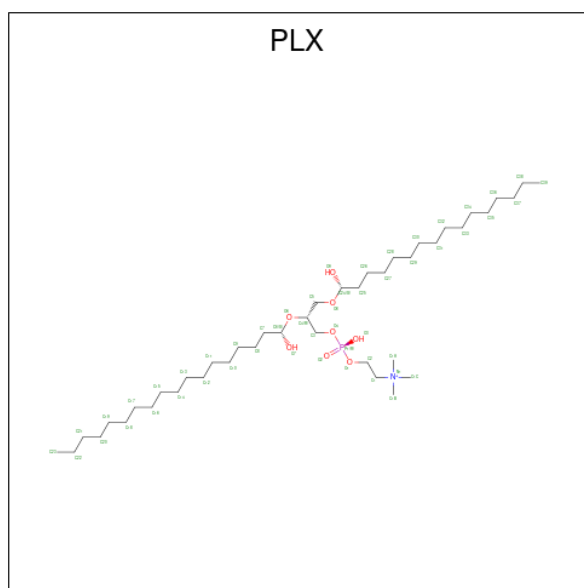
Mol	Chain	Residues	Atoms					AltConf
47	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	W	1	Total	C	N	O	P	0
			41	31	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
47	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	l	1	Total	C	N	O	P	0
			40	30	1	8	1	
47	l	1	Total	C	N	O	P	0
			50	40	1	8	1	
47	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
47	r	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	s	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 48 is (9R,11S)-9-([[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



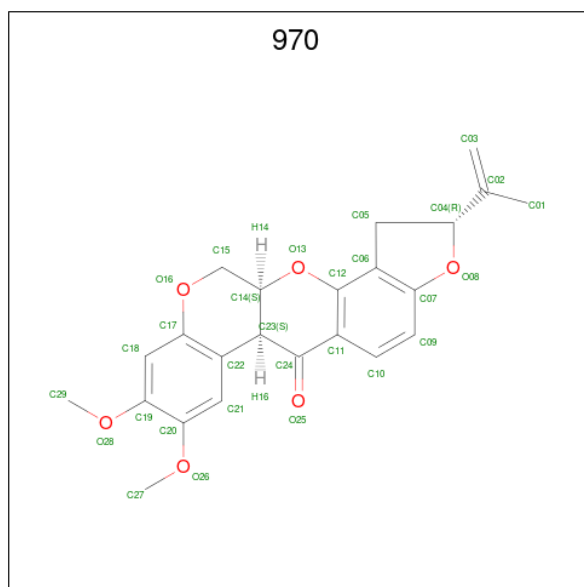
Mol	Chain	Residues	Atoms					AltConf
48	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	e	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	g	1	Total	C	N	O	P	0
			52	42	1	8	1	

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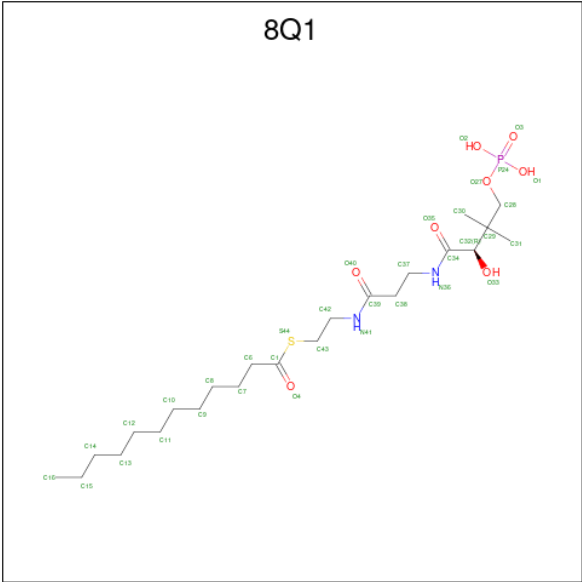
Mol	Chain	Residues	Atoms					AltConf
48	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 49 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).



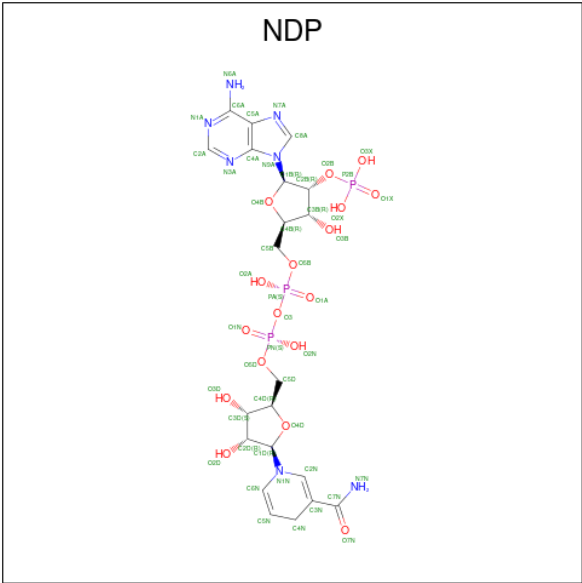
Mol	Chain	Residues	Atoms			AltConf
49	C	1	Total	C	O	0
			29	23	6	

- Molecule 50 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



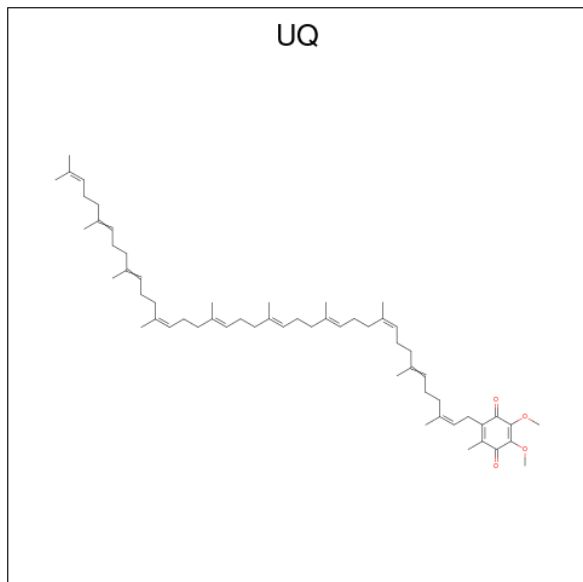
Mol	Chain	Residues	Atoms						AltConf
50	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
50	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

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



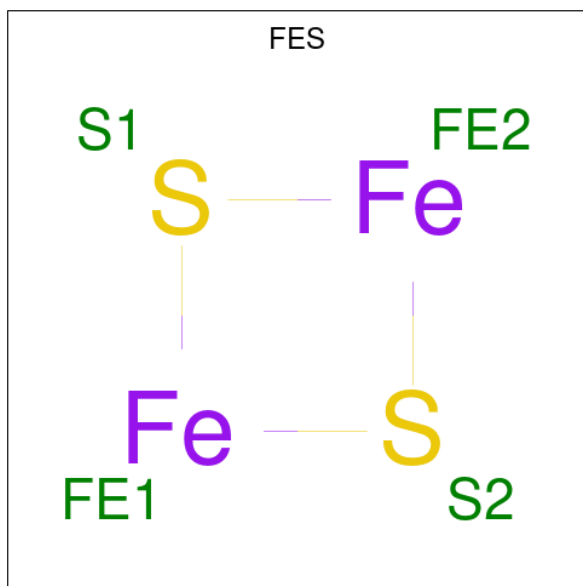
Mol	Chain	Residues	Atoms					AltConf
51	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 52 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
52	J	1	Total	C	O	0
			33	29	4	
52	s	1	Total	C	O	0
			38	34	4	

- Molecule 53 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

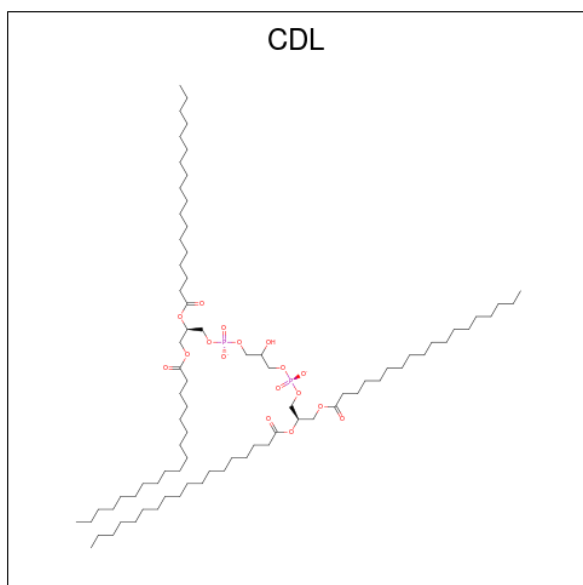


Mol	Chain	Residues	Atoms			AltConf
53	M	1	Total	Fe	S	0
			4	2	2	
53	O	1	Total	Fe	S	0
			4	2	2	

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

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

- Molecule 55 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
55	S	1	Total	C	O	P	0
			51	32	17	2	
55	V	1	Total	C	O	P	0
			94	75	17	2	
55	V	1	Total	C	O	P	0
			100	81	17	2	
55	a	1	Total	C	O	P	0
			100	81	17	2	
55	l	1	Total	C	O	P	0
			99	80	17	2	
55	l	1	Total	C	O	P	0
			100	81	17	2	

Continued on next page...

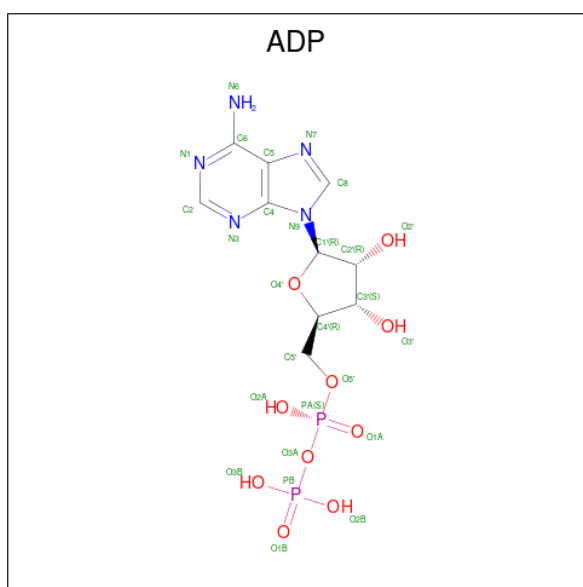
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
55	n	1	Total	C	O	P	0
			55	36	17	2	
55	r	1	Total	C	O	P	0
			99	80	17	2	

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

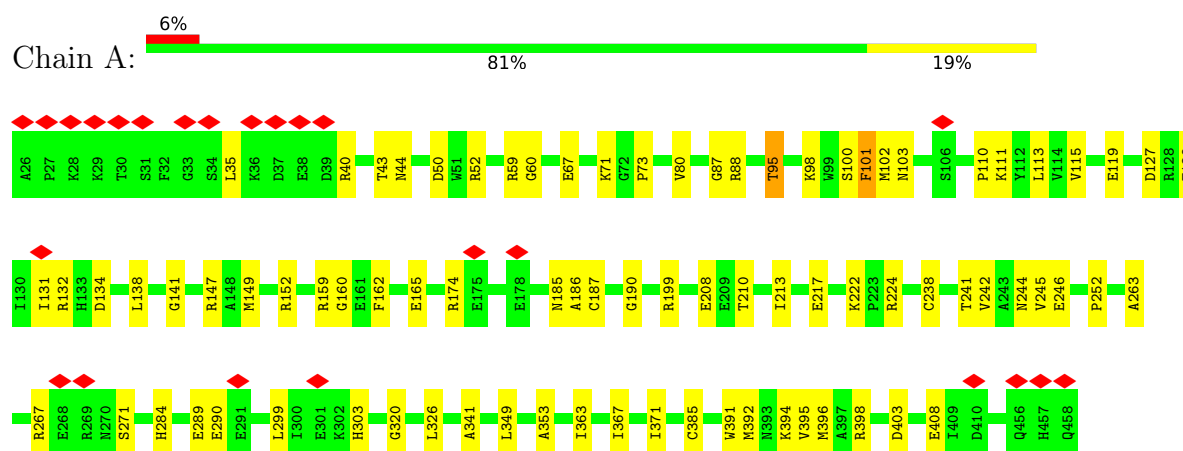


Mol	Chain	Residues	Atoms					AltConf
57	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

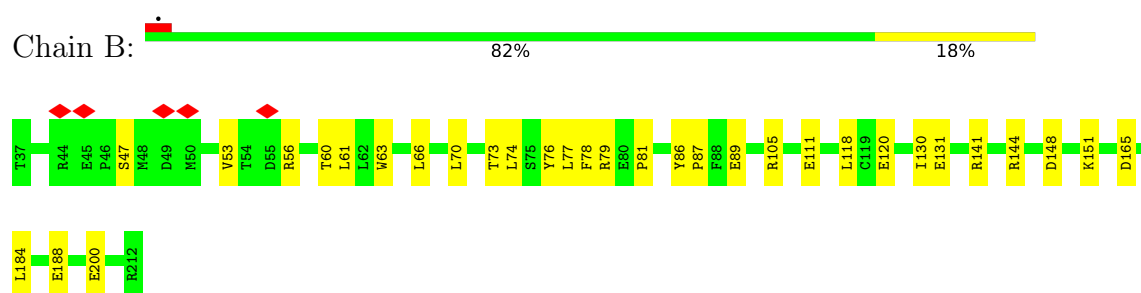
3 Residue-property plots

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.

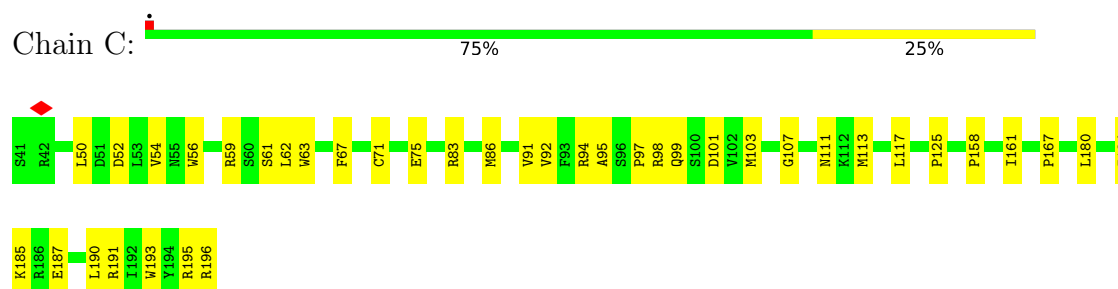
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



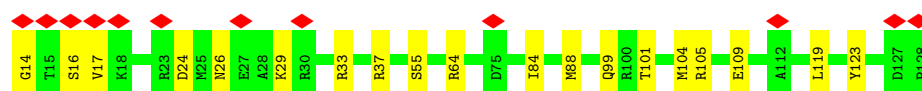
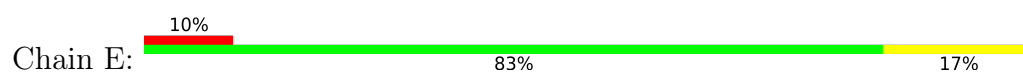
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



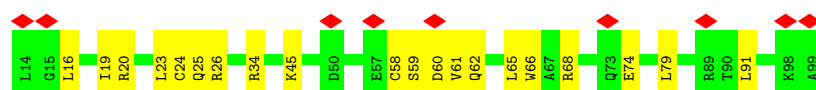
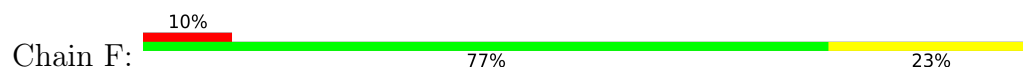
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



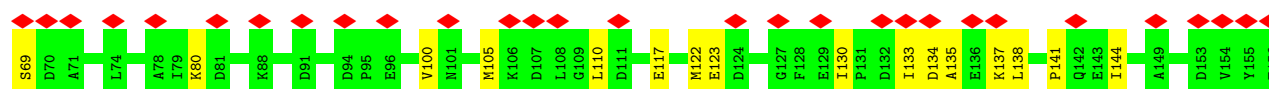
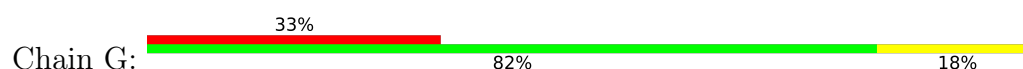
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



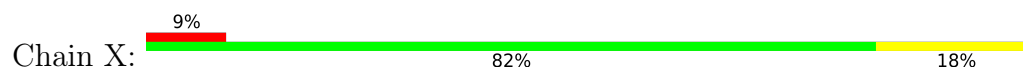
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



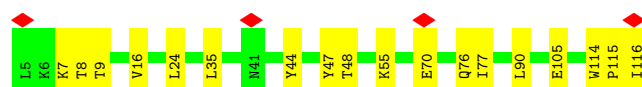
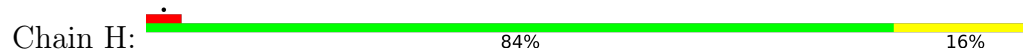
- Molecule 6: Acyl carrier protein



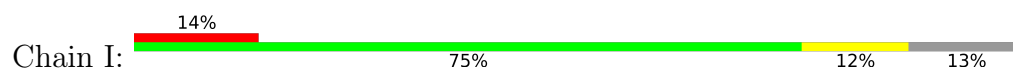
- Molecule 6: Acyl carrier protein



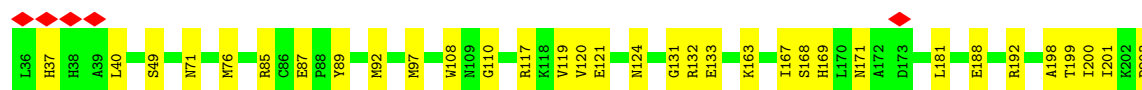
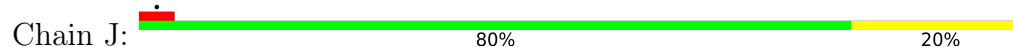
- Molecule 7: Complex I subunit B13

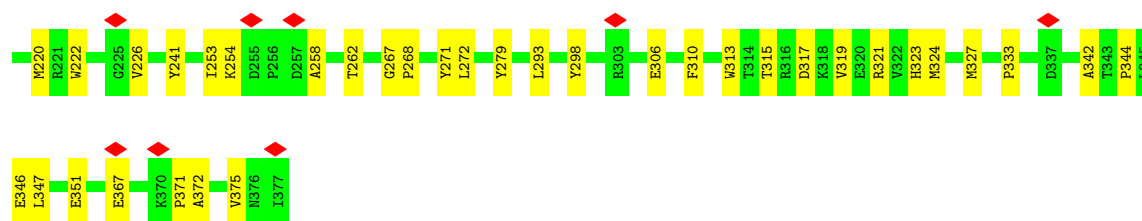


- Molecule 8: Complex I-B14.5a

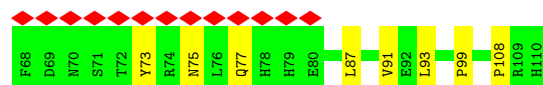
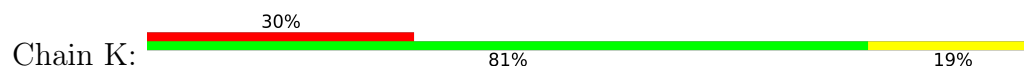


- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

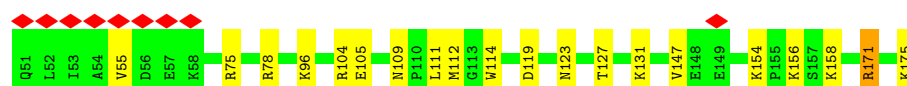
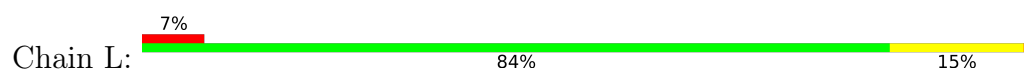




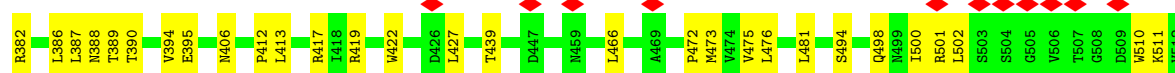
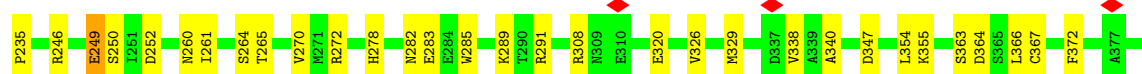
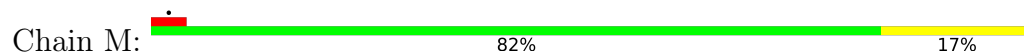
• Molecule 10: Complex I-9kD



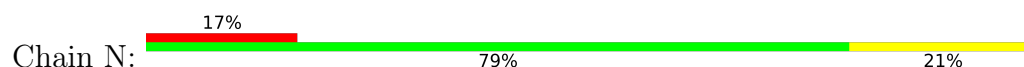
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

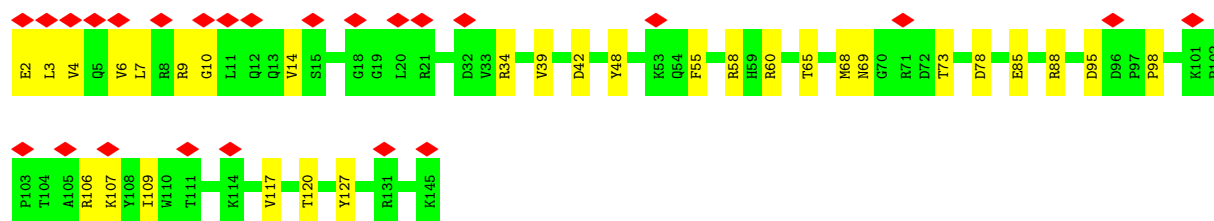


• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

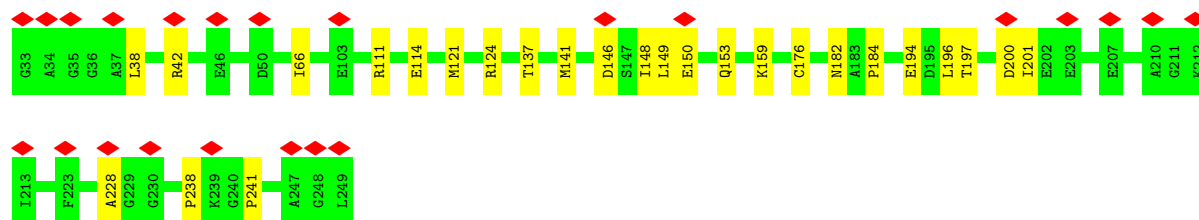
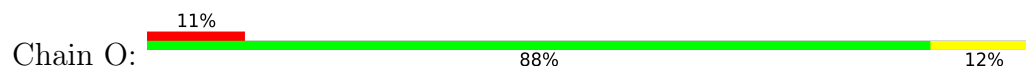


• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

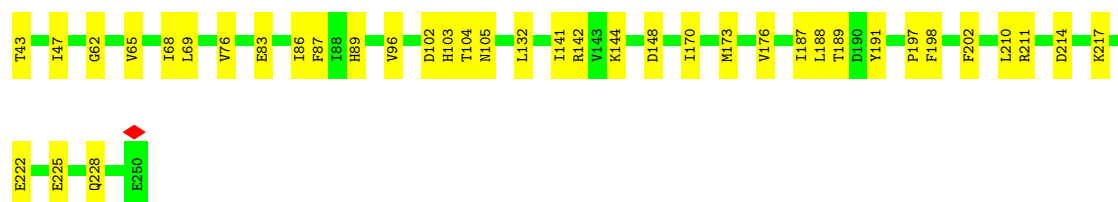
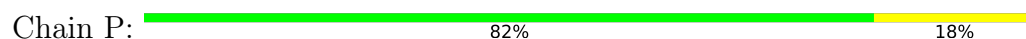




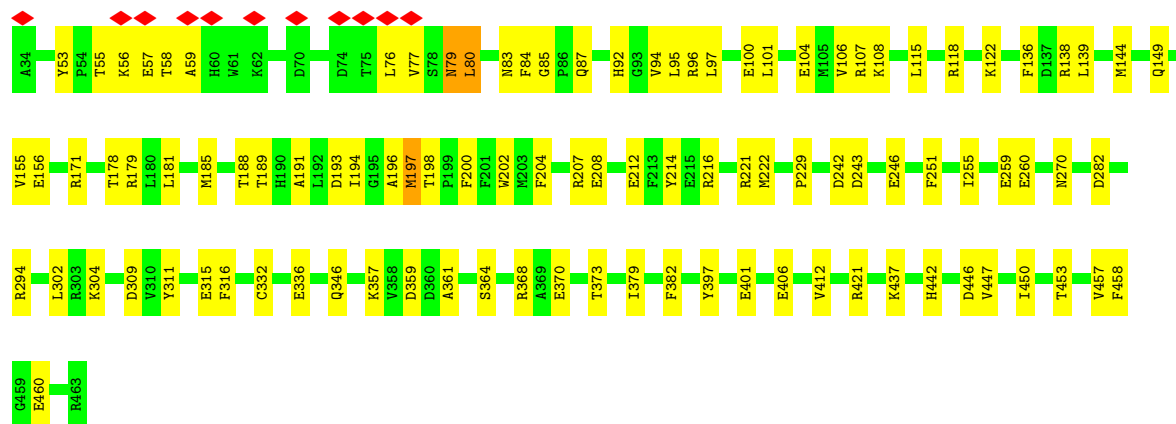
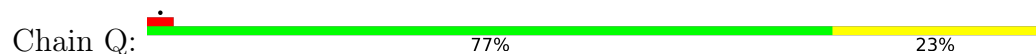
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 15: Complex I-30kD

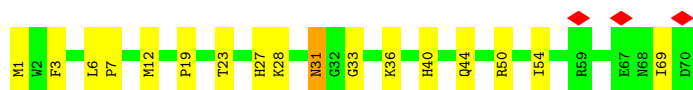


- Molecule 16: Complex I-49kD

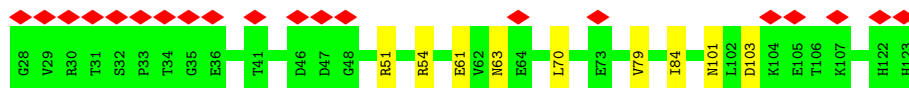
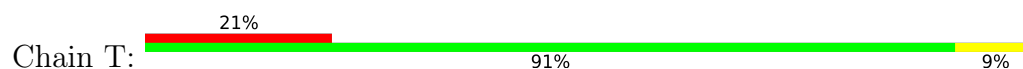


- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

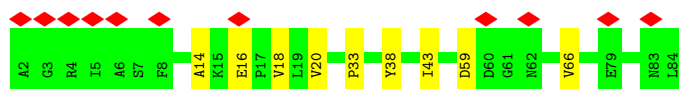
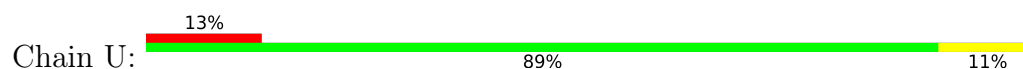




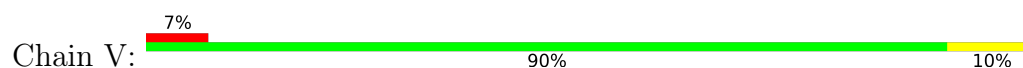
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



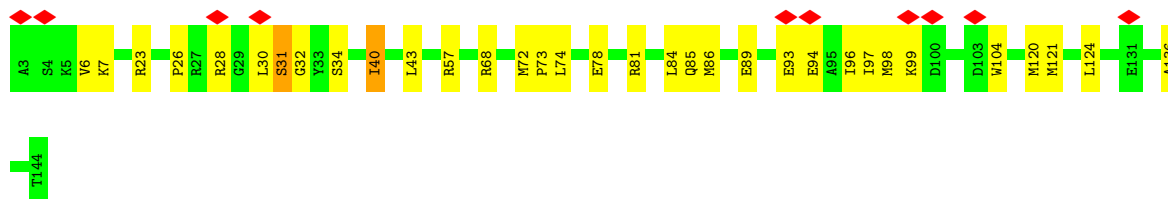
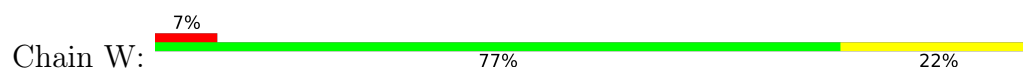
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



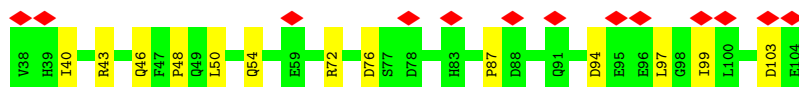
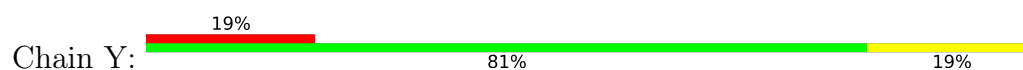
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



- Molecule 21: Complex I-B16.6



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

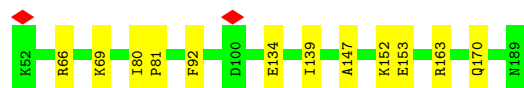


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

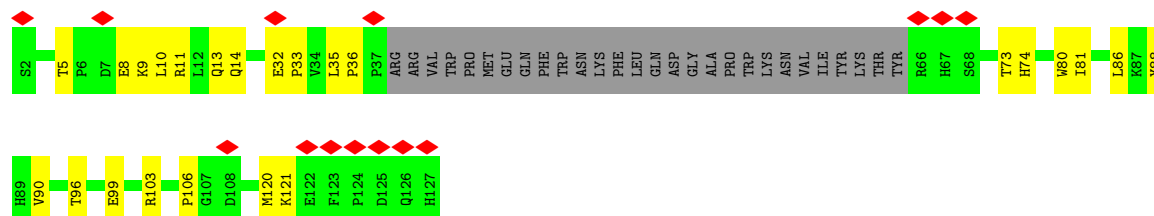




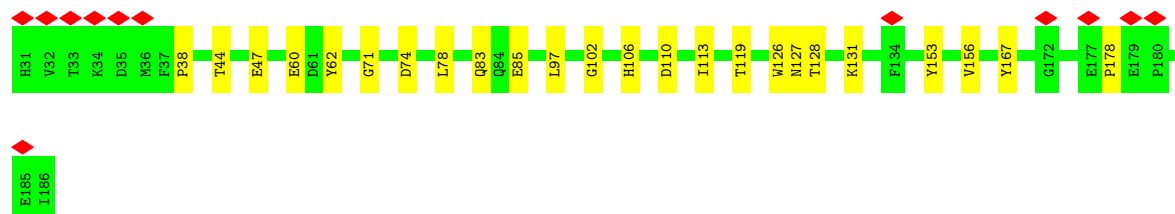
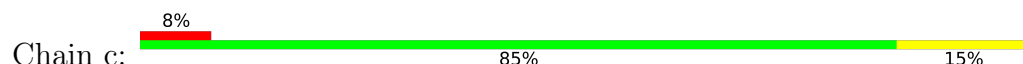
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



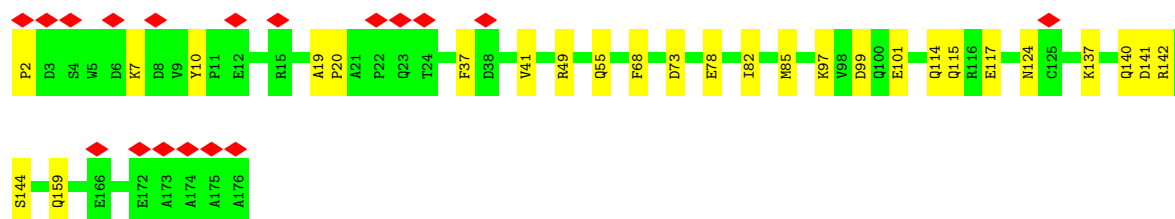
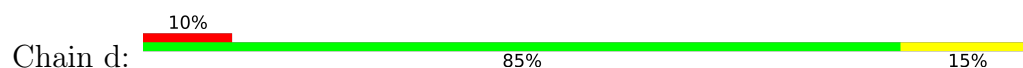
- Molecule 25: Complex I-B17



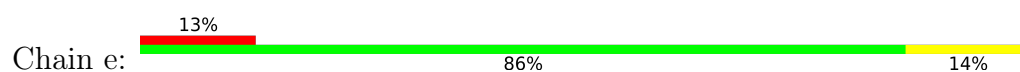
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



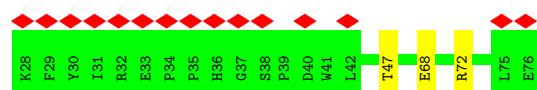
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



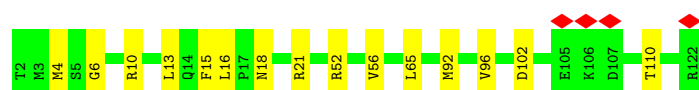
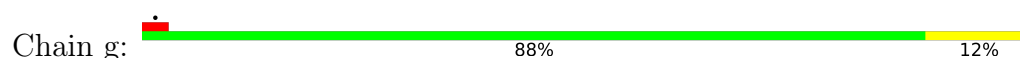
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



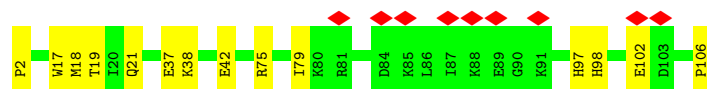
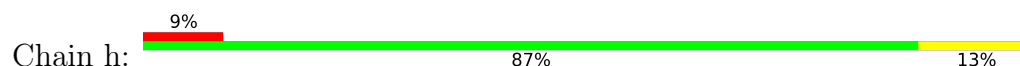
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



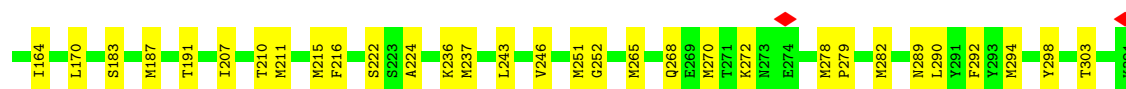
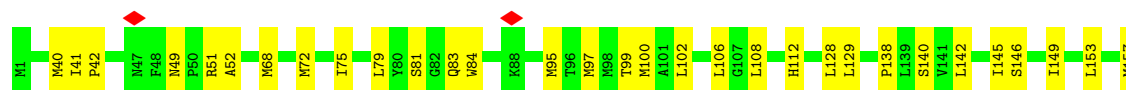
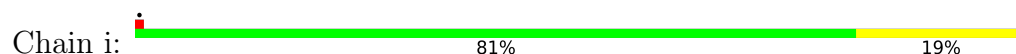
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



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



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

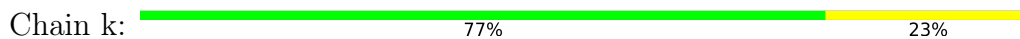


- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

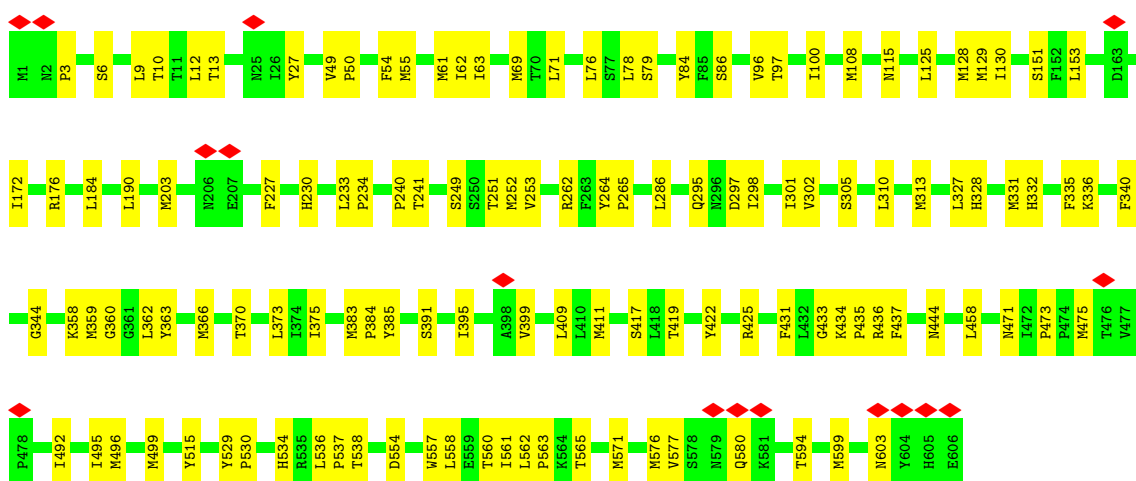
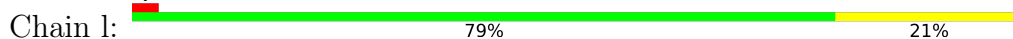




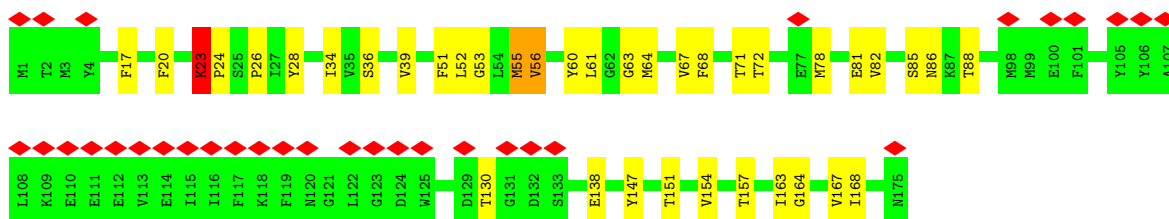
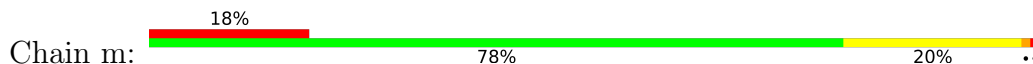
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L



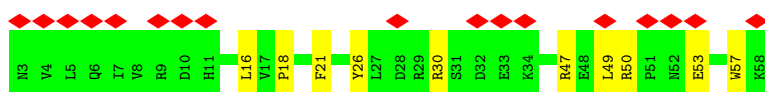
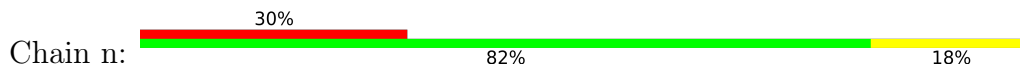
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5



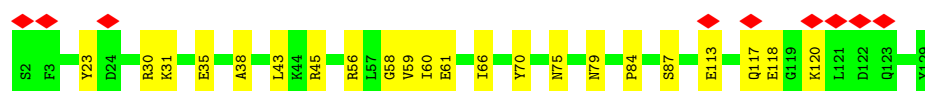
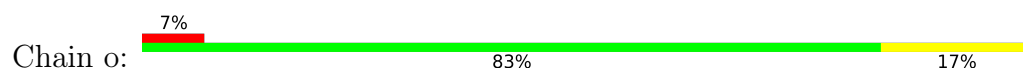
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6



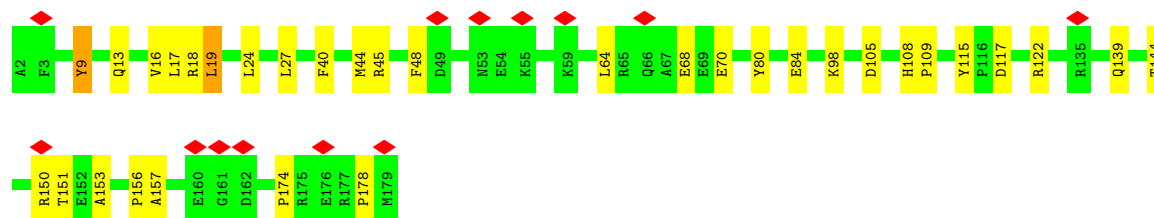
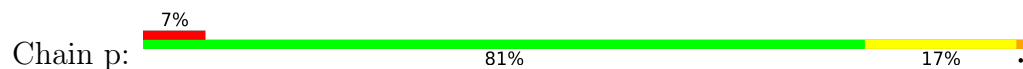
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



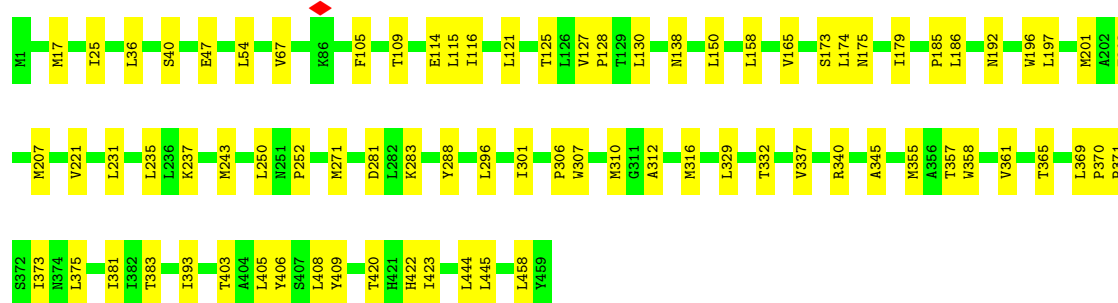
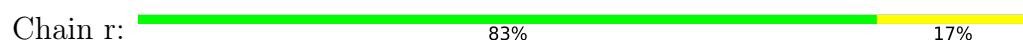
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



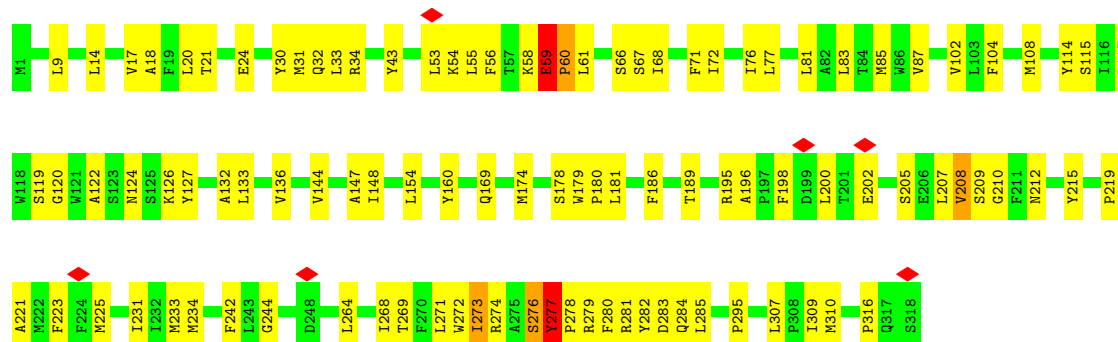
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



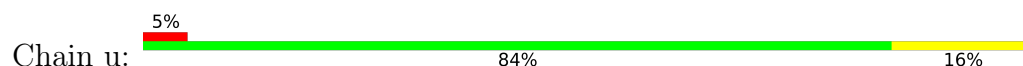
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4



- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

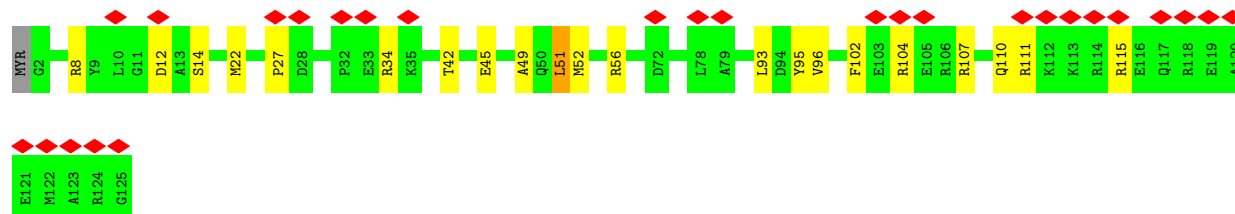
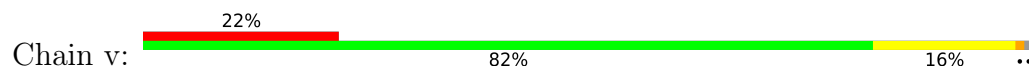


- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

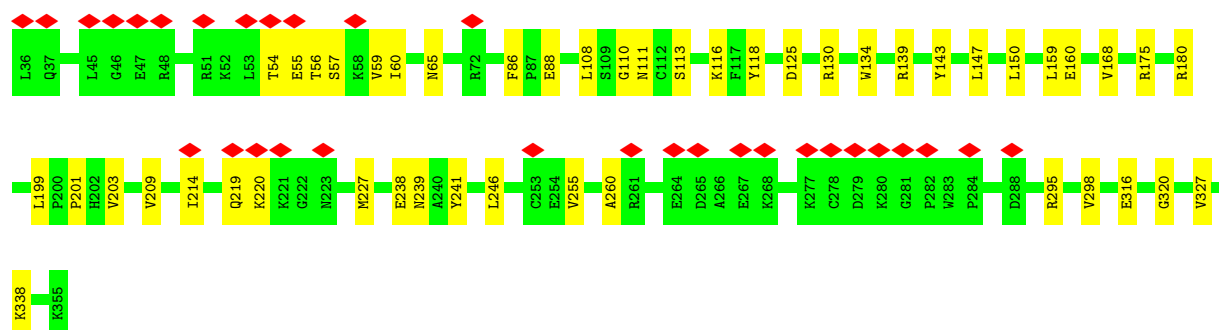
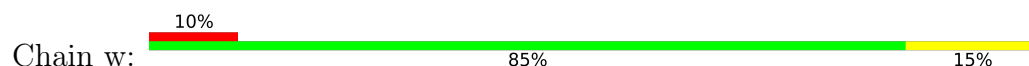




- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- 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	39380	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	0.242	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	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: 970, FMN, 8Q1, 2MR, ADP, ZN, UQ, PEE, NDP, MG, SF4, CDL, FES, PLX

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/3400	0.35	0/4596
2	B	0.19	0/1423	0.39	0/1930
3	C	0.23	0/1278	0.45	0/1729
4	E	0.15	0/995	0.35	0/1340
5	F	0.20	0/698	0.44	0/940
6	G	0.15	0/702	0.41	0/952
6	X	0.12	0/711	0.28	0/963
7	H	0.17	0/929	0.39	0/1258
8	I	0.14	0/798	0.35	0/1079
9	J	0.16	0/2828	0.36	2/3834 (0.1%)
10	K	0.12	0/377	0.27	0/509
11	L	0.16	0/1039	0.34	0/1403
12	M	0.16	0/5380	0.36	0/7290
13	N	0.12	0/1245	0.31	0/1694
14	O	0.15	0/1711	0.36	0/2328
15	P	0.18	0/1789	0.37	0/2436
16	Q	0.22	0/3528	0.44	1/4784 (0.0%)
17	S	0.15	0/581	0.39	0/781
18	T	0.12	0/755	0.28	0/1018
19	U	0.12	0/660	0.28	0/908
20	V	0.13	0/1042	0.26	0/1411
21	W	0.19	0/1198	0.43	0/1617
22	Y	0.13	0/610	0.31	0/836
23	Z	0.11	0/660	0.28	0/892
24	a	0.13	0/1184	0.30	0/1603
25	b	0.16	0/844	0.38	0/1149
26	c	0.13	0/1371	0.32	0/1875
27	d	0.14	0/1494	0.29	0/2015
28	e	0.13	0/891	0.29	0/1210
29	f	0.11	0/385	0.25	0/522
30	g	0.14	0/1031	0.31	0/1394
31	h	0.14	0/889	0.31	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.17	0/2773	0.35	0/3768
33	j	0.27	0/938	0.64	2/1281 (0.2%)
34	k	0.18	0/759	0.40	0/1029
35	l	0.16	0/4947	0.34	0/6728
36	m	0.22	0/1323	0.52	2/1797 (0.1%)
37	n	0.14	0/491	0.29	0/663
38	o	0.14	0/1092	0.31	0/1481
39	p	0.16	0/1590	0.34	0/2155
40	r	0.17	0/3723	0.34	0/5078
41	s	0.24	0/2571	0.61	7/3517 (0.2%)
42	u	0.14	0/1436	0.34	0/1938
43	v	0.12	0/1052	0.35	2/1411 (0.1%)
44	w	0.14	0/2642	0.30	0/3579
All	All	0.17	0/67763	0.37	16/91911 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	s	277	TYR	CA-C-N	10.70	130.66	119.85
41	s	277	TYR	C-N-CA	10.70	130.66	119.85
41	s	276	SER	N-CA-C	8.35	120.39	111.28
36	m	23	LYS	CA-C-N	6.95	128.53	119.84
36	m	23	LYS	C-N-CA	6.95	128.53	119.84
33	j	49	LEU	CA-C-N	6.37	126.40	119.90
33	j	49	LEU	C-N-CA	6.37	126.40	119.90
16	Q	197	MET	N-CA-C	6.26	118.10	111.28
9	J	267	GLY	CA-C-N	5.85	125.54	119.05
9	J	267	GLY	C-N-CA	5.85	125.54	119.05
41	s	277	TYR	N-CA-C	5.69	118.99	109.09
41	s	59	GLU	CA-C-N	5.39	126.57	119.84
41	s	59	GLU	C-N-CA	5.39	126.57	119.84
43	v	51	LEU	CA-C-N	5.25	133.38	122.41
43	v	51	LEU	C-N-CA	5.25	133.38	122.41
41	s	273	ILE	N-CA-C	5.05	115.82	110.72

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	3324	0	3281	63	0
2	B	1392	0	1323	41	0
3	C	1247	0	1251	48	0
4	E	971	0	975	16	0
5	F	687	0	700	15	0
6	G	690	0	669	17	0
6	X	699	0	682	12	0
7	H	910	0	950	14	0
8	I	780	0	808	20	0
9	J	2751	0	2773	47	0
10	K	366	0	338	11	0
11	L	1016	0	1016	22	0
12	M	5292	0	5322	76	0
13	N	1204	0	1162	21	0
14	O	1671	0	1673	19	0
15	P	1738	0	1693	28	0
16	Q	3450	0	3380	96	0
17	S	566	0	561	22	0
18	T	741	0	702	7	0
19	U	639	0	631	9	0
20	V	1021	0	1025	9	0
21	W	1167	0	1155	28	0
22	Y	584	0	529	11	0
23	Z	641	0	620	6	0
24	a	1151	0	1164	10	0
25	b	819	0	835	21	0
26	c	1315	0	1208	16	0
27	d	1461	0	1429	22	0
28	e	867	0	817	12	0
29	f	377	0	353	4	0
30	g	1000	0	994	15	0
31	h	867	0	871	14	0
32	i	2710	0	2874	48	0
33	j	914	0	951	60	0
34	k	748	0	799	34	0
35	l	4816	0	4955	94	0
36	m	1290	0	1256	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	n	479	0	486	8	0
38	o	1062	0	1072	22	0
39	p	1534	0	1470	33	0
40	r	3631	0	3839	61	0
41	s	2498	0	2592	113	0
42	u	1398	0	1374	21	0
43	v	1028	0	982	15	0
44	w	2582	0	2536	30	0
45	A	8	0	0	2	0
45	B	16	0	0	0	0
45	C	8	0	0	3	0
45	M	16	0	0	0	0
46	A	31	0	19	5	0
47	B	51	0	82	7	0
47	W	41	0	59	3	0
47	j	51	0	82	3	0
47	l	136	0	200	10	0
47	r	51	0	82	5	0
47	s	47	0	71	11	0
48	C	52	0	88	10	0
48	a	52	0	88	2	0
48	e	52	0	88	6	0
48	g	52	0	88	7	0
48	j	52	0	88	2	0
48	r	52	0	88	5	0
49	C	29	0	0	0	0
50	G	35	0	0	1	0
50	X	35	0	0	1	0
51	J	48	0	24	3	0
52	J	33	0	39	4	0
52	s	38	0	47	7	0
53	M	4	0	0	0	0
53	O	4	0	0	1	0
54	M	1	0	0	0	0
55	S	51	0	46	15	0
55	V	194	0	294	15	0
55	a	100	0	156	3	0
55	l	199	0	307	18	0
55	n	55	0	54	1	0
55	r	99	0	151	4	0
56	T	1	0	0	0	0
57	w	27	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	67815	0	68328	1140	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 (1140) 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)
51:J:401:NDP:O4D	51:J:401:NDP:C4D	1.68	1.20
33:j:27:LEU:CD2	41:s:60:PRO:HD2	1.73	1.18
33:j:27:LEU:HD21	41:s:60:PRO:HD2	1.17	1.13
11:L:78:ARG:NH2	12:M:249:GLU:HG3	1.64	1.12
36:m:55:MET:HE3	36:m:55:MET:HA	1.30	1.09
6:G:69:SER:N	16:Q:57:GLU:HB3	1.74	1.03
41:s:85:MET:HE1	41:s:108:MET:HB3	1.40	1.01
38:o:30:ARG:NE	39:p:9:TYR:CE2	2.28	1.00
48:C:302:PLX:H362	48:C:302:PLX:H322	1.44	0.98
3:C:59:ARG:HH21	3:C:185:LYS:HB2	1.25	0.97
33:j:48:ARG:HG3	36:m:78:MET:O	1.63	0.97
33:j:27:LEU:HD21	41:s:60:PRO:CD	1.94	0.96
33:j:27:LEU:HD23	41:s:59:GLU:HB2	1.46	0.96
16:Q:79:ASN:ND2	16:Q:107:ARG:HG3	1.81	0.95
11:L:78:ARG:HH22	12:M:249:GLU:HG3	1.21	0.94
33:j:73:LEU:HD12	36:m:55:MET:SD	2.08	0.93
1:A:398:ARG:HG2	1:A:403:ASP:HB2	1.49	0.93
3:C:59:ARG:NH2	3:C:185:LYS:HB2	1.85	0.91
3:C:61:SER:O	41:s:54:LYS:HE2	1.70	0.91
16:Q:79:ASN:HD22	16:Q:107:ARG:HG3	1.34	0.91
41:s:200:LEU:HD21	41:s:280:PHE:O	1.70	0.90
33:j:38:GLU:OE2	33:j:43:PRO:HA	1.72	0.89
33:j:48:ARG:HB3	36:m:78:MET:HA	1.54	0.89
34:k:21:MET:O	36:m:23:LYS:HE2	1.71	0.88
48:C:302:PLX:H171	48:C:302:PLX:H212	1.54	0.88
36:m:55:MET:HA	36:m:55:MET:CE	2.04	0.88
4:E:99:GLN:HE22	33:j:42:ASP:H	1.21	0.87
46:A:502:FMN:N1	46:A:502:FMN:O3'	2.08	0.86
38:o:30:ARG:NE	39:p:9:TYR:CD2	2.44	0.85
6:G:69:SER:HA	16:Q:57:GLU:HA	1.59	0.85
35:l:383:MET:HE3	35:l:384:PRO:HD2	1.59	0.85
8:I:25:GLN:HE22	41:s:33:LEU:HD22	1.42	0.84
41:s:56:PHE:CG	47:s:401:PEE:H77	2.13	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:69:SER:N	16:Q:57:GLU:CB	2.39	0.84
3:C:125:PRO:HG2	41:s:58:LYS:HE2	1.59	0.81
2:B:77:LEU:HA	41:s:30:TYR:O	1.81	0.81
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.16	0.80
7:H:7:LYS:HG3	7:H:8:THR:HG23	1.63	0.80
41:s:117:LEU:HD21	41:s:136:VAL:HG23	1.62	0.80
38:o:30:ARG:CZ	39:p:9:TYR:CD2	2.65	0.80
1:A:87:GLY:HA3	46:A:502:FMN:O2P	1.80	0.79
3:C:50:LEU:O	3:C:54:VAL:HG23	1.83	0.78
39:p:16:VAL:HG22	39:p:64:LEU:HD13	1.66	0.77
3:C:117:LEU:HD12	3:C:117:LEU:O	1.83	0.77
35:l:190:LEU:HD23	40:r:383:THR:HG21	1.67	0.77
36:m:34:ILE:HD11	41:s:114:TYR:CE2	2.21	0.77
41:s:277:TYR:CB	41:s:278:PRO:HD2	2.15	0.76
33:j:48:ARG:CB	36:m:78:MET:HA	2.16	0.76
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.67	0.76
40:r:237:LYS:HD2	40:r:316:MET:HB3	1.68	0.76
33:j:33:LYS:CD	41:s:61:LEU:HD21	2.15	0.76
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.68	0.75
47:W:201:PEE:H58	41:s:108:MET:HE1	1.69	0.75
3:C:56:TRP:HZ3	41:s:53:LEU:HD12	1.50	0.75
35:l:363:TYR:HA	35:l:370:THR:HG21	1.67	0.74
1:A:100:SER:O	1:A:103:ASN:N	2.20	0.74
41:s:277:TYR:HB3	41:s:278:PRO:HD2	1.68	0.74
32:i:236:LYS:HG3	32:i:237:MET:HG3	1.69	0.74
1:A:152:ARG:NH2	10:K:99:PRO:O	2.21	0.73
4:E:99:GLN:NE2	33:j:42:ASP:H	1.86	0.73
9:J:49:SER:OG	15:P:225:GLU:HG2	1.88	0.73
33:j:20:ILE:HG21	47:s:401:PEE:C43	2.18	0.73
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.70	0.73
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.71	0.73
16:Q:92:HIS:NE2	16:Q:193:ASP:OD2	2.20	0.73
3:C:59:ARG:NH2	3:C:185:LYS:CB	2.51	0.73
33:j:20:ILE:HG21	47:s:401:PEE:H70	1.71	0.73
41:s:66:SER:HB2	41:s:122:ALA:O	1.88	0.73
3:C:158:PRO:HB2	9:J:92:MET:HE3	1.71	0.72
32:i:207:ILE:HG22	32:i:211:MET:HE2	1.72	0.72
33:j:47:ALA:HB3	41:s:124:ASN:OD1	1.89	0.72
17:S:1:MET:HE2	55:S:101:CDL:HA22	1.70	0.72
48:C:302:PLX:H322	48:C:302:PLX:C36	2.19	0.72
2:B:47:SER:O	2:B:56:ARG:NH2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:n:26:TYR:HH	37:n:30:ARG:HH21	1.36	0.72
35:l:295:GLN:O	35:l:425:ARG:NH1	2.22	0.72
17:S:1:MET:HG3	55:S:101:CDL:HA21	1.70	0.72
1:A:60:GLY:HA2	14:O:241:PRO:HA	1.72	0.71
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.23	0.71
18:T:79:VAL:HG11	18:T:84:ILE:HD13	1.73	0.71
33:j:67:LEU:HD21	34:k:68:ALA:HB2	1.73	0.71
11:L:123:ASN:OD1	12:M:246:ARG:NH2	2.24	0.70
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.73	0.70
33:j:33:LYS:HD3	41:s:61:LEU:HD21	1.72	0.70
44:w:57:SER:HB3	44:w:150:LEU:HD11	1.72	0.70
3:C:92:VAL:HG11	52:s:402:UQ:H103	1.73	0.70
35:l:473:PRO:HG2	35:l:475:MET:HE2	1.73	0.70
1:A:385:CYS:HB3	45:A:501:SF4:S2	2.30	0.70
1:A:100:SER:O	1:A:102:MET:N	2.24	0.70
9:J:344:PRO:HG2	9:J:347:LEU:HD13	1.74	0.69
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.74	0.69
41:s:85:MET:HB3	41:s:233:MET:HG3	1.74	0.69
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.75	0.69
32:i:49:ASN:O	32:i:52:ALA:N	2.26	0.69
8:I:25:GLN:NE2	41:s:33:LEU:HD22	2.07	0.69
16:Q:185:MET:HE3	16:Q:189:THR:HG21	1.75	0.68
17:S:7:PRO:HG3	55:S:101:CDL:C75	2.24	0.68
1:A:43:THR:HG21	14:O:238:PRO:HB3	1.75	0.68
38:o:30:ARG:CZ	39:p:9:TYR:HD2	2.05	0.67
8:I:25:GLN:NE2	41:s:33:LEU:CD2	2.57	0.67
9:J:192:ARG:NH1	9:J:198:ALA:O	2.27	0.67
33:j:73:LEU:CD1	36:m:55:MET:HE1	2.24	0.67
2:B:200:GLU:HG3	13:N:88:ARG:HD3	1.76	0.67
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.77	0.67
16:Q:294:ARG:NH2	16:Q:401:GLU:OE2	2.28	0.67
5:F:24:CYS:HA	5:F:58:CYS:HB3	1.77	0.67
2:B:70:LEU:HD23	41:s:276:SER:OG	1.95	0.66
36:m:52:LEU:O	36:m:56:VAL:HG12	1.95	0.66
1:A:80:VAL:HG11	1:A:95:THR:HG22	1.76	0.66
1:A:159:ARG:NH2	14:O:176:CYS:O	2.28	0.66
16:Q:79:ASN:HB3	16:Q:101:LEU:O	1.96	0.66
33:j:20:ILE:HG21	47:s:401:PEE:C42	2.25	0.66
4:E:101:THR:O	4:E:105:ARG:HG3	1.95	0.66
30:g:56:VAL:HG21	40:r:17:MET:HE1	1.78	0.66
33:j:18:VAL:HG11	41:s:76:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ARG:CG	1:A:403:ASP:HB2	2.24	0.66
11:L:105:GLU:HA	12:M:611:THR:HG21	1.77	0.66
33:j:67:LEU:CD2	34:k:68:ALA:HB2	2.26	0.66
17:S:3:PHE:HB3	55:S:101:CDL:OA9	1.97	0.65
4:E:37:ARG:NH2	6:G:123:GLU:OE2	2.29	0.65
12:M:161:GLU:OE2	14:O:42:ARG:NH2	2.29	0.65
16:Q:80:LEU:HD12	41:s:126:LYS:HD3	1.78	0.65
21:W:121:MET:HE2	21:W:136:ALA:HB1	1.78	0.65
24:a:152:LYS:HD3	30:g:96:VAL:HG21	1.79	0.65
2:B:184:LEU:HB3	11:L:112:MET:HE2	1.78	0.65
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.29	0.65
12:M:308:ARG:NH2	12:M:578:PRO:O	2.30	0.65
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.29	0.65
38:o:30:ARG:HE	39:p:9:TYR:HE2	1.41	0.65
47:l:704:PEE:H28	47:l:704:PEE:H73	1.79	0.65
41:s:56:PHE:CD2	47:s:401:PEE:H77	2.32	0.65
44:w:54:THR:HG23	44:w:56:THR:HG22	1.79	0.65
41:s:195:ARG:HD3	41:s:231:ILE:HD11	1.78	0.65
16:Q:144:MET:HE3	16:Q:222:MET:HB2	1.78	0.65
16:Q:193:ASP:O	41:s:205:SER:HB3	1.97	0.64
36:m:72:THR:HG21	41:s:133:LEU:HD21	1.79	0.64
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.78	0.64
1:A:52:ARG:HH21	10:K:77:GLN:HG2	1.62	0.64
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.31	0.64
9:J:188:GLU:HG3	9:J:200:ILE:HD13	1.78	0.64
12:M:94:MET:HE2	12:M:100:TRP:HH2	1.63	0.64
33:j:67:LEU:CD2	34:k:68:ALA:CB	2.75	0.64
55:l:703:CDL:H431	55:l:703:CDL:H642	1.80	0.64
16:Q:55:THR:HG22	16:Q:57:GLU:H	1.61	0.64
47:l:704:PEE:H68	47:l:704:PEE:H22	1.79	0.64
7:H:70:GLU:OE2	8:I:103:ARG:NH2	2.31	0.64
16:Q:185:MET:HE3	16:Q:189:THR:CG2	2.27	0.64
38:o:75:ASN:O	38:o:79:ASN:ND2	2.31	0.63
9:J:71:ASN:HB2	9:J:97:MET:HE2	1.80	0.63
17:S:1:MET:HG3	55:S:101:CDL:CA2	2.27	0.63
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.79	0.63
3:C:59:ARG:HH21	3:C:185:LYS:CB	2.08	0.63
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.80	0.63
13:N:2:GLU:HG3	13:N:4:VAL:HG12	1.80	0.63
12:M:406:ASN:ND2	12:M:688:GLN:O	2.30	0.63
38:o:118:GLU:O	38:o:120:LYS:NZ	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:85:GLY:O	33:j:39:CYS:HB2	1.98	0.63
35:l:10:THR:HA	35:l:13:THR:HG22	1.79	0.63
16:Q:270:ASN:HB3	41:s:284:GLN:NE2	2.14	0.62
25:b:14:GLN:HE22	39:p:157:ALA:HB3	1.62	0.62
48:C:302:PLX:H212	48:C:302:PLX:C17	2.29	0.62
7:H:9:THR:O	7:H:76:GLN:NE2	2.31	0.62
33:j:73:LEU:N	33:j:74:PRO:HD2	2.14	0.62
4:E:84:ILE:HG22	4:E:88:MET:HE3	1.80	0.62
16:Q:85:GLY:O	33:j:39:CYS:CB	2.48	0.62
44:w:168:VAL:HG21	44:w:241:TYR:CE1	2.35	0.62
1:A:98:LYS:NZ	1:A:242:VAL:O	2.28	0.62
1:A:40:ARG:NH1	1:A:289:GLU:O	2.33	0.62
17:S:3:PHE:HE2	55:S:101:CDL:OA3	1.82	0.62
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.82	0.62
4:E:64:ARG:NH1	6:G:117:GLU:OE2	2.33	0.62
40:r:337:VAL:HG11	40:r:345:ALA:HB2	1.81	0.61
1:A:222:LYS:O	11:L:175:LYS:NZ	2.31	0.61
6:X:117:GLU:OE2	39:p:45:ARG:NH1	2.33	0.61
39:p:105:ASP:OD1	39:p:122:ARG:NH1	2.32	0.61
14:O:38:LEU:O	14:O:124:ARG:NH2	2.33	0.61
6:X:136:GLU:OE2	39:p:18:ARG:NH1	2.33	0.61
1:A:127:ASP:O	1:A:131:ILE:HG12	2.00	0.61
36:m:23:LYS:N	36:m:24:PRO:HD3	2.15	0.61
41:s:200:LEU:HD23	41:s:279:ARG:HD3	1.82	0.61
3:C:92:VAL:HG21	52:s:402:UQ:C10	2.31	0.61
48:C:302:PLX:H171	48:C:302:PLX:C21	2.26	0.61
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.83	0.61
32:i:270:MET:HE3	32:i:279:PRO:HG3	1.81	0.61
35:l:495:ILE:HG22	35:l:499:MET:HE2	1.81	0.61
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.81	0.61
40:r:231:LEU:HD23	40:r:235:LEU:HD12	1.81	0.61
16:Q:202:TRP:HE1	41:s:32:GLN:HA	1.65	0.61
34:k:31:LEU:HD21	36:m:67:VAL:HG11	1.83	0.61
38:o:59:VAL:HG22	40:r:423:ILE:HG12	1.83	0.61
35:l:577:VAL:O	35:l:580:GLN:NE2	2.29	0.61
35:l:419:THR:HA	35:l:422:TYR:CE2	2.36	0.60
36:m:23:LYS:HB2	36:m:23:LYS:NZ	2.16	0.60
2:B:111:GLU:O	2:B:141:ARG:NH1	2.35	0.60
12:M:59:GLN:HE21	12:M:62:ARG:HH12	1.48	0.60
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.28	0.60
27:d:101:GLU:OE2	28:e:115:GLN:NE2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:h:18:MET:HE3	34:k:56:ALA:HA	1.82	0.60
44:w:116:LYS:NZ	44:w:125:ASP:OD2	2.34	0.60
22:Y:97:LEU:HB3	43:v:104:ARG:HB2	1.82	0.60
12:M:224:ASP:OD2	12:M:291:ARG:NH1	2.35	0.60
30:g:4:MET:O	30:g:10:ARG:NH1	2.33	0.60
9:J:76:MET:HE1	9:J:254:LYS:HD3	1.83	0.60
12:M:472:PRO:O	12:M:510:TRP:NE1	2.29	0.60
16:Q:77:VAL:O	16:Q:77:VAL:HG23	2.00	0.60
33:j:20:ILE:HG21	47:s:401:PEE:H73	1.83	0.60
33:j:20:ILE:CG2	47:s:401:PEE:H70	2.32	0.60
36:m:28:TYR:CZ	36:m:82:VAL:HG12	2.37	0.60
11:L:78:ARG:NH2	12:M:249:GLU:CG	2.54	0.60
42:u:152:PRO:O	42:u:153:GLU:HG2	2.02	0.60
55:S:101:CDL:H512	55:S:101:CDL:H722	1.83	0.60
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.35	0.60
20:V:44:LYS:NZ	55:V:201:CDL:OB4	2.33	0.60
43:v:51:LEU:O	43:v:52:MET:HG3	2.01	0.60
9:J:317:ASP:OD2	9:J:321:ARG:NH1	2.34	0.59
7:H:9:THR:HG23	7:H:16:VAL:HG22	1.84	0.59
1:A:394:LYS:NZ	12:M:156:GLY:O	2.34	0.59
5:F:20:ARG:HB2	5:F:66:TRP:HB2	1.85	0.59
13:N:68:MET:HG3	13:N:69:ASN:H	1.67	0.59
40:r:370:PRO:HG3	40:r:375:LEU:HD22	1.84	0.59
16:Q:80:LEU:CD1	41:s:126:LYS:HD3	2.31	0.59
20:V:17:GLU:OE1	20:V:20:ARG:NH1	2.31	0.59
25:b:80:TRP:CD1	27:d:41:VAL:HG23	2.37	0.59
25:b:80:TRP:HD1	27:d:41:VAL:HG23	1.68	0.59
37:n:47:ARG:NH2	37:n:53:GLU:OE2	2.36	0.59
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	1.85	0.59
17:S:12:MET:HE3	41:s:20:LEU:HB2	1.84	0.59
41:s:221:ALA:O	41:s:225:MET:HG3	2.03	0.59
12:M:217:GLU:HG2	12:M:218:LEU:HG	1.85	0.58
21:W:85:GLN:O	21:W:89:GLU:HG3	2.03	0.58
33:j:63:LEU:HD21	36:m:63:GLY:HA2	1.85	0.58
2:B:63:TRP:CE3	47:B:303:PEE:H62	2.37	0.58
5:F:68:ARG:NH2	12:M:364:ASP:OD2	2.36	0.58
41:s:77:LEU:HD23	41:s:115:SER:HB3	1.85	0.58
46:A:502:FMN:HO3'	46:A:502:FMN:C2	2.12	0.58
16:Q:104:GLU:HB2	41:s:282:TYR:OH	2.04	0.58
27:d:114:GLN:HG3	35:l:203:MET:HG2	1.84	0.58
35:l:286:LEU:HD22	35:l:411:MET:SD	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:191:ARG:HB3	3:C:195:ARG:HH12	1.69	0.58
3:C:191:ARG:HB3	3:C:195:ARG:NH1	2.18	0.58
17:S:3:PHE:CD1	55:S:101:CDL:H531	2.39	0.58
39:p:19:LEU:HD12	39:p:19:LEU:O	2.03	0.58
44:w:118:TYR:OH	57:w:401:ADP:O2'	2.22	0.58
17:S:3:PHE:CE2	55:S:101:CDL:OA3	2.57	0.58
24:a:134:GLU:OE1	37:n:57:TRP:NE1	2.23	0.58
40:r:312:ALA:O	40:r:316:MET:HG3	2.04	0.58
48:a:202:PLX:H92	40:r:40:SER:HB3	1.85	0.58
25:b:9:LYS:HG2	25:b:13:GLN:HE22	1.69	0.58
36:m:26:PRO:HB2	36:m:71:THR:HG21	1.86	0.58
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.85	0.58
16:Q:95:LEU:HB2	16:Q:458:PHE:CE2	2.39	0.57
22:Y:97:LEU:HD12	43:v:107:ARG:HH21	1.69	0.57
34:k:23:ARG:NH1	36:m:81:GLU:OE1	2.36	0.57
39:p:151:THR:HG22	39:p:153:ALA:H	1.69	0.57
9:J:306:GLU:HG2	9:J:315:THR:HG22	1.86	0.57
13:N:117:VAL:O	13:N:120:THR:OG1	2.22	0.57
30:g:13:LEU:HA	48:g:201:PLX:H32	1.87	0.57
43:v:27:PRO:O	43:v:34:ARG:NH1	2.37	0.57
6:G:80:LYS:HE2	6:G:100:VAL:HG21	1.86	0.57
44:w:111:ASN:O	44:w:130:ARG:HD2	2.04	0.57
1:A:217:GLU:OE2	1:A:224:ARG:NH2	2.37	0.57
2:B:148:ASP:HB3	2:B:151:LYS:HB2	1.86	0.57
21:W:98:MET:HE3	31:h:79:ILE:HD13	1.84	0.57
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.38	0.57
16:Q:83:ASN:O	41:s:127:TYR:OH	2.21	0.57
21:W:84:LEU:HD12	42:u:57:LEU:HD21	1.87	0.57
35:l:128:MET:HE1	35:l:252:MET:HA	1.87	0.57
44:w:168:VAL:HG21	44:w:241:TYR:HE1	1.70	0.57
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.86	0.57
15:P:69:LEU:HD22	15:P:96:VAL:HG22	1.86	0.57
40:r:307:TRP:HA	40:r:310:MET:HE2	1.86	0.57
35:l:359:MET:O	35:l:436:ARG:NH2	2.38	0.56
2:B:61:LEU:HD21	19:U:18:VAL:HG22	1.87	0.56
3:C:92:VAL:HG21	52:s:402:UQ:H103	1.87	0.56
14:O:150:GLU:OE2	14:O:150:GLU:N	2.38	0.56
17:S:3:PHE:CD2	55:S:101:CDL:HA61	2.40	0.56
12:M:388:ASN:ND2	12:M:513:MET:O	2.38	0.56
30:g:52:ARG:NH2	44:w:338:LYS:O	2.38	0.56
1:A:50:ASP:O	1:A:59:ARG:NH2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:TRP:HE3	47:B:303:PEE:H62	1.70	0.56
3:C:161:ILE:HG13	3:C:180:LEU:HB2	1.87	0.56
10:K:108:PRO:HG3	11:L:171:ARG:HD2	1.86	0.56
3:C:190:LEU:HD22	47:s:401:PEE:H13	1.88	0.56
8:I:14:TRP:NE1	21:W:28:ARG:NH2	2.54	0.56
9:J:310:PHE:HE1	47:s:401:PEE:H15	1.71	0.56
31:h:18:MET:HE1	34:k:59:MET:HB3	1.87	0.56
32:i:268:GLN:HA	40:r:165:VAL:HG11	1.87	0.56
9:J:133:GLU:OE1	9:J:321:ARG:NH2	2.39	0.56
12:M:389:THR:O	12:M:390:THR:OG1	2.21	0.56
16:Q:242:ASP:O	16:Q:246:GLU:HG2	2.06	0.56
3:C:103:MET:CE	3:C:117:LEU:HD11	2.36	0.56
2:B:73:THR:O	41:s:31:MET:HG2	2.06	0.56
5:F:24:CYS:CA	5:F:58:CYS:HB3	2.36	0.56
55:a:201:CDL:H751	28:e:103:SER:HB2	1.87	0.56
12:M:136:GLU:OE2	12:M:272:ARG:NH2	2.38	0.55
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.88	0.55
35:l:71:LEU:HD12	40:r:310:MET:HE1	1.87	0.55
9:J:49:SER:OG	15:P:225:GLU:CG	2.54	0.55
16:Q:457:VAL:HG13	16:Q:460:GLU:HG2	1.88	0.55
33:j:71:LEU:O	36:m:147:TYR:OH	2.22	0.55
36:m:68:PHE:CE1	41:s:117:LEU:HD22	2.41	0.55
5:F:65:LEU:HD11	5:F:91:LEU:HD21	1.87	0.55
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.87	0.55
39:p:9:TYR:CD1	39:p:9:TYR:N	2.73	0.55
16:Q:194:ILE:HG22	41:s:278:PRO:HB2	1.87	0.55
35:l:375:ILE:HD12	35:l:458:LEU:HD11	1.89	0.55
1:A:113:LEU:HD13	1:A:149:MET:HE1	1.87	0.55
3:C:59:ARG:HH22	3:C:185:LYS:HG3	1.71	0.55
6:G:135:ALA:HA	6:G:138:LEU:HD13	1.89	0.55
21:W:89:GLU:O	21:W:93:GLU:HG2	2.07	0.55
1:A:391:TRP:O	1:A:395:VAL:HG23	2.06	0.55
9:J:199:THR:OG1	9:J:258:ALA:O	2.22	0.55
40:r:403:THR:HA	40:r:406:TYR:CE2	2.41	0.55
1:A:263:ALA:HA	1:A:271:SER:HB3	1.87	0.55
1:A:100:SER:C	1:A:102:MET:N	2.65	0.55
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.88	0.55
48:C:302:PLX:C17	48:C:302:PLX:C21	2.85	0.55
6:G:138:LEU:HD23	6:G:144:ILE:HG12	1.88	0.55
12:M:390:THR:HA	12:M:600:GLU:HG2	1.87	0.55
38:o:45:ARG:HH12	39:p:144:THR:HG21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:127:VAL:HG23	40:r:128:PRO:HD3	1.89	0.55
25:b:103:ARG:NH1	43:v:49:ALA:O	2.41	0.54
35:l:327:LEU:O	35:l:331:MET:HG2	2.07	0.54
10:K:108:PRO:CG	11:L:171:ARG:HD2	2.37	0.54
11:L:158:LYS:NZ	12:M:69:LEU:O	2.35	0.54
14:O:111:ARG:NH1	14:O:114:GLU:OE2	2.40	0.54
55:l:703:CDL:H561	55:l:703:CDL:H342	1.89	0.54
40:r:201:MET:HE2	47:r:501:PEE:H77	1.88	0.54
1:A:185:ASN:C	1:A:187:CYS:H	2.16	0.54
32:i:252:GLY:HA3	32:i:290:LEU:HD13	1.89	0.54
40:r:185:PRO:HB3	40:r:252:PRO:HD3	1.87	0.54
16:Q:193:ASP:O	41:s:205:SER:CB	2.55	0.54
21:W:74:LEU:O	21:W:78:GLU:HG3	2.08	0.54
40:r:243:MET:HB3	40:r:301:ILE:HG21	1.88	0.54
3:C:63:TRP:CD2	41:s:54:LYS:NZ	2.76	0.54
35:l:55:MET:HE2	35:l:471:ASN:HB3	1.89	0.54
1:A:100:SER:O	1:A:101:PHE:C	2.48	0.54
4:E:119:LEU:HD11	12:M:628:GLU:HG2	1.89	0.54
1:A:67:GLU:O	1:A:71:LYS:HG2	2.08	0.54
30:g:15:PHE:O	30:g:16:LEU:HD22	2.07	0.54
40:r:420:THR:HB	40:r:423:ILE:HD12	1.90	0.54
24:a:66:ARG:HA	24:a:69:LYS:HE3	1.90	0.53
32:i:84:TRP:HH2	34:k:59:MET:HE3	1.73	0.53
33:j:27:LEU:HD22	41:s:60:PRO:HD2	1.82	0.53
47:r:501:PEE:H71	47:r:501:PEE:H34	1.90	0.53
41:s:178:SER:HB2	41:s:181:LEU:HD12	1.89	0.53
13:N:127:TYR:OH	18:T:61:GLU:O	2.22	0.53
16:Q:79:ASN:CB	16:Q:101:LEU:O	2.56	0.53
16:Q:179:ARG:NH2	16:Q:401:GLU:O	2.36	0.53
55:l:702:CDL:H822	55:l:702:CDL:H631	1.90	0.53
1:A:102:MET:SD	1:A:241:THR:OG1	2.60	0.53
35:l:515:TYR:OH	39:p:70:GLU:OE2	2.21	0.53
3:C:52:ASP:HB3	48:C:302:PLX:H251	1.90	0.53
9:J:323:HIS:O	9:J:323:HIS:CG	2.60	0.53
11:L:75:ARG:NH1	11:L:119:ASP:OD1	2.35	0.53
12:M:282:ASN:O	12:M:283:GLU:HG2	2.08	0.53
41:s:85:MET:HE1	41:s:108:MET:CB	2.25	0.53
8:I:40:LYS:HB3	21:W:7:LYS:H	1.73	0.53
12:M:285:TRP:HB2	12:M:413:LEU:HD11	1.90	0.53
21:W:40:ILE:HD13	21:W:40:ILE:N	2.24	0.53
33:j:73:LEU:HD12	36:m:55:MET:CE	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:367:CYS:HB2	12:M:533:GLY:O	2.09	0.53
32:i:128:LEU:HD12	32:i:216:PHE:HB3	1.91	0.53
36:m:26:PRO:HB2	36:m:71:THR:CG2	2.39	0.53
31:h:106:PRO:HG2	42:u:17:GLU:HB3	1.91	0.53
41:s:207:LEU:O	41:s:209:SER:N	2.41	0.53
3:C:71:CYS:HB3	45:C:301:SF4:S4	2.46	0.53
3:C:98:ARG:HA	3:C:125:PRO:HD3	1.90	0.53
27:d:137:LYS:NZ	27:d:141:ASP:OD2	2.42	0.53
44:w:246:LEU:HD22	44:w:255:VAL:HG11	1.90	0.53
12:M:476:LEU:HD21	12:M:481:LEU:HD21	1.91	0.52
3:C:59:ARG:NH2	3:C:185:LYS:CG	2.72	0.52
34:k:65:VAL:HG11	36:m:157:THR:HG23	1.90	0.52
35:l:227:PHE:O	35:l:230:HIS:ND1	2.42	0.52
3:C:117:LEU:HD12	3:C:117:LEU:C	2.34	0.52
16:Q:55:THR:CG2	16:Q:56:LYS:N	2.72	0.52
32:i:84:TRP:CH2	34:k:59:MET:HE3	2.44	0.52
34:k:23:ARG:HD3	36:m:23:LYS:O	2.09	0.52
39:p:9:TYR:N	39:p:9:TYR:HD1	2.06	0.52
42:u:83:THR:HA	42:u:86:TRP:CD1	2.43	0.52
39:p:139:GLN:NE2	39:p:156:PRO:O	2.36	0.52
16:Q:80:LEU:HD23	16:Q:101:LEU:HB2	1.91	0.52
16:Q:198:THR:HG23	41:s:32:GLN:HG2	1.91	0.52
27:d:115:GLN:HG2	35:l:62:ILE:HG12	1.90	0.52
48:g:201:PLX:H12	31:h:2:PRO:HD2	1.92	0.52
32:i:102:LEU:HD13	32:i:142:LEU:HG	1.92	0.52
33:j:67:LEU:HG	34:k:68:ALA:CB	2.39	0.52
32:i:268:GLN:NE2	32:i:272:LYS:HE3	2.25	0.52
36:m:20:PHE:CD1	36:m:20:PHE:C	2.88	0.52
41:s:281:ARG:NH1	41:s:283:ASP:OD1	2.42	0.52
33:j:63:LEU:O	33:j:67:LEU:HD23	2.10	0.52
34:k:38:LEU:HB2	36:m:60:TYR:CZ	2.45	0.52
40:r:306:PRO:HB3	40:r:458:LEU:HD12	1.92	0.52
43:v:22:MET:HE1	43:v:102:PHE:HA	1.92	0.52
27:d:10:TYR:OH	28:e:123:GLU:OE2	2.26	0.52
48:j:202:PLX:H341	48:j:202:PLX:H152	1.92	0.52
35:l:370:THR:HG22	35:l:431:PHE:CD1	2.45	0.52
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.92	0.52
3:C:184:ILE:O	3:C:187:GLU:HG2	2.10	0.52
35:l:233:LEU:HB3	35:l:234:PRO:HD3	1.92	0.52
42:u:77:HIS:CE1	42:u:115:LEU:HD21	2.45	0.52
1:A:185:ASN:OD1	1:A:190:GLY:N	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:87:LEU:O	10:K:91:VAL:HG23	2.10	0.52
17:S:28:LYS:O	17:S:33:GLY:N	2.43	0.52
27:d:140:GLN:O	27:d:144:SER:HB2	2.08	0.52
36:m:23:LYS:HB2	36:m:23:LYS:HZ2	1.74	0.52
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.45	0.52
41:s:102:VAL:HG23	41:s:160:TYR:O	2.09	0.52
42:u:157:ASP:OD1	42:u:158:LEU:N	2.43	0.52
24:a:139:ILE:HG23	40:r:54:LEU:HD23	1.92	0.51
32:i:79:LEU:HB2	34:k:47:ILE:HD13	1.92	0.51
6:G:141:PRO:HA	6:G:144:ILE:HD12	1.92	0.51
9:J:272:LEU:HD11	9:J:375:VAL:HG11	1.92	0.51
12:M:264:SER:HB2	12:M:272:ARG:HG2	1.92	0.51
36:m:28:TYR:CE2	36:m:82:VAL:HG12	2.46	0.51
2:B:81:PRO:HB3	41:s:34:ARG:C	2.35	0.51
9:J:222:TRP:HB3	52:J:402:UQ:H152	1.91	0.51
16:Q:85:GLY:C	33:j:39:CYS:HB3	2.35	0.51
1:A:185:ASN:O	1:A:187:CYS:N	2.44	0.51
3:C:95:ALA:HB1	41:s:208:VAL:HG13	1.91	0.51
10:K:73:TYR:CZ	10:K:75:ASN:HB3	2.45	0.51
11:L:114:TRP:HB3	15:P:228:GLN:HG3	1.93	0.51
2:B:79:ARG:NE	8:I:20:LEU:CD2	2.74	0.51
19:U:33:PRO:HA	41:s:310:MET:HG2	1.92	0.51
55:V:201:CDL:H661	35:l:594:THR:HG23	1.92	0.51
6:X:155:TYR:CD2	6:X:156:GLU:HG3	2.46	0.51
27:d:97:LYS:NZ	40:r:47:GLU:OE2	2.37	0.51
32:i:222:SER:O	32:i:224:ALA:N	2.44	0.51
35:l:538:THR:HA	47:l:704:PEE:H59	1.91	0.51
5:F:61:VAL:HG23	5:F:62:GLN:H	1.76	0.51
17:S:69:ILE:HD11	42:u:20:VAL:HG13	1.92	0.51
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.32	0.51
15:P:43:THR:HA	15:P:47:ILE:HD12	1.93	0.51
21:W:68:ARG:CZ	21:W:72:MET:HE2	2.41	0.51
26:c:153:TYR:OH	43:v:8:ARG:NH1	2.44	0.51
48:g:201:PLX:H233	32:i:207:ILE:HD13	1.92	0.51
36:m:34:ILE:CD1	41:s:114:TYR:CE2	2.94	0.51
1:A:267:ARG:HH12	1:A:341:ALA:HB2	1.76	0.51
22:Y:103:ASP:OD1	22:Y:103:ASP:N	2.42	0.51
12:M:388:ASN:HB3	12:M:511:LYS:HD3	1.92	0.51
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.92	0.51
18:T:51:ARG:HG2	18:T:54:ARG:HH21	1.76	0.51
55:V:202:CDL:H712	55:V:202:CDL:H521	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:60:ASN:HD22	35:l:433:GLY:H	1.58	0.51
32:i:100:MET:HE3	32:i:153:LEU:HD21	1.92	0.51
35:l:358:LYS:HG3	39:p:80:TYR:CE1	2.46	0.51
45:C:301:SF4:S2	16:Q:138:ARG:HG2	2.51	0.50
32:i:298:TYR:O	32:i:303:THR:OG1	2.29	0.50
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.46	0.50
40:r:130:LEU:HD22	40:r:150:LEU:HD13	1.92	0.50
40:r:373:ILE:HD11	40:r:444:LEU:HD23	1.93	0.50
47:r:501:PEE:H81	48:r:502:PLX:H393	1.93	0.50
1:A:44:ASN:HB3	1:A:134:ASP:OD1	2.12	0.50
4:E:24:ASP:OD2	4:E:26:ASN:ND2	2.43	0.50
2:B:77:LEU:HA	41:s:30:TYR:C	2.37	0.50
6:G:122:MET:HE3	6:G:144:ILE:HG21	1.93	0.50
9:J:37:HIS:CD2	9:J:40:LEU:HD12	2.46	0.50
44:w:180:ARG:NH1	44:w:316:GLU:OE2	2.44	0.50
11:L:109:ASN:ND2	11:L:111:LEU:O	2.41	0.50
16:Q:282:ASP:OD2	16:Q:437:LYS:NZ	2.39	0.50
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.47	0.50
55:l:702:CDL:H621	55:l:702:CDL:H432	1.93	0.50
1:A:129:GLU:HA	1:A:132:ARG:HG2	1.93	0.50
16:Q:208:GLU:OE2	16:Q:221:ARG:NH2	2.45	0.50
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.47	0.50
55:l:702:CDL:H371	40:r:369:LEU:HD23	1.94	0.50
44:w:219:GLN:NE2	44:w:227:MET:SD	2.85	0.50
8:I:14:TRP:CE2	21:W:28:ARG:NH2	2.80	0.50
37:n:26:TYR:OH	37:n:30:ARG:NH2	2.20	0.50
2:B:70:LEU:HG	41:s:277:TYR:OH	2.12	0.50
32:i:294:MET:HE2	40:r:130:LEU:HD21	1.94	0.50
35:l:362:LEU:HD22	35:l:366:MET:HE2	1.93	0.50
36:m:23:LYS:N	36:m:24:PRO:CD	2.75	0.50
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.25	0.50
9:J:293:LEU:HD23	9:J:298:TYR:HB2	1.94	0.50
16:Q:55:THR:HG22	16:Q:56:LYS:N	2.25	0.50
18:T:51:ARG:HG2	18:T:54:ARG:NH2	2.26	0.50
5:F:58:CYS:SG	5:F:59:SER:N	2.85	0.49
33:j:33:LYS:CG	41:s:61:LEU:HD11	2.42	0.49
55:a:201:CDL:H852	48:e:201:PLX:H232	1.94	0.49
34:k:76:SER:O	34:k:79:VAL:HG12	2.11	0.49
35:l:562:LEU:HB3	35:l:563:PRO:HD3	1.92	0.49
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.52	0.49
7:H:116:ILE:HD12	11:L:127:THR:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.94	0.49
5:F:25:GLN:HG2	5:F:26:ARG:HD3	1.94	0.49
32:i:153:LEU:HG	32:i:157:MET:HE2	1.94	0.49
34:k:28:SER:HB3	36:m:23:LYS:HG2	1.94	0.49
55:r:503:CDL:H332	55:r:503:CDL:H231	1.93	0.49
2:B:120:GLU:HB2	2:B:130:ILE:HD12	1.93	0.49
35:l:108:MET:CE	35:l:240:PRO:HB3	2.43	0.49
35:l:253:VAL:HB	35:l:310:LEU:HD11	1.94	0.49
1:A:210:THR:HB	1:A:224:ARG:H	1.76	0.49
38:o:30:ARG:CZ	39:p:9:TYR:CE2	2.92	0.49
39:p:64:LEU:O	39:p:68:GLU:HG2	2.12	0.49
2:B:60:THR:HG23	47:B:303:PEE:O1P	2.12	0.49
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.48	0.49
14:O:137:THR:O	14:O:141:MET:N	2.44	0.49
32:i:215:MET:HB2	32:i:251:MET:HE1	1.94	0.49
5:F:61:VAL:HG23	5:F:62:GLN:N	2.27	0.49
7:H:90:LEU:HB2	15:P:102:ASP:HB3	1.93	0.49
9:J:222:TRP:CD1	52:J:402:UQ:H101	2.48	0.49
33:j:65:PHE:HA	33:j:68:GLU:HG3	1.95	0.49
47:j:201:PEE:H26	41:s:295:PRO:HB3	1.93	0.49
36:m:164:GLY:O	36:m:168:ILE:HG12	2.13	0.49
40:r:221:VAL:HA	40:r:283:LYS:HD3	1.95	0.49
1:A:320:GLY:HA2	1:A:353:ALA:H	1.77	0.49
4:E:55:SER:HB2	9:J:367:GLU:OE2	2.13	0.49
6:X:120:MET:HE1	39:p:24:LEU:HB3	1.95	0.49
32:i:75:ILE:HD12	34:k:40:LEU:HD22	1.95	0.49
32:i:99:THR:HG22	32:i:157:MET:HE1	1.95	0.49
2:B:105:ARG:NH2	18:T:63:ASN:OD1	2.46	0.49
12:M:265:THR:HG22	12:M:270:VAL:HA	1.95	0.49
13:N:42:ASP:HB2	13:N:48:TYR:HE1	1.78	0.49
18:T:101:ASN:ND2	18:T:103:ASP:OD2	2.45	0.49
24:a:153:GLU:HG3	30:g:92:MET:HE2	1.95	0.49
32:i:170:LEU:HD23	32:i:292:PHE:HB3	1.93	0.49
32:i:246:VAL:HG21	55:r:503:CDL:H362	1.95	0.49
35:l:69:MET:HE2	35:l:76:LEU:HD12	1.95	0.49
42:u:59:GLU:N	42:u:59:GLU:OE1	2.46	0.49
1:A:35:LEU:HD21	1:A:290:GLU:HA	1.95	0.48
1:A:80:VAL:CG1	1:A:95:THR:HG22	2.42	0.48
13:N:3:LEU:O	13:N:7:LEU:HG	2.13	0.48
20:V:40:SER:HA	55:V:201:CDL:HB61	1.95	0.48
55:V:201:CDL:H512	35:l:576:MET:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:68:MET:HE1	34:k:37:MET:SD	2.53	0.48
33:j:73:LEU:N	33:j:74:PRO:CD	2.75	0.48
35:l:27:TYR:O	35:l:115:ASN:ND2	2.44	0.48
35:l:599:MET:O	35:l:603:ASN:HB3	2.13	0.48
40:r:329:LEU:O	40:r:332:THR:OG1	2.28	0.48
9:J:168:SER:OG	9:J:169:HIS:N	2.46	0.48
12:M:419:ARG:NH1	12:M:439:THR:O	2.46	0.48
15:P:214:ASP:O	15:P:217:LYS:NZ	2.44	0.48
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.48	0.48
8:I:42:PRO:HB3	21:W:6:VAL:HG21	1.96	0.48
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.96	0.48
41:s:14:LEU:HD21	41:s:83:LEU:HD21	1.94	0.48
48:C:302:PLX:H221	48:C:302:PLX:H172	1.94	0.48
12:M:49:VAL:HG13	12:M:102:ILE:HD13	1.95	0.48
14:O:149:LEU:O	14:O:153:GLN:HG2	2.13	0.48
16:Q:397:TYR:OH	16:Q:406:GLU:OE2	2.27	0.48
21:W:93:GLU:O	21:W:97:ILE:HD12	2.13	0.48
21:W:121:MET:HE3	36:m:130:THR:HB	1.96	0.48
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.96	0.48
3:C:99:GLN:NE2	41:s:212:ASN:O	2.47	0.48
12:M:466:LEU:HD13	12:M:500:ILE:HD11	1.94	0.48
25:b:10:LEU:O	25:b:14:GLN:HG3	2.14	0.48
48:e:201:PLX:H202	55:l:702:CDL:H812	1.95	0.48
48:g:201:PLX:H232	32:i:210:THR:HG21	1.95	0.48
33:j:53:MET:HE3	33:j:56:PHE:HA	1.94	0.48
8:I:69:VAL:O	15:P:76:VAL:HB	2.14	0.48
55:V:202:CDL:H732	38:o:87:SER:HB3	1.95	0.48
21:W:94:GLU:HG2	31:h:79:ILE:HD12	1.96	0.48
41:s:174:MET:HB3	41:s:242:PHE:HA	1.94	0.48
5:F:65:LEU:HB2	5:F:79:LEU:HD11	1.95	0.48
32:i:265:MET:HE2	32:i:343:LEU:HD21	1.96	0.48
35:l:373:LEU:HD22	35:l:431:PHE:HE2	1.78	0.48
41:s:144:VAL:O	41:s:148:ILE:HD12	2.13	0.48
41:s:186:PHE:O	41:s:189:THR:OG1	2.31	0.48
2:B:53:VAL:HG13	19:U:14:ALA:HA	1.94	0.48
32:i:72:MET:HE2	34:k:12:PHE:CG	2.49	0.48
33:j:38:GLU:OE2	33:j:43:PRO:CA	2.55	0.48
33:j:93:PHE:CZ	33:j:97:LEU:HD11	2.48	0.48
48:r:502:PLX:H101	48:r:502:PLX:H72	1.51	0.48
44:w:54:THR:O	44:w:55:GLU:HG3	2.14	0.48
12:M:340:ALA:HB3	12:M:366:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:65:VAL:HG11	15:P:86:ILE:HD13	1.96	0.48
16:Q:85:GLY:O	33:j:39:CYS:HB3	2.13	0.48
17:S:3:PHE:HD2	55:S:101:CDL:HA61	1.78	0.48
55:S:101:CDL:H711	41:s:43:TYR:OH	2.13	0.48
21:W:68:ARG:O	21:W:72:MET:HG3	2.14	0.48
22:Y:76:ASP:O	35:l:385:TYR:OH	2.21	0.48
24:a:163:ARG:NH1	30:g:102:ASP:OD2	2.44	0.48
35:l:190:LEU:HD21	40:r:307:TRP:CH2	2.49	0.48
42:u:80:GLU:HB2	42:u:81:PRO:HD3	1.95	0.48
1:A:102:MET:O	1:A:111:LYS:NZ	2.42	0.47
26:c:60:GLU:OE1	26:c:60:GLU:N	2.47	0.47
55:l:703:CDL:H612	55:l:703:CDL:H641	1.62	0.47
37:n:50:ARG:HB2	37:n:53:GLU:HG2	1.96	0.47
12:M:501:ARG:HH12	12:M:666:GLN:HB3	1.79	0.47
15:P:173:MET:HE3	15:P:188:LEU:HB2	1.96	0.47
26:c:71:GLY:HA2	38:o:79:ASN:HB2	1.95	0.47
33:j:67:LEU:HD21	34:k:68:ALA:CB	2.40	0.47
35:l:108:MET:HE3	35:l:240:PRO:HB3	1.94	0.47
35:l:313:MET:HG3	35:l:328:HIS:HD2	1.79	0.47
55:l:703:CDL:H351	55:l:703:CDL:H382	1.50	0.47
43:v:12:ASP:OD1	43:v:14:SER:OG	2.30	0.47
44:w:86:PHE:HB2	44:w:159:LEU:HD23	1.96	0.47
12:M:354:LEU:HD22	12:M:548:LEU:HD22	1.96	0.47
35:l:78:LEU:HD11	55:l:702:CDL:H261	1.96	0.47
48:r:502:PLX:H122	48:r:502:PLX:H92	1.51	0.47
7:H:35:LEU:HD11	7:H:48:THR:HG22	1.97	0.47
9:J:132:ARG:NH2	51:J:401:NDP:O2X	2.47	0.47
13:N:34:ARG:HH12	13:N:58:ARG:HB3	1.80	0.47
16:Q:259:GLU:OE1	21:W:23:ARG:NH1	2.39	0.47
35:l:529:TYR:HB3	35:l:530:PRO:HD3	1.96	0.47
38:o:23:TYR:OH	39:p:68:GLU:HG3	2.15	0.47
38:o:56:ARG:NH1	38:o:58:GLY:O	2.47	0.47
41:s:189:THR:HG22	41:s:234:MET:HE3	1.97	0.47
4:E:99:GLN:HE22	33:j:42:ASP:N	2.01	0.47
6:G:69:SER:HA	16:Q:57:GLU:CA	2.37	0.47
9:J:167:ILE:HD13	9:J:201:ILE:HB	1.96	0.47
13:N:85:GLU:HB2	13:N:98:PRO:HB3	1.95	0.47
16:Q:95:LEU:HD22	16:Q:458:PHE:HZ	1.80	0.47
22:Y:43:ARG:HB3	22:Y:46:GLN:HB2	1.97	0.47
22:Y:50:LEU:HB3	22:Y:54:GLN:HE21	1.79	0.47
55:a:201:CDL:H541	47:l:705:PEE:H16	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:47:THR:HG23	30:g:65:LEU:HD22	1.96	0.47
34:k:4:VAL:O	34:k:8:ILE:HG12	2.14	0.47
55:r:503:CDL:H342	55:r:503:CDL:H181	1.97	0.47
41:s:277:TYR:CB	41:s:278:PRO:CD	2.86	0.47
44:w:88:GLU:HG3	44:w:139:ARG:HH12	1.79	0.47
16:Q:94:VAL:O	16:Q:94:VAL:HG23	2.14	0.47
6:X:112:SER:CB	39:p:17:LEU:HD11	2.45	0.47
35:l:366:MET:O	35:l:370:THR:HG23	2.15	0.47
34:k:21:MET:O	36:m:23:LYS:CE	2.54	0.47
36:m:61:LEU:O	41:s:114:TYR:OH	2.32	0.47
41:s:264:LEU:O	41:s:268:ILE:HG12	2.14	0.47
1:A:115:VAL:HG11	1:A:138:LEU:HD11	1.97	0.47
3:C:111:ASN:CG	15:P:210:LEU:HD13	2.39	0.47
9:J:313:TRP:CD2	52:J:402:UQ:H72	2.50	0.47
16:Q:185:MET:CE	16:Q:189:THR:HG21	2.45	0.47
17:S:6:LEU:HD11	55:S:101:CDL:H322	1.96	0.47
40:r:365:THR:HG21	40:r:444:LEU:HD13	1.97	0.47
41:s:117:LEU:HD21	41:s:136:VAL:CG2	2.39	0.47
44:w:60:ILE:HG12	44:w:203:VAL:HB	1.96	0.47
3:C:196:ARG:HB2	9:J:85:ARG:HH12	1.80	0.46
48:e:201:PLX:H21	47:l:705:PEE:H3	1.96	0.46
12:M:213:MET:HB3	12:M:215:MET:HG2	1.97	0.46
21:W:120:MET:O	21:W:121:MET:HB3	2.15	0.46
41:s:55:LEU:HD13	41:s:221:ALA:HB2	1.97	0.46
2:B:78:PHE:HB2	8:I:12:ARG:HG2	1.97	0.46
2:B:79:ARG:NH2	8:I:20:LEU:HD21	2.30	0.46
3:C:61:SER:CB	41:s:54:LYS:CE	2.93	0.46
6:G:130:ILE:HG22	6:G:135:ALA:HB2	1.97	0.46
8:I:18:ARG:HH22	16:Q:260:GLU:HG3	1.79	0.46
9:J:272:LEU:HD12	9:J:272:LEU:N	2.30	0.46
32:i:95:MET:HE1	32:i:145:ILE:HD12	1.97	0.46
35:l:69:MET:HE3	35:l:71:LEU:HD21	1.95	0.46
44:w:220:LYS:HB2	44:w:220:LYS:HE3	1.66	0.46
5:F:59:SER:OG	5:F:60:ASP:N	2.48	0.46
16:Q:100:GLU:OE1	16:Q:108:LYS:HB3	2.16	0.46
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.96	0.46
55:l:702:CDL:H811	55:l:702:CDL:H841	1.64	0.46
41:s:56:PHE:CE2	47:s:401:PEE:H81	2.51	0.46
3:C:113:MET:SD	16:Q:115:LEU:HD23	2.56	0.46
13:N:107:LYS:HE3	18:T:70:LEU:HD22	1.97	0.46
33:j:68:GLU:OE2	33:j:98:LEU:HD13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:18:GLY:O	36:m:23:LYS:CE	2.63	0.46
2:B:188:GLU:HG3	13:N:127:TYR:OH	2.15	0.46
47:j:201:PEE:H59	47:j:201:PEE:H64	1.75	0.46
12:M:395:GLU:OE2	12:M:417:ARG:NH1	2.48	0.46
13:N:55:PHE:CE1	13:N:58:ARG:HG3	2.51	0.46
16:Q:136:PHE:HA	16:Q:139:LEU:HD12	1.97	0.46
26:c:102:GLY:HA3	38:o:43:LEU:HD22	1.96	0.46
28:e:97:ILE:O	28:e:101:LEU:HB2	2.14	0.46
32:i:278:MET:O	32:i:282:MET:HG3	2.16	0.46
40:r:281:ASP:OD1	40:r:340:ARG:HB3	2.15	0.46
1:A:392:MET:O	1:A:396:MET:HG2	2.15	0.46
3:C:107:GLY:HA2	45:C:301:SF4:S1	2.55	0.46
27:d:73:ASP:OD1	27:d:73:ASP:N	2.48	0.46
55:n:101:CDL:H741	55:n:101:CDL:H711	1.70	0.46
6:G:133:ILE:O	6:G:134:ASP:OD1	2.34	0.46
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.97	0.46
55:V:201:CDL:H762	55:V:201:CDL:H401	1.97	0.46
21:W:40:ILE:HG22	21:W:40:ILE:O	2.15	0.46
21:W:73:PRO:HG2	42:u:40:ASN:HB3	1.96	0.46
21:W:81:ARG:HH21	42:u:60:GLY:C	2.24	0.46
22:Y:43:ARG:HD3	22:Y:48:PRO:HA	1.98	0.46
48:j:202:PLX:H281	48:j:202:PLX:H311	1.72	0.46
55:l:702:CDL:H312	55:l:702:CDL:HA61	1.69	0.46
2:B:79:ARG:NE	8:I:20:LEU:HD23	2.31	0.46
3:C:63:TRP:CE2	41:s:54:LYS:NZ	2.80	0.46
5:F:20:ARG:NH2	5:F:74:GLU:OE2	2.49	0.46
12:M:64:CYS:O	12:M:184:ARG:NH2	2.28	0.46
15:P:173:MET:HE1	15:P:189:THR:HG23	1.98	0.46
16:Q:357:LYS:HD3	16:Q:364:SER:HB3	1.98	0.46
26:c:78:LEU:HD12	26:c:106:HIS:HA	1.98	0.46
41:s:202:GLU:HA	41:s:210:GLY:HA3	1.98	0.46
9:J:87:GLU:HG3	9:J:89:TYR:H	1.81	0.45
9:J:268:PRO:HD3	9:J:342:ALA:HB1	1.97	0.45
26:c:156:VAL:HG11	43:v:95:TYR:CZ	2.51	0.45
27:d:85:MET:HE2	27:d:85:MET:HB3	1.79	0.45
32:i:41:ILE:HG13	34:k:73:LEU:HD21	1.96	0.45
32:i:146:SER:HA	32:i:149:ILE:HD12	1.97	0.45
43:v:111:ARG:O	43:v:115:ARG:HG2	2.16	0.45
44:w:175:ARG:HH22	44:w:239:ASN:HD22	1.64	0.45
16:Q:185:MET:O	16:Q:189:THR:HG23	2.16	0.45
35:l:561:ILE:HG13	35:l:562:LEU:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:82:VAL:HG22	36:m:85:SER:HB3	1.98	0.45
38:o:38:ALA:HB2	39:p:150:ARG:HD3	1.99	0.45
9:J:375:VAL:HG23	9:J:375:VAL:O	2.16	0.45
16:Q:155:VAL:HB	16:Q:229:PRO:HB3	1.99	0.45
48:g:201:PLX:H112	48:g:201:PLX:H81	1.46	0.45
2:B:61:LEU:HD23	47:B:303:PEE:O4	2.16	0.45
12:M:29:SER:OG	12:M:30:ASN:N	2.50	0.45
13:N:65:THR:O	13:N:73:THR:OG1	2.32	0.45
16:Q:450:ILE:HA	16:Q:453:THR:HG22	1.98	0.45
9:J:181:LEU:CD1	9:J:324:MET:HE1	2.47	0.45
28:e:98:VAL:HG22	40:r:36:LEU:HB2	1.98	0.45
35:l:305:SER:HB2	35:l:422:TYR:CE1	2.52	0.45
35:l:530:PRO:O	35:l:534:HIS:HB2	2.16	0.45
40:r:138:ASN:C	40:r:138:ASN:HD22	2.23	0.45
41:s:102:VAL:HG11	41:s:154:LEU:HD11	1.99	0.45
3:C:59:ARG:HH22	3:C:185:LYS:CG	2.29	0.45
3:C:83:ARG:NH1	16:Q:212:GLU:OE2	2.30	0.45
14:O:197:THR:H	14:O:200:ASP:HB2	1.81	0.45
16:Q:198:THR:CG2	16:Q:202:TRP:CZ2	3.00	0.45
27:d:2:PRO:O	27:d:7:LYS:NZ	2.39	0.45
35:l:86:SER:OG	35:l:262:ARG:NH2	2.47	0.45
47:l:704:PEE:H58	47:l:704:PEE:H53	1.76	0.45
10:K:108:PRO:CG	11:L:171:ARG:CD	2.95	0.45
29:f:72:ARG:NH2	30:g:18:ASN:OD1	2.50	0.45
33:j:73:LEU:HD12	36:m:55:MET:HE1	1.95	0.45
36:m:64:MET:HB2	41:s:114:TYR:OH	2.17	0.45
1:A:320:GLY:HA3	1:A:349:LEU:O	2.17	0.45
9:J:168:SER:O	9:J:203:PRO:HD2	2.17	0.45
12:M:260:ASN:ND2	12:M:278:HIS:HD2	2.15	0.45
12:M:494:SER:OG	12:M:669:ASN:ND2	2.47	0.45
16:Q:79:ASN:HB3	16:Q:101:LEU:C	2.42	0.45
16:Q:188:THR:HB	16:Q:200:PHE:HA	1.99	0.45
55:V:202:CDL:H142	55:V:202:CDL:H111	1.71	0.45
47:W:201:PEE:H42	47:W:201:PEE:H35	1.76	0.45
26:c:38:PRO:HG2	38:o:70:TYR:HD2	1.81	0.45
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.99	0.45
55:l:703:CDL:H542	55:l:703:CDL:H512	1.77	0.45
44:w:110:GLY:HA2	44:w:134:TRP:CE2	2.52	0.45
3:C:86:MET:HE3	3:C:91:VAL:HG12	1.99	0.45
17:S:3:PHE:CE1	55:S:101:CDL:H521	2.52	0.45
31:h:19:THR:HA	32:i:84:TRP:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:560:THR:O	35:l:565:THR:OG1	2.34	0.45
40:r:115:LEU:HD12	40:r:174:LEU:HD22	1.99	0.45
44:w:143:TYR:OH	44:w:199:LEU:O	2.27	0.45
1:A:160:GLY:O	1:A:199:ARG:NH2	2.49	0.45
1:A:244:ASN:OD1	1:A:245:VAL:N	2.50	0.45
3:C:75:GLU:OE2	16:Q:221:ARG:NH1	2.49	0.45
13:N:6:VAL:HG12	13:N:9:ARG:NH2	2.32	0.45
21:W:96:ILE:O	21:W:99:LYS:HE3	2.16	0.45
35:l:295:GLN:HB2	35:l:301:ILE:HG12	1.99	0.45
41:s:198:PHE:CD1	41:s:285:LEU:HD13	2.51	0.45
3:C:62:LEU:O	3:C:91:VAL:HA	2.17	0.44
55:V:202:CDL:H742	55:V:202:CDL:H601	1.99	0.44
25:b:90:VAL:O	25:b:96:THR:OG1	2.31	0.44
48:g:201:PLX:H101	48:g:201:PLX:H132	1.57	0.44
35:l:176:ARG:HA	35:l:176:ARG:HD3	1.76	0.44
35:l:435:PRO:HB3	35:l:437:PHE:CZ	2.51	0.44
36:m:51:PHE:O	36:m:55:MET:HB2	2.17	0.44
36:m:138:GLU:OE1	36:m:138:GLU:N	2.51	0.44
39:p:98:LYS:HG2	39:p:178:PRO:HG3	1.98	0.44
40:r:203:PHE:O	40:r:207:MET:HG2	2.16	0.44
1:A:88:ARG:C	1:A:244:ASN:HD22	2.25	0.44
1:A:299:LEU:HD12	1:A:303:HIS:HD2	1.82	0.44
12:M:140:GLN:HG2	16:Q:379:ILE:HG23	1.98	0.44
16:Q:370:GLU:HA	16:Q:373:THR:HG22	1.99	0.44
6:X:118:ILE:O	6:X:122:MET:HG2	2.16	0.44
23:Z:53:TYR:CE1	35:l:434:LYS:HG3	2.53	0.44
26:c:167:TYR:CD2	26:c:178:PRO:HG3	2.52	0.44
48:g:201:PLX:H361	48:g:201:PLX:H311	1.98	0.44
35:l:331:MET:HG3	35:l:391:SER:HB3	1.99	0.44
55:l:702:CDL:H452	40:r:445:LEU:HB3	2.00	0.44
36:m:163:ILE:O	36:m:167:VAL:HG23	2.17	0.44
40:r:114:GLU:HG2	40:r:175:ASN:HA	1.99	0.44
8:I:25:GLN:HE22	41:s:33:LEU:CD2	2.15	0.44
12:M:59:GLN:NE2	12:M:62:ARG:HH12	2.15	0.44
12:M:576:GLY:HA2	12:M:579:MET:HE3	1.99	0.44
16:Q:178:THR:OG1	16:Q:214:TYR:OH	2.35	0.44
19:U:43:ILE:HG12	33:j:84:LEU:HB2	1.99	0.44
21:W:94:GLU:OE2	21:W:104:TRP:NE1	2.42	0.44
22:Y:72:ARG:HB3	35:l:385:TYR:CD1	2.52	0.44
25:b:5:THR:OG1	25:b:8:GLU:HG3	2.18	0.44
13:N:78:ASP:OD1	13:N:78:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:86:MET:SD	21:W:124:LEU:HB3	2.58	0.44
6:X:93:ILE:HG21	6:X:98:LEU:HD13	1.99	0.44
25:b:99:GLU:HG2	35:l:61:MET:HG2	1.99	0.44
28:e:57:GLU:OE1	44:w:320:GLY:HA3	2.16	0.44
28:e:76:TYR:HB2	28:e:83:ASP:OD1	2.17	0.44
35:l:554:ASP:OD2	40:r:288:TYR:OH	2.29	0.44
3:C:67:PHE:CD1	16:Q:87:GLN:HG2	2.53	0.44
14:O:148:ILE:HD12	14:O:184:PRO:HB2	1.99	0.44
24:a:92:PHE:HD1	27:d:55:GLN:HE21	1.66	0.44
31:h:75:ARG:O	31:h:79:ILE:HG12	2.18	0.44
36:m:55:MET:HE3	36:m:55:MET:CA	2.20	0.44
38:o:60:ILE:HD12	40:r:422:HIS:HB2	1.99	0.44
40:r:271:MET:HE2	40:r:271:MET:HA	2.00	0.44
1:A:284:HIS:ND1	14:O:228:ALA:HB3	2.33	0.44
47:B:303:PEE:H61	47:B:303:PEE:H55	1.66	0.44
10:K:108:PRO:HG2	11:L:171:ARG:CD	2.48	0.44
16:Q:156:GLU:OE2	16:Q:171:ARG:NH2	2.49	0.44
19:U:16:GLU:O	19:U:20:VAL:HG23	2.18	0.44
19:U:66:VAL:O	42:u:130:LYS:HE3	2.18	0.44
43:v:42:THR:OG1	43:v:45:GLU:HG3	2.17	0.44
1:A:326:LEU:HD23	1:A:367:ILE:HD11	1.99	0.44
6:G:105:MET:HG3	6:G:110:LEU:O	2.18	0.44
8:I:8:ILE:O	8:I:12:ARG:HG3	2.18	0.44
31:h:2:PRO:HA	32:i:140:SER:HB2	2.00	0.44
35:l:249:SER:HG	35:l:340:PHE:HD2	1.66	0.44
41:s:17:VAL:O	41:s:21:THR:HG23	2.18	0.44
47:s:401:PEE:H82	47:s:401:PEE:H74	1.88	0.44
1:A:88:ARG:HG3	1:A:246:GLU:HG2	1.99	0.44
3:C:101:ASP:OD1	41:s:58:LYS:NZ	2.36	0.44
3:C:167:PRO:HG3	16:Q:222:MET:SD	2.57	0.44
9:J:220:MET:HE3	9:J:226:VAL:HG13	2.00	0.44
12:M:250:SER:O	12:M:261:ILE:HG12	2.18	0.44
55:V:202:CDL:H312	38:o:84:PRO:HB3	1.99	0.44
27:d:159:GLN:NE2	28:e:142:PHE:O	2.38	0.44
35:l:492:ILE:O	35:l:496:MET:HG2	2.18	0.44
36:m:53:GLY:HA2	36:m:56:VAL:HG12	2.00	0.44
3:C:61:SER:CB	41:s:54:LYS:HE3	2.48	0.44
16:Q:197:MET:CE	52:s:402:UQ:HM32	2.48	0.44
16:Q:198:THR:HG21	16:Q:202:TRP:CZ2	2.53	0.44
16:Q:442:HIS:HB3	16:Q:446:ASP:HB2	1.99	0.44
24:a:147:ALA:HB2	40:r:173:SER:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:40:MET:HE1	32:i:129:LEU:HD22	1.99	0.44
48:C:302:PLX:C36	48:C:302:PLX:C32	2.89	0.43
27:d:99:ASP:OD2	27:d:142:ARG:NH1	2.51	0.43
31:h:38:LYS:HE2	31:h:42:GLU:OE2	2.18	0.43
32:i:324:LYS:HA	32:i:324:LYS:HD3	1.89	0.43
35:l:128:MET:HE3	35:l:251:THR:HG22	1.99	0.43
2:B:63:TRP:N	2:B:63:TRP:CD1	2.84	0.43
2:B:81:PRO:HA	41:s:33:LEU:O	2.19	0.43
47:B:303:PEE:H21	47:B:303:PEE:H15	1.76	0.43
7:H:116:ILE:HG21	11:L:96:LYS:HD2	2.00	0.43
16:Q:53:TYR:HB3	35:l:571:MET:HE3	2.00	0.43
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	1.99	0.43
20:V:37:SER:O	20:V:41:ILE:HG12	2.18	0.43
25:b:11:ARG:HB2	39:p:156:PRO:HB3	1.99	0.43
34:k:76:SER:OG	36:m:168:ILE:HD12	2.18	0.43
35:l:69:MET:HG3	35:l:71:LEU:CD2	2.47	0.43
55:l:702:CDL:H611	55:l:702:CDL:H581	1.67	0.43
40:r:186:LEU:HD23	40:r:192:ASN:HB3	2.00	0.43
40:r:306:PRO:O	40:r:310:MET:HG3	2.18	0.43
41:s:179:TRP:CG	41:s:180:PRO:HD3	2.53	0.43
52:s:402:UQ:H221	52:s:402:UQ:H262	1.66	0.43
2:B:63:TRP:HB3	2:B:66:LEU:HB2	2.00	0.43
2:B:70:LEU:O	41:s:272:TRP:NE1	2.47	0.43
48:C:302:PLX:C17	48:C:302:PLX:H221	2.48	0.43
9:J:298:TYR:CE2	9:J:319:VAL:HG22	2.53	0.43
16:Q:315:GLU:O	16:Q:346:GLN:NE2	2.49	0.43
44:w:295:ARG:HA	44:w:298:VAL:HG22	2.00	0.43
11:L:104:ARG:HA	11:L:104:ARG:HD3	1.80	0.43
20:V:39:TYR:HB3	55:V:201:CDL:H712	2.01	0.43
32:i:49:ASN:O	32:i:51:ARG:N	2.50	0.43
2:B:63:TRP:CE3	47:B:303:PEE:C38	3.02	0.43
5:F:45:LYS:HA	5:F:45:LYS:HD2	1.78	0.43
12:M:149:ASP:OD2	12:M:150:ARG:NH1	2.51	0.43
14:O:146:ASP:O	14:O:150:GLU:OE2	2.37	0.43
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	2.00	0.43
26:c:44:THR:OG1	26:c:47:GLU:HG3	2.18	0.43
35:l:54:PHE:CZ	35:l:84:TYR:HB2	2.53	0.43
35:l:395:ILE:O	35:l:399:VAL:HG23	2.18	0.43
40:r:357:THR:O	40:r:361:VAL:HG23	2.17	0.43
42:u:45:LEU:HD22	42:u:131:VAL:HB	2.01	0.43
42:u:100:CYS:HB2	42:u:103:GLN:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLY:HA2	1:A:252:PRO:HD3	2.01	0.43
9:J:119:VAL:HG23	9:J:120:VAL:HG13	2.01	0.43
15:P:197:PRO:HA	15:P:202:PHE:CG	2.54	0.43
17:S:31:ASN:CG	17:S:36:LYS:HB2	2.44	0.43
25:b:121:LYS:HD3	25:b:121:LYS:O	2.19	0.43
31:h:17:TRP:CD1	31:h:17:TRP:H	2.36	0.43
35:l:249:SER:OG	35:l:336:LYS:HG3	2.18	0.43
40:r:406:TYR:O	40:r:409:TYR:HB3	2.19	0.43
43:v:93:LEU:HA	43:v:96:VAL:HG12	1.99	0.43
44:w:147:LEU:HD23	44:w:147:LEU:HA	1.90	0.43
7:H:47:TYR:HE1	8:I:92:LYS:O	2.01	0.43
12:M:208:THR:OG1	12:M:210:ILE:O	2.32	0.43
16:Q:309:ASP:C	16:Q:311:TYR:H	2.26	0.43
17:S:19:PRO:HB3	41:s:9:LEU:HD12	2.01	0.43
24:a:80:ILE:HB	24:a:81:PRO:HD3	2.01	0.43
26:c:85:GLU:OE1	26:c:119:THR:OG1	2.33	0.43
34:k:18:GLY:O	36:m:23:LYS:HE3	2.19	0.43
34:k:45:THR:HG23	36:m:52:LEU:HD13	2.01	0.43
35:l:332:HIS:HA	35:l:335:PHE:CZ	2.53	0.43
35:l:399:VAL:HG12	35:l:409:LEU:HD13	2.01	0.43
47:l:701:PEE:H14	47:l:701:PEE:H20	1.69	0.43
38:o:113:GLU:O	38:o:117:GLN:HG2	2.18	0.43
1:A:160:GLY:HA3	14:O:121:MET:HE1	2.00	0.43
9:J:40:LEU:HD13	9:J:124:ASN:ND2	2.32	0.43
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.99	0.43
48:a:202:PLX:H22	48:a:202:PLX:H1C3	1.73	0.43
28:e:72:ASP:OD1	28:e:72:ASP:N	2.47	0.43
40:r:116:ILE:HG13	42:u:168:PHE:CD1	2.54	0.43
40:r:237:LYS:HA	40:r:237:LYS:HD3	1.94	0.43
41:s:68:ILE:O	41:s:72:ILE:HG12	2.18	0.43
1:A:213:ILE:O	1:A:217:GLU:HG3	2.18	0.43
41:s:215:TYR:HD1	41:s:219:PRO:HB2	1.83	0.43
52:s:402:UQ:H152	52:s:402:UQ:H121	1.81	0.43
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.54	0.43
9:J:37:HIS:CD2	9:J:40:LEU:HB2	2.54	0.43
19:U:59:ASP:OD2	42:u:130:LYS:HD3	2.18	0.43
6:X:89:LEU:HD22	23:Z:47:ARG:HB3	2.01	0.43
50:X:201:8Q1:O2	39:p:13:GLN:OE1	2.36	0.43
23:Z:27:THR:HB	23:Z:53:TYR:HD2	1.83	0.43
25:b:99:GLU:HG2	35:l:61:MET:HE2	2.01	0.43
32:i:243:LEU:HD23	55:r:503:CDL:H361	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:12:LEU:HD22	35:l:129:MET:HB3	2.01	0.43
40:r:296:LEU:HG	40:r:381:ILE:HG21	2.01	0.43
41:s:67:SER:O	41:s:71:PHE:HB2	2.19	0.43
44:w:108:LEU:HD23	44:w:327:VAL:HG13	2.01	0.43
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.65	0.42
9:J:117:ARG:O	9:J:121:GLU:HG3	2.19	0.42
12:M:355:LYS:HG3	12:M:366:LEU:HD13	2.01	0.42
25:b:106:PRO:HG2	25:b:120:MET:HE2	2.01	0.42
44:w:88:GLU:N	44:w:160:GLU:HG3	2.34	0.42
1:A:326:LEU:HD22	1:A:363:ILE:HD11	2.02	0.42
15:P:62:GLY:HA3	15:P:76:VAL:HG11	2.00	0.42
16:Q:198:THR:CG2	16:Q:202:TRP:CE2	3.02	0.42
16:Q:304:LYS:NZ	16:Q:316:PHE:O	2.41	0.42
20:V:43:LEU:HD13	55:V:201:CDL:H522	2.01	0.42
23:Z:27:THR:HB	23:Z:53:TYR:CD2	2.54	0.42
25:b:32:GLU:HB2	25:b:33:PRO:HD3	2.01	0.42
2:B:61:LEU:CD2	19:U:18:VAL:HG22	2.49	0.42
9:J:241:TYR:OH	9:J:351:GLU:OE2	2.32	0.42
12:M:689:LEU:HD23	12:M:689:LEU:HA	1.92	0.42
15:P:191:TYR:OH	16:Q:96:ARG:NH1	2.51	0.42
25:b:88:TYR:CE1	27:d:49:ARG:HG2	2.54	0.42
27:d:37:PHE:CD2	35:l:3:PRO:HB3	2.55	0.42
48:e:201:PLX:H362	40:r:67:VAL:HG12	2.01	0.42
35:l:332:HIS:HA	35:l:335:PHE:CE2	2.54	0.42
39:p:27:LEU:HD11	39:p:40:PHE:HB3	2.01	0.42
1:A:73:PRO:HD3	1:A:147:ARG:NH2	2.35	0.42
6:G:69:SER:CA	16:Q:57:GLU:HB3	2.47	0.42
13:N:60:ARG:HH22	13:N:95:ASP:HA	1.84	0.42
24:a:170:GLN:HB2	30:g:6:GLY:O	2.19	0.42
48:e:201:PLX:H111	55:l:702:CDL:H641	2.01	0.42
40:r:174:LEU:HA	40:r:179:ILE:HD11	2.01	0.42
40:r:174:LEU:HD23	40:r:179:ILE:HD11	2.01	0.42
48:r:502:PLX:H1C3	48:r:502:PLX:H22	1.70	0.42
1:A:119:GLU:O	1:A:159:ARG:NH1	2.52	0.42
9:J:108:TRP:HZ3	9:J:110:GLY:HA2	1.84	0.42
14:O:196:LEU:HD13	14:O:201:ILE:HD13	2.02	0.42
16:Q:55:THR:H	16:Q:58:THR:HB	1.84	0.42
17:S:40:HIS:N	17:S:44:GLN:OE1	2.50	0.42
55:V:201:CDL:H372	55:V:201:CDL:H341	1.52	0.42
37:n:16:LEU:HD23	37:n:16:LEU:HA	1.91	0.42
44:w:59:VAL:HG12	44:w:201:PRO:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:SER:C	1:A:102:MET:H	2.27	0.42
3:C:193:TRP:HA	3:C:196:ARG:HG2	2.01	0.42
11:L:131:LYS:HD2	11:L:147:VAL:HG11	2.01	0.42
16:Q:55:THR:O	16:Q:59:ALA:N	2.49	0.42
21:W:57:ARG:HB3	41:s:316:PRO:HG3	2.00	0.42
26:c:110:ASP:HA	26:c:113:ILE:HG23	2.00	0.42
27:d:82:ILE:HD12	27:d:82:ILE:HA	1.92	0.42
33:j:67:LEU:HD13	33:j:67:LEU:HA	1.77	0.42
47:j:201:PEE:H22	47:j:201:PEE:H27	1.89	0.42
34:k:25:HIS:ND1	34:k:88:ASP:OD1	2.39	0.42
35:l:151:SER:HB2	35:l:252:MET:SD	2.60	0.42
36:m:86:ASN:OD1	36:m:88:THR:HG22	2.20	0.42
42:u:38:LYS:HB3	42:u:39:PRO:HD3	2.01	0.42
12:M:329:MET:HG2	12:M:565:PHE:CG	2.54	0.42
55:V:202:CDL:H872	35:l:558:LEU:HD21	2.01	0.42
32:i:81:SER:O	32:i:83:GLN:N	2.50	0.42
40:r:355:MET:HE2	40:r:358:TRP:HD1	1.85	0.42
5:F:16:LEU:HD11	5:F:19:ILE:HD11	2.00	0.42
7:H:44:TYR:HB2	15:P:68:ILE:HG23	2.02	0.42
7:H:105:GLU:HB3	15:P:89:HIS:CD2	2.54	0.42
11:L:154:LYS:O	11:L:156:LYS:NZ	2.51	0.42
13:N:10:GLY:O	13:N:14:VAL:HG23	2.20	0.42
29:f:68:GLU:HG2	30:g:21:ARG:HE	1.85	0.42
33:j:67:LEU:HG	34:k:68:ALA:HB3	2.02	0.42
35:l:297:ASP:O	35:l:301:ILE:HG13	2.20	0.42
35:l:417:SER:OG	55:l:703:CDL:H581	2.20	0.42
43:v:52:MET:O	43:v:56:ARG:HG3	2.19	0.42
9:J:163:LYS:NZ	9:J:253:ILE:O	2.35	0.42
14:O:159:LYS:HA	14:O:159:LYS:HD3	1.65	0.42
15:P:87:PHE:CE2	15:P:144:LYS:HE3	2.55	0.42
25:b:86:LEU:HD11	35:l:9:LEU:HD12	2.01	0.42
27:d:68:PHE:CE1	28:e:114:MET:HE1	2.55	0.42
41:s:18:ALA:O	41:s:21:THR:OG1	2.28	0.42
9:J:279:TYR:HB2	9:J:372:ALA:HB2	2.02	0.42
12:M:77:MET:HE2	12:M:117:MET:HE2	2.01	0.42
12:M:326:VAL:HG13	12:M:567:ILE:HD13	2.02	0.42
16:Q:332:CYS:O	16:Q:336:GLU:HG3	2.20	0.42
28:e:129:ARG:HG2	28:e:134:LEU:HD12	2.01	0.42
35:l:241:THR:HG21	35:l:344:GLY:HA3	2.00	0.42
43:v:107:ARG:HA	43:v:110:GLN:HG3	2.01	0.42
1:A:110:PRO:O	1:A:238:CYS:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:ARG:NE	8:I:20:LEU:HD21	2.34	0.41
3:C:97:PRO:HG2	33:j:37:TYR:CE2	2.55	0.41
7:H:24:LEU:HD23	7:H:24:LEU:HA	1.89	0.41
52:J:402:UQ:H151	52:J:402:UQ:H171	1.59	0.41
20:V:85:ASP:HA	20:V:126:LYS:NZ	2.35	0.41
6:X:103:HIS:O	6:X:107:ASP:HB2	2.20	0.41
32:i:97:MET:HE3	35:l:599:MET:HE3	2.02	0.41
33:j:67:LEU:CG	34:k:68:ALA:HB2	2.50	0.41
41:s:269:THR:O	41:s:273:ILE:HG13	2.20	0.41
41:s:307:LEU:HA	41:s:310:MET:HE3	2.02	0.41
44:w:113:SER:HB3	44:w:116:LYS:HB3	2.02	0.41
4:E:29:LYS:HE2	50:G:201:8Q1:O35	2.20	0.41
6:G:134:ASP:HA	6:G:137:LYS:NZ	2.35	0.41
12:M:591:GLU:HG3	12:M:610:VAL:HG23	2.03	0.41
12:M:666:GLN:HG3	12:M:667:GLN:OE1	2.20	0.41
16:Q:156:GLU:HG3	16:Q:229:PRO:O	2.20	0.41
17:S:50:ARG:O	17:S:54:ILE:HG12	2.19	0.41
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.85	0.41
22:Y:94:ASP:HA	22:Y:99:ILE:HD13	2.03	0.41
25:b:81:ILE:HG23	47:l:705:PEE:H58	2.01	0.41
26:c:127:ASN:O	26:c:131:LYS:HE2	2.20	0.41
32:i:268:GLN:HG3	42:u:168:PHE:CE2	2.55	0.41
34:k:37:MET:HE2	34:k:67:ALA:HB2	2.00	0.41
39:p:84:GLU:OE1	39:p:84:GLU:N	2.53	0.41
40:r:105:PHE:O	40:r:109:THR:OG1	2.31	0.41
40:r:197:LEU:HD13	47:r:501:PEE:H70	2.01	0.41
3:C:61:SER:CB	41:s:54:LYS:HE2	2.50	0.41
5:F:23:LEU:HD12	5:F:34:ARG:HG2	2.02	0.41
16:Q:270:ASN:HB3	41:s:284:GLN:HE22	1.81	0.41
20:V:66:ILE:HD11	20:V:101:LEU:HD13	2.02	0.41
31:h:97:HIS:HB2	31:h:102:GLU:HB2	2.02	0.41
34:k:56:ALA:O	34:k:59:MET:HG3	2.20	0.41
35:l:130:ILE:HD13	55:l:702:CDL:H252	2.02	0.41
35:l:557:TRP:O	35:l:561:ILE:HG12	2.20	0.41
36:m:163:ILE:HD13	36:m:163:ILE:HA	1.92	0.41
41:s:81:LEU:O	41:s:85:MET:HG2	2.20	0.41
41:s:196:ALA:HB3	41:s:274:ARG:HA	2.02	0.41
12:M:234:LYS:HB3	12:M:235:PRO:HD3	2.02	0.41
12:M:511:LYS:HE2	12:M:663:ASN:HB2	2.02	0.41
55:V:202:CDL:H781	55:V:202:CDL:H812	1.78	0.41
21:W:84:LEU:HD13	42:u:8:PRO:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:g:10:ARG:NH2	32:i:347:ASN:O	2.47	0.41
47:l:705:PEE:H60	47:l:705:PEE:H55	1.86	0.41
4:E:33:ARG:O	4:E:37:ARG:HG3	2.21	0.41
8:I:28:TYR:HA	13:N:55:PHE:HA	2.03	0.41
9:J:40:LEU:HD23	9:J:40:LEU:HA	1.79	0.41
12:M:386:LEU:HD23	12:M:386:LEU:HA	1.89	0.41
15:P:103:HIS:CD2	15:P:105:ASN:HB2	2.55	0.41
15:P:197:PRO:O	16:Q:122:LYS:NZ	2.45	0.41
15:P:211:ARG:NH2	15:P:222:GLU:OE2	2.49	0.41
16:Q:200:PHE:CD1	16:Q:200:PHE:C	2.98	0.41
17:S:1:MET:HE3	17:S:1:MET:HB3	2.00	0.41
37:n:49:LEU:HD22	37:n:53:GLU:HG3	2.03	0.41
4:E:14:GLY:C	4:E:16:SER:H	2.29	0.41
6:G:69:SER:N	16:Q:57:GLU:HB2	2.27	0.41
12:M:475:VAL:HG22	12:M:514:ASN:HB2	2.03	0.41
12:M:498:GLN:HG3	12:M:502:LEU:HD23	2.02	0.41
6:X:112:SER:O	6:X:116:VAL:HG23	2.21	0.41
25:b:73:THR:HG23	25:b:74:HIS:ND1	2.36	0.41
32:i:112:HIS:CE1	32:i:164:ILE:HD13	2.55	0.41
39:p:44:MET:HE3	39:p:48:PHE:CE1	2.56	0.41
41:s:104:PHE:CE1	41:s:108:MET:HE3	2.55	0.41
1:A:98:LYS:HE3	46:A:502:FMN:O3P	2.20	0.41
17:S:23:THR:HG22	17:S:27:HIS:CD2	2.56	0.41
26:c:62:TYR:OH	26:c:74:ASP:OD1	2.36	0.41
31:h:21:GLN:HG2	31:h:37:GLU:OE1	2.21	0.41
32:i:183:SER:O	32:i:187:MET:HG2	2.20	0.41
33:j:87:MET:HE1	41:s:309:ILE:HD11	2.02	0.41
35:l:172:ILE:HG21	40:r:408:LEU:HD12	2.02	0.41
1:A:367:ILE:O	1:A:371:ILE:HG12	2.21	0.41
9:J:171:ASN:OD1	9:J:327:MET:HG3	2.21	0.41
10:K:108:PRO:HG2	11:L:171:ARG:HD3	2.03	0.41
12:M:50:LEU:O	12:M:54:GLU:HG2	2.20	0.41
12:M:624:ARG:NH1	12:M:628:GLU:OE1	2.37	0.41
13:N:39:VAL:N	13:N:48:TYR:O	2.54	0.41
14:O:137:THR:HB	53:O:301:FES:S2	2.61	0.41
20:V:95:CYS:HA	20:V:115:CYS:HA	2.02	0.41
6:X:80:LYS:HE3	6:X:80:LYS:HB3	1.86	0.41
22:Y:40:ILE:HD11	35:l:444:ASN:HB2	2.03	0.41
35:l:6:SER:O	35:l:10:THR:OG1	2.24	0.41
37:n:18:PRO:O	37:n:21:PHE:HB3	2.21	0.41
41:s:120:GLY:HA3	41:s:132:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:65:ASN:HD22	44:w:238:GLU:HG3	1.86	0.41
2:B:74:LEU:HA	41:s:31:MET:HE2	2.03	0.41
3:C:103:MET:HE1	3:C:117:LEU:HD11	2.03	0.41
12:M:382:ARG:HE	12:M:527:ASP:CG	2.29	0.41
12:M:647:GLU:HB2	12:M:654:VAL:HG11	2.02	0.41
15:P:170:ILE:HG22	15:P:176:VAL:HB	2.03	0.41
17:S:1:MET:HE2	55:S:101:CDL:CA2	2.46	0.41
47:W:201:PEE:H20	47:W:201:PEE:H14	1.74	0.41
22:Y:87:PRO:HG3	43:v:96:VAL:HG23	2.03	0.41
25:b:35:LEU:HA	25:b:36:PRO:HD3	1.98	0.41
26:c:126:TRP:C	26:c:128:THR:H	2.27	0.41
27:d:19:ALA:HA	27:d:20:PRO:HD3	1.96	0.41
27:d:117:GLU:OE1	27:d:124:ASN:ND2	2.37	0.41
29:f:68:GLU:OE2	29:f:72:ARG:HG3	2.21	0.41
32:i:106:LEU:HG	32:i:138:PRO:HB2	2.03	0.41
33:j:68:GLU:CD	33:j:98:LEU:HD13	2.45	0.41
33:j:75:LEU:HD23	33:j:75:LEU:HA	1.93	0.41
33:j:90:MET:SD	36:m:151:THR:HG23	2.61	0.41
35:l:63:ILE:O	35:l:79:SER:HA	2.21	0.41
35:l:96:VAL:O	35:l:100:ILE:HG12	2.21	0.41
36:m:36:SER:HA	36:m:39:VAL:HG22	2.03	0.41
40:r:121:LEU:O	40:r:125:THR:HG23	2.21	0.41
40:r:158:LEU:HD23	40:r:158:LEU:HA	1.91	0.41
47:r:501:PEE:H68	47:r:501:PEE:H62	1.91	0.41
44:w:110:GLY:HA2	44:w:134:TRP:CD2	2.56	0.41
44:w:209:VAL:HB	44:w:214:ILE:HD11	2.02	0.41
7:H:55:LYS:HE3	15:P:104:THR:HG21	2.02	0.41
9:J:262:THR:O	9:J:333:PRO:HD2	2.21	0.41
12:M:289:LYS:HE2	12:M:694:PHE:O	2.21	0.41
16:Q:251:PHE:O	16:Q:255:ILE:HG13	2.21	0.41
33:j:67:LEU:HG	34:k:68:ALA:HB2	2.03	0.41
33:j:94:LEU:HD13	36:m:154:VAL:HG13	2.02	0.41
38:o:61:GLU:OE2	38:o:66:ILE:HD11	2.21	0.41
2:B:118:LEU:HD11	16:Q:382:PHE:CE2	2.56	0.40
9:J:92:MET:HE3	9:J:92:MET:HB3	1.97	0.40
12:M:338:VAL:O	12:M:363:SER:OG	2.29	0.40
27:d:78:GLU:HA	30:g:110:THR:HA	2.03	0.40
35:l:128:MET:CE	35:l:252:MET:HA	2.51	0.40
35:l:184:LEU:HD13	40:r:393:ILE:HG21	2.03	0.40
35:l:561:ILE:HG13	35:l:562:LEU:N	2.36	0.40
47:l:704:PEE:H55	40:r:405:LEU:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:o:31:LYS:O	38:o:35:GLU:HG2	2.20	0.40
52:s:402:UQ:H203	52:s:402:UQ:H172	1.83	0.40
2:B:70:LEU:HD23	41:s:276:SER:CB	2.51	0.40
2:B:77:LEU:HD13	41:s:31:MET:HG3	2.02	0.40
4:E:104:MET:HE3	4:E:109:GLU:OE2	2.21	0.40
9:J:131:GLY:O	51:J:401:NDP:H51A	2.22	0.40
10:K:87:LEU:HD22	14:O:66:ILE:HD11	2.03	0.40
12:M:198:THR:HG21	12:M:209:TYR:HB2	2.03	0.40
12:M:372:PHE:H	12:M:532:PRO:HB2	1.86	0.40
12:M:394:VAL:HG22	12:M:473:MET:HE1	2.03	0.40
21:W:93:GLU:HG3	31:h:98:HIS:CD2	2.56	0.40
48:e:201:PLX:H221	48:e:201:PLX:H191	1.91	0.40
30:g:92:MET:O	30:g:96:VAL:HG23	2.21	0.40
35:l:49:VAL:HB	35:l:50:PRO:HD3	2.03	0.40
39:p:108:HIS:CD2	39:p:109:PRO:HD2	2.56	0.40
41:s:169:GLN:HB2	41:s:244:GLY:HA3	2.03	0.40
2:B:76:TYR:CD2	41:s:33:LEU:HD13	2.57	0.40
4:E:17:VAL:HG21	11:L:55:VAL:HG12	2.03	0.40
8:I:33:LYS:HD3	8:I:33:LYS:HA	1.77	0.40
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.51	0.40
15:P:173:MET:HB3	15:P:198:PHE:HB2	2.02	0.40
25:b:32:GLU:OE2	39:p:117:ASP:HB2	2.21	0.40
26:c:83:GLN:NE2	26:c:97:LEU:O	2.54	0.40
26:c:167:TYR:CG	26:c:178:PRO:HG3	2.57	0.40
32:i:207:ILE:O	32:i:211:MET:HG3	2.21	0.40
33:j:69:ILE:HD12	41:s:147:ALA:CB	2.50	0.40
35:l:153:LEU:HD23	35:l:153:LEU:HA	1.91	0.40
35:l:298:ILE:O	35:l:302:VAL:HG23	2.21	0.40
55:l:702:CDL:H411	40:r:371:PRO:HD2	2.04	0.40
42:u:56:CYS:HB2	42:u:59:GLU:OE1	2.22	0.40
19:U:38:TYR:HB2	41:s:310:MET:O	2.21	0.40
25:b:32:GLU:HB3	39:p:115:TYR:HD1	1.86	0.40
33:j:73:LEU:CD1	36:m:55:MET:SD	2.96	0.40
33:j:73:LEU:HD23	33:j:73:LEU:HA	1.89	0.40
3:C:94:ARG:HG2	3:C:99:GLN:HB2	2.03	0.40
12:M:422:TRP:HA	12:M:427:LEU:HB3	2.02	0.40
15:P:148:ASP:OD1	15:P:148:ASP:N	2.54	0.40
48:r:502:PLX:H312	48:r:502:PLX:H342	1.91	0.40
41:s:59:GLU:HA	41:s:60:PRO:HD3	1.84	0.40
41:s:119:SER:HG	41:s:223:PHE:HZ	1.65	0.40
44:w:209:VAL:HG22	44:w:260:ALA:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	417 (97%)	12 (3%)	2 (0%)	24	59
2	B	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
3	C	154/156 (99%)	147 (96%)	7 (4%)	0	100	100
4	E	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
5	F	84/86 (98%)	79 (94%)	5 (6%)	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%)	102 (93%)	7 (6%)	1 (1%)	14	47
8	I	93/112 (83%)	80 (86%)	13 (14%)	0	100	100
9	J	340/342 (99%)	329 (97%)	11 (3%)	0	100	100
10	K	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
11	L	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
12	M	688/690 (100%)	660 (96%)	28 (4%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	201 (94%)	14 (6%)	0	100	100
15	P	206/208 (99%)	197 (96%)	9 (4%)	0	100	100
16	Q	427/430 (99%)	410 (96%)	17 (4%)	0	100	100
17	S	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
18	T	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
19	U	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
20	V	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
21	W	140/142 (99%)	129 (92%)	8 (6%)	3 (2%)	5	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	Y	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
23	Z	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
24	a	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
25	b	94/126 (75%)	86 (92%)	8 (8%)	0	100	100
26	c	154/156 (99%)	143 (93%)	11 (7%)	0	100	100
27	d	173/175 (99%)	172 (99%)	1 (1%)	0	100	100
28	e	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
29	f	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
30	g	119/121 (98%)	112 (94%)	7 (6%)	0	100	100
31	h	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
32	i	345/347 (99%)	332 (96%)	13 (4%)	0	100	100
33	j	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
34	k	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
35	l	604/606 (100%)	582 (96%)	22 (4%)	0	100	100
36	m	173/175 (99%)	160 (92%)	13 (8%)	0	100	100
37	n	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
38	o	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
39	p	176/178 (99%)	170 (97%)	5 (3%)	1 (1%)	21	56
40	r	457/459 (100%)	453 (99%)	4 (1%)	0	100	100
41	s	316/318 (99%)	309 (98%)	5 (2%)	2 (1%)	21	56
42	u	169/171 (99%)	162 (96%)	6 (4%)	1 (1%)	21	56
43	v	122/125 (98%)	117 (96%)	5 (4%)	0	100	100
44	w	318/320 (99%)	307 (96%)	11 (4%)	0	100	100
All	All	8174/8313 (98%)	7858 (96%)	306 (4%)	10 (0%)	49	79

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	PHE
21	W	32	GLY
1	A	186	ALA
21	W	31	SER
7	H	77	ILE
21	W	26	PRO

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Mol	Chain	Res	Type
39	p	174	PRO
41	s	60	PRO
42	u	152	PRO
41	s	208	VAL

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	345/346 (100%)	344 (100%)	1 (0%)	86	88
2	B	146/151 (97%)	146 (100%)	0	100	100
3	C	131/132 (99%)	131 (100%)	0	100	100
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	75/76 (99%)	75 (100%)	0	100	100
6	G	75/81 (93%)	75 (100%)	0	100	100
6	X	78/81 (96%)	78 (100%)	0	100	100
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	87 (100%)	0	100	100
9	J	296/296 (100%)	295 (100%)	1 (0%)	86	88
10	K	42/42 (100%)	42 (100%)	0	100	100
11	L	113/113 (100%)	112 (99%)	1 (1%)	70	81
12	M	579/580 (100%)	577 (100%)	2 (0%)	86	88
13	N	130/130 (100%)	130 (100%)	0	100	100
14	O	183/183 (100%)	183 (100%)	0	100	100
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	368/370 (100%)	365 (99%)	3 (1%)	73	82
17	S	57/58 (98%)	56 (98%)	1 (2%)	51	74
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	68/69 (99%)	68 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	V	101/101 (100%)	101 (100%)	0	100	100
21	W	122/123 (99%)	118 (97%)	4 (3%)	33	65
22	Y	62/62 (100%)	62 (100%)	0	100	100
23	Z	62/62 (100%)	62 (100%)	0	100	100
24	a	121/121 (100%)	121 (100%)	0	100	100
25	b	90/119 (76%)	90 (100%)	0	100	100
26	c	141/141 (100%)	141 (100%)	0	100	100
27	d	155/155 (100%)	155 (100%)	0	100	100
28	e	96/96 (100%)	96 (100%)	0	100	100
29	f	35/45 (78%)	35 (100%)	0	100	100
30	g	108/108 (100%)	108 (100%)	0	100	100
31	h	93/93 (100%)	93 (100%)	0	100	100
32	i	311/311 (100%)	311 (100%)	0	100	100
33	j	100/100 (100%)	99 (99%)	1 (1%)	68	80
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	540/540 (100%)	540 (100%)	0	100	100
36	m	128/141 (91%)	125 (98%)	3 (2%)	44	70
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	113/113 (100%)	113 (100%)	0	100	100
39	p	159/159 (100%)	157 (99%)	2 (1%)	61	78
40	r	410/410 (100%)	410 (100%)	0	100	100
41	s	273/275 (99%)	271 (99%)	2 (1%)	76	83
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	104/111 (94%)	104 (100%)	0	100	100
44	w	281/283 (99%)	281 (100%)	0	100	100
All	All	7144/7240 (99%)	7123 (100%)	21 (0%)	84	88

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	THR
9	J	271	TYR
11	L	171	ARG

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Mol	Chain	Res	Type
12	M	249	GLU
12	M	252	ASP
16	Q	76	LEU
16	Q	79	ASN
16	Q	80	LEU
17	S	31	ASN
21	W	30	LEU
21	W	31	SER
21	W	34	SER
21	W	40	ILE
33	j	69	ILE
36	m	23	LYS
36	m	55	MET
36	m	56	VAL
39	p	9	TYR
39	p	19	LEU
41	s	59	GLU
41	s	277	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	381	GLN
3	C	179	GLN
4	E	58	GLN
4	E	99	GLN
4	E	126	HIS
5	F	80	ASN
7	H	83	GLN
8	I	25	GLN
8	I	47	HIS
9	J	37	HIS
9	J	128	ASN
9	J	269	ASN
11	L	71	HIS
12	M	123	ASN
12	M	278	HIS
12	M	304	GLN
12	M	453	GLN
12	M	604	GLN
13	N	91	HIS
14	O	41	HIS

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Mol	Chain	Res	Type
14	O	48	ASN
14	O	187	GLN
15	P	55	HIS
15	P	75	GLN
15	P	124	ASN
15	P	164	ASN
17	S	31	ASN
17	S	68	ASN
18	T	120	GLN
20	V	134	GLN
21	W	90	ASN
23	Z	21	GLN
23	Z	60	ASN
24	a	170	GLN
25	b	67	HIS
27	d	55	GLN
28	e	86	ASN
28	e	145	ASN
29	f	61	GLN
31	h	70	GLN
31	h	97	HIS
32	i	47	ASN
32	i	112	HIS
32	i	134	GLN
32	i	172	GLN
32	i	174	GLN
33	j	83	ASN
34	k	57	ASN
34	k	91	GLN
35	l	59	GLN
35	l	135	ASN
35	l	192	HIS
35	l	199	GLN
35	l	470	ASN
35	l	479	ASN
36	m	175	ASN
39	p	13	GLN
40	r	175	ASN
40	r	338	HIS
41	s	250	HIS
41	s	284	GLN
42	u	30	HIS

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Mol	Chain	Res	Type
43	v	44	GLN
43	v	82	HIS
43	v	84	GLN
44	w	188	ASN
44	w	323	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	2MR	Q	118	16	10,12,13	2.03	1 (10%)	5,13,15	6.07	3 (60%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.71	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	12.38	130.83	119.48
16	Q	118	2MR	CD-NE-CZ	4.25	131.35	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.20	130.51	123.65

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 2 are monoatomic - leaving 38 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	$\# Z > 2$
55	CDL	l	702	-	98,98,99	1.11	8 (8%)	104,110,111	0.91	4 (3%)
52	UQ	J	402	-	33,33,63	3.53	9 (27%)	42,43,79	2.78	15 (35%)
48	PLX	g	201	-	51,51,51	1.20	4 (7%)	53,59,59	0.65	1 (1%)
47	PEE	l	701	-	39,39,50	1.33	6 (15%)	42,44,55	1.11	3 (7%)
47	PEE	l	705	-	45,45,50	1.24	6 (13%)	48,50,55	0.97	2 (4%)
50	8Q1	G	201	6	32,34,34	1.62	6 (18%)	39,43,43	1.68	5 (12%)
55	CDL	r	503	-	98,98,99	1.11	8 (8%)	104,110,111	0.87	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	PEE	W	201	-	40,40,50	1.16	5 (12%)	43,45,55	1.04	2 (4%)
47	PEE	s	401	-	46,46,50	1.23	6 (13%)	49,51,55	1.00	2 (4%)
55	CDL	a	201	-	99,99,99	1.11	8 (8%)	105,111,111	0.86	4 (3%)
48	PLX	j	202	-	51,51,51	1.20	4 (7%)	53,59,59	0.62	1 (1%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-
55	CDL	S	101	-	50,50,99	1.43	9 (18%)	56,62,111	1.20	4 (7%)
49	970	C	303	-	33,33,33	4.89	16 (48%)	48,50,50	2.95	22 (45%)
45	SF4	A	501	1	0,12,12	-	-	-	-	-
45	SF4	B	302	2	0,12,12	-	-	-	-	-
53	FES	O	301	14	0,4,4	-	-	-	-	-
48	PLX	C	302	-	51,51,51	0.61	0	53,59,59	0.74	1 (1%)
47	PEE	l	704	-	49,49,50	1.19	6 (12%)	52,54,55	0.95	2 (3%)
46	FMN	A	502	-	33,33,33	1.43	6 (18%)	48,50,50	1.30	8 (16%)
48	PLX	a	202	-	51,51,51	1.21	4 (7%)	53,59,59	0.60	1 (1%)
53	FES	M	803	12	0,4,4	-	-	-	-	-
55	CDL	n	101	-	54,54,99	1.38	9 (16%)	60,66,111	1.10	4 (6%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
55	CDL	V	201	-	93,93,99	1.14	9 (9%)	99,105,111	0.89	4 (4%)
55	CDL	V	202	-	99,99,99	1.11	8 (8%)	105,111,111	0.89	4 (3%)
55	CDL	l	703	-	99,99,99	1.11	8 (8%)	105,111,111	0.88	4 (3%)
47	PEE	j	201	-	50,50,50	1.18	6 (12%)	53,55,55	0.96	2 (3%)
48	PLX	e	201	-	51,51,51	1.21	5 (9%)	53,59,59	0.55	1 (1%)
47	PEE	r	501	-	50,50,50	1.18	6 (12%)	53,55,55	0.98	2 (3%)
45	SF4	C	301	3	0,12,12	-	-	-	-	-
48	PLX	r	502	-	51,51,51	1.21	5 (9%)	53,59,59	0.61	1 (1%)
50	8Q1	X	201	-	32,34,34	1.61	6 (18%)	39,43,43	1.60	6 (15%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
51	NDP	J	401	-	51,52,52	4.28	25 (49%)	71,80,80	2.22	14 (19%)
47	PEE	B	303	-	50,50,50	1.18	6 (12%)	53,55,55	1.01	2 (3%)
52	UQ	s	402	-	38,38,63	3.63	11 (28%)	48,49,79	2.75	17 (35%)
57	ADP	w	401	-	28,29,29	3.18	9 (32%)	43,45,45	1.91	9 (20%)

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
55	CDL	l	702	-	-	54/109/109/110	-
52	UQ	J	402	-	-	11/27/51/87	0/1/1/1
48	PLX	g	201	-	-	36/55/55/55	-
47	PEE	l	701	-	-	24/43/43/54	-
47	PEE	l	705	-	-	26/49/49/54	-
50	8Q1	G	201	6	-	17/41/41/41	-
55	CDL	r	503	-	-	55/109/109/110	-
47	PEE	W	201	-	-	25/44/44/54	-
47	PEE	s	401	-	-	24/50/50/54	-
55	CDL	a	201	-	-	58/110/110/110	-
48	PLX	j	202	-	-	31/55/55/55	-
45	SF4	M	801	12	-	-	0/6/5/5
55	CDL	S	101	-	-	33/61/61/110	-
49	970	C	303	-	-	4/8/41/41	0/5/5/5
45	SF4	A	501	1	-	-	0/6/5/5
45	SF4	B	302	2	-	-	0/6/5/5
53	FES	O	301	14	-	-	0/1/1/1
48	PLX	C	302	-	-	20/55/55/55	-
47	PEE	l	704	-	-	28/53/53/54	-
46	FMN	A	502	-	-	7/18/18/18	0/3/3/3
48	PLX	a	202	-	-	30/55/55/55	-
53	FES	M	803	12	-	-	0/1/1/1
55	CDL	n	101	-	-	29/65/65/110	-
45	SF4	B	301	2	-	-	0/6/5/5
55	CDL	V	201	-	-	61/104/104/110	-
55	CDL	V	202	-	-	59/110/110/110	-
55	CDL	l	703	-	-	47/110/110/110	-
47	PEE	j	201	-	-	24/54/54/54	-
48	PLX	e	201	-	-	30/55/55/55	-
47	PEE	r	501	-	-	25/54/54/54	-
45	SF4	C	301	3	-	-	0/6/5/5
48	PLX	r	502	-	-	22/55/55/55	-
50	8Q1	X	201	-	-	21/41/41/41	-
45	SF4	M	802	12	-	-	0/6/5/5
51	NDP	J	401	-	-	9/34/77/77	0/5/5/5
47	PEE	B	303	-	-	22/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	UQ	s	402	-	-	12/33/57/87	0/1/1/1
57	ADP	w	401	-	-	6/16/32/32	0/3/3/3

All (224) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	C	303	970	O16-C17	17.54	1.57	1.37
51	J	401	NDP	C3B-C2B	-13.17	1.24	1.53
49	C	303	970	O25-C24	11.48	1.37	1.22
51	J	401	NDP	O4D-C4D	10.76	1.68	1.45
52	s	402	UQ	C18-C19	10.04	1.56	1.33
52	J	402	UQ	C18-C19	9.97	1.56	1.33
51	J	401	NDP	C3D-C4D	-9.95	1.27	1.53
52	J	402	UQ	C13-C14	9.69	1.55	1.33
52	s	402	UQ	C13-C14	9.60	1.55	1.33
52	s	402	UQ	C23-C24	9.36	1.54	1.33
49	C	303	970	C23-C24	9.31	1.61	1.52
52	s	402	UQ	C8-C9	9.29	1.54	1.33
52	J	402	UQ	C8-C9	9.14	1.54	1.33
57	w	401	ADP	C3'-C4'	-8.97	1.30	1.53
51	J	401	NDP	O4B-C4B	-7.95	1.27	1.45
57	w	401	ADP	O4'-C4'	7.70	1.62	1.45
52	J	402	UQ	C23-C24	7.52	1.54	1.32
49	C	303	970	C14-C23	-7.51	1.45	1.52
51	J	401	NDP	C2N-C3N	7.36	1.55	1.35
52	s	402	UQ	C28-C29	7.33	1.54	1.32
51	J	401	NDP	C6N-C5N	7.22	1.55	1.33
51	J	401	NDP	PN-O3	6.68	1.66	1.59
57	w	401	ADP	PA-O3A	6.66	1.66	1.59
49	C	303	970	O08-C07	6.65	1.47	1.37
51	J	401	NDP	PA-O3	5.79	1.65	1.59
51	J	401	NDP	P2B-O2B	5.77	1.69	1.59
51	J	401	NDP	C6A-N6A	5.71	1.48	1.34
57	w	401	ADP	C6-N6	5.40	1.48	1.34
51	J	401	NDP	C3B-C4B	5.35	1.66	1.53
49	C	303	970	C05-C04	-5.28	1.46	1.54
51	J	401	NDP	C6N-N1N	5.08	1.49	1.37
51	J	401	NDP	O4D-C1D	-5.07	1.30	1.42
50	X	201	8Q1	C34-N36	5.05	1.45	1.33
50	G	201	8Q1	C39-N41	5.05	1.45	1.33
50	X	201	8Q1	C39-N41	5.02	1.45	1.33
49	C	303	970	O13-C12	4.99	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	C	303	970	C03-C02	4.98	1.53	1.34
50	G	201	8Q1	C34-N36	4.95	1.45	1.33
46	A	502	FMN	C9A-C5A	4.88	1.49	1.41
51	J	401	NDP	C1B-N9A	-4.64	1.33	1.46
51	J	401	NDP	O4B-C1B	4.61	1.52	1.42
57	w	401	ADP	O4'-C1'	-4.51	1.31	1.42
51	J	401	NDP	O2D-C2D	-4.07	1.32	1.43
47	s	401	PEE	C18-C19	3.84	1.53	1.31
47	l	701	PEE	C18-C19	3.83	1.53	1.31
47	l	704	PEE	C18-C19	3.81	1.53	1.31
47	j	201	PEE	C18-C19	3.81	1.53	1.31
47	B	303	PEE	C18-C19	3.81	1.53	1.31
47	l	705	PEE	C18-C19	3.81	1.53	1.31
51	J	401	NDP	C7N-N7N	3.80	1.44	1.33
47	r	501	PEE	C18-C19	3.79	1.53	1.31
47	W	201	PEE	C18-C19	3.79	1.53	1.31
47	r	501	PEE	C39-C38	3.74	1.53	1.31
47	s	401	PEE	C39-C38	3.74	1.53	1.31
47	B	303	PEE	C39-C38	3.73	1.52	1.31
47	l	705	PEE	C39-C38	3.73	1.52	1.31
47	l	701	PEE	C39-C38	3.72	1.52	1.31
47	j	201	PEE	C39-C38	3.69	1.52	1.31
47	l	704	PEE	C39-C38	3.69	1.52	1.31
49	C	303	970	C15-C14	3.53	1.57	1.51
55	l	703	CDL	OA8-CA7	3.48	1.43	1.33
55	n	101	CDL	OA8-CA7	3.47	1.43	1.33
55	V	201	CDL	OA8-CA7	3.45	1.43	1.33
55	l	702	CDL	OA8-CA7	3.44	1.43	1.33
49	C	303	970	C11-C24	3.42	1.54	1.48
55	S	101	CDL	OA8-CA7	3.42	1.43	1.33
55	a	201	CDL	OA8-CA7	3.40	1.43	1.33
55	V	202	CDL	OA8-CA7	3.40	1.43	1.33
57	w	401	ADP	C8-N9	-3.35	1.31	1.37
55	r	503	CDL	OA8-CA7	3.34	1.43	1.33
46	A	502	FMN	C8-C7	3.26	1.48	1.40
51	J	401	NDP	C8A-N9A	-3.25	1.32	1.37
57	w	401	ADP	O2'-C2'	-3.19	1.35	1.43
55	S	101	CDL	OA6-CA5	3.16	1.43	1.34
55	S	101	CDL	OB8-CB7	3.11	1.42	1.33
55	a	201	CDL	OB6-CB5	3.10	1.43	1.34
49	C	303	970	O16-C15	3.09	1.52	1.44
51	J	401	NDP	C5A-N7A	-3.08	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	V	201	CDL	OA6-CA5	3.07	1.42	1.34
55	r	503	CDL	OB6-CB5	3.05	1.42	1.34
55	a	201	CDL	OB8-CB7	3.03	1.42	1.33
55	l	702	CDL	OB8-CB7	3.02	1.42	1.33
55	r	503	CDL	OB8-CB7	3.00	1.42	1.33
55	V	201	CDL	OB6-CB5	3.00	1.42	1.34
55	S	101	CDL	OB6-CB5	2.99	1.42	1.34
55	l	703	CDL	OB8-CB7	2.98	1.42	1.33
55	l	703	CDL	OB6-CB5	2.98	1.42	1.34
55	n	101	CDL	OB6-CB5	2.97	1.42	1.34
55	V	202	CDL	OB6-CB5	2.96	1.42	1.34
55	a	201	CDL	OA6-CA5	2.96	1.42	1.34
55	V	201	CDL	OB8-CB7	2.95	1.42	1.33
52	J	402	UQ	C6-C1	2.95	1.54	1.46
57	w	401	ADP	O3'-C3'	2.95	1.50	1.43
48	g	201	PLX	O6-C4	-2.95	1.40	1.44
55	V	202	CDL	OB8-CB7	2.94	1.41	1.33
55	l	703	CDL	OA6-CA5	2.94	1.42	1.34
55	V	202	CDL	OA6-CA5	2.94	1.42	1.34
55	n	101	CDL	OB8-CB7	2.94	1.41	1.33
55	n	101	CDL	OA6-CA5	2.93	1.42	1.34
55	l	702	CDL	OB6-CB5	2.93	1.42	1.34
55	l	702	CDL	OA6-CA5	2.88	1.42	1.34
51	J	401	NDP	O3D-C3D	2.86	1.50	1.43
55	r	503	CDL	OA6-CA5	2.85	1.42	1.34
48	r	502	PLX	O6-C4	-2.85	1.41	1.44
51	J	401	NDP	C7N-C3N	2.84	1.54	1.48
48	a	202	PLX	O6-C4	-2.83	1.41	1.44
48	e	201	PLX	O6-C4	-2.76	1.41	1.44
52	s	402	UQ	C6-C1	2.73	1.54	1.46
49	C	303	970	C12-C06	2.69	1.43	1.39
46	A	502	FMN	C4-N3	-2.68	1.33	1.38
47	B	303	PEE	O2-C2	-2.67	1.40	1.46
55	r	503	CDL	OA6-CA4	-2.66	1.40	1.46
49	C	303	970	C09-C07	2.66	1.45	1.39
55	l	702	CDL	OA6-CA4	-2.63	1.40	1.46
47	l	705	PEE	O2-C2	-2.62	1.40	1.46
47	j	201	PEE	O2-C2	-2.61	1.40	1.46
47	r	501	PEE	O2-C2	-2.61	1.40	1.46
48	j	202	PLX	O6-C4	-2.60	1.41	1.44
55	V	202	CDL	OA6-CA4	-2.59	1.40	1.46
47	s	401	PEE	O2-C2	-2.58	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	n	101	CDL	OA6-CA4	-2.58	1.40	1.46
47	W	201	PEE	O2-C2	-2.57	1.40	1.46
47	l	705	PEE	O3-C30	2.54	1.40	1.33
55	a	201	CDL	OA6-CA4	-2.53	1.40	1.46
55	l	703	CDL	OA6-CA4	-2.52	1.40	1.46
47	l	704	PEE	O2-C2	-2.51	1.40	1.46
51	J	401	NDP	O2B-C2B	2.49	1.52	1.44
48	e	201	PLX	C7-C6	2.48	1.55	1.50
47	j	201	PEE	O3-C30	2.47	1.40	1.33
47	l	701	PEE	O3-C30	2.47	1.40	1.33
55	l	703	CDL	OB6-CB4	-2.44	1.40	1.46
47	s	401	PEE	O3-C30	2.44	1.40	1.33
47	l	704	PEE	O3-C30	2.43	1.40	1.33
48	j	202	PLX	C7-C6	2.43	1.55	1.50
57	w	401	ADP	C5-N7	-2.41	1.34	1.39
50	G	201	8Q1	O35-C34	-2.41	1.18	1.23
47	B	303	PEE	O3-C30	2.41	1.40	1.33
55	V	202	CDL	OB6-CB4	-2.41	1.40	1.46
50	X	201	8Q1	C1-S44	2.41	1.81	1.76
55	l	702	CDL	OB6-CB4	-2.40	1.40	1.46
50	G	201	8Q1	C1-S44	2.40	1.81	1.76
47	l	701	PEE	O2-C2	-2.40	1.41	1.46
50	G	201	8Q1	O40-C39	-2.39	1.18	1.23
48	a	202	PLX	C7-C6	2.39	1.55	1.50
47	r	501	PEE	O3-C30	2.38	1.40	1.33
48	r	502	PLX	C7-C6	2.38	1.55	1.50
47	W	201	PEE	O3-C30	2.37	1.40	1.33
48	g	201	PLX	C7-C6	2.37	1.55	1.50
52	s	402	UQ	C7-C8	2.35	1.54	1.50
55	n	101	CDL	OB6-CB4	-2.34	1.41	1.46
55	S	101	CDL	OB6-CB4	-2.34	1.41	1.46
47	l	701	PEE	O2-C10	2.33	1.40	1.34
55	V	201	CDL	OB6-CB4	-2.33	1.41	1.46
52	J	402	UQ	C7-C8	2.32	1.54	1.50
50	X	201	8Q1	O35-C34	-2.31	1.19	1.23
50	X	201	8Q1	O40-C39	-2.31	1.18	1.23
55	V	201	CDL	PB2-OB5	2.30	1.68	1.59
55	a	201	CDL	OB6-CB4	-2.30	1.41	1.46
55	V	201	CDL	PB2-OB2	2.29	1.68	1.59
46	A	502	FMN	C5A-N5	-2.29	1.35	1.39
47	l	704	PEE	O3-C3	-2.28	1.40	1.45
50	G	201	8Q1	C6-C1	2.28	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	l	704	PEE	O2-C10	2.27	1.40	1.34
47	s	401	PEE	O2-C10	2.27	1.40	1.34
55	V	202	CDL	PB2-OB2	2.27	1.68	1.59
50	X	201	8Q1	C6-C1	2.26	1.53	1.50
55	V	201	CDL	OA6-CA4	-2.26	1.41	1.46
55	r	503	CDL	PB2-OB2	2.25	1.68	1.59
55	r	503	CDL	OB6-CB4	-2.25	1.41	1.46
55	S	101	CDL	PB2-OB5	2.24	1.68	1.59
55	l	703	CDL	PB2-OB2	2.24	1.68	1.59
55	S	101	CDL	OA6-CA4	-2.24	1.41	1.46
47	j	201	PEE	O2-C10	2.24	1.40	1.34
55	n	101	CDL	PB2-OB2	2.24	1.68	1.59
47	B	303	PEE	O2-C10	2.23	1.40	1.34
51	J	401	NDP	C2D-C3D	2.23	1.59	1.53
48	j	202	PLX	P1-O4	2.23	1.68	1.59
55	r	503	CDL	PB2-OB5	2.22	1.68	1.59
55	a	201	CDL	PB2-OB2	2.22	1.68	1.59
55	l	703	CDL	PB2-OB5	2.22	1.68	1.59
49	C	303	970	C05-C06	-2.21	1.48	1.51
47	r	501	PEE	O3-C3	-2.21	1.40	1.45
51	J	401	NDP	O7N-C7N	-2.21	1.19	1.24
48	a	202	PLX	P1-O4	2.21	1.68	1.59
47	l	705	PEE	O2-C10	2.21	1.40	1.34
55	a	201	CDL	PB2-OB5	2.21	1.68	1.59
55	n	101	CDL	PB2-OB5	2.20	1.68	1.59
55	V	202	CDL	PB2-OB5	2.20	1.68	1.59
47	l	701	PEE	O3-C3	-2.19	1.40	1.45
47	r	501	PEE	O2-C10	2.19	1.40	1.34
55	S	101	CDL	PB2-OB2	2.18	1.67	1.59
55	l	702	CDL	PB2-OB2	2.18	1.67	1.59
55	l	702	CDL	PB2-OB5	2.18	1.67	1.59
47	W	201	PEE	O2-C10	2.18	1.40	1.34
47	j	201	PEE	O3-C3	-2.17	1.40	1.45
52	J	402	UQ	O4-C4	-2.15	1.18	1.23
48	e	201	PLX	P1-O4	2.15	1.67	1.59
47	W	201	PEE	O3-C3	-2.15	1.40	1.45
51	J	401	NDP	PA-O5B	2.15	1.67	1.59
48	r	502	PLX	P1-O4	2.15	1.67	1.59
48	g	201	PLX	P1-O4	2.13	1.67	1.59
52	s	402	UQ	O4-C4	-2.13	1.18	1.23
47	B	303	PEE	O3-C3	-2.13	1.40	1.45
52	J	402	UQ	O3-CM3	-2.12	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	s	401	PEE	O3-C3	-2.12	1.40	1.45
46	A	502	FMN	C4A-N5	2.12	1.35	1.30
48	j	202	PLX	P1-O1	2.11	1.67	1.59
48	r	502	PLX	P1-O1	2.11	1.67	1.59
49	C	303	970	O26-C20	2.10	1.40	1.37
52	s	402	UQ	O3-CM3	-2.10	1.40	1.45
52	s	402	UQ	C21-C19	2.08	1.55	1.51
49	C	303	970	C04-C02	2.07	1.52	1.50
48	g	201	PLX	P1-O1	2.05	1.67	1.59
47	l	705	PEE	O3-C3	-2.04	1.40	1.45
55	S	101	CDL	C11-CA5	2.04	1.56	1.50
48	a	202	PLX	P1-O1	2.04	1.67	1.59
48	e	201	PLX	C1-C2	2.04	1.57	1.51
52	J	402	UQ	C21-C19	2.03	1.55	1.51
55	V	201	CDL	C11-CA5	2.03	1.56	1.50
48	r	502	PLX	C25-C24	2.03	1.55	1.50
48	e	201	PLX	P1-O1	2.02	1.67	1.59
52	s	402	UQ	O1-C1	-2.02	1.18	1.23
55	n	101	CDL	C11-CA5	2.02	1.56	1.50
46	A	502	FMN	C2-N3	-2.00	1.34	1.39

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	C	303	970	O25-C24-C23	-8.98	108.57	120.99
49	C	303	970	O25-C24-C11	-8.64	108.82	122.18
52	s	402	UQ	C7-C8-C9	-8.03	113.00	126.83
52	J	402	UQ	C7-C8-C9	-7.88	113.26	126.83
51	J	401	NDP	C3N-C2N-N1N	-7.83	111.70	123.20
51	J	401	NDP	C1D-N1N-C2N	-7.29	109.13	121.14
49	C	303	970	O08-C07-C06	-7.28	108.65	112.99
50	G	201	8Q1	C6-C1-S44	6.56	121.22	113.40
52	s	402	UQ	C22-C23-C24	-6.28	113.25	127.62
52	s	402	UQ	C12-C13-C14	-6.27	113.27	127.62
52	J	402	UQ	C12-C13-C14	-6.16	113.52	127.62
52	J	402	UQ	C17-C18-C19	-6.13	113.60	127.62
51	J	401	NDP	C6N-N1N-C2N	-6.06	112.84	119.32
52	s	402	UQ	C17-C18-C19	-5.97	113.96	127.62
50	X	201	8Q1	C6-C1-S44	5.88	120.41	113.40
49	C	303	970	C06-C05-C04	5.67	106.42	101.45
51	J	401	NDP	C1D-N1N-C6N	-5.59	108.96	120.77
51	J	401	NDP	C5A-C4A-N3A	-5.50	119.15	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	w	401	ADP	C5-C4-N3	-5.49	119.16	126.72
52	J	402	UQ	C10-C9-C8	-4.70	111.56	123.63
57	w	401	ADP	N3-C2-N1	-4.63	121.58	128.58
52	s	402	UQ	C27-C28-C29	-4.46	112.77	127.64
52	J	402	UQ	C22-C23-C24	-4.42	112.91	127.64
57	w	401	ADP	N3-C4-N9	4.36	134.57	127.17
52	s	402	UQ	C10-C9-C8	-4.33	112.52	123.63
49	C	303	970	C01-C02-C03	-4.29	111.67	121.38
55	S	101	CDL	OA6-CA5-C11	4.28	120.75	111.48
52	s	402	UQ	C25-C24-C23	-4.27	112.66	123.63
55	S	101	CDL	OB6-CB5-C51	4.15	120.47	111.48
51	J	401	NDP	N3A-C2A-N1A	-4.10	122.38	128.58
47	r	501	PEE	O2-C10-C11	4.07	120.29	111.48
47	l	701	PEE	O2-C10-C11	4.07	120.28	111.48
55	a	201	CDL	OB6-CB5-C51	4.04	120.22	111.48
55	V	202	CDL	OA6-CA5-C11	4.01	120.16	111.48
47	W	201	PEE	O2-C10-C11	4.01	120.15	111.48
55	V	201	CDL	OA6-CA5-C11	4.01	120.15	111.48
49	C	303	970	O08-C07-C09	4.00	131.72	123.85
55	l	702	CDL	OB6-CB5-C51	4.00	120.13	111.48
55	l	702	CDL	OA6-CA5-C11	4.00	120.13	111.48
55	l	703	CDL	OB6-CB5-C51	4.00	120.12	111.48
55	V	201	CDL	OB6-CB5-C51	3.97	120.06	111.48
52	s	402	UQ	C20-C19-C18	-3.96	113.46	123.63
55	l	703	CDL	OA6-CA5-C11	3.95	120.02	111.48
55	V	202	CDL	OB6-CB5-C51	3.94	120.00	111.48
47	B	303	PEE	O2-C10-C11	3.94	120.00	111.48
52	J	402	UQ	C15-C14-C13	-3.93	113.53	123.63
55	n	101	CDL	OA6-CA5-C11	3.92	119.97	111.48
51	J	401	NDP	N3A-C4A-N9A	3.90	133.80	127.17
55	r	503	CDL	OA6-CA5-C11	3.89	119.89	111.48
52	J	402	UQ	C7-C6-C5	-3.87	118.26	124.89
50	G	201	8Q1	O4-C1-C6	-3.87	119.52	123.98
47	j	201	PEE	O2-C10-C11	3.87	119.84	111.48
47	s	401	PEE	O2-C10-C11	3.84	119.79	111.48
55	r	503	CDL	OB6-CB5-C51	3.84	119.79	111.48
55	n	101	CDL	OB6-CB5-C51	3.80	119.70	111.48
47	l	704	PEE	O2-C10-C11	3.79	119.68	111.48
52	J	402	UQ	C20-C19-C18	-3.75	114.00	123.63
52	J	402	UQ	C11-C9-C8	-3.74	112.76	121.17
50	X	201	8Q1	O4-C1-C6	-3.73	119.68	123.98
55	a	201	CDL	OA6-CA5-C11	3.70	119.48	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	C	303	970	C04-C02-C03	-3.69	112.31	120.38
52	J	402	UQ	C16-C14-C13	-3.65	112.97	121.17
52	s	402	UQ	C15-C14-C13	-3.64	114.28	123.63
47	l	705	PEE	O2-C10-C11	3.64	119.35	111.48
52	J	402	UQ	C21-C19-C18	-3.64	113.00	121.17
52	s	402	UQ	C26-C24-C23	-3.63	113.02	121.17
57	w	401	ADP	N9-C8-N7	-3.59	108.84	113.94
57	w	401	ADP	C2-N3-C4	3.58	120.57	111.83
51	J	401	NDP	C2A-N3A-C4A	3.57	120.54	111.83
52	s	402	UQ	C21-C19-C18	-3.54	113.22	121.17
52	J	402	UQ	C7-C6-C1	3.39	122.46	118.52
49	C	303	970	C09-C07-C06	-3.37	119.63	123.21
52	s	402	UQ	C11-C9-C8	-3.29	113.78	121.17
52	s	402	UQ	C30-C29-C28	-3.29	112.78	122.66
57	w	401	ADP	C4-N9-C8	3.26	109.17	105.74
57	w	401	ADP	C5-N7-C8	3.23	108.52	103.45
49	C	303	970	C22-C23-C14	3.22	114.25	109.64
52	J	402	UQ	C25-C24-C23	-3.22	112.99	122.66
52	s	402	UQ	C31-C29-C28	-3.17	113.14	122.66
51	J	401	NDP	C4A-C5A-N7A	-3.15	106.98	110.58
47	B	303	PEE	O3-C30-C31	3.13	121.39	111.83
49	C	303	970	O28-C19-C20	3.09	119.60	115.40
52	J	402	UQ	C26-C24-C23	-3.08	113.40	122.66
49	C	303	970	C05-C04-C02	-3.06	110.86	115.53
49	C	303	970	O26-C20-C19	3.03	119.51	115.40
51	J	401	NDP	N9A-C8A-N7A	-3.03	109.64	113.94
50	X	201	8Q1	C37-C38-C39	3.01	117.41	112.39
51	J	401	NDP	C5A-N7A-C8A	2.97	108.12	103.45
57	w	401	ADP	C4-C5-N7	-2.95	107.21	110.58
49	C	303	970	O13-C14-C23	2.91	115.34	112.44
55	n	101	CDL	OA8-CA7-C31	2.89	119.92	111.15
55	V	202	CDL	OB8-CB7-C71	2.86	120.56	111.83
55	l	702	CDL	OA8-CA7-C31	2.82	120.43	111.83
55	S	101	CDL	OA8-CA7-C31	2.80	120.37	111.83
55	l	703	CDL	OB8-CB7-C71	2.80	120.36	111.83
47	l	704	PEE	O3-C30-C31	2.79	120.36	111.83
55	n	101	CDL	OB8-CB7-C71	2.79	120.33	111.83
47	r	501	PEE	O3-C30-C31	2.78	120.32	111.83
55	V	201	CDL	OB8-CB7-C71	2.78	120.31	111.83
52	J	402	UQ	CM5-C5-C6	-2.78	119.88	124.45
52	s	402	UQ	C16-C14-C13	-2.78	114.93	121.17
47	s	401	PEE	O3-C30-C31	2.78	120.30	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	a	201	CDL	OB8-CB7-C71	2.78	120.30	111.83
47	l	705	PEE	O3-C30-C31	2.75	120.23	111.83
47	j	201	PEE	O3-C30-C31	2.74	120.18	111.83
47	W	201	PEE	O3-C30-C31	2.74	120.17	111.83
55	l	702	CDL	OB8-CB7-C71	2.73	120.16	111.83
55	S	101	CDL	OB8-CB7-C71	2.73	120.15	111.83
55	l	703	CDL	OA8-CA7-C31	2.71	120.10	111.83
55	r	503	CDL	OB8-CB7-C71	2.71	120.09	111.83
50	G	201	8Q1	O4-C1-S44	-2.69	119.26	122.68
55	r	503	CDL	OA8-CA7-C31	2.67	119.96	111.83
47	l	701	PEE	O3-C30-C31	2.66	119.95	111.83
55	V	202	CDL	OA8-CA7-C31	2.61	119.80	111.83
46	A	502	FMN	C4A-C10-N1	-2.58	118.26	124.59
55	a	201	CDL	OA8-CA7-C31	2.58	119.69	111.83
48	g	201	PLX	C1A-N1-C1	2.57	120.14	109.91
46	A	502	FMN	C5A-C9A-N10	2.53	120.25	117.97
55	V	201	CDL	OA8-CA7-C31	2.52	119.53	111.83
51	J	401	NDP	C2B-C3B-C4B	2.50	107.38	101.99
52	s	402	UQ	C7-C6-C5	-2.48	120.63	124.89
48	r	502	PLX	C1A-N1-C1	2.46	119.71	109.91
48	a	202	PLX	C1A-N1-C1	2.46	119.70	109.91
50	X	201	8Q1	C43-S44-C1	2.44	109.05	101.84
49	C	303	970	C21-C22-C17	2.43	120.50	117.09
48	j	202	PLX	C1A-N1-C1	2.42	119.55	109.91
52	s	402	UQ	CM5-C5-C6	-2.42	120.47	124.45
50	G	201	8Q1	C38-C39-N41	2.41	120.73	116.34
49	C	303	970	C11-C12-C06	-2.39	119.54	123.22
48	C	302	PLX	C2-C1-N1	-2.38	108.20	115.82
46	A	502	FMN	C4-C4A-N5	2.37	121.48	118.21
51	J	401	NDP	C4A-N9A-C8A	2.34	108.20	105.74
47	l	701	PEE	C20-C19-C18	-2.34	112.32	126.42
51	J	401	NDP	C2B-C1B-N9A	-2.33	109.92	113.75
49	C	303	970	O28-C19-C18	-2.29	120.13	124.08
50	G	201	8Q1	C37-C38-C39	2.26	116.17	112.39
49	C	303	970	O16-C17-C22	-2.24	120.43	122.83
46	A	502	FMN	C9A-C5A-N5	-2.23	120.09	122.45
46	A	502	FMN	O4-C4-C4A	-2.23	120.65	126.53
49	C	303	970	C01-C02-C04	-2.22	111.51	116.45
50	X	201	8Q1	O4-C1-S44	-2.18	119.90	122.68
48	e	201	PLX	C1A-N1-C1	2.18	118.58	109.91
46	A	502	FMN	C4A-C4-N3	2.12	118.65	113.25
49	C	303	970	C07-C06-C12	2.11	120.73	118.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	X	201	8Q1	C32-C34-N36	2.10	120.46	116.48
46	A	502	FMN	C10-N1-C2	2.08	121.35	116.85
46	A	502	FMN	C4-N3-C2	-2.08	121.95	125.64
57	w	401	ADP	C2'-C3'-C4'	2.07	106.61	102.61
49	C	303	970	C29-O28-C19	-2.06	114.49	117.51
49	C	303	970	C21-C22-C23	-2.06	117.11	121.12
49	C	303	970	O26-C20-C21	-2.02	120.60	124.08

There are no chirality outliers.

All (850) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C1'-C2'-C3'-O3'
46	A	502	FMN	C1'-C2'-C3'-C4'
47	B	303	PEE	C11-C10-O2-C2
47	W	201	PEE	C1-O3P-P-O2P
47	W	201	PEE	C1-O3P-P-O1P
47	W	201	PEE	C1-O3P-P-O4P
47	W	201	PEE	C4-O4P-P-O2P
47	W	201	PEE	O4P-C4-C5-N
47	j	201	PEE	C1-O3P-P-O1P
47	j	201	PEE	C1-O3P-P-O4P
47	j	201	PEE	C4-O4P-P-O3P
47	l	701	PEE	C1-O3P-P-O1P
47	l	701	PEE	C1-O3P-P-O4P
47	l	701	PEE	C4-O4P-P-O3P
47	l	701	PEE	C4-O4P-P-O2P
47	l	704	PEE	C4-O4P-P-O3P
47	l	705	PEE	C1-O3P-P-O1P
47	r	501	PEE	C1-O3P-P-O2P
47	r	501	PEE	C1-O3P-P-O1P
47	r	501	PEE	C1-O3P-P-O4P
48	C	302	PLX	C2-O1-P1-O4
48	C	302	PLX	C2-O1-P1-O3
48	C	302	PLX	N1-C1-C2-O1
48	a	202	PLX	O7-C6-O6-C4
48	a	202	PLX	C3-O4-P1-O2
48	a	202	PLX	C3-O4-P1-O3
48	a	202	PLX	C2-O1-P1-O4
48	a	202	PLX	C2-O1-P1-O2

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Mol	Chain	Res	Type	Atoms
48	a	202	PLX	C2-O1-P1-O3
48	e	201	PLX	O7-C6-O6-C4
48	e	201	PLX	O9-C24-O8-C5
48	g	201	PLX	O7-C6-O6-C4
48	g	201	PLX	C3-O4-P1-O2
48	g	201	PLX	C2-O1-P1-O4
48	g	201	PLX	C2-O1-P1-O2
48	g	201	PLX	C2-O1-P1-O3
48	j	202	PLX	O7-C6-C7-C8
48	j	202	PLX	C3-O4-P1-O1
48	j	202	PLX	C2-O1-P1-O4
48	j	202	PLX	C2-O1-P1-O2
48	j	202	PLX	O9-C24-O8-C5
48	r	502	PLX	O6-C6-C7-C8
48	r	502	PLX	O9-C24-C25-C26
49	C	303	970	C03-C02-C04-C05
49	C	303	970	C03-C02-C04-O08
50	G	201	8Q1	O27-C28-C29-C30
50	G	201	8Q1	O27-C28-C29-C31
50	G	201	8Q1	C28-C29-C32-C34
50	G	201	8Q1	C30-C29-C32-C34
50	G	201	8Q1	C30-C29-C32-O33
50	G	201	8Q1	C31-C29-C32-C34
50	G	201	8Q1	O33-C32-C34-N36
50	G	201	8Q1	C42-C43-S44-C1
50	X	201	8Q1	O4-C1-S44-C43
50	X	201	8Q1	C6-C1-S44-C43
50	X	201	8Q1	C28-C29-C32-C34
50	X	201	8Q1	C31-C29-C32-C34
50	X	201	8Q1	O33-C32-C34-N36
50	X	201	8Q1	C42-C43-S44-C1
50	X	201	8Q1	C28-O27-P24-O3
50	X	201	8Q1	C28-O27-P24-O2
50	X	201	8Q1	C28-O27-P24-O1
51	J	401	NDP	C5B-O5B-PA-O1A
51	J	401	NDP	C2N-C3N-C7N-N7N
52	J	402	UQ	C1-C6-C7-C8
52	J	402	UQ	C5-C6-C7-C8
52	J	402	UQ	C7-C8-C9-C10
52	J	402	UQ	C12-C13-C14-C16
52	s	402	UQ	C7-C8-C9-C11
52	s	402	UQ	C17-C18-C19-C21

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Mol	Chain	Res	Type	Atoms
52	s	402	UQ	C18-C19-C21-C22
52	s	402	UQ	C22-C23-C24-C26
55	S	101	CDL	O1-C1-CB2-OB2
55	S	101	CDL	CA2-OA2-PA1-OA4
55	S	101	CDL	CA2-OA2-PA1-OA5
55	S	101	CDL	C11-CA5-OA6-CA4
55	S	101	CDL	CB2-OB2-PB2-OB3
55	S	101	CDL	CB3-OB5-PB2-OB2
55	S	101	CDL	CB3-OB5-PB2-OB3
55	V	201	CDL	O1-C1-CA2-OA2
55	V	201	CDL	CA2-OA2-PA1-OA3
55	V	201	CDL	CA2-OA2-PA1-OA4
55	V	201	CDL	CA2-OA2-PA1-OA5
55	V	201	CDL	OA7-CA5-OA6-CA4
55	V	201	CDL	CB2-OB2-PB2-OB3
55	V	201	CDL	CB2-OB2-PB2-OB4
55	V	201	CDL	CB2-OB2-PB2-OB5
55	V	201	CDL	CB3-OB5-PB2-OB2
55	V	201	CDL	CB3-OB5-PB2-OB4
55	V	202	CDL	CA2-C1-CB2-OB2
55	V	202	CDL	OA6-CA4-CA6-OA8
55	V	202	CDL	CB2-OB2-PB2-OB3
55	V	202	CDL	CB2-OB2-PB2-OB5
55	V	202	CDL	CB3-OB5-PB2-OB2
55	V	202	CDL	CB3-OB5-PB2-OB3
55	V	202	CDL	CB3-OB5-PB2-OB4
55	V	202	CDL	OB6-CB4-CB6-OB8
55	a	201	CDL	CB2-OB2-PB2-OB3
55	a	201	CDL	CB2-OB2-PB2-OB4
55	a	201	CDL	CB2-OB2-PB2-OB5
55	a	201	CDL	CB3-OB5-PB2-OB2
55	a	201	CDL	CB3-OB5-PB2-OB3
55	a	201	CDL	CB3-OB5-PB2-OB4
55	a	201	CDL	C51-CB5-OB6-CB4
55	l	702	CDL	O1-C1-CA2-OA2
55	l	702	CDL	OA6-CA4-CA6-OA8
55	l	702	CDL	OA9-CA7-OA8-CA6
55	l	702	CDL	C31-CA7-OA8-CA6
55	l	702	CDL	CB2-OB2-PB2-OB4
55	l	702	CDL	CB2-OB2-PB2-OB5
55	l	702	CDL	CB3-OB5-PB2-OB2
55	l	702	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
55	l	703	CDL	O1-C1-CB2-OB2
55	l	703	CDL	CB2-OB2-PB2-OB3
55	l	703	CDL	CB2-OB2-PB2-OB4
55	l	703	CDL	CB2-OB2-PB2-OB5
55	l	703	CDL	CB3-OB5-PB2-OB3
55	l	703	CDL	CB3-OB5-PB2-OB4
55	n	101	CDL	CB2-C1-CA2-OA2
55	n	101	CDL	CA2-OA2-PA1-OA4
55	n	101	CDL	CA2-OA2-PA1-OA5
55	n	101	CDL	OA5-CA3-CA4-OA6
55	n	101	CDL	CB2-OB2-PB2-OB3
55	n	101	CDL	CB2-OB2-PB2-OB4
55	n	101	CDL	CB2-OB2-PB2-OB5
55	n	101	CDL	CB3-OB5-PB2-OB2
55	n	101	CDL	CB3-OB5-PB2-OB4
55	r	503	CDL	CB2-C1-CA2-OA2
55	r	503	CDL	CA2-OA2-PA1-OA3
55	r	503	CDL	CA2-OA2-PA1-OA5
55	r	503	CDL	CA3-OA5-PA1-OA2
55	r	503	CDL	CA3-OA5-PA1-OA3
55	r	503	CDL	CB3-OB5-PB2-OB3
55	r	503	CDL	C51-CB5-OB6-CB4
57	w	401	ADP	C5'-O5'-PA-O1A
57	w	401	ADP	C5'-O5'-PA-O2A
57	w	401	ADP	C5'-O5'-PA-O3A
47	B	303	PEE	O4-C10-O2-C2
47	j	201	PEE	O4-C10-O2-C2
47	l	704	PEE	O4-C10-O2-C2
47	s	401	PEE	O4-C10-O2-C2
55	S	101	CDL	OA7-CA5-OA6-CA4
55	r	503	CDL	OB7-CB5-OB6-CB4
47	j	201	PEE	C11-C10-O2-C2
47	s	401	PEE	C11-C10-O2-C2
55	V	201	CDL	C11-CA5-OA6-CA4
47	l	704	PEE	C31-C30-O3-C3
47	l	705	PEE	C31-C30-O3-C3
55	V	201	CDL	C31-CA7-OA8-CA6
55	l	703	CDL	C71-CB7-OB8-CB6
52	s	402	UQ	C7-C8-C9-C10
47	j	201	PEE	C17-C18-C19-C20
47	r	501	PEE	C17-C18-C19-C20
47	l	705	PEE	O5-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	OB7-CB5-OB6-CB4
55	S	101	CDL	O1-C1-CA2-OA2
55	l	702	CDL	O1-C1-CB2-OB2
55	n	101	CDL	O1-C1-CA2-OA2
55	n	101	CDL	O1-C1-CB2-OB2
55	r	503	CDL	O1-C1-CA2-OA2
47	l	704	PEE	O5-C30-O3-C3
47	l	701	PEE	C11-C10-O2-C2
47	l	704	PEE	C11-C10-O2-C2
55	V	201	CDL	OA9-CA7-OA8-CA6
55	l	703	CDL	OB9-CB7-OB8-CB6
52	J	402	UQ	C14-C16-C17-C18
52	s	402	UQ	C14-C16-C17-C18
55	V	202	CDL	C37-C38-C39-C40
47	l	705	PEE	C37-C38-C39-C40
48	r	502	PLX	C9-C10-C11-C12
48	r	502	PLX	C7-C8-C9-C10
55	S	101	CDL	CA2-C1-CB2-OB2
55	a	201	CDL	CA2-C1-CB2-OB2
55	l	702	CDL	CA2-C1-CB2-OB2
55	l	703	CDL	CA2-C1-CB2-OB2
55	n	101	CDL	CA2-C1-CB2-OB2
47	j	201	PEE	C31-C30-O3-C3
47	l	701	PEE	C31-C30-O3-C3
55	r	503	CDL	C71-CB7-OB8-CB6
48	g	201	PLX	C11-C10-C9-C8
52	J	402	UQ	C13-C14-C16-C17
55	n	101	CDL	C71-C72-C73-C74
48	g	201	PLX	C10-C11-C12-C13
55	V	201	CDL	C62-C63-C64-C65
55	V	202	CDL	CB7-C71-C72-C73
55	l	703	CDL	CA7-C31-C32-C33
55	l	703	CDL	CB5-C51-C52-C53
55	V	202	CDL	O1-C1-CB2-OB2
47	l	701	PEE	O5-C30-O3-C3
55	S	101	CDL	CB7-C71-C72-C73
52	J	402	UQ	C22-C23-C24-C26
55	r	503	CDL	OB9-CB7-OB8-CB6
47	l	701	PEE	O4-C10-O2-C2
48	g	201	PLX	O6-C4-C5-O8
55	a	201	CDL	C71-CB7-OB8-CB6
55	V	201	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
48	j	202	PLX	C28-C29-C30-C31
47	l	701	PEE	C11-C12-C13-C14
55	S	101	CDL	CA7-C31-C32-C33
55	a	201	CDL	CA5-C11-C12-C13
55	l	703	CDL	C17-C18-C19-C20
48	j	202	PLX	C13-C14-C15-C16
55	V	202	CDL	C11-C12-C13-C14
55	l	702	CDL	C81-C82-C83-C84
52	s	402	UQ	C27-C28-C29-C31
48	j	202	PLX	C32-C33-C34-C35
55	l	703	CDL	C39-C40-C41-C42
55	l	703	CDL	C12-C13-C14-C15
55	V	201	CDL	CB7-C71-C72-C73
55	n	101	CDL	CB7-C71-C72-C73
55	r	503	CDL	CB7-C71-C72-C73
55	l	702	CDL	CA7-C31-C32-C33
55	l	702	CDL	CB7-C71-C72-C73
47	r	501	PEE	C12-C13-C14-C15
55	l	703	CDL	C35-C36-C37-C38
55	l	703	CDL	C51-C52-C53-C54
55	V	202	CDL	O1-C1-CA2-OA2
55	a	201	CDL	O1-C1-CB2-OB2
55	l	702	CDL	C71-CB7-OB8-CB6
47	j	201	PEE	O5-C30-O3-C3
47	W	201	PEE	C10-C11-C12-C13
47	s	401	PEE	C30-C31-C32-C33
55	n	101	CDL	CB5-C51-C52-C53
55	V	201	CDL	C34-C35-C36-C37
47	l	701	PEE	C17-C18-C19-C20
46	A	502	FMN	O2'-C2'-C3'-O3'
47	l	701	PEE	C10-C11-C12-C13
48	r	502	PLX	C31-C32-C33-C34
55	V	201	CDL	C71-CB7-OB8-CB6
46	A	502	FMN	O2'-C2'-C3'-C4'
47	B	303	PEE	C34-C35-C36-C37
51	J	401	NDP	C2D-C1D-N1N-C6N
48	C	302	PLX	C15-C16-C17-C18
55	S	101	CDL	CB2-C1-CA2-OA2
55	V	201	CDL	CB2-C1-CA2-OA2
55	l	702	CDL	CB2-C1-CA2-OA2
47	W	201	PEE	C31-C30-O3-C3
47	r	501	PEE	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	C34-C35-C36-C37
55	l	702	CDL	C34-C35-C36-C37
48	j	202	PLX	O6-C6-C7-C8
55	V	201	CDL	C51-CB5-OB6-CB4
48	g	201	PLX	C17-C18-C19-C20
48	C	302	PLX	C9-C10-C11-C12
55	V	201	CDL	OB7-CB5-OB6-CB4
47	B	303	PEE	C17-C18-C19-C20
55	l	703	CDL	C41-C42-C43-C44
55	a	201	CDL	OB9-CB7-OB8-CB6
55	l	703	CDL	CA5-C11-C12-C13
55	V	202	CDL	C57-C58-C59-C60
55	l	702	CDL	OB9-CB7-OB8-CB6
55	l	702	CDL	OA5-CA3-CA4-OA6
55	r	503	CDL	C51-C52-C53-C54
55	l	703	CDL	C61-C62-C63-C64
55	V	201	CDL	OB9-CB7-OB8-CB6
47	s	401	PEE	C42-C43-C44-C45
47	W	201	PEE	C11-C12-C13-C14
48	j	202	PLX	C7-C8-C9-C10
55	V	201	CDL	C17-C18-C19-C20
47	l	704	PEE	C30-C31-C32-C33
48	g	201	PLX	C25-C26-C27-C28
55	V	201	CDL	C56-C57-C58-C59
55	V	202	CDL	C14-C15-C16-C17
55	V	202	CDL	C55-C56-C57-C58
48	C	302	PLX	O9-C24-C25-C26
48	g	201	PLX	O9-C24-C25-C26
48	r	502	PLX	O7-C6-C7-C8
48	a	202	PLX	C9-C10-C11-C12
48	e	201	PLX	C13-C14-C15-C16
48	e	201	PLX	C10-C11-C12-C13
48	g	201	PLX	C14-C15-C16-C17
55	S	101	CDL	C71-C72-C73-C74
55	V	202	CDL	C17-C18-C19-C20
55	V	202	CDL	C52-C53-C54-C55
55	n	101	CDL	C55-C56-C57-C58
55	r	503	CDL	C31-C32-C33-C34
55	r	503	CDL	C32-C33-C34-C35
48	a	202	PLX	C28-C29-C30-C31
55	l	703	CDL	C74-C75-C76-C77
55	V	201	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
47	l	705	PEE	C22-C23-C24-C25
48	j	202	PLX	C11-C12-C13-C14
55	l	702	CDL	C62-C63-C64-C65
55	l	703	CDL	C32-C33-C34-C35
48	g	201	PLX	C9-C10-C11-C12
48	j	202	PLX	C25-C26-C27-C28
55	V	201	CDL	C35-C36-C37-C38
55	l	702	CDL	C59-C60-C61-C62
55	l	702	CDL	C35-C36-C37-C38
55	l	702	CDL	C52-C53-C54-C55
55	n	101	CDL	C52-C53-C54-C55
51	J	401	NDP	O4B-C4B-C5B-O5B
55	a	201	CDL	C22-C23-C24-C25
55	a	201	CDL	C35-C36-C37-C38
55	l	702	CDL	C58-C59-C60-C61
55	r	503	CDL	C80-C81-C82-C83
48	j	202	PLX	C16-C17-C18-C19
55	r	503	CDL	C73-C74-C75-C76
55	V	201	CDL	CB3-CB4-CB6-OB8
47	l	704	PEE	C21-C22-C23-C24
47	l	705	PEE	C14-C15-C16-C17
48	g	201	PLX	C7-C8-C9-C10
55	V	202	CDL	C12-C13-C14-C15
55	a	201	CDL	C17-C18-C19-C20
55	n	101	CDL	C73-C74-C75-C76
55	r	503	CDL	C14-C15-C16-C17
55	V	202	CDL	CA7-C31-C32-C33
47	j	201	PEE	C21-C22-C23-C24
48	e	201	PLX	C14-C15-C16-C17
48	j	202	PLX	C14-C15-C16-C17
55	V	201	CDL	C55-C56-C57-C58
55	V	202	CDL	C41-C42-C43-C44
55	a	201	CDL	C23-C24-C25-C26
55	a	201	CDL	C62-C63-C64-C65
55	l	702	CDL	C71-C72-C73-C74
47	W	201	PEE	O5-C30-O3-C3
47	l	701	PEE	C32-C33-C34-C35
55	V	202	CDL	C82-C83-C84-C85
55	l	702	CDL	C75-C76-C77-C78
47	l	704	PEE	C31-C32-C33-C34
48	e	201	PLX	C28-C29-C30-C31
55	V	202	CDL	C59-C60-C61-C62

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Mol	Chain	Res	Type	Atoms
47	B	303	PEE	C11-C12-C13-C14
48	g	201	PLX	C30-C31-C32-C33
47	r	501	PEE	C11-C10-O2-C2
48	a	202	PLX	C13-C14-C15-C16
55	r	503	CDL	C43-C44-C45-C46
47	s	401	PEE	C32-C33-C34-C35
48	a	202	PLX	C33-C34-C35-C36
48	r	502	PLX	C27-C28-C29-C30
55	l	703	CDL	C75-C76-C77-C78
55	r	503	CDL	C41-C42-C43-C44
48	r	502	PLX	C14-C15-C16-C17
48	r	502	PLX	C11-C10-C9-C8
47	l	701	PEE	C13-C14-C15-C16
48	g	201	PLX	C32-C33-C34-C35
48	j	202	PLX	C18-C19-C20-C21
55	r	503	CDL	C52-C53-C54-C55
52	s	402	UQ	C13-C14-C16-C17
47	s	401	PEE	C33-C34-C35-C36
55	a	201	CDL	C32-C33-C34-C35
48	j	202	PLX	C33-C34-C35-C36
55	V	201	CDL	C38-C39-C40-C41
55	l	702	CDL	C11-C12-C13-C14
47	l	705	PEE	C33-C34-C35-C36
48	e	201	PLX	C25-C26-C27-C28
55	l	702	CDL	C37-C38-C39-C40
55	l	703	CDL	C64-C65-C66-C67
47	W	201	PEE	C12-C13-C14-C15
55	V	202	CDL	C61-C62-C63-C64
55	V	202	CDL	C36-C37-C38-C39
55	l	702	CDL	C56-C57-C58-C59
55	V	202	CDL	C51-CB5-OB6-CB4
55	l	702	CDL	C11-CA5-OA6-CA4
47	B	303	PEE	C20-C21-C22-C23
55	S	101	CDL	C11-C12-C13-C14
47	l	701	PEE	C35-C36-C37-C38
47	l	704	PEE	C39-C40-C41-C42
47	s	401	PEE	C19-C20-C21-C22
55	S	101	CDL	C51-C52-C53-C54
55	l	703	CDL	C11-C12-C13-C14
51	J	401	NDP	O4D-C4D-C5D-O5D
55	V	201	CDL	C44-C45-C46-C47
48	a	202	PLX	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
48	j	202	PLX	C10-C11-C12-C13
55	V	201	CDL	C11-C12-C13-C14
48	C	302	PLX	C7-C8-C9-C10
48	g	201	PLX	C11-C12-C13-C14
55	V	201	CDL	C74-C75-C76-C77
55	a	201	CDL	C82-C83-C84-C85
55	l	702	CDL	C82-C83-C84-C85
48	g	201	PLX	C2-C1-N1-C1A
47	s	401	PEE	C34-C35-C36-C37
55	V	201	CDL	C33-C34-C35-C36
47	r	501	PEE	C32-C33-C34-C35
55	n	101	CDL	C54-C55-C56-C57
55	V	201	CDL	C52-C53-C54-C55
47	l	704	PEE	C10-C11-C12-C13
47	r	501	PEE	O4-C10-O2-C2
55	V	202	CDL	OB7-CB5-OB6-CB4
47	l	704	PEE	O3P-C1-C2-O2
47	B	303	PEE	C23-C24-C25-C26
55	r	503	CDL	C55-C56-C57-C58
47	s	401	PEE	C13-C14-C15-C16
47	B	303	PEE	C14-C15-C16-C17
55	V	201	CDL	OB6-CB4-CB6-OB8
47	l	705	PEE	C31-C32-C33-C34
50	X	201	8Q1	C6-C7-C8-C9
55	V	201	CDL	C75-C76-C77-C78
55	V	202	CDL	C35-C36-C37-C38
48	a	202	PLX	C27-C28-C29-C30
55	a	201	CDL	C60-C61-C62-C63
48	a	202	PLX	C25-C26-C27-C28
48	r	502	PLX	C12-C13-C14-C15
55	V	201	CDL	C78-C79-C80-C81
55	l	703	CDL	C56-C57-C58-C59
55	n	101	CDL	C56-C57-C58-C59
55	a	201	CDL	C18-C19-C20-C21
55	l	702	CDL	C73-C74-C75-C76
47	l	704	PEE	C11-C12-C13-C14
55	V	201	CDL	C51-C52-C53-C54
55	r	503	CDL	C11-C12-C13-C14
55	l	702	CDL	C24-C25-C26-C27
48	e	201	PLX	C11-C12-C13-C14
55	a	201	CDL	C75-C76-C77-C78
55	l	702	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
47	B	303	PEE	C21-C22-C23-C24
48	e	201	PLX	C11-C10-C9-C8
50	G	201	8Q1	O33-C32-C34-O35
47	r	501	PEE	C15-C16-C17-C18
47	r	501	PEE	C39-C40-C41-C42
52	s	402	UQ	C27-C28-C29-C30
48	g	201	PLX	C28-C29-C30-C31
55	V	202	CDL	C15-C16-C17-C18
55	S	101	CDL	OA5-CA3-CA4-CA6
55	l	702	CDL	OA5-CA3-CA4-CA6
55	n	101	CDL	OA5-CA3-CA4-CA6
48	a	202	PLX	C11-C12-C13-C14
48	a	202	PLX	C34-C35-C36-C37
55	V	202	CDL	C75-C76-C77-C78
47	l	705	PEE	C30-C31-C32-C33
48	a	202	PLX	C7-C8-C9-C10
48	r	502	PLX	O8-C24-C25-C26
48	g	201	PLX	C27-C28-C29-C30
55	V	201	CDL	C59-C60-C61-C62
48	e	201	PLX	C27-C28-C29-C30
47	l	704	PEE	C42-C43-C44-C45
48	a	202	PLX	C30-C31-C32-C33
55	l	703	CDL	C73-C74-C75-C76
47	W	201	PEE	C1-C2-C3-O3
47	l	705	PEE	C1-C2-C3-O3
47	s	401	PEE	C1-C2-C3-O3
48	g	201	PLX	C3-C4-C5-O8
55	V	201	CDL	CA3-CA4-CA6-OA8
55	V	202	CDL	CB3-CB4-CB6-OB8
55	l	702	CDL	CA3-CA4-CA6-OA8
55	r	503	CDL	C62-C63-C64-C65
47	B	303	PEE	C15-C16-C17-C18
47	l	704	PEE	C15-C16-C17-C18
55	a	201	CDL	C71-C72-C73-C74
47	W	201	PEE	C24-C25-C26-C27
47	W	201	PEE	C21-C22-C23-C24
48	e	201	PLX	C30-C31-C32-C33
55	V	201	CDL	C15-C16-C17-C18
55	l	702	CDL	OA7-CA5-OA6-CA4
48	j	202	PLX	C27-C28-C29-C30
48	C	302	PLX	C11-C12-C13-C14
48	j	202	PLX	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
55	r	503	CDL	C37-C38-C39-C40
55	V	201	CDL	C53-C54-C55-C56
55	S	101	CDL	CA6-CA4-OA6-CA5
47	l	705	PEE	C13-C14-C15-C16
48	g	201	PLX	C18-C19-C20-C21
55	n	101	CDL	C51-C52-C53-C54
47	B	303	PEE	C35-C36-C37-C38
47	W	201	PEE	C15-C16-C17-C18
48	e	201	PLX	C9-C10-C11-C12
48	j	202	PLX	C31-C32-C33-C34
55	V	201	CDL	C14-C15-C16-C17
47	l	701	PEE	C33-C34-C35-C36
48	r	502	PLX	C16-C17-C18-C19
55	V	202	CDL	CB5-C51-C52-C53
48	r	502	PLX	C10-C11-C12-C13
47	s	401	PEE	C11-C12-C13-C14
48	e	201	PLX	C32-C33-C34-C35
55	V	201	CDL	C73-C74-C75-C76
55	V	202	CDL	CB2-C1-CA2-OA2
47	B	303	PEE	O3P-C1-C2-O2
48	e	201	PLX	C18-C19-C20-C21
55	V	202	CDL	C38-C39-C40-C41
55	V	201	CDL	C32-C33-C34-C35
48	g	201	PLX	C13-C14-C15-C16
47	j	201	PEE	C32-C33-C34-C35
55	l	703	CDL	C59-C60-C61-C62
55	V	202	CDL	C74-C75-C76-C77
48	r	502	PLX	O6-C4-C5-O8
48	g	201	PLX	C2-C1-N1-C1B
47	j	201	PEE	C36-C37-C38-C39
47	r	501	PEE	C36-C37-C38-C39
55	r	503	CDL	C17-C18-C19-C20
55	a	201	CDL	C84-C85-C86-C87
50	G	201	8Q1	C31-C29-C32-O33
50	X	201	8Q1	C30-C29-C32-O33
50	X	201	8Q1	C31-C29-C32-O33
55	r	503	CDL	C15-C16-C17-C18
55	n	101	CDL	C71-CB7-OB8-CB6
55	a	201	CDL	C52-C53-C54-C55
50	G	201	8Q1	C29-C32-C34-O35
55	S	101	CDL	C31-CA7-OA8-CA6
48	C	302	PLX	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
48	g	201	PLX	C16-C17-C18-C19
55	r	503	CDL	C59-C60-C61-C62
47	l	704	PEE	C32-C33-C34-C35
55	a	201	CDL	C31-C32-C33-C34
55	r	503	CDL	C1-CB2-OB2-PB2
55	l	702	CDL	C55-C56-C57-C58
47	l	704	PEE	O3P-C1-C2-C3
55	a	201	CDL	OA5-CA3-CA4-CA6
55	l	703	CDL	OB5-CB3-CB4-CB6
55	r	503	CDL	OB5-CB3-CB4-CB6
48	r	502	PLX	C30-C31-C32-C33
55	V	202	CDL	C60-C61-C62-C63
47	r	501	PEE	C24-C25-C26-C27
55	n	101	CDL	C75-C76-C77-C78
55	l	703	CDL	C44-C45-C46-C47
48	C	302	PLX	C25-C26-C27-C28
48	e	201	PLX	C31-C32-C33-C34
47	B	303	PEE	C38-C39-C40-C41
47	j	201	PEE	C38-C39-C40-C41
55	l	702	CDL	C53-C54-C55-C56
47	r	501	PEE	C40-C41-C42-C43
48	e	201	PLX	C35-C36-C37-C38
55	r	503	CDL	C36-C37-C38-C39
55	V	201	CDL	C40-C41-C42-C43
47	r	501	PEE	C1-C2-C3-O3
48	e	201	PLX	C3-C4-C5-O8
48	j	202	PLX	C3-C4-C5-O8
55	a	201	CDL	C42-C43-C44-C45
47	j	201	PEE	C23-C24-C25-C26
55	a	201	CDL	C61-C62-C63-C64
48	g	201	PLX	C12-C13-C14-C15
55	a	201	CDL	C15-C16-C17-C18
55	a	201	CDL	OB5-CB3-CB4-OB6
55	l	703	CDL	OB5-CB3-CB4-OB6
47	W	201	PEE	C11-C10-O2-C2
55	r	503	CDL	C82-C83-C84-C85
55	a	201	CDL	C44-C45-C46-C47
55	V	201	CDL	C54-C55-C56-C57
47	W	201	PEE	O2-C2-C3-O3
47	l	701	PEE	O2-C2-C3-O3
48	C	302	PLX	O6-C4-C5-O8
48	j	202	PLX	O6-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
55	S	101	CDL	OB6-CB4-CB6-OB8
55	r	503	CDL	C12-C13-C14-C15
47	W	201	PEE	C13-C14-C15-C16
55	l	702	CDL	C33-C34-C35-C36
55	a	201	CDL	C14-C15-C16-C17
55	l	702	CDL	CB5-C51-C52-C53
55	r	503	CDL	CA5-C11-C12-C13
48	g	201	PLX	C2-C1-N1-C1C
48	r	502	PLX	C25-C26-C27-C28
47	j	201	PEE	C11-C12-C13-C14
47	r	501	PEE	C38-C39-C40-C41
55	S	101	CDL	C31-C32-C33-C34
55	V	202	CDL	C78-C79-C80-C81
47	j	201	PEE	C44-C45-C46-C47
55	a	201	CDL	CB5-C51-C52-C53
55	V	201	CDL	C64-C65-C66-C67
47	B	303	PEE	O3P-C1-C2-C3
47	l	701	PEE	O3P-C1-C2-C3
47	r	501	PEE	O3P-C1-C2-C3
55	a	201	CDL	OB5-CB3-CB4-CB6
55	l	703	CDL	OA5-CA3-CA4-CA6
55	a	201	CDL	C54-C55-C56-C57
47	B	303	PEE	C36-C37-C38-C39
47	l	704	PEE	C13-C14-C15-C16
57	w	401	ADP	PA-O3A-PB-O1B
55	n	101	CDL	OB9-CB7-OB8-CB6
55	l	703	CDL	C40-C41-C42-C43
48	e	201	PLX	C33-C34-C35-C36
48	e	201	PLX	C16-C17-C18-C19
55	V	201	CDL	CA6-CA4-OA6-CA5
47	l	704	PEE	C19-C20-C21-C22
47	s	401	PEE	C15-C16-C17-C18
55	S	101	CDL	OA9-CA7-OA8-CA6
47	W	201	PEE	O4-C10-O2-C2
47	l	705	PEE	O3P-C1-C2-O2
47	r	501	PEE	O3P-C1-C2-O2
48	j	202	PLX	O4-C3-C4-O6
55	V	201	CDL	OA5-CA3-CA4-OA6
55	V	202	CDL	OA5-CA3-CA4-OA6
55	a	201	CDL	OA5-CA3-CA4-OA6
55	l	703	CDL	OA5-CA3-CA4-OA6
55	r	503	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	C40-C41-C42-C43
48	a	202	PLX	C3-C4-C5-O8
55	V	202	CDL	CA3-CA4-CA6-OA8
55	a	201	CDL	C37-C38-C39-C40
50	X	201	8Q1	C30-C29-C32-C34
47	l	705	PEE	O2-C2-C3-O3
47	r	501	PEE	O2-C2-C3-O3
47	s	401	PEE	O2-C2-C3-O3
55	V	201	CDL	OA6-CA4-CA6-OA8
55	l	702	CDL	C38-C39-C40-C41
48	a	202	PLX	C35-C36-C37-C38
55	l	702	CDL	C17-C18-C19-C20
48	j	202	PLX	C7-C6-O6-C4
50	G	201	8Q1	C6-C7-C8-C9
51	J	401	NDP	O4D-C1D-N1N-C6N
47	l	705	PEE	C11-C10-O2-C2
48	a	202	PLX	C32-C33-C34-C35
48	r	502	PLX	C11-C12-C13-C14
55	V	202	CDL	C54-C55-C56-C57
47	j	201	PEE	C42-C43-C44-C45
55	a	201	CDL	C11-C12-C13-C14
55	V	202	CDL	C39-C40-C41-C42
55	V	202	CDL	C62-C63-C64-C65
55	l	702	CDL	C31-C32-C33-C34
48	C	302	PLX	C25-C24-O8-C5
48	a	202	PLX	C25-C24-O8-C5
48	g	201	PLX	C25-C24-O8-C5
50	X	201	8Q1	O33-C32-C34-O35
55	a	201	CDL	C73-C74-C75-C76
55	V	201	CDL	C32-C31-CA7-OA8
55	V	201	CDL	C71-C72-C73-C74
55	l	703	CDL	C62-C63-C64-C65
47	l	705	PEE	O3P-C1-C2-C3
48	e	201	PLX	O4-C3-C4-C5
48	j	202	PLX	O4-C3-C4-C5
55	S	101	CDL	OB5-CB3-CB4-CB6
55	V	201	CDL	OA5-CA3-CA4-CA6
55	V	202	CDL	OA5-CA3-CA4-CA6
55	V	202	CDL	OB5-CB3-CB4-CB6
47	W	201	PEE	C23-C24-C25-C26
47	l	705	PEE	O4-C10-O2-C2
55	l	703	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
50	X	201	8Q1	O27-C28-C29-C31
55	V	201	CDL	C43-C44-C45-C46
55	r	503	CDL	C39-C40-C41-C42
48	a	202	PLX	C11-C10-C9-C8
55	V	202	CDL	C64-C65-C66-C67
48	C	302	PLX	O8-C24-C25-C26
47	l	701	PEE	O3P-C1-C2-O2
48	e	201	PLX	O4-C3-C4-O6
55	S	101	CDL	OA5-CA3-CA4-OA6
50	G	201	8Q1	C13-C14-C15-C16
55	l	703	CDL	C15-C16-C17-C18
48	g	201	PLX	C33-C34-C35-C36
55	l	702	CDL	C51-CB5-OB6-CB4
51	J	401	NDP	C2N-C3N-C7N-O7N
47	B	303	PEE	C13-C14-C15-C16
55	l	703	CDL	C43-C44-C45-C46
55	a	201	CDL	C51-C52-C53-C54
47	s	401	PEE	C12-C13-C14-C15
48	r	502	PLX	C3-C4-C5-O8
48	a	202	PLX	C14-C15-C16-C17
50	G	201	8Q1	O27-C28-C29-C32
50	X	201	8Q1	O27-C28-C29-C32
47	s	401	PEE	C43-C44-C45-C46
46	A	502	FMN	C2'-C1'-N10-C10
47	B	303	PEE	C4-O4P-P-O1P
47	W	201	PEE	C4-O4P-P-O3P
47	W	201	PEE	C4-O4P-P-O1P
47	j	201	PEE	C1-O3P-P-O2P
47	j	201	PEE	C4-O4P-P-O2P
47	l	701	PEE	C1-O3P-P-O2P
47	l	704	PEE	C4-O4P-P-O2P
47	l	705	PEE	C1-O3P-P-O4P
47	s	401	PEE	C1-O3P-P-O2P
48	a	202	PLX	C3-O4-P1-O1
48	e	201	PLX	C3-C4-O6-C6
48	e	201	PLX	C5-C4-O6-C6
48	g	201	PLX	C3-O4-P1-O1
48	g	201	PLX	C3-O4-P1-O3
48	j	202	PLX	C3-O4-P1-O2
48	j	202	PLX	C2-O1-P1-O3
48	r	502	PLX	C3-C4-O6-C6
48	r	502	PLX	C5-C4-O6-C6

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Mol	Chain	Res	Type	Atoms
50	G	201	8Q1	C28-C29-C32-O33
50	X	201	8Q1	C28-C29-C32-O33
55	S	101	CDL	CB2-OB2-PB2-OB4
55	S	101	CDL	CB2-OB2-PB2-OB5
55	S	101	CDL	CB3-OB5-PB2-OB4
55	V	201	CDL	CB3-OB5-PB2-OB3
55	V	202	CDL	CB2-OB2-PB2-OB4
55	a	201	CDL	CA2-OA2-PA1-OA3
55	l	702	CDL	CA2-OA2-PA1-OA3
55	l	702	CDL	CB3-OB5-PB2-OB4
55	l	703	CDL	CA3-OA5-PA1-OA3
55	l	703	CDL	CB3-OB5-PB2-OB2
55	n	101	CDL	CB3-OB5-PB2-OB3
55	r	503	CDL	CA2-OA2-PA1-OA4
55	r	503	CDL	CB2-OB2-PB2-OB3
55	r	503	CDL	CB2-OB2-PB2-OB4
55	r	503	CDL	CB2-OB2-PB2-OB5
55	r	503	CDL	CB3-OB5-PB2-OB2
55	r	503	CDL	CB3-OB5-PB2-OB4
52	J	402	UQ	C15-C14-C16-C17
55	n	101	CDL	C72-C71-CB7-OB8
47	W	201	PEE	C22-C23-C24-C25
48	C	302	PLX	C28-C29-C30-C31
55	l	702	CDL	OB7-CB5-OB6-CB4
55	r	503	CDL	C74-C75-C76-C77
47	l	705	PEE	C18-C19-C20-C21
47	r	501	PEE	C18-C19-C20-C21
47	l	704	PEE	C3-C2-O2-C10
47	l	705	PEE	C32-C33-C34-C35
47	B	303	PEE	C44-C45-C46-C47
48	a	202	PLX	C26-C27-C28-C29
50	X	201	8Q1	C12-C13-C14-C15
47	j	201	PEE	C30-C31-C32-C33
52	s	402	UQ	C23-C24-C26-C27
47	B	303	PEE	C42-C43-C44-C45
55	r	503	CDL	C76-C77-C78-C79
48	a	202	PLX	O6-C4-C5-O8
48	e	201	PLX	O6-C4-C5-O8
47	l	701	PEE	C18-C19-C20-C21
47	r	501	PEE	C13-C14-C15-C16
55	V	202	CDL	C22-C23-C24-C25
47	l	705	PEE	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
55	S	101	CDL	CB3-CB4-CB6-OB8
47	l	704	PEE	C40-C41-C42-C43
47	l	705	PEE	C34-C35-C36-C37
55	l	703	CDL	C53-C54-C55-C56
51	J	401	NDP	C3D-C4D-C5D-O5D
47	l	705	PEE	C38-C39-C40-C41
55	n	101	CDL	C74-C75-C76-C77
55	l	702	CDL	C54-C55-C56-C57
55	a	201	CDL	C33-C34-C35-C36
52	s	402	UQ	C12-C11-C9-C10
48	a	202	PLX	O9-C24-C25-C26
48	g	201	PLX	O7-C6-C7-C8
47	l	704	PEE	C36-C37-C38-C39
55	V	202	CDL	C31-C32-C33-C34
47	s	401	PEE	C31-C30-O3-C3
55	V	202	CDL	C32-C31-CA7-OA8
47	r	501	PEE	C16-C17-C18-C19
47	W	201	PEE	C20-C21-C22-C23
47	j	201	PEE	C34-C35-C36-C37
49	C	303	970	C20-C19-O28-C29
47	B	303	PEE	C12-C13-C14-C15
47	l	704	PEE	C41-C42-C43-C44
50	G	201	8Q1	C29-C32-C34-N36
47	l	705	PEE	C16-C17-C18-C19
48	C	302	PLX	C30-C31-C32-C33
47	s	401	PEE	O5-C30-O3-C3
55	l	703	CDL	C72-C73-C74-C75
55	r	503	CDL	C42-C43-C44-C45
48	g	201	PLX	C6-C7-C8-C9
55	a	201	CDL	C16-C17-C18-C19
55	n	101	CDL	C1-CB2-OB2-PB2
55	l	703	CDL	C82-C83-C84-C85
55	V	201	CDL	C31-C32-C33-C34
55	S	101	CDL	C52-C53-C54-C55
55	r	503	CDL	C21-C22-C23-C24
47	l	704	PEE	C38-C39-C40-C41
47	r	501	PEE	C21-C22-C23-C24
48	j	202	PLX	C17-C18-C19-C20
55	l	702	CDL	C84-C85-C86-C87
55	S	101	CDL	OB5-CB3-CB4-OB6
55	V	201	CDL	OB5-CB3-CB4-OB6
55	l	702	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
55	r	503	CDL	C13-C14-C15-C16
55	a	201	CDL	C31-CA7-OA8-CA6
55	V	201	CDL	CA4-CA3-OA5-PA1
47	j	201	PEE	C37-C38-C39-C40
48	j	202	PLX	C9-C10-C11-C12
55	r	503	CDL	C61-C62-C63-C64
55	l	703	CDL	C34-C35-C36-C37
55	r	503	CDL	OA6-CA4-CA6-OA8
52	s	402	UQ	C22-C23-C24-C25
55	l	703	CDL	OB7-CB5-OB6-CB4
47	l	704	PEE	C34-C35-C36-C37
48	a	202	PLX	O6-C6-C7-C8
48	e	201	PLX	O8-C24-C25-C26
55	V	202	CDL	C24-C25-C26-C27
50	X	201	8Q1	C9-C10-C11-C12
55	a	201	CDL	OA9-CA7-OA8-CA6
47	l	701	PEE	C16-C17-C18-C19
55	V	202	CDL	C81-C82-C83-C84
52	J	402	UQ	C12-C11-C9-C10
55	l	702	CDL	CB4-CB3-OB5-PB2
55	S	101	CDL	C12-C13-C14-C15
48	e	201	PLX	C24-C25-C26-C27
47	j	201	PEE	C40-C41-C42-C43
55	V	201	CDL	C57-C58-C59-C60
47	l	701	PEE	C1-C2-C3-O3
55	r	503	CDL	C20-C21-C22-C23
48	C	302	PLX	O7-C6-C7-C8
55	l	703	CDL	C14-C15-C16-C17
55	V	202	CDL	OB5-CB3-CB4-OB6
50	G	201	8Q1	N36-C37-C38-C39
47	B	303	PEE	C18-C19-C20-C21
48	g	201	PLX	C31-C32-C33-C34
47	s	401	PEE	C37-C38-C39-C40
55	a	201	CDL	CA7-C31-C32-C33
55	a	201	CDL	C76-C77-C78-C79
48	a	202	PLX	C12-C13-C14-C15
47	s	401	PEE	C38-C39-C40-C41
47	l	704	PEE	C33-C34-C35-C36
48	j	202	PLX	C26-C27-C28-C29
55	V	202	CDL	C13-C14-C15-C16
55	V	201	CDL	C72-C73-C74-C75
48	e	201	PLX	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
47	W	201	PEE	C16-C17-C18-C19
47	s	401	PEE	C36-C37-C38-C39
55	a	201	CDL	C64-C65-C66-C67
47	l	705	PEE	C21-C22-C23-C24
57	w	401	ADP	PA-O3A-PB-O2B
57	w	401	ADP	PA-O3A-PB-O3B
47	r	501	PEE	C14-C15-C16-C17
55	V	202	CDL	C71-C72-C73-C74
55	a	201	CDL	C58-C59-C60-C61
48	g	201	PLX	O4-C3-C4-O6
47	W	201	PEE	C34-C35-C36-C37
47	l	705	PEE	C23-C24-C25-C26
55	l	703	CDL	C57-C58-C59-C60
47	l	701	PEE	C38-C39-C40-C41
55	V	202	CDL	C58-C59-C60-C61
47	B	303	PEE	C16-C17-C18-C19
47	l	704	PEE	C18-C19-C20-C21
48	a	202	PLX	C6-C7-C8-C9
55	l	702	CDL	C72-C71-CB7-OB8
55	l	703	CDL	C51-CB5-OB6-CB4
51	J	401	NDP	C3B-C4B-C5B-O5B
55	r	503	CDL	C56-C57-C58-C59
47	s	401	PEE	O3-C30-C31-C32
47	l	704	PEE	C22-C23-C24-C25
55	V	202	CDL	C34-C35-C36-C37
55	S	101	CDL	C72-C71-CB7-OB8
55	a	201	CDL	C12-C11-CA5-OA6
55	V	202	CDL	C76-C77-C78-C79
55	r	503	CDL	C72-C73-C74-C75
47	j	201	PEE	O3-C30-C31-C32
48	C	302	PLX	C3-C4-C5-O8
47	r	501	PEE	C44-C45-C46-C47
48	j	202	PLX	C25-C24-O8-C5
52	J	402	UQ	C7-C8-C9-C11
48	r	502	PLX	C35-C36-C37-C38
55	r	503	CDL	C54-C55-C56-C57
55	r	503	CDL	C72-C71-CB7-OB8
55	a	201	CDL	C32-C31-CA7-OA8
50	X	201	8Q1	O27-C28-C29-C30
48	C	302	PLX	C10-C11-C12-C13
48	e	201	PLX	C2-C1-N1-C1B
50	X	201	8Q1	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
55	V	202	CDL	C77-C78-C79-C80
55	l	702	CDL	C72-C71-CB7-OB9
48	r	502	PLX	O4-C3-C4-O6
52	J	402	UQ	C22-C23-C24-C25
48	e	201	PLX	C2-C1-N1-C1C
55	a	201	CDL	C12-C11-CA5-OA7
48	C	302	PLX	O9-C24-O8-C5
47	s	401	PEE	O5-C30-C31-C32
48	g	201	PLX	C4-C5-O8-C24
55	a	201	CDL	C36-C37-C38-C39
55	S	101	CDL	C72-C71-CB7-OB9
47	s	401	PEE	C44-C45-C46-C47
55	r	503	CDL	C72-C71-CB7-OB9
48	e	201	PLX	C2-C1-N1-C1A
48	C	302	PLX	C18-C19-C20-C21
47	j	201	PEE	O5-C30-C31-C32
55	l	702	CDL	C12-C11-CA5-OA6
47	l	705	PEE	C10-C11-C12-C13
55	a	201	CDL	C32-C31-CA7-OA9
55	V	202	CDL	C52-C51-CB5-OB6
49	C	303	970	C18-C19-O28-C29
47	l	701	PEE	O3-C30-C31-C32

There are no ring outliers.

32 monomers are involved in 149 short contacts:

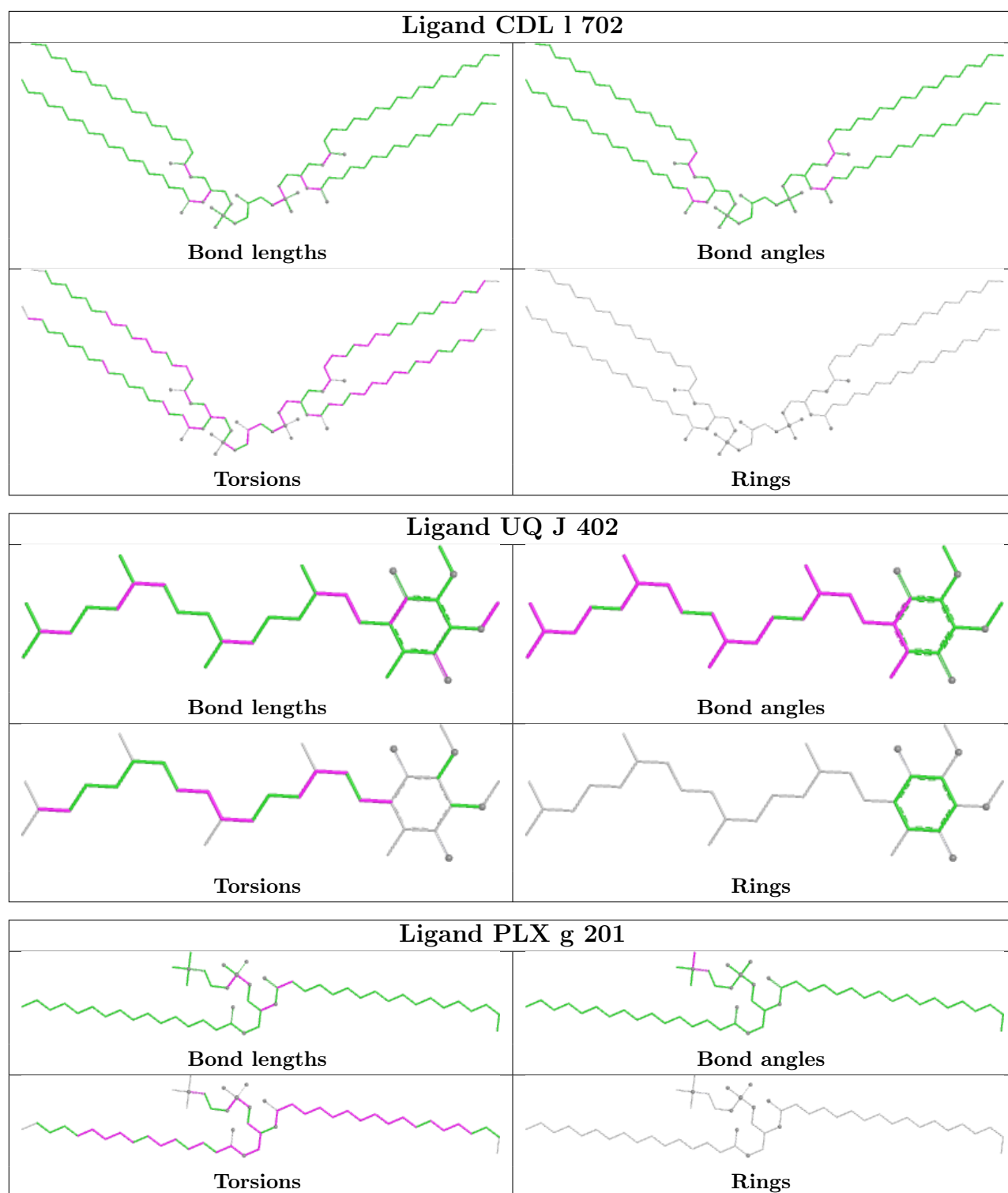
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	l	702	CDL	12	0
52	J	402	UQ	4	0
48	g	201	PLX	7	0
47	l	701	PEE	1	0
47	l	705	PEE	4	0
50	G	201	8Q1	1	0
55	r	503	CDL	4	0
47	W	201	PEE	3	0
47	s	401	PEE	11	0
55	a	201	CDL	3	0
48	j	202	PLX	2	0
55	S	101	CDL	15	0
45	A	501	SF4	2	0
53	O	301	FES	1	0
48	C	302	PLX	10	0

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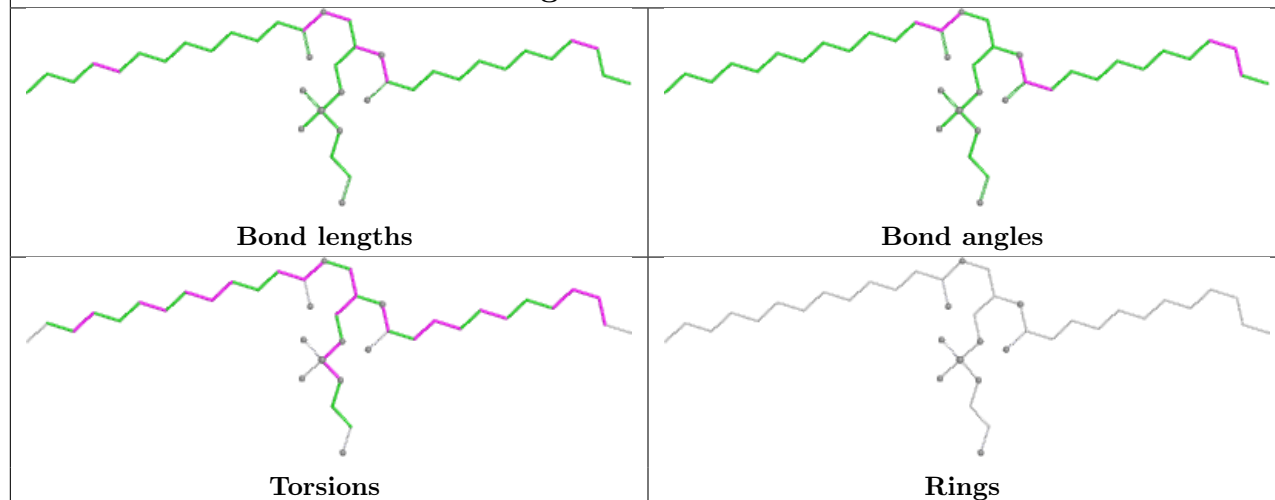
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	l	704	PEE	5	0
46	A	502	FMN	5	0
48	a	202	PLX	2	0
55	n	101	CDL	1	0
55	V	201	CDL	8	0
55	V	202	CDL	7	0
55	l	703	CDL	6	0
47	j	201	PEE	3	0
48	e	201	PLX	6	0
47	r	501	PEE	5	0
45	C	301	SF4	3	0
48	r	502	PLX	5	0
50	X	201	8Q1	1	0
51	J	401	NDP	3	0
47	B	303	PEE	7	0
52	s	402	UQ	7	0
57	w	401	ADP	1	0

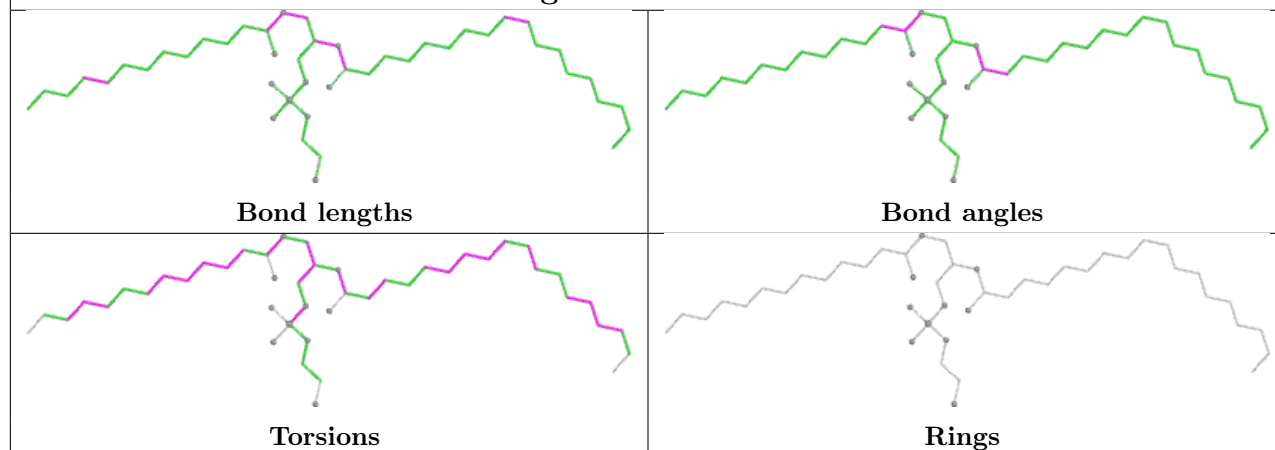
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



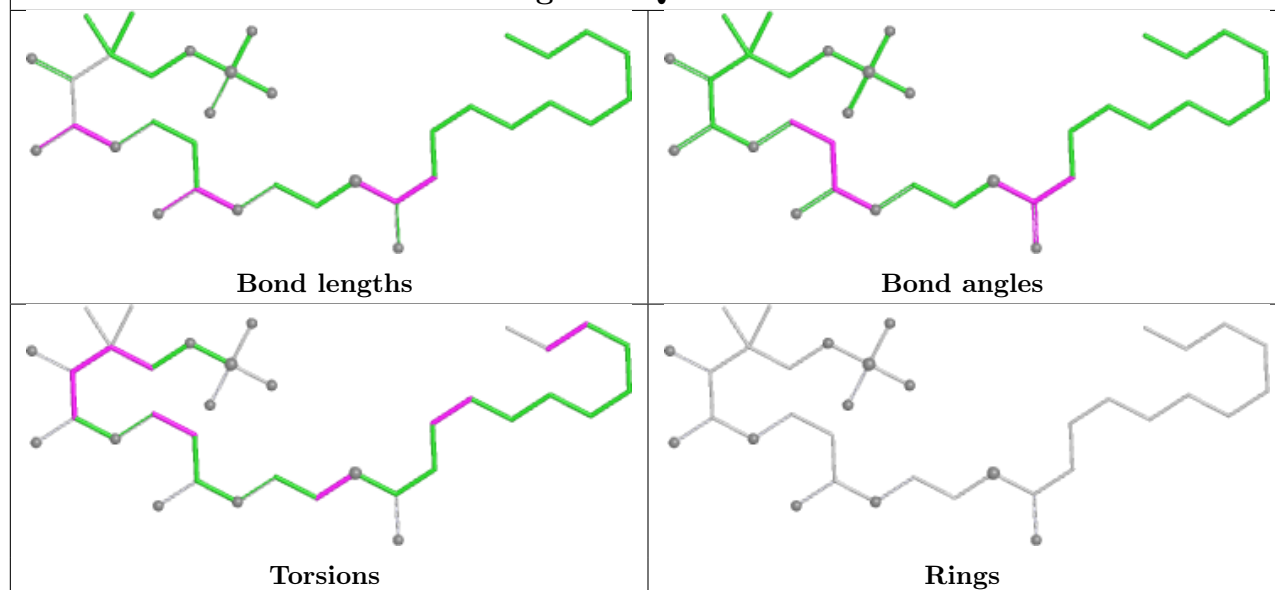
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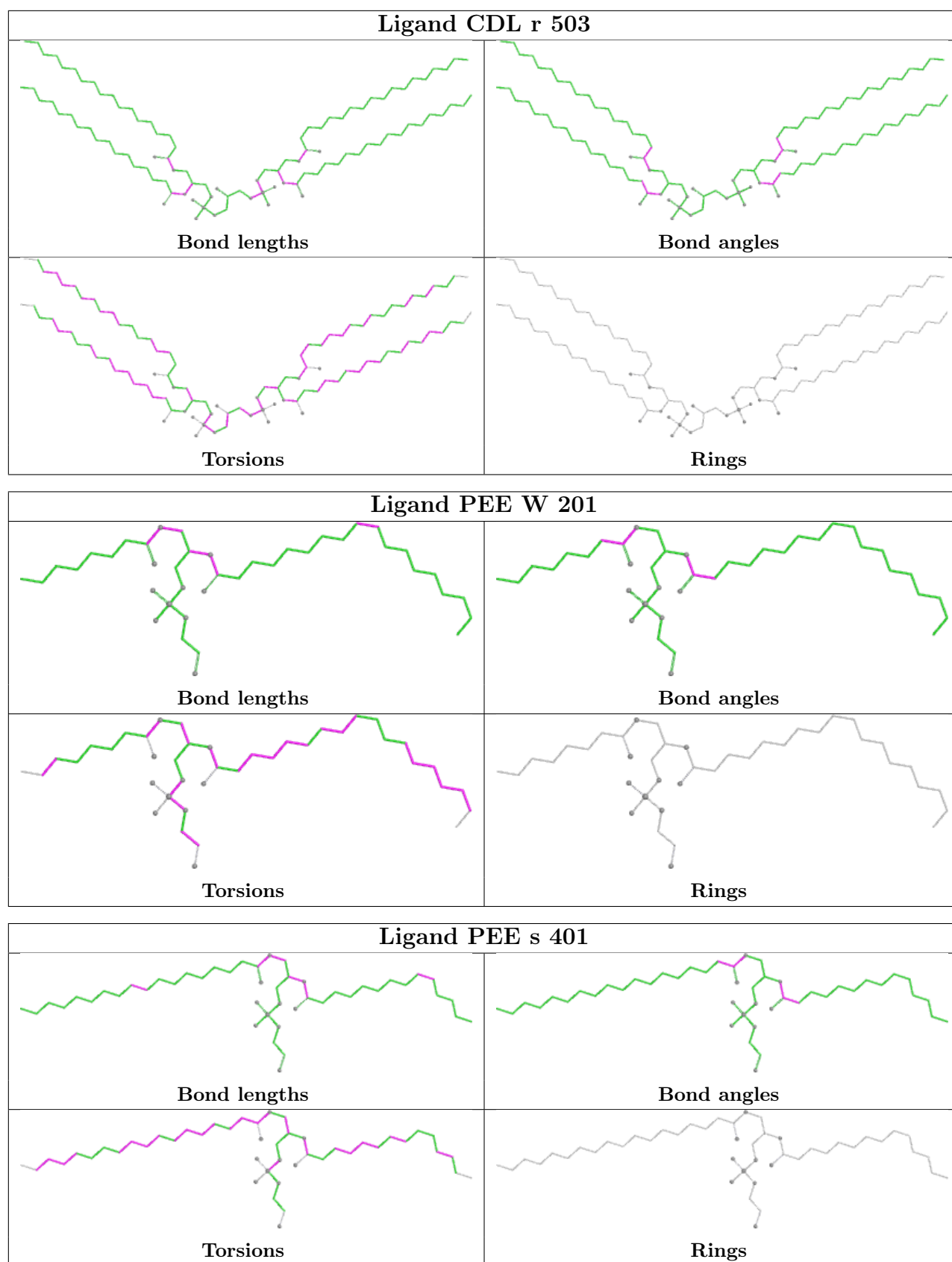


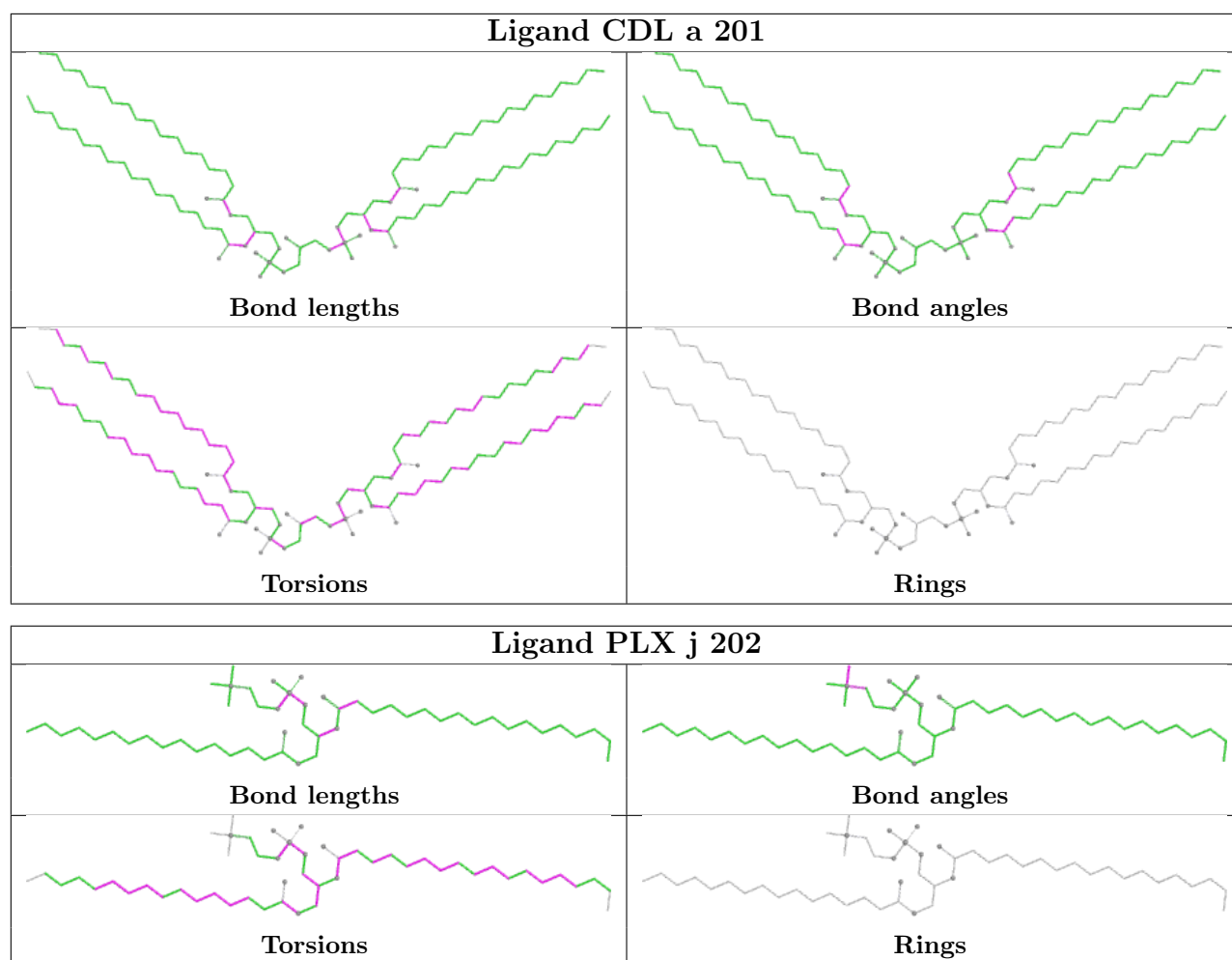
Ligand PEE 1 705

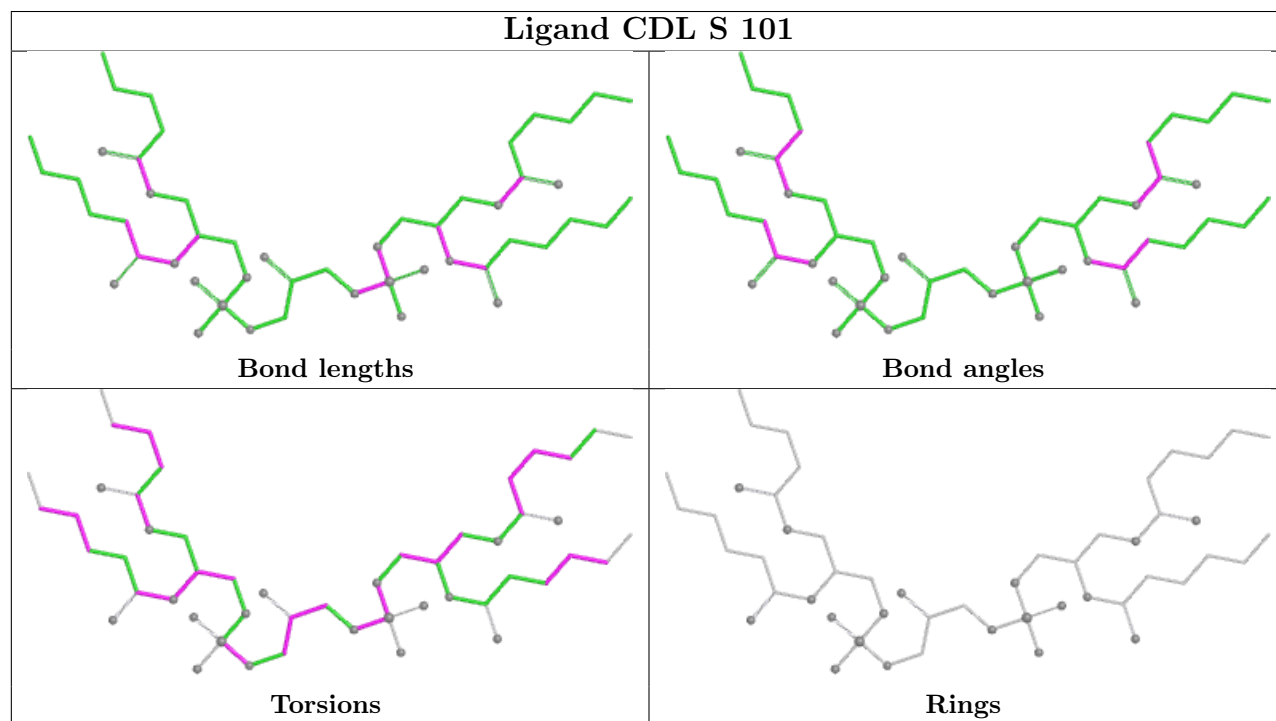
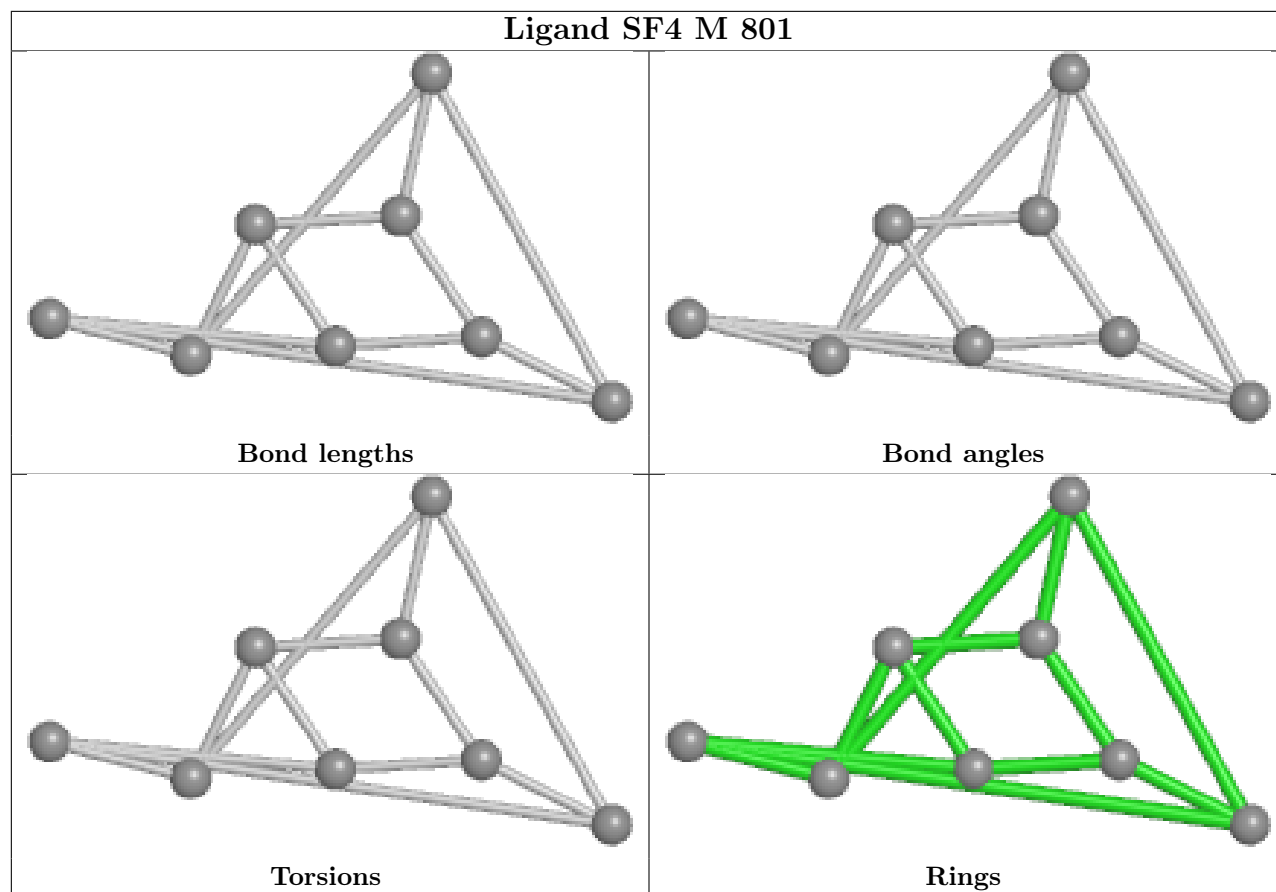


Ligand 8Q1 G 201

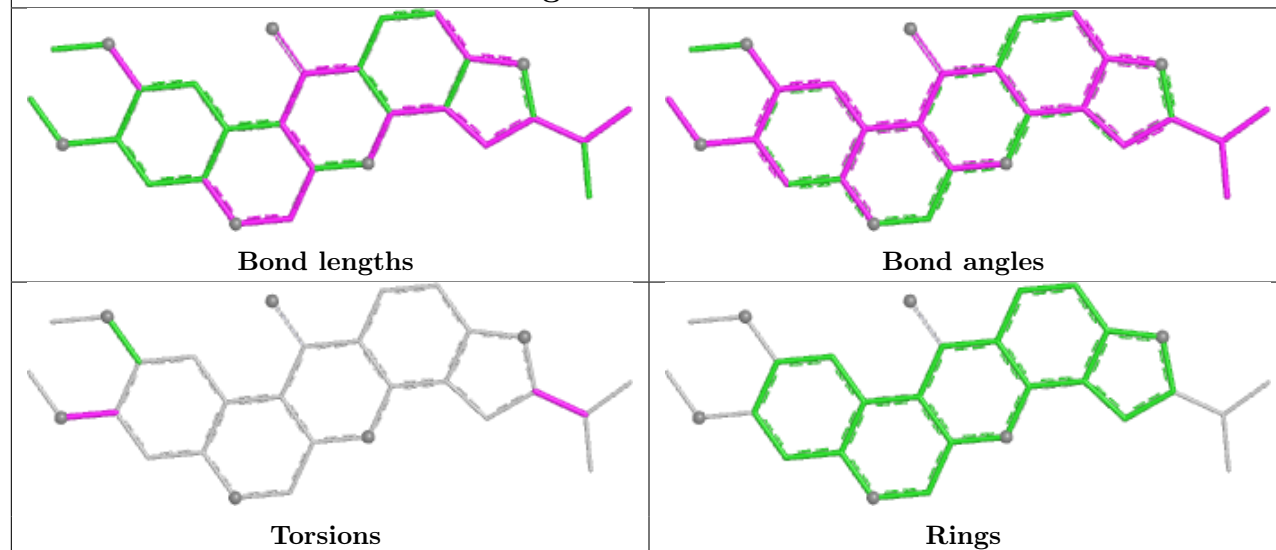




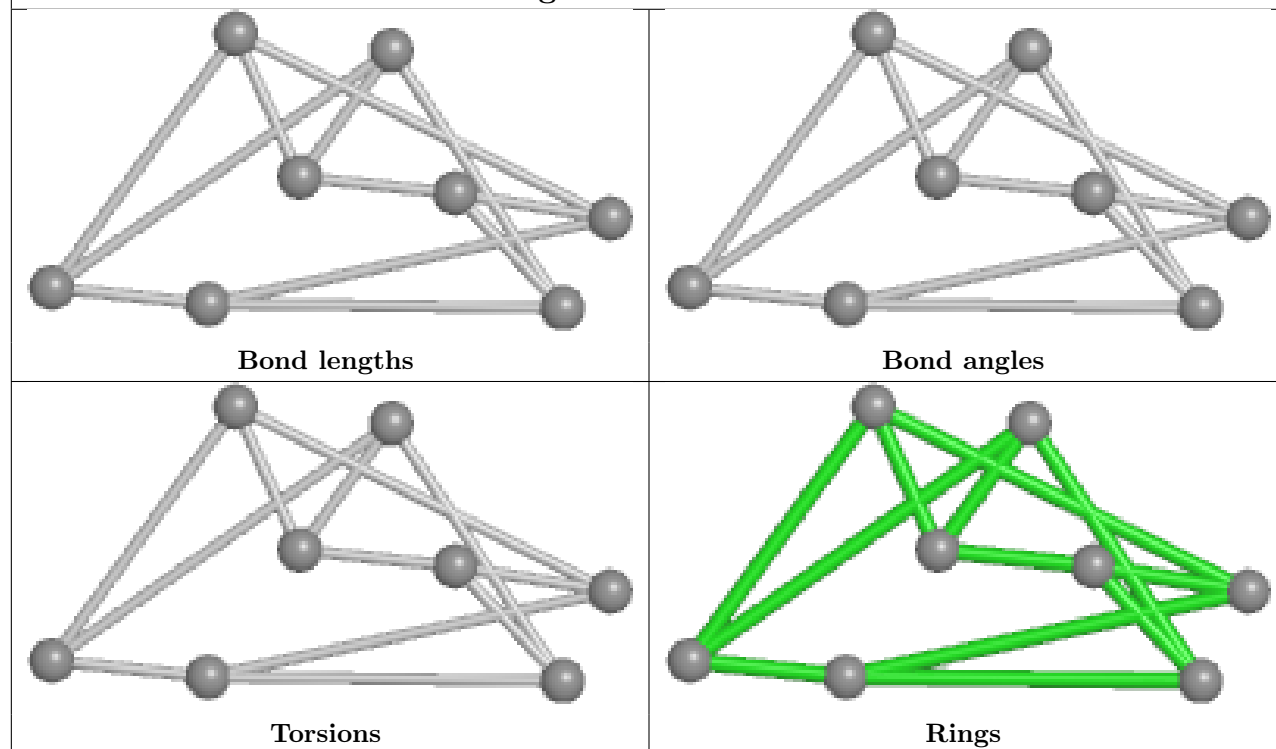




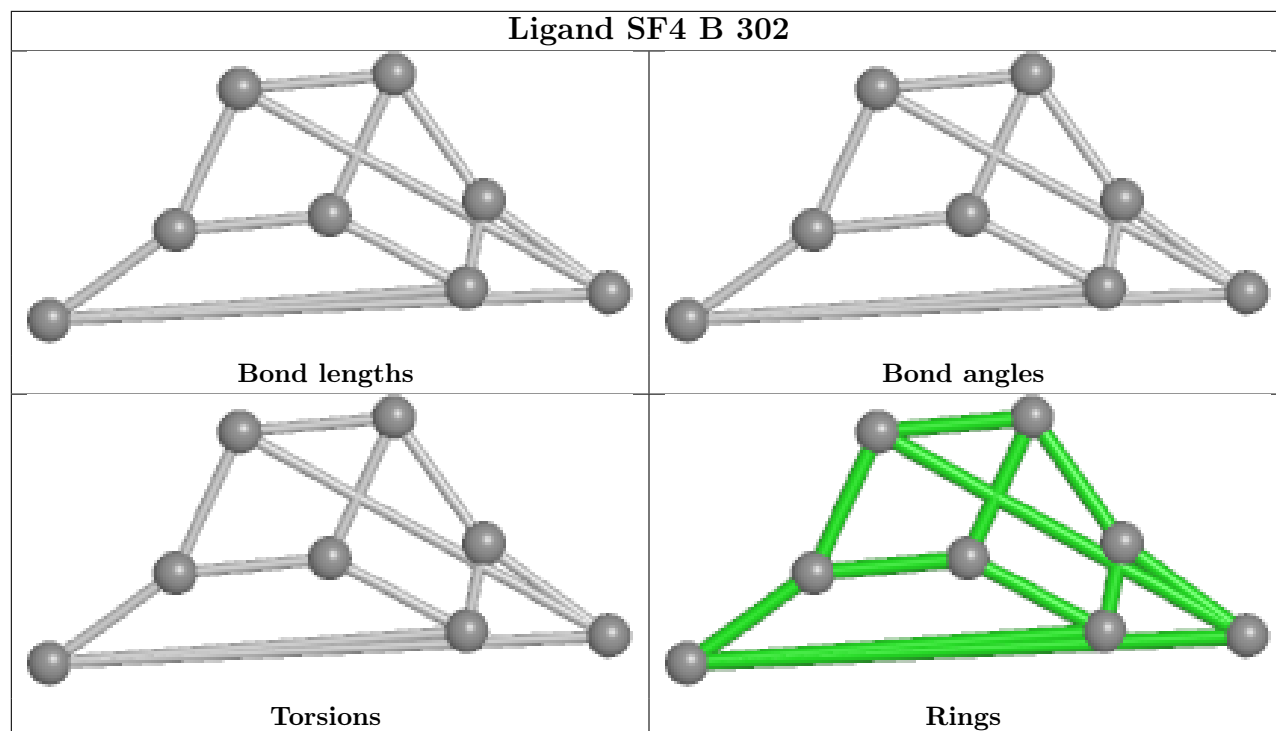
Ligand 970 C 303



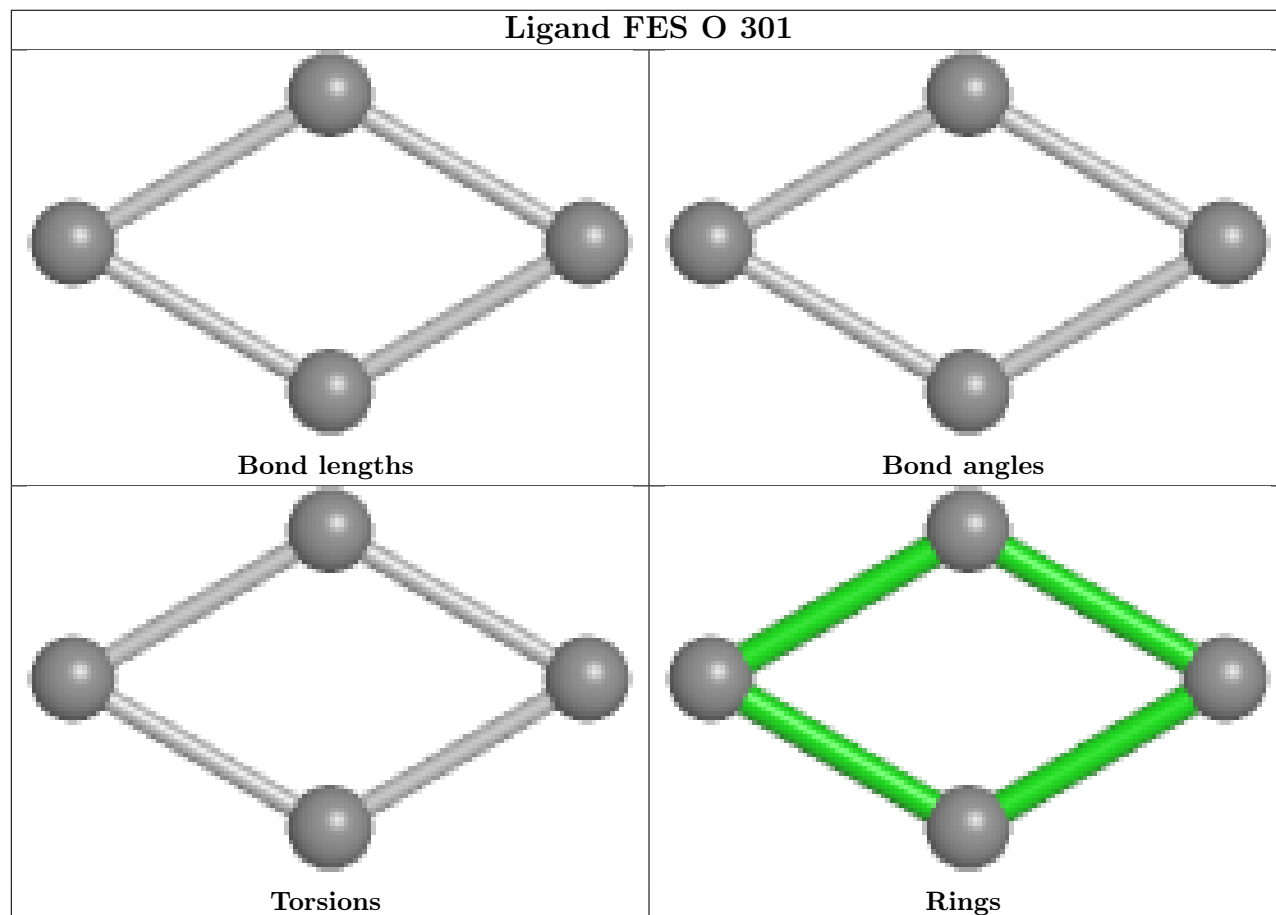
Ligand SF4 A 501

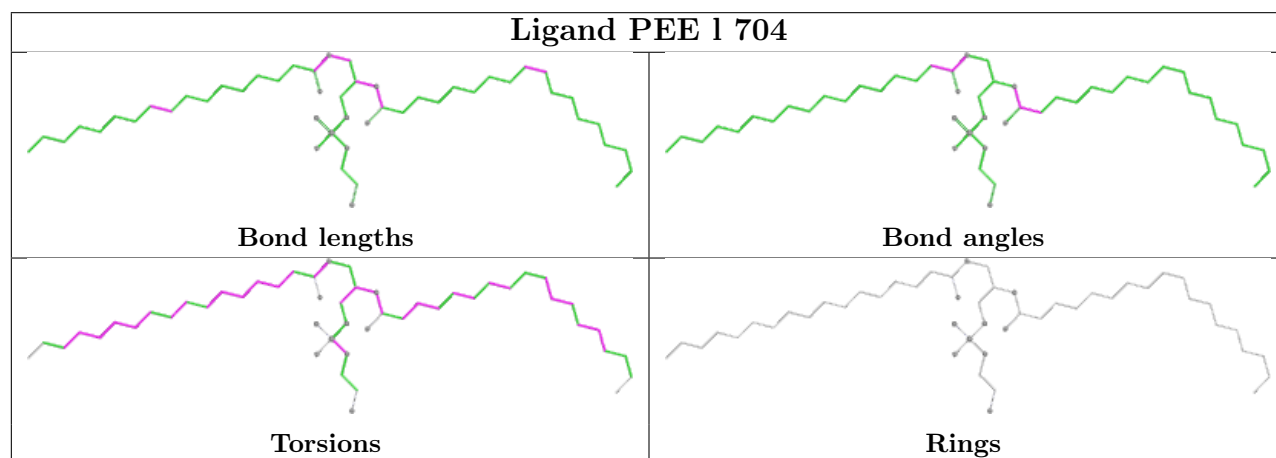
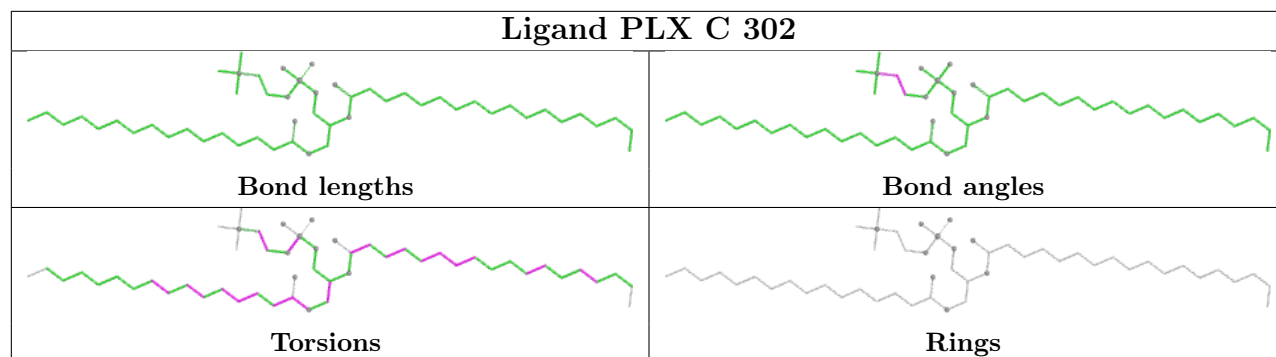


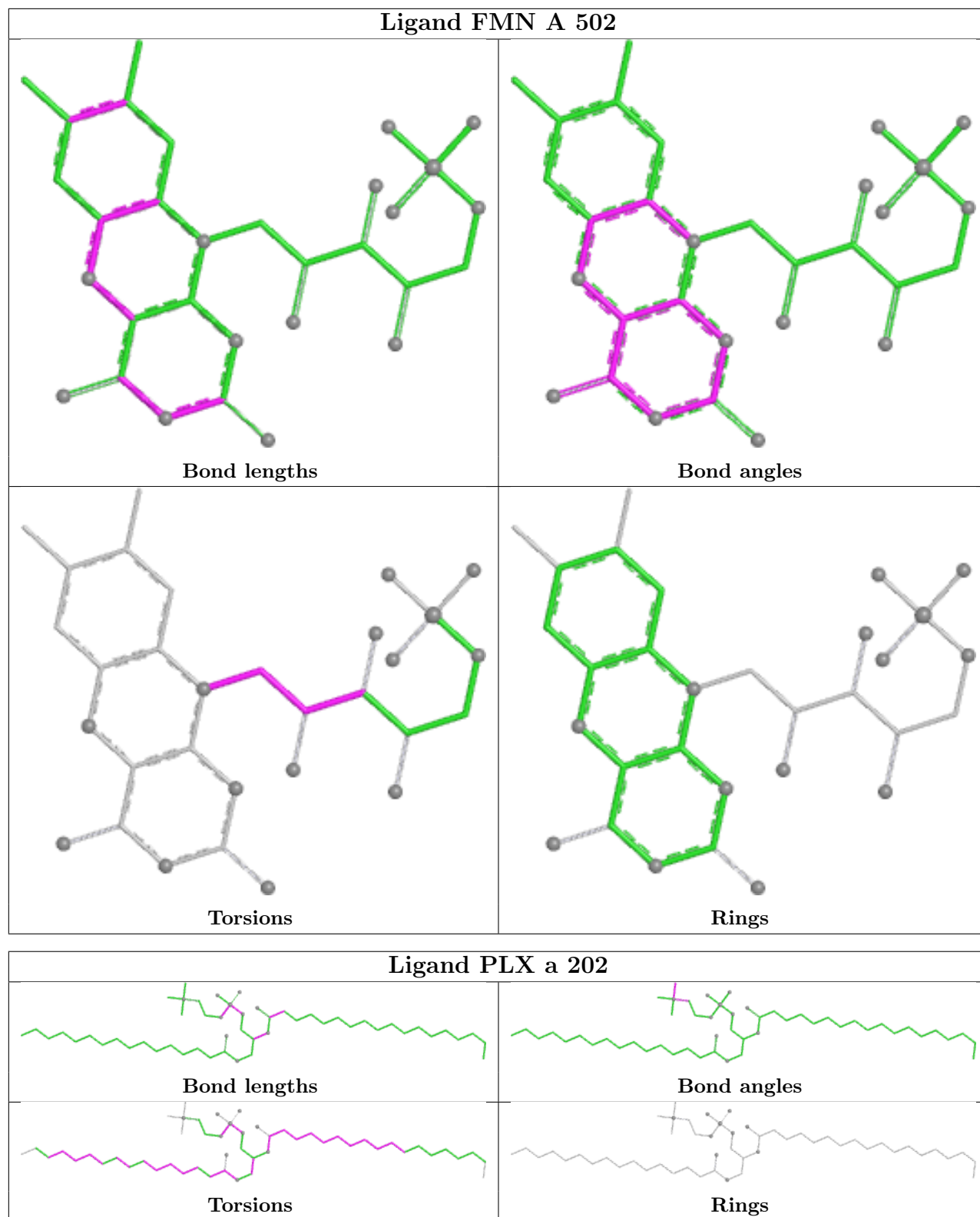
Ligand SF4 B 302

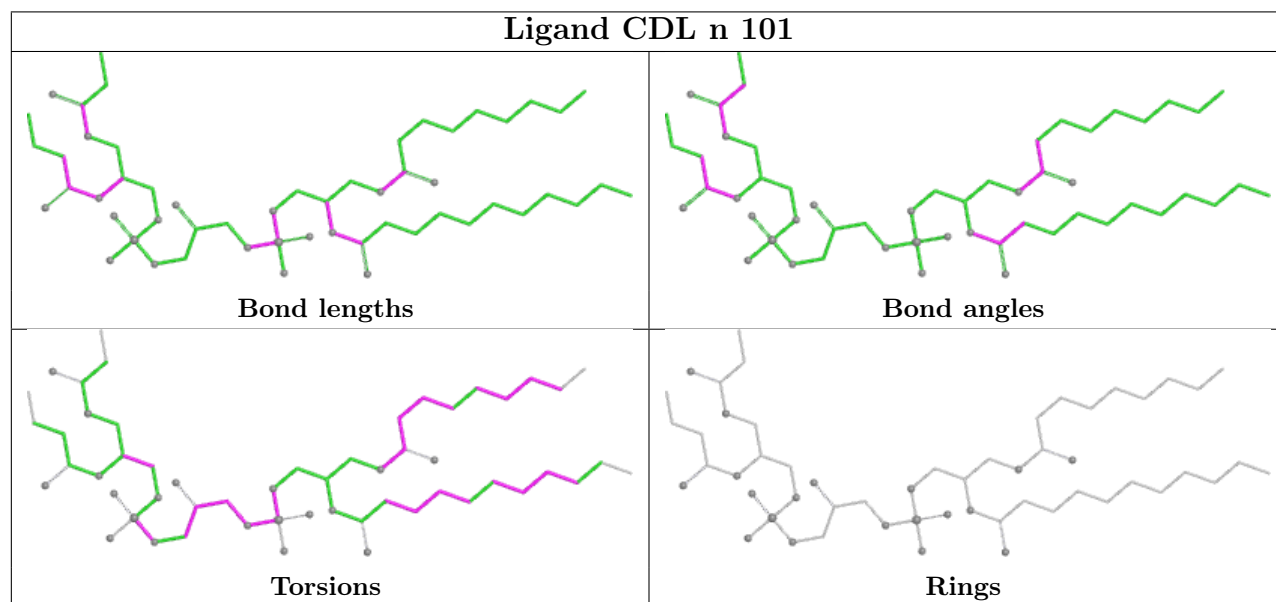
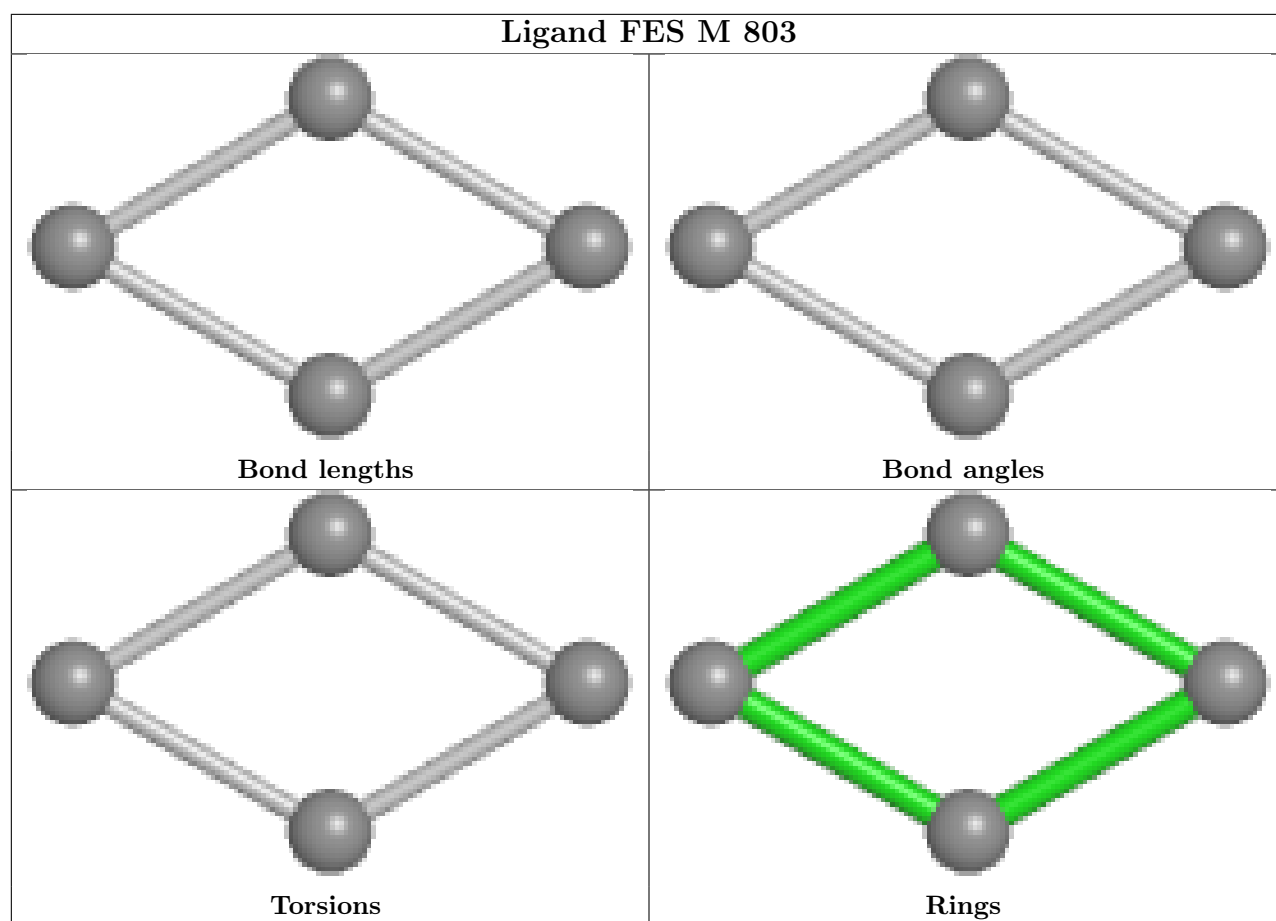


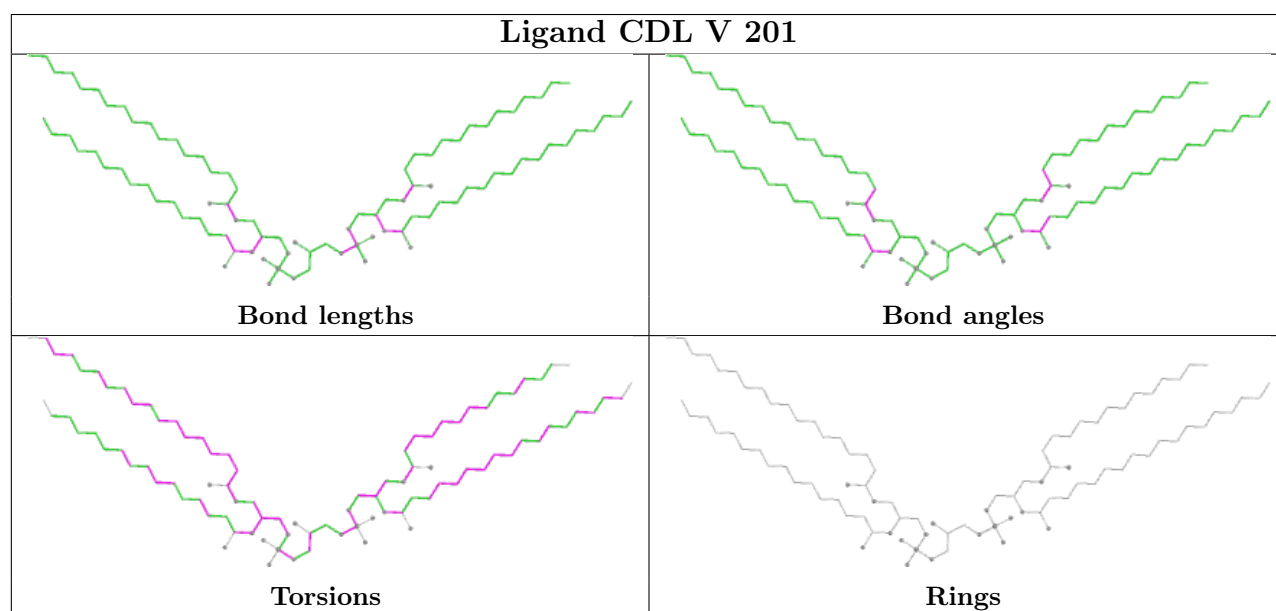
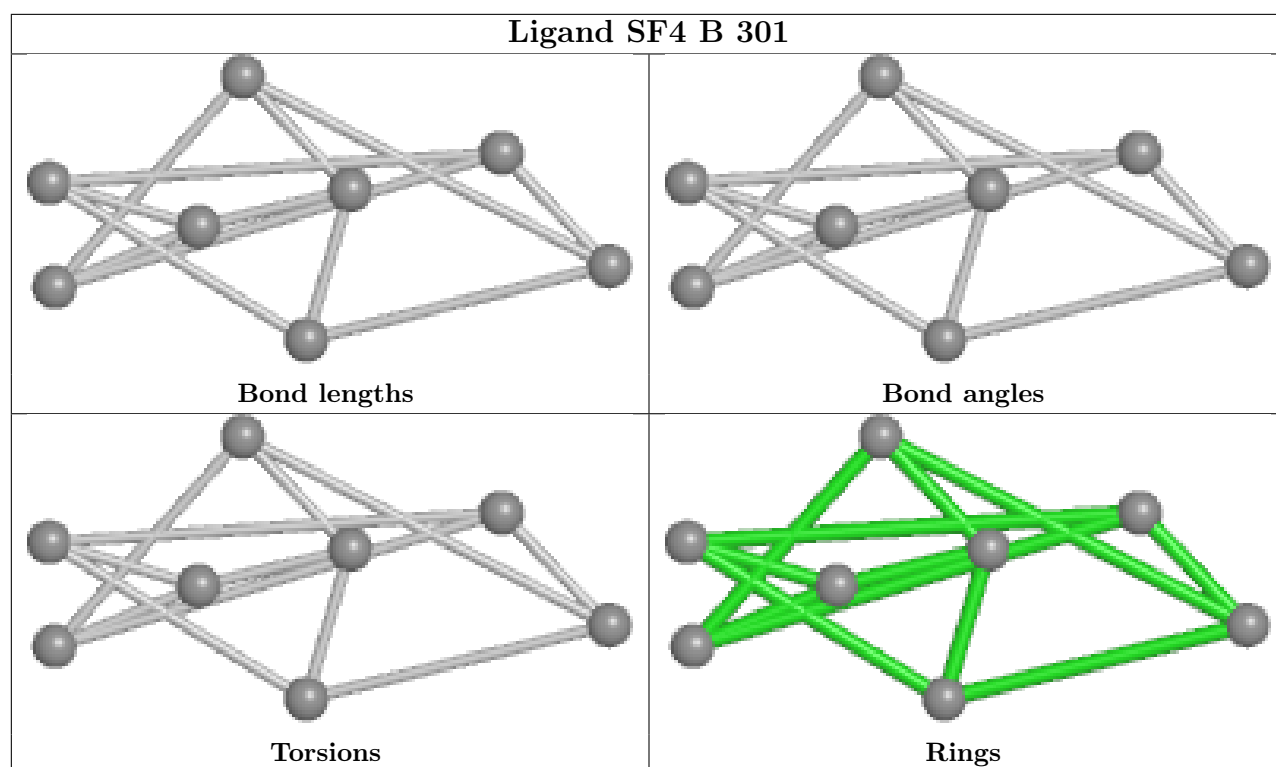
Ligand FES O 301

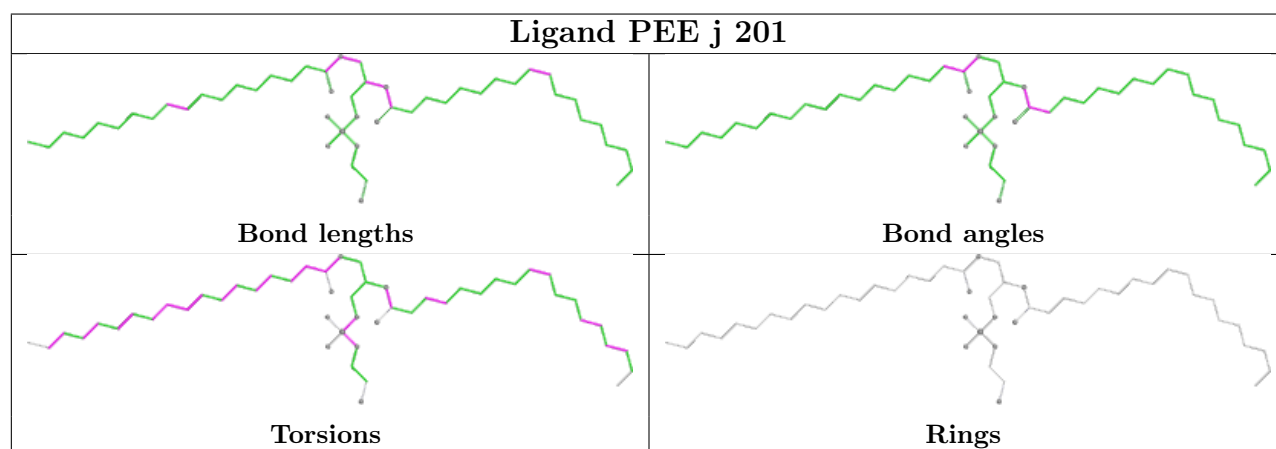
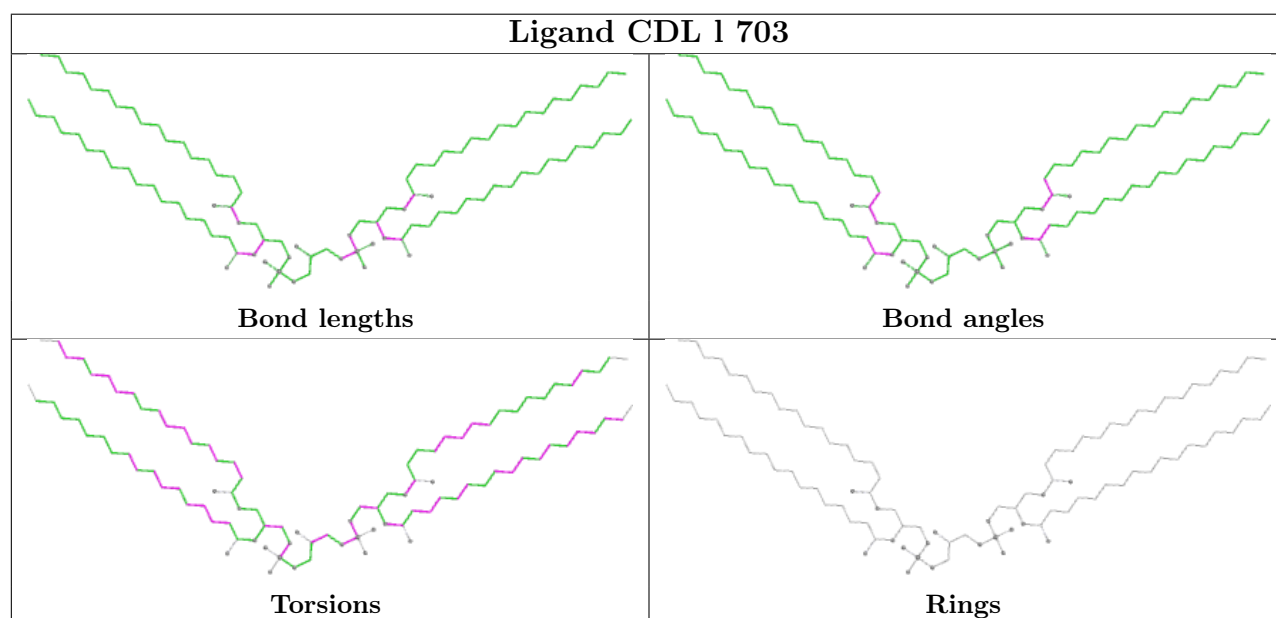
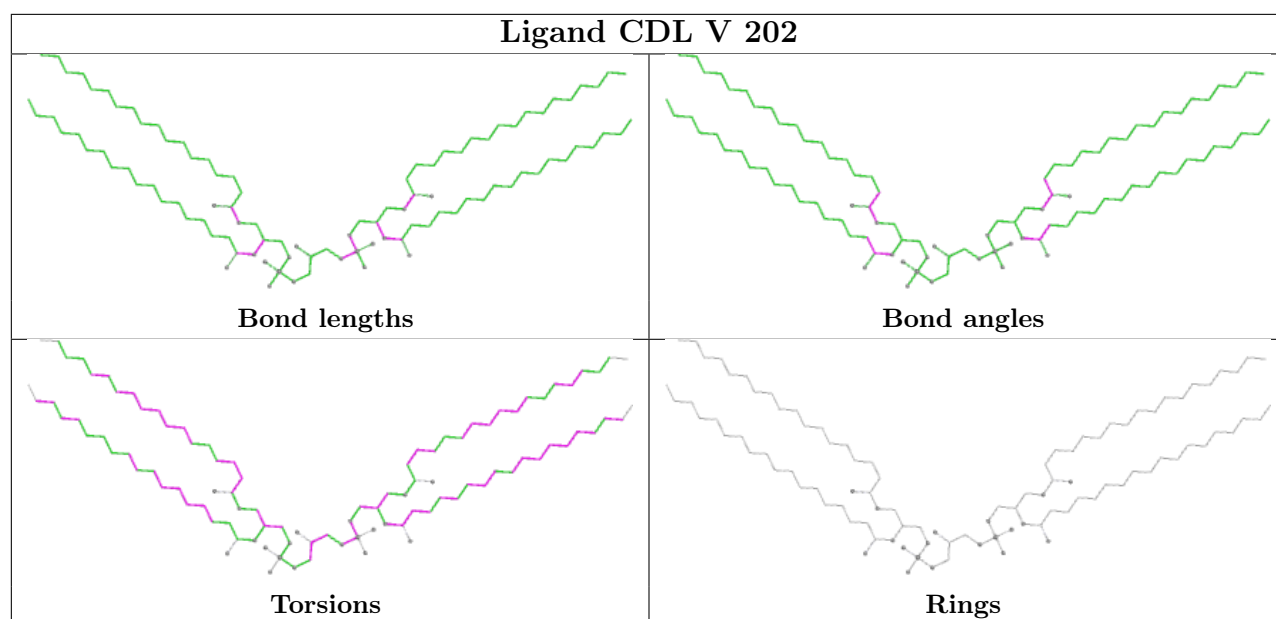


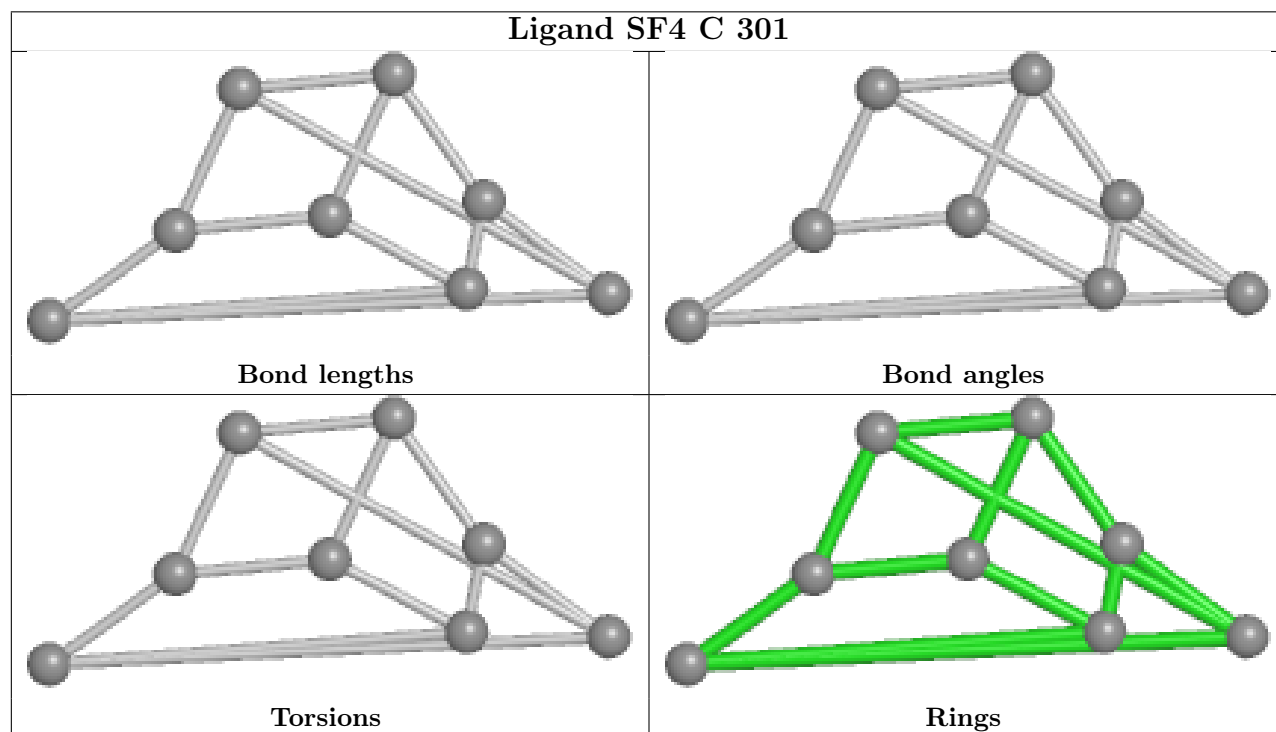
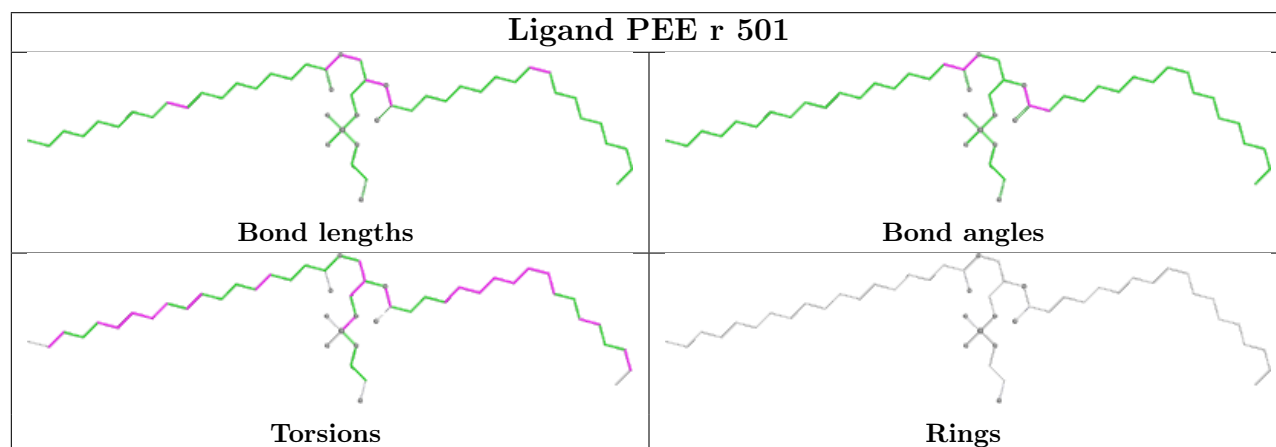


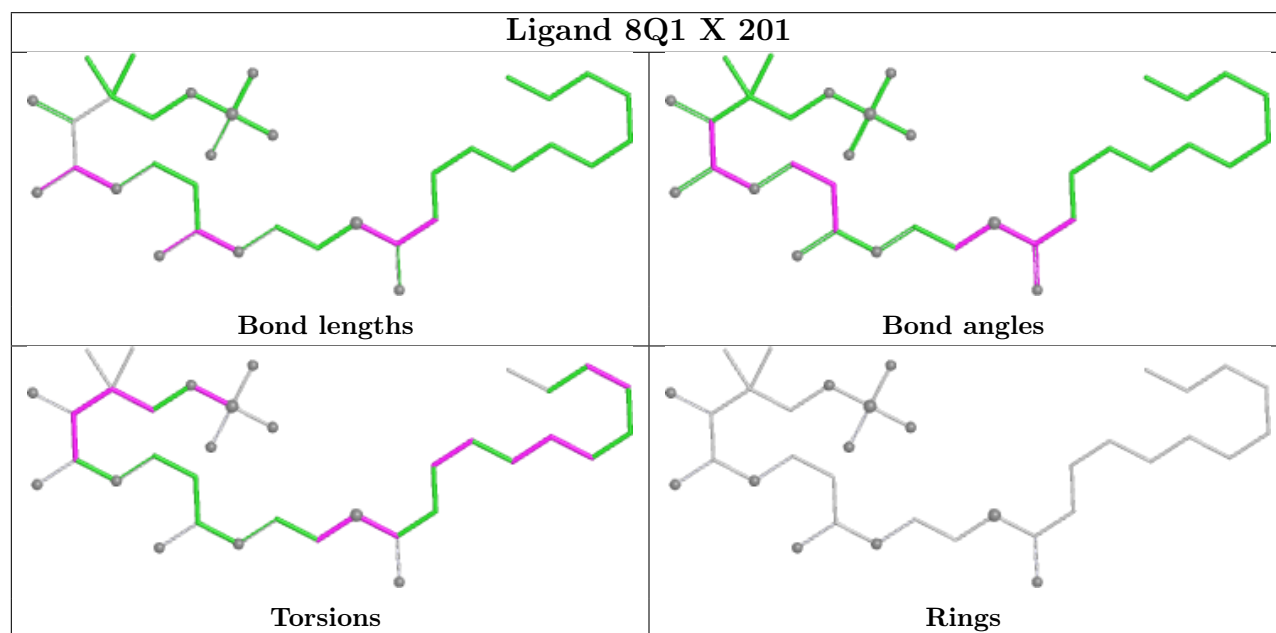
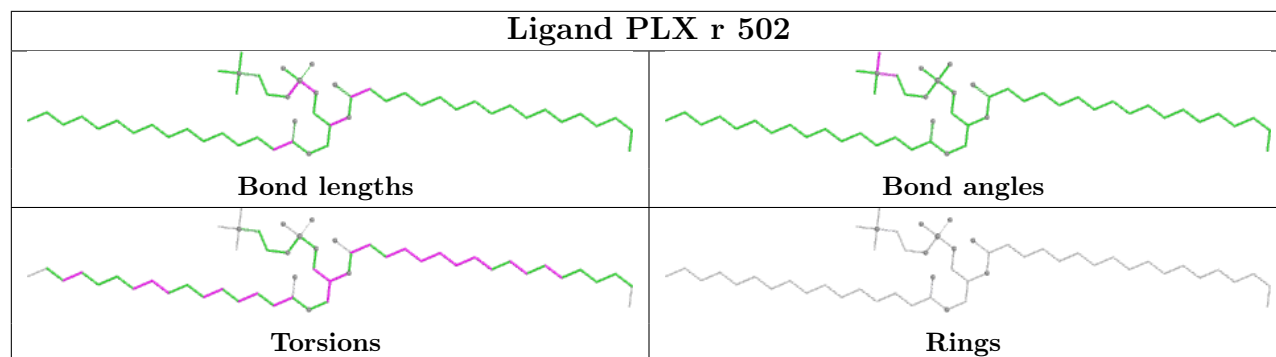


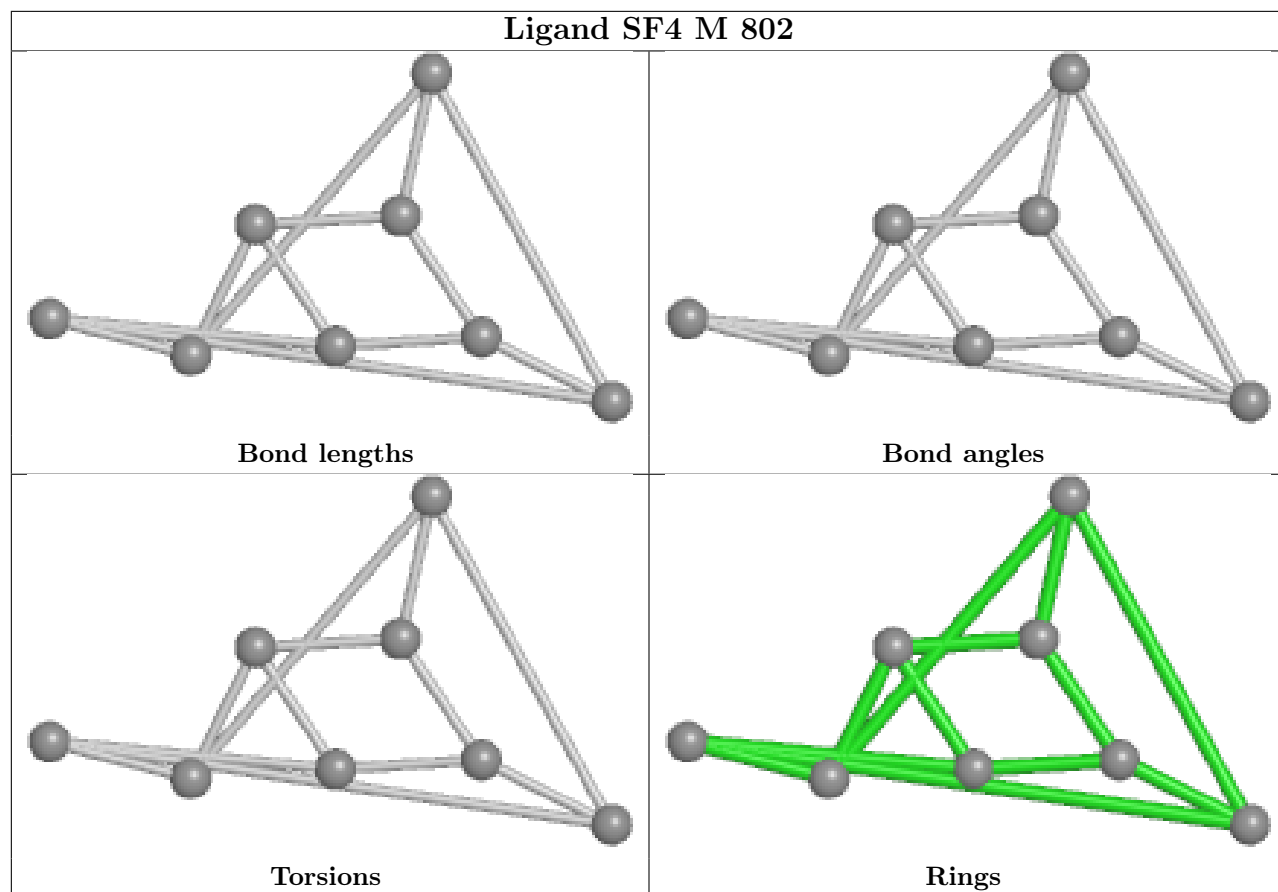




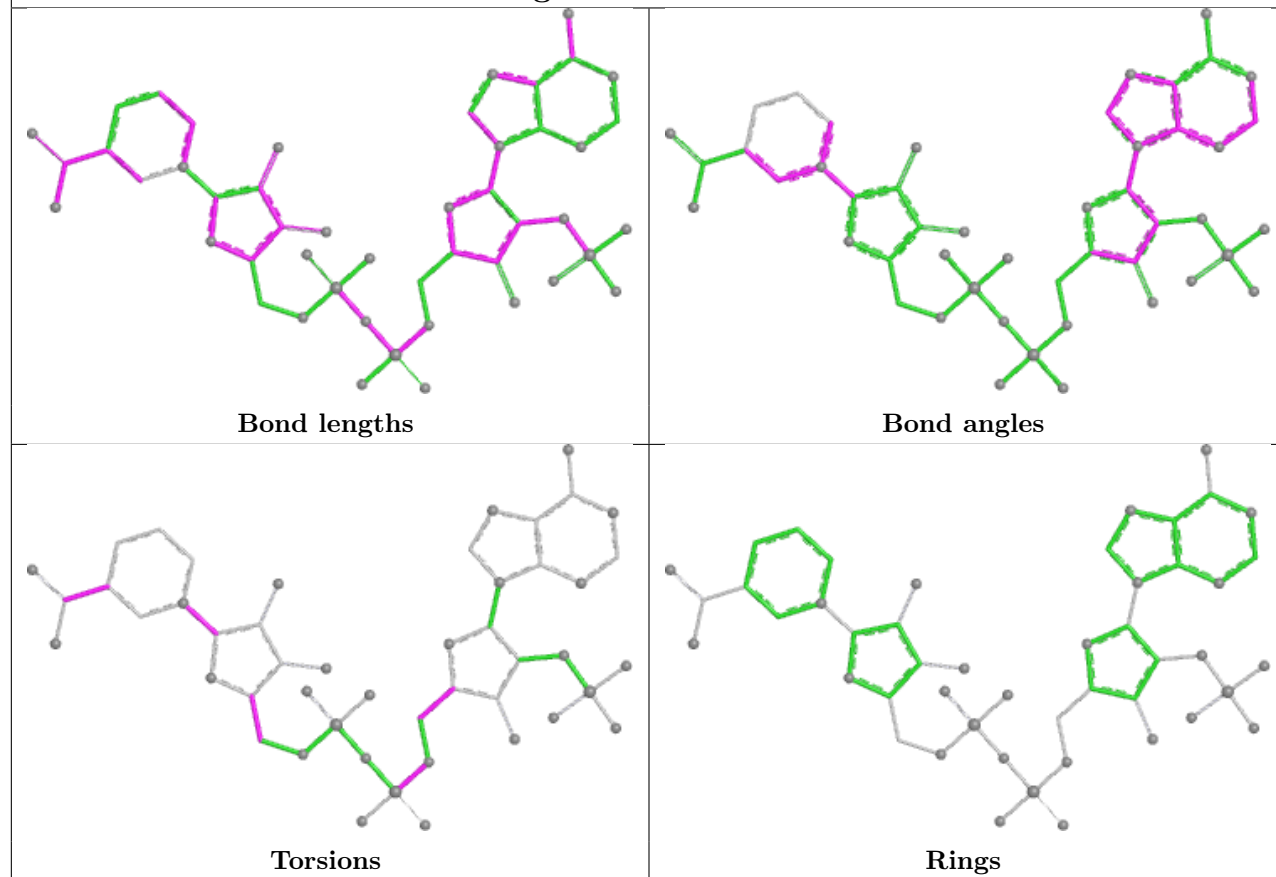




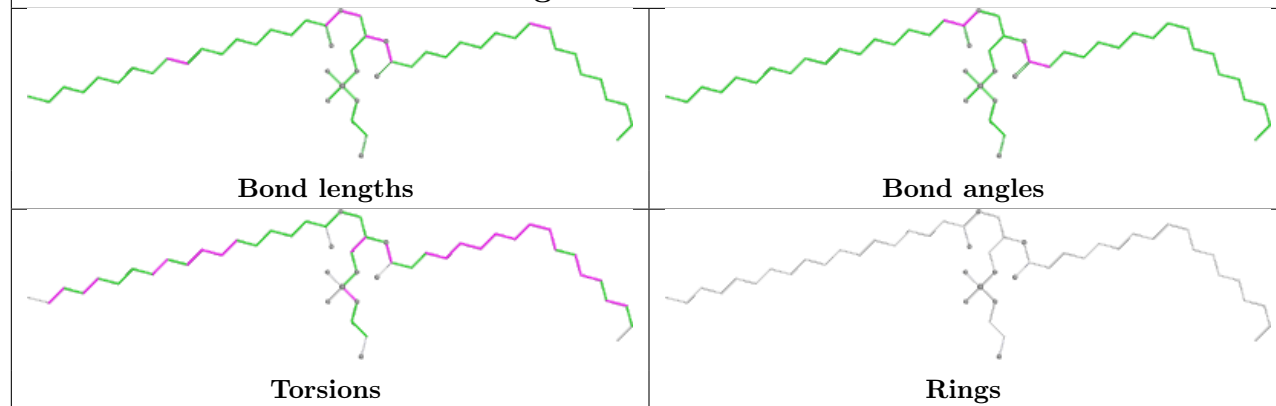


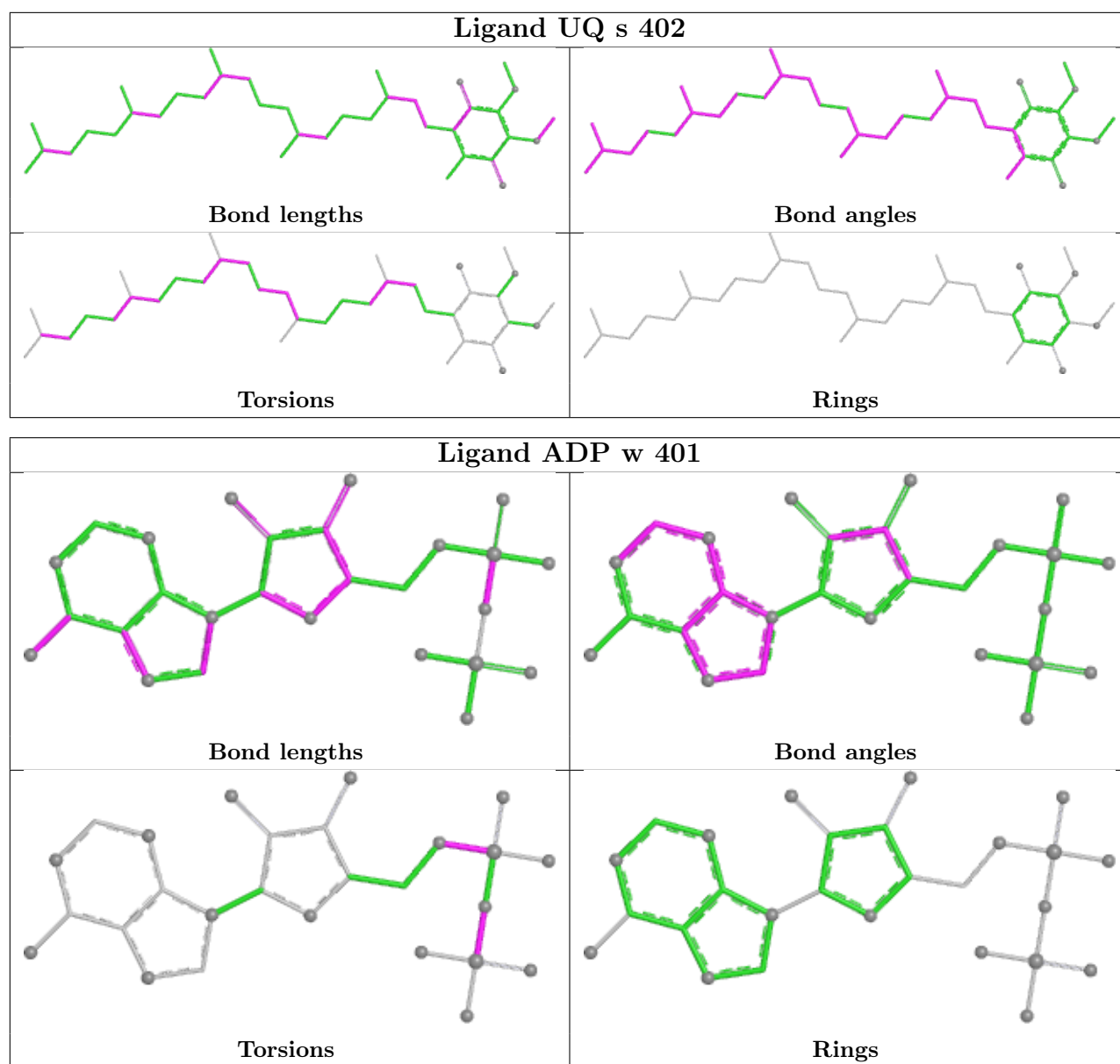


Ligand NDP J 401



Ligand PEE B 303





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.

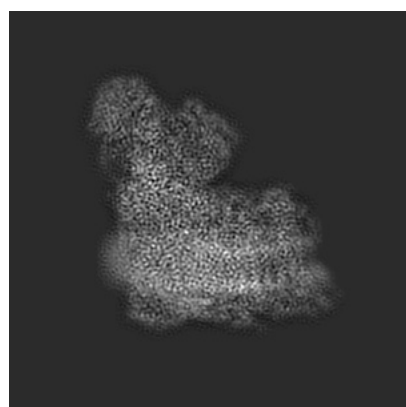
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32256. These allow visual inspection of the internal detail of the map and identification of artifacts.

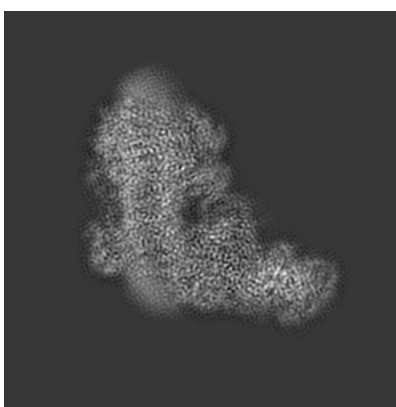
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

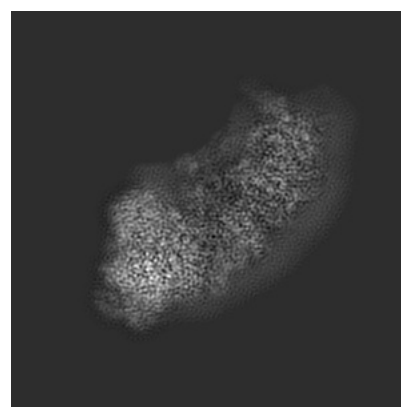
6.1.1 Primary map



X



Y

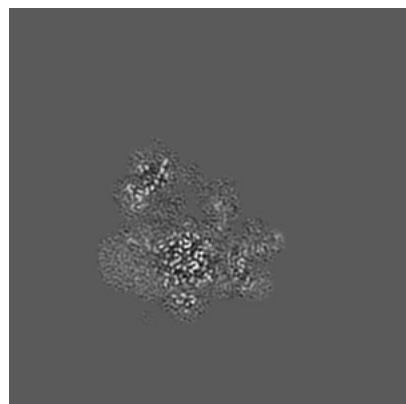


Z

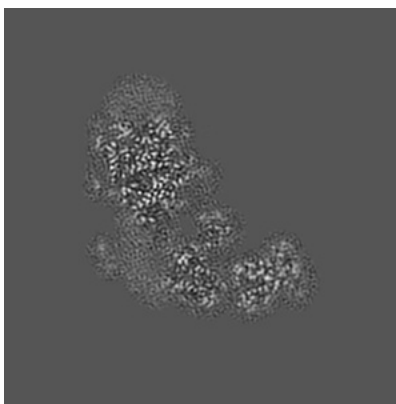
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

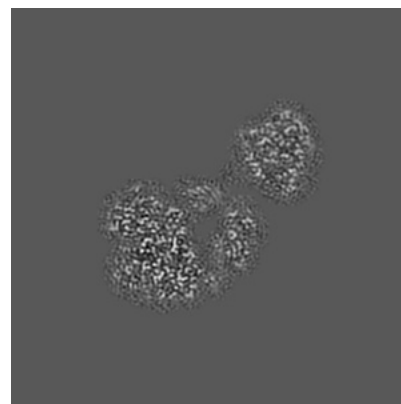
6.2.1 Primary map



X Index: 155



Y Index: 155



Z Index: 155

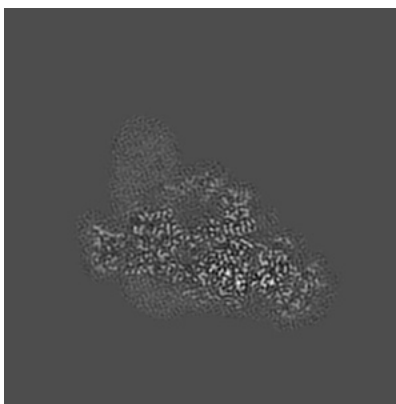
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

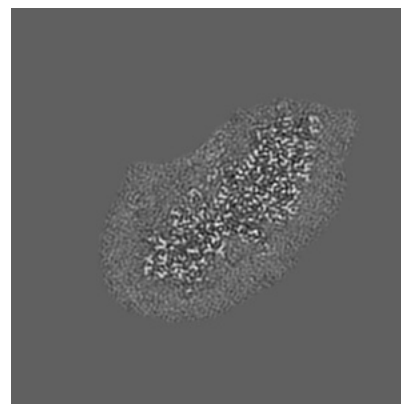
6.3.1 Primary map



X Index: 105



Y Index: 112

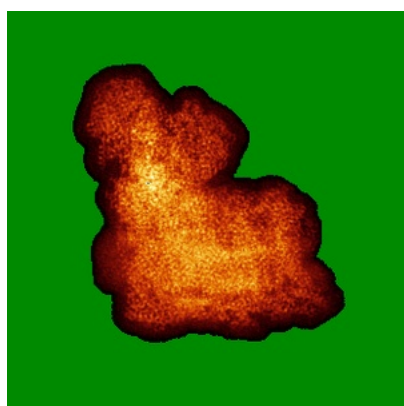


Z Index: 123

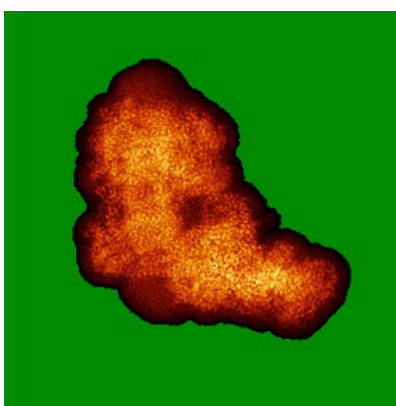
The images above show the largest variance slices of the map in three orthogonal directions.

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

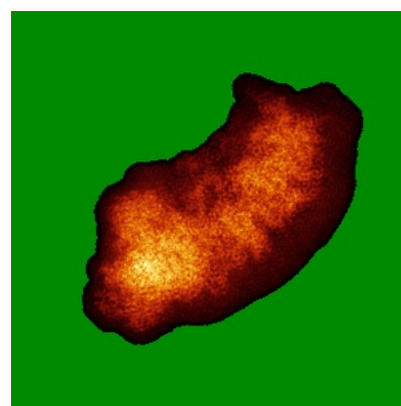
6.4.1 Primary map



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

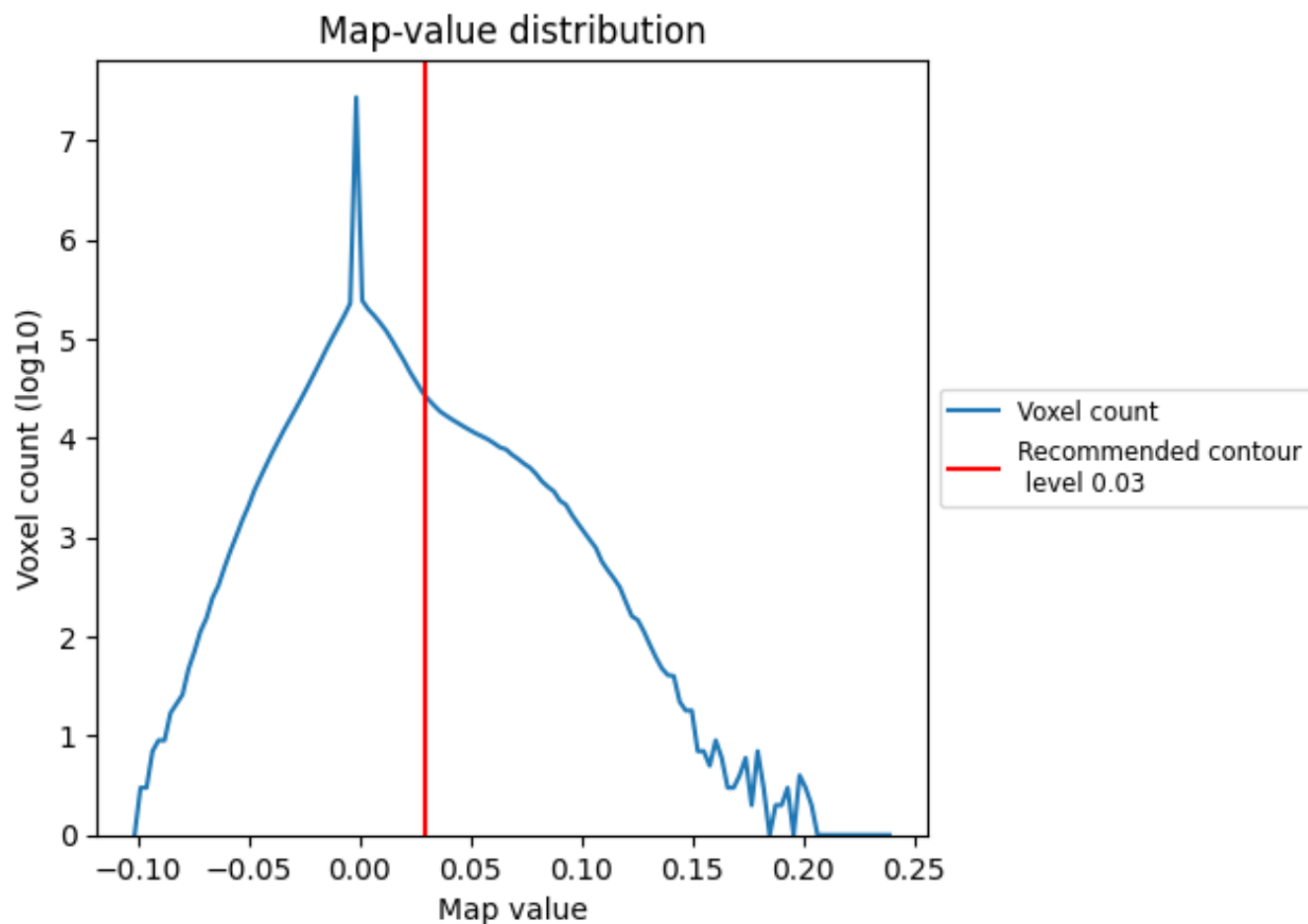
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

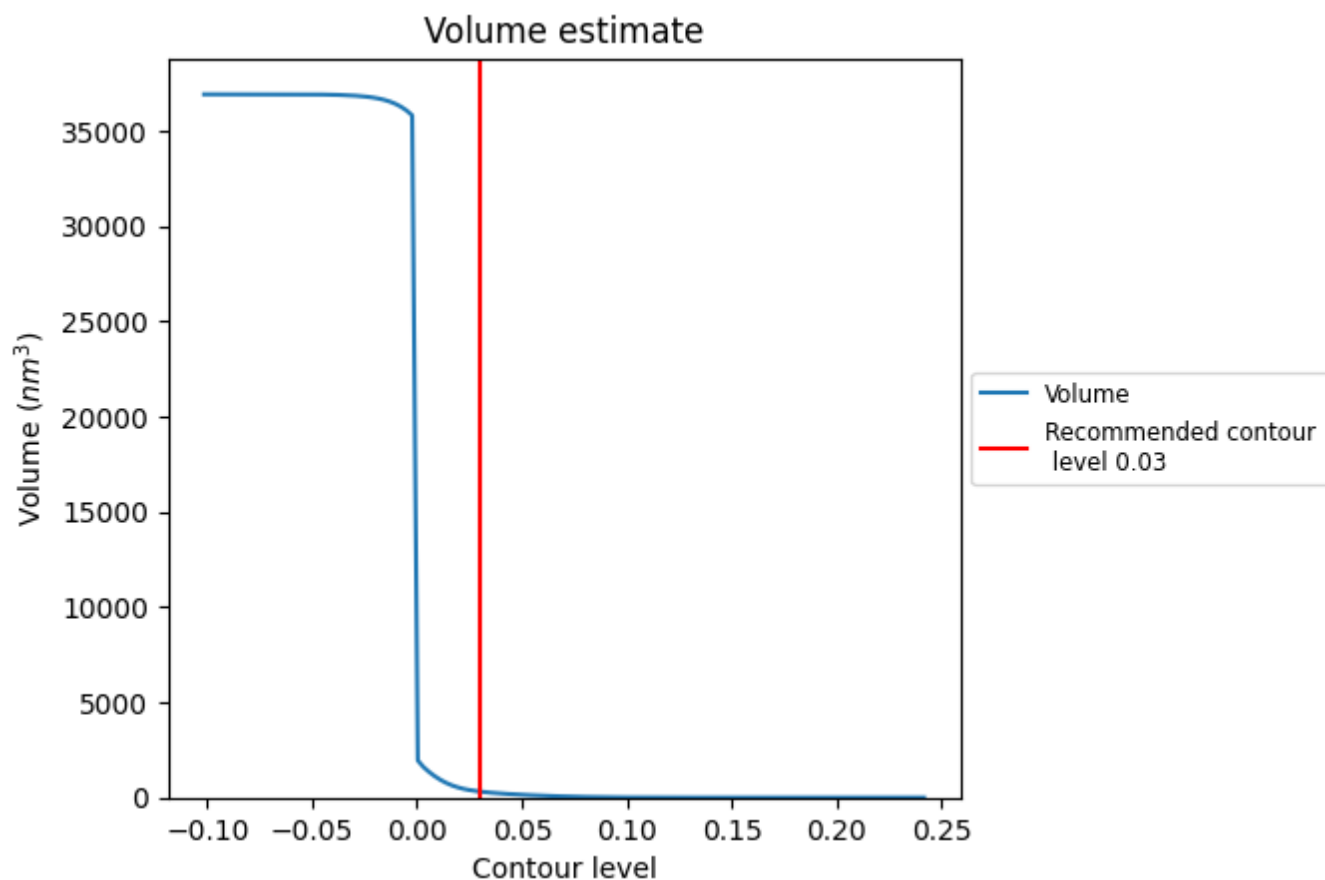
This section contains the results of statistical analysis of the map.

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.

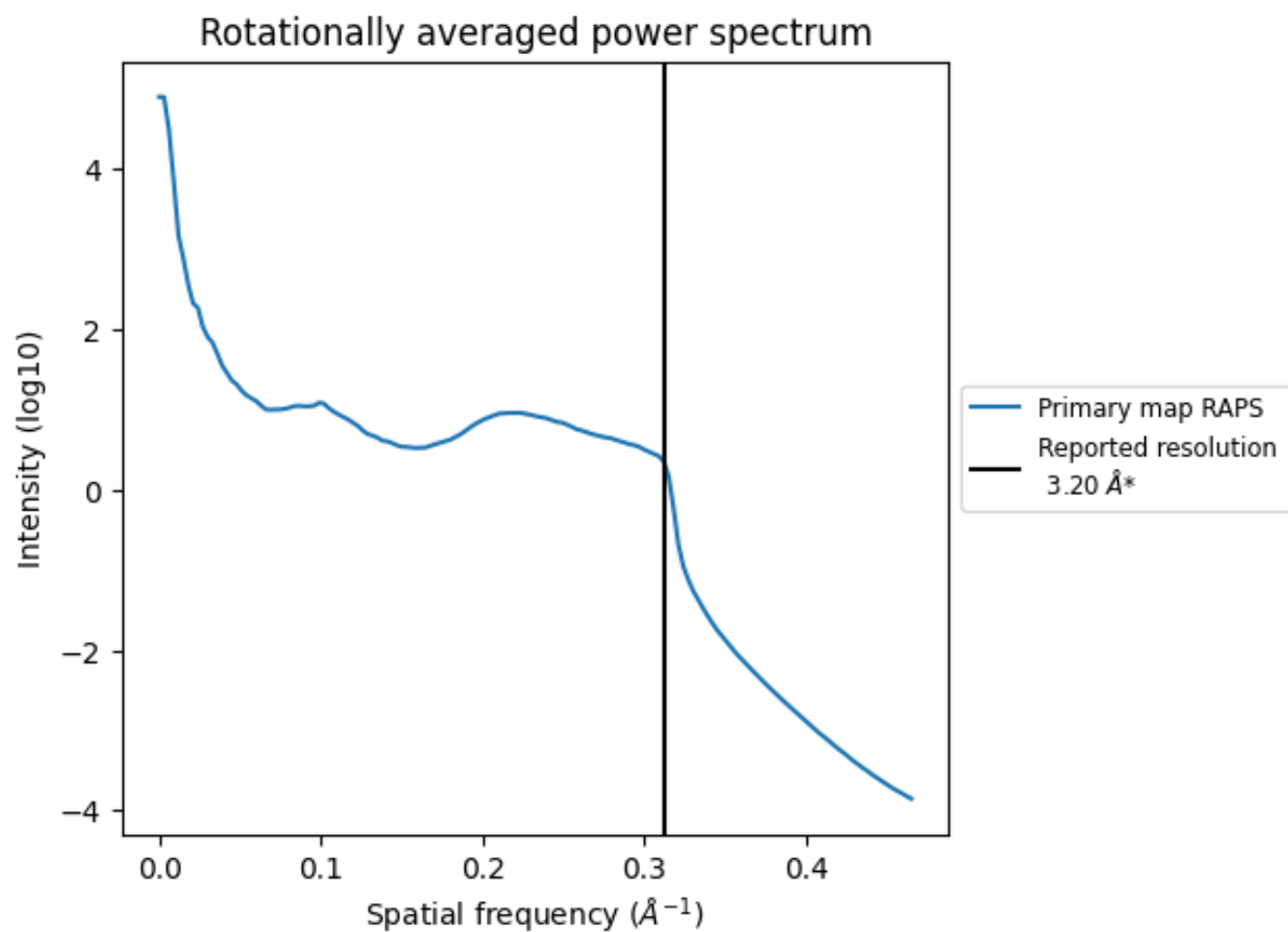
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 314 nm^3 ; this corresponds to an approximate mass of 283 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 0.312 Å⁻¹

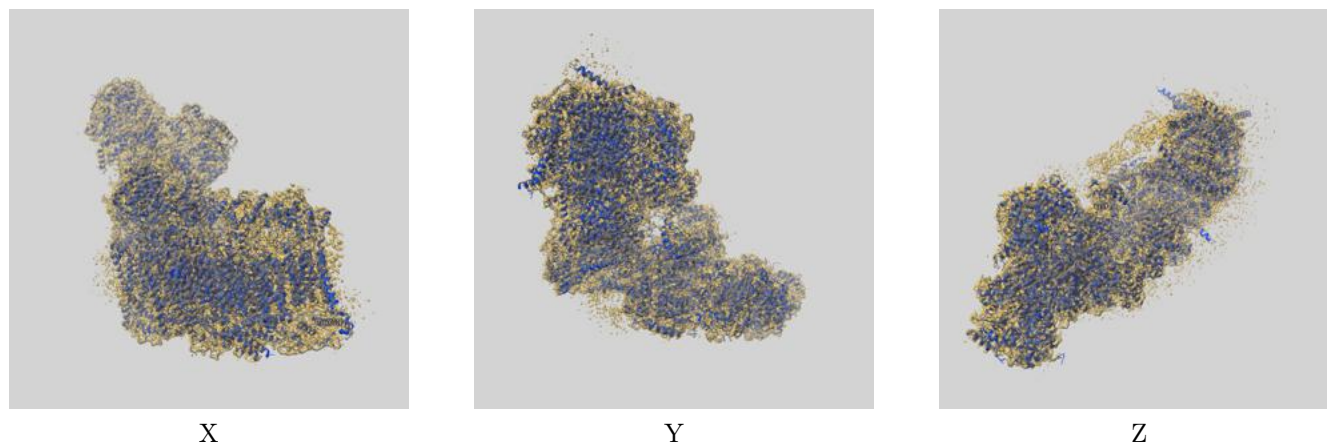
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

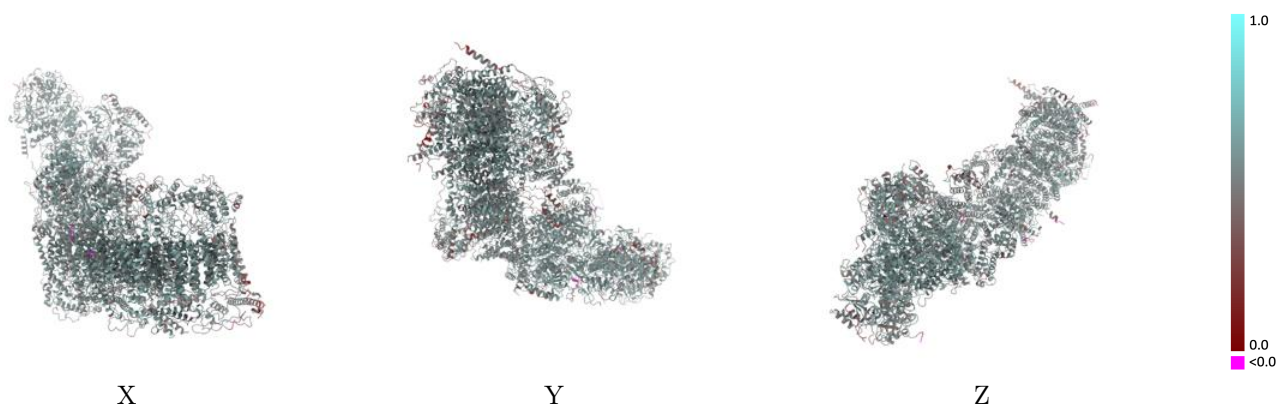
This section contains information regarding the fit between EMDB map EMD-32256 and PDB model 7W1U. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.03 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](#)

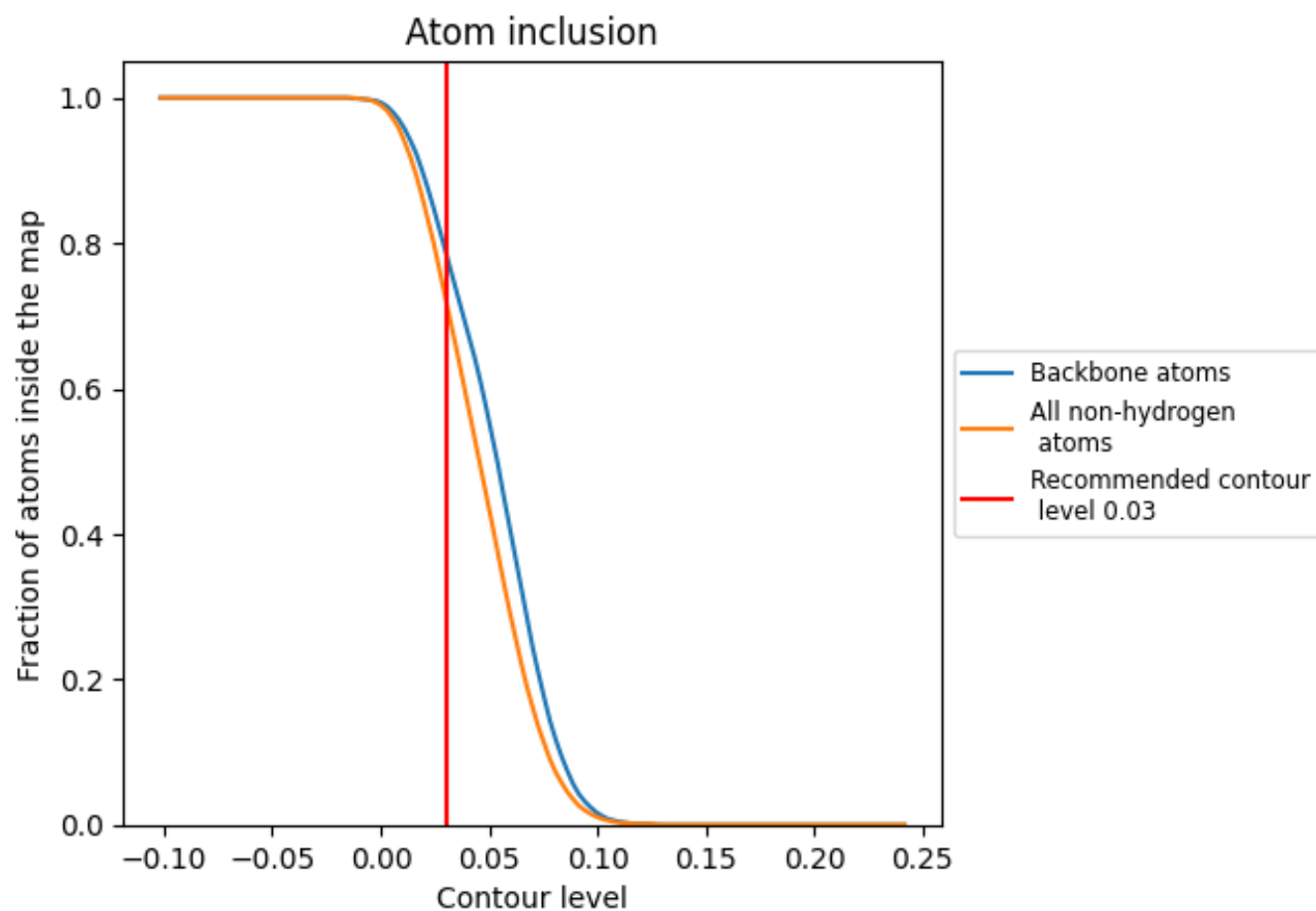


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 72% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7250	 0.5370
A	 0.7170	 0.5350
B	 0.8380	 0.5850
C	 0.8330	 0.5880
E	 0.7470	 0.5460
F	 0.6260	 0.4730
G	 0.5050	 0.4210
H	 0.7230	 0.5270
I	 0.6570	 0.5150
J	 0.7410	 0.5400
K	 0.5130	 0.4610
L	 0.7480	 0.5540
M	 0.7600	 0.5530
N	 0.6330	 0.5220
O	 0.6700	 0.5110
P	 0.8330	 0.5890
Q	 0.8200	 0.5800
S	 0.7200	 0.5270
T	 0.6010	 0.5060
U	 0.6740	 0.5100
V	 0.6180	 0.5150
W	 0.7070	 0.5300
X	 0.6650	 0.5090
Y	 0.6200	 0.4710
Z	 0.5740	 0.4500
a	 0.7220	 0.5510
b	 0.6650	 0.4900
c	 0.7240	 0.5260
d	 0.6990	 0.5190
e	 0.6560	 0.5150
f	 0.5310	 0.4430
g	 0.7500	 0.5440
h	 0.6940	 0.5170
i	 0.8020	 0.5740
j	 0.7120	 0.5490



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Chain	Atom inclusion	Q-score
k	 0.7830	 0.5650
l	 0.7380	 0.5450
m	 0.6520	 0.5050
n	 0.5530	 0.4720
o	 0.7020	 0.5260
p	 0.7310	 0.5310
r	 0.7810	 0.5710
s	 0.7580	 0.5380
u	 0.7260	 0.5340
v	 0.6150	 0.4700
w	 0.6890	 0.5220