



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 11:11 AM JST

PDB ID : 7W2R / pdb_00007w2r
EMDB ID : EMD-32265
Title : Active state CI from DQ-NADH dataset, Subclass 1
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-24
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

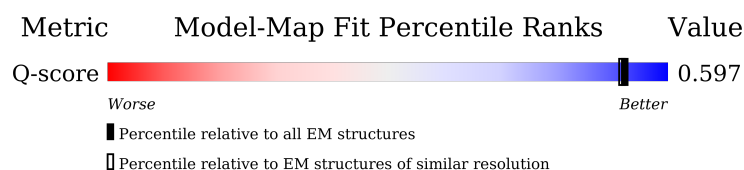
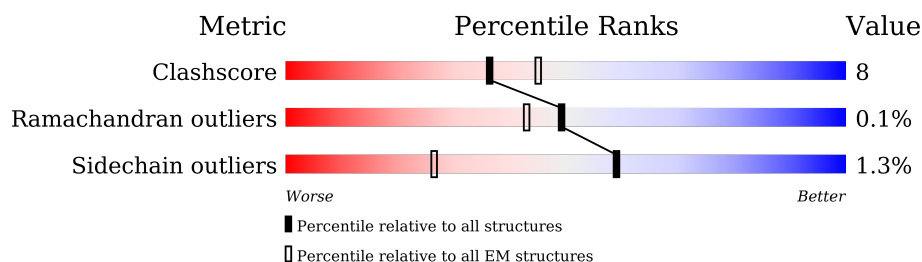
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	176	
3	C	156	
4	E	115	

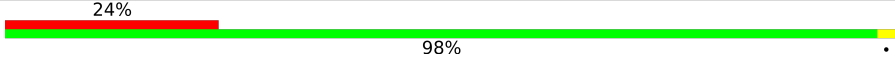
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Mol	Chain	Length	Quality of chain
5	F	86	
6	G	88	
6	X	88	
7	H	112	
8	I	112	
9	J	342	
10	K	43	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	67	
23	Z	80	
24	a	138	
25	b	126	
26	c	156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

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Mol	Chain	Length	Quality of chain
29	f	49	
30	g	122	
31	h	105	
32	i	347	
33	j	115	
34	k	98	
35	l	606	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	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	C	301	-	-	X	-

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 68128 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	86	Total	C	N	O	S	0	0
			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
			693	447	102	139	5		
6	X	88	Total	C	N	O	S	0	0
			693	447	103	138	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
			5296	3320	923	1014	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
			1732	1121	295	314	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			559	361	102	91	5		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	175	Total	C	N	O	S	0	0
			1459	915	265	271	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
			378	246	65	67		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	606	Total	C	N	O	S	0	0
			4800	3182	744	823	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
			1277	852	187	225	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
			2508	1678	385	424	21		

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

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

- Molecule 43 is a protein called 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.

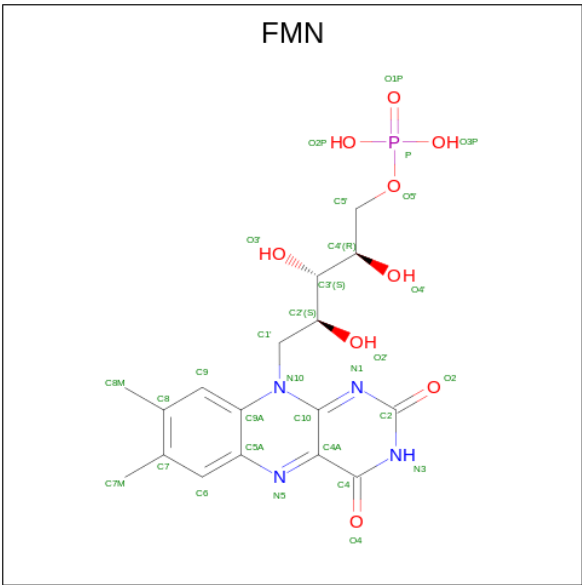
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2579	1642	438	489	10		

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



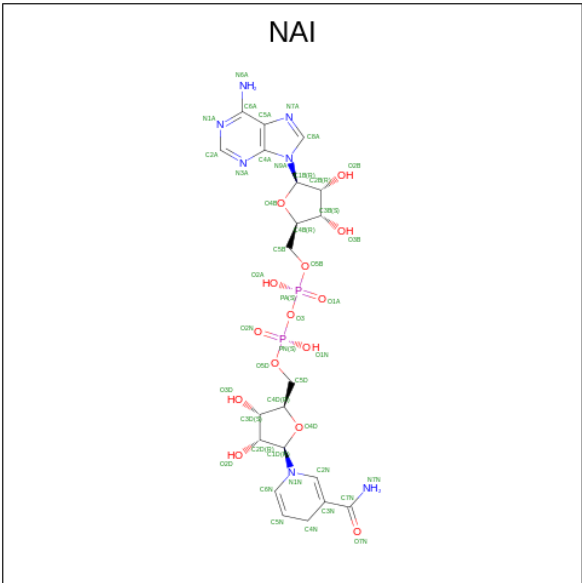
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

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



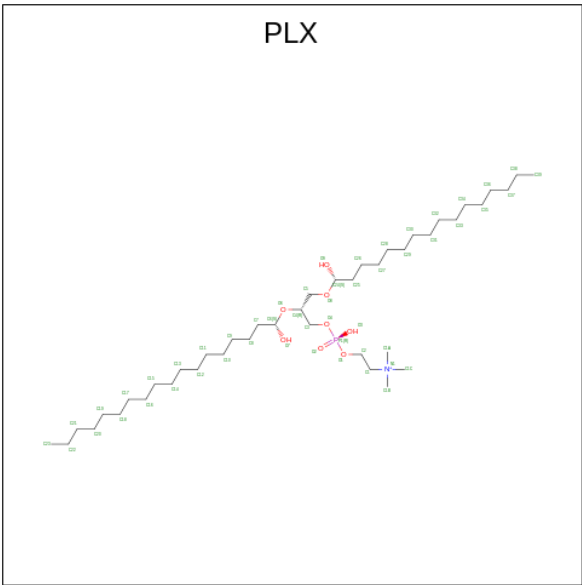
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

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



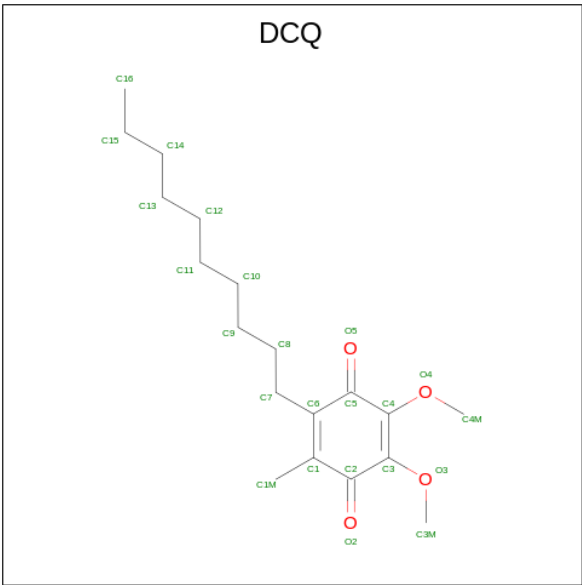
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	V	1	Total	C	N	O	P	0
			40	30	1	8	1	
48	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	b	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	l	1	Total	C	N	O	P	0
			51	41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

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



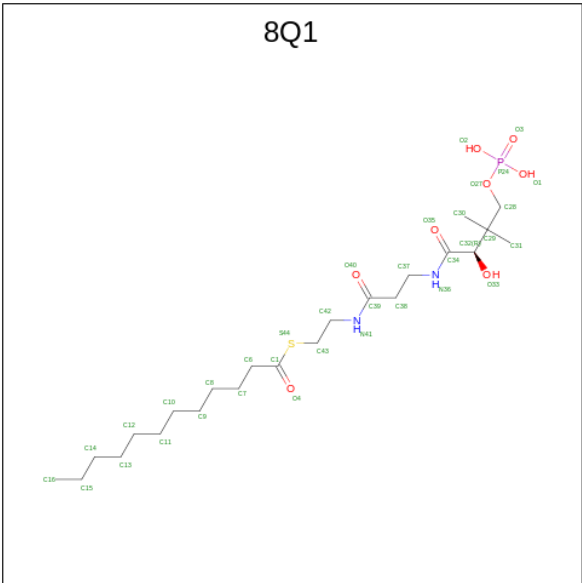
Mol	Chain	Residues	Atoms					AltConf
49	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	J	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42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

- Molecule 50 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (CCD ID: DCQ) (formula: C₁₉H₃₀O₄) (labeled as "Ligand of Interest" by depositor).



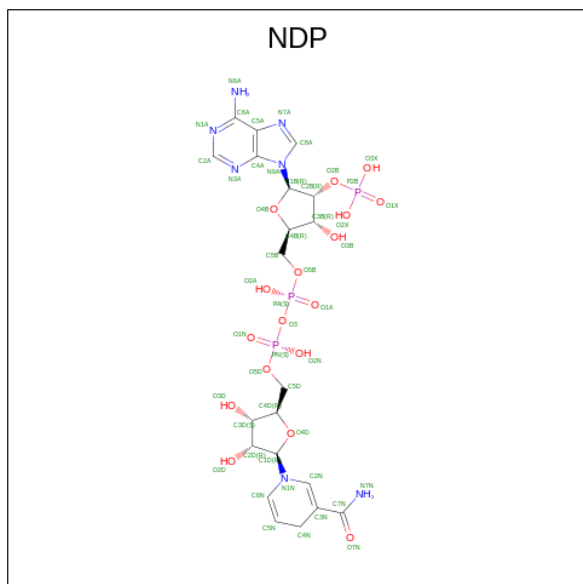
Mol	Chain	Residues	Atoms			AltConf
50	C	1	Total	C	O	0
			23	19	4	

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



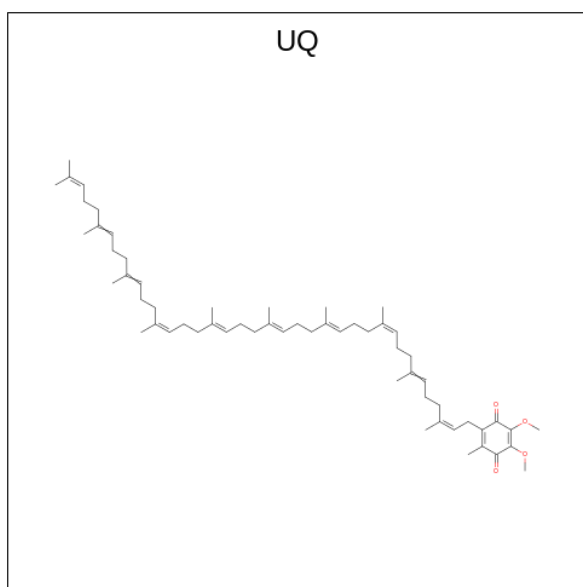
Mol	Chain	Residues	Atoms						AltConf
51	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
51	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 52 is 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).



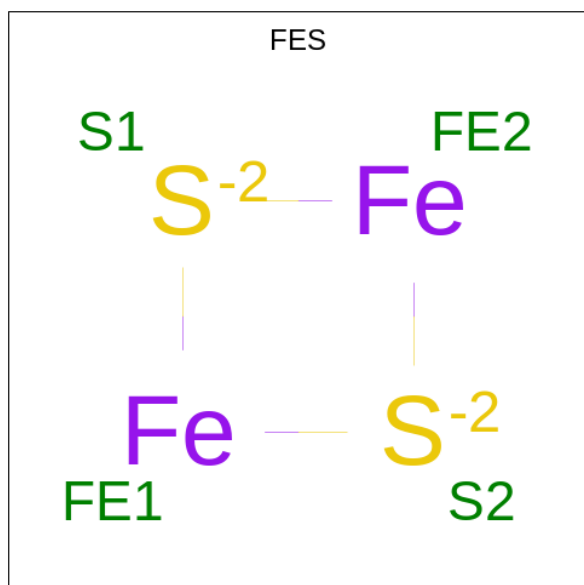
Mol	Chain	Residues	Atoms					AltConf
52	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 53 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
53	J	1	Total	C	O	0
			33	29	4	
53	s	1	Total	C	O	0
			38	34	4	

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

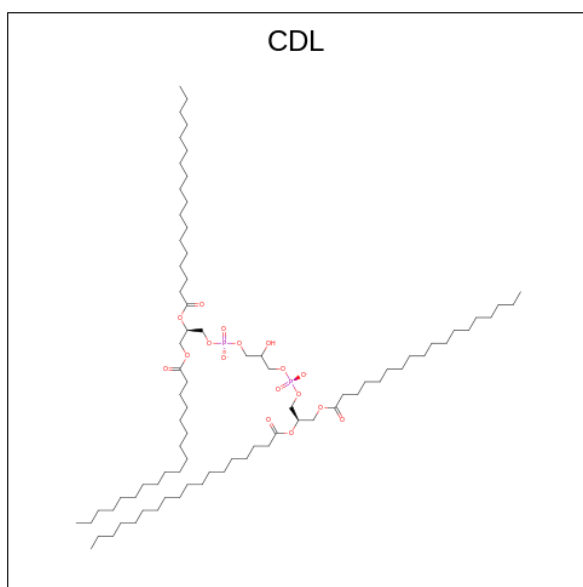


Mol	Chain	Residues	Atoms			AltConf
54	M	1	Total	Fe	S	0
			4	2	2	
54	O	1	Total	Fe	S	0
			4	2	2	

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 56 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

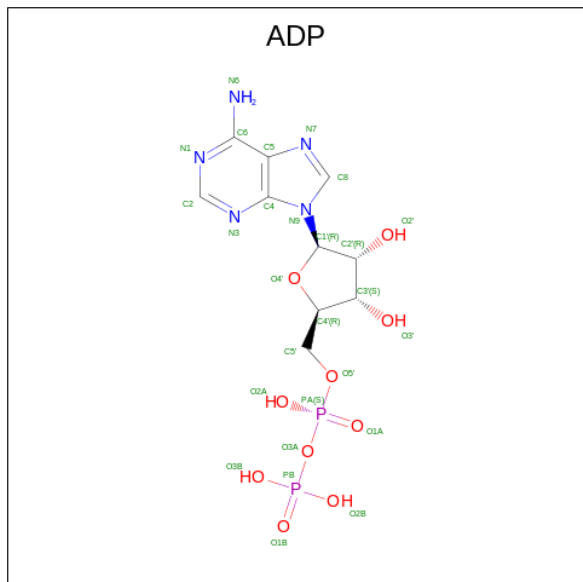


Mol	Chain	Residues	Atoms				AltConf
56	N	1	Total	C	O	P	0
			51	32	17	2	
56	V	1	Total	C	O	P	0
			94	75	17	2	
56	a	1	Total	C	O	P	0
			100	81	17	2	
56	i	1	Total	C	O	P	0
			87	68	17	2	
56	k	1	Total	C	O	P	0
			100	81	17	2	
56	l	1	Total	C	O	P	0
			99	80	17	2	
56	n	1	Total	C	O	P	0
			55	36	17	2	
56	o	1	Total	C	O	P	0
			100	81	17	2	
56	r	1	Total	C	O	P	0
			100	81	17	2	
56	s	1	Total	C	O	P	0
			89	70	17	2	

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

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

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

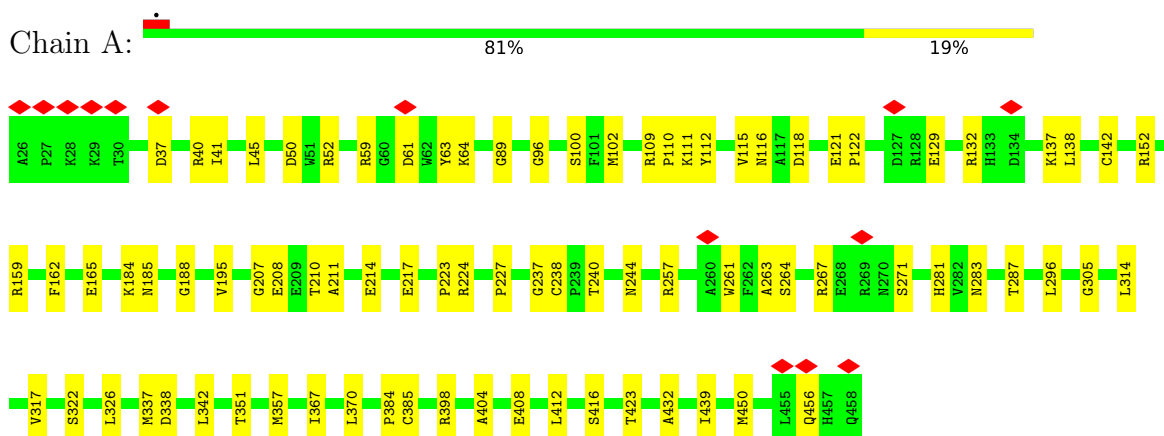


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	w	1	27	10	5	10	2	0

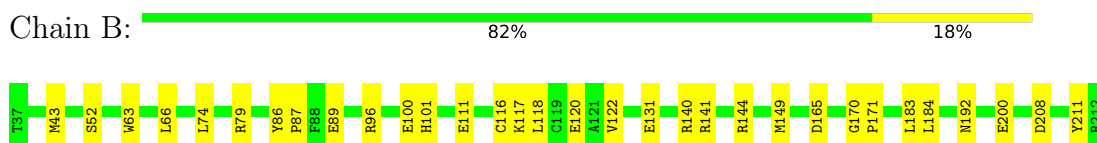
3 Residue-property plots

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

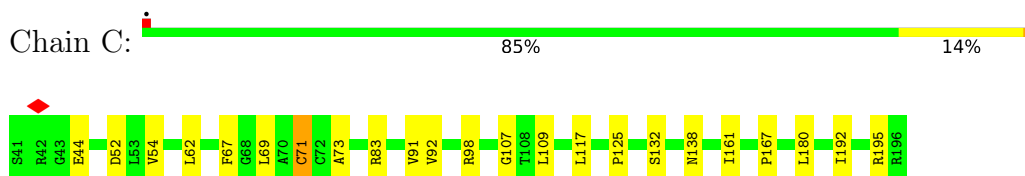
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



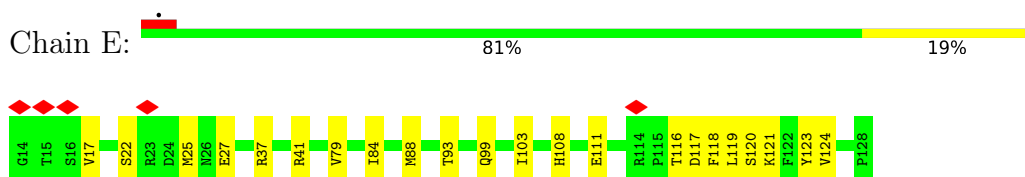
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



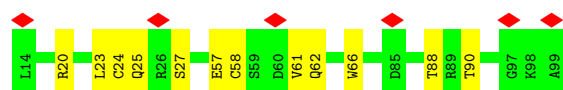
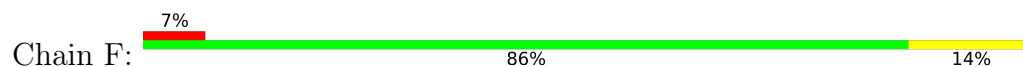
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



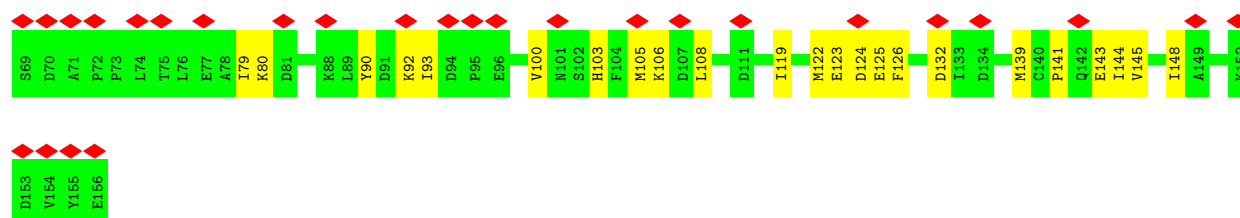
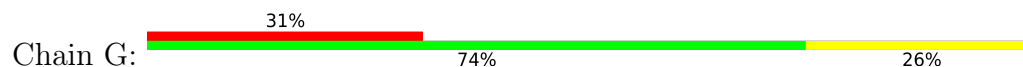
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



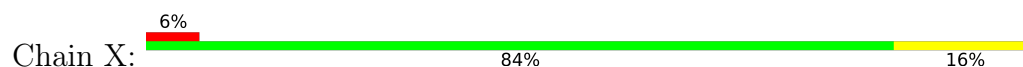
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



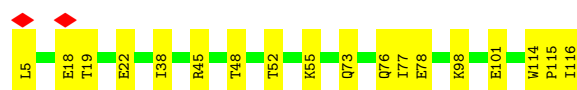
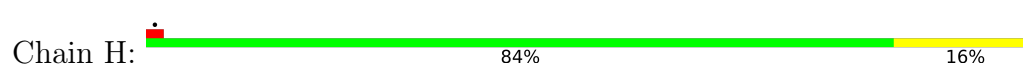
- Molecule 6: Acyl carrier protein



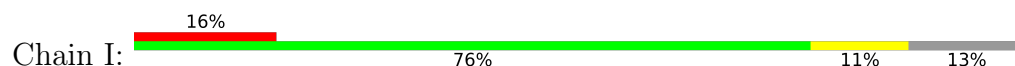
- Molecule 6: Acyl carrier protein



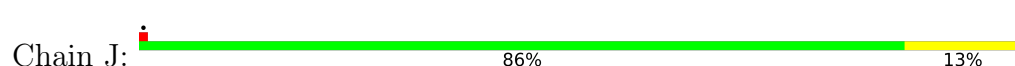
- Molecule 7: Complex I subunit B13

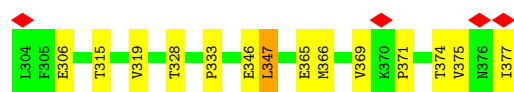


- Molecule 8: Complex I-B14.5a

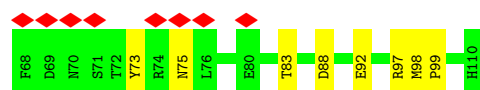
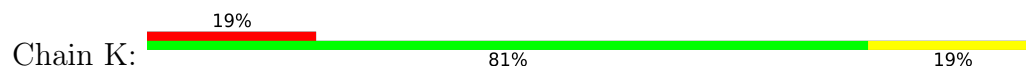


- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

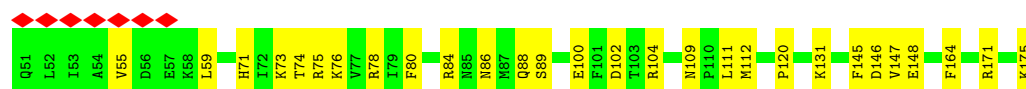
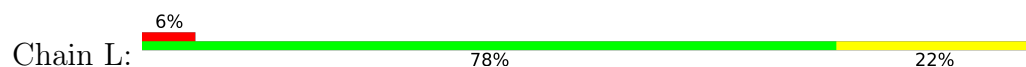




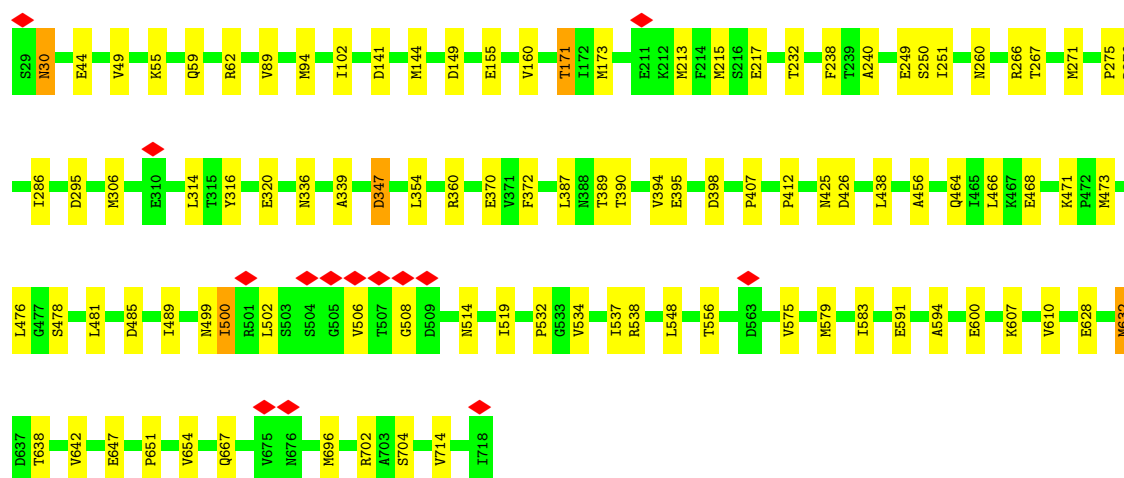
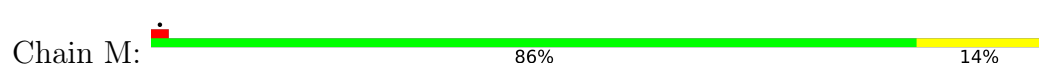
• Molecule 10: Complex I-9kD



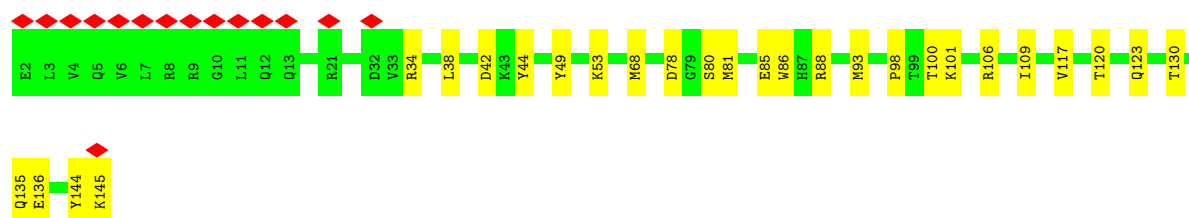
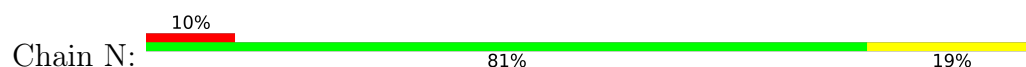
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



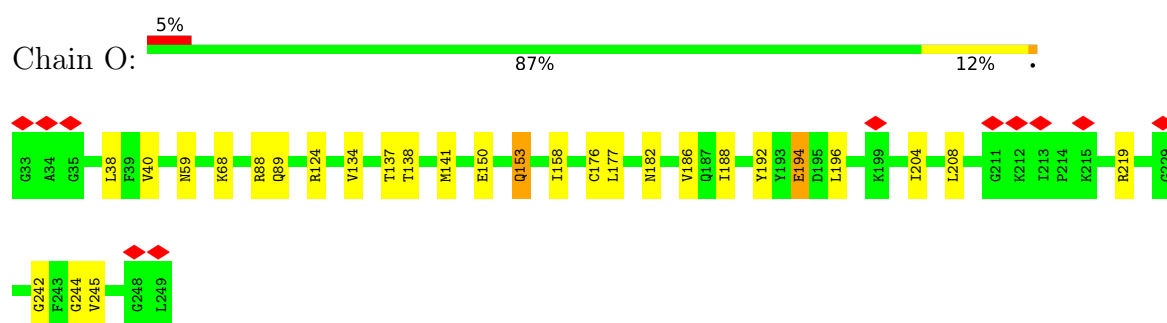
• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



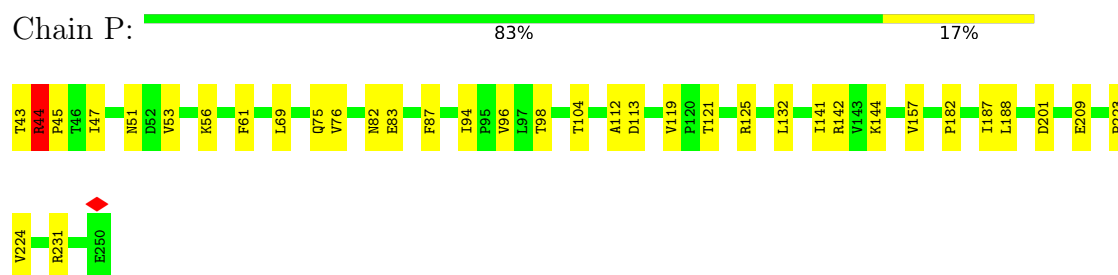
• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



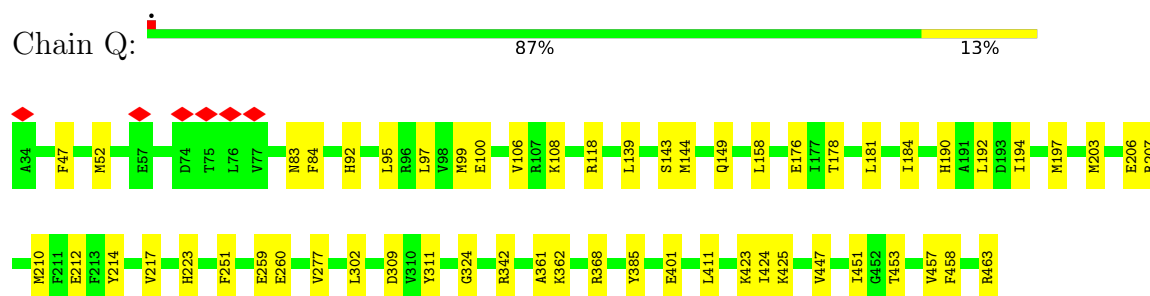
• Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



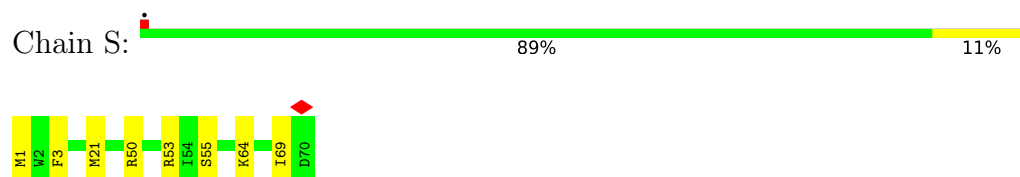
- Molecule 15: Complex I-30kD



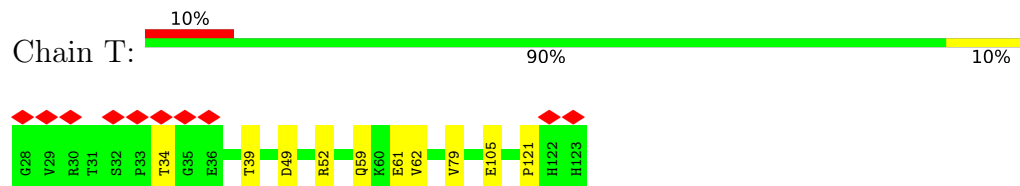
- Molecule 16: Complex I-49kD



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



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

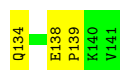
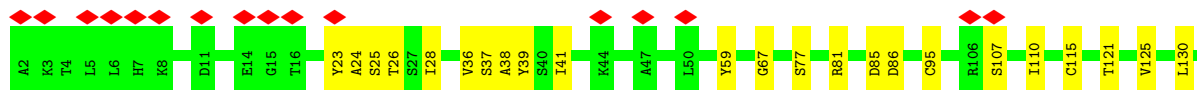
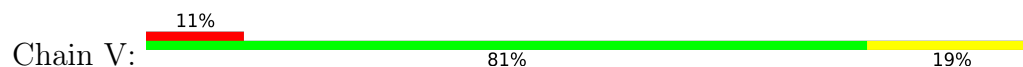


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3





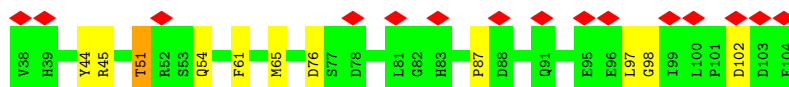
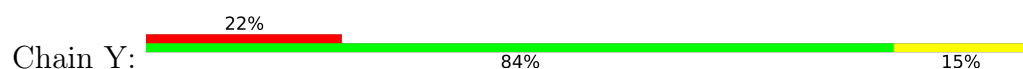
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



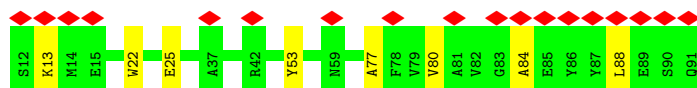
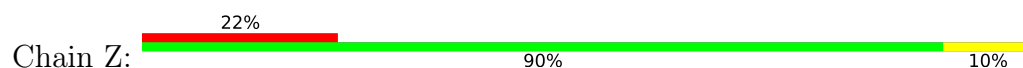
- Molecule 21: Complex I-B16.6



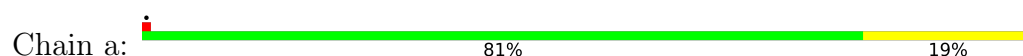
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



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

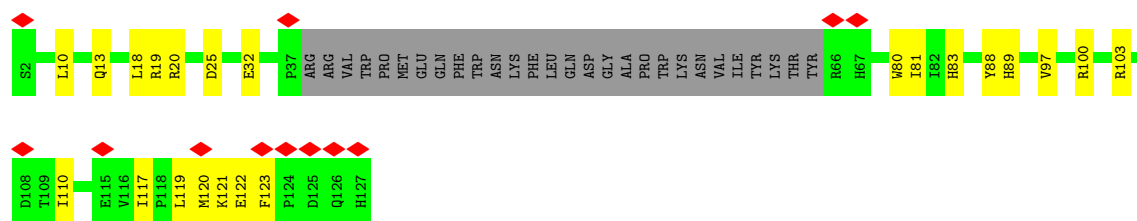


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

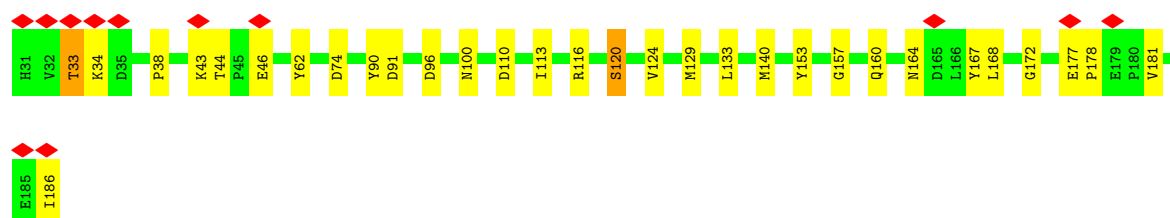
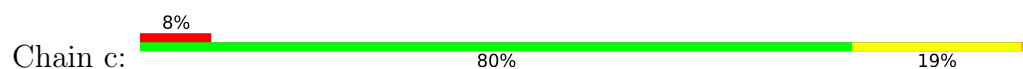


- Molecule 25: Complex I-B17

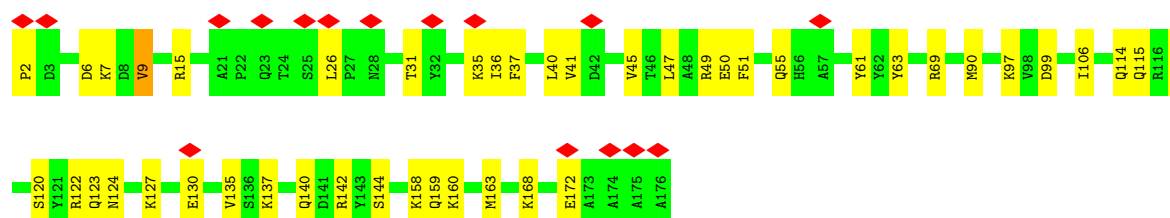
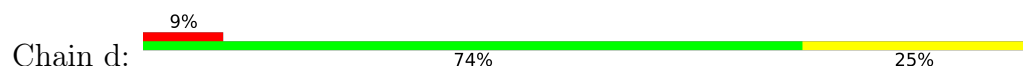




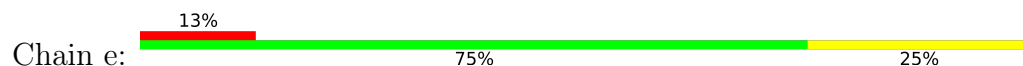
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



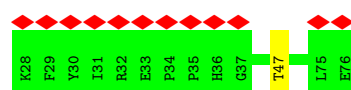
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



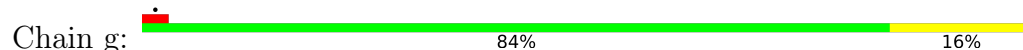
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



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

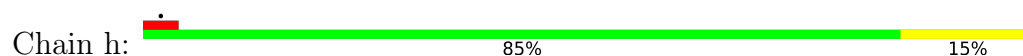


- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

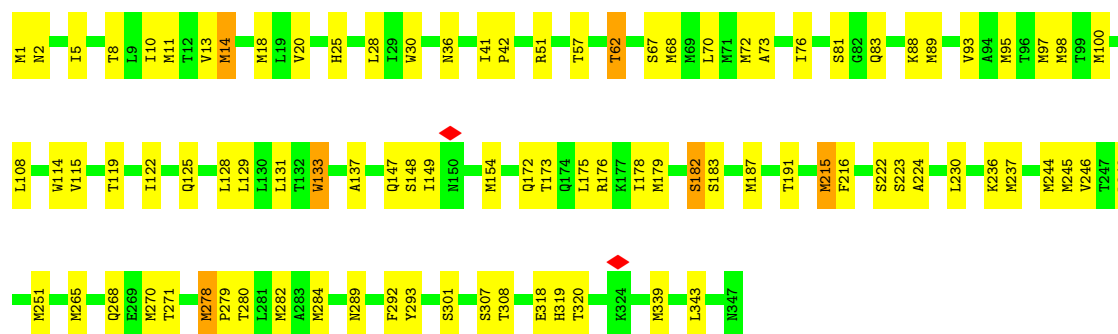




- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

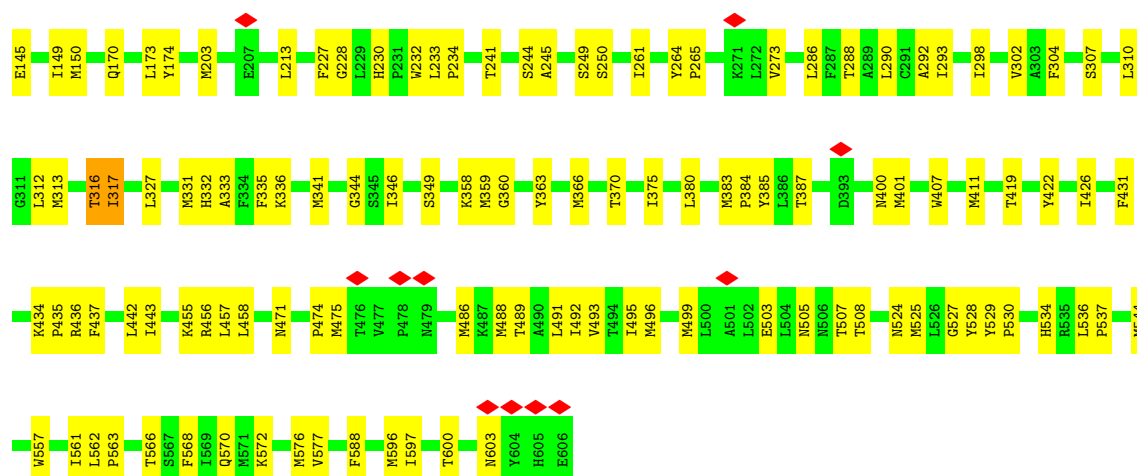


- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

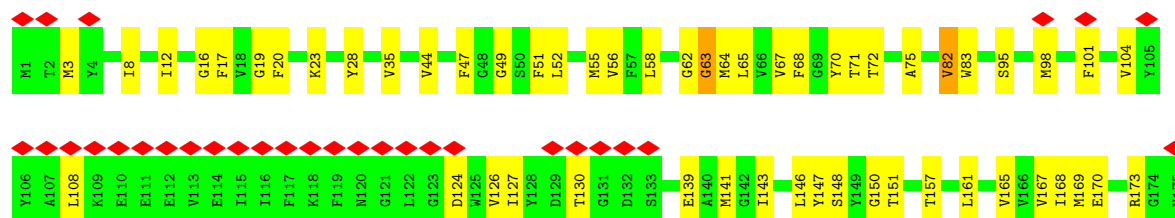


- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

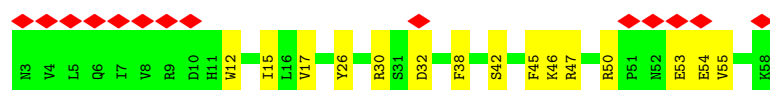
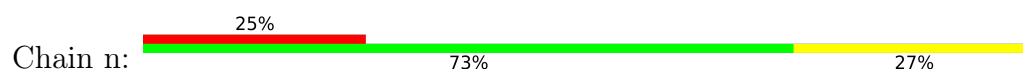




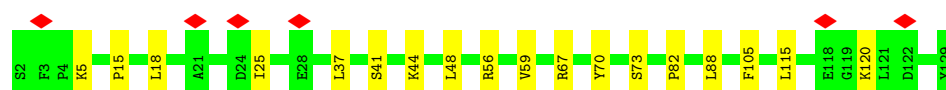
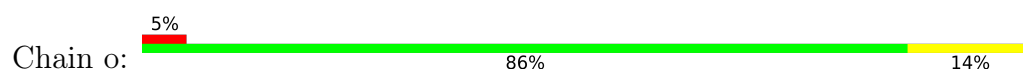
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6



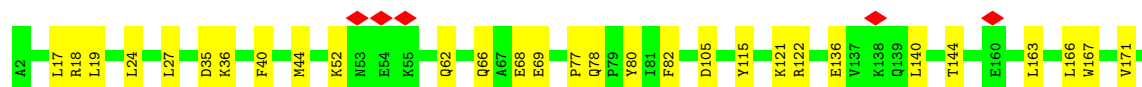
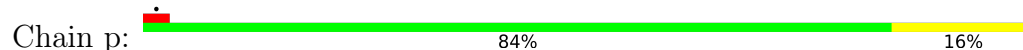
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



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



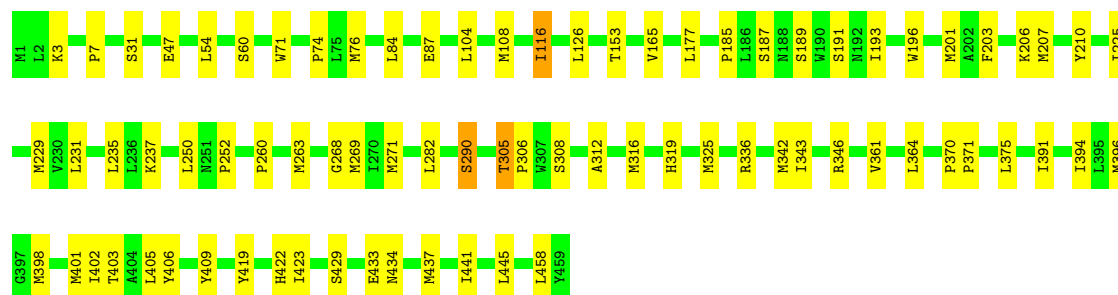
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9





- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r: 83% 17%



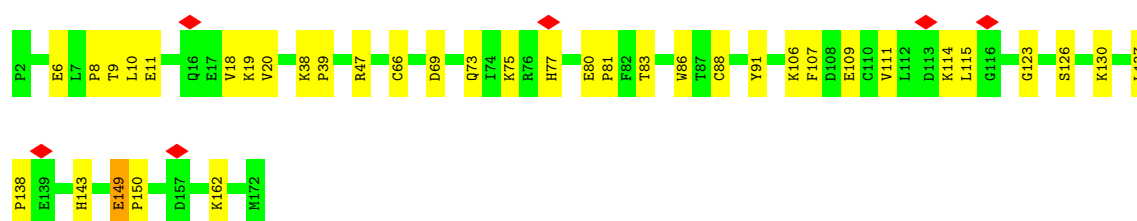
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s: 77% 23%



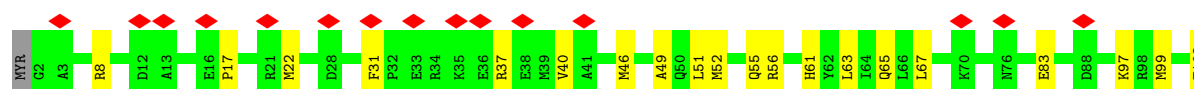
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

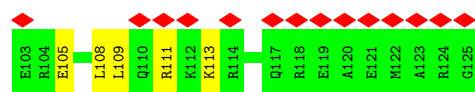
Chain u: 78% 21%



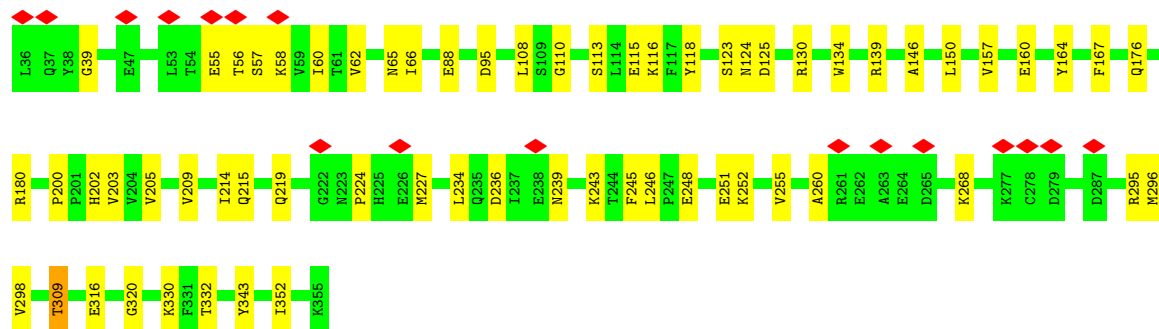
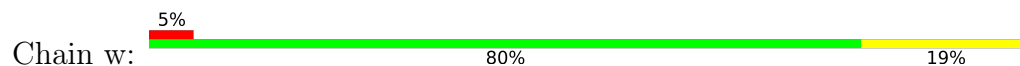
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v: 23% 79% 20%





- 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	85858	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	0.175	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0267	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: FES, ZN, CDL, PEE, NAI, DCQ, 8Q1, FMN, SF4, NDP, PLX, ADP, MG, 2MR, UQ

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	0.14	0/3406	0.30	0/4603
2	B	0.16	0/1443	0.31	0/1952
3	C	0.17	0/1279	0.32	0/1730
4	E	0.16	0/995	0.33	0/1340
5	F	0.16	0/698	0.36	0/940
6	G	0.14	0/705	0.35	0/956
6	X	0.12	0/704	0.29	0/953
7	H	0.16	0/929	0.36	0/1258
8	I	0.15	0/798	0.36	0/1079
9	J	0.14	0/2828	0.31	0/3834
10	K	0.11	0/377	0.26	0/509
11	L	0.18	0/1039	0.45	2/1403 (0.1%)
12	M	0.15	0/5384	0.32	0/7295
13	N	0.13	0/1245	0.32	0/1694
14	O	0.13	0/1711	0.33	0/2328
15	P	0.18	0/1783	0.44	2/2429 (0.1%)
16	Q	0.17	0/3538	0.31	0/4796
17	S	0.23	0/574	0.42	0/772
18	T	0.12	0/755	0.30	0/1018
19	U	0.13	0/664	0.28	0/912
20	V	0.12	0/1042	0.24	0/1411
21	W	0.15	0/1192	0.29	0/1610
22	Y	0.17	0/610	0.41	0/836
23	Z	0.11	0/660	0.31	0/892
24	a	0.15	0/1184	0.30	0/1603
25	b	0.17	0/844	0.39	0/1149
26	c	0.16	0/1371	0.37	0/1875
27	d	0.16	0/1492	0.42	2/2012 (0.1%)
28	e	0.13	0/891	0.34	0/1210
29	f	0.12	0/386	0.23	0/523
30	g	0.13	0/1036	0.28	0/1401
31	h	0.13	0/889	0.30	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.19	0/2773	0.40	1/3768 (0.0%)
33	j	0.22	0/938	0.58	2/1281 (0.2%)
34	k	0.17	0/759	0.31	0/1029
35	l	0.15	0/4929	0.34	0/6704
36	m	0.24	0/1309	0.56	2/1780 (0.1%)
37	n	0.14	0/491	0.30	0/663
38	o	0.13	0/1092	0.31	0/1481
39	p	0.13	0/1590	0.28	0/2155
40	r	0.17	0/3723	0.35	0/5078
41	s	0.20	0/2581	0.43	1/3529 (0.0%)
42	u	0.16	0/1436	0.39	0/1938
43	v	0.12	0/1052	0.31	0/1411
44	w	0.14	0/2639	0.33	0/3576
All	All	0.16	0/67764	0.35	12/91906 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	j	73	LEU	CA-C-N	8.00	128.19	119.87
33	j	73	LEU	C-N-CA	8.00	128.19	119.87
15	P	44	ARG	CA-C-N	7.16	127.00	119.05
15	P	44	ARG	C-N-CA	7.16	127.00	119.05
11	L	74	THR	N-CA-C	6.15	118.07	111.36
32	i	133	TRP	N-CA-C	5.82	117.70	111.36
36	m	148	SER	N-CA-C	5.55	117.41	111.36
11	L	73	LYS	N-CA-C	5.51	117.09	111.14
27	d	26	LEU	CA-C-N	5.21	125.12	119.85
27	d	26	LEU	C-N-CA	5.21	125.12	119.85
36	m	63	GLY	N-CA-C	-5.17	106.14	112.77
41	s	192	GLU	N-CA-C	5.13	116.87	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3330	0	3292	60	0
2	B	1412	0	1363	24	0
3	C	1248	0	1254	20	0
4	E	971	0	975	18	0
5	F	687	0	700	5	0
6	G	693	0	671	18	0
6	X	693	0	671	10	0
7	H	910	0	950	11	0
8	I	780	0	808	13	0
9	J	2751	0	2773	26	0
10	K	366	0	338	6	0
11	L	1016	0	1016	21	0
12	M	5296	0	5326	64	0
13	N	1204	0	1162	18	0
14	O	1671	0	1673	15	0
15	P	1732	0	1682	26	0
16	Q	3459	0	3396	41	0
17	S	559	0	553	6	0
18	T	741	0	701	7	0
19	U	643	0	642	10	0
20	V	1021	0	1025	14	0
21	W	1161	0	1144	16	0
22	Y	584	0	529	8	0
23	Z	641	0	620	6	0
24	a	1151	0	1164	27	0
25	b	819	0	835	21	0
26	c	1315	0	1208	25	0
27	d	1459	0	1424	33	0
28	e	867	0	817	21	0
29	f	378	0	356	1	0
30	g	1005	0	999	14	0
31	h	867	0	871	11	0
32	i	2710	0	2874	66	0
33	j	914	0	951	44	0
34	k	748	0	799	32	0
35	l	4800	0	4939	105	0
36	m	1277	0	1239	66	0
37	n	479	0	486	14	0
38	o	1062	0	1072	17	0
39	p	1534	0	1470	24	0
40	r	3631	0	3839	59	0
41	s	2508	0	2607	60	0
42	u	1398	0	1374	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	v	1028	0	982	24	0
44	w	2579	0	2529	44	0
45	A	8	0	0	1	0
45	B	16	0	0	0	0
45	C	8	0	0	2	0
45	M	16	0	0	0	0
46	A	31	0	19	6	0
47	A	44	0	27	5	0
48	B	51	0	82	2	0
48	C	47	0	71	1	0
48	V	40	0	54	3	0
48	W	41	0	59	2	0
48	b	46	0	69	4	0
48	j	51	0	82	6	0
48	l	51	0	82	3	0
48	r	51	0	82	2	0
48	s	41	0	59	3	0
49	C	52	0	88	2	0
49	J	52	0	88	1	0
49	a	52	0	88	3	0
49	g	52	0	88	8	0
49	j	52	0	88	2	0
49	r	104	0	176	8	0
50	C	23	0	30	3	0
51	G	35	0	0	0	0
51	X	35	0	0	0	0
52	J	48	0	25	3	0
53	J	33	0	39	3	0
53	s	38	0	47	5	0
54	M	4	0	0	0	0
54	O	4	0	0	0	0
55	M	1	0	0	0	0
56	N	51	0	46	0	0
56	V	94	0	138	8	0
56	a	100	0	156	8	0
56	i	87	0	124	3	0
56	k	100	0	156	4	0
56	l	99	0	151	13	0
56	n	55	0	54	2	0
56	o	100	0	156	7	0
56	r	100	0	156	7	0
56	s	89	0	125	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	T	1	0	0	0	0
58	w	27	0	11	2	0
All	All	68128	0	68815	1056	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 (1056) 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)
15:P:44:ARG:CB	15:P:45:PRO:HD2	1.63	1.29
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.17
52:J:401:NDP:O4D	52:J:401:NDP:C4D	1.68	1.11
15:P:44:ARG:CB	15:P:45:PRO:CD	2.32	1.07
33:j:73:LEU:HD12	36:m:55:MET:SD	2.01	1.00
36:m:55:MET:HE3	36:m:55:MET:HA	1.43	1.00
36:m:64:MET:HE2	36:m:64:MET:HA	1.45	0.98
11:L:76:LYS:HE3	11:L:146:ASP:OD2	1.69	0.93
41:s:21:THR:HG21	53:s:403:UQ:H13	1.51	0.92
4:E:117:ASP:OD1	4:E:120:SER:HB2	1.78	0.84
4:E:108:HIS:HB3	4:E:111:GLU:OE2	1.77	0.84
33:j:63:LEU:O	33:j:67:LEU:HD23	1.80	0.81
16:Q:83:ASN:HB2	33:j:38:GLU:HG2	1.63	0.81
11:L:76:LYS:CE	11:L:146:ASP:OD2	2.30	0.80
32:i:236:LYS:HG3	32:i:237:MET:HG3	1.63	0.80
36:m:49:GLY:HA2	36:m:139:GLU:OE1	1.81	0.80
35:l:400:ASN:HB3	35:l:486:MET:HE3	1.63	0.79
36:m:55:MET:HE1	36:m:58:LEU:HD23	1.64	0.79
36:m:82:VAL:HG11	56:s:402:CDL:HB31	1.63	0.79
1:A:184:LYS:HD2	10:K:98:MET:HE1	1.64	0.77
1:A:121:GLU:HG2	47:A:503:NAI:H42N	1.66	0.77
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.67	0.75
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.67	0.74
33:j:108:GLN:HB2	36:m:169:MET:HE1	1.69	0.73
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.21	0.73
36:m:64:MET:HA	36:m:64:MET:CE	2.18	0.72
36:m:141:MET:HE2	36:m:141:MET:HA	1.69	0.72
31:h:59:GLU:N	31:h:59:GLU:OE1	2.21	0.72
32:i:278:MET:O	32:i:282:MET:HG3	1.89	0.72
12:M:213:MET:HG2	12:M:215:MET:HG2	1.73	0.71
33:j:74:PRO:HB3	36:m:143:ILE:HG22	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:97:MET:HA	32:i:100:MET:HE2	1.73	0.71
56:a:201:CDL:H171	56:a:201:CDL:H712	1.73	0.71
56:l:701:CDL:H331	56:l:701:CDL:H142	1.73	0.71
56:l:701:CDL:H432	56:l:701:CDL:H621	1.71	0.71
12:M:89:VAL:HB	12:M:94:MET:HE3	1.73	0.70
1:A:50:ASP:O	1:A:59:ARG:NH2	2.23	0.70
44:w:176:GLN:NE2	44:w:236:ASP:OD2	2.24	0.70
14:O:38:LEU:O	14:O:124:ARG:NH2	2.25	0.70
36:m:51:PHE:HB3	36:m:139:GLU:OE2	1.92	0.70
35:l:150:MET:HE1	56:l:701:CDL:H132	1.73	0.69
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.25	0.69
14:O:182:ASN:HB3	14:O:194:GLU:HB2	1.74	0.69
33:j:69:ILE:HD13	41:s:147:ALA:HB3	1.73	0.69
33:j:67:LEU:HD21	34:k:68:ALA:HB2	1.73	0.69
33:j:67:LEU:HG	34:k:68:ALA:CB	2.22	0.69
1:A:152:ARG:NH2	10:K:99:PRO:O	2.26	0.68
33:j:67:LEU:CD2	34:k:68:ALA:HB2	2.23	0.68
11:L:109:ASN:ND2	11:L:111:LEU:O	2.27	0.68
16:Q:47:PHE:HD1	16:Q:52:MET:HE1	1.58	0.68
44:w:108:LEU:HD21	44:w:330:LYS:HD3	1.75	0.68
9:J:192:ARG:NH1	9:J:198:ALA:O	2.27	0.68
25:b:83:HIS:HD2	27:d:45:VAL:HG21	1.59	0.67
41:s:21:THR:HG21	53:s:403:UQ:C13	2.23	0.67
32:i:128:LEU:C	32:i:128:LEU:HD23	2.19	0.67
4:E:117:ASP:OD1	4:E:120:SER:CB	2.43	0.67
33:j:73:LEU:N	33:j:74:PRO:CD	2.58	0.66
32:i:215:MET:HG2	32:i:251:MET:HE1	1.76	0.66
12:M:696:MET:HG2	12:M:702:ARG:HA	1.79	0.65
35:l:102:GLU:OE2	35:l:456:ARG:NH2	2.27	0.65
2:B:184:LEU:HB3	11:L:112:MET:HE2	1.78	0.65
40:r:336:ARG:HH22	40:r:429:SER:HA	1.62	0.65
56:a:201:CDL:H191	56:a:201:CDL:H732	1.78	0.65
56:r:504:CDL:H401	56:r:504:CDL:H221	1.79	0.64
41:s:77:LEU:HD23	41:s:115:SER:HB3	1.79	0.64
4:E:84:ILE:O	4:E:88:MET:HG3	1.96	0.64
33:j:69:ILE:HD11	41:s:144:VAL:HA	1.77	0.64
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.77	0.64
30:g:15:PHE:HB2	49:g:201:PLX:H6	1.80	0.64
33:j:73:LEU:CD1	36:m:55:MET:SD	2.83	0.64
44:w:246:LEU:HD12	44:w:255:VAL:HG11	1.79	0.64
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:499:MET:O	35:l:503:GLU:HG2	1.97	0.64
41:s:85:MET:HE3	41:s:105:MET:HE3	1.79	0.63
1:A:61:ASP:OD1	1:A:137:LYS:NZ	2.31	0.63
20:V:81:ARG:NH2	20:V:86:ASP:OD2	2.30	0.63
20:V:107:SER:HB3	20:V:110:ILE:HB	1.80	0.63
35:l:525:MET:HE2	39:p:77:PRO:HB3	1.80	0.63
34:k:37:MET:HE1	34:k:63:LEU:HG	1.80	0.63
38:o:15:PRO:HG2	38:o:18:LEU:HD12	1.79	0.63
38:o:59:VAL:HG22	40:r:423:ILE:HG12	1.81	0.63
40:r:104:LEU:HG	40:r:108:MET:HE2	1.80	0.63
40:r:271:MET:HE2	40:r:271:MET:HA	1.81	0.63
11:L:80:PHE:HE1	11:L:100:GLU:HG2	1.64	0.62
24:a:78:THR:HG21	28:e:96:SER:HA	1.81	0.62
37:n:50:ARG:HB2	37:n:53:GLU:HG2	1.80	0.62
34:k:23:ARG:HG3	36:m:23:LYS:HE2	1.79	0.62
44:w:65:ASN:OD1	44:w:66:ILE:N	2.29	0.62
33:j:71:LEU:O	33:j:74:PRO:HD2	1.99	0.62
3:C:73:ALA:HB3	50:C:304:DCQ:H4MB	1.81	0.62
11:L:75:ARG:HD2	11:L:104:ARG:NH2	2.14	0.62
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.81	0.62
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.82	0.62
25:b:88:TYR:CE1	27:d:49:ARG:HG2	2.35	0.62
40:r:312:ALA:O	40:r:316:MET:HG3	2.00	0.62
42:u:9:THR:HG22	42:u:11:GLU:H	1.65	0.62
40:r:290:SER:HB2	40:r:319:HIS:HE2	1.65	0.61
44:w:125:ASP:O	44:w:130:ARG:NH2	2.33	0.61
40:r:306:PRO:HB3	40:r:458:LEU:HD12	1.82	0.61
33:j:92:LEU:HD22	41:s:302:MET:HG2	1.81	0.61
1:A:227:PRO:HD2	12:M:94:MET:SD	2.40	0.61
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.82	0.61
12:M:249:GLU:HG2	12:M:276:ARG:HD3	1.82	0.61
26:c:153:TYR:OH	43:v:8:ARG:NH1	2.34	0.61
35:l:524:ASN:HD21	39:p:78:GLN:HB2	1.66	0.61
36:m:71:THR:HA	36:m:75:ALA:HB3	1.82	0.61
6:G:103:HIS:CD2	6:G:106:LYS:HD3	2.36	0.60
14:O:59:ASN:ND2	14:O:89:GLN:OE1	2.28	0.60
23:Z:25:GLU:OE2	23:Z:25:GLU:N	2.34	0.60
41:s:142:TYR:CZ	41:s:192:GLU:HG2	2.36	0.60
1:A:263:ALA:HA	1:A:271:SER:HB3	1.84	0.60
19:U:26:GLY:HA3	48:j:201:PEE:H38	1.84	0.60
48:l:702:PEE:H62	40:r:401:MET:HE1	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:298:TYR:HD2	9:J:319:VAL:HG13	1.66	0.60
40:r:201:MET:HE3	48:r:501:PEE:H76	1.84	0.60
32:i:73:ALA:HB2	32:i:97:MET:HB3	1.83	0.60
32:i:265:MET:O	32:i:268:GLN:HG3	2.01	0.60
44:w:118:TYR:OH	58:w:401:ADP:O2'	2.20	0.60
36:m:55:MET:HE3	36:m:58:LEU:HB3	1.83	0.60
35:l:290:LEU:HD12	35:l:293:ILE:HD11	1.84	0.60
36:m:62:GLY:HA2	36:m:65:LEU:HB3	1.84	0.60
9:J:36:LEU:HD23	9:J:41:ILE:HG12	1.83	0.59
28:e:140:ASN:HD22	28:e:144:PRO:HG3	1.67	0.59
56:a:201:CDL:H111	48:b:201:PEE:H60	1.84	0.59
26:c:129:MET:HB3	35:l:528:TYR:CG	2.37	0.59
6:G:105:MET:HB3	6:G:106:LYS:HD2	1.83	0.59
33:j:1:MET:HA	33:j:1:MET:HE3	1.84	0.59
32:i:149:ILE:HG21	32:i:154:MET:HG3	1.83	0.59
3:C:44:GLU:OE2	3:C:195:ARG:NE	2.33	0.59
34:k:13:ALA:HB1	56:k:101:CDL:H821	1.85	0.59
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.85	0.59
32:i:68:MET:HE2	32:i:68:MET:HA	1.85	0.59
41:s:195:ARG:HD3	41:s:231:ILE:HD11	1.84	0.59
35:l:366:MET:HE2	35:l:443:ILE:HG23	1.83	0.59
28:e:72:ASP:OD1	28:e:72:ASP:N	2.36	0.59
42:u:81:PRO:HG3	42:u:106:LYS:HE2	1.84	0.59
1:A:121:GLU:HG2	47:A:503:NAI:C4N	2.33	0.58
41:s:85:MET:SD	41:s:108:MET:CB	2.91	0.58
6:X:90:TYR:OH	6:X:114:ASP:OD1	2.21	0.58
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.34	0.58
6:G:141:PRO:O	6:G:145:VAL:HG23	2.03	0.58
38:o:56:ARG:NH1	40:r:422:HIS:O	2.32	0.58
40:r:153:THR:HG23	40:r:206:LYS:HD3	1.84	0.58
41:s:253:GLU:O	41:s:257:ILE:HG13	2.04	0.58
42:u:137:LEU:HD22	42:u:138:PRO:HD2	1.85	0.58
35:l:228:GLY:HA3	48:l:702:PEE:H38	1.85	0.58
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.31	0.58
25:b:103:ARG:NH1	43:v:49:ALA:O	2.37	0.58
41:s:145:THR:HG21	41:s:289:LEU:HD12	1.84	0.58
32:i:11:MET:HE3	56:i:401:CDL:H581	1.86	0.58
41:s:259:PHE:O	41:s:263:THR:HG23	2.03	0.58
34:k:2:PRO:HG3	36:m:127:ILE:HD13	1.85	0.57
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.37	0.57
12:M:591:GLU:HG2	12:M:610:VAL:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:157:VAL:HG21	15:P:182:PRO:HD3	1.86	0.57
48:W:201:PEE:H45	56:s:402:CDL:H561	1.87	0.57
35:l:596:MET:O	35:l:600:THR:HG23	2.04	0.57
42:u:69:ASP:O	42:u:73:GLN:HG3	2.03	0.57
34:k:21:MET:HE1	56:k:101:CDL:H582	1.85	0.57
43:v:83:GLU:H	43:v:83:GLU:CD	2.12	0.57
4:E:17:VAL:HG21	11:L:55:VAL:HG22	1.86	0.57
17:S:53:ARG:HG2	31:h:104:PRO:HB2	1.86	0.57
32:i:68:MET:HE1	34:k:37:MET:SD	2.45	0.57
36:m:55:MET:HA	36:m:55:MET:CE	2.21	0.57
3:C:132:SER:OG	3:C:138:ASN:OD1	2.21	0.57
40:r:189:SER:HA	49:r:502:PLX:H1B3	1.87	0.57
32:i:30:TRP:HD1	32:i:70:LEU:HD23	1.69	0.57
32:i:265:MET:HE2	32:i:343:LEU:HD21	1.86	0.57
35:l:261:ILE:HG13	35:l:317:ILE:HD11	1.87	0.57
26:c:38:PRO:HG2	38:o:70:TYR:HD2	1.70	0.56
44:w:343:TYR:HA	44:w:352:ILE:CD1	2.35	0.56
2:B:79:ARG:HA	8:I:12:ARG:HH11	1.70	0.56
15:P:209:GLU:HG2	15:P:224:VAL:HA	1.86	0.56
24:a:106:VAL:HG13	37:m:50:ARG:HH21	1.70	0.56
35:l:505:ASN:O	35:l:508:THR:OG1	2.21	0.56
36:m:64:MET:HE2	36:m:64:MET:CA	2.28	0.56
43:v:46:MET:HE3	43:v:56:ARG:HB3	1.87	0.56
44:w:245:PHE:HD2	44:w:246:LEU:HD22	1.71	0.56
1:A:214:GLU:OE1	11:L:175:LYS:NZ	2.25	0.56
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.86	0.56
30:g:4:MET:O	30:g:10:ARG:NH1	2.37	0.56
38:o:82:PRO:HB2	56:o:201:CDL:HB4	1.87	0.56
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.40	0.56
33:j:67:LEU:HG	34:k:68:ALA:HB3	1.86	0.56
35:l:14:ILE:HD11	35:l:43:ALA:HB2	1.88	0.56
41:s:138:GLN:NE2	41:s:191:ALA:O	2.33	0.56
6:G:103:HIS:CE1	6:G:139:MET:HB3	2.40	0.56
6:G:143:GLU:OE1	6:G:143:GLU:N	2.29	0.56
24:a:149:LEU:HD11	42:u:162:LYS:HE2	1.87	0.56
35:l:7:LEU:HD22	35:l:46:LEU:HD11	1.87	0.56
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.87	0.56
16:Q:52:MET:HE2	32:i:173:THR:HG22	1.86	0.56
2:B:200:GLU:HG3	13:N:88:ARG:HD3	1.87	0.56
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.87	0.56
32:i:182:SER:HB2	32:i:293:TYR:OH	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:67:LEU:CD2	34:k:68:ALA:CB	2.84	0.56
41:s:85:MET:SD	41:s:108:MET:HB2	2.46	0.56
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.88	0.56
35:l:27:TYR:O	35:l:115:ASN:ND2	2.36	0.56
33:j:60:ILE:HG22	36:m:168:ILE:HD12	1.88	0.55
42:u:77:HIS:CD2	42:u:115:LEU:HD21	2.41	0.55
9:J:87:GLU:HG3	9:J:89:TYR:H	1.72	0.55
21:W:121:MET:HE3	36:m:130:THR:HB	1.88	0.55
32:i:88:LYS:HG2	32:i:148:SER:HB2	1.87	0.55
48:s:401:PEE:H26	56:s:402:CDL:H162	1.88	0.55
33:j:67:LEU:HD12	34:k:65:VAL:HA	1.87	0.55
50:C:304:DCQ:H3M	16:Q:457:VAL:HG22	1.88	0.55
56:V:201:CDL:H771	56:V:201:CDL:H401	1.88	0.55
24:a:135:LYS:NZ	37:n:32:ASP:OD1	2.26	0.55
27:d:15:ARG:O	27:d:15:ARG:HG2	2.06	0.55
6:G:139:MET:HE2	6:G:139:MET:HA	1.88	0.55
32:i:131:LEU:HD12	32:i:216:PHE:HE2	1.71	0.55
39:p:140:LEU:O	39:p:144:THR:OG1	2.24	0.55
26:c:157:GLY:HA2	43:v:22:MET:HE2	1.87	0.55
33:j:68:GLU:HG3	33:j:98:LEU:HD13	1.89	0.55
35:l:173:LEU:HD12	40:r:405:LEU:HD21	1.88	0.55
41:s:236:ALA:HA	41:s:263:THR:HG22	1.89	0.55
9:J:199:THR:OG1	9:J:258:ALA:O	2.23	0.55
12:M:59:GLN:HE21	12:M:62:ARG:HH12	1.53	0.55
16:Q:84:PHE:HB2	16:Q:99:MET:HE2	1.87	0.55
6:X:155:TYR:HA	25:b:20:ARG:HD3	1.89	0.55
11:L:84:ARG:NH1	11:L:88:GLN:O	2.40	0.55
32:i:20:VAL:HG11	32:i:137:ALA:HB1	1.89	0.55
4:E:41:ARG:NH1	6:G:124:ASP:OD1	2.40	0.54
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.43	0.54
6:G:106:LYS:HD2	6:G:106:LYS:N	2.22	0.54
15:P:43:THR:HA	15:P:47:ILE:HD12	1.89	0.54
15:P:69:LEU:HD13	15:P:96:VAL:HG22	1.89	0.54
42:u:83:THR:HA	42:u:86:TRP:CD1	2.41	0.54
36:m:72:THR:HG21	41:s:133:LEU:HD21	1.88	0.54
40:r:343:ILE:O	40:r:346:ARG:NH1	2.41	0.54
12:M:556:THR:HA	12:M:579:MET:HE1	1.87	0.54
7:H:48:THR:O	7:H:52:THR:OG1	2.20	0.54
56:V:201:CDL:H321	35:l:576:MET:HE1	1.89	0.54
9:J:192:ARG:NH2	9:J:262:THR:OG1	2.40	0.54
9:J:347:LEU:HD13	9:J:366:MET:HE1	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:375:ILE:HD12	35:l:458:LEU:HD11	1.89	0.54
41:s:157:ASN:ND2	41:s:159:SER:O	2.38	0.54
22:Y:87:PRO:HD2	43:v:99:MET:HE1	1.90	0.54
36:m:19:GLY:HA3	56:s:402:CDL:H772	1.88	0.54
3:C:83:ARG:NH1	16:Q:212:GLU:OE2	2.36	0.54
32:i:131:LEU:HD12	32:i:216:PHE:CE2	2.43	0.54
56:r:504:CDL:H201	56:r:504:CDL:H351	1.89	0.54
48:V:202:PEE:H7	35:l:568:PHE:HE2	1.73	0.54
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.43	0.54
42:u:149:GLU:HG2	42:u:150:PRO:HD2	1.90	0.54
12:M:370:GLU:HG3	12:M:519:ILE:HG13	1.90	0.53
27:d:47:LEU:HA	27:d:50:GLU:HG3	1.88	0.53
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.89	0.53
12:M:320:GLU:CD	12:M:320:GLU:H	2.15	0.53
30:g:36:MET:HE1	49:g:201:PLX:H393	1.88	0.53
41:s:85:MET:SD	41:s:108:MET:HB3	2.49	0.53
35:l:250:SER:HB2	35:l:333:ALA:HA	1.89	0.53
38:o:5:LYS:NZ	39:p:69:GLU:OE1	2.36	0.53
56:s:402:CDL:H362	56:s:402:CDL:H201	1.90	0.53
44:w:343:TYR:HA	44:w:352:ILE:HD11	1.89	0.53
12:M:667:GLN:OE1	12:M:667:GLN:N	2.40	0.53
35:l:173:LEU:HG	40:r:401:MET:HE3	1.90	0.53
43:v:17:PRO:HB3	43:v:105:GLU:HG2	1.90	0.53
18:T:39:THR:HG22	18:T:62:VAL:HG22	1.91	0.53
33:j:63:LEU:HD21	36:m:63:GLY:HA2	1.88	0.53
24:a:163:ARG:NH1	30:g:102:ASP:OD2	2.34	0.53
31:h:24:GLU:OE1	31:h:28:LYS:NZ	2.40	0.53
1:A:404:ALA:HB3	1:A:450:MET:HE2	1.90	0.53
32:i:222:SER:O	32:i:224:ALA:N	2.42	0.53
2:B:117:LYS:NZ	2:B:120:GLU:OE2	2.42	0.53
24:a:95:GLU:OE2	56:a:201:CDL:O1	2.23	0.53
27:d:115:GLN:HG2	35:l:62:ILE:HG12	1.91	0.53
35:l:227:PHE:O	35:l:230:HIS:ND1	2.36	0.53
1:A:398:ARG:NH2	1:A:408:GLU:OE2	2.40	0.52
3:C:125:PRO:HG2	41:s:58:LYS:HE3	1.90	0.52
2:B:101:HIS:ND1	2:B:149:MET:HE1	2.24	0.52
11:L:71:HIS:CE1	11:L:120:PRO:HD2	2.45	0.52
21:W:50:MET:HG3	41:s:177:THR:HG21	1.90	0.52
22:Y:102:ASP:HA	43:v:111:ARG:HH11	1.75	0.52
25:b:100:ARG:HD3	35:l:60:GLU:HB2	1.91	0.52
33:j:71:LEU:O	36:m:147:TYR:OH	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:l:701:CDL:H452	40:r:445:LEU:HB3	1.91	0.52
36:m:124:ASP:O	36:m:127:ILE:HG12	2.08	0.52
7:H:38:ILE:O	7:H:45:ARG:NH1	2.34	0.52
14:O:188:ILE:HG21	14:O:208:LEU:HD21	1.90	0.52
15:P:53:VAL:HA	15:P:56:LYS:HD2	1.91	0.52
21:W:58:ARG:O	21:W:62:ILE:HG13	2.09	0.52
4:E:120:SER:O	4:E:124:VAL:HG22	2.10	0.52
33:j:113:TRP:HZ2	41:s:286:MET:HE3	1.73	0.52
56:l:701:CDL:H391	40:r:371:PRO:HD2	1.91	0.52
44:w:316:GLU:N	44:w:316:GLU:OE2	2.43	0.52
33:j:67:LEU:CG	34:k:68:ALA:HB2	2.39	0.52
36:m:52:LEU:O	36:m:56:VAL:HG12	2.09	0.52
41:s:79:LEU:HD22	41:s:222:MET:HG2	1.90	0.52
14:O:204:ILE:HD11	14:O:219:ARG:HD2	1.92	0.52
31:h:69:ARG:O	31:h:73:MET:HG3	2.09	0.52
32:i:8:THR:HG23	56:i:401:CDL:H791	1.91	0.52
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.91	0.52
40:r:403:THR:HA	40:r:406:TYR:CE2	2.44	0.52
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.92	0.52
44:w:200:PRO:HG3	44:w:252:LYS:HD2	1.92	0.52
16:Q:178:THR:OG1	16:Q:214:TYR:OH	2.24	0.52
36:m:64:MET:HE1	36:m:67:VAL:HG21	1.92	0.52
44:w:245:PHE:CD2	44:w:246:LEU:HD22	2.44	0.52
1:A:211:ALA:HB2	1:A:223:PRO:HG3	1.91	0.52
9:J:179:ARG:NH1	9:J:179:ARG:HB2	2.24	0.52
44:w:60:ILE:HG12	44:w:203:VAL:HB	1.91	0.52
21:W:120:MET:HB3	21:W:123:GLU:HG3	1.92	0.52
56:a:201:CDL:OA4	25:b:89:HIS:NE2	2.36	0.52
35:l:233:LEU:HB3	35:l:234:PRO:HD3	1.91	0.52
6:X:116:VAL:HG21	39:p:17:LEU:HD12	1.91	0.52
33:j:78:ALA:C	33:j:80:GLN:H	2.17	0.52
35:l:213:LEU:HB3	35:l:273:VAL:HG11	1.92	0.52
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.92	0.51
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.92	0.51
12:M:44:GLU:H	12:M:44:GLU:CD	2.18	0.51
13:N:100:THR:C	13:N:101:LYS:HD2	2.35	0.51
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.92	0.51
2:B:120:GLU:OE1	15:P:231:ARG:NH1	2.44	0.51
3:C:69:LEU:HB2	3:C:107:GLY:HA3	1.91	0.51
6:G:79:ILE:HG22	6:G:145:VAL:HG13	1.91	0.51
32:i:230:LEU:HD11	32:i:244:MET:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:145:GLU:O	35:l:149:ILE:HG22	2.11	0.51
12:M:370:GLU:OE2	12:M:478:SER:OG	2.25	0.51
12:M:407:PRO:HD2	12:M:438:LEU:HD21	1.92	0.51
28:e:63:ASP:N	28:e:63:ASP:OD1	2.39	0.51
35:l:419:THR:HA	35:l:422:TYR:CE2	2.46	0.51
37:n:47:ARG:NH2	37:n:53:GLU:OE2	2.43	0.51
41:s:205:SER:OG	41:s:279:ARG:NH1	2.35	0.51
33:j:69:ILE:HD13	41:s:147:ALA:CB	2.40	0.51
34:k:65:VAL:HG11	36:m:157:THR:HG23	1.91	0.51
56:o:201:CDL:H662	56:o:201:CDL:H611	1.93	0.51
41:s:307:LEU:HA	41:s:310:MET:HE2	1.91	0.51
43:v:51:LEU:HD13	43:v:63:LEU:HD23	1.92	0.51
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.43	0.51
30:g:19:GLU:O	30:g:22:SER:OG	2.27	0.51
49:g:201:PLX:H361	49:g:201:PLX:H311	1.92	0.51
36:m:51:PHE:CB	36:m:139:GLU:OE2	2.58	0.51
12:M:390:THR:HA	12:M:600:GLU:HG2	1.93	0.51
12:M:506:VAL:HG12	12:M:508:GLY:H	1.76	0.51
28:e:76:TYR:HB2	28:e:83:ASP:OD1	2.11	0.51
35:l:359:MET:O	35:l:436:ARG:NH2	2.43	0.51
16:Q:47:PHE:CD1	16:Q:52:MET:HE1	2.43	0.51
20:V:85:ASP:HB3	20:V:130:LEU:HD21	1.93	0.51
24:a:160:MET:HE2	24:a:167:PRO:HD2	1.92	0.51
26:c:168:LEU:HA	26:c:172:GLY:HA2	1.93	0.51
9:J:262:THR:O	9:J:333:PRO:HD2	2.11	0.51
16:Q:206:GLU:O	16:Q:210:MET:HG3	2.11	0.51
28:e:73:SER:O	28:e:75:GLY:N	2.44	0.51
34:k:27:MET:HE1	36:m:70:TYR:HB3	1.92	0.51
40:r:269:MET:HE1	40:r:396:MET:SD	2.51	0.51
10:K:83:THR:HG23	14:O:88:ARG:HH11	1.76	0.51
32:i:270:MET:HE1	32:i:282:MET:SD	2.50	0.51
36:m:170:GLU:CD	36:m:173:ARG:HH21	2.19	0.50
1:A:224:ARG:HG2	11:L:164:PHE:CZ	2.46	0.50
2:B:100:GLU:O	2:B:170:GLY:N	2.35	0.50
16:Q:100:GLU:HG3	16:Q:108:LYS:HB3	1.94	0.50
25:b:19:ARG:HA	39:p:171:VAL:HG13	1.93	0.50
38:o:105:PHE:CD2	40:r:263:MET:HE1	2.47	0.50
43:v:83:GLU:OE2	43:v:83:GLU:N	2.30	0.50
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.47	0.50
40:r:185:PRO:HB3	40:r:252:PRO:HD3	1.93	0.50
40:r:231:LEU:HD23	40:r:235:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:40:LYS:HB3	21:W:7:LYS:H	1.77	0.50
25:b:110:ILE:HD11	25:b:117:ILE:HD11	1.94	0.50
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.46	0.50
7:H:73:GLN:OE1	7:H:73:GLN:HA	2.11	0.50
13:N:123:GLN:O	18:T:59:GLN:NE2	2.44	0.50
14:O:134:VAL:HG22	14:O:186:VAL:HG22	1.93	0.50
26:c:124:VAL:HG23	35:l:525:MET:HE1	1.93	0.50
27:d:97:LYS:NZ	40:r:47:GLU:HG3	2.26	0.50
36:m:51:PHE:CD1	36:m:143:ILE:HD13	2.47	0.50
40:r:406:TYR:O	40:r:409:TYR:HB3	2.12	0.50
1:A:261:TRP:O	1:A:264:SER:OG	2.29	0.50
12:M:275:PRO:HG3	12:M:286:ILE:HG12	1.93	0.50
26:c:133:LEU:HD13	35:l:527:GLY:O	2.12	0.50
39:p:105:ASP:OD1	39:p:122:ARG:NH1	2.25	0.50
13:N:144:TYR:CZ	13:N:145:LYS:HD2	2.47	0.50
56:a:201:CDL:H541	48:b:201:PEE:H16	1.93	0.50
35:l:488:MET:O	35:l:492:ILE:HG13	2.12	0.50
1:A:112:TYR:O	1:A:240:THR:HA	2.11	0.50
12:M:306:MET:HB2	12:M:583:ILE:HB	1.93	0.50
30:g:52:ARG:NH1	32:i:318:GLU:OE1	2.45	0.49
35:l:170:GLN:OE1	35:l:534:HIS:NE2	2.45	0.49
4:E:108:HIS:CB	4:E:111:GLU:OE2	2.56	0.49
24:a:134:GLU:HG2	37:n:38:PHE:O	2.11	0.49
49:g:201:PLX:H312	49:g:201:PLX:H211	1.94	0.49
32:i:93:VAL:HG13	35:l:603:ASN:HD21	1.77	0.49
36:m:55:MET:HE3	36:m:55:MET:CA	2.31	0.49
42:u:114:LYS:C	42:u:115:LEU:HD23	2.36	0.49
44:w:57:SER:HB3	44:w:150:LEU:HD11	1.95	0.49
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.26	0.49
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.46	0.49
11:L:78:ARG:HD2	12:M:607:LYS:HE2	1.94	0.49
56:V:201:CDL:H641	35:l:597:ILE:HG21	1.93	0.49
24:a:166:GLY:O	24:a:170:GLN:NE2	2.42	0.49
35:l:566:THR:O	35:l:570:GLN:HG2	2.12	0.49
41:s:123:SER:HB3	41:s:214:GLU:HG3	1.94	0.49
46:A:502:FMN:N1	46:A:502:FMN:O3'	2.28	0.49
13:N:78:ASP:OD2	13:N:80:SER:OG	2.24	0.49
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	1.94	0.49
35:l:245:ALA:O	35:l:249:SER:OG	2.30	0.49
41:s:179:TRP:O	41:s:183:MET:HG3	2.13	0.49
1:A:63:TYR:CD2	1:A:64:LYS:HG2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLY:O	47:A:503:NAI:H2N	2.13	0.49
1:A:281:HIS:HD2	1:A:357:MET:HA	1.76	0.49
33:j:18:VAL:HG23	41:s:222:MET:HE1	1.95	0.49
35:l:349:SER:HB2	35:l:366:MET:HE1	1.94	0.49
41:s:142:TYR:CE1	41:s:192:GLU:HG2	2.47	0.49
44:w:39:GLY:HA2	44:w:296:MET:HE1	1.94	0.49
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.48	0.49
8:I:70:MET:O	8:I:70:MET:SD	2.71	0.49
38:o:105:PHE:HD2	40:r:263:MET:HE1	1.78	0.49
6:G:93:ILE:HG12	6:G:108:LEU:HD22	1.94	0.49
9:J:129:LEU:HD23	9:J:167:ILE:HG13	1.95	0.49
33:j:95:LEU:HD13	41:s:302:MET:HG3	1.95	0.49
35:l:292:ALA:HB2	35:l:304:PHE:HB3	1.94	0.49
43:v:51:LEU:O	43:v:52:MET:HG3	2.13	0.49
1:A:122:PRO:HA	14:O:176:CYS:SG	2.53	0.49
7:H:55:LYS:NZ	15:P:104:THR:HG21	2.27	0.49
27:d:69:ARG:NH2	37:n:46:LYS:O	2.35	0.49
35:l:34:ASN:OD1	35:l:105:MET:HE1	2.13	0.49
1:A:118:ASP:O	1:A:159:ARG:HD2	2.12	0.49
16:Q:190:HIS:O	16:Q:194:ILE:HG12	2.12	0.49
16:Q:192:LEU:HD12	16:Q:197:MET:HA	1.94	0.49
35:l:69:MET:HG2	35:l:76:LEU:HD12	1.95	0.49
35:l:310:LEU:HD23	35:l:313:MET:HE3	1.94	0.49
36:m:82:VAL:HG12	36:m:83:TRP:H	1.77	0.49
44:w:248:GLU:OE1	44:w:248:GLU:N	2.45	0.49
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.95	0.48
21:W:94:GLU:OE2	21:W:104:TRP:NE1	2.38	0.48
31:h:86:LEU:HB3	31:h:92:TYR:HB3	1.95	0.48
42:u:83:THR:HA	42:u:86:TRP:NE1	2.28	0.48
12:M:266:ARG:HG2	12:M:267:THR:HG23	1.95	0.48
12:M:466:LEU:HD13	12:M:500:ILE:HD11	1.94	0.48
18:T:105:GLU:OE2	18:T:105:GLU:N	2.32	0.48
32:i:248:LEU:HD23	32:i:251:MET:HE3	1.95	0.48
56:l:701:CDL:H342	56:l:701:CDL:H372	1.62	0.48
44:w:58:LYS:O	44:w:60:ILE:HG13	2.12	0.48
1:A:338:ASP:OD1	1:A:338:ASP:N	2.43	0.48
35:l:529:TYR:HB3	35:l:530:PRO:HD3	1.95	0.48
40:r:433:GLU:O	40:r:437:MET:HG2	2.13	0.48
41:s:108:MET:N	41:s:108:MET:HE2	2.29	0.48
1:A:337:MET:SD	1:A:342:LEU:HD11	2.53	0.48
46:A:502:FMN:N5	47:A:503:NAI:H4N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:73:LEU:N	33:j:74:PRO:HD3	2.26	0.48
1:A:45:LEU:HD21	1:A:287:THR:HG22	1.94	0.48
2:B:116:CYS:SG	2:B:118:LEU:HG	2.53	0.48
56:a:201:CDL:H361	56:a:201:CDL:H392	1.55	0.48
35:l:474:PRO:HD2	43:v:67:LEU:HD21	1.96	0.48
1:A:257:ARG:HD3	14:O:244:GLY:HA3	1.94	0.48
4:E:25:MET:HE1	4:E:79:VAL:HG21	1.96	0.48
12:M:250:SER:OG	12:M:251:ILE:N	2.43	0.48
25:b:121:LYS:HD3	43:v:40:VAL:HA	1.95	0.48
27:d:114:GLN:HG3	35:l:203:MET:HG2	1.94	0.48
28:e:120:ARG:O	28:e:124:ARG:HG3	2.13	0.48
35:l:286:LEU:HD13	35:l:411:MET:SD	2.53	0.48
40:r:31:SER:HB2	40:r:74:PRO:HG3	1.96	0.48
44:w:295:ARG:HA	44:w:298:VAL:HG22	1.96	0.48
9:J:306:GLU:HG2	9:J:315:THR:HG22	1.95	0.48
12:M:389:THR:O	12:M:390:THR:OG1	2.26	0.48
24:a:114:LYS:HB2	27:d:63:TYR:CE1	2.48	0.48
56:i:401:CDL:H312	56:i:401:CDL:HA62	1.63	0.48
33:j:68:GLU:HG2	36:m:161:LEU:HD13	1.95	0.48
39:p:68:GLU:OE1	39:p:68:GLU:HA	2.14	0.48
4:E:37:ARG:NH2	6:G:132:ASP:OD1	2.47	0.48
9:J:168:SER:O	9:J:203:PRO:HD2	2.13	0.48
11:L:75:ARG:CD	11:L:104:ARG:NH2	2.76	0.48
20:V:25:SER:OG	20:V:67:GLY:O	2.25	0.48
20:V:38:ALA:HB2	56:k:101:CDL:H251	1.95	0.48
28:e:114:MET:HA	28:e:114:MET:HE2	1.95	0.48
40:r:104:LEU:HD21	56:r:504:CDL:H861	1.96	0.48
49:j:202:PLX:H311	49:j:202:PLX:H282	1.48	0.48
39:p:27:LEU:HD22	39:p:44:MET:HG3	1.95	0.48
3:C:71:CYS:HB2	45:C:301:SF4:S4	2.54	0.48
32:i:175:LEU:O	32:i:179:MET:HG2	2.14	0.48
56:l:701:CDL:H591	56:l:701:CDL:H332	1.96	0.48
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.49	0.48
1:A:244:ASN:N	46:A:502:FMN:O3P	2.45	0.47
2:B:74:LEU:HB2	41:s:272:TRP:CZ2	2.48	0.47
12:M:213:MET:CG	12:M:215:MET:HG2	2.43	0.47
53:s:403:UQ:H221	53:s:403:UQ:H262	1.66	0.47
2:B:111:GLU:O	2:B:141:ARG:NH1	2.47	0.47
7:H:22:GLU:OE2	7:H:22:GLU:N	2.25	0.47
8:I:12:ARG:HB3	8:I:20:LEU:HD12	1.95	0.47
11:L:76:LYS:HE2	11:L:146:ASP:OD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:24:ALA:O	20:V:28:ILE:HG13	2.14	0.47
34:k:4:VAL:O	34:k:8:ILE:HG12	2.14	0.47
35:l:562:LEU:HB3	35:l:563:PRO:HD3	1.95	0.47
36:m:8:ILE:O	36:m:12:ILE:HG12	2.13	0.47
56:r:504:CDL:H782	56:r:504:CDL:H232	1.96	0.47
49:g:201:PLX:H12	31:h:2:PRO:HD2	1.96	0.47
35:l:561:ILE:HG13	35:l:562:LEU:H	1.79	0.47
25:b:18:LEU:HD11	39:p:163:LEU:HD22	1.97	0.47
26:c:38:PRO:HD3	38:o:67:ARG:HG2	1.96	0.47
32:i:115:VAL:O	32:i:119:THR:OG1	2.26	0.47
33:j:67:LEU:HG	34:k:68:ALA:HB2	1.92	0.47
33:j:67:LEU:CG	34:k:68:ALA:CB	2.91	0.47
34:k:46:LEU:HD22	36:m:47:PHE:CD2	2.49	0.47
35:l:298:ILE:O	35:l:302:VAL:HG23	2.15	0.47
44:w:224:PRO:HA	44:w:227:MET:HG3	1.96	0.47
1:A:195:VAL:O	10:K:97:ARG:NH1	2.47	0.47
15:P:75:GLN:HB3	15:P:87:PHE:CD1	2.50	0.47
27:d:2:PRO:O	27:d:7:LYS:NZ	2.31	0.47
35:l:241:THR:HG21	35:l:344:GLY:HA3	1.96	0.47
35:l:503:GLU:O	35:l:507:THR:HG23	2.15	0.47
41:s:32:GLN:OE1	41:s:34:ARG:NH2	2.47	0.47
48:s:401:PEE:H31	56:s:402:CDL:H222	1.97	0.47
43:v:22:MET:HE1	43:v:102:PHE:HA	1.96	0.47
7:H:116:ILE:HG12	15:P:121:THR:HG21	1.96	0.47
40:r:191:SER:HB3	48:r:501:PEE:H2	1.97	0.47
42:u:18:VAL:HG12	42:u:20:VAL:HG22	1.95	0.47
1:A:214:GLU:OE2	1:A:224:ARG:HD2	2.14	0.47
9:J:61:ALA:HA	9:J:66:GLY:HA3	1.97	0.47
12:M:215:MET:HG3	12:M:714:VAL:HG12	1.97	0.47
13:N:68:MET:SD	13:N:81:MET:HG2	2.54	0.47
21:W:68:ARG:O	21:W:72:MET:HG3	2.15	0.47
25:b:81:ILE:HG23	48:b:201:PEE:H58	1.95	0.47
27:d:137:LYS:HE3	27:d:137:LYS:HB3	1.67	0.47
49:g:201:PLX:H351	32:i:339:MET:HB2	1.95	0.47
35:l:358:LYS:HG3	39:p:80:TYR:CE1	2.50	0.47
35:l:401:MET:HE3	35:l:401:MET:HB3	1.79	0.47
36:m:55:MET:CE	36:m:58:LEU:HB3	2.45	0.47
56:n:101:CDL:H581	56:n:101:CDL:H552	1.53	0.47
42:u:81:PRO:HB3	42:u:106:LYS:HG2	1.97	0.47
8:I:69:VAL:O	15:P:76:VAL:HB	2.15	0.47
9:J:375:VAL:O	9:J:375:VAL:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:53:TYR:CE2	35:l:434:LYS:HG3	2.50	0.47
28:e:126:VAL:O	28:e:130:GLU:HG2	2.14	0.47
33:j:63:LEU:CD2	36:m:63:GLY:HA2	2.44	0.47
35:l:55:MET:HG2	35:l:471:ASN:O	2.15	0.47
44:w:209:VAL:HG22	44:w:260:ALA:HB2	1.97	0.47
22:Y:76:ASP:O	35:l:385:TYR:OH	2.24	0.47
28:e:55:LEU:HD11	44:w:320:GLY:HA2	1.96	0.47
35:l:41:SER:O	35:l:45:THR:HG22	2.15	0.47
35:l:332:HIS:HA	35:l:335:PHE:CZ	2.50	0.47
42:u:80:GLU:HB2	42:u:81:PRO:HD3	1.96	0.47
44:w:115:GLU:OE2	44:w:115:GLU:N	2.41	0.47
49:C:303:PLX:H1C3	49:C:303:PLX:H21	1.72	0.47
9:J:117:ARG:O	9:J:121:GLU:HG3	2.14	0.47
12:M:295:ASP:OD1	12:M:704:SER:OG	2.29	0.47
12:M:464:GLN:O	12:M:468:GLU:HG3	2.14	0.47
12:M:638:THR:O	12:M:642:VAL:HG23	2.15	0.47
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.80	0.47
36:m:35:VAL:HA	56:s:402:CDL:H631	1.97	0.47
42:u:91:TYR:C	42:u:91:TYR:CD2	2.92	0.47
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.47	0.46
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.95	0.46
12:M:339:ALA:HB1	12:M:537:ILE:HD12	1.97	0.46
16:Q:447:VAL:O	16:Q:451:ILE:HG13	2.15	0.46
21:W:84:LEU:HD13	42:u:8:PRO:HG2	1.97	0.46
21:W:115:ARG:HB3	42:u:143:HIS:HB2	1.97	0.46
26:c:62:TYR:OH	26:c:74:ASP:OD1	2.32	0.46
36:m:104:VAL:O	36:m:108:LEU:HD22	2.14	0.46
38:o:88:LEU:HD11	56:o:201:CDL:H331	1.97	0.46
39:p:52:LYS:HE2	39:p:52:LYS:HB3	1.79	0.46
1:A:296:LEU:HD21	1:A:317:VAL:HG11	1.97	0.46
24:a:152:LYS:HD3	30:g:96:VAL:HG21	1.96	0.46
28:e:97:ILE:O	28:e:101:LEU:HB2	2.15	0.46
32:i:62:THR:HG21	32:i:114:TRP:CD1	2.51	0.46
12:M:306:MET:HE3	12:M:316:TYR:CE1	2.51	0.46
17:S:50:ARG:NH1	42:u:20:VAL:O	2.41	0.46
25:b:88:TYR:CZ	27:d:49:ARG:HG2	2.50	0.46
9:J:109:ASN:HB3	9:J:112:ASP:HB3	1.97	0.46
19:U:28:LEU:HD22	19:U:32:LEU:HG	1.97	0.46
24:a:137:MET:CE	37:n:42:SER:HB3	2.45	0.46
33:j:28:ASN:O	33:j:33:LYS:HE3	2.16	0.46
1:A:102:MET:O	1:A:111:LYS:NZ	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:VAL:HG11	1:A:138:LEU:HD11	1.98	0.46
8:I:105:GLU:OE1	8:I:105:GLU:HA	2.16	0.46
12:M:171:THR:HG23	12:M:173:MET:HG2	1.98	0.46
12:M:372:PHE:H	12:M:532:PRO:HB2	1.81	0.46
20:V:37:SER:O	20:V:41:ILE:HG12	2.15	0.46
27:d:90:MET:SD	40:r:47:GLU:HB3	2.56	0.46
27:d:127:LYS:O	27:d:130:GLU:HG3	2.16	0.46
32:i:57:THR:HA	34:k:77:LEU:HD13	1.96	0.46
32:i:88:LYS:HG3	32:i:147:GLN:HG2	1.96	0.46
40:r:325:MET:HE3	40:r:441:ILE:HB	1.97	0.46
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.50	0.46
19:U:32:LEU:HD23	19:U:32:LEU:HA	1.82	0.46
40:r:237:LYS:HB3	40:r:316:MET:HE3	1.96	0.46
44:w:139:ARG:HH12	58:w:401:ADP:HN61	1.64	0.46
1:A:326:LEU:HD23	1:A:367:ILE:HD11	1.97	0.46
24:a:95:GLU:HB3	24:a:114:LYS:HG2	1.97	0.46
34:k:25:HIS:ND1	34:k:88:ASP:OD1	2.38	0.46
1:A:109:ARG:NH1	1:A:237:GLY:O	2.47	0.46
9:J:37:HIS:CE1	18:T:49:ASP:HA	2.51	0.46
32:i:268:GLN:O	32:i:271:THR:OG1	2.34	0.46
35:l:489:THR:O	35:l:493:VAL:HG22	2.16	0.46
11:L:102:ASP:OD1	11:L:102:ASP:N	2.49	0.46
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.97	0.46
19:U:69:HIS:CE1	19:U:71:GLN:HG3	2.50	0.46
6:X:120:MET:HE1	39:p:24:LEU:HB3	1.98	0.46
26:c:90:TYR:HE2	26:c:100:ASN:HD21	1.64	0.46
33:j:73:LEU:O	41:s:160:TYR:OH	2.28	0.46
34:k:24:SER:HB3	34:k:89:TYR:CD1	2.51	0.46
56:l:701:CDL:H312	56:l:701:CDL:HA61	1.71	0.46
56:o:201:CDL:H371	56:o:201:CDL:H401	1.73	0.46
13:N:85:GLU:HG2	13:N:86:TRP:H	1.81	0.46
35:l:491:LEU:O	35:l:495:ILE:HG12	2.16	0.46
40:r:394:ILE:O	40:r:398:MET:HG3	2.16	0.46
52:J:401:NDP:H2N	52:J:401:NDP:H2D	1.74	0.45
2:B:96:ARG:HG2	2:B:208:ASP:OD2	2.16	0.45
6:G:119:ILE:O	6:G:123:GLU:HG3	2.16	0.45
15:P:51:ASN:HB3	15:P:82:ASN:ND2	2.31	0.45
49:g:201:PLX:H102	49:g:201:PLX:H71	1.65	0.45
12:M:144:MET:O	16:Q:362:LYS:HE3	2.16	0.45
32:i:89:MET:HE1	32:i:98:MET:HE2	1.97	0.45
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:118:PHE:CD1	4:E:118:PHE:C	2.95	0.45
5:F:61:VAL:HG23	5:F:62:GLN:H	1.80	0.45
24:a:140:LEU:HD21	40:r:177:LEU:HB3	1.98	0.45
26:c:96:ASP:N	26:c:96:ASP:OD1	2.50	0.45
39:p:19:LEU:HD13	39:p:68:GLU:OE1	2.17	0.45
41:s:204:GLU:CD	41:s:204:GLU:H	2.25	0.45
42:u:38:LYS:HB3	42:u:39:PRO:HD3	1.99	0.45
1:A:118:ASP:HB3	46:A:502:FMN:O4	2.16	0.45
28:e:87:MET:HE3	28:e:87:MET:HB3	1.88	0.45
32:i:89:MET:HG3	32:i:95:MET:SD	2.55	0.45
32:i:280:THR:O	32:i:284:MET:HG2	2.17	0.45
56:o:201:CDL:H872	56:o:201:CDL:H841	1.82	0.45
44:w:180:ARG:NH1	44:w:316:GLU:OE1	2.45	0.45
8:I:62:GLU:OE2	15:P:47:ILE:HD13	2.15	0.45
20:V:39:TYR:CZ	56:V:201:CDL:H592	2.52	0.45
48:j:201:PEE:H60	48:j:201:PEE:H55	1.73	0.45
1:A:210:THR:HB	1:A:224:ARG:H	1.81	0.45
8:I:46:SER:O	8:I:52:ASN:ND2	2.46	0.45
48:V:202:PEE:H57	48:V:202:PEE:H13	1.98	0.45
36:m:165:VAL:O	36:m:168:ILE:HG12	2.16	0.45
38:o:37:LEU:O	38:o:41:SER:OG	2.29	0.45
41:s:307:LEU:HB3	41:s:308:PRO:HD3	1.99	0.45
11:L:80:PHE:CE1	11:L:100:GLU:HG2	2.49	0.45
13:N:85:GLU:HB2	13:N:98:PRO:HB3	1.99	0.45
15:P:119:VAL:HG12	15:P:121:THR:HG22	1.98	0.45
26:c:168:LEU:HB3	27:d:123:GLN:HE21	1.82	0.45
27:d:31:THR:HG22	27:d:35:LYS:NZ	2.32	0.45
27:d:168:LYS:O	27:d:172:GLU:HG3	2.16	0.45
30:g:13:LEU:HD23	49:g:201:PLX:H32	1.99	0.45
32:i:215:MET:HE1	32:i:244:MET:SD	2.57	0.45
33:j:67:LEU:HD13	33:j:67:LEU:HA	1.87	0.45
35:l:141:PHE:HE2	40:r:375:LEU:HD11	1.81	0.45
35:l:312:LEU:O	35:l:316:THR:HG22	2.17	0.45
37:n:30:ARG:NE	56:n:101:CDL:OA4	2.50	0.45
1:A:314:LEU:HD11	1:A:317:VAL:HG23	1.97	0.45
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.98	0.45
3:C:67:PHE:CZ	3:C:117:LEU:HD12	2.52	0.45
5:F:23:LEU:O	5:F:57:GLU:HA	2.17	0.45
49:J:403:PLX:H92	49:J:403:PLX:H122	1.78	0.45
22:Y:44:TYR:O	22:Y:45:ARG:HB2	2.17	0.45
24:a:69:LYS:HB2	24:a:69:LYS:HE2	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:31:THR:HG22	27:d:35:LYS:HZ2	1.81	0.45
32:i:172:GLN:HB2	32:i:178:ILE:HG13	1.99	0.45
32:i:307:SER:OG	32:i:308:THR:N	2.49	0.45
35:l:69:MET:SD	35:l:71:LEU:HD11	2.56	0.45
40:r:370:PRO:HB3	40:r:375:LEU:HD22	1.99	0.45
3:C:107:GLY:HA2	45:C:301:SF4:S1	2.57	0.45
9:J:163:LYS:NZ	9:J:253:ILE:O	2.39	0.45
17:S:69:ILE:HD11	42:u:75:LYS:HD2	1.99	0.45
21:W:43:LEU:HG	41:s:179:TRP:NE1	2.32	0.45
22:Y:51:THR:H	22:Y:54:GLN:HE21	1.64	0.45
26:c:91:ASP:O	38:o:44:LYS:NZ	2.49	0.45
33:j:78:ALA:O	33:j:80:GLN:N	2.50	0.45
41:s:117:LEU:HD21	41:s:136:VAL:HG23	1.99	0.45
44:w:88:GLU:N	44:w:160:GLU:HG3	2.32	0.45
44:w:309:THR:O	44:w:309:THR:OG1	2.31	0.45
10:K:88:ASP:O	10:K:92:GLU:HG3	2.17	0.44
12:M:55:LYS:HB3	12:M:55:LYS:HE2	1.49	0.44
16:Q:176:GLU:OE2	16:Q:311:TYR:OH	2.21	0.44
24:a:139:ILE:HG23	40:r:54:LEU:HD23	1.99	0.44
27:d:99:ASP:OD2	27:d:142:ARG:NH1	2.50	0.44
27:d:160:LYS:HE2	28:e:147:ILE:HG23	1.99	0.44
32:i:51:ARG:HG2	34:k:96:LEU:HD21	1.99	0.44
56:o:201:CDL:H331	56:o:201:CDL:H361	1.59	0.44
56:s:402:CDL:H771	56:s:402:CDL:H801	1.80	0.44
1:A:296:LEU:HD13	1:A:337:MET:HE2	1.99	0.44
1:A:416:SER:HB2	1:A:432:ALA:HB1	1.98	0.44
6:G:80:LYS:NZ	6:G:100:VAL:HG21	2.33	0.44
28:e:92:PHE:O	28:e:96:SER:HB2	2.16	0.44
32:i:95:MET:HE2	32:i:149:ILE:HG12	1.99	0.44
34:k:31:LEU:HD21	36:m:67:VAL:HG11	1.99	0.44
2:B:43:MET:HE3	2:B:43:MET:HA	1.99	0.44
12:M:360:ARG:HG2	12:M:360:ARG:HH11	1.83	0.44
35:l:488:MET:HE3	35:l:488:MET:HB3	1.87	0.44
41:s:55:LEU:HD13	41:s:221:ALA:HB2	2.00	0.44
53:s:403:UQ:H152	53:s:403:UQ:H121	1.82	0.44
44:w:164:TYR:O	44:w:167:PHE:CE1	2.70	0.44
44:w:246:LEU:CD1	44:w:255:VAL:HG11	2.46	0.44
3:C:161:ILE:HG13	3:C:180:LEU:HB2	2.00	0.44
15:P:187:ILE:HG23	15:P:188:LEU:HG	2.00	0.44
24:a:160:MET:HE2	24:a:166:GLY:HA3	1.99	0.44
35:l:327:LEU:O	35:l:331:MET:HG2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:561:ILE:HG13	35:l:562:LEU:N	2.33	0.44
36:m:126:VAL:HG23	36:m:127:ILE:HG23	1.98	0.44
2:B:192:ASN:ND2	18:T:61:GLU:OE2	2.51	0.44
13:N:117:VAL:O	13:N:120:THR:OG1	2.28	0.44
21:W:85:GLN:HG2	42:u:10:LEU:HD22	1.99	0.44
26:c:167:TYR:CD2	26:c:178:PRO:HG3	2.52	0.44
32:i:89:MET:HE3	32:i:95:MET:HA	2.00	0.44
35:l:341:MET:HE1	35:l:457:LEU:HD12	1.98	0.44
44:w:62:VAL:HA	44:w:205:VAL:HB	2.00	0.44
44:w:146:ALA:HB1	44:w:157:VAL:HG21	1.98	0.44
2:B:171:PRO:HB3	13:N:93:MET:HE1	1.98	0.44
48:B:303:PEE:H14	48:B:303:PEE:H20	1.71	0.44
6:G:80:LYS:HZ2	6:G:100:VAL:HG21	1.83	0.44
7:H:76:GLN:O	7:H:78:GLU:N	2.49	0.44
13:N:42:ASP:HB3	13:N:44:TYR:H	1.81	0.44
48:W:201:PEE:H28	48:W:201:PEE:H57	2.00	0.44
35:l:544:MET:HE2	35:l:544:MET:HA	2.00	0.44
40:r:3:LYS:HB3	40:r:3:LYS:HE2	1.71	0.44
12:M:354:LEU:HD22	12:M:548:LEU:HD22	2.00	0.44
14:O:242:GLY:HA2	14:O:245:VAL:HG23	2.00	0.44
56:l:701:CDL:H202	56:l:701:CDL:H231	1.84	0.44
39:p:136:GLU:OE2	39:p:167:TRP:NE1	2.49	0.44
42:u:114:LYS:O	42:u:115:LEU:HD23	2.18	0.44
44:w:248:GLU:O	44:w:251:GLU:HG3	2.17	0.44
6:G:126:PHE:CE2	6:G:148:ILE:HD13	2.53	0.44
11:L:131:LYS:HD2	11:L:147:VAL:HG11	2.00	0.44
12:M:476:LEU:HD21	12:M:481:LEU:HD21	2.00	0.44
32:i:13:VAL:O	32:i:36:ASN:ND2	2.50	0.44
34:k:37:MET:HE2	34:k:67:ALA:HB2	2.00	0.44
35:l:530:PRO:O	35:l:534:HIS:HB2	2.16	0.44
39:p:27:LEU:HD21	39:p:40:PHE:HB3	1.99	0.44
42:u:39:PRO:HG2	42:u:66:CYS:SG	2.58	0.44
1:A:37:ASP:OD1	1:A:40:ARG:NH1	2.51	0.44
1:A:217:GLU:CD	11:L:171:ARG:HH22	2.25	0.44
48:V:202:PEE:H7	35:l:568:PHE:CE2	2.53	0.44
32:i:93:VAL:HG13	35:l:603:ASN:ND2	2.33	0.44
35:l:435:PRO:HB3	35:l:437:PHE:CZ	2.53	0.44
37:n:54:GLU:HG3	37:n:55:VAL:HG22	1.99	0.44
49:r:502:PLX:H72	49:r:502:PLX:H101	1.52	0.44
41:s:198:PHE:CD1	41:s:285:LEU:HD13	2.52	0.44
1:A:96:GLY:O	1:A:100:SER:OG	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.82	0.43
12:M:394:VAL:HG22	12:M:473:MET:HE1	1.99	0.43
35:l:49:VAL:HB	35:l:50:PRO:HD3	1.99	0.43
40:r:76:MET:HA	40:r:229:MET:HE1	1.98	0.43
19:U:28:LEU:HD23	19:U:28:LEU:HA	1.81	0.43
24:a:184:LYS:HB3	31:h:30:PRO:HB3	2.00	0.43
25:b:80:TRP:HD1	27:d:41:VAL:HG13	1.83	0.43
48:b:201:PEE:H38	35:l:66:TRP:HZ3	1.84	0.43
32:i:81:SER:O	32:i:83:GLN:N	2.48	0.43
56:k:101:CDL:H131	56:k:101:CDL:H161	1.84	0.43
35:l:407:TRP:O	35:l:411:MET:HG2	2.18	0.43
3:C:192:ILE:HG21	9:J:86:CYS:HA	1.98	0.43
17:S:1:MET:HB2	17:S:3:PHE:CZ	2.53	0.43
19:U:78:LEU:HD12	42:u:123:GLY:HA3	2.00	0.43
56:r:504:CDL:H802	56:r:504:CDL:H831	1.89	0.43
44:w:268:LYS:HD2	44:w:268:LYS:HA	1.63	0.43
4:E:116:THR:HA	4:E:121:LYS:HE3	2.00	0.43
17:S:55:SER:O	17:S:64:LYS:NZ	2.51	0.43
19:U:33:PRO:HA	41:s:310:MET:HG2	2.00	0.43
27:d:122:ARG:HA	27:d:122:ARG:HD3	1.84	0.43
32:i:1:MET:HE2	36:m:170:GLU:HG3	1.99	0.43
38:o:88:LEU:HG	56:o:201:CDL:H572	1.99	0.43
12:M:456:ALA:O	12:M:499:ASN:ND2	2.51	0.43
26:c:186:ILE:HG22	43:v:97:LYS:HG3	2.00	0.43
32:i:128:LEU:C	32:i:128:LEU:CD2	2.89	0.43
34:k:20:LEU:HD23	35:l:588:PHE:HD2	1.84	0.43
35:l:475:MET:SD	43:v:52:MET:HE3	2.58	0.43
36:m:16:GLY:HA2	56:s:402:CDL:H791	2.01	0.43
39:p:35:ASP:OD1	39:p:36:LYS:N	2.50	0.43
40:r:225:ILE:HG13	40:r:229:MET:HE2	2.01	0.43
42:u:47:ARG:HA	42:u:47:ARG:HD2	1.79	0.43
44:w:95:ASP:OD1	44:w:95:ASP:N	2.51	0.43
1:A:283:ASN:ND2	1:A:305:GLY:O	2.51	0.43
3:C:109:LEU:HD13	3:C:117:LEU:HD13	2.01	0.43
13:N:85:GLU:HG2	13:N:86:TRP:N	2.33	0.43
13:N:135:GLN:NE2	13:N:136:GLU:O	2.45	0.43
19:U:38:TYR:HD1	19:U:41:TYR:HD2	1.66	0.43
26:c:177:GLU:OE1	26:c:177:GLU:HA	2.19	0.43
33:j:78:ALA:C	33:j:80:GLN:N	2.76	0.43
36:m:65:LEU:HD23	36:m:65:LEU:C	2.43	0.43
41:s:9:LEU:O	41:s:13:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:119:LEU:HD11	12:M:628:GLU:HG2	2.00	0.43
12:M:30:ASN:OD1	12:M:30:ASN:N	2.37	0.43
12:M:395:GLU:O	12:M:425:ASN:ND2	2.51	0.43
27:d:51:PHE:O	27:d:55:GLN:HG2	2.19	0.43
31:h:17:TRP:CZ2	36:m:150:GLY:HA2	2.54	0.43
39:p:62:GLN:NE2	39:p:66:GLN:OE1	2.42	0.43
40:r:84:LEU:HD22	40:r:87:GLU:HG3	2.00	0.43
41:s:81:LEU:HD13	41:s:81:LEU:HA	1.87	0.43
6:G:125:GLU:HG3	6:G:126:PHE:CD2	2.54	0.43
12:M:651:PRO:O	12:M:654:VAL:HG22	2.19	0.43
15:P:132:LEU:HB2	15:P:141:ILE:HG22	2.01	0.43
16:Q:139:LEU:HD13	16:Q:424:ILE:HG21	2.00	0.43
56:V:201:CDL:H532	35:l:577:VAL:HG22	2.00	0.43
24:a:94:GLY:O	27:d:61:TYR:OH	2.36	0.43
49:a:202:PLX:H1C3	49:a:202:PLX:H22	1.82	0.43
28:e:55:LEU:HD23	28:e:57:GLU:HB2	2.00	0.43
32:i:183:SER:O	32:i:187:MET:HG2	2.19	0.43
37:n:42:SER:OG	37:n:45:PHE:HB2	2.18	0.43
38:o:48:LEU:HB3	39:p:166:LEU:HD13	2.00	0.43
3:C:98:ARG:NH2	33:j:35:SER:O	2.52	0.43
11:L:88:GLN:NE2	12:M:141:ASP:OD2	2.35	0.43
11:L:89:SER:O	12:M:59:GLN:NE2	2.51	0.43
12:M:632:MET:H	12:M:632:MET:HG2	1.64	0.43
14:O:137:THR:HG22	14:O:138:THR:H	1.84	0.43
16:Q:99:MET:HE3	16:Q:99:MET:HB2	1.81	0.43
6:X:88:LYS:HE2	6:X:88:LYS:HB2	1.75	0.43
22:Y:98:GLY:HA3	43:v:31:PHE:CE2	2.53	0.43
27:d:159:GLN:O	27:d:163:MET:HG3	2.17	0.43
48:j:201:PEE:H59	48:j:201:PEE:H64	1.67	0.43
34:k:58:MET:SD	36:m:146:LEU:HD13	2.58	0.43
41:s:63:PRO:HB2	41:s:66:SER:HB3	2.00	0.43
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.75	0.43
9:J:135:GLU:HG2	9:J:140:ASP:HA	2.01	0.43
12:M:260:ASN:HD22	12:M:260:ASN:N	2.15	0.43
24:a:165:ASP:OD1	24:a:165:ASP:N	2.36	0.43
26:c:140:MET:HE1	35:l:411:MET:SD	2.58	0.43
49:j:202:PLX:H342	49:j:202:PLX:H372	1.77	0.43
40:r:346:ARG:O	40:r:419:TYR:HA	2.19	0.43
4:E:111:GLU:OE1	15:P:223:PRO:HD3	2.19	0.42
35:l:12:LEU:HD22	35:l:129:MET:HB3	2.01	0.42
49:r:502:PLX:H51	49:r:502:PLX:H6	1.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:215:GLN:O	44:w:219:GLN:HG2	2.18	0.42
44:w:219:GLN:HA	44:w:227:MET:HE3	2.00	0.42
12:M:398:ASP:OD2	12:M:471:LYS:N	2.47	0.42
15:P:113:ASP:OD1	16:Q:423:LYS:NZ	2.50	0.42
16:Q:184:ILE:HD11	16:Q:251:PHE:CE1	2.54	0.42
6:X:116:VAL:CG2	39:p:17:LEU:HD12	2.49	0.42
29:f:47:THR:HG23	30:g:65:LEU:HD22	2.01	0.42
35:l:346:ILE:HD11	35:l:431:PHE:CZ	2.54	0.42
40:r:203:PHE:O	40:r:207:MET:HG2	2.19	0.42
1:A:322:SER:HB2	1:A:370:LEU:HD22	2.01	0.42
4:E:99:GLN:CD	33:j:41:PHE:HD1	2.28	0.42
13:N:38:LEU:HD12	13:N:49:TYR:CE2	2.55	0.42
20:V:121:THR:O	20:V:125:VAL:HG23	2.19	0.42
24:a:137:MET:HE2	37:n:42:SER:HB3	2.00	0.42
56:a:201:CDL:H612	35:l:9:LEU:HD12	2.00	0.42
32:i:270:MET:HE3	32:i:279:PRO:HG3	2.01	0.42
35:l:244:SER:O	35:l:249:SER:HB3	2.19	0.42
35:l:557:TRP:O	35:l:561:ILE:HG12	2.20	0.42
44:w:113:SER:HB3	44:w:116:LYS:HB3	2.01	0.42
1:A:398:ARG:HH22	1:A:408:GLU:CD	2.25	0.42
3:C:62:LEU:O	3:C:91:VAL:HA	2.19	0.42
14:O:177:LEU:O	14:O:192:TYR:OH	2.35	0.42
17:S:21:MET:HG3	41:s:256:THR:HG21	2.02	0.42
44:w:214:ILE:HG21	44:w:234:LEU:HD22	2.02	0.42
7:H:98:LYS:O	7:H:101:GLU:HG3	2.19	0.42
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.49	0.42
14:O:137:THR:O	14:O:141:MET:N	2.48	0.42
25:b:10:LEU:O	25:b:13:GLN:HG3	2.19	0.42
25:b:119:LEU:HD22	25:b:119:LEU:H	1.85	0.42
32:i:246:VAL:HG11	56:r:504:CDL:H392	2.00	0.42
35:l:61:MET:HE2	35:l:61:MET:HB2	1.78	0.42
35:l:383:MET:SD	35:l:384:PRO:HD2	2.60	0.42
35:l:572:LYS:HD2	35:l:572:LYS:HA	1.57	0.42
38:o:105:PHE:CE1	40:r:391:ILE:HB	2.55	0.42
41:s:59:GLU:O	41:s:59:GLU:HG3	2.19	0.42
41:s:146:LEU:HD12	41:s:188:SER:HB3	2.02	0.42
7:H:5:LEU:N	7:H:18:GLU:OE2	2.52	0.42
10:K:73:TYR:CZ	10:K:75:ASN:HB3	2.55	0.42
12:M:240:ALA:HB2	12:M:271:MET:HE2	2.01	0.42
16:Q:277:VAL:HA	16:Q:324:GLY:O	2.19	0.42
25:b:120:MET:O	25:b:120:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:43:LYS:HE2	26:c:43:LYS:HB2	1.83	0.42
35:l:60:GLU:HG2	35:l:83:ASP:HA	2.01	0.42
36:m:101:PHE:CD1	36:m:101:PHE:C	2.97	0.42
41:s:222:MET:HA	41:s:225:MET:HE3	2.00	0.42
44:w:110:GLY:HA2	44:w:134:TRP:CD2	2.54	0.42
1:A:214:GLU:CD	1:A:224:ARG:HD2	2.44	0.42
3:C:167:PRO:HD3	16:Q:223:HIS:CD2	2.54	0.42
6:G:90:TYR:HE1	6:G:92:LYS:HB2	1.84	0.42
9:J:283:VAL:HG22	9:J:369:VAL:HG11	2.02	0.42
18:T:79:VAL:O	18:T:121:PRO:HD3	2.19	0.42
20:V:23:TYR:O	20:V:26:THR:HG22	2.19	0.42
24:a:169:TYR:CZ	30:g:3:MET:HG3	2.55	0.42
26:c:33:THR:OG1	26:c:34:LYS:N	2.52	0.42
32:i:2:ASN:HB3	32:i:5:ILE:HG12	2.02	0.42
35:l:336:LYS:HA	35:l:336:LYS:HD3	1.80	0.42
1:A:41:ILE:O	1:A:137:LYS:HE3	2.19	0.42
1:A:110:PRO:O	1:A:238:CYS:HB3	2.20	0.42
8:I:18:ARG:NH2	16:Q:260:GLU:OE2	2.42	0.42
11:L:145:PHE:HD2	11:L:147:VAL:HG23	1.85	0.42
12:M:49:VAL:HG13	12:M:102:ILE:HD13	2.02	0.42
23:Z:13:LYS:HA	23:Z:13:LYS:HD2	1.87	0.42
37:n:12:TRP:O	37:n:15:ILE:HG12	2.19	0.42
40:r:305:THR:O	40:r:308:SER:OG	2.27	0.42
41:s:179:TRP:CG	41:s:180:PRO:HD3	2.55	0.42
1:A:115:VAL:HG21	1:A:142:CYS:SG	2.60	0.42
1:A:267:ARG:NH1	1:A:338:ASP:OD2	2.51	0.42
3:C:92:VAL:HG11	53:s:403:UQ:H103	2.02	0.42
53:J:402:UQ:H202	53:J:402:UQ:H221	1.92	0.42
20:V:138:GLU:HG2	20:V:139:PRO:HD2	2.01	0.42
22:Y:61:PHE:CZ	35:l:455:LYS:HG3	2.55	0.42
24:a:95:GLU:HB3	24:a:114:LYS:CG	2.50	0.42
48:j:201:PEE:H35	48:j:201:PEE:H30	1.89	0.42
34:k:38:LEU:O	34:k:42:ILE:HG12	2.19	0.42
38:o:115:LEU:HG	38:o:120:LYS:O	2.20	0.42
43:v:113:LYS:HE3	43:v:113:LYS:HB3	1.91	0.42
7:H:19:THR:HB	7:H:22:GLU:OE1	2.20	0.42
9:J:85:ARG:NH2	52:J:401:NDP:O3X	2.45	0.42
19:U:38:TYR:CD1	19:U:41:TYR:HD2	2.37	0.42
49:a:202:PLX:H162	28:e:105:PHE:HB2	2.02	0.42
26:c:160:GLN:OE1	43:v:37:ARG:NH1	2.53	0.42
27:d:158:LYS:HG3	30:g:118:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:25:HIS:HB3	32:i:28:LEU:HD23	2.01	0.42
33:j:57:LEU:HD21	36:m:169:MET:SD	2.60	0.42
33:j:83:ASN:OD1	33:j:83:ASN:N	2.53	0.42
40:r:71:TRP:CG	49:r:503:PLX:H341	2.54	0.42
40:r:361:VAL:HG11	40:r:441:ILE:HG12	2.02	0.42
40:r:398:MET:O	40:r:402:ILE:HG13	2.19	0.42
41:s:77:LEU:HD12	48:s:401:PEE:H40	2.01	0.42
12:M:306:MET:HB3	12:M:314:LEU:HD22	2.02	0.41
13:N:53:LYS:HB3	13:N:53:LYS:HE3	1.81	0.41
18:T:34:THR:OG1	18:T:52:ARG:NH1	2.53	0.41
6:X:129:GLU:HB2	39:p:82:PHE:CD2	2.55	0.41
25:b:25:ASP:OD1	39:p:121:LYS:HD3	2.19	0.41
41:s:102:VAL:HG11	41:s:154:LEU:HD11	2.01	0.41
44:w:110:GLY:HA2	44:w:134:TRP:CE2	2.55	0.41
44:w:239:ASN:O	44:w:243:LYS:HB2	2.19	0.41
56:V:201:CDL:H352	56:V:201:CDL:H322	1.65	0.41
24:a:127:ASP:OD1	49:a:202:PLX:H12	2.19	0.41
26:c:44:THR:HG22	26:c:46:GLU:H	1.85	0.41
27:d:127:LYS:HB3	27:d:127:LYS:HE2	1.77	0.41
28:e:154:ASP:OD1	28:e:154:ASP:N	2.54	0.41
36:m:95:SER:O	36:m:98:MET:HG3	2.20	0.41
6:G:122:MET:HE3	6:G:144:ILE:HD13	2.02	0.41
14:O:153:GLN:HG3	14:O:158:ILE:O	2.20	0.41
16:Q:158:LEU:HD23	16:Q:158:LEU:HA	1.91	0.41
25:b:97:VAL:HG22	35:l:63:ILE:HG23	2.02	0.41
35:l:40:VAL:HG21	35:l:101:MET:HE3	2.02	0.41
56:l:701:CDL:H272	56:l:701:CDL:H241	1.86	0.41
36:m:63:GLY:O	36:m:67:VAL:HG23	2.21	0.41
8:I:97:PRO:HD3	15:P:61:PHE:CE1	2.55	0.41
36:m:49:GLY:CA	36:m:139:GLU:OE1	2.59	0.41
40:r:282:LEU:HD13	40:r:342:MET:HG3	2.02	0.41
43:v:52:MET:HB2	43:v:55:GLN:HB2	2.03	0.41
43:v:65:GLN:OE1	43:v:65:GLN:HA	2.19	0.41
44:w:55:GLU:O	44:w:55:GLU:HG2	2.19	0.41
1:A:456:GLN:OE1	1:A:456:GLN:C	2.64	0.41
16:Q:342:ARG:HD2	21:W:21:TYR:CZ	2.55	0.41
19:U:66:VAL:O	42:u:130:LYS:HE3	2.20	0.41
25:b:122:GLU:O	25:b:122:GLU:OE2	2.38	0.41
27:d:140:GLN:O	27:d:144:SER:HB2	2.20	0.41
28:e:73:SER:C	28:e:75:GLY:H	2.28	0.41
35:l:79:SER:HB3	35:l:135:ASN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:174:TYR:CD2	35:l:232:TRP:HB3	2.55	0.41
35:l:264:TYR:CG	35:l:265:PRO:HD3	2.55	0.41
56:l:701:CDL:H801	49:r:503:PLX:H181	2.03	0.41
40:r:116:ILE:HD13	40:r:116:ILE:HA	1.83	0.41
41:s:233:MET:HE3	41:s:233:MET:HB3	1.75	0.41
44:w:58:LYS:HA	44:w:202:HIS:CG	2.56	0.41
3:C:67:PHE:HZ	3:C:117:LEU:HD12	1.86	0.41
53:J:402:UQ:H71	53:J:402:UQ:HM53	1.74	0.41
15:P:112:ALA:O	16:Q:425:LYS:HE3	2.21	0.41
24:a:100:ASP:OD1	24:a:100:ASP:N	2.54	0.41
27:d:117:GLU:HG3	27:d:124:ASN:HB2	2.03	0.41
32:i:128:LEU:HD23	32:i:128:LEU:O	2.20	0.41
48:l:702:PEE:H59	48:l:702:PEE:H53	1.94	0.41
36:m:141:MET:HE2	36:m:141:MET:CA	2.43	0.41
40:r:210:TYR:CG	40:r:268:GLY:HA3	2.55	0.41
50:C:304:DCQ:H3MB	16:Q:92:HIS:ND1	2.36	0.41
4:E:93:THR:HG23	4:E:103:ILE:HD11	2.03	0.41
16:Q:144:MET:HE2	16:Q:144:MET:HB2	2.01	0.41
20:V:59:TYR:CD1	56:V:201:CDL:H112	2.56	0.41
6:X:71:ALA:HB2	35:l:442:LEU:HD11	2.03	0.41
26:c:120:SER:H	26:c:120:SER:HG	1.65	0.41
27:d:36:ILE:O	27:d:40:LEU:HB2	2.20	0.41
32:i:10:ILE:O	32:i:14:MET:HG3	2.20	0.41
34:k:28:SER:HB3	36:m:23:LYS:HG2	2.03	0.41
56:l:701:CDL:H611	56:l:701:CDL:H581	1.67	0.41
38:o:25:ILE:HD12	38:o:25:ILE:C	2.45	0.41
40:r:260:PRO:HG3	49:r:502:PLX:H131	2.03	0.41
1:A:412:LEU:HD23	1:A:439:ILE:HD11	2.03	0.41
2:B:149:MET:HB2	2:B:183:LEU:O	2.21	0.41
9:J:365:GLU:H	9:J:365:GLU:CD	2.28	0.41
28:e:51:PRO:HB3	44:w:124:ASN:O	2.21	0.41
34:k:30:LEU:O	34:k:34:GLU:HG2	2.19	0.41
40:r:364:LEU:HD23	40:r:364:LEU:HA	1.86	0.41
43:v:83:GLU:CD	43:v:83:GLU:N	2.76	0.41
1:A:185:ASN:ND2	1:A:188:GLY:HA2	2.36	0.41
2:B:144:ARG:HB2	13:N:130:THR:HG23	2.02	0.41
5:F:20:ARG:HB2	5:F:66:TRP:HB2	2.03	0.41
5:F:24:CYS:N	5:F:58:CYS:SG	2.94	0.41
8:I:40:LYS:CB	21:W:7:LYS:H	2.34	0.41
12:M:171:THR:HG23	12:M:173:MET:CE	2.51	0.41
12:M:347:ASP:OD1	12:M:347:ASP:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:534:VAL:HG23	12:M:538:ARG:HE	1.86	0.41
15:P:94:ILE:O	15:P:98:THR:OG1	2.31	0.41
16:Q:143:SER:HA	16:Q:178:THR:HG22	2.03	0.41
21:W:134:LEU:HD21	36:m:3:MET:HG3	2.03	0.41
22:Y:65:MET:SD	35:l:375:ILE:HG12	2.61	0.41
25:b:32:GLU:HB3	39:p:115:TYR:HD1	1.86	0.41
26:c:110:ASP:OD1	26:c:110:ASP:N	2.53	0.41
28:e:55:LEU:CD2	28:e:57:GLU:HB2	2.51	0.41
31:h:17:TRP:CD1	31:h:17:TRP:H	2.39	0.41
32:i:41:ILE:HG13	34:k:73:LEU:HD21	2.03	0.41
32:i:129:LEU:HD12	32:i:133:TRP:HB3	2.01	0.41
34:k:24:SER:HB3	34:k:89:TYR:CE1	2.56	0.41
35:l:10:THR:O	35:l:14:ILE:HG23	2.21	0.41
35:l:288:THR:HG21	35:l:307:SER:HB3	2.03	0.41
36:m:28:TYR:HB3	36:m:83:TRP:CH2	2.56	0.41
36:m:68:PHE:CD1	36:m:68:PHE:C	2.99	0.41
49:r:502:PLX:H121	49:r:502:PLX:H92	1.86	0.41
56:s:402:CDL:H171	56:s:402:CDL:H141	1.87	0.41
42:u:107:PHE:O	42:u:111:VAL:HG22	2.20	0.41
44:w:123:SER:OG	44:w:125:ASP:OD1	2.30	0.41
3:C:52:ASP:HB3	49:C:303:PLX:H251	2.03	0.41
3:C:54:VAL:HG21	48:C:302:PEE:H55	2.02	0.41
9:J:83:PRO:HA	9:J:106:MET:O	2.20	0.41
26:c:113:ILE:HD11	26:c:116:ARG:HD2	2.03	0.41
27:d:106:ILE:HG13	27:d:135:VAL:HG21	2.03	0.41
32:i:271:THR:HG21	40:r:165:VAL:HG23	2.03	0.41
41:s:105:MET:HE2	41:s:105:MET:HB3	1.94	0.41
5:F:23:LEU:C	5:F:58:CYS:SG	3.04	0.40
53:J:402:UQ:H101	53:J:402:UQ:H121	1.72	0.40
14:O:196:LEU:HD23	14:O:196:LEU:HA	1.95	0.40
15:P:75:GLN:HB3	15:P:87:PHE:HD1	1.86	0.40
15:P:87:PHE:CE2	15:P:144:LYS:HE2	2.55	0.40
20:V:67:GLY:HA2	56:V:201:CDL:H221	2.02	0.40
24:a:67:PHE:CE2	40:r:434:ASN:HB3	2.56	0.40
27:d:37:PHE:CD2	35:l:3:PRO:HB3	2.57	0.40
30:g:109:LYS:HB3	30:g:113:GLU:HG3	2.03	0.40
36:m:44:VAL:HG12	36:m:49:GLY:O	2.20	0.40
40:r:193:ILE:HD13	49:r:502:PLX:H102	2.02	0.40
41:s:207:LEU:O	41:s:209:SER:N	2.54	0.40
12:M:485:ASP:O	12:M:489:ILE:HD12	2.21	0.40
12:M:647:GLU:HB2	12:M:654:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:184:ILE:HG12	16:Q:203:MET:HE3	2.02	0.40
26:c:164:ASN:HA	26:c:181:VAL:HG22	2.02	0.40
30:g:45:LEU:HB3	56:r:504:CDL:H731	2.03	0.40
30:g:48:ASN:HB3	30:g:55:VAL:HA	2.03	0.40
32:i:72:MET:HE2	32:i:76:ILE:HG13	2.03	0.40
32:i:122:ILE:O	32:i:176:ARG:NH1	2.51	0.40
56:l:701:CDL:H861	56:l:701:CDL:H572	2.03	0.40
37:n:26:TYR:CZ	37:n:30:ARG:HD2	2.56	0.40
41:s:213:VAL:HG13	41:s:214:GLU:HG2	2.03	0.40
42:u:19:LYS:HE3	42:u:19:LYS:HB2	1.58	0.40
8:I:40:LYS:HA	8:I:40:LYS:HD2	1.68	0.40
9:J:271:TYR:CE2	9:J:374:THR:HG22	2.57	0.40
16:Q:158:LEU:HD12	16:Q:411:LEU:HD23	2.03	0.40
27:d:6:ASP:HB3	27:d:9:VAL:HG23	2.03	0.40
28:e:109:LEU:HD23	28:e:109:LEU:HA	1.97	0.40
32:i:125:GLN:OE1	32:i:125:GLN:N	2.53	0.40
48:j:201:PEE:H22	48:j:201:PEE:H27	1.90	0.40
35:l:363:TYR:CD1	35:l:370:THR:HG21	2.56	0.40
36:m:51:PHE:O	36:m:55:MET:HB2	2.21	0.40
1:A:116:ASN:ND2	1:A:207:GLY:O	2.35	0.40
48:B:303:PEE:H16	41:s:293:PHE:CE1	2.56	0.40
16:Q:259:GLU:HG2	21:W:25:LEU:HD11	2.02	0.40
20:V:95:CYS:HA	20:V:115:CYS:HA	2.02	0.40
6:X:132:ASP:OD2	39:p:18:ARG:HG2	2.21	0.40
23:Z:84:ALA:O	23:Z:88:LEU:HB2	2.21	0.40
40:r:398:MET:HG3	40:r:398:MET:H	1.68	0.40
1:A:129:GLU:OE1	1:A:132:ARG:HD3	2.22	0.40
3:C:98:ARG:HA	3:C:125:PRO:HD3	2.02	0.40
4:E:22:SER:HB3	4:E:27:GLU:HB2	2.04	0.40
12:M:44:GLU:OE2	12:M:44:GLU:N	2.38	0.40
15:P:125:ARG:NH2	15:P:201:ASP:OD1	2.47	0.40
23:Z:77:ALA:O	23:Z:80:VAL:HG12	2.21	0.40
24:a:174:ILE:HG21	31:h:20:ILE:HG21	2.02	0.40
25:b:123:PHE:CE1	43:v:61:HIS:HB2	2.56	0.40
31:h:51:ARG:NH2	31:h:55:GLU:OE1	2.51	0.40
32:i:131:LEU:HD23	32:i:131:LEU:HA	1.84	0.40
32:i:245:MET:HB2	32:i:301:SER:OG	2.21	0.40
33:j:90:MET:HE3	36:m:151:THR:HG23	2.04	0.40
48:j:201:PEE:H51	48:j:201:PEE:H56	1.89	0.40
37:n:17:VAL:HG13	40:r:7:PRO:HB3	2.02	0.40
43:v:108:LEU:HD23	43:v:108:LEU:HA	1.90	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%)	421 (98%)	10 (2%)	0	100	100
2	B	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
3	C	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
4	E	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
5	F	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
6	G	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
6	X	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
7	H	110/112 (98%)	105 (96%)	4 (4%)	1 (1%)	14	41
8	I	93/112 (83%)	85 (91%)	8 (9%)	0	100	100
9	J	340/342 (99%)	329 (97%)	10 (3%)	1 (0%)	36	65
10	K	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	672 (98%)	16 (2%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	204 (95%)	11 (5%)	0	100	100
15	P	206/208 (99%)	200 (97%)	5 (2%)	1 (0%)	24	54
16	Q	427/430 (99%)	416 (97%)	11 (3%)	0	100	100
17	S	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
18	T	94/96 (98%)	92 (98%)	2 (2%)	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%)	134 (96%)	6 (4%)	0	100	100

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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%)	77 (99%)	1 (1%)	0	100	100
24	a	136/138 (99%)	134 (98%)	2 (2%)	0	100	100
25	b	94/126 (75%)	89 (95%)	5 (5%)	0	100	100
26	c	154/156 (99%)	144 (94%)	10 (6%)	0	100	100
27	d	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
28	e	102/104 (98%)	97 (95%)	5 (5%)	0	100	100
29	f	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
30	g	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
31	h	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
32	i	345/347 (99%)	335 (97%)	10 (3%)	0	100	100
33	j	113/115 (98%)	108 (96%)	3 (3%)	2 (2%)	6	25
34	k	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
35	l	604/606 (100%)	583 (96%)	21 (4%)	0	100	100
36	m	173/175 (99%)	160 (92%)	13 (8%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
39	p	176/178 (99%)	168 (96%)	8 (4%)	0	100	100
40	r	457/459 (100%)	449 (98%)	8 (2%)	0	100	100
41	s	316/318 (99%)	303 (96%)	12 (4%)	1 (0%)	36	65
42	u	169/171 (99%)	164 (97%)	5 (3%)	0	100	100
43	v	122/125 (98%)	117 (96%)	5 (4%)	0	100	100
44	w	318/320 (99%)	310 (98%)	8 (2%)	0	100	100
All	All	8175/8314 (98%)	7913 (97%)	256 (3%)	6 (0%)	49	77

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	P	44	ARG
7	H	77	ILE
33	j	79	SER
9	J	38	HIS
33	j	40	GLY
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	346/346 (100%)	344 (99%)	2 (1%)	78	93
2	B	151/151 (100%)	150 (99%)	1 (1%)	76	92
3	C	132/132 (100%)	131 (99%)	1 (1%)	73	90
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	75/76 (99%)	71 (95%)	4 (5%)	20	52
6	G	76/81 (94%)	76 (100%)	0	100	100
6	X	75/81 (93%)	71 (95%)	4 (5%)	20	52
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%)	293 (99%)	3 (1%)	68	89
10	K	42/42 (100%)	42 (100%)	0	100	100
11	L	113/113 (100%)	110 (97%)	3 (3%)	39	73
12	M	580/580 (100%)	568 (98%)	12 (2%)	47	77
13	N	130/130 (100%)	130 (100%)	0	100	100
14	O	183/183 (100%)	178 (97%)	5 (3%)	39	73
15	P	189/190 (100%)	189 (100%)	0	100	100
16	Q	370/370 (100%)	368 (100%)	2 (0%)	81	93
17	S	55/58 (95%)	55 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	98 (97%)	3 (3%)	36	70
21	W	121/123 (98%)	120 (99%)	1 (1%)	73	90
22	Y	62/62 (100%)	60 (97%)	2 (3%)	34	68
23	Z	62/62 (100%)	62 (100%)	0	100	100
24	a	121/121 (100%)	120 (99%)	1 (1%)	73	90
25	b	90/119 (76%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	c	141/141 (100%)	139 (99%)	2 (1%)	59	85
27	d	154/155 (99%)	152 (99%)	2 (1%)	61	86
28	e	96/96 (100%)	95 (99%)	1 (1%)	68	89
29	f	36/45 (80%)	36 (100%)	0	100	100
30	g	108/109 (99%)	107 (99%)	1 (1%)	70	90
31	h	93/93 (100%)	91 (98%)	2 (2%)	45	77
32	i	311/311 (100%)	301 (97%)	10 (3%)	34	68
33	j	100/100 (100%)	99 (99%)	1 (1%)	68	89
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	537/540 (99%)	529 (98%)	8 (2%)	57	84
36	m	126/141 (89%)	125 (99%)	1 (1%)	73	90
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	113/113 (100%)	112 (99%)	1 (1%)	70	90
39	p	159/159 (100%)	159 (100%)	0	100	100
40	r	410/410 (100%)	404 (98%)	6 (2%)	57	84
41	s	275/275 (100%)	272 (99%)	3 (1%)	65	88
42	u	153/153 (100%)	148 (97%)	5 (3%)	33	67
43	v	104/111 (94%)	103 (99%)	1 (1%)	68	89
44	w	280/283 (99%)	277 (99%)	3 (1%)	65	88
All	All	7145/7241 (99%)	7054 (99%)	91 (1%)	59	86

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	351	THR
2	B	52	SER
3	C	71	CYS
5	F	25	GLN
5	F	27	SER
5	F	88	THR
5	F	90	THR
9	J	328	THR
9	J	347	LEU
9	J	377	ILE

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Mol	Chain	Res	Type
11	L	59	LEU
11	L	86	ASN
11	L	148	GLU
12	M	30	ASN
12	M	160	VAL
12	M	171	THR
12	M	232	THR
12	M	336	ASN
12	M	347	ASP
12	M	426	ASP
12	M	500	ILE
12	M	502	LEU
12	M	575	VAL
12	M	632	MET
12	M	636	TYR
14	O	40	VAL
14	O	68	LYS
14	O	150	GLU
14	O	153	GLN
14	O	194	GLU
16	Q	217	VAL
16	Q	453	THR
20	V	36	VAL
20	V	77	SER
20	V	134	GLN
21	W	96	ILE
6	X	75	THR
6	X	91	ASP
6	X	105	MET
6	X	140	CYS
22	Y	51	THR
22	Y	97	LEU
24	a	54	LEU
26	c	33	THR
26	c	120	SER
27	d	9	VAL
27	d	120	SER
28	e	139	SER
30	g	2	THR
31	h	21	GLN
31	h	75	ARG
32	i	14	MET

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Mol	Chain	Res	Type
32	i	18	MET
32	i	62	THR
32	i	67	SER
32	i	182	SER
32	i	215	MET
32	i	223	SER
32	i	278	MET
32	i	319	HIS
32	i	320	THR
33	j	101	SER
35	l	9	LEU
35	l	71	LEU
35	l	316	THR
35	l	317	ILE
35	l	380	LEU
35	l	387	THR
35	l	426	ILE
35	l	496	MET
36	m	82	VAL
38	o	73	SER
40	r	60	SER
40	r	116	ILE
40	r	126	LEU
40	r	187	SER
40	r	290	SER
40	r	305	THR
41	s	21	THR
41	s	28	LEU
41	s	156	MET
42	u	6	GLU
42	u	88	CYS
42	u	109	GLU
42	u	126	SER
42	u	149	GLU
43	v	109	LEU
44	w	56	THR
44	w	309	THR
44	w	332	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	ASN
1	A	344	GLN
1	A	393	ASN
4	E	58	GLN
5	F	48	ASN
5	F	62	GLN
6	G	115	GLN
9	J	122	HIS
9	J	295	HIS
9	J	323	HIS
10	K	70	ASN
10	K	106	GLN
11	L	71	HIS
12	M	164	ASN
12	M	202	ASN
12	M	260	ASN
12	M	278	HIS
12	M	669	ASN
13	N	5	GLN
13	N	113	HIS
14	O	90	ASN
14	O	182	ASN
15	P	55	HIS
15	P	63	GLN
15	P	75	GLN
15	P	77	GLN
15	P	82	ASN
15	P	131	ASN
15	P	196	HIS
16	Q	38	GLN
16	Q	162	GLN
16	Q	223	HIS
18	T	74	GLN
18	T	120	GLN
19	U	83	ASN
21	W	76	GLN
22	Y	54	GLN
23	Z	21	GLN
26	c	100	ASN
26	c	154	GLN
27	d	55	GLN
27	d	123	GLN
27	d	131	GLN

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Mol	Chain	Res	Type
27	d	134	GLN
29	f	62	HIS
30	g	90	HIS
32	i	63	GLN
32	i	152	ASN
32	i	197	ASN
32	i	221	HIS
34	k	57	ASN
35	l	135	ASN
35	l	199	GLN
35	l	205	ASN
35	l	270	ASN
35	l	296	ASN
35	l	309	GLN
35	l	446	ASN
35	l	447	ASN
35	l	470	ASN
35	l	524	ASN
35	l	603	ASN
36	m	175	ASN
37	n	6	GLN
40	r	175	ASN
40	r	251	ASN
40	r	304	GLN
40	r	366	ASN
40	r	450	ASN
41	s	247	HIS
41	s	287	HIS
42	u	99	HIS
43	v	44	GLN
44	w	85	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	2MR	Q	118	16	10,12,13	1.99	1 (10%)	5,13,15	6.00	3 (60%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.66	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	12.33	130.79	119.48
16	Q	118	2MR	CD-NE-CZ	4.07	131.03	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.15	130.82	123.86

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 45 ligands modelled in this entry, 2 are monoatomic - leaving 43 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$
49	PLX	j	202	-	51,51,51	1.14	4 (7%)	55,59,59	0.60	1 (1%)
47	NAI	A	503	-	45,48,48	3.90	20 (44%)	60,73,73	1.79	13 (21%)
46	FMN	A	502	-	33,33,33	1.10	2 (6%)	48,50,50	1.26	8 (16%)
45	SF4	A	501	1	0,12,12	-	-	-	-	-
51	8Q1	G	201	-	31,34,34	1.70	6 (19%)	40,43,43	1.63	6 (15%)
48	PEE	V	202	-	39,39,50	1.31	6 (15%)	41,44,55	1.03	2 (4%)
52	NDP	J	401	-	49,52,52	4.39	23 (46%)	66,80,80	2.18	13 (19%)
50	DCQ	C	304	-	23,23,23	1.32	5 (21%)	26,29,29	0.99	1 (3%)
56	CDL	n	101	-	54,54,99	1.36	8 (14%)	60,66,111	1.11	4 (6%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
54	FES	O	301	14	0,4,4	-	-	-	-	-
49	PLX	g	201	-	51,51,51	1.14	3 (5%)	55,59,59	0.61	1 (1%)
48	PEE	B	303	-	50,50,50	1.16	6 (12%)	53,55,55	1.01	2 (3%)
54	FES	M	803	12	0,4,4	-	-	-	-	-
56	CDL	o	201	-	99,99,99	1.09	8 (8%)	105,111,111	0.87	4 (3%)
48	PEE	s	401	-	40,40,50	1.15	5 (12%)	43,45,55	1.01	2 (4%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-
49	PLX	J	403	-	51,51,51	1.15	3 (5%)	55,59,59	0.59	1 (1%)
45	SF4	C	301	3	0,12,12	-	-	-	-	-
48	PEE	C	302	-	46,46,50	1.20	6 (13%)	49,51,55	1.01	2 (4%)
48	PEE	l	702	-	50,50,50	1.15	6 (12%)	53,55,55	0.94	2 (3%)
56	CDL	i	401	-	86,86,99	1.15	8 (9%)	92,98,111	0.91	4 (4%)
56	CDL	V	201	-	93,93,99	1.11	9 (9%)	99,105,111	0.89	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	PLX	a	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.58	1 (1%)
49	PLX	r	502	-	51,51,51	1.14	4 (7%)	55,59,59	0.65	1 (1%)
56	CDL	r	504	-	99,99,99	1.08	8 (8%)	105,111,111	0.88	4 (3%)
58	ADP	w	401	-	27,29,29	2.97	8 (29%)	42,45,45	2.07	11 (26%)
53	UQ	J	402	-	33,33,63	3.45	8 (24%)	40,43,79	2.77	13 (32%)
48	PEE	W	201	-	40,40,50	1.14	5 (12%)	43,45,55	1.00	2 (4%)
56	CDL	N	201	-	50,50,99	1.41	8 (16%)	56,62,111	1.13	4 (7%)
56	CDL	a	201	-	99,99,99	1.09	8 (8%)	105,111,111	0.86	4 (3%)
56	CDL	l	701	-	98,98,99	1.08	8 (8%)	104,110,111	0.90	4 (3%)
48	PEE	b	201	-	45,45,50	1.22	6 (13%)	48,50,55	1.02	2 (4%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
48	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	1.00	2 (3%)
49	PLX	C	303	-	51,51,51	1.14	3 (5%)	55,59,59	0.59	1 (1%)
56	CDL	k	101	-	99,99,99	1.09	8 (8%)	105,111,111	0.83	4 (3%)
49	PLX	r	503	-	51,51,51	1.14	3 (5%)	55,59,59	0.53	1 (1%)
48	PEE	j	201	-	50,50,50	1.15	6 (12%)	53,55,55	0.96	2 (3%)
51	8Q1	X	201	-	31,34,34	1.70	5 (16%)	40,43,43	1.57	6 (15%)
53	UQ	s	403	-	38,38,63	3.53	11 (28%)	46,49,79	2.86	16 (34%)
45	SF4	B	302	2	0,12,12	-	-	-	-	-
56	CDL	s	402	-	88,88,99	1.13	8 (9%)	94,100,111	0.92	4 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	PLX	j	202	-	-	34/55/55/55	-
47	NAI	A	503	-	-	9/29/72/72	0/5/5/5
46	FMN	A	502	-	-	7/18/18/18	0/3/3/3
45	SF4	A	501	1	-	-	0/6/5/5
51	8Q1	G	201	-	-	9/41/41/41	-
48	PEE	V	202	-	-	20/43/43/54	-
52	NDP	J	401	-	-	9/34/77/77	0/4/5/5
50	DCQ	C	304	-	-	3/14/38/38	0/1/1/1
56	CDL	n	101	-	-	29/65/65/110	-
45	SF4	B	301	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	FES	O	301	14	-	-	0/1/1/1
49	PLX	g	201	-	-	29/55/55/55	-
48	PEE	B	303	-	-	28/54/54/54	-
54	FES	M	803	12	-	-	0/1/1/1
56	CDL	o	201	-	-	58/110/110/110	-
48	PEE	s	401	-	-	21/44/44/54	-
45	SF4	M	801	12	-	-	0/6/5/5
49	PLX	J	403	-	-	31/55/55/55	-
45	SF4	C	301	3	-	-	0/6/5/5
48	PEE	C	302	-	-	24/50/50/54	-
48	PEE	l	702	-	-	29/54/54/54	-
56	CDL	i	401	-	-	49/97/97/110	-
56	CDL	V	201	-	-	60/104/104/110	-
49	PLX	a	202	-	-	26/55/55/55	-
49	PLX	r	502	-	-	26/55/55/55	-
56	CDL	r	504	-	-	62/110/110/110	-
58	ADP	w	401	-	-	4/16/32/32	0/3/3/3
53	UQ	J	402	-	-	16/27/51/87	0/1/1/1
48	PEE	W	201	-	-	17/44/44/54	-
56	CDL	N	201	-	-	35/61/61/110	-
56	CDL	a	201	-	-	54/110/110/110	-
56	CDL	l	701	-	-	66/109/109/110	-
48	PEE	b	201	-	-	23/49/49/54	-
45	SF4	M	802	12	-	-	0/6/5/5
48	PEE	r	501	-	-	27/54/54/54	-
49	PLX	C	303	-	-	27/55/55/55	-
56	CDL	k	101	-	-	64/110/110/110	-
49	PLX	r	503	-	-	31/55/55/55	-
48	PEE	j	201	-	-	21/54/54/54	-
51	8Q1	X	201	-	-	8/41/41/41	-
53	UQ	s	403	-	-	13/33/57/87	0/1/1/1
45	SF4	B	302	2	-	-	0/6/5/5
56	CDL	s	402	-	-	52/99/99/110	-

All (245) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	J	401	NDP	C3B-C2B	-13.11	1.23	1.52
52	J	401	NDP	C6N-C5N	12.49	1.55	1.33
52	J	401	NDP	O4D-C4D	10.58	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.31	1.26	1.53
52	J	401	NDP	C3D-C4D	-9.92	1.27	1.53
53	J	402	UQ	C18-C19	9.61	1.56	1.33
53	s	403	UQ	C18-C19	9.59	1.56	1.33
53	s	403	UQ	C13-C14	9.23	1.55	1.33
53	J	402	UQ	C13-C14	9.20	1.55	1.33
47	A	503	NAI	O4B-C1B	9.10	1.63	1.42
53	s	403	UQ	C23-C24	9.06	1.54	1.33
53	J	402	UQ	C8-C9	8.92	1.54	1.33
53	s	403	UQ	C8-C9	8.92	1.54	1.33
58	w	401	ADP	C3'-C4'	-8.89	1.30	1.53
47	A	503	NAI	O4B-C4B	-8.31	1.26	1.45
52	J	401	NDP	O4B-C4B	-7.91	1.27	1.45
53	J	402	UQ	C23-C24	7.87	1.55	1.32
58	w	401	ADP	O4'-C4'	7.70	1.62	1.45
53	s	403	UQ	C28-C29	7.63	1.54	1.32
47	A	503	NAI	C2D-C1D	-7.62	1.29	1.53
52	J	401	NDP	C2N-C3N	7.25	1.55	1.34
47	A	503	NAI	C2B-C1B	-7.20	1.30	1.53
47	A	503	NAI	O4D-C4D	6.82	1.60	1.45
47	A	503	NAI	C2D-C3D	5.94	1.69	1.53
52	J	401	NDP	C6A-N6A	5.85	1.48	1.34
47	A	503	NAI	C7N-N7N	5.74	1.48	1.33
58	w	401	ADP	C6-N6	5.57	1.48	1.34
52	J	401	NDP	P2B-O2B	5.55	1.69	1.59
51	X	201	8Q1	C34-N36	5.49	1.45	1.33
51	G	201	8Q1	C34-N36	5.43	1.45	1.33
47	A	503	NAI	O4D-C1D	5.40	1.54	1.42
51	X	201	8Q1	C39-N41	5.38	1.45	1.33
51	G	201	8Q1	C39-N41	5.37	1.45	1.33
52	J	401	NDP	C3B-C4B	5.28	1.66	1.53
47	A	503	NAI	C6A-N6A	5.19	1.47	1.34
47	A	503	NAI	C4N-C3N	-5.07	1.40	1.49
52	J	401	NDP	O4D-C1D	-4.86	1.30	1.42
52	J	401	NDP	C6N-N1N	4.84	1.49	1.37
52	J	401	NDP	O4B-C1B	4.62	1.52	1.42
47	A	503	NAI	O2B-C2B	4.51	1.53	1.43
52	J	401	NDP	C1B-N9A	-4.51	1.33	1.46
58	w	401	ADP	O4'-C1'	-4.51	1.31	1.42
52	J	401	NDP	O2D-C2D	-4.24	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	J	401	NDP	C7N-N7N	4.13	1.44	1.33
47	A	503	NAI	C6N-C5N	3.87	1.40	1.33
48	B	303	PEE	C18-C19	3.74	1.53	1.31
48	C	302	PEE	C18-C19	3.73	1.53	1.31
48	r	501	PEE	C18-C19	3.73	1.53	1.31
48	V	202	PEE	C18-C19	3.73	1.53	1.31
48	l	702	PEE	C18-C19	3.73	1.53	1.31
48	b	201	PEE	C18-C19	3.72	1.53	1.31
46	A	502	FMN	C4A-N5	3.72	1.38	1.30
48	s	401	PEE	C18-C19	3.71	1.53	1.31
48	W	201	PEE	C18-C19	3.71	1.53	1.31
48	j	201	PEE	C18-C19	3.70	1.53	1.31
48	b	201	PEE	C39-C38	3.66	1.53	1.31
48	V	202	PEE	C39-C38	3.66	1.53	1.31
48	r	501	PEE	C39-C38	3.65	1.52	1.31
48	C	302	PEE	C39-C38	3.63	1.52	1.31
48	j	201	PEE	C39-C38	3.63	1.52	1.31
48	B	303	PEE	C39-C38	3.62	1.52	1.31
48	l	702	PEE	C39-C38	3.62	1.52	1.31
47	A	503	NAI	C7N-C3N	3.55	1.56	1.48
56	l	701	CDL	OA8-CA7	3.52	1.43	1.33
56	n	101	CDL	OA8-CA7	3.48	1.43	1.33
56	i	401	CDL	OA8-CA7	3.48	1.43	1.33
56	o	201	CDL	OA8-CA7	3.48	1.43	1.33
56	a	201	CDL	OA8-CA7	3.47	1.43	1.33
56	N	201	CDL	OA8-CA7	3.46	1.43	1.33
56	k	101	CDL	OA8-CA7	3.45	1.43	1.33
56	s	402	CDL	OA8-CA7	3.43	1.43	1.33
56	V	201	CDL	OA8-CA7	3.40	1.43	1.33
56	r	504	CDL	OA8-CA7	3.37	1.43	1.33
58	w	401	ADP	O2'-C2'	-3.33	1.35	1.43
47	A	503	NAI	C4N-C5N	-3.32	1.40	1.48
58	w	401	ADP	C8-N9	-3.20	1.31	1.37
56	V	201	CDL	OA6-CA5	3.15	1.43	1.34
56	k	101	CDL	OA6-CA5	3.10	1.43	1.34
58	w	401	ADP	O3'-C3'	3.09	1.50	1.43
52	J	401	NDP	C8A-N9A	-3.09	1.32	1.37
56	r	504	CDL	OB6-CB5	3.06	1.42	1.34
56	a	201	CDL	OB8-CB7	3.06	1.42	1.33
56	k	101	CDL	OB6-CB5	3.04	1.42	1.34
56	o	201	CDL	OA6-CA5	3.04	1.42	1.34
56	i	401	CDL	OB6-CB5	3.03	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	a	201	CDL	OB6-CB5	3.02	1.42	1.34
56	N	201	CDL	OB6-CB5	3.02	1.42	1.34
56	i	401	CDL	OB8-CB7	3.01	1.42	1.33
56	n	101	CDL	OB8-CB7	3.01	1.42	1.33
56	N	201	CDL	OB8-CB7	3.01	1.42	1.33
56	n	101	CDL	OB6-CB5	3.01	1.42	1.34
56	s	402	CDL	OB6-CB5	3.00	1.42	1.34
56	i	401	CDL	OA6-CA5	3.00	1.42	1.34
56	r	504	CDL	OB8-CB7	3.00	1.42	1.33
52	J	401	NDP	O3D-C3D	2.99	1.50	1.43
56	s	402	CDL	OA6-CA5	2.98	1.42	1.34
56	V	201	CDL	OB8-CB7	2.98	1.42	1.33
56	N	201	CDL	OA6-CA5	2.98	1.42	1.34
56	l	701	CDL	OB6-CB5	2.97	1.42	1.34
56	o	201	CDL	OB8-CB7	2.96	1.42	1.33
56	o	201	CDL	OB6-CB5	2.96	1.42	1.34
56	k	101	CDL	OB8-CB7	2.95	1.42	1.33
56	l	701	CDL	OB8-CB7	2.94	1.41	1.33
52	J	401	NDP	C5A-N7A	-2.94	1.33	1.39
56	V	201	CDL	OB6-CB5	2.93	1.42	1.34
56	a	201	CDL	OA6-CA5	2.93	1.42	1.34
52	J	401	NDP	C7N-C3N	2.91	1.54	1.48
56	n	101	CDL	OA6-CA5	2.90	1.42	1.34
56	r	504	CDL	OA6-CA5	2.87	1.42	1.34
56	l	701	CDL	OA6-CA5	2.87	1.42	1.34
56	s	402	CDL	OB8-CB7	2.84	1.41	1.33
53	J	402	UQ	C6-C1	2.79	1.54	1.46
49	g	201	PLX	O6-C4	-2.69	1.41	1.44
49	r	503	PLX	O6-C4	-2.69	1.41	1.44
49	C	303	PLX	O6-C4	-2.66	1.41	1.44
53	s	403	UQ	C6-C1	2.66	1.54	1.46
47	A	503	NAI	C8A-N9A	-2.65	1.32	1.37
49	a	202	PLX	O6-C4	-2.64	1.41	1.44
49	J	403	PLX	O6-C4	-2.57	1.41	1.44
49	j	202	PLX	O6-C4	-2.54	1.41	1.44
48	j	201	PEE	O2-C2	-2.51	1.40	1.46
47	A	503	NAI	O3B-C3B	-2.50	1.37	1.43
53	J	402	UQ	C7-C8	2.50	1.54	1.50
48	V	202	PEE	O3-C30	2.48	1.40	1.33
53	s	403	UQ	C7-C8	2.47	1.54	1.50
48	B	303	PEE	O2-C2	-2.47	1.40	1.46
48	s	401	PEE	O3-C30	2.47	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	W	201	PEE	O3-C30	2.47	1.40	1.33
48	C	302	PEE	O2-C2	-2.46	1.40	1.46
56	a	201	CDL	OA6-CA4	-2.46	1.40	1.46
56	l	701	CDL	OA6-CA4	-2.46	1.40	1.46
48	B	303	PEE	O3-C30	2.46	1.40	1.33
48	C	302	PEE	O3-C30	2.46	1.40	1.33
56	n	101	CDL	OA6-CA4	-2.42	1.40	1.46
48	r	501	PEE	O2-C2	-2.42	1.40	1.46
49	r	502	PLX	O6-C4	-2.41	1.41	1.44
51	X	201	8Q1	C1-S44	2.41	1.82	1.76
56	r	504	CDL	OA6-CA4	-2.41	1.40	1.46
48	l	702	PEE	O3-C30	2.41	1.40	1.33
48	j	201	PEE	O3-C30	2.40	1.40	1.33
48	l	702	PEE	O2-C2	-2.40	1.40	1.46
48	W	201	PEE	O2-C2	-2.40	1.40	1.46
49	a	202	PLX	C7-C6	2.40	1.55	1.50
51	G	201	8Q1	C1-S44	2.40	1.81	1.76
48	s	401	PEE	O2-C2	-2.40	1.40	1.46
56	s	402	CDL	OA6-CA4	-2.39	1.40	1.46
47	A	503	NAI	PN-O5D	2.38	1.68	1.59
56	o	201	CDL	OA6-CA4	-2.38	1.40	1.46
49	g	201	PLX	C7-C6	2.35	1.55	1.50
48	r	501	PEE	O3-C30	2.35	1.40	1.33
49	j	202	PLX	C7-C6	2.35	1.55	1.50
49	r	502	PLX	C7-C6	2.35	1.55	1.50
48	b	201	PEE	O2-C10	2.34	1.40	1.34
49	C	303	PLX	C7-C6	2.34	1.55	1.50
52	J	401	NDP	O2B-C2B	2.33	1.52	1.44
48	b	201	PEE	O3-C30	2.33	1.40	1.33
49	r	503	PLX	C7-C6	2.33	1.55	1.50
46	A	502	FMN	C10-N1	2.32	1.38	1.33
48	V	202	PEE	O2-C10	2.32	1.40	1.34
48	l	702	PEE	O2-C10	2.32	1.40	1.34
52	J	401	NDP	C2D-C3D	2.31	1.59	1.53
56	i	401	CDL	OA6-CA4	-2.31	1.40	1.46
56	N	201	CDL	OA6-CA4	-2.30	1.40	1.46
49	J	403	PLX	C7-C6	2.30	1.55	1.50
48	b	201	PEE	O2-C2	-2.29	1.40	1.46
51	G	201	8Q1	O40-C39	-2.28	1.18	1.23
48	B	303	PEE	O2-C10	2.27	1.40	1.34
48	V	202	PEE	O2-C2	-2.27	1.40	1.46
48	W	201	PEE	O2-C10	2.27	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	w	401	ADP	C5-N7	-2.26	1.34	1.39
47	A	503	NAI	C5B-C4B	2.26	1.58	1.51
51	X	201	8Q1	O35-C34	-2.25	1.18	1.23
51	G	201	8Q1	O35-C34	-2.25	1.18	1.23
51	X	201	8Q1	O40-C39	-2.25	1.18	1.23
50	C	304	DCQ	C6-C5	2.24	1.52	1.46
48	r	501	PEE	O2-C10	2.24	1.40	1.34
56	o	201	CDL	PB2-OB2	2.24	1.68	1.59
56	V	201	CDL	OB6-CB4	-2.23	1.41	1.46
56	V	201	CDL	PB2-OB2	2.23	1.68	1.59
52	J	401	NDP	O7N-C7N	-2.22	1.19	1.24
56	i	401	CDL	PB2-OB2	2.22	1.68	1.59
48	j	201	PEE	O2-C10	2.21	1.40	1.34
48	C	302	PEE	O2-C10	2.20	1.40	1.34
56	r	504	CDL	PB2-OB2	2.20	1.68	1.59
48	s	401	PEE	O2-C10	2.20	1.40	1.34
56	i	401	CDL	PB2-OB5	2.19	1.68	1.59
56	l	701	CDL	PB2-OB5	2.19	1.68	1.59
49	j	202	PLX	P1-O4	2.19	1.68	1.59
56	r	504	CDL	PB2-OB5	2.19	1.68	1.59
56	V	201	CDL	PB2-OB5	2.18	1.68	1.59
56	l	701	CDL	OB6-CB4	-2.18	1.41	1.46
48	r	501	PEE	O3-C3	-2.18	1.40	1.45
56	o	201	CDL	OB6-CB4	-2.18	1.41	1.46
56	N	201	CDL	PB2-OB2	2.17	1.68	1.59
56	s	402	CDL	PB2-OB2	2.17	1.68	1.59
56	n	101	CDL	OB6-CB4	-2.16	1.41	1.46
56	N	201	CDL	PB2-OB5	2.16	1.68	1.59
48	l	702	PEE	O3-C3	-2.16	1.40	1.45
56	o	201	CDL	PB2-OB5	2.16	1.68	1.59
56	n	101	CDL	PB2-OB2	2.16	1.68	1.59
48	W	201	PEE	O3-C3	-2.16	1.40	1.45
50	C	304	DCQ	O4-C4M	-2.15	1.40	1.45
48	B	303	PEE	O3-C3	-2.15	1.40	1.45
56	n	101	CDL	PB2-OB5	2.15	1.68	1.59
56	a	201	CDL	PB2-OB2	2.15	1.68	1.59
48	b	201	PEE	O3-C3	-2.15	1.40	1.45
56	a	201	CDL	OB6-CB4	-2.15	1.41	1.46
56	a	201	CDL	PB2-OB5	2.15	1.68	1.59
56	k	101	CDL	PB2-OB2	2.15	1.68	1.59
56	l	701	CDL	PB2-OB2	2.15	1.68	1.59
56	k	101	CDL	OB6-CB4	-2.15	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	s	402	CDL	OB6-CB4	-2.14	1.41	1.46
56	k	101	CDL	PB2-OB5	2.14	1.68	1.59
49	a	202	PLX	P1-O4	2.14	1.68	1.59
56	k	101	CDL	OA6-CA4	-2.14	1.41	1.46
49	r	502	PLX	P1-O4	2.13	1.67	1.59
48	V	202	PEE	O3-C3	-2.13	1.40	1.45
49	J	403	PLX	P1-O4	2.13	1.67	1.59
53	J	402	UQ	O4-C4	-2.13	1.18	1.23
50	C	304	DCQ	O5-C5	-2.13	1.18	1.23
53	s	403	UQ	O4-C4	-2.13	1.18	1.23
56	i	401	CDL	OB6-CB4	-2.12	1.41	1.46
49	g	201	PLX	P1-O4	2.12	1.67	1.59
48	j	201	PEE	O3-C3	-2.11	1.40	1.45
56	N	201	CDL	OB6-CB4	-2.11	1.41	1.46
50	C	304	DCQ	O3-C3M	-2.10	1.40	1.45
56	s	402	CDL	PB2-OB5	2.10	1.67	1.59
53	s	403	UQ	O1-C1	-2.10	1.18	1.23
51	G	201	8Q1	C6-C1	2.09	1.53	1.50
49	C	303	PLX	P1-O4	2.09	1.67	1.59
49	r	503	PLX	P1-O4	2.08	1.67	1.59
56	r	504	CDL	OB6-CB4	-2.08	1.41	1.46
50	C	304	DCQ	O2-C2	-2.08	1.18	1.23
56	V	201	CDL	C11-CA5	2.06	1.56	1.50
56	V	201	CDL	OA6-CA4	-2.06	1.41	1.46
49	r	502	PLX	P1-O1	2.05	1.67	1.59
49	j	202	PLX	P1-O1	2.05	1.67	1.59
53	s	403	UQ	C21-C19	2.05	1.55	1.51
48	C	302	PEE	O3-C3	-2.05	1.40	1.45
53	J	402	UQ	C21-C19	2.04	1.55	1.51
48	s	401	PEE	O3-C3	-2.04	1.40	1.45
47	A	503	NAI	C5A-N7A	-2.03	1.35	1.39
53	s	403	UQ	O3-CM3	-2.03	1.40	1.45
49	a	202	PLX	C25-C24	2.01	1.55	1.50
52	J	401	NDP	PA-O5B	2.01	1.67	1.59

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	J	401	NDP	C3N-C2N-N1N	-9.38	109.70	123.10
53	s	403	UQ	C7-C8-C9	-8.04	113.41	126.79
53	J	402	UQ	C7-C8-C9	-7.25	114.72	126.79
51	G	201	8Q1	C6-C1-S44	6.29	120.77	113.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	J	402	UQ	C12-C13-C14	-6.19	112.76	127.66
53	J	402	UQ	C17-C18-C19	-6.06	113.07	127.66
52	J	401	NDP	C1D-N1N-C2N	-5.95	111.21	121.11
52	J	401	NDP	C5A-C4A-N3A	-5.92	119.03	126.75
53	s	403	UQ	C12-C13-C14	-5.88	113.51	127.66
53	s	403	UQ	C22-C23-C24	-5.85	113.58	127.66
47	A	503	NAI	C5A-C4A-N3A	-5.83	119.14	126.75
51	X	201	8Q1	C6-C1-S44	5.80	120.20	113.46
53	s	403	UQ	C17-C18-C19	-5.76	113.78	127.66
58	w	401	ADP	C5-C4-N3	-5.72	119.29	126.75
53	J	402	UQ	C10-C9-C8	-4.80	111.36	123.68
52	J	401	NDP	C1D-N1N-C6N	-4.63	110.85	120.83
53	s	403	UQ	C10-C9-C8	-4.60	111.88	123.68
58	w	401	ADP	N3-C2-N1	-4.52	121.53	128.60
53	s	403	UQ	C27-C28-C29	-4.45	112.53	127.75
53	J	402	UQ	C15-C14-C13	-4.43	112.32	123.68
58	w	401	ADP	N3-C4-N9	4.38	134.30	127.08
53	s	403	UQ	C25-C24-C23	-4.33	112.57	123.68
53	J	402	UQ	C16-C14-C13	-4.32	112.38	121.12
47	A	503	NAI	N3A-C2A-N1A	-4.30	121.88	128.60
53	s	403	UQ	C21-C19-C18	-4.22	112.58	121.12
53	J	402	UQ	C11-C9-C8	-4.21	112.60	121.12
52	J	401	NDP	N3A-C4A-N9A	4.17	133.95	127.08
48	s	401	PEE	O2-C10-C11	4.17	120.48	111.50
47	A	503	NAI	N3A-C4A-N9A	4.16	133.94	127.08
53	J	402	UQ	C22-C23-C24	-4.15	113.56	127.75
56	N	201	CDL	OB6-CB5-C51	4.13	120.40	111.50
56	l	701	CDL	OB6-CB5-C51	4.12	120.39	111.50
56	o	201	CDL	OB6-CB5-C51	4.12	120.37	111.50
56	s	402	CDL	OB6-CB5-C51	4.11	120.35	111.50
53	J	402	UQ	C20-C19-C18	-4.08	113.20	123.68
48	r	501	PEE	O2-C10-C11	4.06	120.26	111.50
53	s	403	UQ	C11-C9-C8	-4.05	112.93	121.12
56	a	201	CDL	OB6-CB5-C51	4.05	120.22	111.50
56	i	401	CDL	OA6-CA5-C11	4.04	120.22	111.50
56	n	101	CDL	OB6-CB5-C51	4.04	120.22	111.50
56	i	401	CDL	OB6-CB5-C51	4.04	120.21	111.50
53	s	403	UQ	C20-C19-C18	-4.02	113.36	123.68
56	o	201	CDL	OA6-CA5-C11	4.02	120.16	111.50
56	r	504	CDL	OA6-CA5-C11	4.01	120.15	111.50
48	V	202	PEE	O2-C10-C11	4.01	120.14	111.50
56	r	504	CDL	OB6-CB5-C51	4.01	120.14	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	V	201	CDL	OA6-CA5-C11	4.00	120.12	111.50
56	n	101	CDL	OA6-CA5-C11	3.99	120.11	111.50
52	J	401	NDP	N3A-C2A-N1A	-3.99	122.36	128.60
56	k	101	CDL	OB6-CB5-C51	3.98	120.07	111.50
53	s	403	UQ	C16-C14-C13	-3.97	113.08	121.12
56	V	201	CDL	OB6-CB5-C51	3.97	120.06	111.50
56	s	402	CDL	OA6-CA5-C11	3.97	120.06	111.50
48	b	201	PEE	O2-C10-C11	3.97	120.05	111.50
53	s	403	UQ	C26-C24-C23	-3.97	113.09	121.12
48	C	302	PEE	O2-C10-C11	3.96	120.03	111.50
48	W	201	PEE	O2-C10-C11	3.95	120.02	111.50
53	J	402	UQ	C21-C19-C18	-3.95	113.12	121.12
56	N	201	CDL	OA6-CA5-C11	3.93	119.96	111.50
48	B	303	PEE	O2-C10-C11	3.89	119.89	111.50
47	A	503	NAI	C2A-N3A-C4A	3.87	120.90	111.75
56	l	701	CDL	OA6-CA5-C11	3.86	119.82	111.50
48	j	201	PEE	O2-C10-C11	3.84	119.79	111.50
51	G	201	8Q1	C37-C38-C39	3.84	118.75	112.36
53	s	403	UQ	C15-C14-C13	-3.83	113.85	123.68
58	w	401	ADP	N9-C8-N7	-3.81	108.70	113.91
51	G	201	8Q1	O4-C1-C6	-3.78	119.53	123.99
48	l	702	PEE	O2-C10-C11	3.77	119.62	111.50
56	a	201	CDL	OA6-CA5-C11	3.77	119.62	111.50
58	w	401	ADP	C2-N3-C4	3.75	120.61	111.75
52	J	401	NDP	C2A-N3A-C4A	3.74	120.58	111.75
47	A	503	NAI	C5A-N7A-C8A	3.67	108.72	103.51
58	w	401	ADP	C5-N7-C8	3.62	108.65	103.51
51	X	201	8Q1	O4-C1-C6	-3.61	119.73	123.99
53	s	403	UQ	C31-C29-C28	-3.38	112.89	122.65
47	A	503	NAI	N9A-C8A-N7A	-3.37	109.30	113.91
46	A	502	FMN	C4-N3-C2	-3.35	119.44	125.64
56	k	101	CDL	OA6-CA5-C11	3.35	118.73	111.50
53	s	403	UQ	C30-C29-C28	-3.35	112.98	122.65
53	J	402	UQ	C25-C24-C23	-3.29	113.14	122.65
51	X	201	8Q1	C37-C38-C39	3.26	117.79	112.36
52	J	401	NDP	C5A-N7A-C8A	3.26	108.14	103.51
47	A	503	NAI	C3D-C2D-C1D	3.26	107.61	101.43
58	w	401	ADP	C4-N9-C8	3.21	109.21	105.73
47	A	503	NAI	C4A-C5A-N7A	-3.19	106.73	110.62
52	J	401	NDP	N9A-C8A-N7A	-3.17	109.57	113.91
56	n	101	CDL	OA8-CA7-C31	3.10	119.51	111.38
53	J	402	UQ	C26-C24-C23	-3.09	113.73	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	w	401	ADP	C4'-O4'-C1'	-3.03	102.79	109.47
52	J	401	NDP	C4A-C5A-N7A	-2.98	106.99	110.62
58	w	401	ADP	C4-C5-N7	-2.94	107.04	110.62
48	B	303	PEE	O3-C30-C31	2.84	120.81	111.91
47	A	503	NAI	C2D-C3D-C4D	2.79	108.06	102.64
56	l	701	CDL	OA8-CA7-C31	2.78	120.62	111.91
48	r	501	PEE	O3-C30-C31	2.77	120.61	111.91
46	A	502	FMN	C4A-C4-N3	2.77	120.23	113.19
48	l	702	PEE	O3-C30-C31	2.75	120.53	111.91
53	J	402	UQ	CM5-C5-C6	-2.74	119.93	124.40
48	b	201	PEE	O3-C30-C31	2.74	120.51	111.91
56	V	201	CDL	OB8-CB7-C71	2.73	120.49	111.91
56	k	101	CDL	OA8-CA7-C31	2.73	120.47	111.91
56	i	401	CDL	OA8-CA7-C31	2.72	120.45	111.91
56	a	201	CDL	OB8-CB7-C71	2.71	120.40	111.91
56	r	504	CDL	OB8-CB7-C71	2.68	120.32	111.91
48	C	302	PEE	O3-C30-C31	2.67	120.28	111.91
56	o	201	CDL	OB8-CB7-C71	2.65	120.22	111.91
56	r	504	CDL	OA8-CA7-C31	2.65	120.21	111.91
56	n	101	CDL	OB8-CB7-C71	2.63	120.15	111.91
56	N	201	CDL	OB8-CB7-C71	2.63	120.15	111.91
56	a	201	CDL	OA8-CA7-C31	2.62	120.14	111.91
56	s	402	CDL	OA8-CA7-C31	2.62	120.13	111.91
46	A	502	FMN	O4-C4-C4A	-2.62	119.66	126.60
56	s	402	CDL	OB8-CB7-C71	2.61	120.11	111.91
56	k	101	CDL	OB8-CB7-C71	2.61	120.10	111.91
50	C	304	DCQ	C1M-C1-C6	-2.60	120.15	124.40
56	i	401	CDL	OB8-CB7-C71	2.59	120.03	111.91
56	l	701	CDL	OB8-CB7-C71	2.58	120.01	111.91
48	V	202	PEE	O3-C30-C31	2.57	119.97	111.91
48	W	201	PEE	O3-C30-C31	2.56	119.95	111.91
47	A	503	NAI	C4D-O4D-C1D	-2.56	103.83	109.47
56	N	201	CDL	OA8-CA7-C31	2.55	119.92	111.91
52	J	401	NDP	PN-O3-PA	-2.55	124.08	132.83
47	A	503	NAI	PN-O3-PA	-2.53	124.15	132.83
49	r	502	PLX	C1A-N1-C1	2.53	120.25	109.92
48	j	201	PEE	O3-C30-C31	2.52	119.80	111.91
56	V	201	CDL	OA8-CA7-C31	2.50	119.75	111.91
58	w	401	ADP	PA-O3A-PB	-2.50	124.26	132.83
48	s	401	PEE	O3-C30-C31	2.49	119.73	111.91
51	G	201	8Q1	C43-S44-C1	2.45	109.49	101.87
53	s	403	UQ	CM5-C5-C6	-2.42	120.46	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	o	201	CDL	OA8-CA7-C31	2.40	119.45	111.91
47	A	503	NAI	C4A-N9A-C8A	2.40	108.33	105.73
49	g	201	PLX	C1A-N1-C1	2.39	119.71	109.92
46	A	502	FMN	C4A-C10-N1	-2.39	119.20	124.73
46	A	502	FMN	C4A-C10-N10	2.38	119.97	116.48
52	J	401	NDP	C4A-N9A-C8A	2.35	108.28	105.73
51	X	201	8Q1	C38-C39-N41	2.33	120.34	116.42
51	X	201	8Q1	C43-S44-C1	2.31	109.05	101.87
49	j	202	PLX	C1A-N1-C1	2.30	119.34	109.92
49	C	303	PLX	C1A-N1-C1	2.26	119.14	109.92
49	a	202	PLX	C1A-N1-C1	2.25	119.12	109.92
46	A	502	FMN	C9A-C5A-N5	-2.25	119.99	122.43
51	G	201	8Q1	O4-C1-S44	-2.24	119.70	122.61
52	J	401	NDP	C2B-C1B-N9A	-2.24	109.75	113.53
58	w	401	ADP	O4'-C1'-N9	2.24	112.46	108.06
49	J	403	PLX	C1A-N1-C1	2.22	119.01	109.92
46	A	502	FMN	C10-C4A-N5	-2.18	120.24	124.86
51	G	201	8Q1	C38-C39-N41	2.13	120.01	116.42
46	A	502	FMN	C5A-C9A-N10	2.10	120.12	117.95
49	r	503	PLX	C1A-N1-C1	2.07	118.40	109.92
47	A	503	NAI	C3B-C2B-C1B	2.06	105.33	101.43
51	X	201	8Q1	C32-C34-N36	2.03	120.61	116.58

There are no chirality outliers.

All (1021) 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	C3'-C4'-C5'-O5'
46	A	502	FMN	O4'-C4'-C5'-O5'
46	A	502	FMN	C5'-O5'-P-O2P
46	A	502	FMN	C5'-O5'-P-O3P
47	A	503	NAI	PN-O3-PA-O5B
48	C	302	PEE	C1-O3P-P-O1P
48	V	202	PEE	C18-C19-C20-C21
48	V	202	PEE	C11-C10-O2-C2
48	V	202	PEE	C1-O3P-P-O2P
48	V	202	PEE	C1-O3P-P-O1P
48	V	202	PEE	C1-O3P-P-O4P
48	j	201	PEE	C11-C10-O2-C2
48	j	201	PEE	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
48	l	702	PEE	C11-C10-O2-C2
48	l	702	PEE	C4-O4P-P-O3P
48	r	501	PEE	C1-O3P-P-O2P
48	s	401	PEE	C11-C10-O2-C2
48	s	401	PEE	O4P-C4-C5-N
49	C	303	PLX	O6-C4-C5-O8
49	C	303	PLX	C2-O1-P1-O2
49	C	303	PLX	N1-C1-C2-O1
49	C	303	PLX	O9-C24-O8-C5
49	J	403	PLX	O7-C6-C7-C8
49	J	403	PLX	O7-C6-O6-C4
49	J	403	PLX	C5-C4-O6-C6
49	J	403	PLX	C2-O1-P1-O2
49	a	202	PLX	O7-C6-O6-C4
49	a	202	PLX	O9-C24-C25-C26
49	g	201	PLX	C2-O1-P1-O2
49	g	201	PLX	C2-O1-P1-O3
49	g	201	PLX	C25-C24-O8-C5
49	j	202	PLX	O7-C6-C7-C8
49	j	202	PLX	O7-C6-O6-C4
49	j	202	PLX	C3-O4-P1-O2
49	j	202	PLX	C25-C24-O8-C5
49	j	202	PLX	O9-C24-C25-C26
49	r	502	PLX	O7-C6-C7-C8
49	r	502	PLX	C5-C4-O6-C6
49	r	502	PLX	C3-O4-P1-O2
49	r	502	PLX	C2-O1-P1-O2
49	r	502	PLX	C2-O1-P1-O3
49	r	502	PLX	O9-C24-C25-C26
49	r	503	PLX	O7-C6-O6-C4
49	r	503	PLX	C5-C4-O6-C6
49	r	503	PLX	C3-O4-P1-O2
49	r	503	PLX	O9-C24-O8-C5
49	r	503	PLX	O9-C24-C25-C26
51	G	201	8Q1	O4-C1-S44-C43
51	G	201	8Q1	C6-C1-S44-C43
51	G	201	8Q1	N41-C42-C43-S44
51	G	201	8Q1	C28-O27-P24-O3
51	G	201	8Q1	C28-O27-P24-O2
51	G	201	8Q1	C28-O27-P24-O1
51	X	201	8Q1	C42-C43-S44-C1
52	J	401	NDP	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
52	J	401	NDP	O4D-C1D-N1N-C6N
53	J	402	UQ	C7-C8-C9-C11
53	J	402	UQ	C12-C13-C14-C15
53	J	402	UQ	C12-C13-C14-C16
53	J	402	UQ	C14-C16-C17-C18
53	J	402	UQ	C16-C17-C18-C19
53	J	402	UQ	C17-C18-C19-C20
53	J	402	UQ	C17-C18-C19-C21
53	J	402	UQ	C22-C23-C24-C25
53	s	403	UQ	C7-C8-C9-C10
53	s	403	UQ	C7-C8-C9-C11
53	s	403	UQ	C12-C13-C14-C16
53	s	403	UQ	C18-C19-C21-C22
53	s	403	UQ	C22-C23-C24-C26
56	N	201	CDL	CA2-OA2-PA1-OA4
56	N	201	CDL	OA5-CA3-CA4-OA6
56	N	201	CDL	CB2-OB2-PB2-OB3
56	N	201	CDL	CB3-OB5-PB2-OB3
56	V	201	CDL	CA3-OA5-PA1-OA3
56	V	201	CDL	CA3-OA5-PA1-OA4
56	V	201	CDL	C11-CA5-OA6-CA4
56	V	201	CDL	CB2-OB2-PB2-OB3
56	V	201	CDL	CB2-OB2-PB2-OB4
56	V	201	CDL	CB3-OB5-PB2-OB3
56	V	201	CDL	CB3-OB5-PB2-OB4
56	a	201	CDL	CA2-OA2-PA1-OA3
56	a	201	CDL	CA2-OA2-PA1-OA4
56	a	201	CDL	CB2-OB2-PB2-OB3
56	a	201	CDL	CB2-OB2-PB2-OB4
56	a	201	CDL	CB3-OB5-PB2-OB2
56	a	201	CDL	CB3-OB5-PB2-OB3
56	a	201	CDL	CB3-OB5-PB2-OB4
56	i	401	CDL	CB2-C1-CA2-OA2
56	i	401	CDL	CA2-OA2-PA1-OA3
56	i	401	CDL	CA3-OA5-PA1-OA2
56	i	401	CDL	CA3-OA5-PA1-OA3
56	i	401	CDL	CA3-OA5-PA1-OA4
56	i	401	CDL	OA9-CA7-OA8-CA6
56	i	401	CDL	C31-CA7-OA8-CA6
56	i	401	CDL	CB3-OB5-PB2-OB3
56	i	401	CDL	OB6-CB4-CB6-OB8
56	k	101	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
56	k	101	CDL	CB2-OB2-PB2-OB4
56	l	701	CDL	CA2-C1-CB2-OB2
56	l	701	CDL	OA5-CA3-CA4-OA6
56	l	701	CDL	OA9-CA7-OA8-CA6
56	l	701	CDL	C31-CA7-OA8-CA6
56	l	701	CDL	CB2-OB2-PB2-OB3
56	l	701	CDL	CB2-OB2-PB2-OB4
56	l	701	CDL	CB2-OB2-PB2-OB5
56	l	701	CDL	CB3-OB5-PB2-OB3
56	l	701	CDL	CB3-OB5-PB2-OB4
56	n	101	CDL	O1-C1-CA2-OA2
56	n	101	CDL	CB2-C1-CA2-OA2
56	n	101	CDL	CA2-OA2-PA1-OA4
56	n	101	CDL	OA6-CA4-CA6-OA8
56	n	101	CDL	CB2-OB2-PB2-OB3
56	o	201	CDL	CB2-OB2-PB2-OB3
56	o	201	CDL	CB3-OB5-PB2-OB3
56	o	201	CDL	C51-CB5-OB6-CB4
56	r	504	CDL	O1-C1-CA2-OA2
56	r	504	CDL	CA2-OA2-PA1-OA3
56	r	504	CDL	CA3-OA5-PA1-OA2
56	r	504	CDL	CA3-OA5-PA1-OA3
56	r	504	CDL	CB2-OB2-PB2-OB3
56	r	504	CDL	CB2-OB2-PB2-OB4
56	r	504	CDL	CB2-OB2-PB2-OB5
56	r	504	CDL	CB3-OB5-PB2-OB3
56	r	504	CDL	CB3-OB5-PB2-OB4
56	s	402	CDL	OA9-CA7-OA8-CA6
56	s	402	CDL	C31-CA7-OA8-CA6
56	s	402	CDL	C51-CB5-OB6-CB4
58	w	401	ADP	C5'-O5'-PA-O3A
58	w	401	ADP	O4'-C4'-C5'-O5'
48	V	202	PEE	O4-C10-O2-C2
48	b	201	PEE	O4-C10-O2-C2
48	j	201	PEE	O4-C10-O2-C2
48	l	702	PEE	O4-C10-O2-C2
48	s	401	PEE	O4-C10-O2-C2
56	V	201	CDL	OA7-CA5-OA6-CA4
56	o	201	CDL	OB7-CB5-OB6-CB4
56	s	402	CDL	OB7-CB5-OB6-CB4
50	C	304	DCQ	C6-C7-C8-C9
48	l	702	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
48	b	201	PEE	C11-C10-O2-C2
53	J	402	UQ	C12-C11-C9-C8
48	V	202	PEE	C17-C18-C19-C20
48	W	201	PEE	C17-C18-C19-C20
48	j	201	PEE	C17-C18-C19-C20
49	r	502	PLX	C11-C12-C13-C14
53	s	403	UQ	C17-C18-C19-C21
48	l	702	PEE	O5-C30-O3-C3
56	N	201	CDL	O1-C1-CA2-OA2
56	i	401	CDL	O1-C1-CA2-OA2
56	i	401	CDL	O1-C1-CB2-OB2
56	k	101	CDL	O1-C1-CB2-OB2
56	l	701	CDL	O1-C1-CA2-OA2
56	l	701	CDL	O1-C1-CB2-OB2
56	n	101	CDL	O1-C1-CB2-OB2
56	V	201	CDL	C31-CA7-OA8-CA6
56	V	201	CDL	C71-CB7-OB8-CB6
56	a	201	CDL	C51-CB5-OB6-CB4
56	r	504	CDL	C51-CB5-OB6-CB4
49	j	202	PLX	C13-C14-C15-C16
53	s	403	UQ	C27-C28-C29-C31
56	V	201	CDL	OA9-CA7-OA8-CA6
49	g	201	PLX	C9-C10-C11-C12
49	g	201	PLX	C7-C8-C9-C10
49	j	202	PLX	C28-C29-C30-C31
49	r	502	PLX	C9-C10-C11-C12
49	r	502	PLX	C7-C8-C9-C10
56	V	201	CDL	C32-C33-C34-C35
56	o	201	CDL	C33-C34-C35-C36
56	k	101	CDL	C60-C61-C62-C63
58	w	401	ADP	C3'-C4'-C5'-O5'
56	r	504	CDL	OB7-CB5-OB6-CB4
56	k	101	CDL	C62-C63-C64-C65
56	n	101	CDL	C55-C56-C57-C58
56	o	201	CDL	C17-C18-C19-C20
53	J	402	UQ	C13-C14-C16-C17
56	V	201	CDL	OB9-CB7-OB8-CB6
56	V	201	CDL	C62-C63-C64-C65
53	J	402	UQ	C22-C23-C24-C26
48	B	303	PEE	C11-C12-C13-C14
48	l	702	PEE	C33-C34-C35-C36
56	l	701	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
56	l	701	CDL	CB2-C1-CA2-OA2
56	n	101	CDL	CA2-C1-CB2-OB2
56	s	402	CDL	CA2-C1-CB2-OB2
48	r	501	PEE	C41-C42-C43-C44
48	j	201	PEE	C31-C30-O3-C3
56	l	701	CDL	C58-C59-C60-C61
56	V	201	CDL	C59-C60-C61-C62
48	l	702	PEE	O3P-C1-C2-O2
56	s	402	CDL	OA5-CA3-CA4-OA6
56	r	504	CDL	C74-C75-C76-C77
56	s	402	CDL	O1-C1-CB2-OB2
56	a	201	CDL	CB5-C51-C52-C53
56	l	701	CDL	OA6-CA4-CA6-OA8
56	N	201	CDL	CB5-C51-C52-C53
56	l	701	CDL	CB5-C51-C52-C53
56	i	401	CDL	CB7-C71-C72-C73
56	k	101	CDL	CA7-C31-C32-C33
49	J	403	PLX	C9-C10-C11-C12
48	l	702	PEE	C30-C31-C32-C33
56	N	201	CDL	CA7-C31-C32-C33
56	V	201	CDL	CB7-C71-C72-C73
56	n	101	CDL	CB5-C51-C52-C53
56	o	201	CDL	CB7-C71-C72-C73
48	b	201	PEE	C31-C30-O3-C3
48	W	201	PEE	C11-C12-C13-C14
56	a	201	CDL	C36-C37-C38-C39
56	a	201	CDL	OB7-CB5-OB6-CB4
49	g	201	PLX	C2-C1-N1-C1A
53	s	403	UQ	C14-C16-C17-C18
56	l	701	CDL	C34-C35-C36-C37
56	a	201	CDL	CB7-C71-C72-C73
56	a	201	CDL	O1-C1-CA2-OA2
56	k	101	CDL	O1-C1-CA2-OA2
56	o	201	CDL	O1-C1-CB2-OB2
48	j	201	PEE	O5-C30-O3-C3
48	B	303	PEE	C11-C10-O2-C2
56	k	101	CDL	C11-CA5-OA6-CA4
48	B	303	PEE	C1-O3P-P-O4P
48	C	302	PEE	C1-O3P-P-O4P
48	V	202	PEE	C4-O4P-P-O3P
48	j	201	PEE	C1-O3P-P-O4P
48	r	501	PEE	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
49	J	403	PLX	C2-O1-P1-O4
49	a	202	PLX	C3-O4-P1-O1
49	g	201	PLX	C2-O1-P1-O4
49	j	202	PLX	C3-O4-P1-O1
49	r	502	PLX	C2-O1-P1-O4
49	r	503	PLX	C3-O4-P1-O1
56	N	201	CDL	CA2-OA2-PA1-OA5
56	N	201	CDL	CA3-OA5-PA1-OA2
56	N	201	CDL	CB2-OB2-PB2-OB5
56	N	201	CDL	CB3-OB5-PB2-OB2
56	V	201	CDL	CA3-OA5-PA1-OA2
56	V	201	CDL	CB2-OB2-PB2-OB5
56	V	201	CDL	CB3-OB5-PB2-OB2
56	a	201	CDL	CA2-OA2-PA1-OA5
56	a	201	CDL	CB2-OB2-PB2-OB5
56	i	401	CDL	CA2-OA2-PA1-OA5
56	i	401	CDL	CB3-OB5-PB2-OB2
56	k	101	CDL	CA2-OA2-PA1-OA5
56	k	101	CDL	CA3-OA5-PA1-OA2
56	k	101	CDL	CB2-OB2-PB2-OB5
56	l	701	CDL	CB3-OB5-PB2-OB2
56	n	101	CDL	CA2-OA2-PA1-OA5
56	o	201	CDL	CA2-OA2-PA1-OA5
56	o	201	CDL	CB2-OB2-PB2-OB5
56	o	201	CDL	CB3-OB5-PB2-OB2
56	r	504	CDL	CB3-OB5-PB2-OB2
56	s	402	CDL	CB2-OB2-PB2-OB5
48	W	201	PEE	C31-C30-O3-C3
56	V	201	CDL	CA5-C11-C12-C13
56	N	201	CDL	CB2-C1-CA2-OA2
56	a	201	CDL	CB2-C1-CA2-OA2
56	i	401	CDL	CA2-C1-CB2-OB2
56	k	101	CDL	CB2-C1-CA2-OA2
56	o	201	CDL	CA2-C1-CB2-OB2
56	r	504	CDL	CB2-C1-CA2-OA2
48	B	303	PEE	O4-C10-O2-C2
56	k	101	CDL	OA7-CA5-OA6-CA4
49	g	201	PLX	C2-C1-N1-C1B
49	g	201	PLX	O6-C6-C7-C8
49	r	502	PLX	O6-C6-C7-C8
56	o	201	CDL	C37-C38-C39-C40
56	N	201	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
49	a	202	PLX	C17-C18-C19-C20
47	A	503	NAI	C3D-C4D-C5D-O5D
48	r	501	PEE	C11-C12-C13-C14
48	s	401	PEE	C14-C15-C16-C17
49	J	403	PLX	C12-C13-C14-C15
49	r	502	PLX	C11-C10-C9-C8
49	r	503	PLX	C25-C26-C27-C28
56	a	201	CDL	C35-C36-C37-C38
56	i	401	CDL	C76-C77-C78-C79
56	k	101	CDL	C55-C56-C57-C58
56	k	101	CDL	C75-C76-C77-C78
56	l	701	CDL	C71-C72-C73-C74
56	n	101	CDL	C52-C53-C54-C55
56	n	101	CDL	C54-C55-C56-C57
56	o	201	CDL	C59-C60-C61-C62
56	r	504	CDL	C53-C54-C55-C56
56	o	201	CDL	C31-CA7-OA8-CA6
48	B	303	PEE	C42-C43-C44-C45
48	C	302	PEE	C34-C35-C36-C37
48	W	201	PEE	C13-C14-C15-C16
49	a	202	PLX	C7-C8-C9-C10
49	g	201	PLX	C32-C33-C34-C35
49	j	202	PLX	C12-C13-C14-C15
49	r	502	PLX	C27-C28-C29-C30
51	X	201	8Q1	C11-C10-C9-C8
56	i	401	CDL	C55-C56-C57-C58
56	k	101	CDL	C14-C15-C16-C17
56	l	701	CDL	C52-C53-C54-C55
56	s	402	CDL	C82-C83-C84-C85
56	i	401	CDL	CA7-C31-C32-C33
56	l	701	CDL	CA5-C11-C12-C13
48	C	302	PEE	C41-C42-C43-C44
49	C	303	PLX	C14-C15-C16-C17
49	j	202	PLX	C25-C26-C27-C28
56	k	101	CDL	C59-C60-C61-C62
56	l	701	CDL	C62-C63-C64-C65
56	o	201	CDL	C13-C14-C15-C16
49	a	202	PLX	C9-C10-C11-C12
49	r	503	PLX	C13-C14-C15-C16
56	k	101	CDL	C17-C18-C19-C20
56	r	504	CDL	C59-C60-C61-C62
56	s	402	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
48	r	501	PEE	C31-C32-C33-C34
48	s	401	PEE	C23-C24-C25-C26
49	C	303	PLX	C9-C10-C11-C12
56	o	201	CDL	C34-C35-C36-C37
48	V	202	PEE	C30-C31-C32-C33
56	i	401	CDL	CA5-C11-C12-C13
56	l	701	CDL	CB7-C71-C72-C73
48	B	303	PEE	C20-C21-C22-C23
49	g	201	PLX	C33-C34-C35-C36
50	C	304	DCQ	C7-C8-C9-C10
56	V	201	CDL	C52-C53-C54-C55
56	k	101	CDL	C56-C57-C58-C59
56	l	701	CDL	C75-C76-C77-C78
56	s	402	CDL	C17-C18-C19-C20
48	b	201	PEE	O5-C30-O3-C3
49	C	303	PLX	C10-C11-C12-C13
56	a	201	CDL	C62-C63-C64-C65
56	k	101	CDL	C73-C74-C75-C76
56	l	701	CDL	C11-C12-C13-C14
56	o	201	CDL	C73-C74-C75-C76
56	r	504	CDL	C37-C38-C39-C40
56	r	504	CDL	C43-C44-C45-C46
56	r	504	CDL	C55-C56-C57-C58
56	o	201	CDL	CA7-C31-C32-C33
49	J	403	PLX	C10-C11-C12-C13
56	l	701	CDL	C56-C57-C58-C59
56	r	504	CDL	C62-C63-C64-C65
49	a	202	PLX	C14-C15-C16-C17
49	a	202	PLX	C27-C28-C29-C30
49	a	202	PLX	C31-C32-C33-C34
49	j	202	PLX	C33-C34-C35-C36
56	a	201	CDL	C18-C19-C20-C21
56	i	401	CDL	C37-C38-C39-C40
56	i	401	CDL	C59-C60-C61-C62
48	s	401	PEE	C11-C12-C13-C14
49	a	202	PLX	C12-C13-C14-C15
49	g	201	PLX	C13-C14-C15-C16
56	a	201	CDL	C60-C61-C62-C63
56	k	101	CDL	C51-C52-C53-C54
56	k	101	CDL	C71-C72-C73-C74
56	r	504	CDL	C41-C42-C43-C44
56	s	402	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
56	s	402	CDL	C38-C39-C40-C41
56	s	402	CDL	C71-C72-C73-C74
56	k	101	CDL	CB5-C51-C52-C53
56	s	402	CDL	CB7-C71-C72-C73
48	C	302	PEE	C11-C12-C13-C14
49	C	303	PLX	C11-C12-C13-C14
49	C	303	PLX	C27-C28-C29-C30
49	J	403	PLX	C34-C35-C36-C37
49	j	202	PLX	C14-C15-C16-C17
49	r	502	PLX	C30-C31-C32-C33
56	N	201	CDL	C11-C12-C13-C14
56	V	201	CDL	C55-C56-C57-C58
56	k	101	CDL	C39-C40-C41-C42
56	l	701	CDL	C37-C38-C39-C40
56	r	504	CDL	C33-C34-C35-C36
56	r	504	CDL	C75-C76-C77-C78
56	r	504	CDL	C77-C78-C79-C80
56	s	402	CDL	C52-C53-C54-C55
49	C	303	PLX	C17-C18-C19-C20
56	V	201	CDL	C12-C13-C14-C15
56	l	701	CDL	C31-C32-C33-C34
56	n	101	CDL	C51-C52-C53-C54
48	b	201	PEE	C32-C33-C34-C35
49	J	403	PLX	C28-C29-C30-C31
49	g	201	PLX	C12-C13-C14-C15
56	k	101	CDL	C19-C20-C21-C22
56	k	101	CDL	C81-C82-C83-C84
56	o	201	CDL	C83-C84-C85-C86
49	g	201	PLX	C25-C26-C27-C28
49	j	202	PLX	C10-C11-C12-C13
56	a	201	CDL	C21-C22-C23-C24
56	l	701	CDL	C35-C36-C37-C38
56	l	701	CDL	C71-CB7-OB8-CB6
49	j	202	PLX	C11-C12-C13-C14
49	j	202	PLX	C27-C28-C29-C30
49	r	502	PLX	C28-C29-C30-C31
56	i	401	CDL	C14-C15-C16-C17
56	s	402	CDL	C34-C35-C36-C37
49	g	201	PLX	C27-C28-C29-C30
49	g	201	PLX	C30-C31-C32-C33
49	r	502	PLX	C31-C32-C33-C34
56	l	701	CDL	C59-C60-C61-C62

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Mol	Chain	Res	Type	Atoms
56	r	504	CDL	CB5-C51-C52-C53
48	V	202	PEE	C32-C33-C34-C35
49	g	201	PLX	C11-C12-C13-C14
56	i	401	CDL	C73-C74-C75-C76
56	k	101	CDL	C78-C79-C80-C81
56	r	504	CDL	C71-C72-C73-C74
48	b	201	PEE	C12-C13-C14-C15
49	J	403	PLX	C33-C34-C35-C36
56	a	201	CDL	C32-C33-C34-C35
48	W	201	PEE	C10-C11-C12-C13
51	G	201	8Q1	C12-C13-C14-C15
56	o	201	CDL	C55-C56-C57-C58
56	s	402	CDL	C37-C38-C39-C40
48	r	501	PEE	C11-C10-O2-C2
56	V	201	CDL	C73-C74-C75-C76
56	k	101	CDL	C52-C53-C54-C55
49	g	201	PLX	O7-C6-C7-C8
49	g	201	PLX	O9-C24-C25-C26
56	n	101	CDL	C74-C75-C76-C77
56	r	504	CDL	C34-C35-C36-C37
56	s	402	CDL	C35-C36-C37-C38
48	s	401	PEE	C15-C16-C17-C18
48	W	201	PEE	O5-C30-O3-C3
49	j	202	PLX	C9-C10-C11-C12
56	N	201	CDL	O1-C1-CB2-OB2
49	r	503	PLX	C29-C30-C31-C32
49	j	202	PLX	C15-C16-C17-C18
56	l	701	CDL	C14-C15-C16-C17
56	l	701	CDL	C51-C52-C53-C54
48	r	501	PEE	O4-C10-O2-C2
49	C	303	PLX	C33-C34-C35-C36
56	i	401	CDL	C77-C78-C79-C80
56	n	101	CDL	C75-C76-C77-C78
56	o	201	CDL	OA9-CA7-OA8-CA6
49	g	201	PLX	C28-C29-C30-C31
49	r	503	PLX	C11-C10-C9-C8
56	k	101	CDL	C37-C38-C39-C40
49	g	201	PLX	C2-C1-N1-C1C
56	o	201	CDL	C60-C61-C62-C63
56	s	402	CDL	C75-C76-C77-C78
48	B	303	PEE	C31-C30-O3-C3
56	N	201	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
56	N	201	CDL	C51-CB5-OB6-CB4
49	a	202	PLX	C13-C14-C15-C16
56	V	201	CDL	C53-C54-C55-C56
48	B	303	PEE	C12-C13-C14-C15
48	b	201	PEE	C14-C15-C16-C17
49	J	403	PLX	C27-C28-C29-C30
56	l	701	CDL	OB9-CB7-OB8-CB6
56	i	401	CDL	C71-C72-C73-C74
48	C	302	PEE	C35-C36-C37-C38
56	V	201	CDL	OB7-CB5-OB6-CB4
56	k	101	CDL	OB7-CB5-OB6-CB4
56	k	101	CDL	C71-CB7-OB8-CB6
56	o	201	CDL	C71-CB7-OB8-CB6
49	g	201	PLX	C10-C11-C12-C13
49	j	202	PLX	C34-C35-C36-C37
51	X	201	8Q1	C12-C13-C14-C15
56	a	201	CDL	C38-C39-C40-C41
56	k	101	CDL	C64-C65-C66-C67
48	W	201	PEE	C22-C23-C24-C25
48	l	702	PEE	C40-C41-C42-C43
56	o	201	CDL	C56-C57-C58-C59
56	o	201	CDL	C62-C63-C64-C65
49	j	202	PLX	C29-C30-C31-C32
49	r	503	PLX	C17-C18-C19-C20
56	r	504	CDL	C81-C82-C83-C84
56	V	201	CDL	C57-C58-C59-C60
56	V	201	CDL	C76-C77-C78-C79
49	r	502	PLX	C13-C14-C15-C16
49	r	503	PLX	C28-C29-C30-C31
56	s	402	CDL	C19-C20-C21-C22
51	X	201	8Q1	C10-C11-C12-C13
56	N	201	CDL	C51-C52-C53-C54
48	C	302	PEE	C11-C10-O2-C2
56	V	201	CDL	C51-CB5-OB6-CB4
56	a	201	CDL	C11-CA5-OA6-CA4
56	k	101	CDL	C51-CB5-OB6-CB4
56	s	402	CDL	C11-CA5-OA6-CA4
56	V	201	CDL	OB5-CB3-CB4-OB6
48	l	702	PEE	C21-C22-C23-C24
49	J	403	PLX	C7-C8-C9-C10
49	r	502	PLX	C14-C15-C16-C17
56	k	101	CDL	C76-C77-C78-C79

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Mol	Chain	Res	Type	Atoms
56	N	201	CDL	OB7-CB5-OB6-CB4
56	s	402	CDL	OA7-CA5-OA6-CA4
56	k	101	CDL	OB6-CB4-CB6-OB8
56	a	201	CDL	C75-C76-C77-C78
56	n	101	CDL	C72-C73-C74-C75
56	r	504	CDL	C36-C37-C38-C39
56	l	701	CDL	C73-C74-C75-C76
56	r	504	CDL	C82-C83-C84-C85
48	C	302	PEE	C19-C20-C21-C22
48	r	501	PEE	C39-C40-C41-C42
48	W	201	PEE	C12-C13-C14-C15
49	r	503	PLX	C27-C28-C29-C30
56	i	401	CDL	C81-C82-C83-C84
47	A	503	NAI	O4B-C4B-C5B-O5B
49	j	202	PLX	C7-C8-C9-C10
49	r	502	PLX	C25-C26-C27-C28
49	C	303	PLX	C28-C29-C30-C31
48	B	303	PEE	O5-C30-O3-C3
56	k	101	CDL	OB9-CB7-OB8-CB6
56	a	201	CDL	OA7-CA5-OA6-CA4
48	B	303	PEE	C36-C37-C38-C39
48	b	201	PEE	C1-O3P-P-O4P
49	C	303	PLX	C2-O1-P1-O4
49	r	502	PLX	C3-O4-P1-O1
56	o	201	CDL	CA3-OA5-PA1-OA2
48	B	303	PEE	C34-C35-C36-C37
56	a	201	CDL	C11-C12-C13-C14
56	N	201	CDL	OA9-CA7-OA8-CA6
49	J	403	PLX	O4-C3-C4-C5
56	N	201	CDL	OA5-CA3-CA4-CA6
56	a	201	CDL	OB5-CB3-CB4-CB6
56	s	402	CDL	OA5-CA3-CA4-CA6
49	g	201	PLX	C14-C15-C16-C17
56	l	701	CDL	C16-C17-C18-C19
56	r	504	CDL	C84-C85-C86-C87
56	s	402	CDL	C55-C56-C57-C58
56	n	101	CDL	CB7-C71-C72-C73
49	C	303	PLX	C13-C14-C15-C16
56	k	101	CDL	C82-C83-C84-C85
56	r	504	CDL	C83-C84-C85-C86
49	j	202	PLX	C30-C31-C32-C33
56	a	201	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
48	l	702	PEE	C13-C14-C15-C16
56	a	201	CDL	C52-C53-C54-C55
56	i	401	CDL	C62-C63-C64-C65
56	k	101	CDL	C15-C16-C17-C18
56	r	504	CDL	C35-C36-C37-C38
49	J	403	PLX	C30-C31-C32-C33
56	a	201	CDL	C31-C32-C33-C34
56	k	101	CDL	C43-C44-C45-C46
56	o	201	CDL	OB9-CB7-OB8-CB6
49	a	202	PLX	C11-C12-C13-C14
48	W	201	PEE	C1-C2-C3-O3
48	b	201	PEE	C1-C2-C3-O3
49	C	303	PLX	C3-C4-C5-O8
49	g	201	PLX	C3-C4-C5-O8
56	i	401	CDL	CA3-CA4-CA6-OA8
56	i	401	CDL	CB3-CB4-CB6-OB8
56	k	101	CDL	CB3-CB4-CB6-OB8
56	l	701	CDL	C18-C19-C20-C21
56	l	701	CDL	C32-C33-C34-C35
56	s	402	CDL	CB3-CB4-CB6-OB8
56	N	201	CDL	C52-C53-C54-C55
56	s	402	CDL	C12-C13-C14-C15
48	V	202	PEE	C10-C11-C12-C13
56	r	504	CDL	CA5-C11-C12-C13
49	r	503	PLX	C7-C8-C9-C10
56	o	201	CDL	C19-C20-C21-C22
56	r	504	CDL	C13-C14-C15-C16
49	J	403	PLX	O6-C6-C7-C8
48	s	401	PEE	C31-C30-O3-C3
48	j	201	PEE	C36-C37-C38-C39
48	r	501	PEE	C14-C15-C16-C17
49	J	403	PLX	C36-C37-C38-C39
49	a	202	PLX	C16-C17-C18-C19
49	a	202	PLX	C25-C26-C27-C28
56	i	401	CDL	C52-C53-C54-C55
56	s	402	CDL	C15-C16-C17-C18
48	B	303	PEE	C23-C24-C25-C26
49	J	403	PLX	C14-C15-C16-C17
52	J	401	NDP	O4D-C4D-C5D-O5D
56	V	201	CDL	C75-C76-C77-C78
48	r	501	PEE	C10-C11-C12-C13
56	s	402	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
56	k	101	CDL	CA6-CA4-OA6-CA5
56	a	201	CDL	C55-C56-C57-C58
56	r	504	CDL	C14-C15-C16-C17
56	s	402	CDL	C18-C19-C20-C21
49	r	503	PLX	C11-C12-C13-C14
56	V	201	CDL	C14-C15-C16-C17
56	r	504	CDL	C15-C16-C17-C18
46	A	502	FMN	C5'-O5'-P-O1P
56	i	401	CDL	C71-CB7-OB8-CB6
56	r	504	CDL	C71-CB7-OB8-CB6
49	J	403	PLX	O4-C3-C4-O6
56	k	101	CDL	OA5-CA3-CA4-OA6
56	l	701	CDL	OB5-CB3-CB4-OB6
48	r	501	PEE	C17-C18-C19-C20
56	a	201	CDL	OB9-CB7-OB8-CB6
48	l	702	PEE	C32-C33-C34-C35
49	g	201	PLX	O6-C4-C5-O8
56	a	201	CDL	C37-C38-C39-C40
56	a	201	CDL	C84-C85-C86-C87
56	r	504	CDL	C32-C33-C34-C35
48	C	302	PEE	O4-C10-O2-C2
48	s	401	PEE	O5-C30-O3-C3
56	V	201	CDL	C43-C44-C45-C46
56	i	401	CDL	C64-C65-C66-C67
48	l	702	PEE	C31-C32-C33-C34
49	j	202	PLX	C17-C18-C19-C20
56	l	701	CDL	C72-C73-C74-C75
48	j	201	PEE	C41-C42-C43-C44
49	r	503	PLX	C31-C32-C33-C34
52	J	401	NDP	PN-O3-PA-O1A
49	r	502	PLX	C12-C13-C14-C15
56	i	401	CDL	OB9-CB7-OB8-CB6
56	s	402	CDL	OB9-CB7-OB8-CB6
56	V	201	CDL	C33-C34-C35-C36
56	l	701	CDL	C81-C82-C83-C84
56	n	101	CDL	C56-C57-C58-C59
48	b	201	PEE	C37-C38-C39-C40
48	r	501	PEE	C42-C43-C44-C45
47	A	503	NAI	C3B-C4B-C5B-O5B
48	C	302	PEE	O3P-C1-C2-C3
48	l	702	PEE	O3P-C1-C2-C3
56	N	201	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
56	V	201	CDL	OB5-CB3-CB4-CB6
56	l	701	CDL	OA5-CA3-CA4-CA6
56	n	101	CDL	OA5-CA3-CA4-CA6
53	J	402	UQ	C19-C21-C22-C23
48	W	201	PEE	O4P-C4-C5-N
48	j	201	PEE	C40-C41-C42-C43
56	V	201	CDL	C35-C36-C37-C38
56	a	201	CDL	C31-CA7-OA8-CA6
48	b	201	PEE	C13-C14-C15-C16
53	s	403	UQ	C23-C24-C26-C27
56	s	402	CDL	CB5-C51-C52-C53
48	B	303	PEE	C33-C34-C35-C36
48	b	201	PEE	C31-C32-C33-C34
49	C	303	PLX	C16-C17-C18-C19
49	j	202	PLX	C16-C17-C18-C19
56	s	402	CDL	C54-C55-C56-C57
56	o	201	CDL	C12-C13-C14-C15
56	o	201	CDL	C57-C58-C59-C60
48	r	501	PEE	C36-C37-C38-C39
56	k	101	CDL	C84-C85-C86-C87
51	X	201	8Q1	C13-C14-C15-C16
56	k	101	CDL	C54-C55-C56-C57
56	l	701	CDL	C42-C43-C44-C45
49	J	403	PLX	C13-C14-C15-C16
56	a	201	CDL	C73-C74-C75-C76
48	V	202	PEE	C1-C2-C3-O3
48	s	401	PEE	C1-C2-C3-O3
49	r	502	PLX	C3-C4-C5-O8
49	r	503	PLX	C3-C4-C5-O8
56	V	201	CDL	CA3-CA4-CA6-OA8
56	l	701	CDL	CA3-CA4-CA6-OA8
56	n	101	CDL	CA3-CA4-CA6-OA8
56	o	201	CDL	CB3-CB4-CB6-OB8
56	r	504	CDL	CB3-CB4-CB6-OB8
49	r	503	PLX	C10-C11-C12-C13
56	i	401	CDL	C35-C36-C37-C38
48	B	303	PEE	C17-C18-C19-C20
56	a	201	CDL	C44-C45-C46-C47
48	j	201	PEE	C21-C22-C23-C24
56	i	401	CDL	C74-C75-C76-C77
48	C	302	PEE	C20-C21-C22-C23
56	k	101	CDL	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
49	a	202	PLX	C5-C4-O6-C6
56	n	101	CDL	CB2-OB2-PB2-OB5
56	r	504	CDL	CA2-OA2-PA1-OA5
48	r	501	PEE	C40-C41-C42-C43
49	C	303	PLX	O7-C6-C7-C8
56	k	101	CDL	C31-C32-C33-C34
56	N	201	CDL	OB5-CB3-CB4-OB6
48	V	202	PEE	C31-C30-O3-C3
56	r	504	CDL	OB9-CB7-OB8-CB6
49	r	502	PLX	C16-C17-C18-C19
56	V	201	CDL	C51-C52-C53-C54
56	o	201	CDL	C84-C85-C86-C87
56	V	201	CDL	C64-C65-C66-C67
47	A	503	NAI	O4D-C4D-C5D-O5D
56	V	201	CDL	C34-C35-C36-C37
48	b	201	PEE	O2-C2-C3-O3
48	s	401	PEE	O2-C2-C3-O3
49	r	503	PLX	O6-C4-C5-O8
56	o	201	CDL	OB6-CB4-CB6-OB8
56	r	504	CDL	OB6-CB4-CB6-OB8
56	s	402	CDL	OB6-CB4-CB6-OB8
48	B	303	PEE	C38-C39-C40-C41
49	C	303	PLX	C25-C26-C27-C28
49	C	303	PLX	C26-C27-C28-C29
56	k	101	CDL	C13-C14-C15-C16
56	k	101	CDL	CA2-C1-CB2-OB2
56	o	201	CDL	CB2-C1-CA2-OA2
48	C	302	PEE	C12-C13-C14-C15
56	l	701	CDL	C44-C45-C46-C47
56	n	101	CDL	C73-C74-C75-C76
56	V	201	CDL	C1-CB2-OB2-PB2
56	i	401	CDL	C1-CB2-OB2-PB2
56	k	101	CDL	C16-C17-C18-C19
56	k	101	CDL	C79-C80-C81-C82
56	r	504	CDL	C64-C65-C66-C67
51	X	201	8Q1	O4-C1-S44-C43
49	j	202	PLX	C18-C19-C20-C21
48	B	303	PEE	C21-C22-C23-C24
48	l	702	PEE	C44-C45-C46-C47
56	l	701	CDL	C40-C41-C42-C43
56	r	504	CDL	C73-C74-C75-C76
48	s	401	PEE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
49	g	201	PLX	O8-C24-C25-C26
49	r	502	PLX	O8-C24-C25-C26
56	n	101	CDL	C71-C72-C73-C74
56	i	401	CDL	OB5-CB3-CB4-CB6
56	k	101	CDL	OA5-CA3-CA4-CA6
56	l	701	CDL	OB5-CB3-CB4-CB6
56	V	201	CDL	O1-C1-CB2-OB2
56	o	201	CDL	C32-C33-C34-C35
49	r	503	PLX	C26-C27-C28-C29
48	s	401	PEE	C19-C20-C21-C22
48	s	401	PEE	C12-C13-C14-C15
48	B	303	PEE	C31-C32-C33-C34
49	a	202	PLX	C15-C16-C17-C18
49	a	202	PLX	C30-C31-C32-C33
56	o	201	CDL	C18-C19-C20-C21
51	X	201	8Q1	C6-C1-S44-C43
56	V	201	CDL	CA6-CA4-OA6-CA5
56	i	401	CDL	C51-C52-C53-C54
56	k	101	CDL	C18-C19-C20-C21
56	k	101	CDL	C11-C12-C13-C14
56	r	504	CDL	C58-C59-C60-C61
48	B	303	PEE	C15-C16-C17-C18
48	C	302	PEE	C1-C2-C3-O3
49	a	202	PLX	C3-C4-C5-O8
49	j	202	PLX	C7-C6-O6-C4
56	N	201	CDL	CA3-CA4-CA6-OA8
56	k	101	CDL	CA4-CA3-OA5-PA1
56	r	504	CDL	C1-CB2-OB2-PB2
56	a	201	CDL	OA9-CA7-OA8-CA6
48	C	302	PEE	O3P-C1-C2-O2
48	r	501	PEE	O3P-C1-C2-O2
56	i	401	CDL	OB5-CB3-CB4-OB6
56	o	201	CDL	OA5-CA3-CA4-OA6
48	W	201	PEE	C21-C22-C23-C24
56	r	504	CDL	C17-C18-C19-C20
49	J	403	PLX	C24-C25-C26-C27
52	J	401	NDP	C2D-C1D-N1N-C2N
48	l	702	PEE	C24-C25-C26-C27
56	l	701	CDL	CA7-C31-C32-C33
49	r	502	PLX	O6-C4-C5-O8
56	V	201	CDL	OA6-CA4-CA6-OA8
56	s	402	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
48	b	201	PEE	C20-C21-C22-C23
48	C	302	PEE	C32-C33-C34-C35
56	r	504	CDL	C56-C57-C58-C59
56	l	701	CDL	C51-CB5-OB6-CB4
56	n	101	CDL	C53-C54-C55-C56
48	V	202	PEE	O5-C30-O3-C3
48	r	501	PEE	C33-C34-C35-C36
56	a	201	CDL	C34-C35-C36-C37
56	r	504	CDL	C72-C71-CB7-OB8
48	C	302	PEE	C44-C45-C46-C47
48	r	501	PEE	C24-C25-C26-C27
56	s	402	CDL	C84-C85-C86-C87
48	r	501	PEE	C30-C31-C32-C33
56	o	201	CDL	C75-C76-C77-C78
56	s	402	CDL	C59-C60-C61-C62
49	a	202	PLX	C24-C25-C26-C27
49	r	503	PLX	C24-C25-C26-C27
48	j	201	PEE	C4-O4P-P-O3P
56	V	201	CDL	CA2-OA2-PA1-OA5
56	l	701	CDL	CA2-OA2-PA1-OA5
56	s	402	CDL	CB3-OB5-PB2-OB2
48	j	201	PEE	C34-C35-C36-C37
56	r	504	CDL	C51-C52-C53-C54
48	B	303	PEE	C1-O3P-P-O2P
48	B	303	PEE	C1-O3P-P-O1P
48	B	303	PEE	C4-O4P-P-O1P
48	C	302	PEE	C1-O3P-P-O2P
48	V	202	PEE	C4-O4P-P-O1P
48	b	201	PEE	C1-O3P-P-O1P
48	j	201	PEE	C1-O3P-P-O2P
48	l	702	PEE	C4-O4P-P-O2P
48	r	501	PEE	C1-O3P-P-O1P
48	s	401	PEE	C4-O4P-P-O1P
49	C	303	PLX	C2-O1-P1-O3
49	J	403	PLX	C3-O4-P1-O2
49	J	403	PLX	C2-O1-P1-O3
49	a	202	PLX	C3-O4-P1-O2
49	a	202	PLX	C3-O4-P1-O3
49	j	202	PLX	C3-O4-P1-O3
49	r	503	PLX	C3-O4-P1-O3
56	N	201	CDL	CA3-OA5-PA1-OA3
56	N	201	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
56	N	201	CDL	CB2-OB2-PB2-OB4
56	N	201	CDL	CB3-OB5-PB2-OB4
56	i	401	CDL	CB3-OB5-PB2-OB4
56	k	101	CDL	CA2-OA2-PA1-OA3
56	k	101	CDL	CA2-OA2-PA1-OA4
56	k	101	CDL	CA3-OA5-PA1-OA4
56	l	701	CDL	CA2-OA2-PA1-OA3
56	n	101	CDL	CB2-OB2-PB2-OB4
56	o	201	CDL	CA2-OA2-PA1-OA4
56	o	201	CDL	CA3-OA5-PA1-OA3
56	o	201	CDL	CA3-OA5-PA1-OA4
56	o	201	CDL	CB2-OB2-PB2-OB4
56	o	201	CDL	CB3-OB5-PB2-OB4
56	r	504	CDL	CA2-OA2-PA1-OA4
56	s	402	CDL	CB2-OB2-PB2-OB3
56	s	402	CDL	CB2-OB2-PB2-OB4
58	w	401	ADP	C5'-O5'-PA-O2A
49	r	503	PLX	O4-C3-C4-C5
56	V	201	CDL	C15-C16-C17-C18
56	V	201	CDL	C42-C43-C44-C45
56	r	504	CDL	C11-C12-C13-C14
49	J	403	PLX	C25-C24-O8-C5
49	a	202	PLX	C25-C24-O8-C5
49	J	403	PLX	C31-C32-C33-C34
48	B	303	PEE	C30-C31-C32-C33
53	s	403	UQ	C12-C11-C9-C10
49	r	503	PLX	O4-C3-C4-O6
56	a	201	CDL	OB5-CB3-CB4-OB6
56	n	101	CDL	OA5-CA3-CA4-OA6
56	o	201	CDL	C64-C65-C66-C67
49	j	202	PLX	C35-C36-C37-C38
56	o	201	CDL	O1-C1-CA2-OA2
56	s	402	CDL	C14-C15-C16-C17
56	s	402	CDL	C40-C41-C42-C43
48	l	702	PEE	C1-C2-C3-O3
48	r	501	PEE	C1-C2-C3-O3
49	J	403	PLX	N1-C1-C2-O1
56	s	402	CDL	CA3-CA4-CA6-OA8
56	l	701	CDL	OB7-CB5-OB6-CB4
48	V	202	PEE	O2-C2-C3-O3
48	W	201	PEE	O2-C2-C3-O3
48	l	702	PEE	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
48	r	501	PEE	O2-C2-C3-O3
49	j	202	PLX	O6-C4-C5-O8
56	i	401	CDL	OA6-CA4-CA6-OA8
48	C	302	PEE	C16-C17-C18-C19
56	l	701	CDL	C77-C78-C79-C80
56	i	401	CDL	C34-C35-C36-C37
49	r	503	PLX	O8-C24-C25-C26
48	r	501	PEE	C13-C14-C15-C16
56	V	201	CDL	C44-C45-C46-C47
56	l	701	CDL	C54-C55-C56-C57
49	r	503	PLX	C16-C17-C18-C19
48	s	401	PEE	C21-C22-C23-C24
49	g	201	PLX	C36-C37-C38-C39
48	B	303	PEE	C44-C45-C46-C47
49	r	503	PLX	C35-C36-C37-C38
56	o	201	CDL	C51-C52-C53-C54
53	s	403	UQ	C13-C14-C16-C17
49	a	202	PLX	C33-C34-C35-C36
48	b	201	PEE	C34-C35-C36-C37
56	V	201	CDL	C31-C32-C33-C34
56	a	201	CDL	C76-C77-C78-C79
48	l	702	PEE	C1-C2-O2-C10
56	o	201	CDL	OA5-CA3-CA4-CA6
56	l	701	CDL	C24-C25-C26-C27
49	j	202	PLX	C31-C32-C33-C34
56	o	201	CDL	C1-CB2-OB2-PB2
48	j	201	PEE	C37-C38-C39-C40
49	J	403	PLX	C11-C12-C13-C14
53	J	402	UQ	C12-C11-C9-C10
48	W	201	PEE	O4-C10-O2-C2
56	i	401	CDL	C75-C76-C77-C78
48	s	401	PEE	C33-C34-C35-C36
49	C	303	PLX	C18-C19-C20-C21
49	r	503	PLX	C12-C13-C14-C15
49	C	303	PLX	C3-O4-P1-O1
49	J	403	PLX	C3-O4-P1-O1
49	a	202	PLX	C2-O1-P1-O4
49	r	503	PLX	C2-O1-P1-O4
47	A	503	NAI	C2D-C1D-N1N-C2N
52	J	401	NDP	C3D-C4D-C5D-O5D
56	V	201	CDL	C18-C19-C20-C21
48	l	702	PEE	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
47	A	503	NAI	O4D-C1D-N1N-C2N
56	k	101	CDL	C57-C58-C59-C60
56	k	101	CDL	C58-C59-C60-C61
56	l	701	CDL	C82-C83-C84-C85
56	s	402	CDL	C77-C78-C79-C80
56	s	402	CDL	C56-C57-C58-C59
56	V	201	CDL	CA4-CA3-OA5-PA1
56	r	504	CDL	CB4-CB3-OB5-PB2
48	l	702	PEE	C37-C38-C39-C40
56	s	402	CDL	C80-C81-C82-C83
56	V	201	CDL	CA7-C31-C32-C33
48	b	201	PEE	C16-C17-C18-C19
48	j	201	PEE	C38-C39-C40-C41
48	r	501	PEE	C38-C39-C40-C41
52	J	401	NDP	O4B-C4B-C5B-O5B
49	j	202	PLX	C24-C25-C26-C27
56	l	701	CDL	C23-C24-C25-C26
48	W	201	PEE	C11-C10-O2-C2
56	o	201	CDL	OB5-CB3-CB4-OB6
49	C	303	PLX	C11-C10-C9-C8
56	i	401	CDL	C13-C14-C15-C16
51	X	201	8Q1	C11-C12-C13-C14
48	B	303	PEE	C13-C14-C15-C16
48	b	201	PEE	C39-C40-C41-C42
49	g	201	PLX	C11-C10-C9-C8
49	j	202	PLX	O6-C6-C7-C8
48	b	201	PEE	C2-C1-O3P-P
48	s	401	PEE	C16-C17-C18-C19
56	r	504	CDL	C54-C55-C56-C57
56	s	402	CDL	C39-C40-C41-C42
48	j	201	PEE	C30-C31-C32-C33
48	j	201	PEE	C19-C20-C21-C22
49	J	403	PLX	C19-C20-C21-C22
56	l	701	CDL	C36-C37-C38-C39
49	C	303	PLX	C24-C25-C26-C27
49	J	403	PLX	C6-C7-C8-C9
49	j	202	PLX	C3-C4-C5-O8
48	b	201	PEE	C18-C19-C20-C21
53	J	402	UQ	C7-C8-C9-C10
56	o	201	CDL	C39-C40-C41-C42
56	r	504	CDL	C78-C79-C80-C81
56	i	401	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
49	r	503	PLX	C30-C31-C32-C33
48	l	702	PEE	C20-C21-C22-C23
56	V	201	CDL	C38-C39-C40-C41
56	r	504	CDL	C52-C53-C54-C55
56	i	401	CDL	CA4-CA3-OA5-PA1
53	s	403	UQ	C6-C7-C8-C9
56	k	101	CDL	C44-C45-C46-C47
56	a	201	CDL	C82-C83-C84-C85
51	G	201	8Q1	C42-C43-S44-C1
48	C	302	PEE	O2-C2-C3-O3
52	J	401	NDP	O4D-C1D-N1N-C2N
56	V	201	CDL	CA2-C1-CB2-OB2
48	C	302	PEE	C38-C39-C40-C41
56	l	701	CDL	C21-C22-C23-C24
56	l	701	CDL	C80-C81-C82-C83
56	l	701	CDL	C84-C85-C86-C87
56	a	201	CDL	C64-C65-C66-C67
48	V	202	PEE	C2-C1-O3P-P
56	l	701	CDL	C39-C40-C41-C42
56	a	201	CDL	C20-C21-C22-C23
56	r	504	CDL	C76-C77-C78-C79
56	o	201	CDL	C32-C31-CA7-OA8
56	V	201	CDL	C56-C57-C58-C59
56	i	401	CDL	C36-C37-C38-C39
53	s	403	UQ	C22-C23-C24-C25
49	a	202	PLX	C4-C5-O8-C24
49	j	202	PLX	C4-C5-O8-C24
53	J	402	UQ	C5-C6-C7-C8
48	V	202	PEE	C38-C39-C40-C41
49	a	202	PLX	C10-C11-C12-C13
49	j	202	PLX	O8-C24-C25-C26
48	V	202	PEE	O4P-C4-C5-N
56	l	701	CDL	C74-C75-C76-C77
51	G	201	8Q1	C10-C11-C12-C13
49	C	303	PLX	C12-C13-C14-C15
56	n	101	CDL	CA5-C11-C12-C13
56	N	201	CDL	OA6-CA4-CA6-OA8
48	C	302	PEE	C42-C43-C44-C45
56	o	201	CDL	C82-C83-C84-C85
48	V	202	PEE	C16-C17-C18-C19
56	a	201	CDL	C77-C78-C79-C80
56	k	101	CDL	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
56	a	201	CDL	CA5-C11-C12-C13
56	k	101	CDL	C36-C37-C38-C39
53	J	402	UQ	C1-C6-C7-C8
49	C	303	PLX	C31-C32-C33-C34
56	l	701	CDL	C20-C21-C22-C23
56	k	101	CDL	C52-C51-CB5-OB6
48	l	702	PEE	C16-C17-C18-C19
48	l	702	PEE	C36-C37-C38-C39
48	s	401	PEE	C18-C19-C20-C21
48	l	702	PEE	C3-C2-O2-C10
56	r	504	CDL	C60-C61-C62-C63
48	j	201	PEE	C12-C13-C14-C15
56	o	201	CDL	C38-C39-C40-C41
50	C	304	DCQ	C2-C3-O3-C3M
48	C	302	PEE	C15-C16-C17-C18
48	W	201	PEE	C15-C16-C17-C18
56	s	402	CDL	C74-C75-C76-C77
56	V	201	CDL	C78-C79-C80-C81
49	g	201	PLX	C6-C7-C8-C9
48	s	401	PEE	C32-C33-C34-C35
49	r	502	PLX	C33-C34-C35-C36
56	r	504	CDL	C12-C13-C14-C15
48	r	501	PEE	O3P-C1-C2-C3
56	a	201	CDL	C32-C31-CA7-OA8
48	l	702	PEE	C38-C39-C40-C41
48	r	501	PEE	C16-C17-C18-C19
56	i	401	CDL	C54-C55-C56-C57
49	C	303	PLX	O9-C24-C25-C26
49	J	403	PLX	O9-C24-C25-C26
56	o	201	CDL	C78-C79-C80-C81
48	B	303	PEE	C16-C17-C18-C19
48	W	201	PEE	C16-C17-C18-C19
48	r	501	PEE	C18-C19-C20-C21
48	b	201	PEE	C30-C31-C32-C33
56	a	201	CDL	C15-C16-C17-C18
56	N	201	CDL	C12-C11-CA5-OA6
56	s	402	CDL	C12-C11-CA5-OA6
49	r	503	PLX	C32-C33-C34-C35
48	B	303	PEE	C18-C19-C20-C21
56	a	201	CDL	C83-C84-C85-C86
56	o	201	CDL	C15-C16-C17-C18
56	N	201	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
56	l	701	CDL	C72-C71-CB7-OB8
56	V	201	CDL	C36-C37-C38-C39
48	B	303	PEE	C39-C40-C41-C42
48	B	303	PEE	C22-C23-C24-C25
47	A	503	NAI	C2N-C3N-C7N-N7N
48	C	302	PEE	C4-O4P-P-O2P
48	W	201	PEE	C4-O4P-P-O1P
48	b	201	PEE	C1-O3P-P-O2P
48	j	201	PEE	C4-O4P-P-O1P
48	l	702	PEE	C1-O3P-P-O1P
52	J	401	NDP	C2N-C3N-C7N-N7N
56	k	101	CDL	CB3-OB5-PB2-OB3
56	n	101	CDL	CA2-OA2-PA1-OA3
56	n	101	CDL	CA3-OA5-PA1-OA3
56	s	402	CDL	CA2-OA2-PA1-OA3
56	o	201	CDL	OB5-CB3-CB4-CB6
56	r	504	CDL	C80-C81-C82-C83
56	s	402	CDL	C12-C11-CA5-OA7
56	a	201	CDL	C12-C11-CA5-OA6
56	r	504	CDL	OA7-CA5-OA6-CA4
56	a	201	CDL	C72-C73-C74-C75
56	N	201	CDL	C12-C11-CA5-OA7
48	s	401	PEE	C5-C4-O4P-P
56	s	402	CDL	CA6-CA4-OA6-CA5
56	V	201	CDL	C58-C59-C60-C61
47	A	503	NAI	C2D-C1D-N1N-C6N
48	C	302	PEE	O3-C30-C31-C32
56	a	201	CDL	C72-C71-CB7-OB8
48	j	201	PEE	C24-C25-C26-C27
56	V	201	CDL	C19-C20-C21-C22
48	r	501	PEE	O2-C10-C11-C12
56	N	201	CDL	C52-C51-CB5-OB6
56	a	201	CDL	C32-C31-CA7-OA9
48	l	702	PEE	C10-C11-C12-C13
56	N	201	CDL	C72-C71-CB7-OB9
56	l	701	CDL	C72-C71-CB7-OB9
56	o	201	CDL	C76-C77-C78-C79
48	b	201	PEE	O2-C10-C11-C12
56	V	201	CDL	C12-C11-CA5-OA6
56	i	401	CDL	C12-C11-CA5-OA6

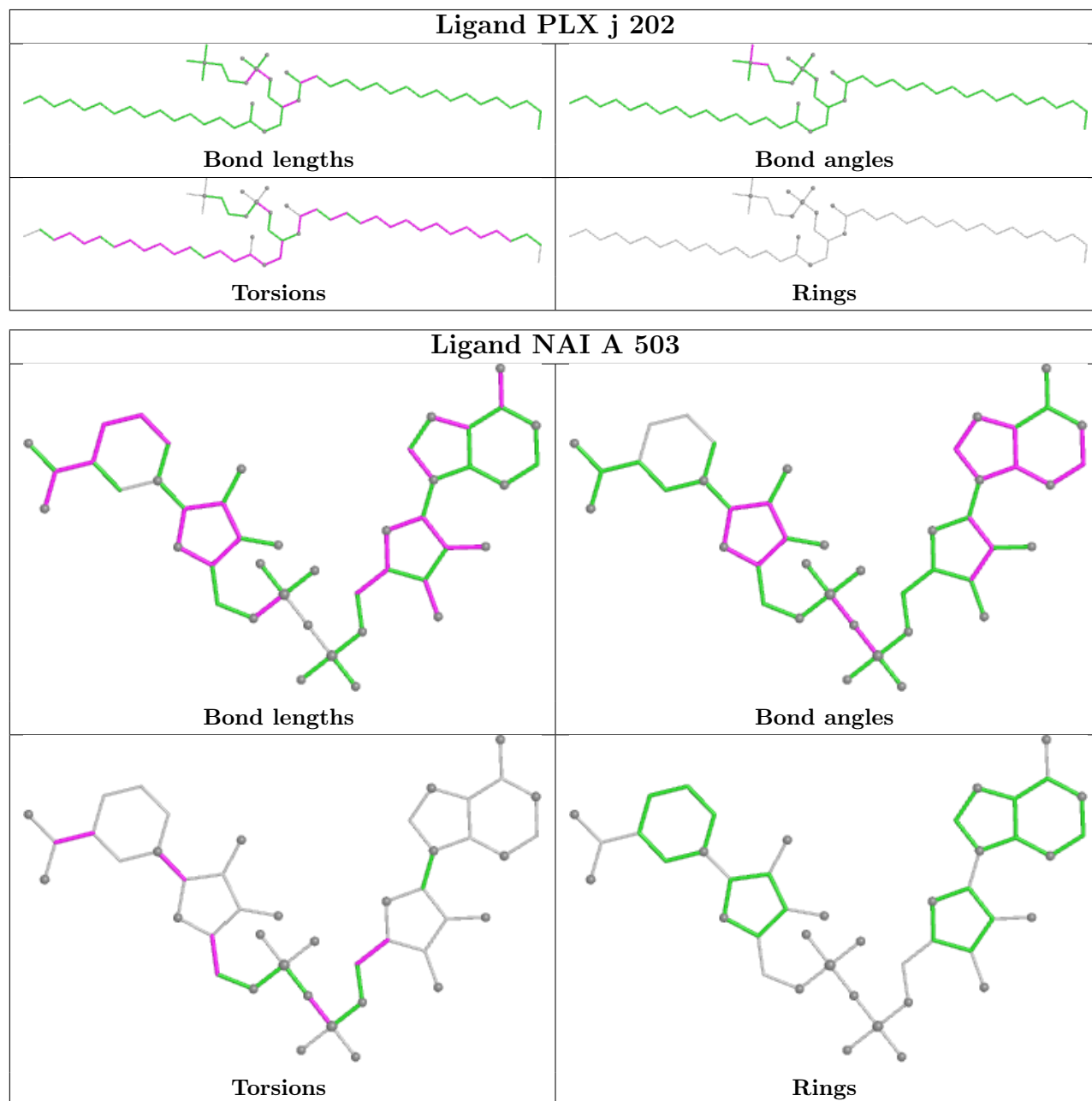
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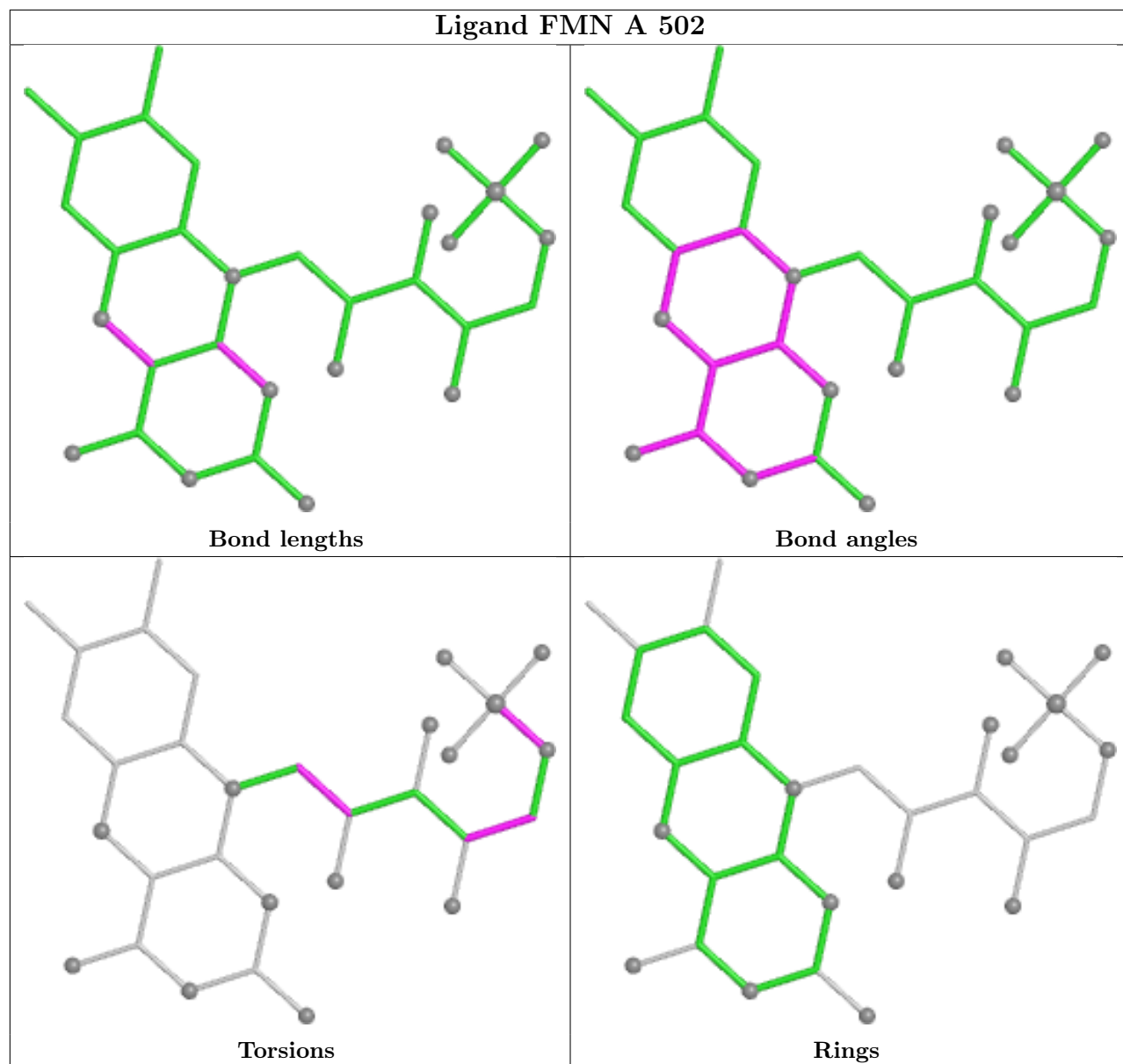
34 monomers are involved in 135 short contacts:

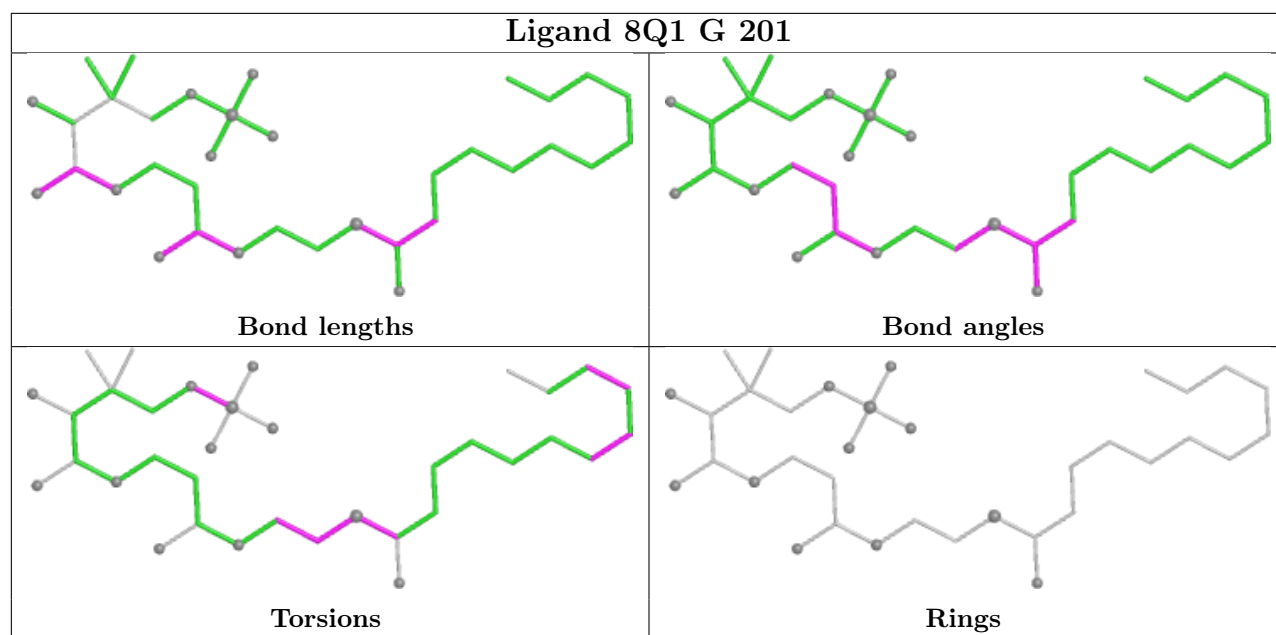
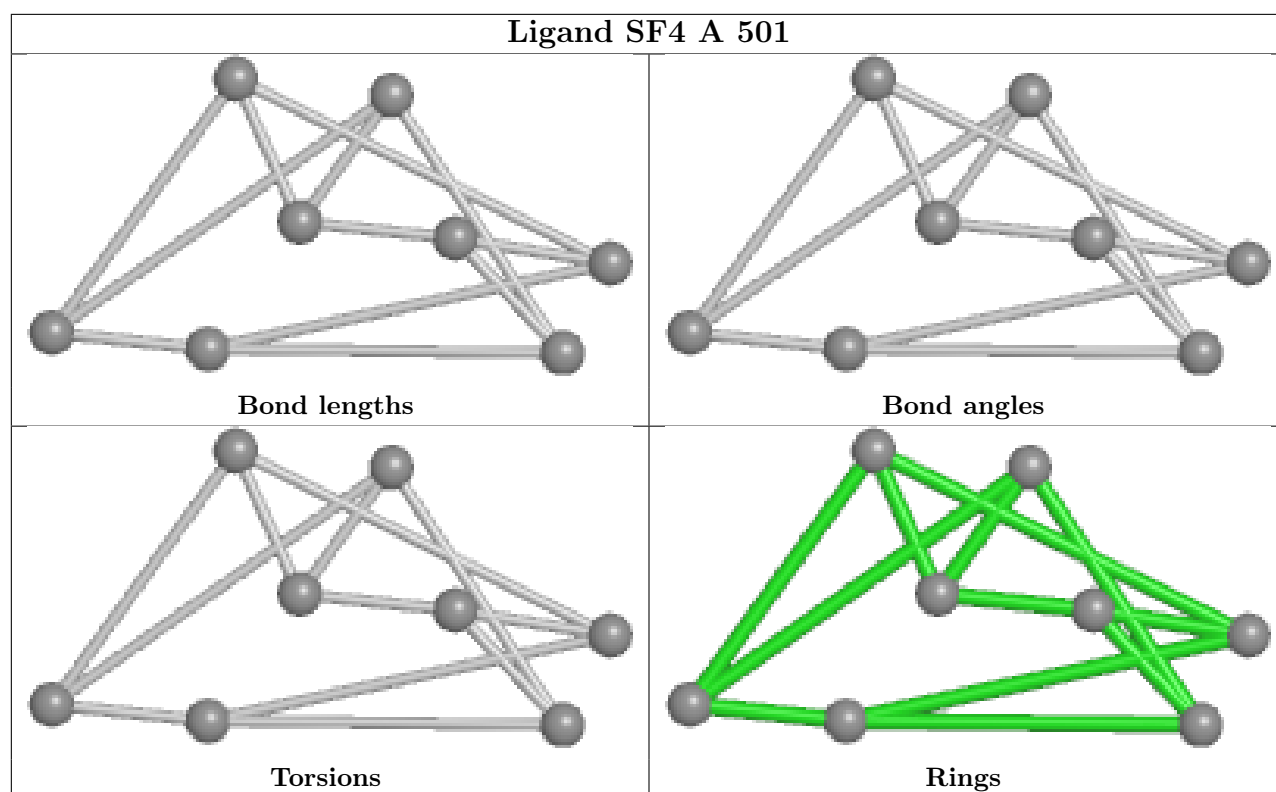
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	j	202	PLX	2	0
47	A	503	NAI	5	0
46	A	502	FMN	6	0
45	A	501	SF4	1	0
48	V	202	PEE	3	0
52	J	401	NDP	3	0
50	C	304	DCQ	3	0
56	n	101	CDL	2	0
49	g	201	PLX	8	0
48	B	303	PEE	2	0
56	o	201	CDL	7	0
48	s	401	PEE	3	0
49	J	403	PLX	1	0
45	C	301	SF4	2	0
48	C	302	PEE	1	0
48	l	702	PEE	3	0
56	i	401	CDL	3	0
56	V	201	CDL	8	0
49	a	202	PLX	3	0
49	r	502	PLX	6	0
56	r	504	CDL	7	0
58	w	401	ADP	2	0
53	J	402	UQ	3	0
48	W	201	PEE	2	0
56	a	201	CDL	8	0
56	l	701	CDL	13	0
48	b	201	PEE	4	0
48	r	501	PEE	2	0
49	C	303	PLX	2	0
56	k	101	CDL	4	0
49	r	503	PLX	2	0
48	j	201	PEE	6	0
53	s	403	UQ	5	0
56	s	402	CDL	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

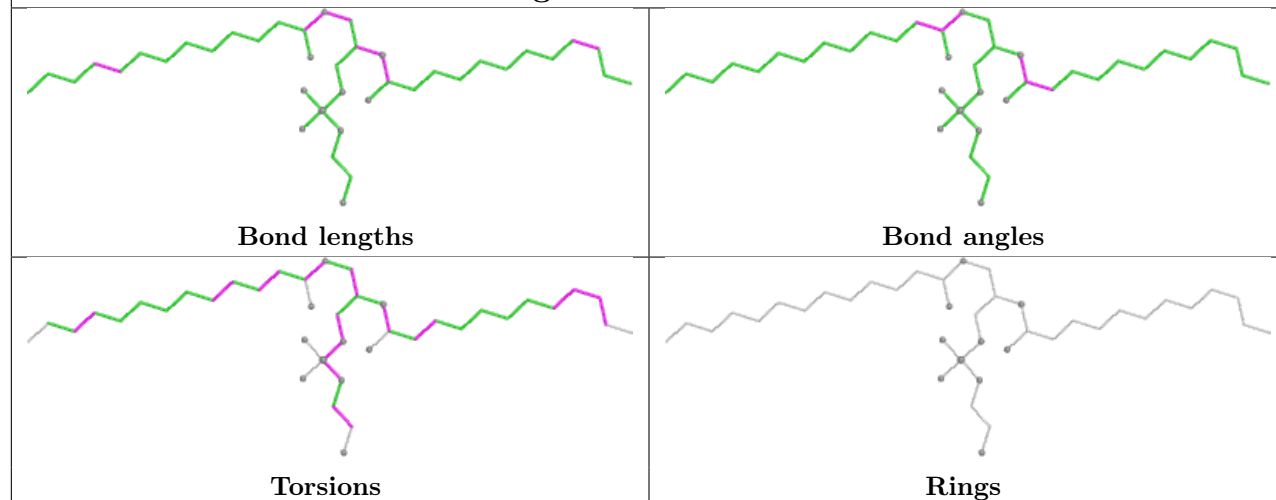
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



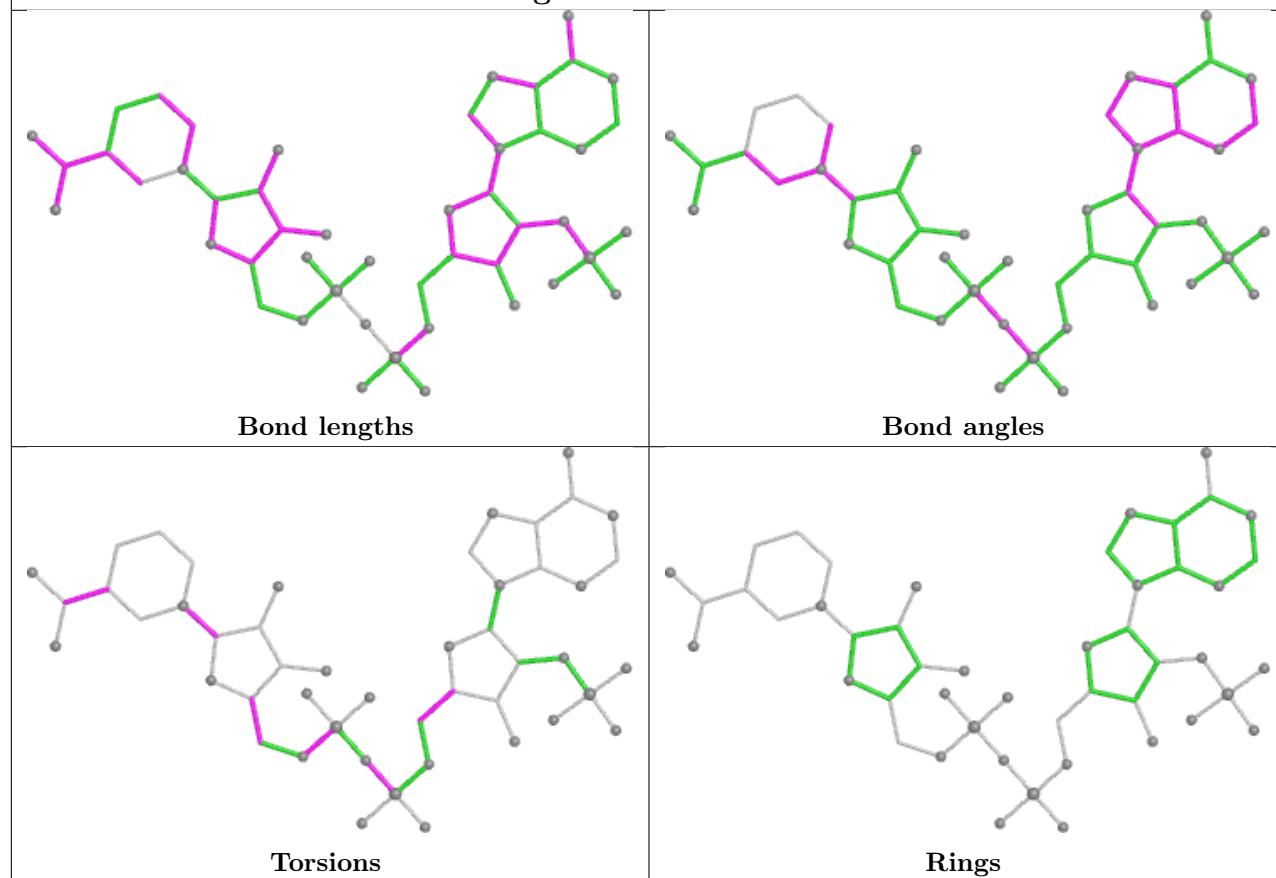


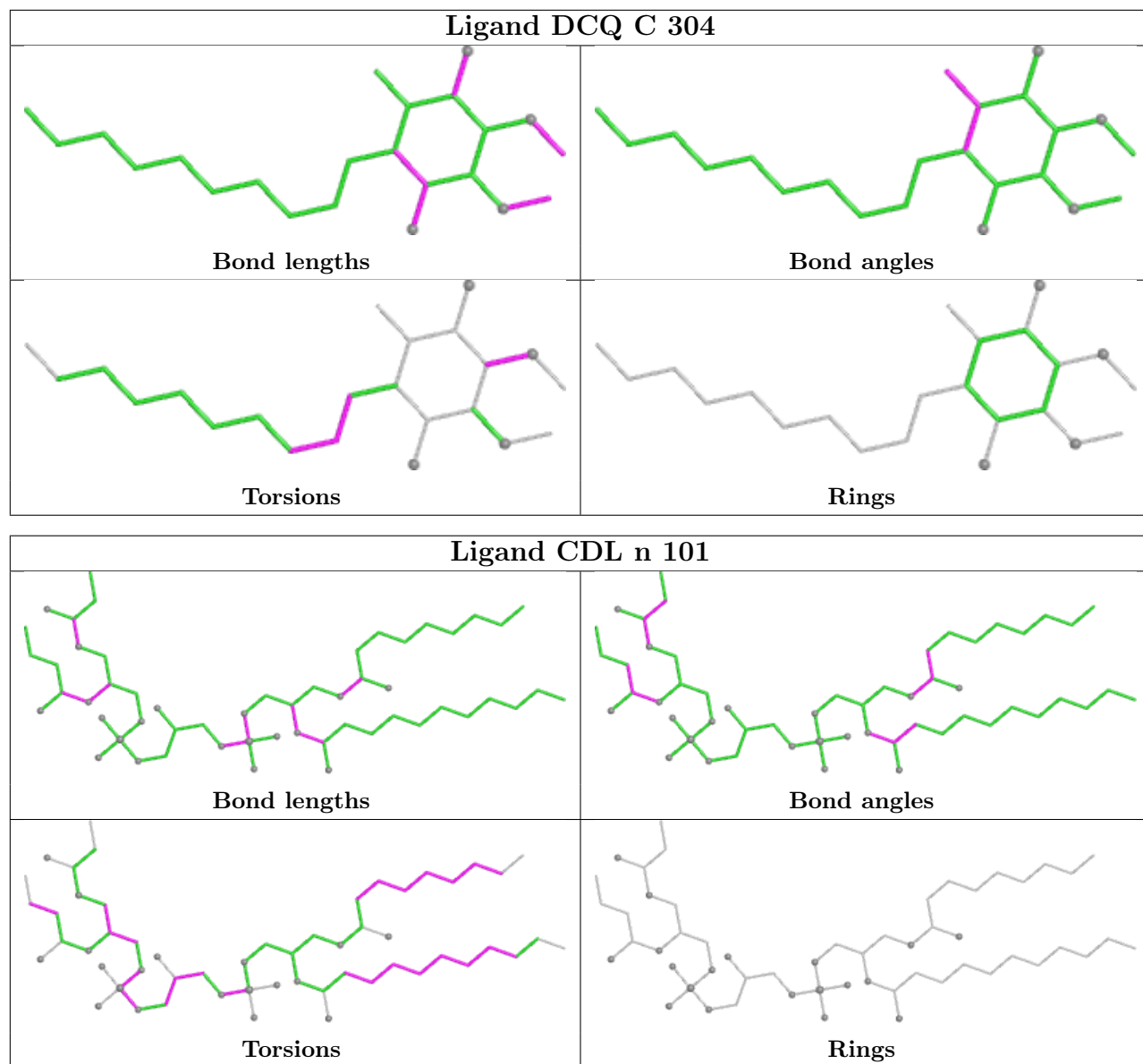


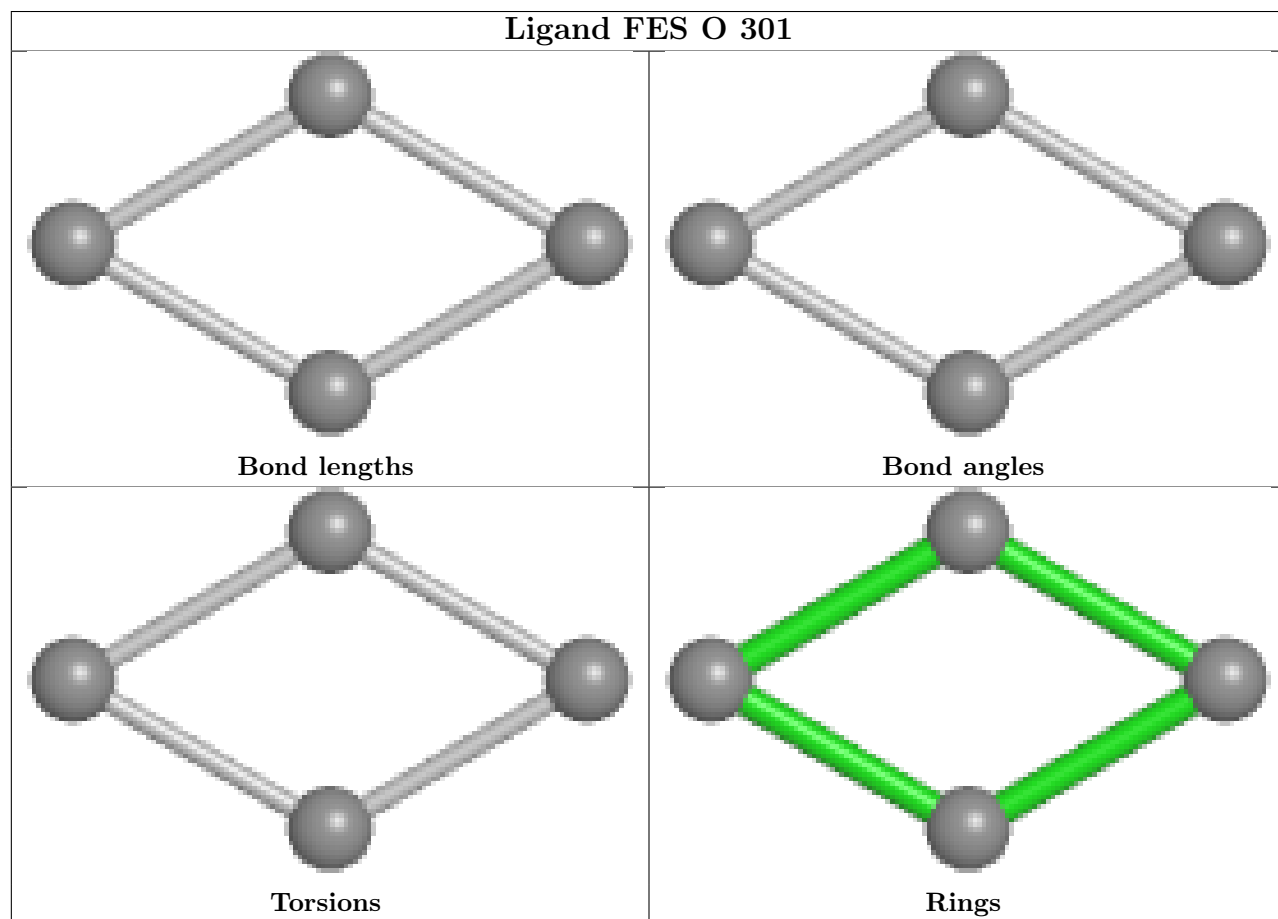
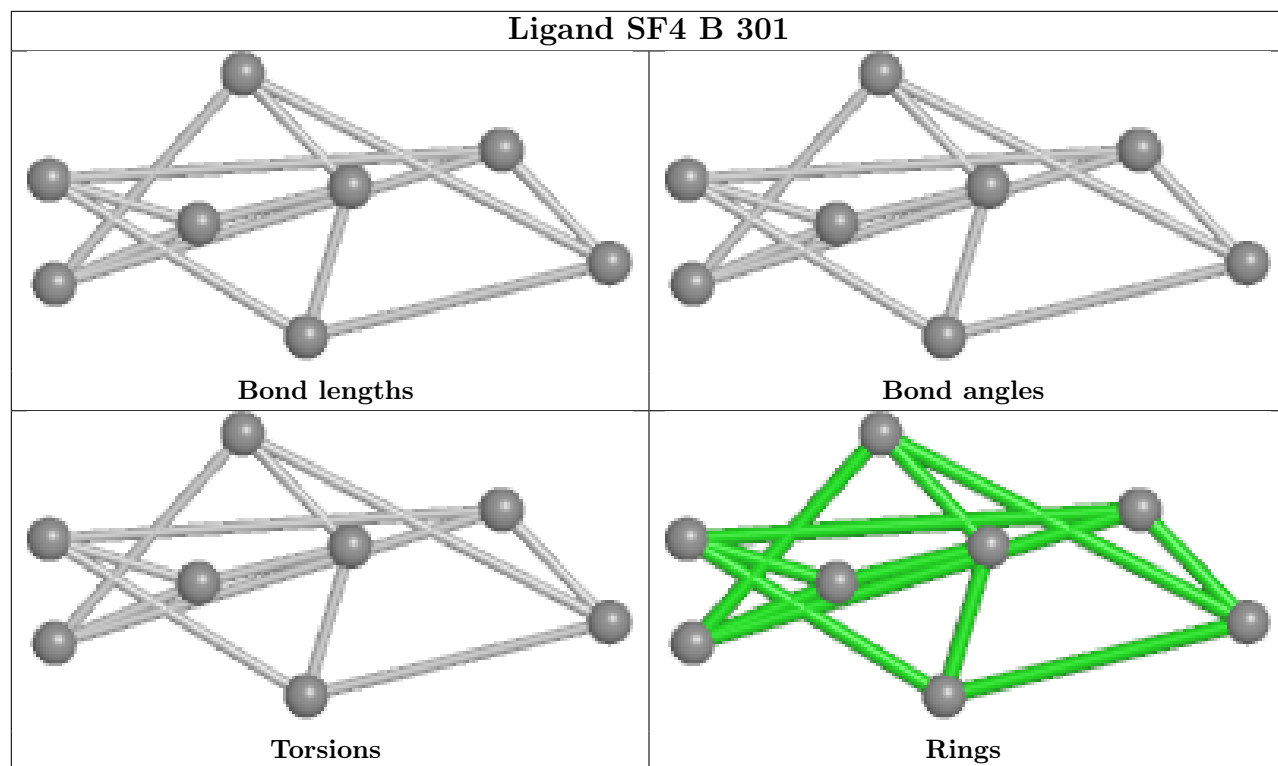
Ligand PEE V 202

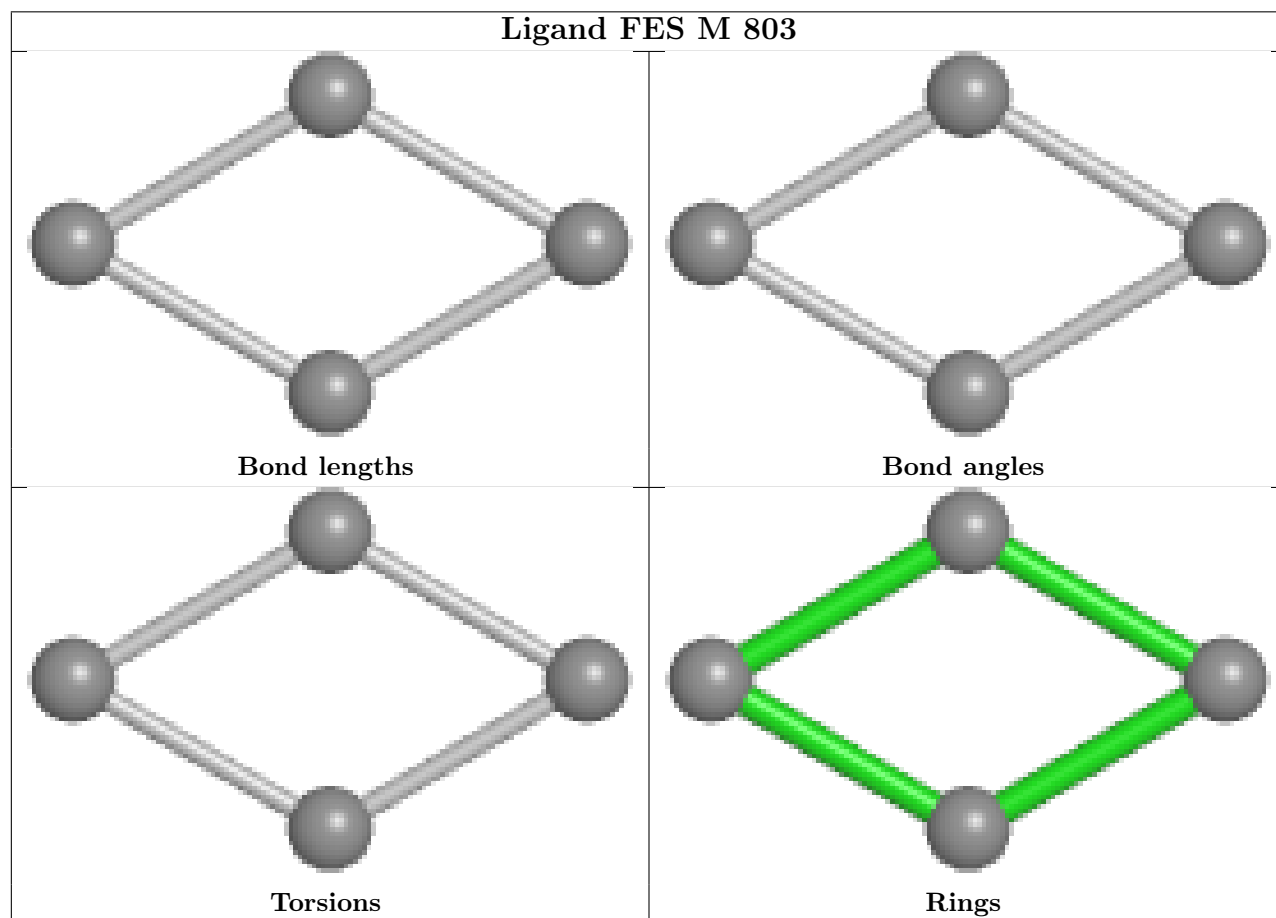
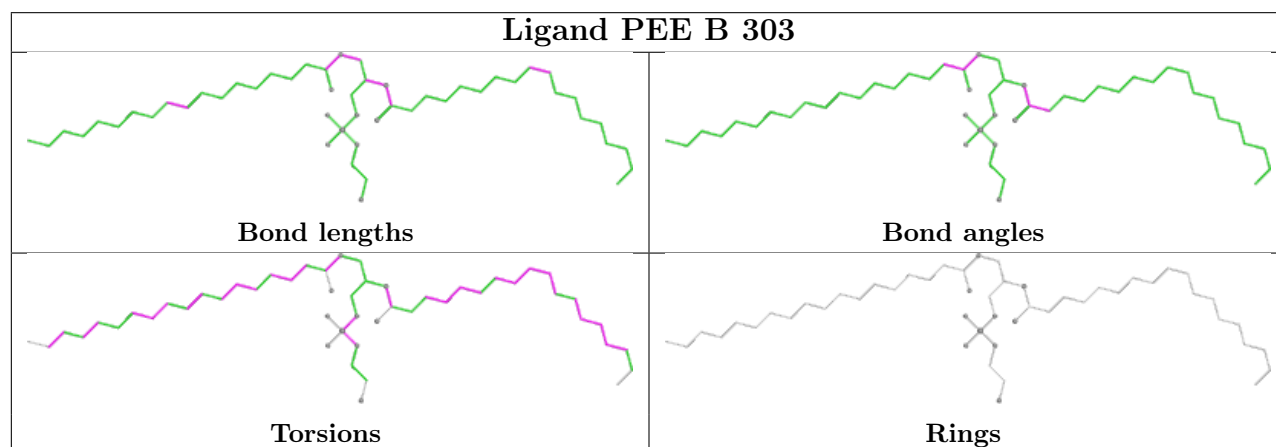


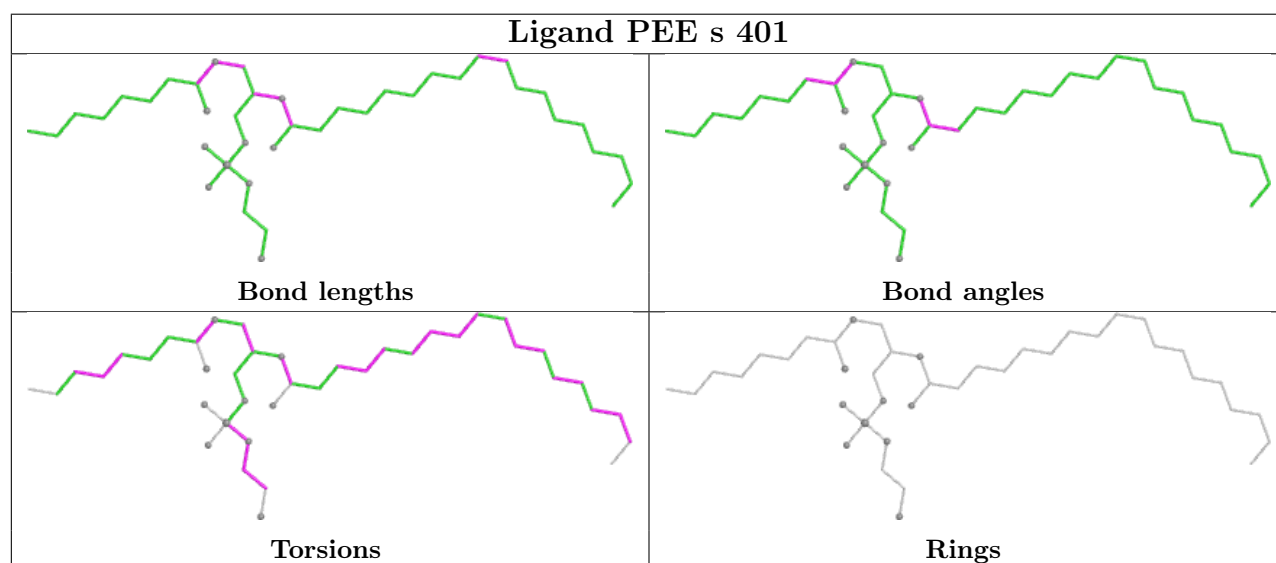
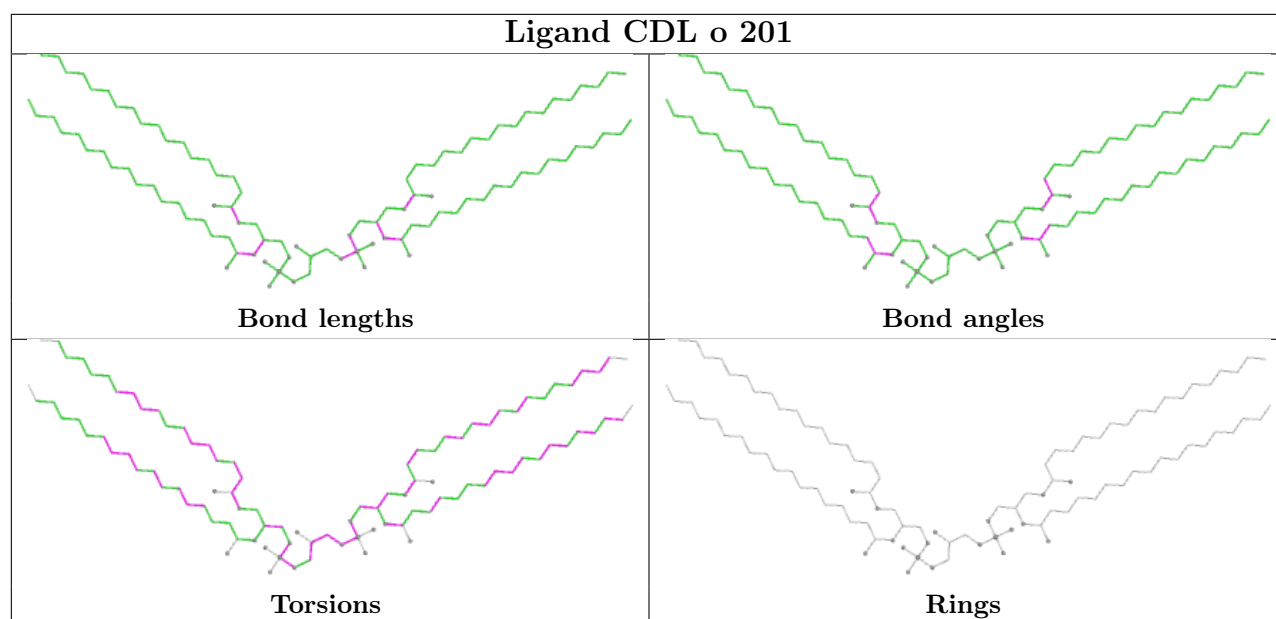
Ligand NDP J 401

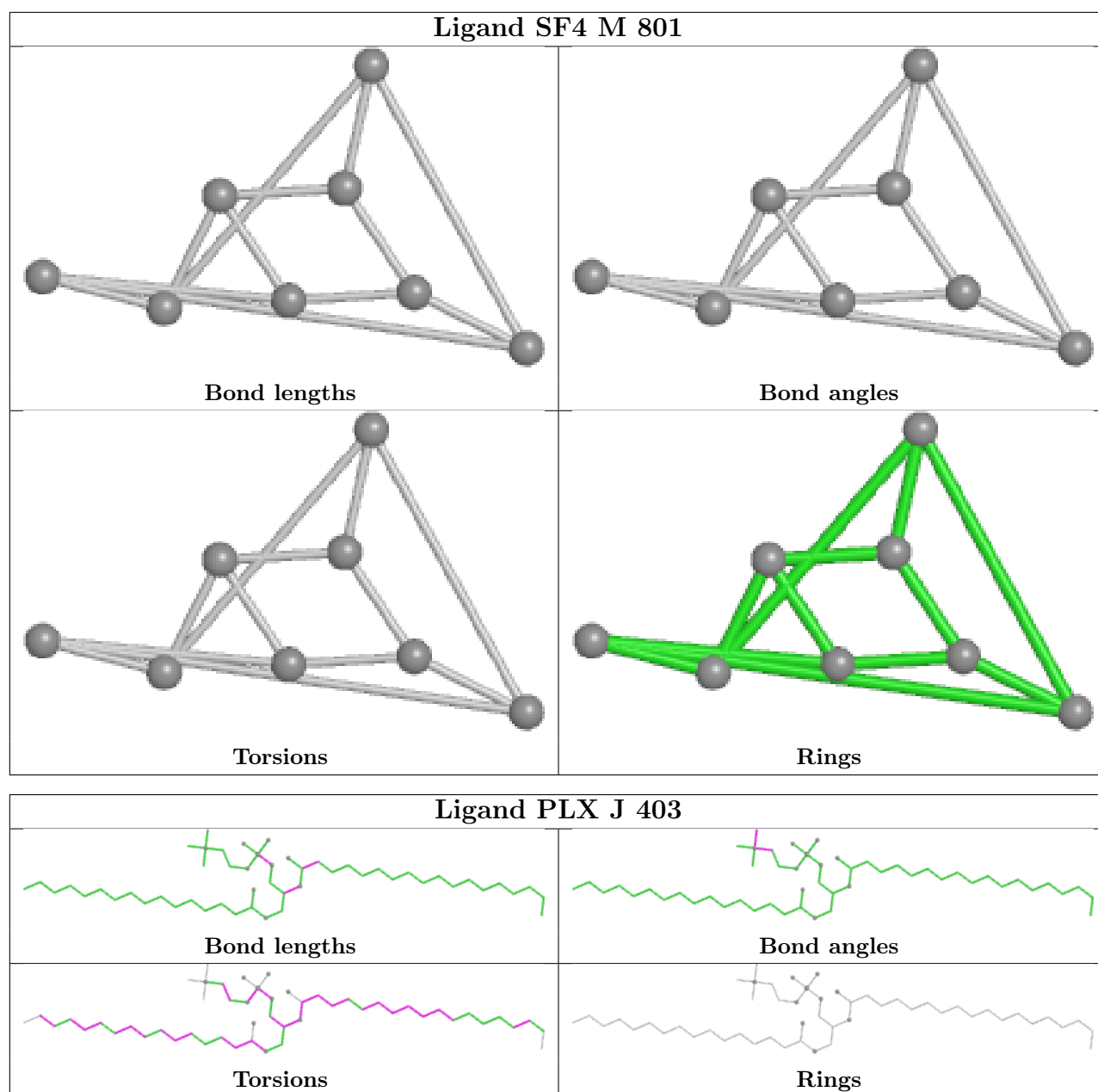


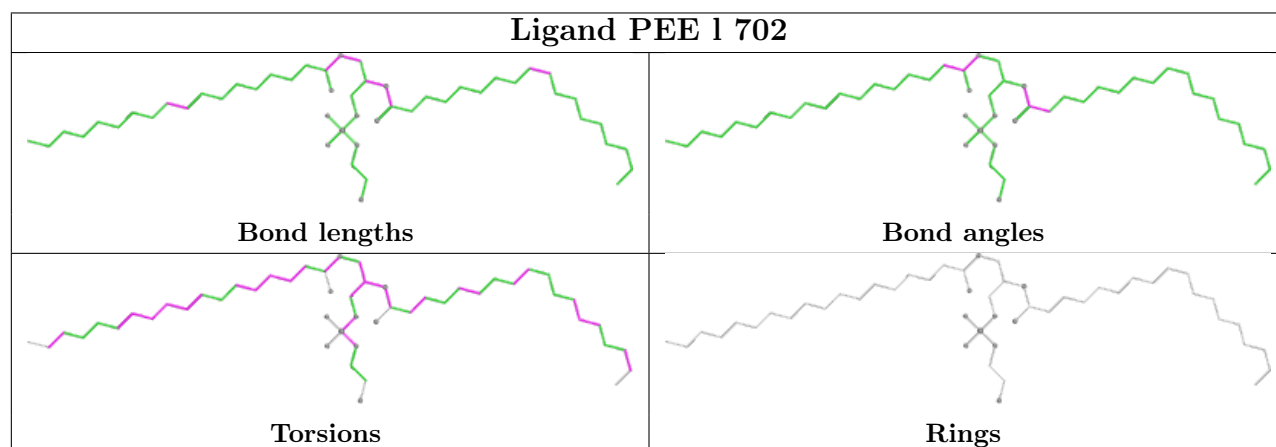
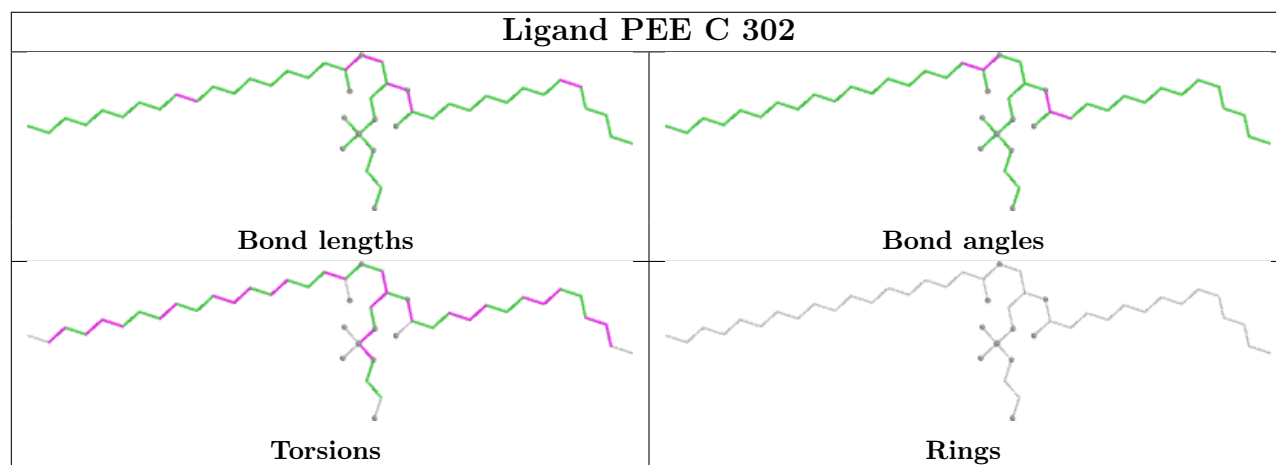
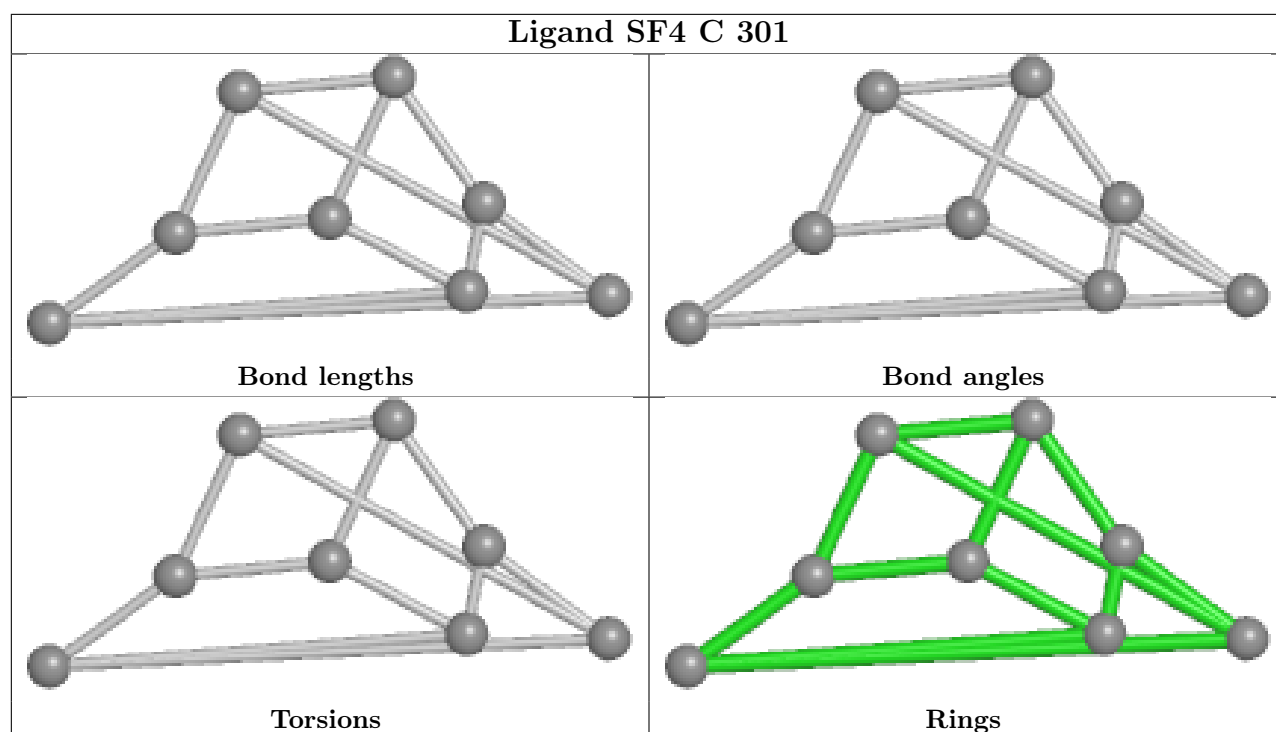


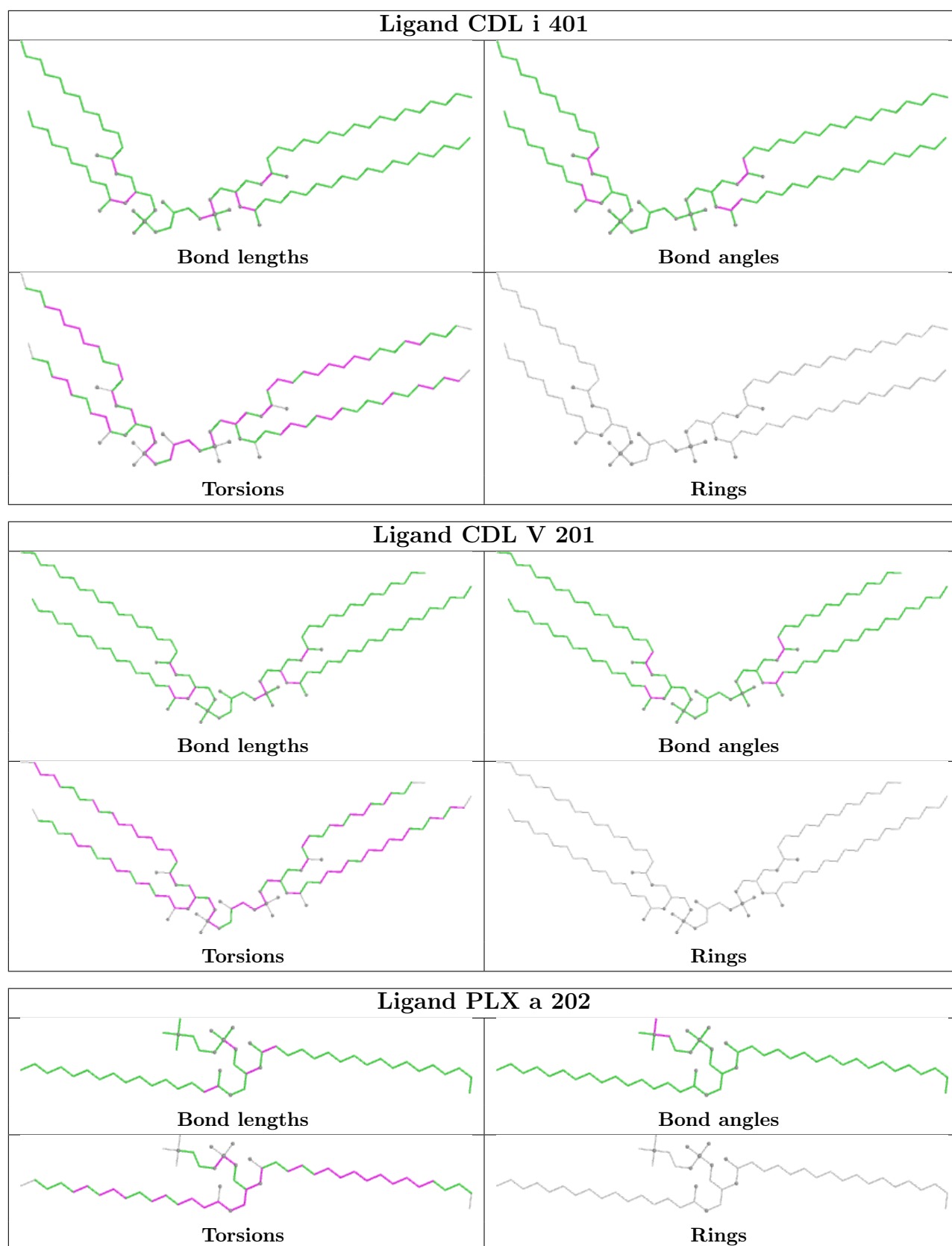


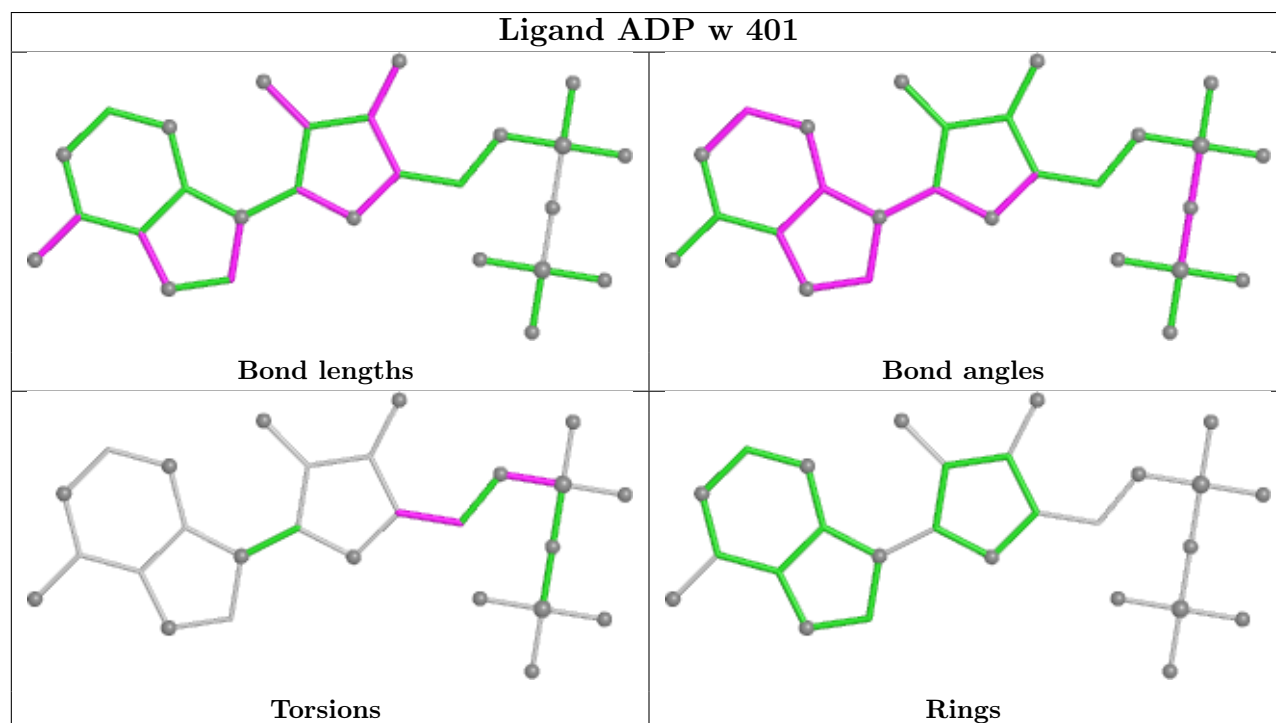
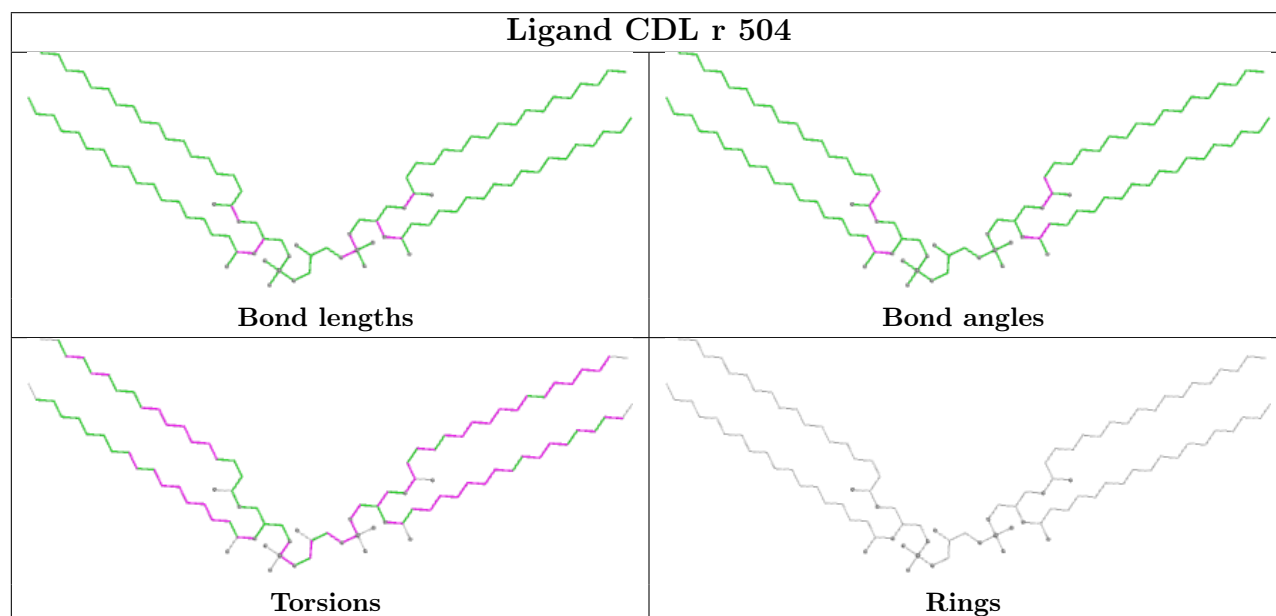
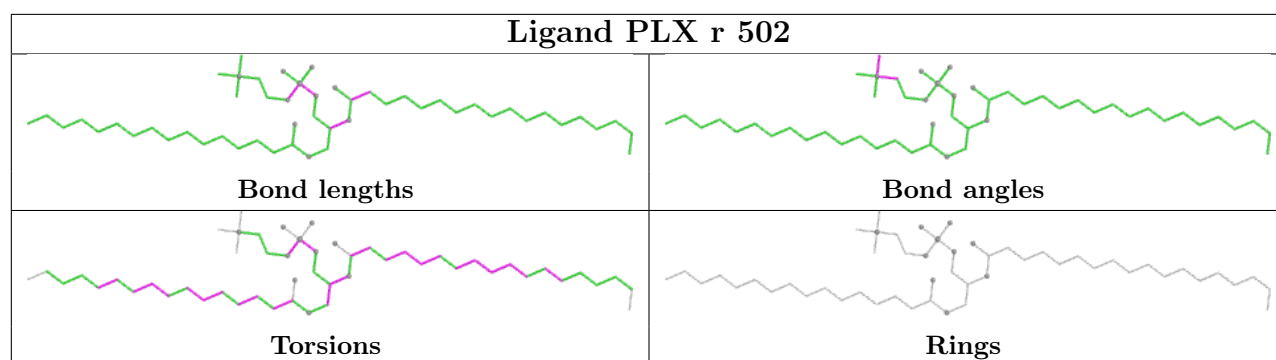


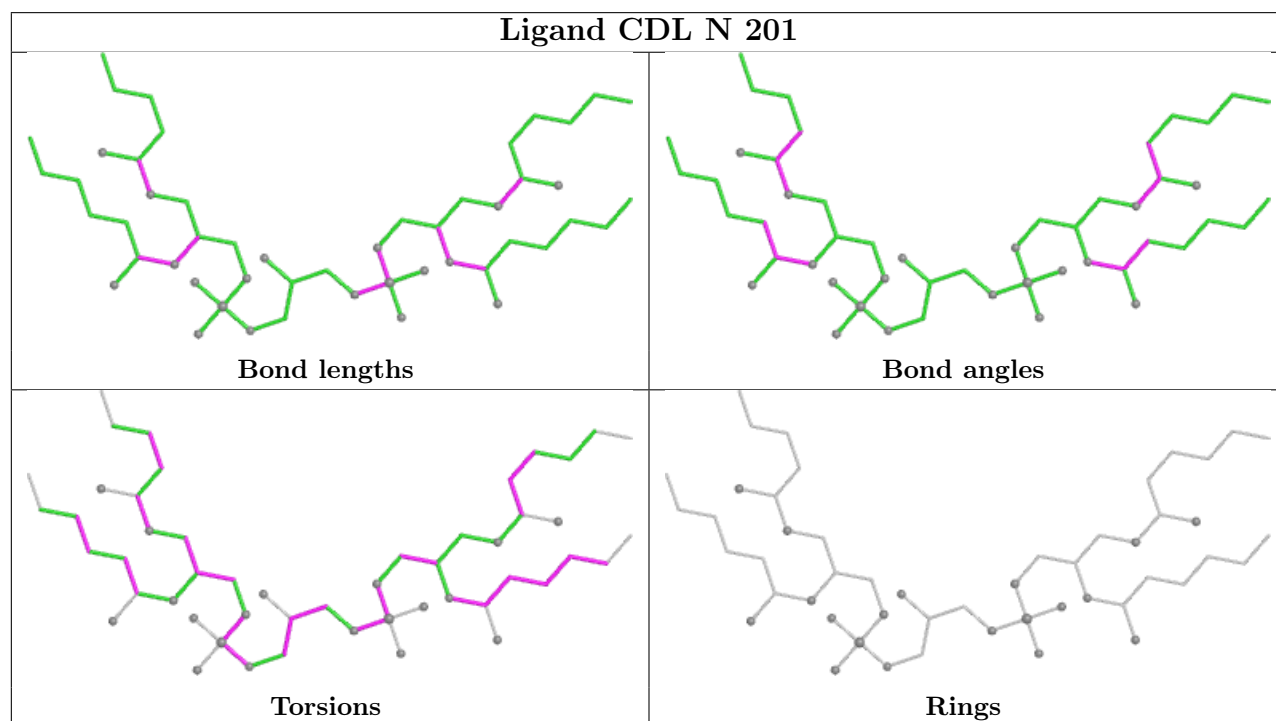
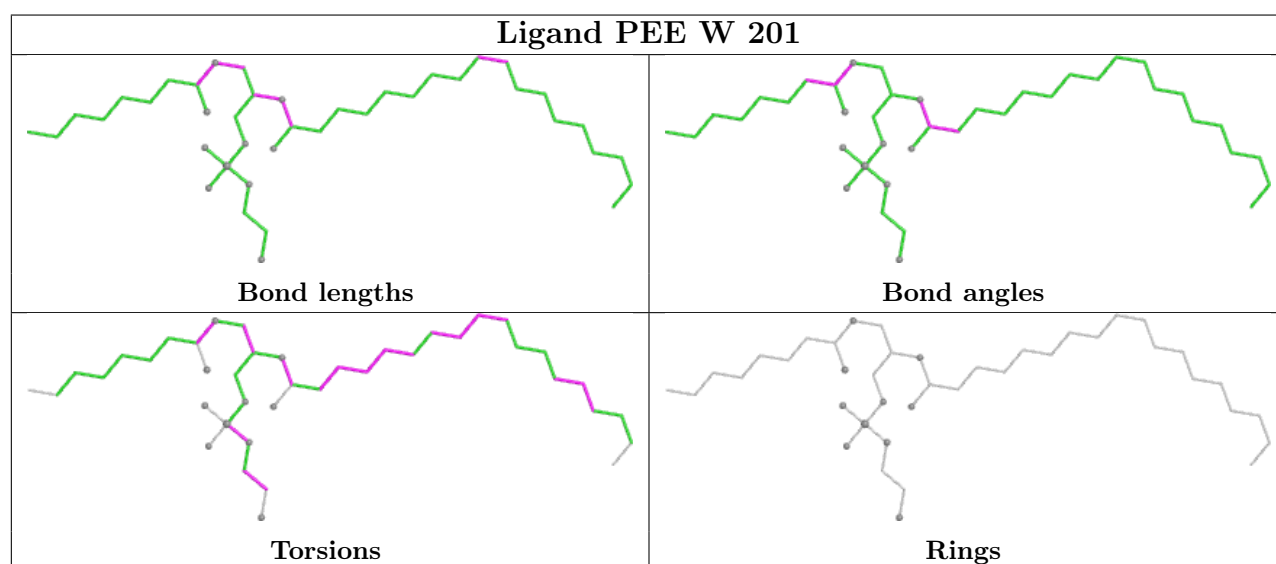
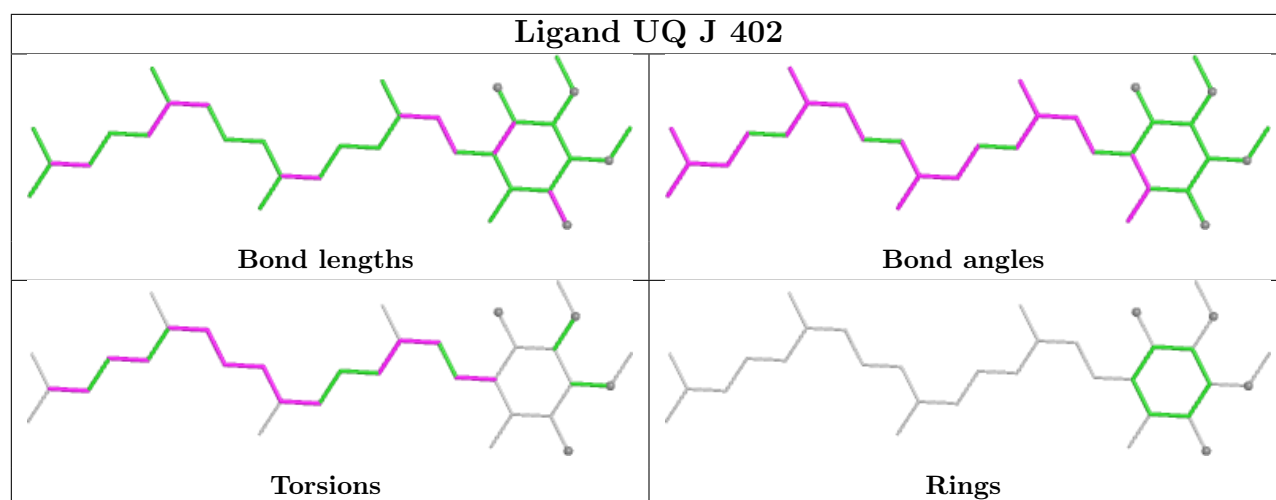


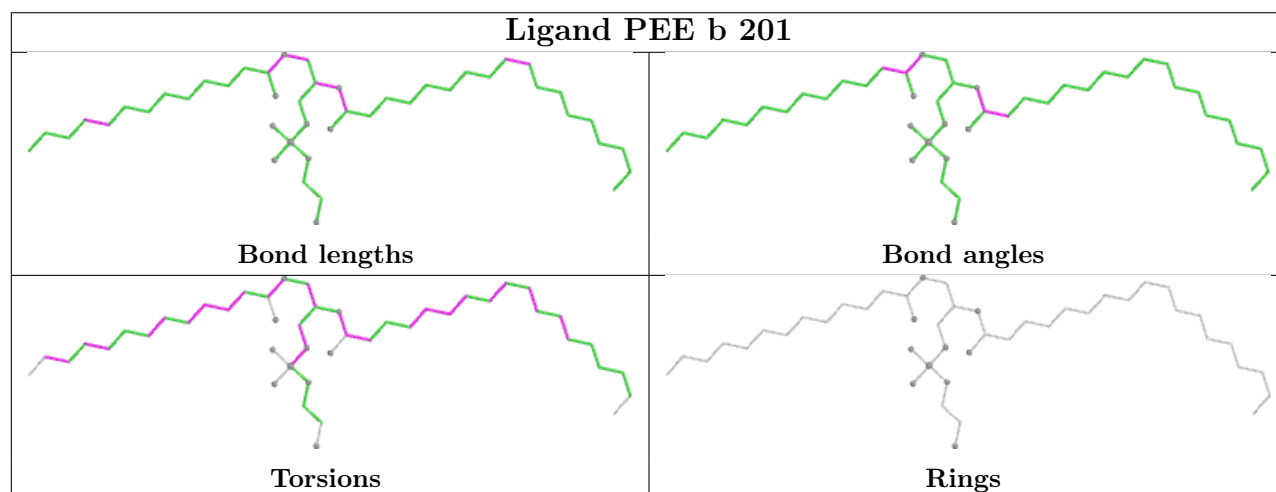
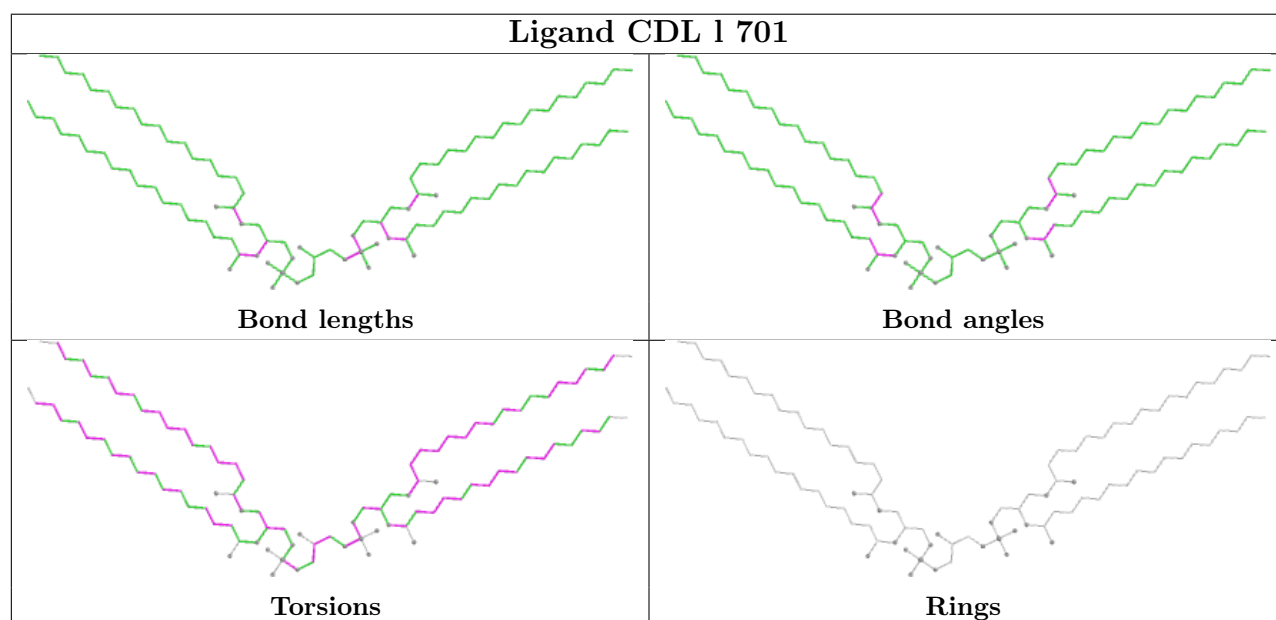
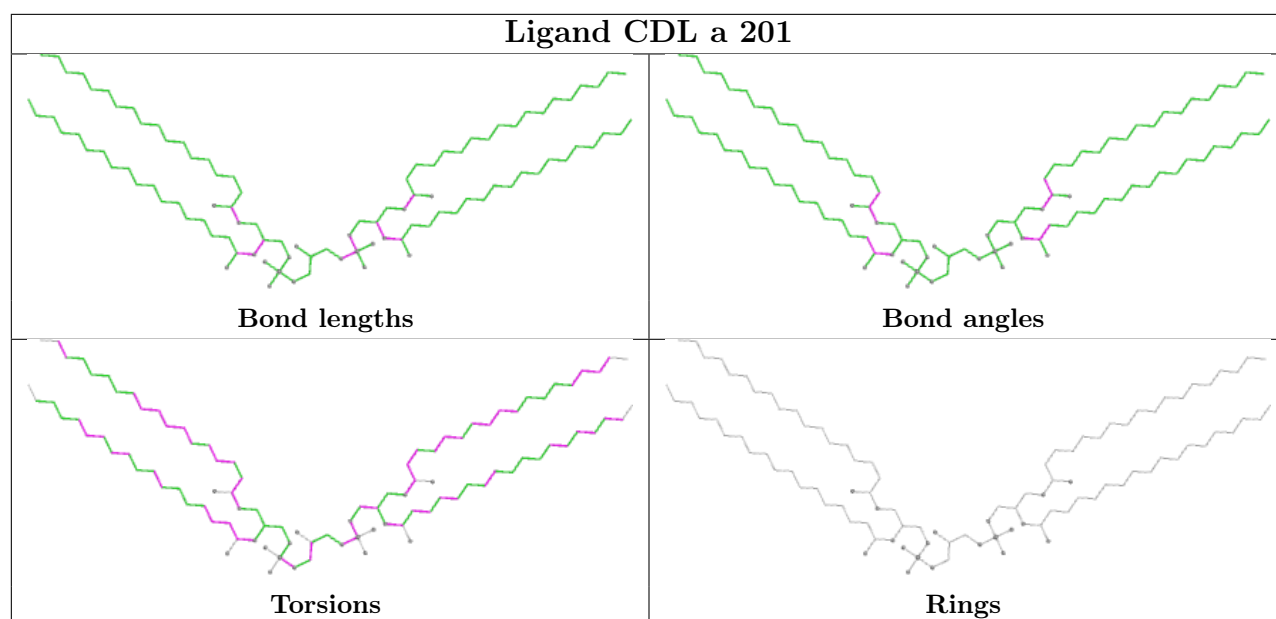


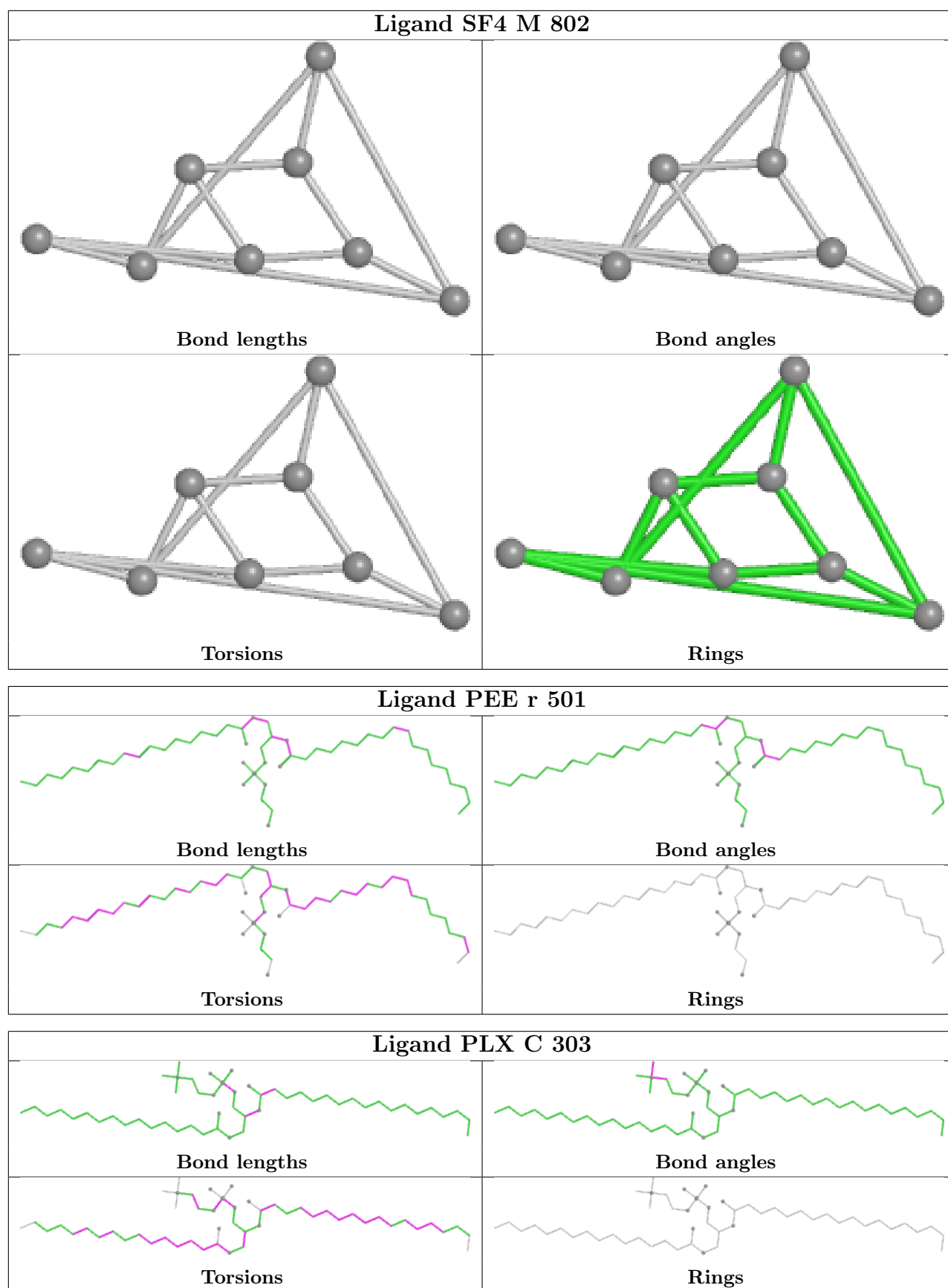


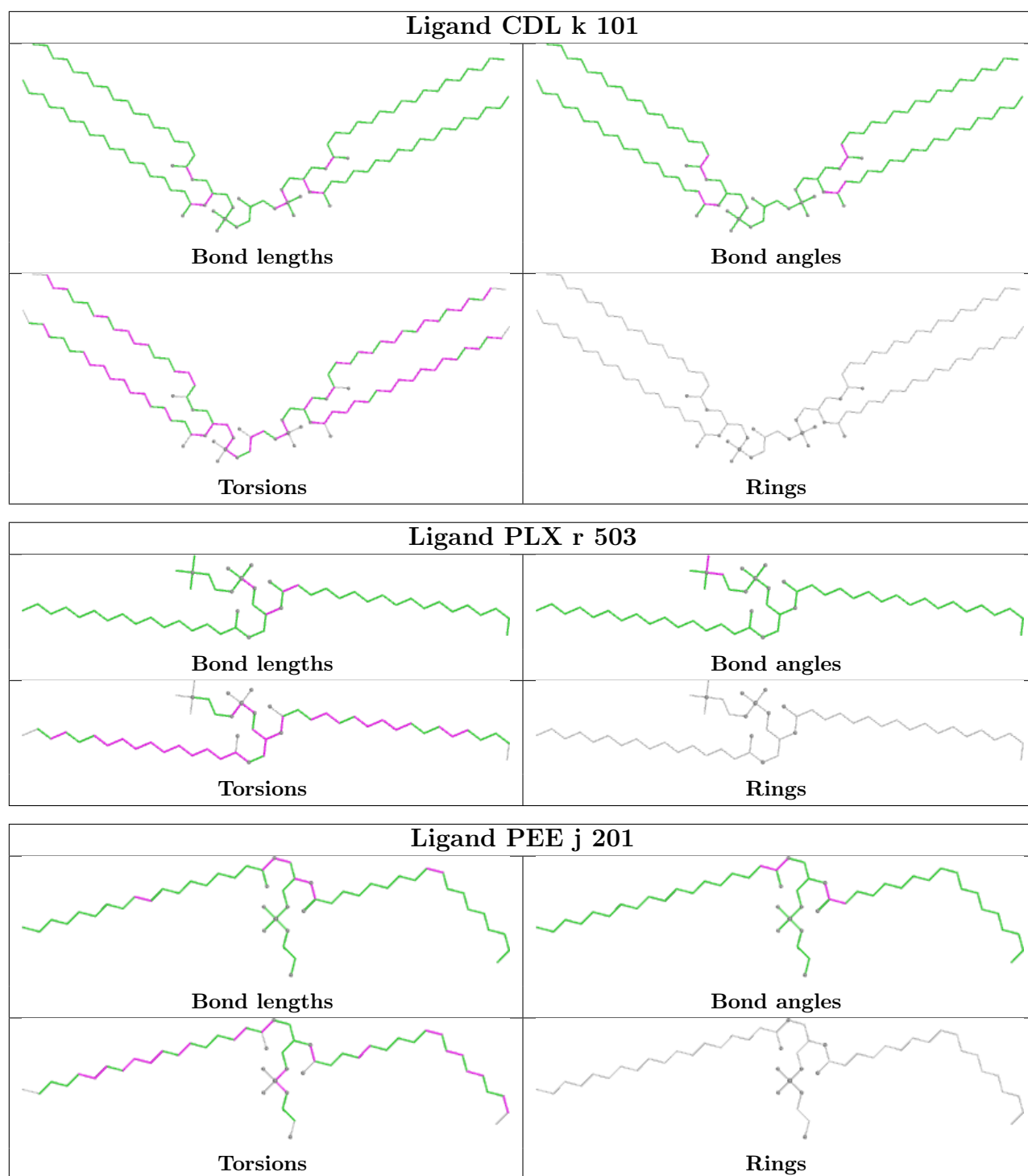


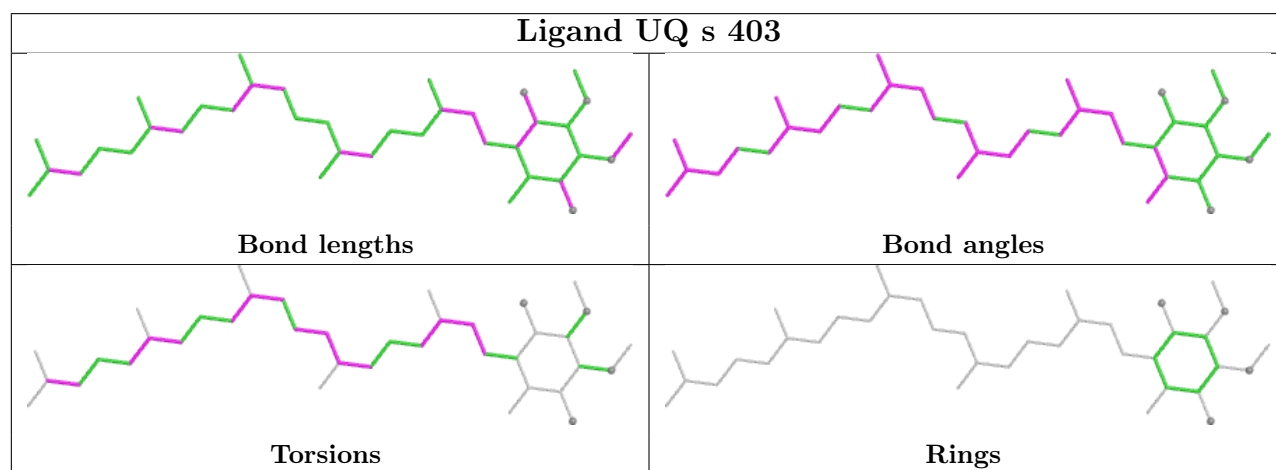
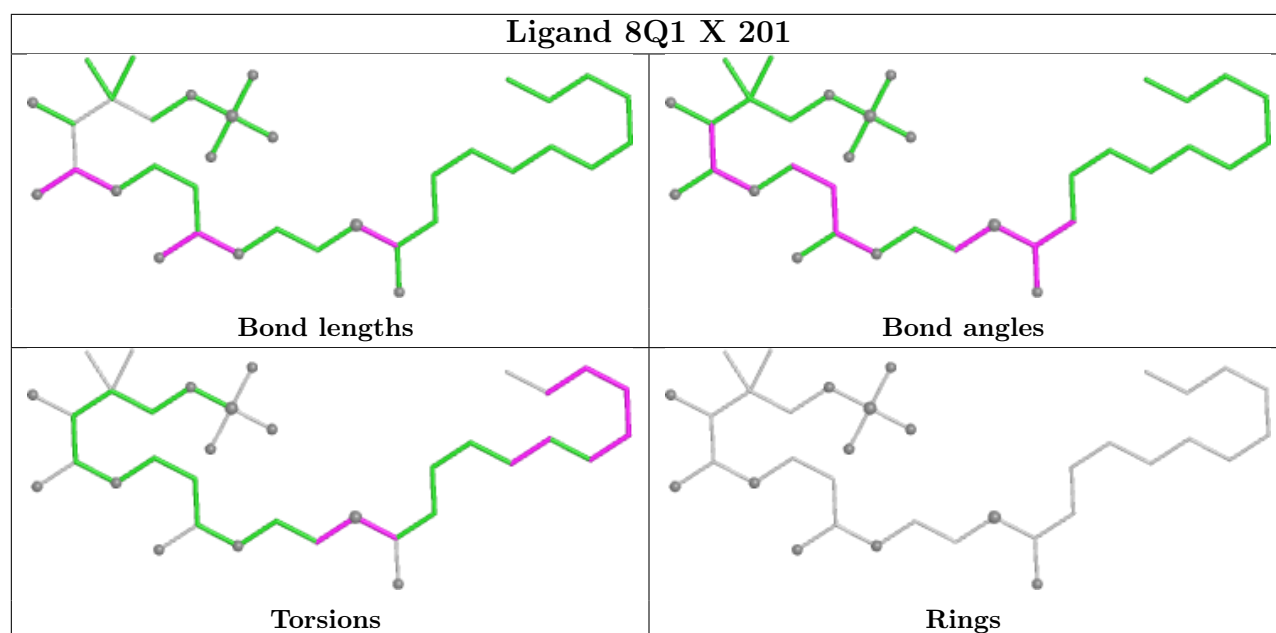


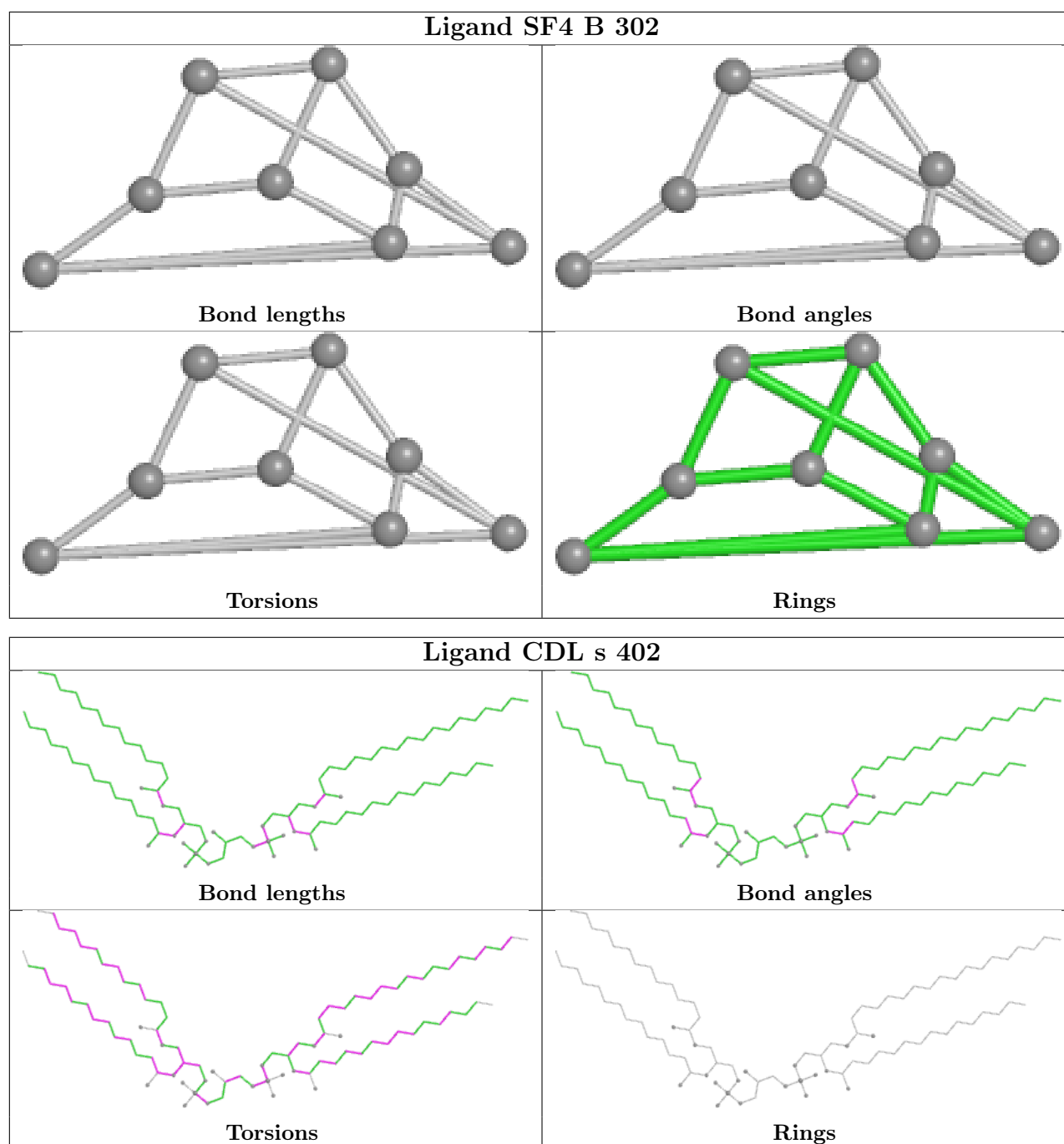












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

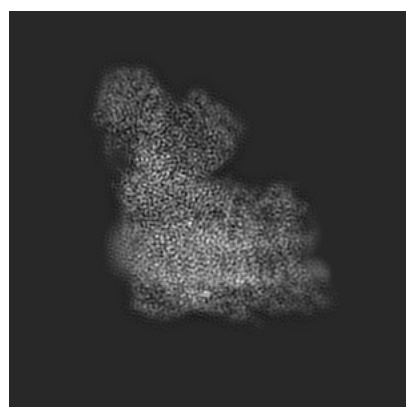
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32265. These allow visual inspection of the internal detail of the map and identification of artifacts.

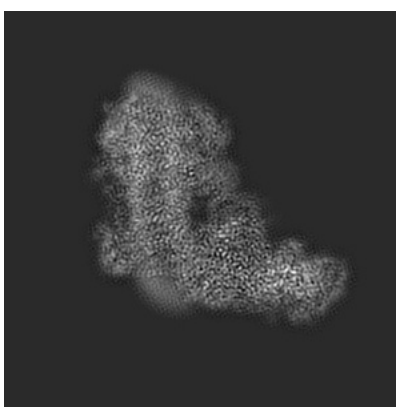
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

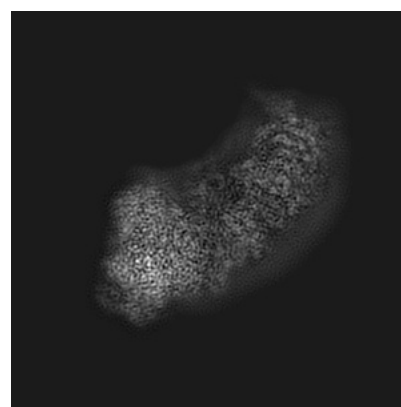
6.1.1 Primary map



X



Y

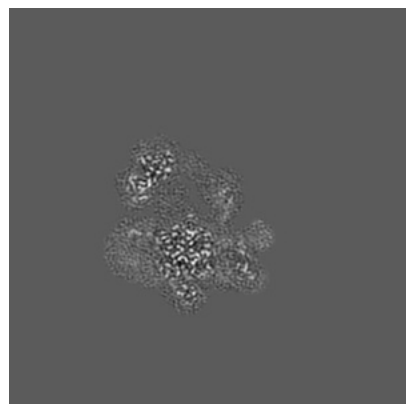


Z

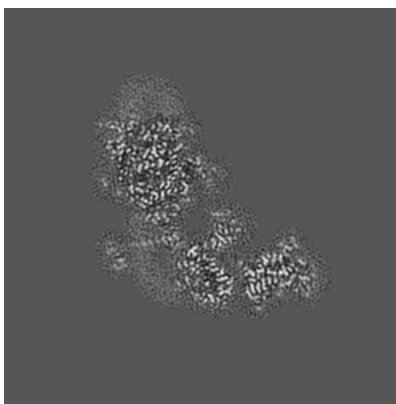
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

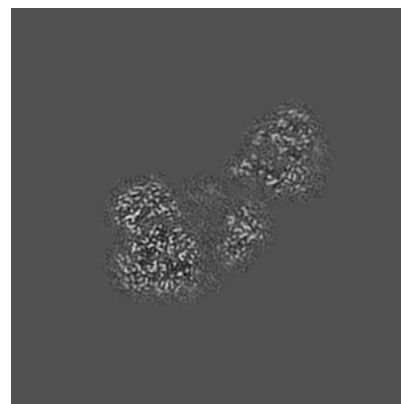
6.2.1 Primary map



X Index: 155



Y Index: 155

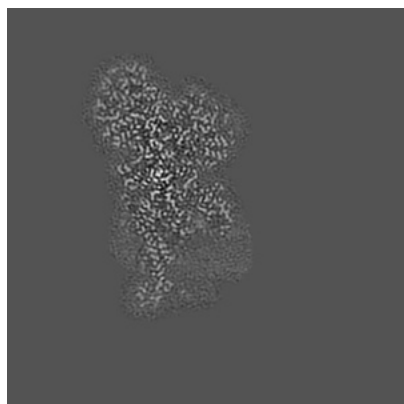


Z Index: 155

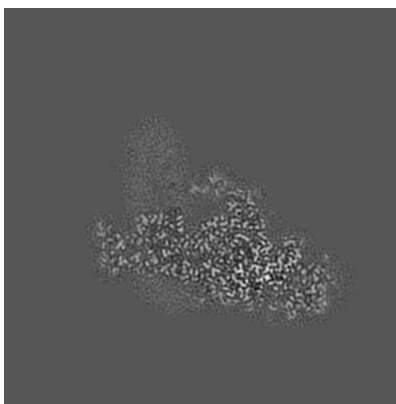
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

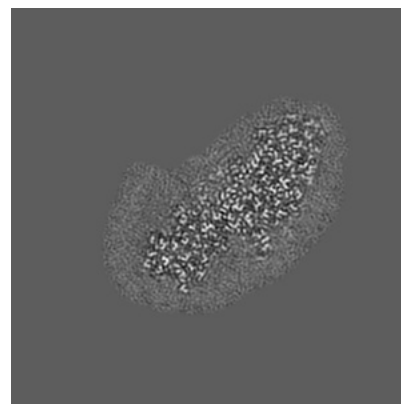
6.3.1 Primary map



X Index: 106



Y Index: 112

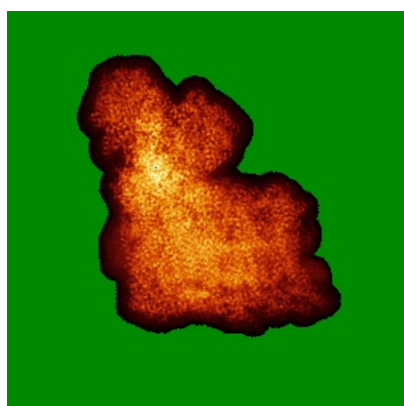


Z Index: 127

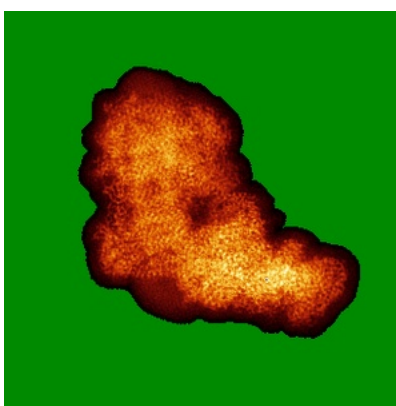
The images above show the largest variance slices of the map in three orthogonal directions.

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

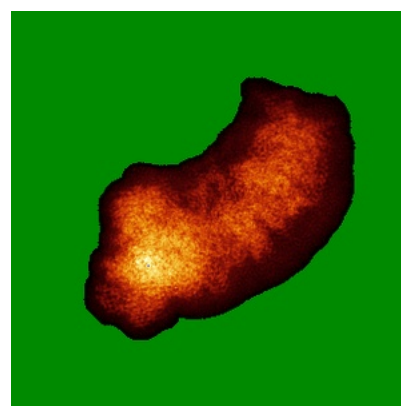
6.4.1 Primary map



X



Y

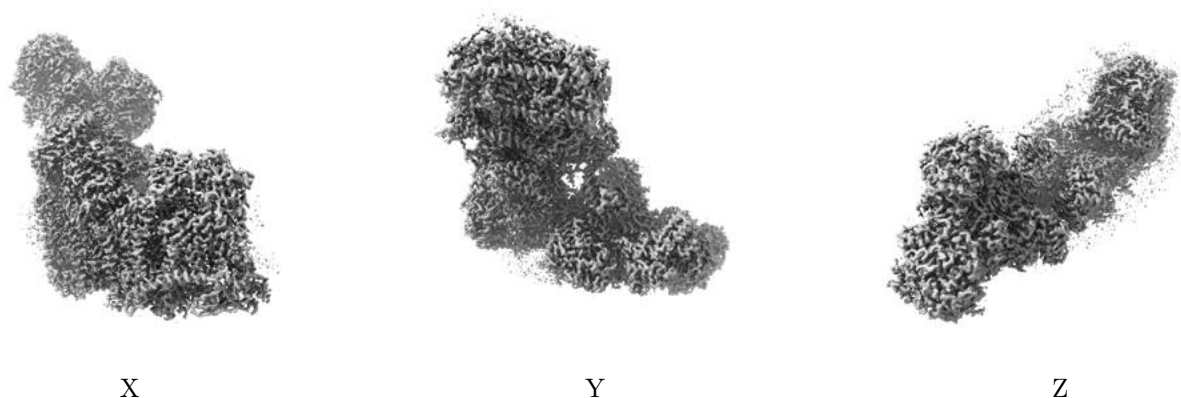


Z

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 0.0267. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

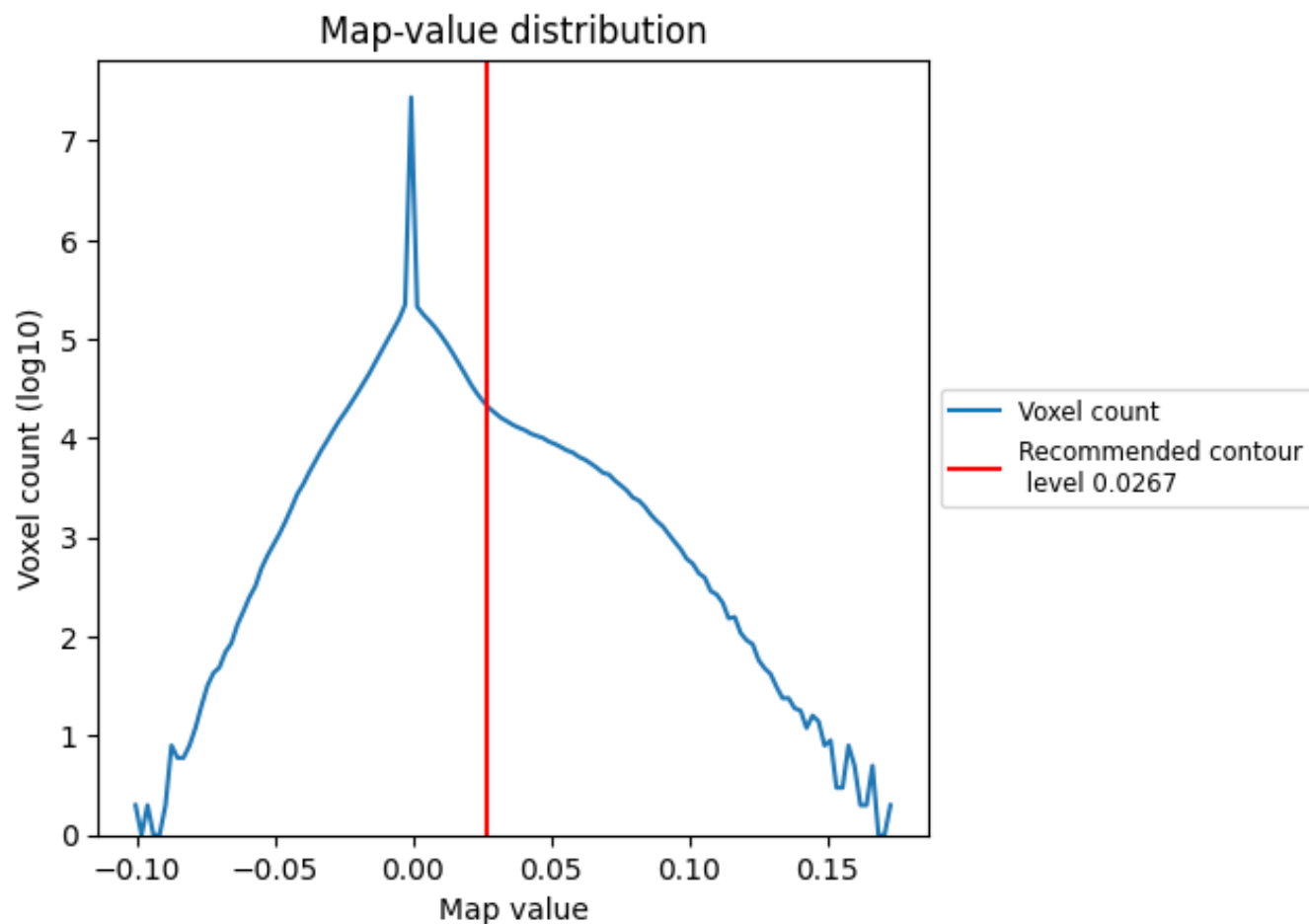
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

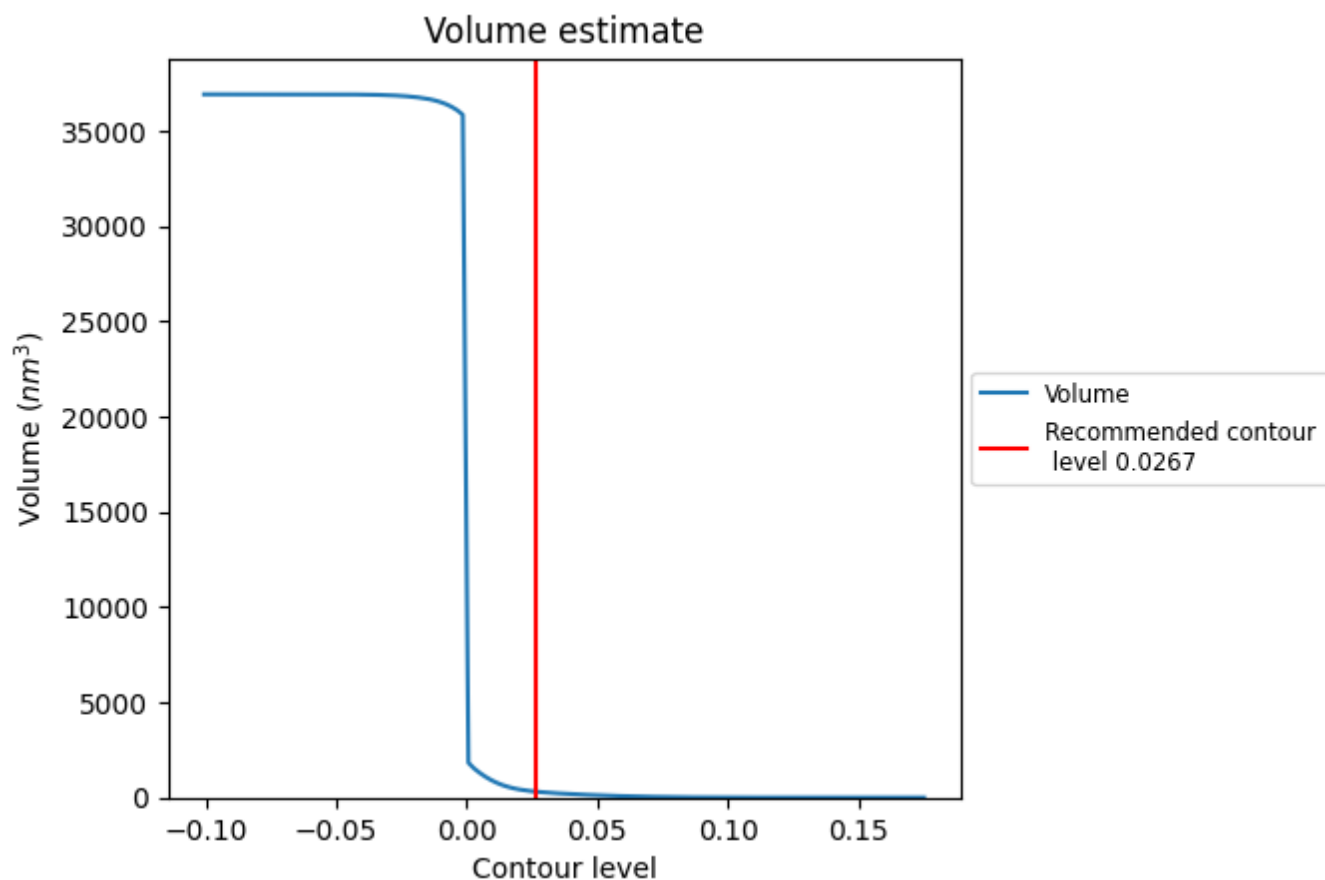
This section contains the results of statistical analysis of the map.

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.

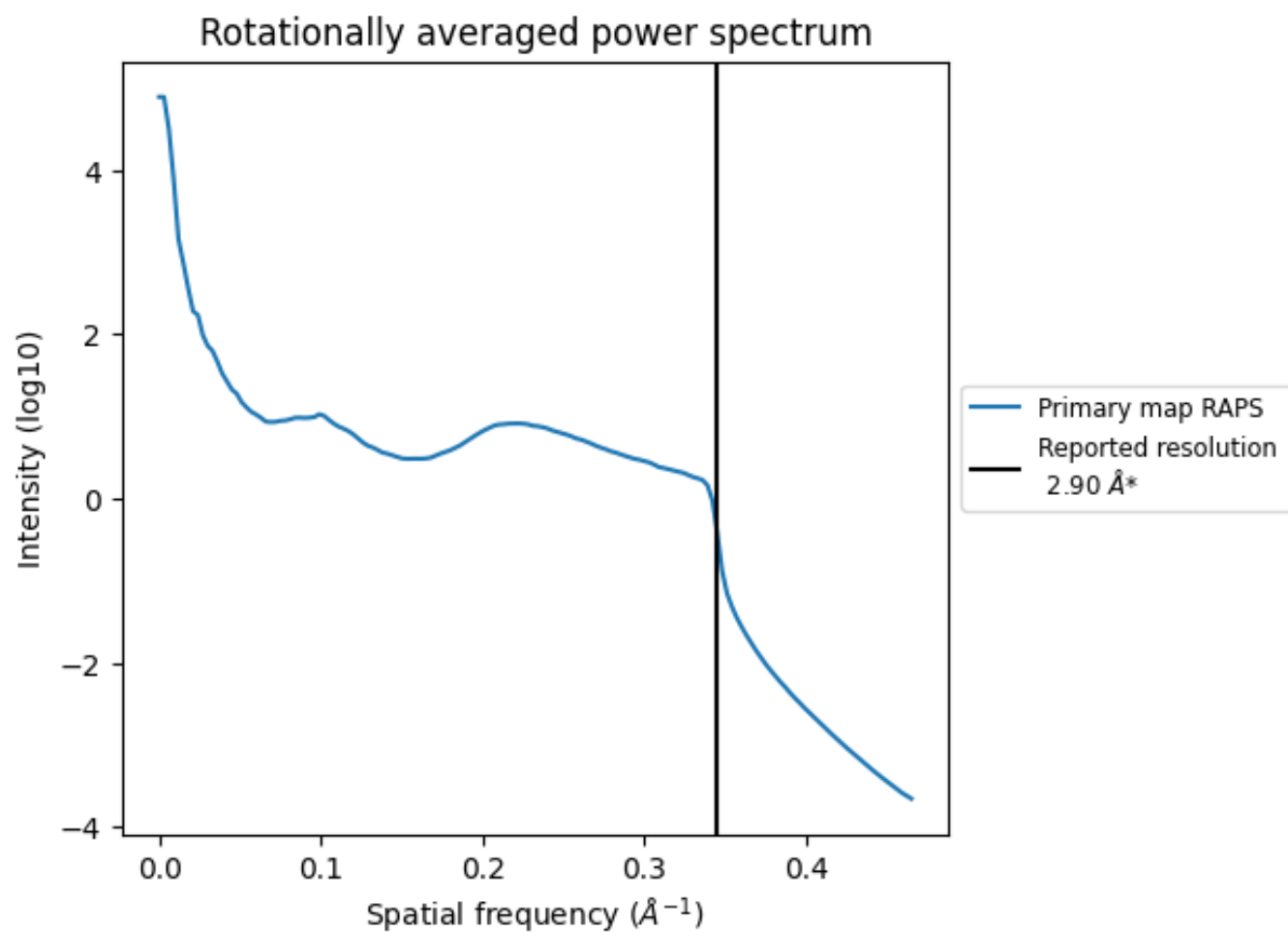
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 308 nm³; this corresponds to an approximate mass of 278 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 0.345 Å⁻¹

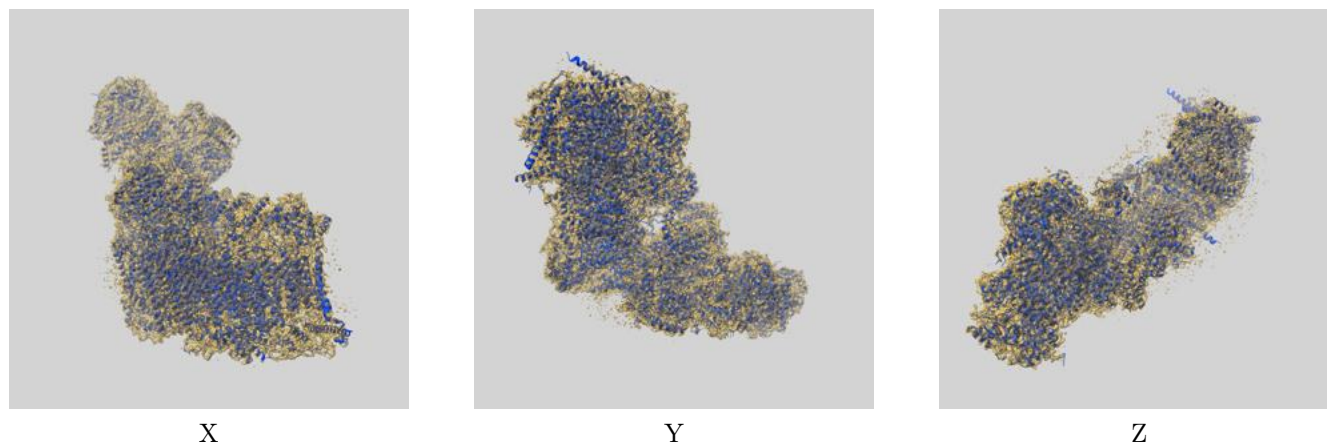
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

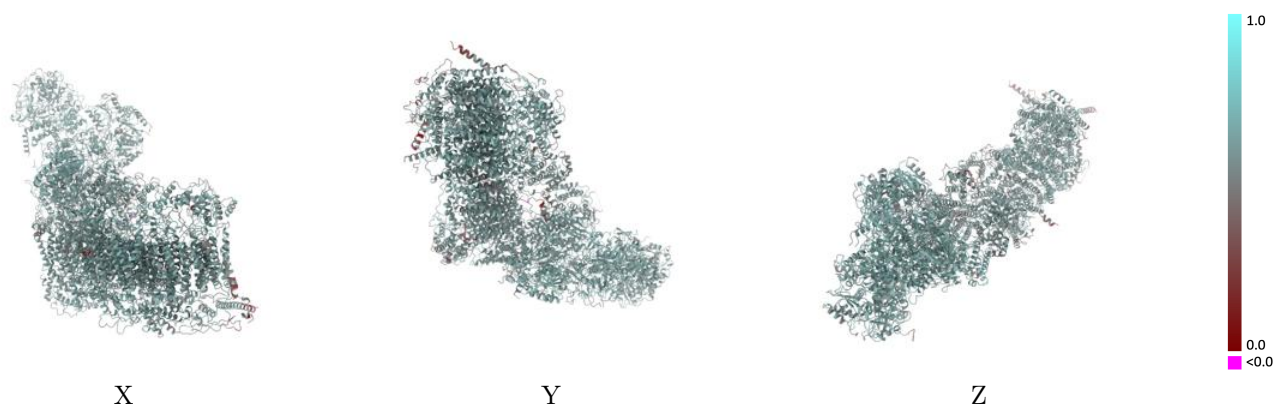
This section contains information regarding the fit between EMDB map EMD-32265 and PDB model 7W2R. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



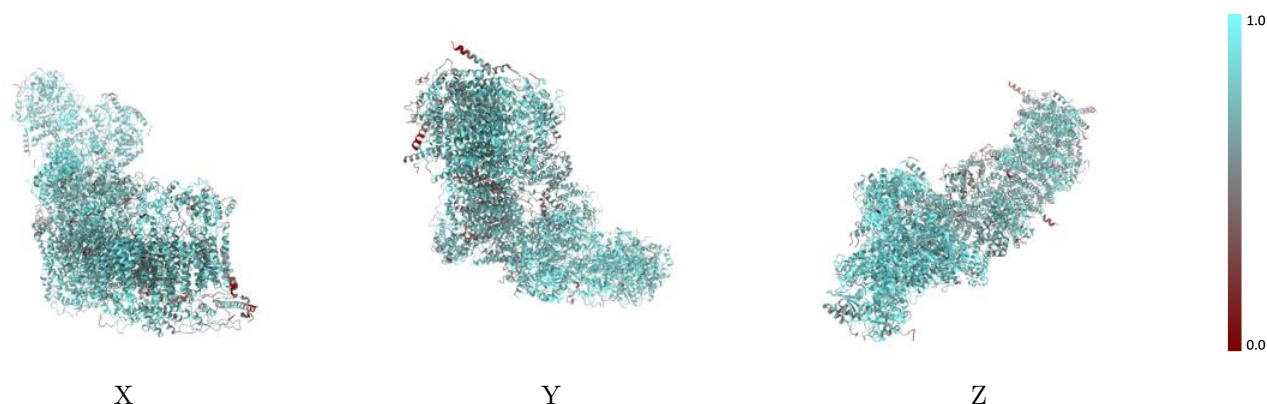
The images above show the 3D surface view of the map at the recommended contour level 0.0267 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



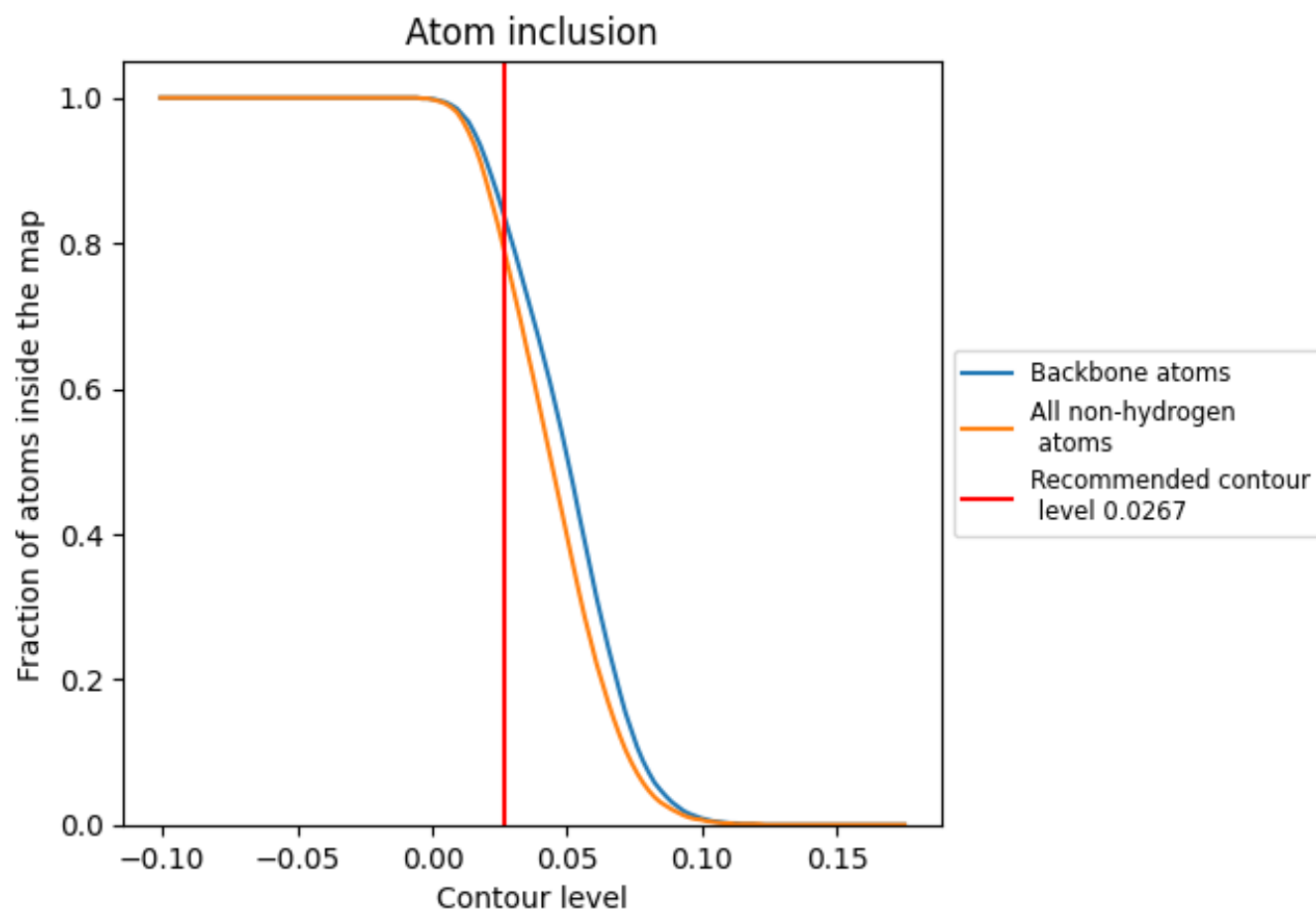
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0267).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0267) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7910	 0.5970
A	 0.8170	 0.5980
B	 0.9140	 0.6370
C	 0.8840	 0.6350
E	 0.8240	 0.6130
F	 0.7510	 0.5730
G	 0.5430	 0.4820
H	 0.8160	 0.6020
I	 0.7130	 0.5830
J	 0.8370	 0.6110
K	 0.6730	 0.5560
L	 0.8540	 0.6240
M	 0.8660	 0.6180
N	 0.7310	 0.5970
O	 0.7560	 0.5840
P	 0.9260	 0.6440
Q	 0.9020	 0.6360
S	 0.8640	 0.6110
T	 0.7640	 0.6010
U	 0.7680	 0.5660
V	 0.6020	 0.5590
W	 0.7770	 0.5830
X	 0.7410	 0.5740
Y	 0.6030	 0.5240
Z	 0.5810	 0.5160
a	 0.7680	 0.5980
b	 0.6570	 0.5450
c	 0.7720	 0.5870
d	 0.7240	 0.5760
e	 0.7150	 0.5690
f	 0.5840	 0.5330
g	 0.8080	 0.6010
h	 0.7840	 0.5850
i	 0.8490	 0.6180
j	 0.7880	 0.6090



Continued on next page...

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Chain	Atom inclusion	Q-score
k	 0.7700	 0.6010
l	 0.7710	 0.5970
m	 0.7160	 0.5650
n	 0.6360	 0.5440
o	 0.7210	 0.5760
p	 0.7740	 0.5900
r	 0.8240	 0.6110
s	 0.8470	 0.6170
u	 0.7860	 0.5870
v	 0.5980	 0.5210
w	 0.7330	 0.5790