



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:07 PM UTC

PDB ID : 7V31 / pdb_00007v31
EMDB ID : EMD-31649
Title : Active state complex I from rotenone dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-08-10
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:

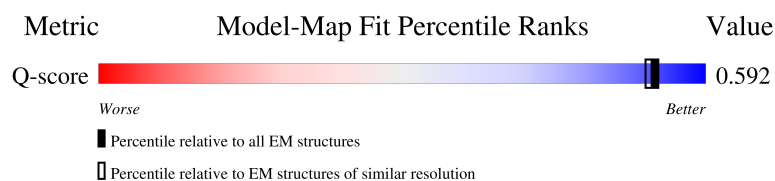
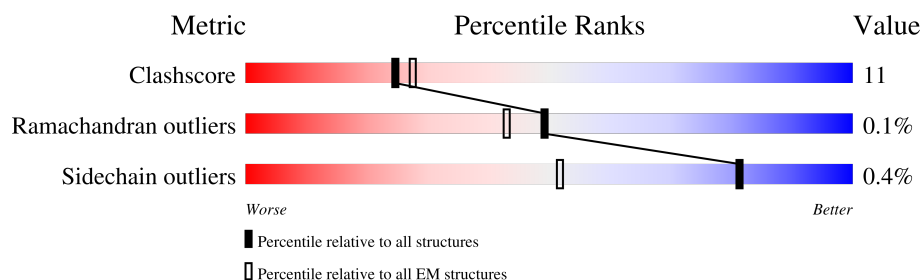
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 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	 78% 22%
2	B	176	 78% 22%
3	C	156	 78% 22%
4	E	115	 86% 13%

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

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Mol	Chain	Length	Quality of chain
29	f	49	
30	g	121	
31	h	105	
32	i	347	
33	j	115	
34	k	98	
35	l	606	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	125	
44	w	320	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	C	301	-	-	X	-
45	SF4	M	802	-	-	X	-
47	PEE	Q	501	-	-	X	-
53	FES	M	803	-	-	X	-
53	FES	O	301	-	-	X	-
55	CDL	s	402	-	-	X	-

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 68204 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
			699	450	103	141	5		

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

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 NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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 NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

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 NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

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

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

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

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

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

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

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

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

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

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	142	Total	C	N	O	S	0	0
			1167	752	200	206	9		

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	104	Total	C	N	O	S	0	0
			867	553	142	168	4		

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	606	Total	C	N	O	S	0	0
			4816	3193	746	826	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	175	Total	C	N	O	S	0	0
			1292	863	188	228	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		

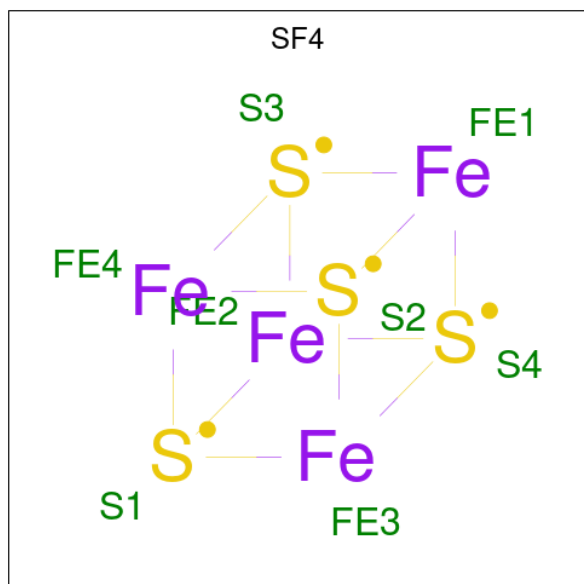
There is a discrepancy between the modelled and reference sequences:

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.

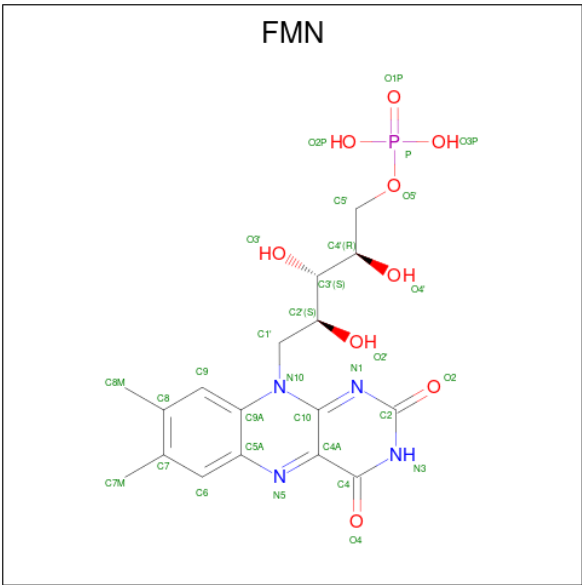
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2586	1646	439	491	10		

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



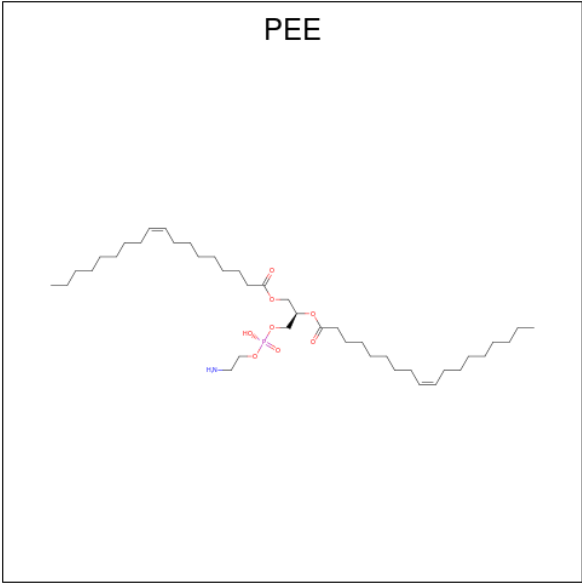
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 47 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



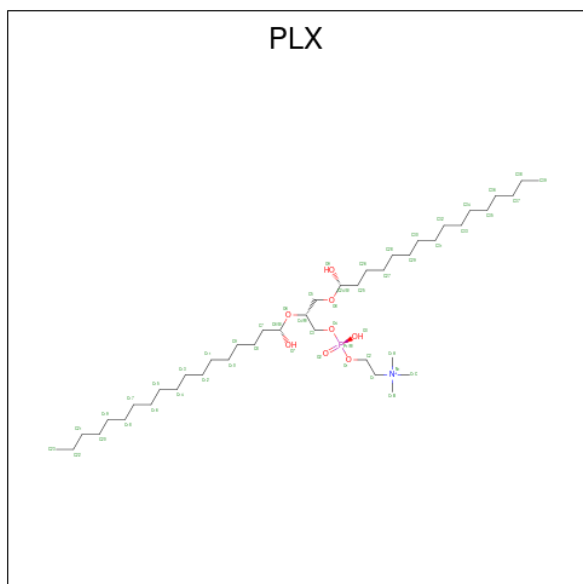
Mol	Chain	Residues	Atoms					AltConf
47	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	Q	1	Total	C	N	O	P	0
			47	37	1	8	1	

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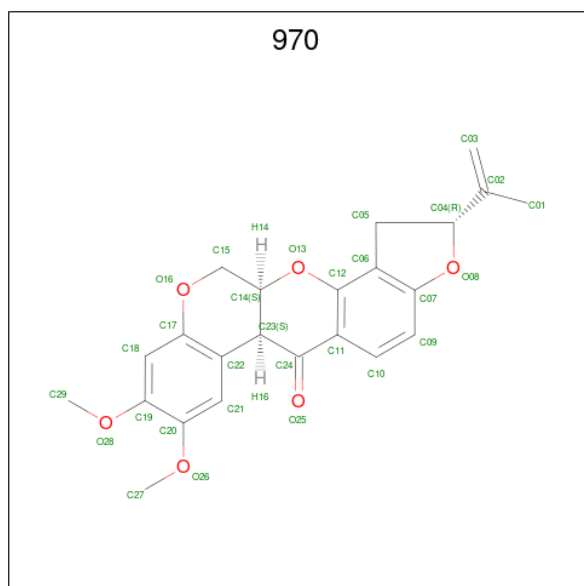
Mol	Chain	Residues	Atoms					AltConf
47	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
47	b	1	Total	C	N	O	P	0
			46	36	1	8	1	
47	f	1	Total	N				0
			1	1				
47	j	1	Total	C	N	O	P	0
			41	31	1	8	1	
47	l	1	Total	C	N	O	P	0
			40	30	1	8	1	
47	l	1	Total	C	N	O	P	0
			50	40	1	8	1	
47	r	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	s	1	Total	C	N	O	P	0
			47	37	1	8	1	
47	v	1	Total	N				0
			1	1				

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



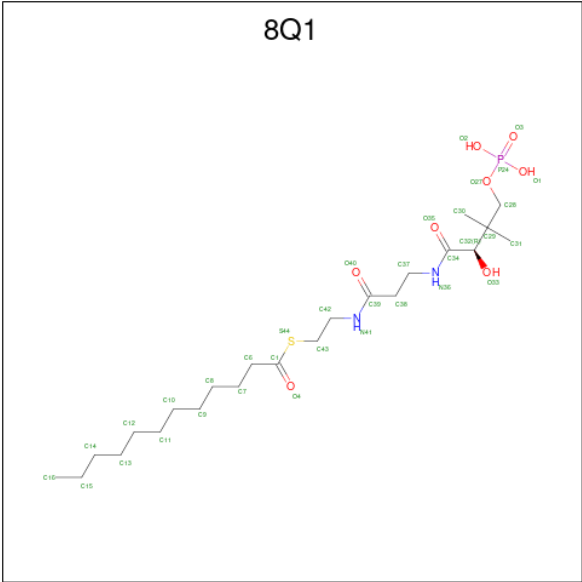
Mol	Chain	Residues	Atoms					AltConf
48	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	J	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	r	1	Total	C	N	O	P	0
			52	42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

- Molecule 49 is (2R,6aS,12aS)-8,9-dimethoxy-2-(prop-1-en-2-yl)-1,2,12,12a-tetrahydrofuro[2',3':7,8][1]benzopyrano[2,3-c][1]benzopyran-6(6aH)-one (CCD ID: 970) (formula: C₂₃H₂₂O₆) (labeled as "Ligand of Interest" by depositor).



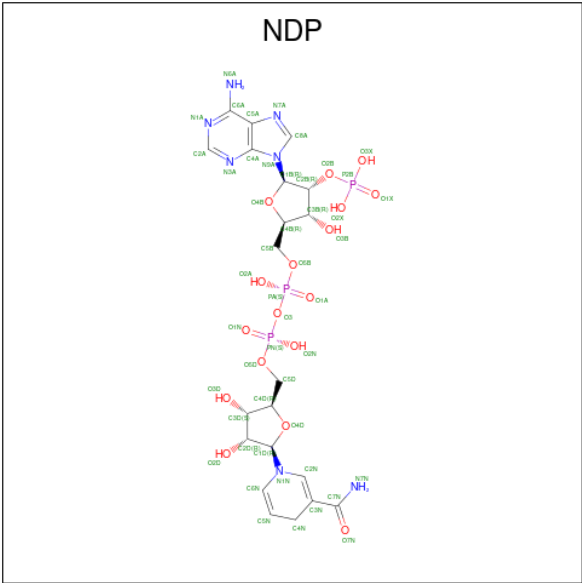
Mol	Chain	Residues	Atoms			AltConf
49	C	1	Total	C	O	0
			29	23	6	

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



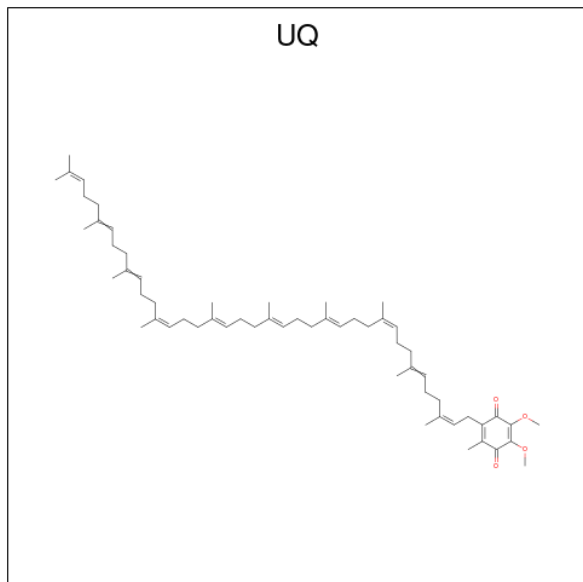
Mol	Chain	Residues	Atoms						AltConf
50	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
50	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

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



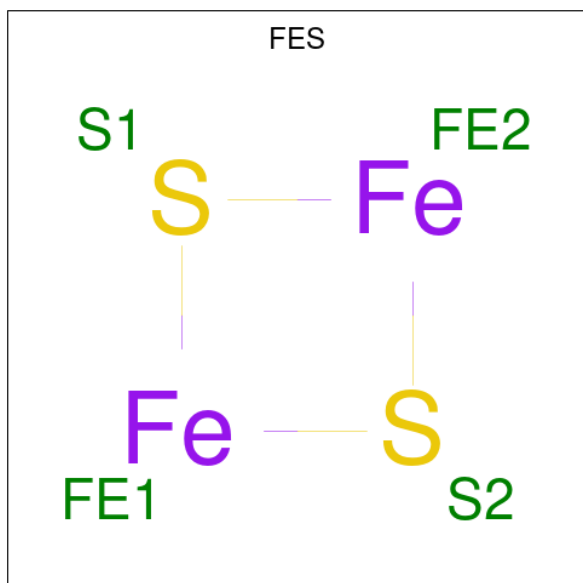
Mol	Chain	Residues	Atoms					AltConf
51	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

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



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

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

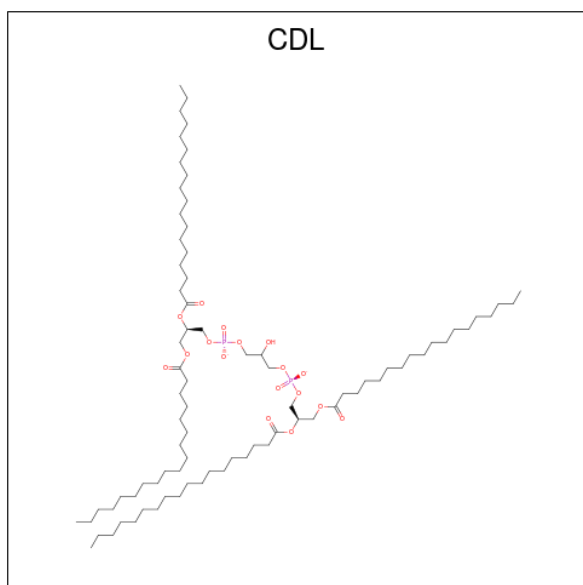


Mol	Chain	Residues	Atoms			AltConf
53	M	1	Total	Fe	S	0
			4	2	2	
53	O	1	Total	Fe	S	0
			4	2	2	

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

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

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



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

Continued on next page...

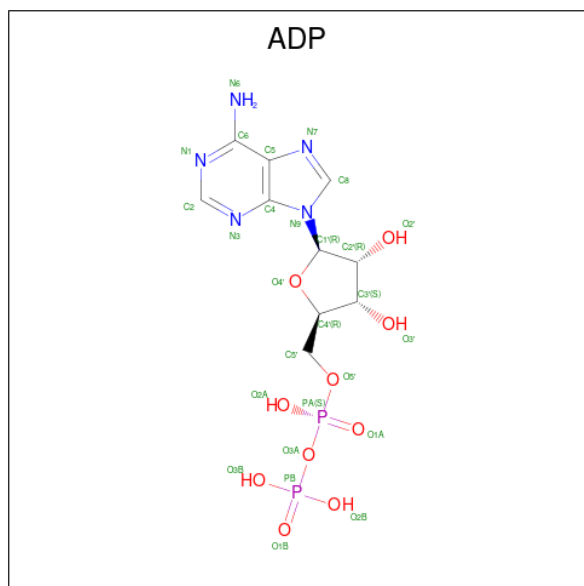
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
55	m	1	Total	C	O	P	0
			95	76	17	2	
55	r	1	Total	C	O	P	0
			99	80	17	2	
55	s	1	Total	C	O	P	0
			89	70	17	2	
55	u	1	Total	C	O	P	0
			55	36	17	2	

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

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

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

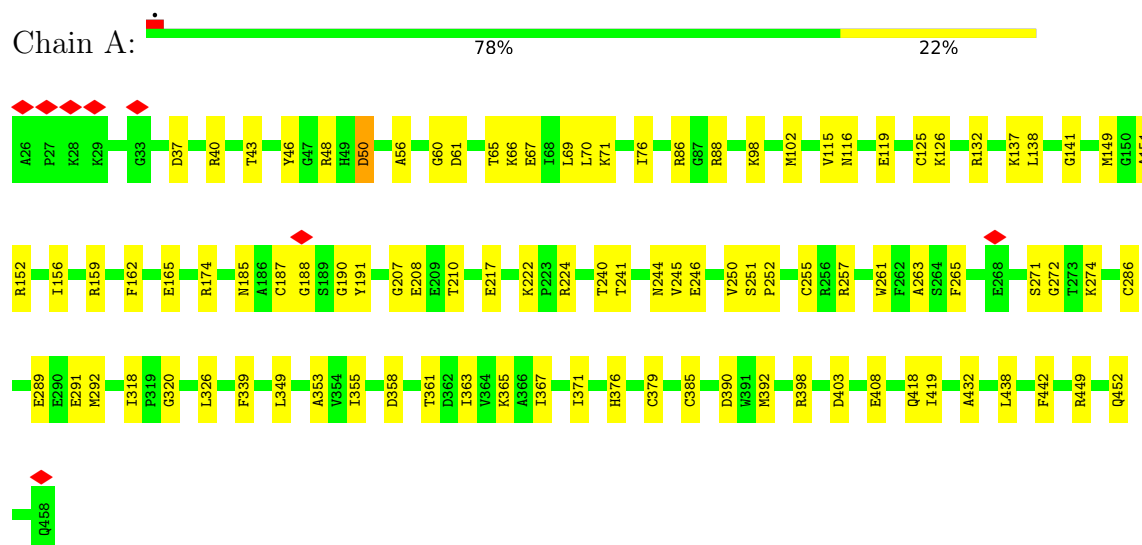


Mol	Chain	Residues	Atoms					AltConf
57	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

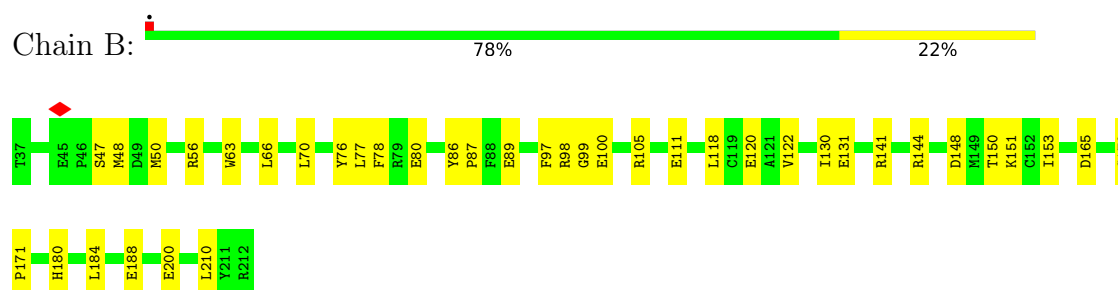
3 Residue-property plots

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

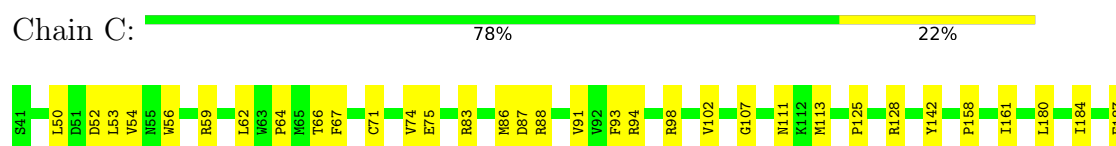
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



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

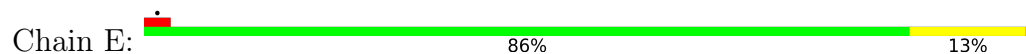


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

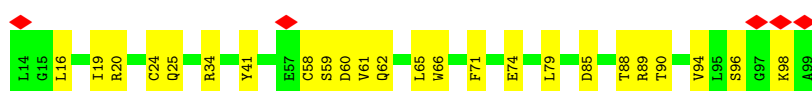




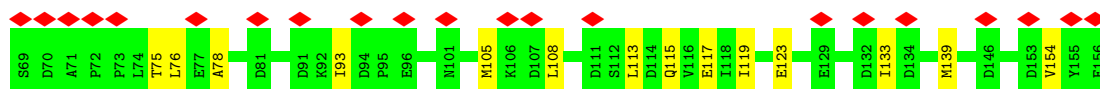
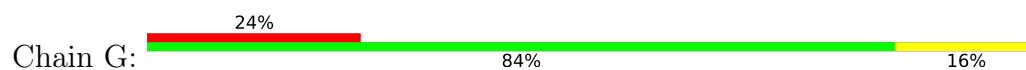
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



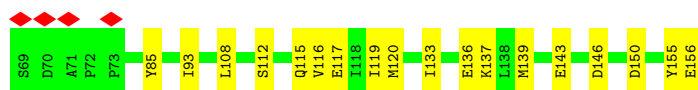
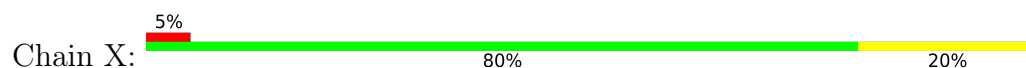
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



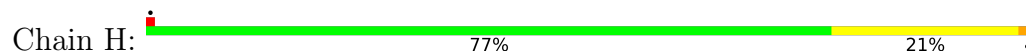
- Molecule 6: Acyl carrier protein



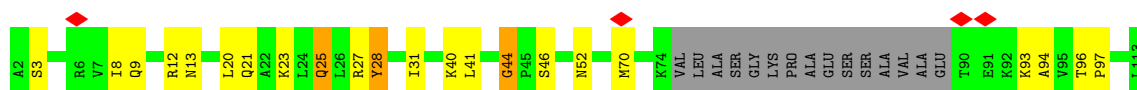
- Molecule 6: Acyl carrier protein



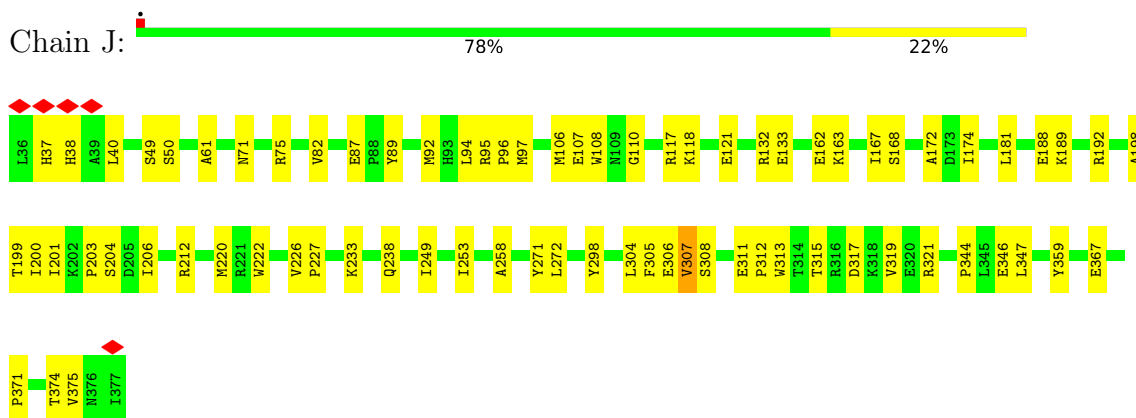
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



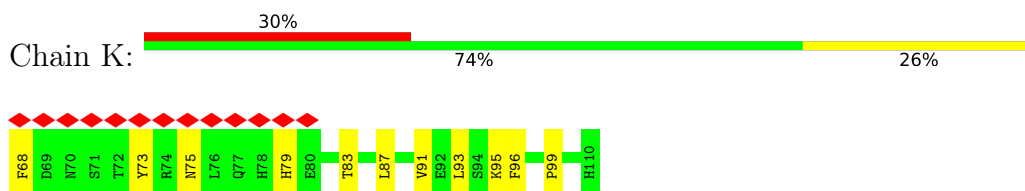
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



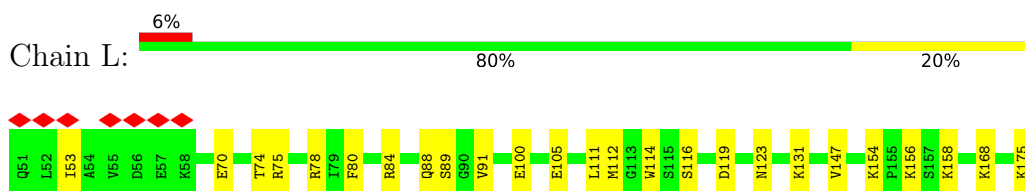
- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial



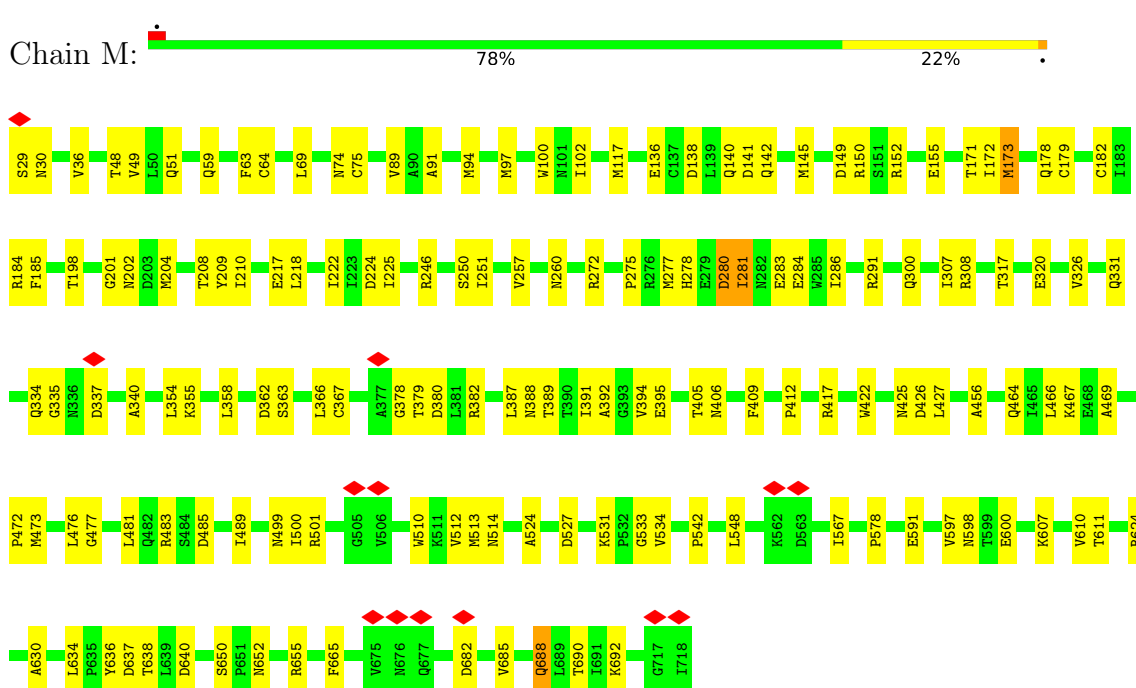
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



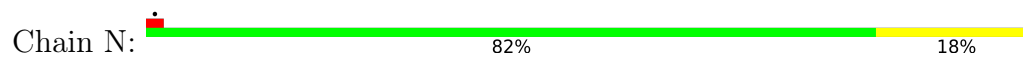
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



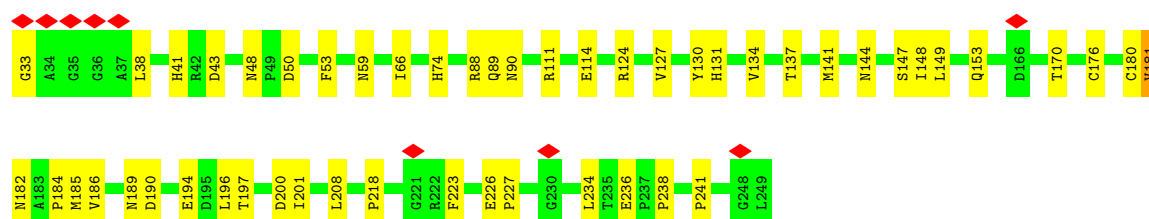
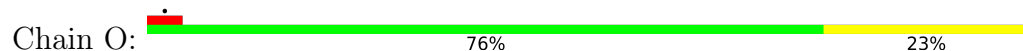
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



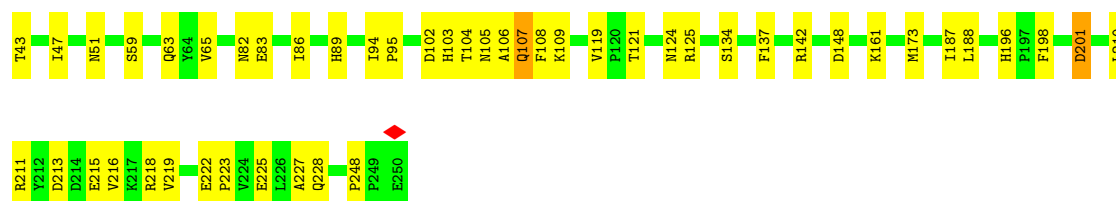
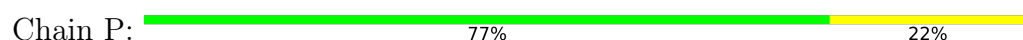
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



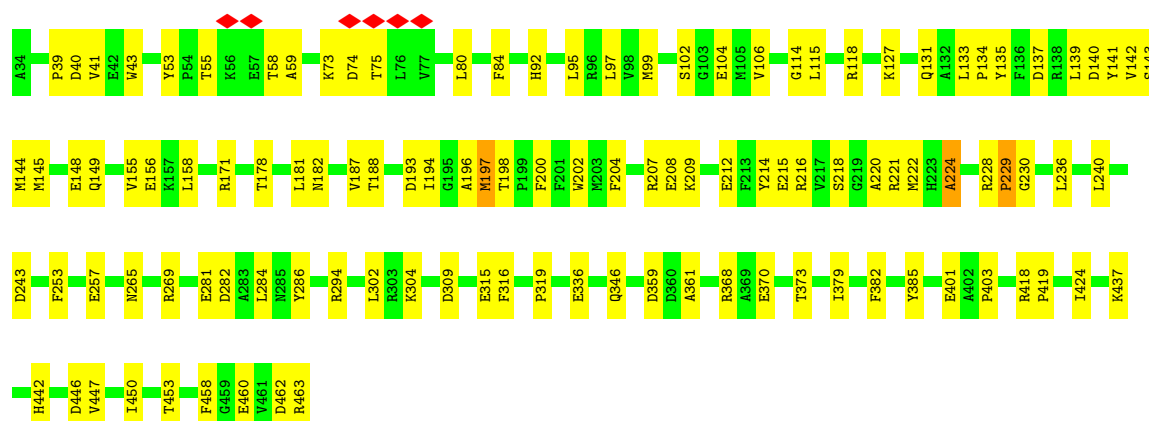
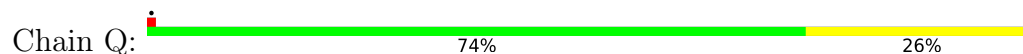
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



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



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

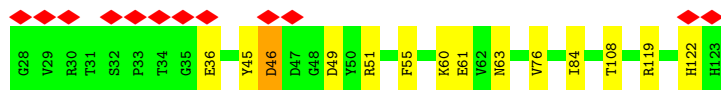
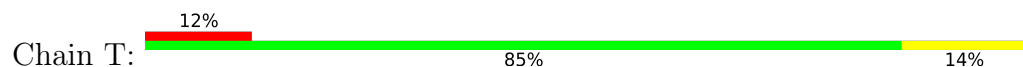


- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

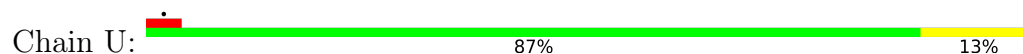




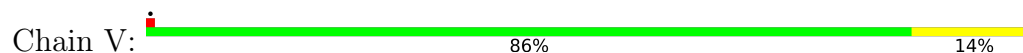
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



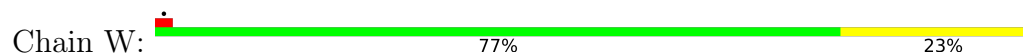
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



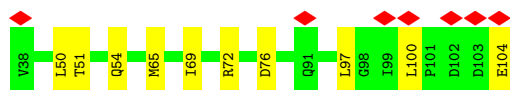
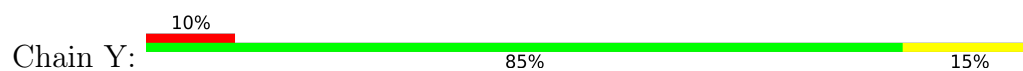
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



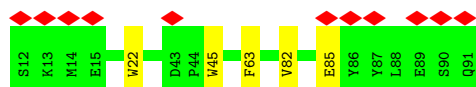
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



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



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



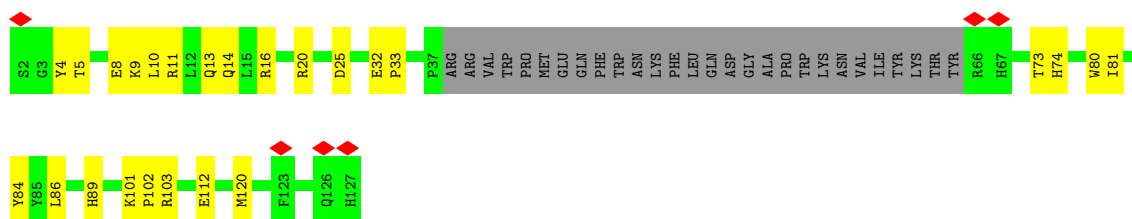
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:  86% 14%



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

Chain b:  5% 58% 20% 22%



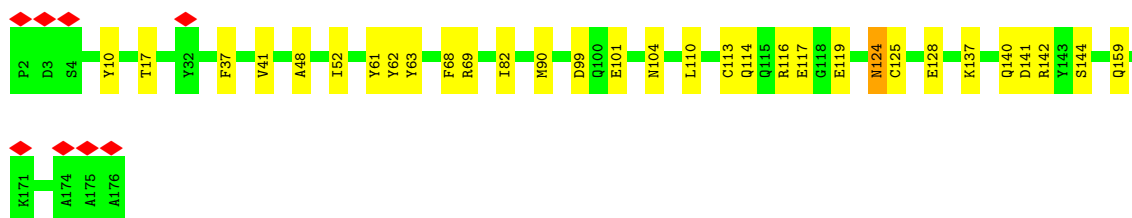
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c:  81% 18%



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

Chain d:  5% 82% 17%

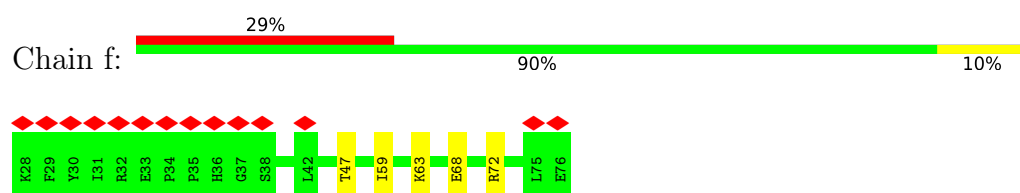


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

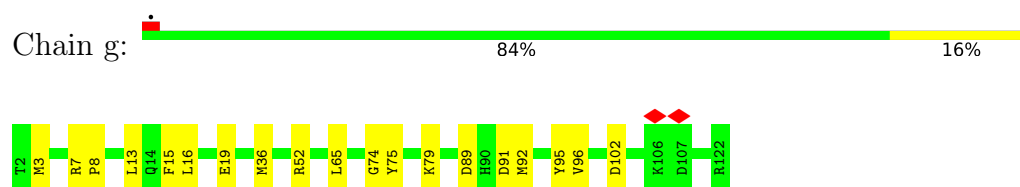
Chain e:  8% 75% 25%



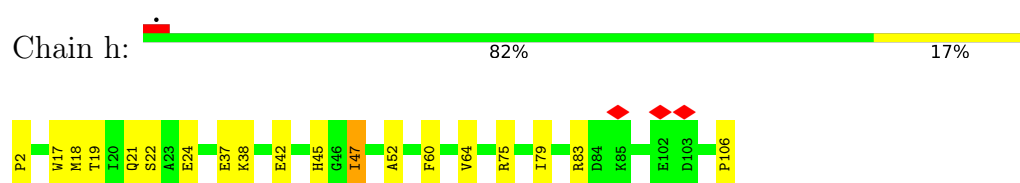
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



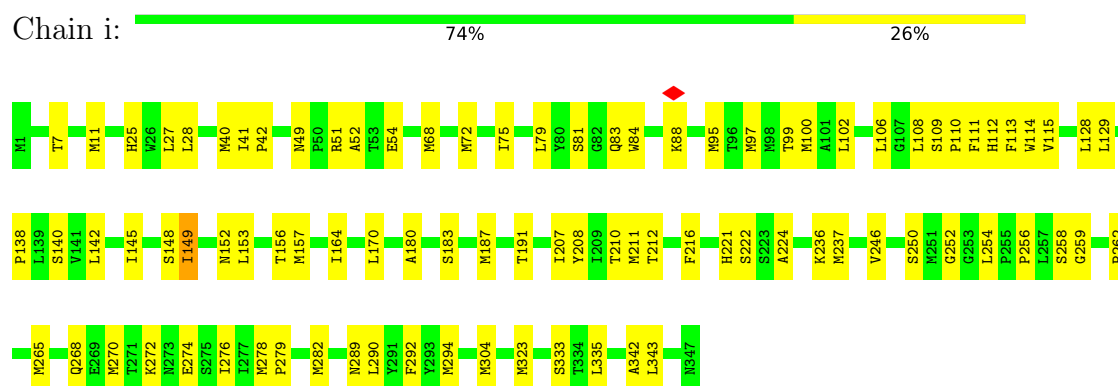
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



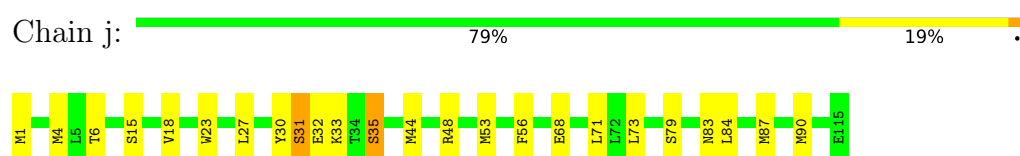
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



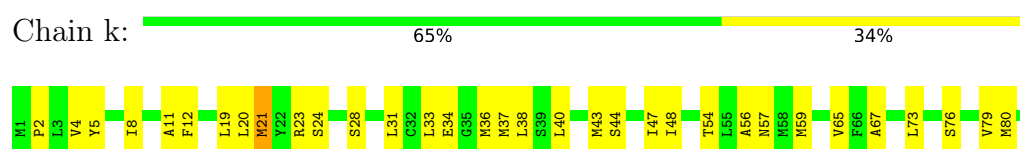
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



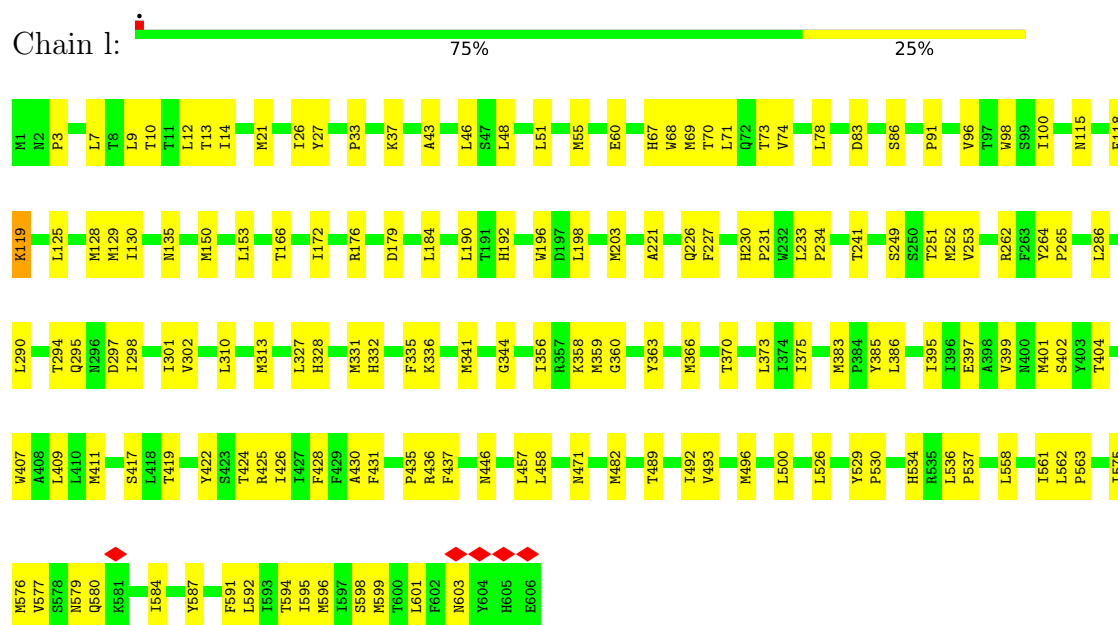
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3



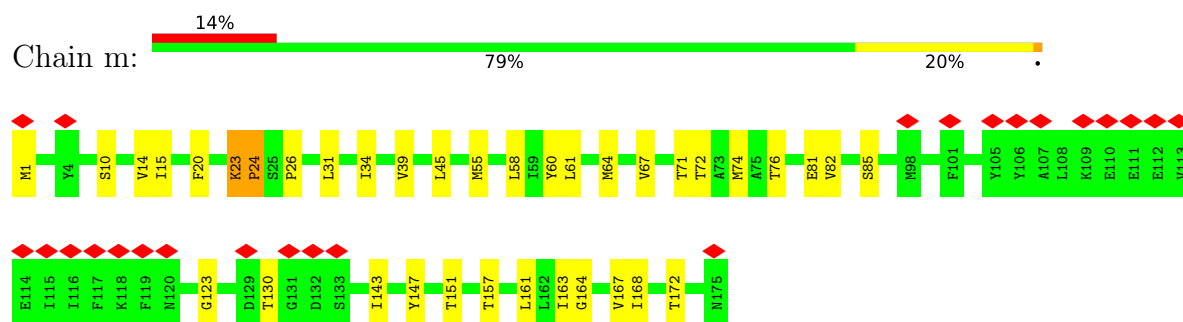
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L



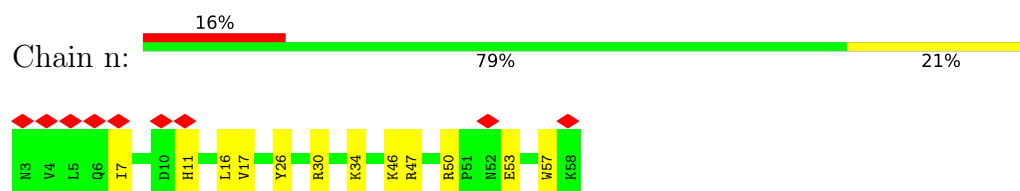
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5



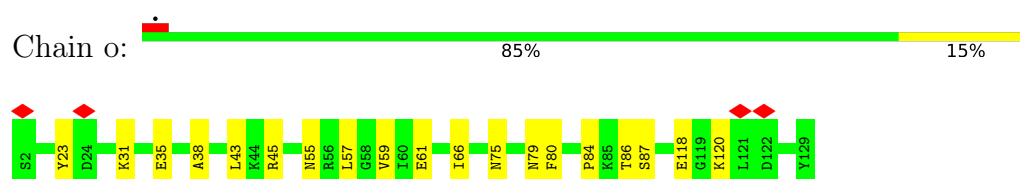
• Molecule 36: NADH-ubiquinone oxidoreductase chain 6



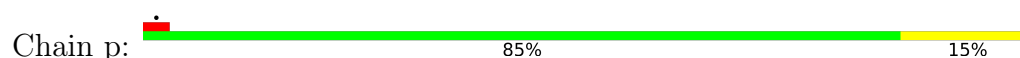
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

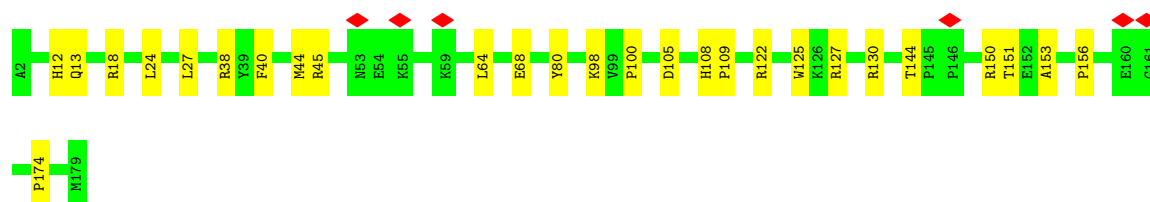


• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



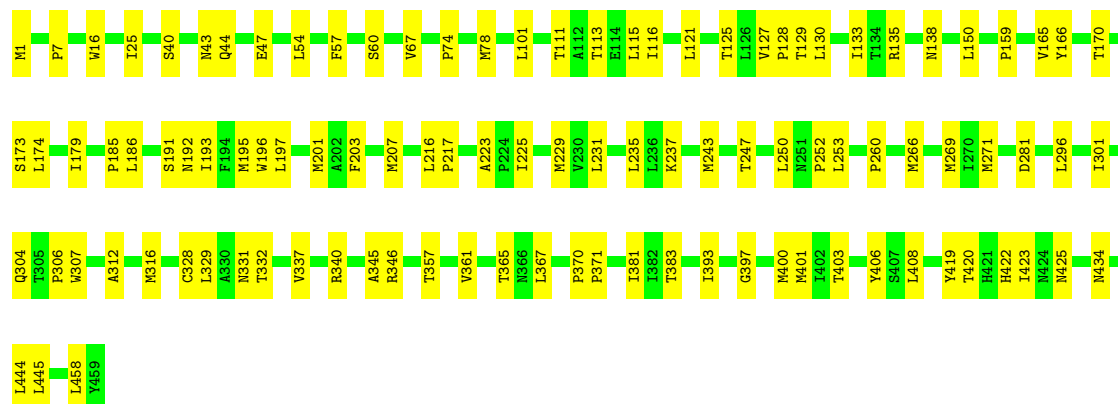
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9





- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r: 77% 23%



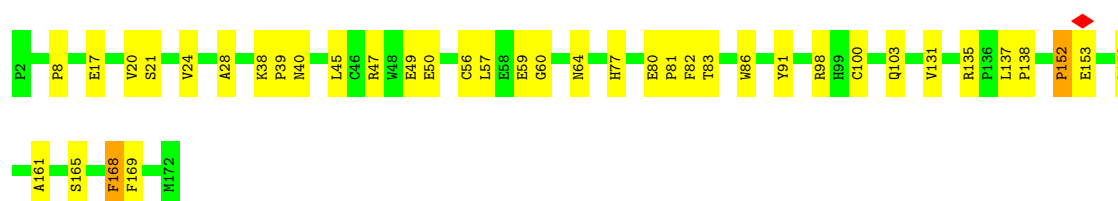
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s: 68% 31%

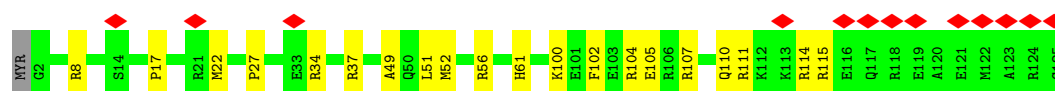
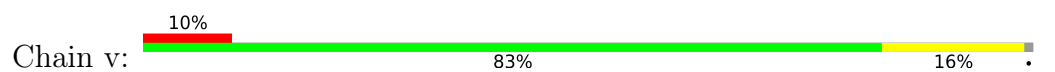


- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

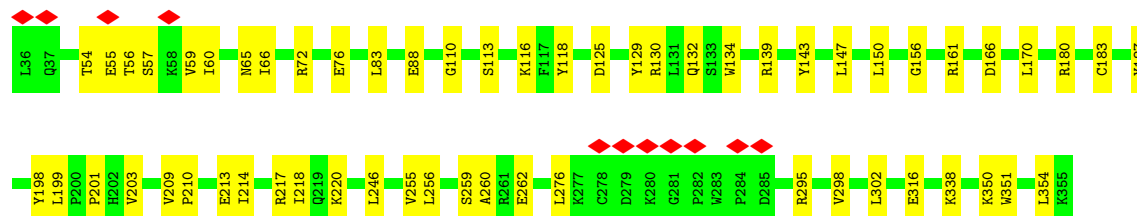
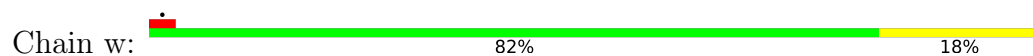
Chain u: 77% 22%



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	111024	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	0.208	Depositor
Minimum map value	-0.124	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0257	Depositor
Map size ($\text{\AA}$)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: CDL, FMN, 970, SF4, PEE, FES, ZN, NDP, MG, UQ, 8Q1, 2MR, ADP, PLX

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.17	0/3406	0.39	0/4603
2	B	0.16	0/1443	0.36	0/1952
3	C	0.22	0/1279	0.43	0/1730
4	E	0.17	0/995	0.41	0/1340
5	F	0.14	0/698	0.40	0/940
6	G	0.14	0/705	0.47	2/956 (0.2%)
6	X	0.16	0/711	0.41	0/963
7	H	0.16	0/929	0.51	1/1258 (0.1%)
8	I	0.26	0/798	0.71	3/1079 (0.3%)
9	J	0.18	0/2828	0.44	1/3834 (0.0%)
10	K	0.09	0/377	0.28	0/509
11	L	0.15	0/1039	0.40	0/1403
12	M	0.23	0/5384	0.57	4/7295 (0.1%)
13	N	0.11	0/1245	0.33	0/1694
14	O	0.18	0/1711	0.45	0/2328
15	P	0.27	0/1789	0.58	3/2436 (0.1%)
16	Q	0.24	0/3538	0.52	5/4796 (0.1%)
17	S	0.23	0/581	0.65	1/781 (0.1%)
18	T	0.14	0/755	0.35	0/1018
19	U	0.10	0/664	0.27	0/912
20	V	0.16	0/1042	0.38	0/1411
21	W	0.16	0/1198	0.42	0/1617
22	Y	0.14	0/610	0.40	0/836
23	Z	0.09	0/660	0.28	0/892
24	a	0.17	0/1184	0.45	1/1603 (0.1%)
25	b	0.17	0/844	0.38	0/1149
26	c	0.14	0/1371	0.51	2/1875 (0.1%)
27	d	0.20	0/1494	0.48	1/2015 (0.0%)
28	e	0.12	0/891	0.32	0/1210
29	f	0.19	0/385	0.42	0/522
30	g	0.15	0/1031	0.37	0/1394
31	h	0.18	0/889	0.53	2/1190 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.18	0/2773	0.48	3/3768 (0.1%)
33	j	0.17	0/938	0.48	3/1281 (0.2%)
34	k	0.24	0/759	0.56	1/1029 (0.1%)
35	l	0.19	0/4947	0.46	3/6728 (0.0%)
36	m	0.20	0/1325	0.53	2/1800 (0.1%)
37	n	0.12	0/491	0.31	0/663
38	o	0.15	0/1092	0.43	1/1481 (0.1%)
39	p	0.10	0/1590	0.29	0/2155
40	r	0.16	0/3723	0.44	4/5078 (0.1%)
41	s	0.19	0/2581	0.47	2/3529 (0.1%)
42	u	0.16	0/1436	0.42	1/1938 (0.1%)
43	v	0.12	0/1052	0.36	0/1411
44	w	0.11	0/2646	0.31	0/3584
All	All	0.18	0/67827	0.45	46/91986 (0.1%)

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	r	250	LEU	N-CA-C	10.60	122.83	111.28
12	M	74	ASN	N-CA-C	10.27	122.56	111.36
26	c	75	TYR	CA-C-N	9.67	129.62	119.85
26	c	75	TYR	C-N-CA	9.67	129.62	119.85
16	Q	197	MET	N-CA-C	9.37	121.57	111.36
36	m	23	LYS	CA-C-N	8.18	130.06	119.84
36	m	23	LYS	C-N-CA	8.18	130.06	119.84
12	M	173	MET	N-CA-C	7.70	120.75	111.82
35	l	192	HIS	N-CA-C	7.60	119.65	111.36
8	I	44	GLY	CA-C-N	7.54	127.42	119.05
8	I	44	GLY	C-N-CA	7.54	127.42	119.05
32	i	114	TRP	N-CA-C	7.40	119.34	111.28
35	l	26	ILE	N-CA-C	-7.36	106.72	113.71
31	h	45	HIS	N-CA-C	7.07	118.99	111.28
34	k	54	THR	N-CA-C	7.05	118.96	111.28
8	I	28	TYR	N-CA-C	6.96	118.66	111.14
16	Q	102	SER	N-CA-C	-6.96	97.38	108.73
15	P	196	HIS	CA-C-N	6.62	126.39	119.05
15	P	196	HIS	C-N-CA	6.62	126.39	119.05
38	o	55	ASN	N-CA-C	6.53	118.40	111.28
33	j	35	SER	CA-C-N	6.26	126.22	119.78
33	j	35	SER	C-N-CA	6.26	126.22	119.78
24	a	163	ARG	N-CA-C	6.15	118.06	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	224	ALA	N-CA-C	6.00	117.82	111.28
9	J	307	VAL	N-CA-C	5.86	116.59	110.62
40	r	422	HIS	N-CA-C	5.70	120.23	113.16
15	P	248	PRO	CA-N-CD	-5.64	104.10	112.00
32	i	113	PHE	N-CA-C	5.62	117.41	111.28
12	M	280	ASP	N-CA-C	5.50	117.36	111.36
41	s	67	SER	N-CA-C	-5.48	100.36	109.46
16	Q	140	ASP	N-CA-C	-5.42	98.37	108.02
31	h	47	ILE	N-CA-C	5.36	116.08	110.62
41	s	217	ALA	CB-CA-C	-5.33	110.42	116.54
7	H	104	VAL	N-CA-C	5.32	116.05	110.62
17	S	34	LYS	N-CA-C	5.29	119.43	112.92
42	u	165	SER	N-CA-C	5.29	117.04	111.28
16	Q	187	VAL	N-CA-C	5.25	115.47	110.53
6	G	133	ILE	CA-C-N	5.23	134.22	125.02
6	G	133	ILE	C-N-CA	5.23	134.22	125.02
40	r	422	HIS	CA-C-N	-5.20	116.25	122.22
40	r	422	HIS	C-N-CA	-5.20	116.25	122.22
33	j	31	SER	N-CA-C	5.18	116.92	111.28
27	d	124	ASN	N-CA-C	5.17	116.92	111.28
32	i	112	HIS	N-CA-C	5.13	119.17	113.01
35	l	74	VAL	N-CA-C	5.10	116.16	109.58
12	M	469	ALA	N-CA-C	5.03	117.59	110.10

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	90	0
2	B	1412	0	1363	35	0
3	C	1248	0	1254	34	0
4	E	971	0	975	13	0
5	F	687	0	700	22	0
6	G	693	0	671	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	X	699	0	682	12	0
7	H	910	0	950	20	0
8	I	780	0	808	30	0
9	J	2751	0	2773	62	0
10	K	366	0	338	9	0
11	L	1016	0	1016	21	0
12	M	5296	0	5329	132	0
13	N	1204	0	1162	25	0
14	O	1671	0	1675	44	0
15	P	1738	0	1693	39	0
16	Q	3459	0	3396	112	0
17	S	566	0	561	25	0
18	T	741	0	702	11	0
19	U	643	0	642	9	0
20	V	1021	0	1025	14	0
21	W	1167	0	1155	28	0
22	Y	584	0	529	11	0
23	Z	641	0	620	5	0
24	a	1151	0	1164	24	0
25	b	819	0	835	24	0
26	c	1315	0	1208	23	0
27	d	1461	0	1431	35	0
28	e	867	0	817	20	0
29	f	377	0	353	3	0
30	g	1000	0	994	19	0
31	h	867	0	873	20	0
32	i	2710	0	2874	78	0
33	j	914	0	951	28	0
34	k	748	0	799	42	0
35	l	4816	0	4955	130	0
36	m	1292	0	1261	46	0
37	n	479	0	486	9	0
38	o	1062	0	1072	18	0
39	p	1534	0	1469	24	0
40	r	3631	0	3839	83	0
41	s	2508	0	2607	107	0
42	u	1398	0	1374	30	0
43	v	1028	0	982	19	0
44	w	2586	0	2542	35	0
45	A	8	0	0	1	0
45	B	16	0	0	0	0
45	C	8	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	M	16	0	0	7	0
46	A	31	0	19	6	0
47	B	51	0	82	3	0
47	Q	47	0	71	23	0
47	U	51	0	82	5	0
47	W	41	0	59	17	0
47	b	46	0	69	10	0
47	f	1	0	0	0	0
47	j	41	0	58	4	0
47	l	90	0	131	10	0
47	r	51	0	82	18	0
47	s	47	0	71	5	0
47	v	1	0	0	0	0
48	C	52	0	88	6	0
48	J	52	0	88	4	0
48	a	52	0	88	2	0
48	g	52	0	88	8	0
48	j	52	0	88	2	0
48	r	104	0	176	10	0
49	C	29	0	0	0	0
50	G	35	0	0	0	0
50	X	35	0	0	5	0
51	J	48	0	23	2	0
52	J	33	0	39	11	0
52	s	38	0	47	6	0
53	M	4	0	0	3	0
53	O	4	0	0	3	0
54	M	1	0	0	0	0
55	N	51	0	46	18	0
55	V	194	0	294	16	0
55	a	100	0	156	8	0
55	l	199	0	307	30	0
55	m	95	0	143	6	0
55	r	99	0	151	9	0
55	s	89	0	125	33	0
55	u	55	0	54	8	0
56	T	1	0	0	0	0
57	w	27	0	11	2	0
All	All	68204	0	68933	1450	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (1450) 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)
41:s:62:ARG:CD	41:s:68:ILE:HD13	1.53	1.36
16:Q:53:TYR:OH	47:Q:501:PEE:C1	1.75	1.34
50:X:201:8Q1:O2	39:p:13:GLN:NE2	1.59	1.32
5:F:71:PHE:CE1	12:M:334:GLN:NE2	1.99	1.29
8:I:23:LYS:HD2	16:Q:253:PHE:CD2	1.67	1.28
41:s:62:ARG:HD2	41:s:68:ILE:CD1	1.63	1.27
5:F:71:PHE:HE1	12:M:334:GLN:NE2	1.30	1.25
8:I:46:SER:O	8:I:52:ASN:ND2	1.68	1.24
27:d:113:CYS:SG	27:d:125:CYS:CB	2.26	1.23
8:I:23:LYS:CE	16:Q:253:PHE:HE2	1.52	1.22
51:J:401:NDP:O4D	51:J:401:NDP:C4D	1.68	1.21
16:Q:53:TYR:OH	47:Q:501:PEE:H2	1.03	1.17
47:W:201:PEE:H38	55:s:402:CDL:C64	1.76	1.15
8:I:23:LYS:CE	16:Q:253:PHE:CE2	2.28	1.14
9:J:220:MET:CE	9:J:227:PRO:HD2	1.79	1.13
8:I:23:LYS:NZ	16:Q:253:PHE:HE2	1.45	1.12
27:d:113:CYS:SG	27:d:125:CYS:HB3	1.91	1.09
8:I:23:LYS:HD2	16:Q:253:PHE:CE2	1.90	1.05
47:b:201:PEE:H3	48:r:503:PLX:H21	1.09	1.05
35:l:599:MET:O	35:l:603:ASN:HB3	1.57	1.03
12:M:179:CYS:SG	45:M:802:SF4:FE1	1.52	1.02
47:W:201:PEE:C23	55:s:402:CDL:C64	2.36	1.02
15:P:125:ARG:NH2	15:P:201:ASP:OD1	1.92	1.00
16:Q:53:TYR:OH	47:Q:501:PEE:H8	1.61	1.00
47:Q:501:PEE:H42	47:Q:501:PEE:H34	1.43	1.00
35:l:596:MET:SD	55:m:201:CDL:C62	2.51	0.98
55:N:201:CDL:H532	55:N:201:CDL:CA7	1.93	0.98
16:Q:141:TYR:O	16:Q:144:MET:SD	2.21	0.98
41:s:73:ILE:HD11	55:s:402:CDL:H202	1.45	0.98
8:I:23:LYS:CD	16:Q:253:PHE:CE2	2.46	0.98
38:o:61:GLU:OE2	38:o:66:ILE:HD11	1.64	0.97
34:k:21:MET:O	36:m:23:LYS:HE3	1.64	0.97
1:A:116:ASN:O	1:A:245:VAL:HG23	1.64	0.97
1:A:48:ARG:HH21	14:O:226:GLU:CD	1.72	0.96
12:M:391:ILE:HG13	12:M:600:GLU:OE2	1.66	0.96
27:d:104:ASN:OD1	35:l:73:THR:O	1.84	0.95
1:A:48:ARG:NH2	14:O:226:GLU:CD	2.24	0.95
47:r:501:PEE:H71	47:r:501:PEE:H34	1.49	0.95
55:a:201:CDL:H512	47:b:201:PEE:H13	1.49	0.95
1:A:125:CYS:SG	14:O:181:VAL:HG22	2.08	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:62:ARG:CG	41:s:68:ILE:HD13	1.98	0.93
8:I:23:LYS:HE3	16:Q:253:PHE:CE2	2.03	0.93
55:s:402:CDL:H852	55:s:402:CDL:C41	1.99	0.93
17:S:31:ASN:ND2	17:S:60:TYR:OH	2.02	0.92
47:b:201:PEE:H3	48:r:503:PLX:C2	1.98	0.92
36:m:23:LYS:NZ	55:m:201:CDL:OB9	2.02	0.92
1:A:392:MET:HE2	1:A:419:ILE:HD12	1.52	0.91
33:j:27:LEU:HD21	41:s:60:PRO:HD2	1.50	0.91
55:s:402:CDL:H852	55:s:402:CDL:H412	1.53	0.91
12:M:389:THR:HG21	12:M:473:MET:HE3	1.53	0.90
55:N:201:CDL:H312	55:N:201:CDL:C54	2.00	0.90
3:C:59:ARG:NH1	48:C:302:PLX:O3	2.04	0.90
33:j:33:LYS:HD3	41:s:61:LEU:HD21	1.54	0.89
1:A:244:ASN:N	46:A:502:FMN:O1P	2.05	0.89
55:a:201:CDL:H512	47:b:201:PEE:C11	2.03	0.89
5:F:71:PHE:CZ	12:M:334:GLN:NE2	2.41	0.88
17:S:34:LYS:O	42:u:91:TYR:O	1.92	0.88
47:Q:501:PEE:H28	47:Q:501:PEE:H36	1.57	0.87
46:A:502:FMN:N1	46:A:502:FMN:O3'	2.08	0.87
32:i:99:THR:HG21	32:i:153:LEU:HD23	1.55	0.87
41:s:221:ALA:O	41:s:225:MET:HG3	1.75	0.86
12:M:389:THR:HG22	12:M:514:ASN:OD1	1.73	0.86
34:k:20:LEU:HD13	35:l:592:LEU:HB2	1.57	0.86
24:a:163:ARG:HH22	30:g:102:ASP:CG	1.83	0.86
33:j:27:LEU:CD2	41:s:60:PRO:HD2	2.06	0.86
8:I:23:LYS:HZ2	16:Q:253:PHE:HE2	1.07	0.86
16:Q:53:TYR:CZ	47:Q:501:PEE:H2	2.11	0.85
24:a:94:GLY:O	27:d:61:TYR:OH	1.93	0.85
47:b:201:PEE:C1	48:r:503:PLX:H21	2.01	0.85
16:Q:144:MET:HG2	16:Q:222:MET:O	1.77	0.85
47:W:201:PEE:H58	41:s:108:MET:HE1	1.59	0.85
34:k:23:ARG:HG3	36:m:23:LYS:HE2	1.59	0.85
14:O:134:VAL:HG23	14:O:186:VAL:HG12	1.58	0.84
55:s:402:CDL:H381	55:s:402:CDL:H742	1.59	0.84
12:M:278:HIS:O	12:M:283:GLU:HA	1.75	0.84
55:u:201:CDL:H581	55:u:201:CDL:H541	1.60	0.84
34:k:79:VAL:HG23	36:m:74:MET:HE1	1.60	0.83
25:b:103:ARG:NH1	43:v:49:ALA:O	2.10	0.83
12:M:690:THR:HG23	12:M:692:LYS:HG2	1.60	0.83
41:s:62:ARG:CD	41:s:68:ILE:CD1	2.38	0.83
12:M:178:GLN:HG2	12:M:204:MET:HE3	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:6:VAL:HG12	13:N:9:ARG:HH21	1.43	0.83
16:Q:53:TYR:HE1	47:Q:501:PEE:H10	1.41	0.83
15:P:125:ARG:HH22	15:P:201:ASP:CG	1.86	0.82
16:Q:53:TYR:OH	47:Q:501:PEE:C3	2.26	0.82
2:B:76:TYR:OH	16:Q:257:GLU:OE1	1.98	0.81
32:i:153:LEU:O	32:i:157:MET:HG3	1.79	0.81
47:Q:501:PEE:H37	47:Q:501:PEE:C37	2.11	0.81
22:Y:97:LEU:HD12	43:v:107:ARG:HH21	1.44	0.81
41:s:62:ARG:HD2	41:s:68:ILE:HD13	0.83	0.81
1:A:126:LYS:NZ	1:A:246:GLU:OE1	2.10	0.81
40:r:191:SER:HB3	47:r:501:PEE:H3	1.63	0.81
47:Q:501:PEE:H34	47:Q:501:PEE:C25	2.10	0.80
9:J:220:MET:HE2	9:J:227:PRO:HD2	1.61	0.80
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.15	0.80
32:i:256:PRO:HB3	55:u:201:CDL:C60	2.12	0.79
1:A:149:MET:HE1	1:A:241:THR:HB	1.64	0.79
21:W:81:ARG:NH2	42:u:64:ASN:OD1	2.14	0.79
7:H:7:LYS:HG3	7:H:8:THR:HG23	1.63	0.79
1:A:149:MET:CE	1:A:241:THR:HB	2.13	0.79
47:r:501:PEE:H81	48:r:502:PLX:H393	1.65	0.78
35:l:401:MET:HE3	35:l:482:MET:HG2	1.64	0.78
40:r:266:MET:HA	40:r:269:MET:HE3	1.65	0.78
25:b:9:LYS:HG2	25:b:13:GLN:HE22	1.49	0.78
32:i:97:MET:SD	35:l:599:MET:HE1	2.24	0.78
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.64	0.78
41:s:62:ARG:CG	41:s:68:ILE:CD1	2.61	0.78
55:N:201:CDL:H532	55:N:201:CDL:C31	2.14	0.77
35:l:190:LEU:HD23	40:r:383:THR:HG21	1.66	0.77
36:m:26:PRO:HB2	36:m:71:THR:HG21	1.66	0.77
15:P:161:LYS:HD2	16:Q:286:TYR:CE1	2.19	0.77
35:l:294:THR:CG2	55:l:703:CDL:HB62	2.15	0.77
12:M:75:CYS:SG	53:M:803:FES:FE2	1.76	0.77
12:M:337:ASP:O	12:M:542:PRO:CB	2.33	0.77
47:W:201:PEE:H37	55:s:402:CDL:C64	2.14	0.77
6:X:150:ASP:OD2	25:b:16:ARG:NH1	2.19	0.76
22:Y:76:ASP:O	35:l:385:TYR:OH	2.03	0.76
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.66	0.76
1:A:48:ARG:NH2	14:O:226:GLU:OE1	2.11	0.76
3:C:158:PRO:HB2	9:J:92:MET:HE3	1.67	0.76
12:M:483:ARG:NH2	12:M:682:ASP:HB3	2.01	0.76
11:L:168:LYS:HE2	11:L:168:LYS:HA	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.68	0.75
5:F:71:PHE:HE1	12:M:334:GLN:HE21	0.77	0.75
15:P:109:LYS:NZ	16:Q:281:GLU:OE2	2.16	0.75
16:Q:53:TYR:HH	47:Q:501:PEE:H2	0.78	0.75
12:M:391:ILE:CG1	12:M:600:GLU:OE2	2.33	0.75
8:I:23:LYS:HD2	16:Q:253:PHE:HD2	1.45	0.75
36:m:72:THR:HG21	41:s:133:LEU:HD21	1.69	0.75
1:A:66:LYS:HE2	1:A:188:GLY:C	2.12	0.74
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.19	0.74
47:l:704:PEE:C11	47:l:704:PEE:H7	2.17	0.74
1:A:152:ARG:NH2	10:K:99:PRO:O	2.20	0.74
26:c:116:ARG:HG2	47:l:704:PEE:H49	1.70	0.74
34:k:80:MET:HE3	36:m:172:THR:HA	1.69	0.74
14:O:185:MET:HB3	14:O:194:GLU:HA	1.69	0.74
55:s:402:CDL:H412	55:s:402:CDL:C85	2.18	0.74
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.21	0.73
47:b:201:PEE:H10	48:r:503:PLX:O2	1.88	0.73
47:l:704:PEE:H7	47:l:704:PEE:H14	1.69	0.73
35:l:601:LEU:O	35:l:601:LEU:HD23	1.88	0.73
55:N:201:CDL:H532	55:N:201:CDL:H312	1.69	0.73
16:Q:53:TYR:HH	47:Q:501:PEE:C1	1.73	0.73
9:J:50:SER:OG	15:P:225:GLU:OE2	2.06	0.73
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.71	0.73
47:Q:501:PEE:H42	47:Q:501:PEE:C21	2.18	0.73
9:J:220:MET:HE3	9:J:227:PRO:HD2	1.69	0.73
35:l:363:TYR:HA	35:l:370:THR:HG21	1.69	0.73
35:l:500:LEU:HD13	55:l:703:CDL:H351	1.71	0.73
12:M:466:LEU:HD13	12:M:500:ILE:HD11	1.71	0.72
47:W:201:PEE:C37	55:s:402:CDL:H632	2.19	0.72
32:i:100:MET:HE2	32:i:153:LEU:HD21	1.71	0.72
55:N:201:CDL:H312	55:N:201:CDL:C53	2.19	0.72
32:i:207:ILE:HG22	32:i:211:MET:HE2	1.72	0.72
27:d:114:GLN:HG3	35:l:203:MET:HG2	1.71	0.72
5:F:41:TYR:OH	12:M:380:ASP:HB3	1.90	0.72
27:d:101:GLU:OE1	28:e:115:GLN:NE2	2.23	0.72
27:d:113:CYS:SG	27:d:125:CYS:HB2	2.27	0.72
41:s:195:ARG:HG3	41:s:231:ILE:HD11	1.72	0.72
17:S:28:LYS:O	17:S:33:GLY:N	2.23	0.71
24:a:163:ARG:NH2	30:g:102:ASP:OD2	2.23	0.71
32:i:236:LYS:HG3	32:i:237:MET:HG3	1.70	0.71
44:w:132:GLN:NE2	44:w:166:ASP:OD1	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLY:HA2	14:O:241:PRO:HA	1.73	0.71
12:M:337:ASP:O	12:M:542:PRO:HB2	1.91	0.71
28:e:130:GLU:HG2	28:e:136:LEU:HD21	1.72	0.71
31:h:38:LYS:HE2	31:h:42:GLU:OE1	1.90	0.71
47:W:201:PEE:H36	36:m:39:VAL:HG13	1.73	0.70
17:S:31:ASN:CG	17:S:36:LYS:HB2	2.17	0.70
16:Q:197:MET:HE1	52:s:403:UQ:HM33	1.73	0.70
36:m:23:LYS:N	36:m:24:PRO:HD3	2.06	0.70
47:W:201:PEE:H49	36:m:45:LEU:CD2	2.20	0.70
47:l:704:PEE:H77	40:r:401:MET:HE1	1.73	0.70
31:h:47:ILE:HD11	31:h:52:ALA:HA	1.73	0.70
14:O:180:CYS:SG	53:O:301:FES:FE2	1.82	0.70
47:r:501:PEE:H34	47:r:501:PEE:C42	2.21	0.70
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.31	0.70
22:Y:72:ARG:HB3	35:l:385:TYR:CD1	2.27	0.70
35:l:60:GLU:HG2	35:l:83:ASP:HA	1.73	0.69
1:A:48:ARG:NH2	14:O:226:GLU:OE2	2.25	0.69
32:i:256:PRO:CB	55:u:201:CDL:C60	2.70	0.69
41:s:174:MET:HB3	41:s:242:PHE:HA	1.71	0.69
3:C:75:GLU:OE1	16:Q:221:ARG:NH1	2.24	0.69
9:J:344:PRO:HG2	9:J:347:LEU:HD13	1.72	0.69
14:O:59:ASN:ND2	14:O:89:GLN:OE1	2.25	0.69
36:m:31:LEU:HD21	55:s:402:CDL:H542	1.72	0.69
9:J:305:PHE:HE1	9:J:313:TRP:CE3	2.11	0.69
12:M:178:GLN:HG2	12:M:204:MET:CE	2.22	0.69
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.73	0.69
35:l:500:LEU:HD12	55:l:703:CDL:H571	1.75	0.69
44:w:118:TYR:OH	57:w:401:ADP:O2'	2.10	0.69
43:v:51:LEU:O	43:v:52:MET:HG3	1.93	0.69
12:M:389:THR:CG2	12:M:473:MET:HE3	2.22	0.69
36:m:26:PRO:HB2	36:m:71:THR:CG2	2.23	0.69
1:A:43:THR:HG21	14:O:238:PRO:HB3	1.74	0.68
2:B:98:ARG:NH2	16:Q:224:ALA:O	2.26	0.68
55:N:201:CDL:H312	55:N:201:CDL:C55	2.23	0.68
12:M:179:CYS:HG	45:M:802:SF4:FE1	1.09	0.68
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.73	0.68
47:r:501:PEE:H68	47:r:501:PEE:H33	1.75	0.68
12:M:278:HIS:CE1	12:M:280:ASP:HB2	2.29	0.68
32:i:254:LEU:HD21	32:i:290:LEU:HD21	1.76	0.68
30:g:7:ARG:HG3	30:g:8:PRO:HD2	1.76	0.67
55:s:402:CDL:H852	55:s:402:CDL:H411	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:83:GLN:HE21	15:P:107:GLN:NE2	1.92	0.67
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.74	0.67
20:V:17:GLU:OE1	20:V:20:ARG:NH1	2.27	0.67
21:W:121:MET:HE2	21:W:136:ALA:HB1	1.76	0.67
41:s:62:ARG:HG3	41:s:68:ILE:CD1	2.25	0.67
1:A:149:MET:CE	1:A:241:THR:CB	2.73	0.67
39:p:105:ASP:OD1	39:p:122:ARG:NH1	2.27	0.67
55:N:201:CDL:H312	55:N:201:CDL:H541	1.77	0.67
47:W:201:PEE:H36	36:m:39:VAL:CG1	2.25	0.67
17:S:34:LYS:O	17:S:35:GLU:HB3	1.96	0.66
31:h:47:ILE:CD1	31:h:52:ALA:HA	2.25	0.66
32:i:276:ILE:HG21	47:r:501:PEE:H14	1.77	0.66
3:C:184:ILE:O	3:C:187:GLU:HG2	1.94	0.66
12:M:308:ARG:NH2	12:M:578:PRO:O	2.28	0.66
2:B:47:SER:O	2:B:56:ARG:NH2	2.28	0.66
3:C:74:VAL:HB	16:Q:222:MET:HE1	1.77	0.66
32:i:49:ASN:O	32:i:52:ALA:N	2.27	0.66
40:r:301:ILE:O	40:r:304:GLN:NE2	2.28	0.66
41:s:24:GLU:OE1	41:s:228:TYR:OH	2.12	0.66
50:X:201:8Q1:O40	39:p:12:HIS:HE1	1.79	0.66
8:I:3:SER:O	55:N:201:CDL:H1	1.94	0.66
8:I:44:GLY:HA3	16:Q:359:ASP:OD2	1.96	0.66
52:J:402:UQ:C26	52:J:402:UQ:H201	2.25	0.66
12:M:277:MET:HA	12:M:283:GLU:O	1.96	0.66
1:A:125:CYS:SG	14:O:181:VAL:CG2	2.84	0.66
9:J:87:GLU:HG3	9:J:89:TYR:H	1.61	0.66
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.29	0.66
38:o:57:LEU:CD2	40:r:425:ASN:HB3	2.25	0.66
47:r:501:PEE:H71	47:r:501:PEE:C21	2.25	0.65
11:L:123:ASN:OD1	12:M:246:ARG:NH2	2.28	0.65
38:o:61:GLU:OE2	38:o:66:ILE:CD1	2.43	0.65
40:r:231:LEU:HD23	40:r:235:LEU:HD12	1.78	0.65
7:H:105:GLU:HB3	15:P:89:HIS:CD2	2.31	0.65
12:M:485:ASP:OD1	12:M:489:ILE:HD11	1.97	0.65
17:S:12:MET:HE3	41:s:20:LEU:HB2	1.78	0.65
18:T:108:THR:HG22	18:T:119:ARG:HD3	1.78	0.65
9:J:359:TYR:HD1	41:s:65:THR:HG22	1.61	0.65
9:J:305:PHE:CE1	9:J:313:TRP:CE3	2.84	0.65
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.78	0.65
8:I:23:LYS:NZ	16:Q:253:PHE:CE2	2.36	0.65
41:s:52:ALA:HB1	47:s:401:PEE:H79	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:34:LYS:O	17:S:35:GLU:CB	2.44	0.65
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.79	0.65
27:d:113:CYS:HG	27:d:125:CYS:CB	1.95	0.65
38:o:57:LEU:HD23	40:r:425:ASN:HB3	1.76	0.65
1:A:159:ARG:NH2	14:O:176:CYS:O	2.29	0.65
12:M:182:CYS:HG	45:M:802:SF4:FE3	1.10	0.64
47:Q:501:PEE:H37	47:Q:501:PEE:H60	1.78	0.64
30:g:7:ARG:CG	30:g:8:PRO:HD2	2.27	0.64
44:w:125:ASP:O	44:w:130:ARG:NH2	2.30	0.64
12:M:75:CYS:HG	53:M:803:FES:FE2	1.14	0.64
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.79	0.64
16:Q:53:TYR:OH	47:Q:501:PEE:C2	2.42	0.64
16:Q:294:ARG:NH2	16:Q:401:GLU:OE2	2.30	0.64
46:A:502:FMN:HO3'	46:A:502:FMN:C2	2.05	0.64
2:B:111:GLU:O	2:B:141:ARG:NH1	2.31	0.64
16:Q:178:THR:HG1	16:Q:214:TYR:HH	1.39	0.64
36:m:61:LEU:O	41:s:114:TYR:OH	2.14	0.64
12:M:278:HIS:O	12:M:283:GLU:CA	2.46	0.64
16:Q:218:SER:CB	16:Q:224:ALA:HB1	2.27	0.64
32:i:100:MET:CE	32:i:153:LEU:HD11	2.28	0.64
24:a:163:ARG:NH1	30:g:102:ASP:OD2	2.30	0.64
25:b:80:TRP:HD1	27:d:41:VAL:HG23	1.63	0.64
9:J:188:GLU:HG3	9:J:200:ILE:HD13	1.79	0.64
12:M:182:CYS:SG	45:M:802:SF4:FE3	1.89	0.64
18:T:46:ASP:N	18:T:46:ASP:OD1	2.29	0.64
26:c:139:PHE:CD2	55:l:703:CDL:H862	2.33	0.64
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.80	0.64
35:l:601:LEU:HD23	35:l:601:LEU:C	2.23	0.63
50:X:201:8Q1:C10	39:p:44:MET:HE1	2.28	0.63
37:n:47:ARG:NH2	37:n:53:GLU:OE2	2.30	0.63
55:l:703:CDL:H321	55:l:703:CDL:H111	1.79	0.63
7:H:101:GLU:HB3	7:H:102:PRO:HD2	1.79	0.63
9:J:71:ASN:HB2	9:J:97:MET:HE2	1.79	0.63
17:S:31:ASN:ND2	17:S:36:LYS:HA	2.13	0.63
40:r:129:THR:HG21	40:r:235:LEU:HD11	1.81	0.63
55:s:402:CDL:H412	55:s:402:CDL:C86	2.29	0.63
44:w:57:SER:HB3	44:w:150:LEU:HD11	1.81	0.63
3:C:83:ARG:NH1	16:Q:212:GLU:OE2	2.26	0.62
11:L:75:ARG:NH1	11:L:119:ASP:OD1	2.30	0.62
33:j:18:VAL:HG11	41:s:76:ILE:HD11	1.79	0.62
1:A:50:ASP:N	1:A:50:ASP:OD1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:136:GLU:OE2	39:p:18:ARG:NH1	2.32	0.62
13:N:9:ARG:NH2	55:N:201:CDL:O1	2.32	0.62
55:a:201:CDL:H512	47:b:201:PEE:H14	1.82	0.62
8:I:96:THR:HB	8:I:97:PRO:HD2	1.81	0.62
12:M:388:ASN:ND2	12:M:513:MET:O	2.32	0.61
20:V:37:SER:O	20:V:41:ILE:HG12	1.99	0.61
48:a:202:PLX:H92	40:r:40:SER:HB3	1.82	0.61
42:u:152:PRO:O	42:u:153:GLU:HG2	1.98	0.61
9:J:49:SER:OG	15:P:225:GLU:HG2	2.01	0.61
24:a:98:LEU:HD12	27:d:63:TYR:O	2.00	0.61
44:w:88:GLU:OE2	44:w:161:ARG:NH1	2.32	0.61
4:E:101:THR:OG1	15:P:219:VAL:O	2.18	0.61
12:M:389:THR:HG22	12:M:514:ASN:CG	2.25	0.61
33:j:27:LEU:HD21	41:s:60:PRO:CD	2.28	0.61
16:Q:315:GLU:O	16:Q:346:GLN:NE2	2.31	0.61
17:S:31:ASN:OD1	17:S:36:LYS:HB2	1.99	0.61
55:u:201:CDL:H581	55:u:201:CDL:C54	2.28	0.61
32:i:110:PRO:HG2	35:l:594:THR:HG21	1.82	0.61
14:O:38:LEU:O	14:O:124:ARG:NH2	2.34	0.61
17:S:28:LYS:HB3	17:S:33:GLY:HA2	1.83	0.61
2:B:200:GLU:HG3	13:N:88:ARG:HD3	1.81	0.61
34:k:44:SER:HB2	34:k:59:MET:HE1	1.83	0.61
37:n:26:TYR:OH	37:n:30:ARG:NH2	2.20	0.61
44:w:54:THR:HG23	44:w:56:THR:HG22	1.83	0.61
12:M:690:THR:CG2	12:M:692:LYS:HG2	2.30	0.61
33:j:27:LEU:HD22	41:s:59:GLU:HG3	1.81	0.61
52:J:402:UQ:HM33	52:J:402:UQ:O2	2.01	0.60
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.82	0.60
32:i:270:MET:HE3	32:i:279:PRO:HG3	1.82	0.60
38:o:75:ASN:O	38:o:79:ASN:ND2	2.33	0.60
42:u:56:CYS:HB2	42:u:59:GLU:OE1	2.00	0.60
1:A:217:GLU:OE2	1:A:224:ARG:NH2	2.34	0.60
9:J:192:ARG:NH1	9:J:198:ALA:O	2.34	0.60
12:M:394:VAL:HG22	12:M:473:MET:HE1	1.83	0.60
13:N:2:GLU:HG3	13:N:4:VAL:HG12	1.81	0.60
24:a:96:ALA:HB2	27:d:61:TYR:CD2	2.36	0.60
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.35	0.60
14:O:197:THR:H	14:O:200:ASP:HB2	1.65	0.60
5:F:24:CYS:HA	5:F:58:CYS:HB3	1.82	0.60
16:Q:104:GLU:HB2	41:s:282:TYR:OH	2.01	0.60
25:b:80:TRP:CD1	27:d:41:VAL:HG23	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:141:VAL:C	24:a:161:ARG:HH11	2.10	0.60
17:S:59:ARG:HB2	17:S:62:VAL:HG23	1.84	0.60
35:l:286:LEU:HD22	35:l:411:MET:SD	2.42	0.60
38:o:118:GLU:O	38:o:120:LYS:NZ	2.34	0.60
9:J:133:GLU:OE1	9:J:212:ARG:HD3	2.02	0.59
12:M:483:ARG:NH2	12:M:682:ASP:O	2.32	0.59
32:i:268:GLN:HA	40:r:165:VAL:HG11	1.83	0.59
11:L:116:SER:OG	15:P:227:ALA:O	2.18	0.59
21:W:140:PHE:O	47:W:201:PEE:H11	2.01	0.59
48:g:201:PLX:H361	48:g:201:PLX:H311	1.84	0.59
4:E:96:VAL:O	4:E:96:VAL:HG23	2.01	0.59
24:a:179:ILE:HG23	31:h:22:SER:HB3	1.83	0.59
7:H:83:GLN:NE2	15:P:107:GLN:NE2	2.50	0.59
6:X:117:GLU:OE2	39:p:45:ARG:NH1	2.36	0.59
26:c:75:TYR:OH	26:c:105:ILE:O	2.15	0.59
40:r:403:THR:HA	40:r:406:TYR:CE2	2.38	0.59
47:B:303:PEE:H7	41:s:288:LEU:HD11	1.83	0.59
52:J:402:UQ:HM23	52:J:402:UQ:O1	2.02	0.59
12:M:48:THR:OG1	12:M:51:GLN:HG3	2.03	0.59
40:r:337:VAL:HG11	40:r:345:ALA:HB2	1.85	0.59
16:Q:53:TYR:HE1	47:Q:501:PEE:C4	2.12	0.59
35:l:10:THR:HA	35:l:13:THR:HG22	1.83	0.59
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.84	0.59
12:M:358:LEU:HB3	12:M:363:SER:HB3	1.85	0.59
27:d:137:LYS:NZ	27:d:141:ASP:OD2	2.35	0.59
34:k:19:LEU:HD23	34:k:36:MET:HE1	1.84	0.59
27:d:128:GLU:N	27:d:128:GLU:OE1	2.36	0.58
32:i:88:LYS:O	32:i:148:SER:CB	2.51	0.58
47:W:201:PEE:C21	47:W:201:PEE:H42	2.32	0.58
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.30	0.58
40:r:196:TRP:HB2	40:r:253:LEU:HD23	1.84	0.58
1:A:185:ASN:ND2	1:A:187:CYS:O	2.37	0.58
13:N:127:TYR:OH	18:T:61:GLU:O	2.17	0.58
47:W:201:PEE:H49	36:m:45:LEU:HD23	1.84	0.58
32:i:41:ILE:HG13	34:k:73:LEU:HD21	1.85	0.58
47:Q:501:PEE:H37	47:Q:501:PEE:H61	1.86	0.58
32:i:95:MET:HE1	32:i:145:ILE:HD12	1.86	0.58
34:k:20:LEU:CD1	35:l:592:LEU:HB2	2.33	0.58
35:l:402:SER:OG	35:l:404:THR:OG1	2.19	0.58
24:a:66:ARG:HA	24:a:69:LYS:HE3	1.86	0.58
11:L:154:LYS:O	11:L:156:LYS:NZ	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:100:MET:HE3	35:l:598:SER:CB	2.33	0.58
40:r:201:MET:HE2	47:r:501:PEE:H77	1.86	0.58
9:J:174:ILE:HD11	9:J:189:LYS:NZ	2.18	0.58
9:J:317:ASP:OD2	9:J:321:ARG:NH1	2.36	0.58
12:M:524:ALA:HB2	12:M:597:VAL:HG23	1.86	0.58
6:X:146:ASP:HB3	25:b:16:ARG:NH1	2.19	0.58
35:l:496:MET:HE3	35:l:496:MET:HA	1.86	0.58
41:s:87:VAL:HG12	41:s:95:LEU:HD23	1.85	0.58
1:A:263:ALA:HA	1:A:271:SER:HB3	1.86	0.58
22:Y:51:THR:OG1	35:l:446:ASN:OD1	2.20	0.58
1:A:61:ASP:OD2	1:A:137:LYS:HG3	2.04	0.58
1:A:418:GLN:HE22	12:M:152:ARG:NH2	2.01	0.58
11:L:114:TRP:HB3	15:P:228:GLN:HG3	1.85	0.58
13:N:68:MET:HG3	13:N:69:ASN:H	1.69	0.58
9:J:306:GLU:HG2	9:J:315:THR:HG22	1.85	0.57
26:c:167:TYR:OH	26:c:173:ASP:OD2	2.22	0.57
30:g:92:MET:O	30:g:96:VAL:HG23	2.04	0.57
32:i:88:LYS:O	32:i:148:SER:HB3	2.02	0.57
3:C:56:TRP:CH2	41:s:50:ALA:HB2	2.40	0.57
27:d:110:LEU:HD11	35:l:203:MET:HE2	1.87	0.57
35:l:397:GLU:HG2	35:l:482:MET:HE1	1.85	0.57
12:M:652:ASN:HA	12:M:655:ARG:HH21	1.69	0.57
55:l:702:CDL:H1O1	40:r:357:THR:HG1	1.49	0.57
3:C:71:CYS:HB3	45:C:301:SF4:S4	2.42	0.57
7:H:38:ILE:O	7:H:45:ARG:NH1	2.36	0.57
12:M:378:GLY:O	12:M:379:THR:HB	2.05	0.57
41:s:202:GLU:HA	41:s:210:GLY:HA3	1.87	0.57
43:v:111:ARG:O	43:v:115:ARG:HG2	2.05	0.57
13:N:34:ARG:HH12	13:N:58:ARG:HB3	1.69	0.57
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.87	0.57
25:b:81:ILE:HG23	47:b:201:PEE:H58	1.86	0.57
33:j:48:ARG:O	36:m:76:THR:OG1	2.19	0.57
34:k:23:ARG:HD3	36:m:23:LYS:O	2.05	0.57
40:r:420:THR:HB	40:r:423:ILE:HD12	1.87	0.57
1:A:40:ARG:NH1	1:A:289:GLU:O	2.37	0.56
9:J:206:ILE:HD12	51:J:401:NDP:C3N	2.35	0.56
9:J:220:MET:CE	9:J:227:PRO:CD	2.70	0.56
36:m:15:ILE:CG2	55:s:402:CDL:H831	2.35	0.56
33:j:71:LEU:O	36:m:147:TYR:OH	2.16	0.56
44:w:116:LYS:NZ	44:w:125:ASP:OD2	2.37	0.56
3:C:54:VAL:HG21	47:s:401:PEE:H55	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:86:MET:HE1	3:C:93:PHE:CD2	2.40	0.56
4:E:84:ILE:HG22	4:E:88:MET:HE3	1.86	0.56
16:Q:188:THR:HB	16:Q:200:PHE:HA	1.87	0.56
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.36	0.56
27:d:110:LEU:CD1	35:l:203:MET:HE2	2.35	0.56
42:u:83:THR:HA	42:u:86:TRP:CD1	2.40	0.56
8:I:25:GLN:O	16:Q:209:LYS:NZ	2.28	0.56
24:a:134:GLU:OE1	37:n:57:TRP:NE1	2.21	0.56
30:g:13:LEU:HA	48:g:201:PLX:H32	1.88	0.56
33:j:53:MET:HE3	33:j:56:PHE:HA	1.86	0.56
35:l:359:MET:O	35:l:436:ARG:NH2	2.39	0.56
47:r:501:PEE:H71	47:r:501:PEE:H29	1.88	0.56
55:s:402:CDL:H812	55:s:402:CDL:H751	1.88	0.56
9:J:307:VAL:O	9:J:308:SER:C	2.47	0.56
9:J:359:TYR:CD1	41:s:65:THR:HG22	2.40	0.56
32:i:294:MET:HE2	40:r:130:LEU:HD21	1.88	0.56
12:M:64:CYS:O	12:M:184:ARG:NH2	2.20	0.56
16:Q:92:HIS:NE2	16:Q:193:ASP:OD2	2.34	0.56
30:g:15:PHE:O	30:g:16:LEU:HD22	2.06	0.56
35:l:184:LEU:HD13	40:r:393:ILE:HG21	1.86	0.56
36:m:23:LYS:N	36:m:24:PRO:CD	2.69	0.56
12:M:281:ILE:HG23	12:M:391:ILE:HD12	1.87	0.56
16:Q:200:PHE:CE2	16:Q:204:PHE:CE2	2.94	0.56
38:o:59:VAL:HG22	40:r:423:ILE:HG23	1.87	0.56
37:n:34:LYS:NZ	55:u:201:CDL:HA22	2.19	0.56
12:M:140:GLN:HG2	16:Q:379:ILE:HG23	1.86	0.55
12:M:389:THR:HG21	12:M:473:MET:CE	2.33	0.55
28:e:143:ASP:OD1	28:e:146:LYS:NZ	2.31	0.55
32:i:265:MET:HE2	32:i:343:LEU:HD21	1.88	0.55
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.41	0.55
34:k:34:GLU:O	36:m:60:TYR:OH	2.19	0.55
47:r:501:PEE:H68	47:r:501:PEE:C21	2.36	0.55
12:M:391:ILE:CD1	12:M:600:GLU:OE2	2.55	0.55
41:s:202:GLU:HG2	41:s:209:SER:O	2.05	0.55
7:H:105:GLU:HA	7:H:105:GLU:OE1	2.07	0.55
25:b:86:LEU:HD11	35:l:9:LEU:HD12	1.89	0.55
35:l:375:ILE:HD12	35:l:458:LEU:HD11	1.87	0.55
40:r:306:PRO:HB3	40:r:458:LEU:HD12	1.88	0.55
24:a:147:ALA:HB2	40:r:173:SER:HB3	1.88	0.55
12:M:472:PRO:O	12:M:510:TRP:NE1	2.35	0.55
33:j:18:VAL:HB	41:s:222:MET:HE1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:56:PHE:CE2	47:s:401:PEE:H81	2.42	0.55
9:J:227:PRO:O	9:J:298:TYR:HE2	1.89	0.55
12:M:379:THR:O	12:M:379:THR:HG22	2.07	0.55
12:M:638:THR:OG1	12:M:640:ASP:OD1	2.21	0.55
8:I:23:LYS:CD	16:Q:253:PHE:CD2	2.59	0.55
9:J:37:HIS:NE2	9:J:40:LEU:HD12	2.21	0.55
33:j:73:LEU:O	41:s:160:TYR:OH	2.22	0.55
55:l:702:CDL:O1	40:r:357:THR:OG1	2.25	0.55
41:s:63:PRO:HB2	41:s:66:SER:HB3	1.89	0.55
41:s:306:SER:O	41:s:310:MET:HG3	2.07	0.55
15:P:105:ASN:O	15:P:137:PHE:CE2	2.60	0.55
17:S:57:VAL:HG11	17:S:62:VAL:HG21	1.89	0.55
21:W:74:LEU:O	21:W:78:GLU:HG3	2.07	0.55
35:l:294:THR:HG23	55:l:703:CDL:HB62	1.89	0.55
11:L:158:LYS:NZ	12:M:69:LEU:O	2.34	0.55
3:C:161:ILE:HG13	3:C:180:LEU:HB2	1.88	0.54
55:N:201:CDL:C55	55:N:201:CDL:C32	2.85	0.54
40:r:57:PHE:CE1	40:r:113:THR:HA	2.42	0.54
40:r:130:LEU:HD22	40:r:150:LEU:HD13	1.88	0.54
41:s:170:GLU:OE2	42:u:98:ARG:NH1	2.40	0.54
16:Q:53:TYR:CZ	47:Q:501:PEE:C1	2.82	0.54
38:o:45:ARG:HH12	39:p:144:THR:HG21	1.72	0.54
41:s:204:GLU:O	41:s:204:GLU:HG2	2.07	0.54
32:i:259:GLY:O	32:i:262:PRO:HD2	2.06	0.54
33:j:33:LYS:CD	41:s:61:LEU:HD21	2.31	0.54
33:j:79:SER:HA	33:j:87:MET:HE2	1.88	0.54
2:B:200:GLU:HG3	13:N:88:ARG:HB2	1.89	0.54
55:N:201:CDL:CA7	55:N:201:CDL:C34	2.86	0.54
35:l:313:MET:HG3	35:l:328:HIS:HD2	1.73	0.54
41:s:62:ARG:HD2	41:s:68:ILE:CG1	2.32	0.54
12:M:36:VAL:HG22	12:M:102:ILE:HD12	1.89	0.54
12:M:331:GLN:NE2	12:M:630:ALA:O	2.40	0.54
47:U:101:PEE:H33	41:s:302:MET:CE	2.37	0.54
35:l:253:VAL:HB	35:l:310:LEU:HD11	1.89	0.54
32:i:102:LEU:HD13	32:i:142:LEU:HG	1.90	0.54
40:r:195:MET:HB2	47:r:501:PEE:O4	2.08	0.54
44:w:217:ARG:HA	44:w:220:LYS:HE3	1.89	0.54
12:M:483:ARG:HD3	12:M:489:ILE:HD11	1.88	0.54
34:k:31:LEU:HD21	36:m:67:VAL:HG11	1.89	0.54
40:r:346:ARG:O	40:r:419:TYR:HA	2.06	0.54
55:N:201:CDL:C31	55:N:201:CDL:C55	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:140:LYS:HD2	32:i:274:GLU:HG2	1.90	0.54
34:k:79:VAL:HG13	34:k:80:MET:HE2	1.90	0.54
55:s:402:CDL:H381	55:s:402:CDL:C74	2.36	0.54
14:O:137:THR:O	14:O:141:MET:N	2.36	0.54
6:X:139:MET:N	6:X:143:GLU:OE1	2.36	0.54
32:i:276:ILE:HG21	47:r:501:PEE:H7	1.90	0.54
34:k:20:LEU:HD13	35:l:592:LEU:CB	2.34	0.54
35:l:241:THR:HG21	35:l:344:GLY:HA3	1.90	0.54
27:d:159:GLN:NE2	28:e:142:PHE:O	2.34	0.54
44:w:54:THR:O	44:w:55:GLU:HG3	2.07	0.54
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.89	0.53
9:J:167:ILE:HD13	9:J:201:ILE:HB	1.89	0.53
34:k:19:LEU:HD22	34:k:33:LEU:CD2	2.39	0.53
55:s:402:CDL:OA7	55:s:402:CDL:HA61	2.08	0.53
11:L:168:LYS:NZ	12:M:426:ASP:OD2	2.28	0.53
12:M:179:CYS:SG	45:M:802:SF4:S4	3.06	0.53
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.90	0.53
26:c:54:LYS:NZ	26:c:74:ASP:OD2	2.40	0.53
1:A:151:ALA:O	1:A:191:TYR:OH	2.21	0.53
5:F:65:LEU:HD12	5:F:79:LEU:HD11	1.91	0.53
33:j:83:ASN:ND2	48:j:202:PLX:O2	2.40	0.53
35:l:327:LEU:O	35:l:331:MET:HG2	2.09	0.53
16:Q:182:ASN:ND2	16:Q:403:PRO:HB2	2.24	0.53
21:W:98:MET:HE3	31:h:79:ILE:HD13	1.89	0.53
28:e:129:ARG:HG2	28:e:134:LEU:HD12	1.89	0.53
32:i:100:MET:HE3	35:l:598:SER:OG	2.09	0.53
34:k:21:MET:O	36:m:23:LYS:CE	2.48	0.53
35:l:55:MET:HE3	35:l:471:ASN:HB3	1.91	0.53
41:s:87:VAL:HG23	41:s:88:PRO:HD3	1.90	0.53
12:M:136:GLU:OE2	12:M:272:ARG:NH2	2.33	0.53
35:l:128:MET:HE1	35:l:252:MET:HA	1.89	0.53
12:M:326:VAL:HG13	12:M:567:ILE:HD13	1.90	0.53
21:W:84:LEU:HD12	42:u:57:LEU:HD21	1.90	0.53
35:l:128:MET:HE3	35:l:251:THR:HG22	1.91	0.53
1:A:418:GLN:HE22	12:M:152:ARG:HH21	1.57	0.53
52:J:402:UQ:C26	52:J:402:UQ:C20	2.87	0.53
19:U:69:HIS:N	19:U:72:ASP:OD2	2.39	0.53
32:i:7:THR:O	32:i:11:MET:HG3	2.09	0.53
32:i:97:MET:SD	35:l:599:MET:CE	2.96	0.53
41:s:14:LEU:HD21	41:s:83:LEU:HD21	1.90	0.53
16:Q:53:TYR:CE1	47:Q:501:PEE:H10	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:174:LEU:HA	40:r:179:ILE:HD11	1.91	0.53
4:E:39:TRP:O	4:E:43:VAL:HG23	2.08	0.53
18:T:45:TYR:HE2	18:T:55:PHE:CE2	2.27	0.53
41:s:81:LEU:O	41:s:85:MET:HG2	2.07	0.53
4:E:64:ARG:NH1	6:G:117:GLU:OE2	2.42	0.52
9:J:117:ARG:O	9:J:121:GLU:HG3	2.08	0.52
12:M:217:GLU:HG2	12:M:218:LEU:HG	1.91	0.52
38:o:59:VAL:HG22	40:r:423:ILE:HG12	1.90	0.52
1:A:326:LEU:HD23	1:A:367:ILE:HD11	1.91	0.52
43:v:27:PRO:O	43:v:34:ARG:NH1	2.42	0.52
11:L:89:SER:O	12:M:59:GLN:NE2	2.39	0.52
17:S:59:ARG:HB3	17:S:61:HIS:CE1	2.45	0.52
12:M:464:GLN:HG3	12:M:467:LYS:NZ	2.24	0.52
16:Q:55:THR:HB	16:Q:58:THR:HB	1.90	0.52
55:l:702:CDL:H822	55:l:702:CDL:H631	1.91	0.52
12:M:250:SER:OG	12:M:251:ILE:N	2.42	0.52
34:k:20:LEU:HD12	35:l:592:LEU:HD13	1.92	0.52
41:s:18:ALA:O	41:s:21:THR:OG1	2.25	0.52
31:h:106:PRO:HG2	42:u:17:GLU:HB3	1.92	0.52
35:l:426:ILE:O	35:l:430:ALA:HB3	2.10	0.52
35:l:492:ILE:O	35:l:496:MET:HG2	2.09	0.52
35:l:370:THR:HG22	35:l:431:PHE:CD1	2.45	0.52
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.92	0.52
41:s:198:PHE:CD1	41:s:285:LEU:HD13	2.44	0.52
1:A:66:LYS:HE2	1:A:188:GLY:O	2.10	0.52
1:A:141:GLY:HA2	1:A:252:PRO:HD3	1.91	0.52
5:F:20:ARG:NH2	5:F:74:GLU:OE2	2.42	0.52
14:O:111:ARG:NH1	14:O:114:GLU:OE2	2.43	0.52
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.91	0.52
34:k:23:ARG:HG2	55:m:201:CDL:HB62	1.92	0.52
44:w:246:LEU:HD22	44:w:255:VAL:HG11	1.92	0.52
8:I:8:ILE:O	8:I:12:ARG:HG3	2.10	0.52
16:Q:197:MET:CE	52:s:403:UQ:HM33	2.40	0.52
27:d:110:LEU:HD11	35:l:203:MET:CE	2.40	0.52
52:J:402:UQ:O1	52:J:402:UQ:H8	2.10	0.51
11:L:70:GLU:O	11:L:74:THR:OG1	2.21	0.51
12:M:340:ALA:HB3	12:M:366:LEU:HD23	1.90	0.51
12:M:367:CYS:HB2	12:M:533:GLY:O	2.09	0.51
14:O:196:LEU:HD13	14:O:201:ILE:HD13	1.91	0.51
40:r:329:LEU:O	40:r:332:THR:OG1	2.28	0.51
1:A:37:ASP:HA	1:A:40:ARG:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:101:LYS:HB2	27:d:116:ARG:O	2.10	0.51
55:u:201:CDL:H741	55:u:201:CDL:H532	1.92	0.51
44:w:59:VAL:HG12	44:w:201:PRO:HB3	1.92	0.51
1:A:390:ASP:CB	12:M:202:ASN:HD22	2.24	0.51
2:B:184:LEU:HB3	11:L:112:MET:HE2	1.91	0.51
5:F:61:VAL:HG23	5:F:62:GLN:H	1.76	0.51
10:K:83:THR:HG23	14:O:88:ARG:HH11	1.76	0.51
10:K:87:LEU:HD22	14:O:66:ILE:HD11	1.91	0.51
16:Q:198:THR:HG22	16:Q:202:TRP:CE2	2.45	0.51
35:l:358:LYS:HG3	39:p:80:TYR:CE1	2.46	0.51
11:L:84:ARG:HD3	11:L:91:VAL:HG12	1.93	0.51
16:Q:131:GLN:O	16:Q:134:PRO:HD2	2.11	0.51
26:c:102:GLY:HA3	38:o:43:LEU:HD22	1.91	0.51
32:i:100:MET:HE1	32:i:153:LEU:HD11	1.92	0.51
34:k:23:ARG:NH1	36:m:81:GLU:OE1	2.41	0.51
44:w:60:ILE:HG12	44:w:203:VAL:HB	1.93	0.51
16:Q:156:GLU:OE2	16:Q:171:ARG:NH2	2.44	0.51
29:f:47:THR:HG23	30:g:65:LEU:HD22	1.93	0.51
35:l:577:VAL:O	35:l:580:GLN:NE2	2.27	0.51
55:V:202:CDL:H742	55:V:202:CDL:H601	1.92	0.51
35:l:27:TYR:O	35:l:115:ASN:ND2	2.41	0.51
9:J:222:TRP:CD1	52:J:402:UQ:C10	2.93	0.51
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.91	0.51
15:P:211:ARG:NH2	15:P:222:GLU:OE2	2.42	0.51
12:M:501:ARG:HH11	12:M:665:PHE:HD2	1.59	0.51
21:W:50:MET:HG2	41:s:156:MET:HE3	1.92	0.51
6:X:137:LYS:HE3	25:b:4:TYR:CD1	2.46	0.51
35:l:294:THR:HG22	55:l:703:CDL:HB62	1.90	0.51
5:F:24:CYS:CA	5:F:58:CYS:HB3	2.41	0.51
35:l:119:LYS:HE3	55:l:702:CDL:OA3	2.11	0.51
35:l:417:SER:OG	55:l:703:CDL:H581	2.11	0.51
44:w:139:ARG:NE	44:w:166:ASP:OD2	2.38	0.51
44:w:213:GLU:CD	44:w:217:ARG:HE	2.18	0.51
12:M:335:GLY:HA2	12:M:362:ASP:O	2.11	0.50
19:U:67:PRO:HB3	19:U:72:ASP:HB2	1.93	0.50
55:V:201:CDL:H661	35:l:594:THR:HG23	1.91	0.50
55:s:402:CDL:H742	55:s:402:CDL:H362	1.92	0.50
1:A:222:LYS:O	11:L:175:LYS:NZ	2.34	0.50
3:C:53:LEU:HB2	48:C:302:PLX:H302	1.93	0.50
9:J:106:MET:HE2	9:J:118:LYS:HD3	1.92	0.50
14:O:149:LEU:O	14:O:153:GLN:HG2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Q:501:PEE:H28	47:Q:501:PEE:C22	2.36	0.50
52:J:402:UQ:C24	52:J:402:UQ:C19	2.89	0.50
12:M:483:ARG:HH22	12:M:682:ASP:HB3	1.73	0.50
55:r:504:CDL:H342	55:r:504:CDL:H181	1.92	0.50
41:s:119:SER:HG	41:s:223:PHE:HZ	1.53	0.50
1:A:149:MET:HE3	1:A:241:THR:CB	2.41	0.50
6:G:115:GLN:O	6:G:119:ILE:HG12	2.11	0.50
7:H:55:LYS:HE3	15:P:104:THR:HG21	1.94	0.50
9:J:233:LYS:HA	9:J:272:LEU:HD23	1.93	0.50
14:O:180:CYS:HG	53:O:301:FES:FE2	1.28	0.50
26:c:75:TYR:CG	26:c:76:PRO:HD2	2.47	0.50
34:k:65:VAL:HG11	36:m:157:THR:HG23	1.92	0.50
35:l:51:LEU:O	35:l:55:MET:HG3	2.11	0.50
1:A:56:ALA:HB1	1:A:61:ASP:HB2	1.94	0.50
47:U:101:PEE:H26	41:s:295:PRO:HB3	1.92	0.50
25:b:5:THR:OG1	25:b:8:GLU:HG3	2.12	0.50
35:l:295:GLN:HB2	35:l:301:ILE:HG12	1.92	0.50
47:l:704:PEE:H77	40:r:401:MET:CE	2.40	0.50
44:w:170:LEU:HD22	44:w:187:TYR:CD1	2.47	0.50
35:l:135:ASN:O	35:l:198:LEU:HG	2.11	0.50
55:s:402:CDL:H212	55:s:402:CDL:H552	1.94	0.50
1:A:392:MET:HE1	1:A:432:ALA:HA	1.93	0.50
3:C:87:ASP:OD2	52:s:403:UQ:HM21	2.12	0.50
15:P:201:ASP:OD1	15:P:201:ASP:N	2.31	0.50
24:a:168:TRP:HB3	30:g:3:MET:HG3	1.94	0.50
55:a:201:CDL:H751	28:e:103:SER:HB2	1.94	0.50
27:d:117:GLU:HG3	27:d:124:ASN:HB3	1.94	0.50
48:g:201:PLX:H232	32:i:210:THR:HG21	1.93	0.50
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.47	0.50
55:l:703:CDL:H431	55:l:703:CDL:H642	1.93	0.50
1:A:244:ASN:HD22	1:A:245:VAL:H	1.59	0.50
16:Q:133:LEU:HB3	16:Q:134:PRO:HD3	1.92	0.50
35:l:130:ILE:HD13	55:l:702:CDL:H252	1.94	0.50
35:l:562:LEU:HB3	35:l:563:PRO:HD3	1.92	0.50
1:A:274:LYS:HB2	1:A:292:MET:SD	2.51	0.50
47:W:201:PEE:C22	36:m:39:VAL:CG1	2.90	0.50
24:a:160:MET:HE2	30:g:95:TYR:CD1	2.47	0.50
40:r:203:PHE:O	40:r:207:MET:HG2	2.11	0.50
40:r:225:ILE:O	40:r:229:MET:HG3	2.12	0.50
42:u:45:LEU:HD22	42:u:131:VAL:HB	1.94	0.50
9:J:174:ILE:HD11	9:J:189:LYS:HZ3	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:304:LEU:HD21	48:J:403:PLX:H282	1.93	0.49
10:K:87:LEU:O	10:K:91:VAL:HG23	2.12	0.49
47:W:201:PEE:C36	41:s:108:MET:HE1	2.38	0.49
26:c:167:TYR:CD2	26:c:178:PRO:HG3	2.46	0.49
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.93	0.49
16:Q:144:MET:CG	16:Q:222:MET:O	2.57	0.49
50:X:201:8Q1:O40	39:p:12:HIS:CE1	2.62	0.49
30:g:52:ARG:NH2	44:w:338:LYS:O	2.46	0.49
36:m:15:ILE:HG22	55:s:402:CDL:H831	1.93	0.49
2:B:100:GLU:O	2:B:170:GLY:N	2.43	0.49
9:J:305:PHE:CE1	9:J:313:TRP:HE3	2.28	0.49
6:X:120:MET:HE1	39:p:24:LEU:HB3	1.94	0.49
31:h:18:MET:HE3	34:k:56:ALA:HA	1.94	0.49
35:l:172:ILE:HG21	40:r:408:LEU:HD12	1.94	0.49
38:o:38:ALA:HB2	39:p:150:ARG:HD3	1.94	0.49
9:J:199:THR:OG1	9:J:258:ALA:O	2.27	0.49
20:V:124:LEU:HD11	47:r:501:PEE:H58	1.94	0.49
35:l:366:MET:O	35:l:370:THR:HG23	2.12	0.49
4:E:111:GLU:OE2	15:P:223:PRO:HD3	2.12	0.49
11:L:84:ARG:NH1	11:L:88:GLN:O	2.46	0.49
32:i:258:SER:OG	32:i:333:SER:O	2.31	0.49
35:l:249:SER:OG	35:l:336:LYS:HG3	2.12	0.49
14:O:180:CYS:SG	53:O:301:FES:S2	3.04	0.49
34:k:37:MET:HE2	34:k:67:ALA:HB2	1.93	0.49
35:l:561:ILE:HG13	35:l:562:LEU:H	1.77	0.49
39:p:151:THR:HG22	39:p:153:ALA:H	1.78	0.49
40:r:243:MET:O	40:r:247:THR:HG23	2.12	0.49
41:s:189:THR:HG22	41:s:234:MET:HE3	1.94	0.49
55:s:402:CDL:H742	55:s:402:CDL:H402	1.94	0.49
1:A:365:LYS:HE3	14:O:141:MET:HE1	1.93	0.49
22:Y:50:LEU:HB3	22:Y:54:GLN:HE21	1.76	0.49
32:i:75:ILE:HD12	34:k:40:LEU:HD22	1.95	0.49
32:i:111:PHE:HA	35:l:591:PHE:CE1	2.47	0.49
2:B:148:ASP:HB3	2:B:151:LYS:HB2	1.95	0.49
5:F:20:ARG:HB2	5:F:66:TRP:HB2	1.95	0.49
9:J:107:GLU:O	9:J:118:LYS:NZ	2.46	0.49
9:J:313:TRP:CE2	52:J:402:UQ:H72	2.48	0.49
26:c:78:LEU:HD12	26:c:106:HIS:HA	1.93	0.49
40:r:197:LEU:HD13	47:r:501:PEE:H70	1.94	0.49
41:s:85:MET:HB3	41:s:233:MET:HG3	1.94	0.49
16:Q:41:VAL:HG23	28:e:55:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:114:GLY:N	16:Q:462:ASP:OD1	2.45	0.49
50:X:201:8Q1:C31	39:p:13:GLN:HG3	2.43	0.49
48:g:201:PLX:H233	32:i:207:ILE:HD13	1.95	0.49
35:l:227:PHE:O	35:l:230:HIS:ND1	2.46	0.49
40:r:57:PHE:HE1	40:r:113:THR:HA	1.77	0.49
3:C:192:ILE:HD13	9:J:87:GLU:N	2.27	0.49
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.48	0.49
52:J:402:UQ:C26	52:J:402:UQ:C19	2.91	0.49
21:W:121:MET:HE3	36:m:130:THR:HB	1.94	0.49
32:i:256:PRO:HB2	55:u:201:CDL:C60	2.43	0.49
6:X:112:SER:O	6:X:116:VAL:HG23	2.13	0.48
35:l:601:LEU:C	35:l:601:LEU:CD2	2.85	0.48
41:s:195:ARG:CG	41:s:231:ILE:HD11	2.40	0.48
1:A:320:GLY:HA2	1:A:353:ALA:H	1.78	0.48
55:V:202:CDL:H312	38:o:84:PRO:HB3	1.94	0.48
22:Y:100:LEU:HD12	22:Y:104:GLU:HG2	1.94	0.48
24:a:163:ARG:CZ	30:g:102:ASP:OD2	2.61	0.48
29:f:68:GLU:OE2	29:f:72:ARG:NE	2.47	0.48
35:l:233:LEU:HB3	35:l:234:PRO:HD3	1.94	0.48
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.47	0.48
12:M:278:HIS:C	12:M:283:GLU:HA	2.37	0.48
21:W:58:ARG:HD2	21:W:58:ARG:HA	1.69	0.48
23:Z:45:TRP:HB2	39:p:38:ARG:HH11	1.79	0.48
26:c:135:GLY:HA3	55:l:703:CDL:H272	1.95	0.48
39:p:64:LEU:O	39:p:68:GLU:HG2	2.13	0.48
4:E:31:ARG:O	4:E:34:GLU:HG2	2.13	0.48
6:G:76:LEU:HD12	6:G:154:VAL:HG12	1.95	0.48
48:J:403:PLX:H272	48:J:403:PLX:H301	1.55	0.48
16:Q:133:LEU:N	16:Q:134:PRO:CD	2.76	0.48
9:J:162:GLU:N	9:J:162:GLU:OE1	2.47	0.48
16:Q:265:ASN:HD21	41:s:277:TYR:HD1	1.61	0.48
31:h:21:GLN:HG2	31:h:37:GLU:OE1	2.14	0.48
40:r:357:THR:O	40:r:361:VAL:HG23	2.13	0.48
44:w:180:ARG:NH1	44:w:316:GLU:OE2	2.46	0.48
11:L:80:PHE:HE1	11:L:100:GLU:HG2	1.78	0.48
16:Q:55:THR:O	16:Q:59:ALA:N	2.40	0.48
18:T:49:ASP:OD1	18:T:51:ARG:NE	2.27	0.48
24:a:139:ILE:HG23	40:r:54:LEU:HD23	1.96	0.48
32:i:222:SER:O	32:i:224:ALA:N	2.47	0.48
55:m:201:CDL:H351	55:m:201:CDL:H222	1.95	0.48
1:A:66:LYS:HZ1	1:A:70:LEU:HD11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:PRO:HG3	2:B:200:GLU:OE2	2.14	0.48
47:B:303:PEE:H61	47:B:303:PEE:H55	1.57	0.48
5:F:58:CYS:SG	5:F:59:SER:N	2.87	0.48
17:S:69:ILE:HD11	42:u:20:VAL:HG13	1.96	0.48
23:Z:63:PHE:CZ	35:l:424:THR:HG23	2.49	0.48
3:C:98:ARG:NH2	33:j:35:SER:O	2.44	0.48
13:N:44:TYR:OH	13:N:113:HIS:N	2.39	0.48
16:Q:133:LEU:CD2	16:Q:228:ARG:HD3	2.44	0.48
55:V:201:CDL:H512	35:l:576:MET:HG2	1.96	0.48
34:k:19:LEU:HD22	34:k:33:LEU:HD23	1.95	0.48
35:l:419:THR:HA	35:l:422:TYR:CE2	2.47	0.48
36:m:164:GLY:O	36:m:168:ILE:HG12	2.14	0.48
41:s:144:VAL:O	41:s:148:ILE:HD12	2.13	0.48
6:X:155:TYR:CD2	6:X:156:GLU:HG3	2.49	0.48
41:s:264:LEU:O	41:s:268:ILE:HG12	2.13	0.48
1:A:56:ALA:O	1:A:61:ASP:HB2	2.13	0.48
1:A:66:LYS:NZ	1:A:70:LEU:HD11	2.29	0.48
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.44	0.48
2:B:184:LEU:O	13:N:124:TYR:OH	2.31	0.48
5:F:25:GLN:O	5:F:34:ARG:NH1	2.47	0.48
21:W:68:ARG:O	21:W:72:MET:HG3	2.14	0.48
24:a:152:LYS:HD3	30:g:96:VAL:HG21	1.95	0.48
15:P:213:ASP:HB3	15:P:216:VAL:HG22	1.96	0.47
16:Q:142:VAL:HG12	16:Q:182:ASN:HA	1.95	0.47
16:Q:144:MET:SD	16:Q:144:MET:N	2.86	0.47
20:V:141:VAL:O	24:a:169:TYR:OH	2.26	0.47
6:X:93:ILE:HG12	6:X:108:LEU:HD23	1.95	0.47
27:d:113:CYS:HG	27:d:125:CYS:HG	1.31	0.47
40:r:115:LEU:HD12	40:r:174:LEU:HD22	1.96	0.47
42:u:50:GLU:OE2	42:u:135:ARG:NH1	2.47	0.47
14:O:134:VAL:HG11	14:O:149:LEU:HD13	1.96	0.47
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.48	0.47
35:l:290:LEU:HD11	55:l:703:CDL:H731	1.96	0.47
35:l:407:TRP:O	35:l:411:MET:HG2	2.13	0.47
55:l:703:CDL:H321	55:l:703:CDL:C11	2.44	0.47
48:J:403:PLX:H32	48:J:403:PLX:H6	1.62	0.47
16:Q:80:LEU:HD21	41:s:126:LYS:HD3	1.96	0.47
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	1.96	0.47
55:V:202:CDL:H732	38:o:87:SER:HB3	1.95	0.47
55:a:201:CDL:OA4	25:b:84:TYR:OH	2.28	0.47
27:d:69:ARG:NH2	37:n:46:LYS:O	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:140:GLN:O	27:d:144:SER:HB2	2.14	0.47
32:i:81:SER:O	32:i:83:GLN:N	2.45	0.47
33:j:27:LEU:HD22	41:s:60:PRO:HD2	1.95	0.47
37:n:50:ARG:HB2	37:n:53:GLU:HG2	1.96	0.47
44:w:295:ARG:HA	44:w:298:VAL:HG22	1.96	0.47
1:A:76:ILE:HG23	1:A:255:CYS:SG	2.54	0.47
1:A:185:ASN:O	1:A:187:CYS:N	2.47	0.47
12:M:688:GLN:HA	12:M:688:GLN:HE21	1.79	0.47
22:Y:65:MET:SD	35:l:375:ILE:HG12	2.55	0.47
55:a:201:CDL:H852	48:r:503:PLX:H232	1.97	0.47
26:c:184:TYR:HB2	43:v:34:ARG:HH21	1.79	0.47
41:s:283:ASP:OD1	41:s:284:GLN:N	2.47	0.47
55:N:201:CDL:OA3	17:S:3:PHE:HE2	1.97	0.47
35:l:395:ILE:O	35:l:399:VAL:HG23	2.14	0.47
3:C:66:THR:OG1	3:C:93:PHE:HB3	2.13	0.47
3:C:142:TYR:CE2	16:Q:135:TYR:CD1	3.02	0.47
12:M:685:VAL:HG23	12:M:685:VAL:O	2.14	0.47
16:Q:182:ASN:HD22	16:Q:403:PRO:HB2	1.78	0.47
25:b:4:TYR:HB2	25:b:9:LYS:HE3	1.96	0.47
48:g:201:PLX:H112	48:g:201:PLX:H81	1.47	0.47
32:i:99:THR:HG21	32:i:153:LEU:CD2	2.37	0.47
40:r:237:LYS:HD2	40:r:316:MET:HB3	1.97	0.47
44:w:209:VAL:HG22	44:w:260:ALA:HB2	1.96	0.47
6:G:113:LEU:O	6:G:117:GLU:HG3	2.15	0.47
8:I:27:ARG:HB3	8:I:31:ILE:CG2	2.44	0.47
12:M:405:THR:HB	12:M:477:GLY:HA3	1.97	0.47
19:U:43:ILE:HG12	33:j:84:LEU:HB2	1.97	0.47
25:b:10:LEU:O	25:b:14:GLN:HG3	2.15	0.47
47:j:201:PEE:H40	41:s:77:LEU:CD1	2.44	0.47
35:l:125:LEU:O	35:l:129:MET:HG2	2.15	0.47
36:m:34:ILE:HG13	36:m:64:MET:HG3	1.96	0.47
40:r:16:TRP:CZ2	55:r:504:CDL:C26	2.97	0.47
41:s:207:LEU:O	41:s:209:SER:N	2.47	0.47
1:A:210:THR:HB	1:A:224:ARG:H	1.79	0.47
7:H:108:PRO:HG2	15:P:124:ASN:HD22	1.79	0.47
48:J:403:PLX:H252	48:J:403:PLX:H281	1.53	0.47
12:M:149:ASP:OD2	12:M:150:ARG:NH1	2.47	0.47
32:i:252:GLY:HA3	32:i:290:LEU:HD13	1.97	0.47
16:Q:370:GLU:HA	16:Q:373:THR:HG22	1.97	0.47
35:l:529:TYR:HB3	35:l:530:PRO:HD3	1.97	0.47
15:P:51:ASN:HB3	15:P:82:ASN:HD21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:265:ASN:O	16:Q:269:ARG:HG3	2.14	0.47
16:Q:319:PRO:HG2	16:Q:336:GLU:HG3	1.97	0.47
19:U:6:ALA:O	19:U:10:LYS:HG2	2.14	0.47
20:V:95:CYS:HA	20:V:115:CYS:HA	1.96	0.47
32:i:128:LEU:HD12	32:i:216:PHE:HB3	1.97	0.47
32:i:304:MET:HE3	40:r:135:ARG:HH22	1.80	0.47
35:l:67:HIS:NE2	35:l:70:THR:OG1	2.43	0.47
40:r:296:LEU:HG	40:r:381:ILE:HG21	1.97	0.47
41:s:68:ILE:HG21	55:s:402:CDL:OA3	2.15	0.47
42:u:80:GLU:HB2	42:u:81:PRO:HD3	1.96	0.47
3:C:86:MET:HE1	3:C:93:PHE:CE2	2.50	0.46
7:H:87:GLU:OE1	15:P:104:THR:OG1	2.33	0.46
8:I:40:LYS:HB3	21:W:7:LYS:H	1.80	0.46
25:b:120:MET:HE3	43:v:61:HIS:HB2	1.96	0.46
26:c:60:GLU:N	26:c:60:GLU:OE2	2.49	0.46
26:c:153:TYR:OH	43:v:8:ARG:NH1	2.48	0.46
28:e:76:TYR:HB2	28:e:83:ASP:OD1	2.15	0.46
32:i:221:HIS:ND1	32:i:323:MET:HE1	2.30	0.46
35:l:14:ILE:HD11	35:l:43:ALA:HA	1.97	0.46
40:r:186:LEU:HD23	40:r:192:ASN:HB3	1.97	0.46
1:A:86:ARG:O	1:A:88:ARG:NH1	2.48	0.46
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.96	0.46
16:Q:40:ASP:OD1	16:Q:40:ASP:N	2.48	0.46
30:g:7:ARG:NH2	30:g:91:ASP:OD1	2.46	0.46
55:l:702:CDL:H581	55:l:702:CDL:H611	1.61	0.46
41:s:179:TRP:CG	41:s:180:PRO:HD3	2.51	0.46
1:A:185:ASN:OD1	1:A:190:GLY:N	2.40	0.46
5:F:85:ASP:O	5:F:89:ARG:HG3	2.15	0.46
9:J:95:ARG:HB2	9:J:96:PRO:HD3	1.98	0.46
19:U:38:TYR:HB2	41:s:310:MET:O	2.15	0.46
21:W:86:MET:SD	21:W:124:LEU:HB3	2.56	0.46
33:j:30:TYR:CD1	33:j:32:GLU:HG2	2.51	0.46
55:l:702:CDL:H452	40:r:445:LEU:HB3	1.97	0.46
43:v:107:ARG:HA	43:v:110:GLN:HG3	1.97	0.46
3:C:88:ARG:HA	41:s:37:PRO:HA	1.96	0.46
15:P:119:VAL:HG12	15:P:121:THR:HG22	1.96	0.46
16:Q:74:ASP:OD1	16:Q:74:ASP:N	2.46	0.46
16:Q:236:LEU:HD22	16:Q:240:LEU:HD23	1.97	0.46
21:W:85:GLN:O	21:W:89:GLU:HG3	2.15	0.46
26:c:97:LEU:HB3	26:c:99:LEU:HD13	1.98	0.46
32:i:79:LEU:HB2	34:k:47:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:373:LEU:HD22	35:l:431:PHE:HE2	1.80	0.46
39:p:127:ARG:HA	39:p:130:ARG:HE	1.81	0.46
15:P:43:THR:HA	15:P:47:ILE:HD12	1.98	0.46
35:l:561:ILE:HG13	35:l:562:LEU:N	2.31	0.46
40:r:225:ILE:HD13	40:r:331:ASN:HB2	1.96	0.46
41:s:73:ILE:HD11	55:s:402:CDL:C20	2.31	0.46
44:w:66:ILE:HA	57:w:401:ADP:O2A	2.15	0.46
1:A:244:ASN:ND2	1:A:245:VAL:H	2.13	0.46
1:A:250:VAL:O	1:A:251:SER:C	2.58	0.46
1:A:265:PHE:HB3	1:A:291:GLU:HG3	1.96	0.46
1:A:272:GLY:O	1:A:292:MET:HG2	2.14	0.46
12:M:257:VAL:O	12:M:598:ASN:OD1	2.33	0.46
12:M:337:ASP:O	12:M:542:PRO:HB3	2.14	0.46
16:Q:127:LYS:O	16:Q:418:ARG:HG3	2.16	0.46
16:Q:137:ASP:OD1	16:Q:148:GLU:CG	2.64	0.46
16:Q:450:ILE:HA	16:Q:453:THR:HG22	1.98	0.46
18:T:76:VAL:HG11	18:T:119:ARG:HE	1.80	0.46
27:d:10:TYR:OH	28:e:123:GLU:OE2	2.31	0.46
31:h:24:GLU:HG3	31:h:24:GLU:O	2.15	0.46
35:l:298:ILE:O	35:l:302:VAL:HG23	2.15	0.46
41:s:102:VAL:HG11	41:s:154:LEU:HD11	1.98	0.46
43:v:111:ARG:HG3	43:v:114:ARG:HH21	1.79	0.46
9:J:174:ILE:HD12	9:J:174:ILE:H	1.81	0.46
33:j:23:TRP:CZ2	47:j:201:PEE:H52	2.51	0.46
40:r:121:LEU:O	40:r:125:THR:HG23	2.15	0.46
1:A:67:GLU:O	1:A:71:LYS:HG2	2.15	0.46
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.51	0.46
7:H:108:PRO:O	7:H:109:ALA:C	2.59	0.46
9:J:359:TYR:HB2	41:s:65:THR:HA	1.98	0.46
15:P:103:HIS:CD2	15:P:105:ASN:HB2	2.51	0.46
55:a:201:CDL:H541	47:b:201:PEE:C12	2.46	0.46
41:s:293:PHE:O	41:s:297:THR:OG1	2.26	0.46
9:J:220:MET:CE	9:J:226:VAL:HG13	2.46	0.46
12:M:29:SER:OG	12:M:30:ASN:N	2.49	0.46
12:M:141:ASP:O	12:M:145:MET:HG2	2.15	0.46
12:M:208:THR:OG1	12:M:210:ILE:O	2.30	0.46
25:b:13:GLN:HA	25:b:16:ARG:HG2	1.97	0.46
35:l:86:SER:OG	35:l:262:ARG:NH2	2.49	0.46
52:s:403:UQ:H221	52:s:403:UQ:H262	1.58	0.46
42:u:169:PHE:HE1	55:u:201:CDL:H551	1.80	0.46
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:48:ASN:ND2	14:O:50:ASP:H	2.14	0.46
55:V:202:CDL:H401	55:V:202:CDL:H371	1.41	0.46
32:i:170:LEU:HD23	32:i:292:PHE:HB3	1.97	0.46
41:s:62:ARG:HG3	41:s:68:ILE:HD11	1.98	0.46
44:w:65:ASN:OD1	44:w:66:ILE:N	2.43	0.46
3:C:94:ARG:HH12	41:s:220:PHE:HZ	1.64	0.45
12:M:89:VAL:HB	12:M:94:MET:HE3	1.97	0.45
15:P:148:ASP:N	15:P:148:ASP:OD1	2.48	0.45
21:W:96:ILE:O	21:W:99:LYS:HE3	2.16	0.45
22:Y:69:ILE:HD13	35:l:383:MET:HE2	1.98	0.45
31:h:2:PRO:HA	32:i:140:SER:HB2	1.98	0.45
39:p:108:HIS:CD2	39:p:109:PRO:HD2	2.51	0.45
47:r:501:PEE:H14	47:r:501:PEE:H7	1.98	0.45
5:F:16:LEU:HD21	5:F:19:ILE:HD11	1.97	0.45
5:F:59:SER:OG	5:F:60:ASP:N	2.49	0.45
9:J:304:LEU:C	9:J:304:LEU:HD23	2.41	0.45
12:M:456:ALA:O	12:M:499:ASN:ND2	2.49	0.45
16:Q:145:MET:HB2	16:Q:178:THR:OG1	2.15	0.45
21:W:94:GLU:HG2	31:h:79:ILE:HD12	1.98	0.45
35:l:332:HIS:HA	35:l:335:PHE:CZ	2.51	0.45
55:l:702:CDL:H811	55:l:702:CDL:H841	1.63	0.45
36:m:82:VAL:HG22	36:m:85:SER:HB3	1.99	0.45
40:r:243:MET:HB3	40:r:301:ILE:HG21	1.98	0.45
55:s:402:CDL:H341	55:s:402:CDL:H371	1.76	0.45
1:A:398:ARG:CG	1:A:403:ASP:HB2	2.46	0.45
9:J:168:SER:O	9:J:203:PRO:HD2	2.16	0.45
9:J:375:VAL:HG23	9:J:375:VAL:O	2.16	0.45
31:h:60:PHE:O	31:h:64:VAL:HG13	2.15	0.45
35:l:341:MET:CE	35:l:457:LEU:HD12	2.47	0.45
40:r:271:MET:HE2	40:r:271:MET:HA	1.98	0.45
55:s:402:CDL:H332	55:s:402:CDL:H182	1.98	0.45
44:w:143:TYR:OH	44:w:199:LEU:O	2.27	0.45
12:M:406:ASN:ND2	12:M:409:PHE:CD2	2.84	0.45
47:W:201:PEE:H20	47:W:201:PEE:H14	1.73	0.45
32:i:40:MET:HE1	32:i:129:LEU:HD22	1.98	0.45
7:H:108:PRO:HG2	15:P:124:ASN:ND2	2.32	0.45
8:I:3:SER:OG	55:N:201:CDL:H1	2.16	0.45
12:M:64:CYS:SG	12:M:75:CYS:SG	3.03	0.45
12:M:464:GLN:HG3	12:M:467:LYS:HZ3	1.82	0.45
34:k:38:LEU:HB2	36:m:60:TYR:CZ	2.51	0.45
40:r:74:PRO:O	40:r:78:MET:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASN:C	1:A:187:CYS:H	2.25	0.45
35:l:166:THR:CG2	47:l:704:PEE:H2	2.46	0.45
35:l:386:LEU:HD23	35:l:386:LEU:HA	1.71	0.45
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.27	0.45
2:B:105:ARG:NH2	18:T:63:ASN:OD1	2.49	0.45
15:P:108:PHE:CD2	15:P:134:SER:HB2	2.51	0.45
22:Y:97:LEU:HD12	43:v:107:ARG:NH2	2.22	0.45
32:i:72:MET:HE2	34:k:12:PHE:CG	2.52	0.45
35:l:575:ILE:O	35:l:579:ASN:ND2	2.38	0.45
40:r:133:ILE:HG12	40:r:223:ALA:HB2	1.99	0.45
3:C:111:ASN:CG	15:P:210:LEU:HD13	2.41	0.45
3:C:128:ARG:NH2	33:j:30:TYR:OH	2.35	0.45
4:E:96:VAL:HG21	33:j:44:MET:HA	1.99	0.45
9:J:220:MET:HE1	9:J:227:PRO:HD2	1.88	0.45
16:Q:53:TYR:OH	47:Q:501:PEE:H3	1.99	0.45
33:j:33:LYS:HD3	41:s:61:LEU:CD2	2.38	0.45
48:r:502:PLX:H101	48:r:502:PLX:H72	1.55	0.45
2:B:50:MET:SD	19:U:10:LYS:HD2	2.57	0.45
12:M:97:MET:HG3	12:M:100:TRP:CZ2	2.52	0.45
12:M:138:ASP:HB3	12:M:142:GLN:HE21	1.82	0.45
12:M:485:ASP:OD1	12:M:489:ILE:CD1	2.64	0.45
12:M:652:ASN:HA	12:M:655:ARG:HE	1.82	0.45
28:e:112:TYR:HD2	40:r:43:ASN:HD21	1.65	0.45
34:k:11:ALA:HB2	36:m:14:VAL:HG22	1.98	0.45
34:k:57:ASN:HB3	36:m:143:ILE:HG13	1.98	0.45
5:F:41:TYR:OH	12:M:380:ASP:CB	2.63	0.45
10:K:95:LYS:HE2	10:K:96:PHE:CZ	2.52	0.45
12:M:392:ALA:HA	12:M:417:ARG:NH1	2.31	0.45
19:U:82:LYS:HA	21:W:59:ARG:HD3	1.99	0.45
55:a:201:CDL:H441	55:a:201:CDL:H411	1.80	0.45
25:b:89:HIS:CD2	47:b:201:PEE:H49	2.51	0.45
47:j:201:PEE:H40	41:s:77:LEU:HD13	1.98	0.45
35:l:176:ARG:HA	35:l:176:ARG:HD3	1.65	0.45
40:r:116:ILE:HG13	42:u:168:PHE:CE1	2.52	0.45
44:w:210:PRO:O	44:w:214:ILE:HG12	2.17	0.45
12:M:278:HIS:O	12:M:283:GLU:N	2.50	0.44
14:O:131:HIS:CD2	14:O:170:THR:HG23	2.52	0.44
14:O:144:ASN:O	14:O:147:SER:OG	2.35	0.44
48:a:202:PLX:H1C3	48:a:202:PLX:H22	1.78	0.44
36:m:15:ILE:HG21	55:s:402:CDL:H831	1.99	0.44
1:A:60:GLY:CA	14:O:241:PRO:HA	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:85:ASP:OD1	5:F:85:ASP:N	2.50	0.44
12:M:483:ARG:HH22	12:M:682:ASP:C	2.25	0.44
16:Q:133:LEU:HD22	16:Q:228:ARG:HD3	2.00	0.44
16:Q:282:ASP:OD2	16:Q:437:LYS:NZ	2.47	0.44
47:U:101:PEE:H59	47:U:101:PEE:H64	1.83	0.44
21:W:120:MET:O	21:W:121:MET:HB3	2.17	0.44
28:e:51:PRO:C	28:e:53:ILE:H	2.24	0.44
31:h:75:ARG:O	31:h:79:ILE:HG12	2.17	0.44
35:l:530:PRO:O	35:l:534:HIS:HB2	2.16	0.44
44:w:256:LEU:HD21	44:w:276:LEU:HD21	1.99	0.44
1:A:257:ARG:NH1	1:A:261:TRP:CZ2	2.84	0.44
2:B:118:LEU:HD11	16:Q:382:PHE:CE2	2.53	0.44
2:B:153:ILE:CG2	3:C:142:TYR:HB2	2.47	0.44
11:L:111:LEU:HD11	13:N:126:PRO:HG2	1.99	0.44
19:U:52:ASN:HD22	24:a:185:THR:HG22	1.83	0.44
55:V:202:CDL:H142	55:V:202:CDL:H111	1.77	0.44
29:f:59:ILE:O	29:f:63:LYS:HG2	2.17	0.44
35:l:7:LEU:HD22	35:l:46:LEU:HD11	1.98	0.44
36:m:1:MET:HG3	36:m:123:GLY:HA2	1.98	0.44
55:r:504:CDL:H612	55:r:504:CDL:H641	1.76	0.44
1:A:71:LYS:HD2	1:A:71:LYS:HA	1.79	0.44
1:A:102:MET:HE2	1:A:149:MET:HE2	2.00	0.44
21:W:128:ARG:HB3	21:W:132:GLU:OE2	2.18	0.44
34:k:4:VAL:O	34:k:8:ILE:HG12	2.17	0.44
35:l:190:LEU:HD21	40:r:307:TRP:CH2	2.51	0.44
35:l:190:LEU:HD22	35:l:196:TRP:CZ2	2.52	0.44
55:r:504:CDL:H761	55:r:504:CDL:H791	1.82	0.44
9:J:38:HIS:HE1	13:N:136:GLU:CD	2.26	0.44
12:M:422:TRP:HA	12:M:427:LEU:HB3	1.99	0.44
28:e:97:ILE:O	28:e:101:LEU:HB2	2.17	0.44
30:g:89:ASP:OD2	42:u:161:ALA:HB1	2.17	0.44
35:l:419:THR:HA	35:l:422:TYR:CZ	2.53	0.44
2:B:80:GLU:OE1	8:I:28:TYR:OH	2.35	0.44
2:B:99:GLY:CA	2:B:170:GLY:O	2.65	0.44
3:C:107:GLY:HA2	45:C:301:SF4:S1	2.57	0.44
32:i:54:GLU:HG3	34:k:93:LEU:HB3	1.99	0.44
35:l:489:THR:O	35:l:493:VAL:HG13	2.17	0.44
35:l:599:MET:O	35:l:603:ASN:CB	2.47	0.44
41:s:67:SER:O	41:s:71:PHE:HB2	2.18	0.44
42:u:59:GLU:OE1	42:u:59:GLU:N	2.47	0.44
1:A:326:LEU:HD22	1:A:363:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:354:LEU:HD22	12:M:548:LEU:HD22	2.00	0.44
12:M:650:SER:OG	12:M:652:ASN:OD1	2.36	0.44
16:Q:228:ARG:C	16:Q:230:GLY:H	2.26	0.44
47:Q:501:PEE:H47	47:r:501:PEE:H39	2.00	0.44
14:O:41:HIS:HE1	14:O:43:ASP:OD1	2.00	0.44
16:Q:304:LYS:NZ	16:Q:316:PHE:O	2.41	0.44
32:i:95:MET:HE2	32:i:149:ILE:HG13	1.99	0.44
32:i:183:SER:O	32:i:187:MET:HG2	2.17	0.44
40:r:281:ASP:OD1	40:r:340:ARG:HB3	2.18	0.44
41:s:55:LEU:HD13	41:s:221:ALA:HB2	1.99	0.44
3:C:52:ASP:HB3	48:C:302:PLX:H251	1.98	0.44
52:J:402:UQ:H203	52:J:402:UQ:H172	1.78	0.44
16:Q:442:HIS:HB3	16:Q:446:ASP:HB2	1.99	0.44
27:d:48:ALA:O	27:d:52:ILE:HG12	2.17	0.44
1:A:250:VAL:C	1:A:252:PRO:HD2	2.43	0.43
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.70	0.43
4:E:65:GLU:O	4:E:69:LYS:HG3	2.18	0.43
7:H:35:LEU:HD11	7:H:48:THR:HG22	2.00	0.43
8:I:44:GLY:CA	16:Q:359:ASP:OD2	2.64	0.43
17:S:57:VAL:O	17:S:58:ASN:CB	2.66	0.43
21:W:84:LEU:HD13	42:u:8:PRO:HG2	1.99	0.43
26:c:135:GLY:HA3	55:l:703:CDL:C27	2.47	0.43
26:c:185:GLU:OE2	43:v:37:ARG:HG3	2.17	0.43
31:h:19:THR:HA	32:i:84:TRP:HB2	2.00	0.43
40:r:419:TYR:CD1	40:r:419:TYR:O	2.70	0.43
41:s:86:TRP:HH2	41:s:232:ILE:HG22	1.83	0.43
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.99	0.43
2:B:48:MET:HA	2:B:48:MET:HE2	2.00	0.43
3:C:113:MET:SD	16:Q:115:LEU:HD23	2.58	0.43
48:C:302:PLX:H102	48:C:302:PLX:C27	2.48	0.43
12:M:512:VAL:O	12:M:514:ASN:ND2	2.51	0.43
32:i:265:MET:HE3	32:i:265:MET:HB3	1.87	0.43
40:r:44:GLN:HG3	40:r:60:SER:HA	2.01	0.43
47:r:501:PEE:H74	47:r:501:PEE:H69	1.75	0.43
41:s:69:SER:HB3	55:s:402:CDL:OB7	2.18	0.43
2:B:70:LEU:HB3	41:s:272:TRP:CZ2	2.53	0.43
55:V:201:CDL:H372	55:V:201:CDL:H341	1.53	0.43
40:r:365:THR:HG21	40:r:444:LEU:HD13	2.01	0.43
40:r:370:PRO:HA	40:r:371:PRO:HA	1.83	0.43
55:s:402:CDL:H742	55:s:402:CDL:C38	2.40	0.43
42:u:28:ALA:HB2	42:u:82:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:198:THR:HG21	12:M:209:TYR:HB2	2.00	0.43
12:M:382:ARG:HE	12:M:527:ASP:CG	2.27	0.43
13:N:10:GLY:O	13:N:14:VAL:HG23	2.18	0.43
14:O:189:ASN:O	14:O:190:ASP:HB2	2.18	0.43
16:Q:139:LEU:HD11	16:Q:424:ILE:HD13	2.01	0.43
47:U:101:PEE:H33	41:s:302:MET:HE1	2.00	0.43
47:W:201:PEE:H55	41:s:108:MET:CE	2.49	0.43
25:b:112:GLU:OE1	27:d:17:THR:HG22	2.18	0.43
35:l:96:VAL:O	35:l:100:ILE:HG12	2.19	0.43
40:r:260:PRO:HG3	48:r:502:PLX:H131	1.99	0.43
55:r:504:CDL:H511	55:r:504:CDL:H541	1.62	0.43
41:s:24:GLU:HG3	41:s:271:LEU:HD22	2.00	0.43
44:w:302:LEU:HD23	44:w:302:LEU:HA	1.90	0.43
2:B:150:THR:HG21	2:B:180:HIS:CD2	2.53	0.43
5:F:85:ASP:HA	5:F:88:THR:HG22	2.01	0.43
7:H:24:LEU:HD12	7:H:77:ILE:HD11	2.00	0.43
12:M:284:GLU:HG2	12:M:284:GLU:O	2.19	0.43
12:M:485:ASP:O	12:M:489:ILE:HG13	2.19	0.43
14:O:218:PRO:HD2	14:O:223:PHE:HA	2.00	0.43
15:P:173:MET:HB3	15:P:198:PHE:HB2	2.01	0.43
16:Q:194:ILE:O	16:Q:194:ILE:HG22	2.18	0.43
27:d:119:GLU:HG2	43:v:52:MET:HA	2.00	0.43
30:g:19:GLU:HG3	42:u:158:LEU:HD22	2.00	0.43
31:h:47:ILE:HD11	31:h:52:ALA:CA	2.46	0.43
33:j:68:GLU:HG2	36:m:161:LEU:HD13	2.00	0.43
35:l:332:HIS:HA	35:l:335:PHE:CE2	2.53	0.43
41:s:119:SER:OG	41:s:223:PHE:HZ	2.01	0.43
41:s:120:GLY:HA2	41:s:128:ALA:HB1	2.01	0.43
55:s:402:CDL:H141	55:s:402:CDL:H171	1.65	0.43
17:S:50:ARG:O	17:S:54:ILE:HG12	2.17	0.43
40:r:101:LEU:HD13	55:r:504:CDL:H441	2.00	0.43
40:r:216:LEU:HB3	40:r:217:PRO:HD3	2.00	0.43
44:w:72:ARG:O	44:w:76:GLU:HG3	2.19	0.43
9:J:220:MET:HE2	9:J:226:VAL:HA	2.00	0.43
13:N:3:LEU:HD11	55:N:201:CDL:H311	2.01	0.43
13:N:85:GLU:HB2	13:N:98:PRO:HB3	2.00	0.43
16:Q:73:LYS:HE2	16:Q:75:THR:HG22	2.01	0.43
35:l:176:ARG:HA	35:l:179:ASP:HB2	2.00	0.43
38:o:31:LYS:O	38:o:35:GLU:HG2	2.19	0.43
41:s:178:SER:HB2	41:s:181:LEU:HD12	2.00	0.43
44:w:83:LEU:HD22	44:w:156:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ASP:HB2	14:O:236:GLU:HB2	2.01	0.43
14:O:134:VAL:CG2	14:O:186:VAL:HG12	2.39	0.43
15:P:94:ILE:HB	15:P:95:PRO:HD3	2.00	0.43
20:V:41:ILE:HG23	20:V:46:PRO:HD3	1.99	0.43
20:V:49:PHE:HA	55:m:201:CDL:HA62	2.01	0.43
22:Y:97:LEU:HB3	43:v:104:ARG:HB2	2.00	0.43
28:e:70:ASN:HB3	28:e:73:SER:HB2	2.01	0.43
48:g:201:PLX:H12	31:h:2:PRO:HD2	2.01	0.43
34:k:48:ILE:HD11	34:k:59:MET:HE3	2.00	0.43
35:l:230:HIS:N	35:l:231:PRO:HD3	2.33	0.43
35:l:428:PHE:CD1	35:l:428:PHE:C	2.97	0.43
40:r:67:VAL:HG12	48:r:503:PLX:H362	2.00	0.43
48:r:502:PLX:H1C3	48:r:502:PLX:H22	1.73	0.43
1:A:418:GLN:NE2	12:M:152:ARG:NH2	2.65	0.43
48:C:302:PLX:H1C3	48:C:302:PLX:O1	2.19	0.43
9:J:108:TRP:CZ3	9:J:110:GLY:HA2	2.54	0.43
12:M:624:ARG:NH2	12:M:637:ASP:OD1	2.47	0.43
26:c:139:PHE:CE2	55:l:703:CDL:H842	2.53	0.43
34:k:28:SER:HB3	36:m:23:LYS:HG2	2.00	0.43
44:w:354:LEU:HD23	44:w:354:LEU:HA	1.90	0.43
11:L:131:LYS:HD2	11:L:147:VAL:HG11	2.00	0.43
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.54	0.43
27:d:82:ILE:HD12	27:d:82:ILE:HA	1.91	0.43
31:h:47:ILE:HD12	31:h:52:ALA:HA	2.00	0.43
32:i:278:MET:O	32:i:282:MET:HG3	2.19	0.43
41:s:267:THR:O	41:s:271:LEU:HG	2.19	0.43
42:u:100:CYS:HB2	42:u:103:GLN:OE1	2.19	0.43
8:I:9:GLN:O	8:I:13:ASN:ND2	2.52	0.42
12:M:63:PHE:CZ	12:M:117:MET:HE1	2.54	0.42
16:Q:84:PHE:HB2	16:Q:99:MET:HE1	2.01	0.42
20:V:39:TYR:HB3	55:V:201:CDL:H712	2.01	0.42
55:V:202:CDL:H792	55:V:202:CDL:H761	1.75	0.42
24:a:96:ALA:HB2	27:d:61:TYR:CE2	2.53	0.42
24:a:98:LEU:CD1	27:d:63:TYR:O	2.67	0.42
25:b:11:ARG:HB2	39:p:156:PRO:HB3	2.01	0.42
34:k:43:MET:O	34:k:47:ILE:HG13	2.19	0.42
37:n:17:VAL:HG13	40:r:7:PRO:HB3	2.01	0.42
40:r:193:ILE:HA	40:r:253:LEU:HD21	2.01	0.42
1:A:379:CYS:C	12:M:201:GLY:H	2.27	0.42
8:I:28:TYR:HA	13:N:55:PHE:HA	2.01	0.42
9:J:222:TRP:CD1	52:J:402:UQ:H101	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:300:GLN:HE21	13:N:137:TRP:HD1	1.67	0.42
13:N:3:LEU:HD13	55:N:201:CDL:OA7	2.18	0.42
30:g:75:TYR:CE2	30:g:79:LYS:HD2	2.54	0.42
43:v:52:MET:O	43:v:56:ARG:HG3	2.18	0.42
1:A:438:LEU:HD12	1:A:442:PHE:HB2	2.02	0.42
48:C:302:PLX:H21	48:C:302:PLX:H1A2	1.72	0.42
7:H:94:MET:HE2	7:H:97:TRP:HE3	1.83	0.42
9:J:204:SER:OG	9:J:238:GLN:O	2.34	0.42
9:J:315:THR:O	9:J:319:VAL:HG23	2.20	0.42
11:L:78:ARG:HD2	12:M:607:LYS:HE2	2.01	0.42
12:M:395:GLU:O	12:M:425:ASN:ND2	2.52	0.42
55:V:201:CDL:H442	55:V:201:CDL:H472	1.81	0.42
32:i:250:SER:O	32:i:259:GLY:HA3	2.18	0.42
35:l:33:PRO:HB3	35:l:118:PHE:CE1	2.54	0.42
35:l:153:LEU:HD23	35:l:153:LEU:HA	1.91	0.42
55:l:702:CDL:H121	55:l:702:CDL:H561	2.00	0.42
40:r:1:MET:O	40:r:1:MET:HG3	2.19	0.42
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.47	0.42
4:E:109:GLU:OE1	15:P:218:ARG:NH2	2.52	0.42
6:G:105:MET:HE1	6:G:139:MET:SD	2.59	0.42
21:W:103:ASP:OD1	21:W:103:ASP:N	2.52	0.42
26:c:79:PRO:C	26:c:81:ARG:H	2.27	0.42
32:i:207:ILE:O	32:i:211:MET:HG3	2.20	0.42
35:l:71:LEU:N	35:l:71:LEU:HD22	2.35	0.42
35:l:176:ARG:HH22	40:r:367:LEU:HD13	1.84	0.42
55:l:703:CDL:H571	55:l:703:CDL:H602	1.93	0.42
36:m:20:PHE:CD1	36:m:20:PHE:C	2.97	0.42
41:s:11:ILE:HB	41:s:12:PRO:HD3	2.02	0.42
41:s:66:SER:HB2	41:s:122:ALA:O	2.19	0.42
41:s:81:LEU:HA	41:s:81:LEU:HD23	1.80	0.42
42:u:38:LYS:HB3	42:u:39:PRO:HD3	2.01	0.42
43:v:17:PRO:HB3	43:v:105:GLU:HG3	2.00	0.42
2:B:120:GLU:HB2	2:B:130:ILE:HD12	2.01	0.42
8:I:93:LYS:HD3	8:I:94:ALA:O	2.20	0.42
9:J:172:ALA:HA	9:J:181:LEU:HB3	2.02	0.42
16:Q:220:ALA:HB3	16:Q:224:ALA:HA	2.01	0.42
21:W:58:ARG:HD3	41:s:316:PRO:HA	2.01	0.42
33:j:90:MET:SD	36:m:151:THR:HG23	2.59	0.42
35:l:341:MET:HE1	35:l:457:LEU:HD12	2.01	0.42
40:r:185:PRO:HB3	40:r:252:PRO:HD3	2.01	0.42
1:A:398:ARG:HG3	1:A:403:ASP:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:PHE:HB2	8:I:12:ARG:HG2	2.00	0.42
9:J:61:ALA:HB3	9:J:82:VAL:HG13	2.01	0.42
12:M:260:ASN:HD21	12:M:278:HIS:HD2	1.67	0.42
16:Q:139:LEU:HD22	16:Q:463:ARG:HG2	2.02	0.42
47:W:201:PEE:H42	47:W:201:PEE:H33	2.01	0.42
32:i:49:ASN:O	32:i:51:ARG:N	2.53	0.42
32:i:100:MET:HE2	32:i:153:LEU:HD11	1.98	0.42
32:i:106:LEU:HG	32:i:138:PRO:HB2	2.01	0.42
32:i:110:PRO:CG	35:l:594:THR:HG21	2.49	0.42
32:i:152:ASN:O	32:i:156:THR:HG22	2.19	0.42
38:o:80:PHE:HE1	38:o:86:THR:HG21	1.85	0.42
1:A:115:VAL:HB	1:A:156:ILE:HG12	2.01	0.42
1:A:115:VAL:HG11	1:A:138:LEU:HD11	2.00	0.42
1:A:320:GLY:HA3	1:A:349:LEU:O	2.20	0.42
47:B:303:PEE:H7	41:s:288:LEU:CD1	2.48	0.42
9:J:271:TYR:CE1	9:J:374:THR:HG22	2.54	0.42
12:M:467:LYS:HE2	12:M:467:LYS:HB3	1.64	0.42
12:M:476:LEU:HD21	12:M:481:LEU:HD21	2.00	0.42
16:Q:158:LEU:HD23	16:Q:158:LEU:HA	1.90	0.42
16:Q:196:ALA:HB2	41:s:278:PRO:HB3	2.02	0.42
20:V:66:ILE:HD11	20:V:101:LEU:HB2	2.00	0.42
55:V:201:CDL:H762	55:V:201:CDL:H401	2.01	0.42
23:Z:45:TRP:HB2	39:p:38:ARG:NH1	2.34	0.42
23:Z:82:VAL:HA	23:Z:85:GLU:HG2	2.01	0.42
24:a:74:TYR:O	28:e:96:SER:OG	2.26	0.42
26:c:161:TYR:HB3	26:c:166:LEU:HG	2.01	0.42
27:d:90:MET:SD	40:r:47:GLU:HB3	2.60	0.42
32:i:99:THR:CG2	32:i:153:LEU:HD23	2.39	0.42
35:l:51:LEU:HD22	35:l:91:PRO:HG3	2.02	0.42
36:m:163:ILE:O	36:m:167:VAL:HG23	2.19	0.42
55:m:201:CDL:H732	55:m:201:CDL:H762	1.90	0.42
41:s:126:LYS:O	41:s:130:ILE:HG13	2.18	0.42
41:s:209:SER:HB3	41:s:213:VAL:HA	2.02	0.42
4:E:55:SER:HB2	9:J:367:GLU:OE2	2.19	0.42
10:K:73:TYR:CZ	10:K:75:ASN:HB3	2.55	0.42
14:O:53:PHE:HD1	14:O:90:ASN:HD22	1.67	0.42
16:Q:139:LEU:O	16:Q:460:GLU:N	2.53	0.42
16:Q:145:MET:HG3	16:Q:214:TYR:OH	2.20	0.42
47:Q:501:PEE:H36	47:Q:501:PEE:C18	2.39	0.42
32:i:208:TYR:CZ	32:i:212:THR:HG21	2.54	0.42
32:i:335:LEU:HD21	55:r:504:CDL:H391	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:221:ALA:HA	35:l:226:GLN:HG2	2.00	0.42
47:l:704:PEE:H66	47:l:704:PEE:H72	1.48	0.42
38:o:23:TYR:OH	39:p:68:GLU:HG3	2.19	0.42
40:r:1:MET:SD	40:r:111:THR:HG21	2.60	0.42
41:s:54:LYS:HE3	41:s:54:LYS:HB3	1.87	0.42
43:v:22:MET:HE1	43:v:102:PHE:HA	2.02	0.42
3:C:50:LEU:O	3:C:54:VAL:HG23	2.20	0.42
3:C:142:TYR:CE2	16:Q:135:TYR:CE1	3.08	0.42
12:M:49:VAL:HB	12:M:91:ALA:HA	2.02	0.42
12:M:534:VAL:HG12	12:M:534:VAL:O	2.20	0.42
17:S:12:MET:HE1	41:s:20:LEU:HD13	2.02	0.42
17:S:65:GLY:HA2	42:u:24:VAL:HG21	2.01	0.42
18:T:84:ILE:HD12	18:T:84:ILE:HA	1.94	0.42
32:i:68:MET:HE1	34:k:37:MET:SD	2.59	0.42
35:l:399:VAL:HG12	35:l:409:LEU:HD13	2.02	0.42
40:r:312:ALA:O	40:r:316:MET:HG3	2.19	0.42
55:s:402:CDL:H742	55:s:402:CDL:C36	2.50	0.42
1:A:149:MET:HE1	1:A:241:THR:CB	2.37	0.42
2:B:188:GLU:HG3	13:N:127:TYR:OH	2.20	0.42
8:I:44:GLY:C	16:Q:359:ASP:OD2	2.62	0.42
12:M:591:GLU:HG3	12:M:610:VAL:HG23	2.02	0.42
14:O:130:TYR:CE1	14:O:208:LEU:HD11	2.54	0.42
24:a:66:ARG:NH1	28:e:72:ASP:HB2	2.35	0.42
32:i:25:HIS:HB3	32:i:28:LEU:HD23	2.01	0.42
34:k:2:PRO:HD2	34:k:5:TYR:CD2	2.54	0.42
35:l:435:PRO:HB3	35:l:437:PHE:CZ	2.55	0.42
55:l:702:CDL:H342	55:l:702:CDL:H372	1.67	0.42
55:l:703:CDL:H421	55:l:703:CDL:H391	1.79	0.42
42:u:47:ARG:HD2	42:u:47:ARG:HA	1.83	0.42
42:u:83:THR:HA	42:u:86:TRP:NE1	2.34	0.42
44:w:259:SER:OG	44:w:262:GLU:HG2	2.19	0.42
1:A:286:CYS:SG	14:O:227:PRO:HG3	2.60	0.41
1:A:376:HIS:NE2	14:O:33:GLY:O	2.50	0.41
1:A:449:ARG:HA	1:A:452:GLN:HG2	2.01	0.41
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.85	0.41
5:F:90:THR:O	5:F:94:VAL:HG23	2.20	0.41
6:G:119:ILE:O	6:G:123:GLU:HG3	2.20	0.41
8:I:20:LEU:O	8:I:23:LYS:O	2.38	0.41
10:K:68:PHE:CZ	14:O:238:PRO:HD2	2.55	0.41
47:U:101:PEE:H35	47:U:101:PEE:H30	1.70	0.41
55:V:202:CDL:H781	55:V:202:CDL:H812	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:71:GLY:HA2	38:o:79:ASN:HB2	2.01	0.41
39:p:98:LYS:O	40:r:419:TYR:HE2	2.03	0.41
41:s:4:ILE:HD12	41:s:4:ILE:H	1.85	0.41
41:s:56:PHE:CD2	47:s:401:PEE:H77	2.55	0.41
2:B:86:TYR:CG	2:B:87:PRO:HA	2.54	0.41
5:F:61:VAL:O	5:F:62:GLN:NE2	2.50	0.41
6:G:75:THR:HG23	6:G:78:ALA:H	1.85	0.41
18:T:119:ARG:HH12	18:T:122:HIS:CD2	2.39	0.41
55:V:202:CDL:H872	35:l:558:LEU:HD21	2.02	0.41
35:l:37:LYS:HD3	35:l:98:TRP:HE1	1.86	0.41
55:s:402:CDL:H202	55:s:402:CDL:H172	1.79	0.41
1:A:318:ILE:HB	1:A:355:ILE:HB	2.01	0.41
2:B:144:ARG:NH1	11:L:112:MET:O	2.33	0.41
12:M:355:LYS:HG3	12:M:366:LEU:HD13	2.02	0.41
47:W:201:PEE:H55	41:s:108:MET:HE1	2.02	0.41
25:b:25:ASP:OD2	39:p:125:TRP:NE1	2.40	0.41
26:c:167:TYR:CG	26:c:178:PRO:HG3	2.55	0.41
27:d:99:ASP:OD2	27:d:142:ARG:NH1	2.53	0.41
32:i:246:VAL:HG11	55:r:504:CDL:H392	2.02	0.41
36:m:15:ILE:CG2	55:s:402:CDL:C83	2.98	0.41
40:r:397:GLY:HA2	40:r:400:MET:HE3	2.01	0.41
3:C:62:LEU:O	3:C:91:VAL:HA	2.21	0.41
8:I:70:MET:CE	15:P:63:GLN:HG2	2.50	0.41
13:N:29:ARG:NH2	13:N:64:TYR:O	2.49	0.41
17:S:54:ILE:HD11	42:u:21:SER:HA	2.01	0.41
21:W:30:LEU:HG	21:W:31:SER:H	1.85	0.41
21:W:73:PRO:HG2	42:u:40:ASN:HB3	2.00	0.41
25:b:16:ARG:O	25:b:20:ARG:HG3	2.21	0.41
27:d:68:PHE:CE1	28:e:114:MET:HE1	2.56	0.41
32:i:115:VAL:HG12	32:i:180:ALA:HB1	2.01	0.41
34:k:76:SER:HA	34:k:79:VAL:HG12	2.02	0.41
35:l:68:TRP:CZ3	35:l:69:MET:HE2	2.55	0.41
35:l:297:ASP:O	35:l:301:ILE:HG13	2.20	0.41
40:r:127:VAL:CG2	40:r:128:PRO:HD3	2.51	0.41
41:s:213:VAL:HG13	41:s:214:GLU:HG2	2.02	0.41
9:J:75:ARG:NH2	15:P:215:GLU:OE1	2.53	0.41
12:M:185:PHE:CD1	12:M:185:PHE:C	2.98	0.41
14:O:148:ILE:HD12	14:O:184:PRO:HB2	2.02	0.41
17:S:48:MET:HE1	21:W:143:TYR:CZ	2.55	0.41
32:i:27:LEU:HD22	34:k:59:MET:HG2	2.02	0.41
35:l:356:ILE:HD11	35:l:425:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:534:HIS:CD2	47:l:704:PEE:O2P	2.73	0.41
41:s:2:PHE:O	41:s:6:ILE:HG13	2.21	0.41
41:s:24:GLU:HA	41:s:271:LEU:HD13	2.03	0.41
47:s:401:PEE:H80	52:s:403:UQ:H222	2.03	0.41
55:s:402:CDL:H412	55:s:402:CDL:H861	2.02	0.41
3:C:67:PHE:HZ	3:C:113:MET:HE2	1.86	0.41
3:C:83:ARG:CZ	16:Q:208:GLU:HG2	2.51	0.41
11:L:105:GLU:HA	12:M:611:THR:HG21	2.01	0.41
12:M:275:PRO:HG3	12:M:286:ILE:HG12	2.02	0.41
16:Q:84:PHE:HB2	16:Q:99:MET:CE	2.51	0.41
16:Q:155:VAL:HB	16:Q:229:PRO:HB3	2.02	0.41
16:Q:284:LEU:HD23	16:Q:284:LEU:HA	1.96	0.41
26:c:126:TRP:C	26:c:128:THR:H	2.28	0.41
32:i:246:VAL:HG21	55:r:504:CDL:H362	2.02	0.41
47:j:201:PEE:H30	55:s:402:CDL:H221	1.03	0.41
34:k:19:LEU:CD2	34:k:33:LEU:CD2	2.99	0.41
34:k:76:SER:O	34:k:79:VAL:HG12	2.20	0.41
1:A:358:ASP:OD1	1:A:361:THR:OG1	2.39	0.41
2:B:153:ILE:HG22	3:C:142:TYR:HB2	2.03	0.41
12:M:75:CYS:SG	53:M:803:FES:S1	3.19	0.41
12:M:179:CYS:SG	45:M:802:SF4:S3	3.06	0.41
26:c:186:ILE:HD11	43:v:104:ARG:HD2	2.03	0.41
48:g:201:PLX:H352	32:i:342:ALA:HB3	2.02	0.41
33:j:1:MET:HA	33:j:4:MET:HE3	2.02	0.41
44:w:113:SER:HB3	44:w:116:LYS:HB3	2.03	0.41
44:w:129:TYR:CD1	44:w:183:CYS:HB3	2.55	0.41
3:C:125:PRO:HG2	41:s:58:LYS:NZ	2.36	0.41
4:E:19:PRO:HB3	11:L:53:ILE:HG21	2.03	0.41
7:H:90:LEU:HB2	15:P:102:ASP:HB3	2.02	0.41
7:H:93:LYS:HB3	7:H:97:TRP:CZ3	2.56	0.41
7:H:94:MET:SD	7:H:99:PRO:HG3	2.61	0.41
8:I:12:ARG:NH2	8:I:21:GLN:HE21	2.18	0.41
17:S:63:THR:HG23	42:u:21:SER:HB2	2.03	0.41
27:d:37:PHE:CD2	35:l:3:PRO:HB3	2.56	0.41
1:A:46:TYR:CD2	14:O:234:LEU:HD12	2.56	0.41
1:A:119:GLU:O	1:A:159:ARG:NH1	2.54	0.41
1:A:339:PHE:CE1	1:A:349:LEU:HD23	2.55	0.41
2:B:77:LEU:HD13	41:s:31:MET:HG3	2.01	0.41
2:B:97:PHE:HB2	16:Q:215:GLU:OE2	2.21	0.41
3:C:64:PRO:HA	3:C:102:VAL:O	2.20	0.41
7:H:81:ILE:O	7:H:85:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:49:VAL:HG13	12:M:102:ILE:HD13	2.02	0.41
12:M:300:GLN:NE2	13:N:137:TRP:HD1	2.18	0.41
12:M:307:ILE:HG23	12:M:317:THR:HG21	2.03	0.41
12:M:406:ASN:ND2	12:M:409:PHE:HD2	2.19	0.41
16:Q:127:LYS:O	16:Q:419:PRO:HD2	2.21	0.41
17:S:31:ASN:ND2	17:S:36:LYS:HB2	2.35	0.41
21:W:94:GLU:OE2	21:W:104:TRP:NE1	2.51	0.41
22:Y:97:LEU:HD21	43:v:100:LYS:HB3	2.03	0.41
24:a:80:ILE:HB	24:a:81:PRO:HD3	2.03	0.41
31:h:17:TRP:CD1	31:h:17:TRP:H	2.38	0.41
35:l:12:LEU:HD22	35:l:129:MET:HB3	2.02	0.41
35:l:78:LEU:HD11	55:l:702:CDL:H261	2.02	0.41
35:l:150:MET:HE3	55:l:702:CDL:H151	2.03	0.41
35:l:526:LEU:HD12	35:l:530:PRO:HG2	2.03	0.41
35:l:584:ILE:HG22	35:l:587:TYR:OH	2.21	0.41
35:l:591:PHE:O	35:l:595:ILE:HG13	2.20	0.41
37:n:7:ILE:O	37:n:11:HIS:N	2.54	0.41
38:o:57:LEU:HD23	38:o:57:LEU:C	2.46	0.41
39:p:27:LEU:HD11	39:p:40:PHE:HB3	2.02	0.41
40:r:159:PRO:HB3	47:r:501:PEE:H25	2.03	0.41
40:r:328:CYS:O	40:r:332:THR:HG23	2.21	0.41
1:A:61:ASP:OD2	1:A:137:LYS:CG	2.69	0.41
12:M:182:CYS:SG	45:M:802:SF4:S2	3.19	0.41
15:P:59:SER:O	15:P:63:GLN:HG3	2.21	0.41
15:P:106:ALA:HB1	15:P:108:PHE:CE1	2.56	0.41
20:V:25:SER:OG	20:V:67:GLY:O	2.35	0.41
55:V:202:CDL:H712	55:V:202:CDL:H521	2.03	0.41
21:W:81:ARG:HH21	42:u:60:GLY:C	2.29	0.41
21:W:97:ILE:HD13	31:h:83:ARG:HB2	2.03	0.41
32:i:79:LEU:HB2	34:k:47:ILE:CD1	2.51	0.41
44:w:147:LEU:HD12	44:w:198:TYR:HD2	1.85	0.41
1:A:207:GLY:HA3	46:A:502:FMN:N5	2.35	0.40
9:J:94:LEU:HA	9:J:97:MET:SD	2.61	0.40
12:M:224:ASP:OD2	12:M:291:ARG:NH2	2.54	0.40
12:M:367:CYS:HA	12:M:531:LYS:O	2.20	0.40
13:N:55:PHE:CE1	13:N:58:ARG:HG3	2.56	0.40
55:N:201:CDL:C55	55:N:201:CDL:H742	2.51	0.40
27:d:62:TYR:CD1	27:d:62:TYR:N	2.88	0.40
34:k:4:VAL:HG13	36:m:10:SER:OG	2.21	0.40
55:l:702:CDL:H621	55:l:702:CDL:H432	2.02	0.40
44:w:110:GLY:HA2	44:w:134:TRP:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:132:ARG:HA	9:J:132:ARG:HD3	1.76	0.40
14:O:127:VAL:HB	14:O:170:THR:HG21	2.04	0.40
18:T:36:GLU:OE1	18:T:60:LYS:NZ	2.48	0.40
18:T:45:TYR:CE2	18:T:55:PHE:CE2	3.08	0.40
20:V:49:PHE:O	20:V:53:VAL:HG23	2.21	0.40
55:V:202:CDL:H392	55:V:202:CDL:H421	1.82	0.40
28:e:90:VAL:HG13	40:r:78:MET:HE2	2.04	0.40
28:e:129:ARG:HD2	28:e:136:LEU:HA	2.03	0.40
33:j:15:SER:HA	33:j:18:VAL:HG12	2.01	0.40
55:l:703:CDL:H641	55:l:703:CDL:H612	1.87	0.40
1:A:98:LYS:NZ	46:A:502:FMN:O3P	2.46	0.40
5:F:96:SER:O	5:F:98:LYS:N	2.50	0.40
13:N:3:LEU:O	13:N:6:VAL:HG22	2.21	0.40
13:N:106:ARG:HB2	13:N:109:ILE:HG13	2.02	0.40
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.85	0.40
28:e:66:LEU:HD23	28:e:66:LEU:HA	1.93	0.40
30:g:36:MET:HG3	30:g:74:GLY:HA3	2.03	0.40
32:i:109:SER:HB3	32:i:164:ILE:HD12	2.04	0.40
33:j:73:LEU:HD12	36:m:55:MET:SD	2.62	0.40
35:l:48:LEU:HD23	35:l:48:LEU:HA	1.95	0.40
47:l:704:PEE:H68	47:l:704:PEE:H22	2.02	0.40
36:m:58:LEU:HD13	41:s:107:ALA:HA	2.03	0.40
39:p:100:PRO:HD3	40:r:419:TYR:CZ	2.56	0.40
40:r:253:LEU:HD12	40:r:253:LEU:HA	1.96	0.40
44:w:350:LYS:HG3	44:w:351:TRP:CD1	2.56	0.40
1:A:367:ILE:O	1:A:371:ILE:HG12	2.22	0.40
6:G:93:ILE:HG23	6:G:108:LEU:HD22	2.04	0.40
9:J:163:LYS:NZ	9:J:253:ILE:O	2.39	0.40
9:J:167:ILE:HD11	9:J:249:ILE:HD11	2.04	0.40
9:J:311:GLU:HA	9:J:312:PRO:HD3	1.84	0.40
55:N:201:CDL:OA7	55:N:201:CDL:HA62	2.16	0.40
15:P:65:VAL:HG11	15:P:86:ILE:HD13	2.03	0.40
17:S:31:ASN:ND2	17:S:60:TYR:HH	2.15	0.40
6:X:115:GLN:O	6:X:119:ILE:HG12	2.22	0.40
25:b:73:THR:HG23	25:b:74:HIS:ND1	2.36	0.40
31:h:47:ILE:CD1	31:h:52:ALA:CA	2.97	0.40
32:i:41:ILE:HD13	32:i:41:ILE:HA	1.94	0.40
32:i:268:GLN:NE2	32:i:272:LYS:HE3	2.36	0.40
47:l:704:PEE:H58	47:l:704:PEE:H53	1.50	0.40
44:w:214:ILE:O	44:w:218:ILE:HG13	2.22	0.40
1:A:65:THR:O	1:A:69:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:LEU:HD23	2:B:210:LEU:HA	1.94	0.40
10:K:79:HIS:O	10:K:79:HIS:ND1	2.48	0.40
12:M:634:LEU:HD13	12:M:636:TYR:OH	2.22	0.40
14:O:185:MET:C	14:O:185:MET:SD	3.05	0.40
17:S:1:MET:HE3	17:S:1:MET:HB3	1.99	0.40
19:U:41:TYR:O	19:U:45:ILE:HG13	2.22	0.40
20:V:22:ALA:O	20:V:26:THR:OG1	2.35	0.40
24:a:67:PHE:CE2	40:r:434:ASN:HB3	2.56	0.40
25:b:32:GLU:HB2	25:b:33:PRO:HD3	2.03	0.40
25:b:101:LYS:HA	25:b:102:PRO:HD3	1.98	0.40
48:g:201:PLX:H132	48:g:201:PLX:H101	1.77	0.40
48:j:202:PLX:H4	48:j:202:PLX:H72	1.77	0.40
35:l:21:MET:HE2	35:l:21:MET:HB3	2.01	0.40
37:n:16:LEU:HD23	37:n:16:LEU:HA	1.94	0.40
40:r:166:TYR:O	40:r:170:THR:HG23	2.22	0.40
41:s:18:ALA:HB2	52:s:403:UQ:H211	2.03	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%)	413 (96%)	18 (4%)	0	100	100
2	B	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
3	C	154/156 (99%)	150 (97%)	4 (3%)	0	100	100
4	E	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
5	F	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
6	G	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
6	X	86/88 (98%)	84 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	110/112 (98%)	103 (94%)	6 (6%)	1 (1%)	14	41
8	I	93/112 (83%)	84 (90%)	8 (9%)	1 (1%)	11	36
9	J	340/342 (99%)	329 (97%)	11 (3%)	0	100	100
10	K	41/43 (95%)	41 (100%)	0	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	663 (96%)	24 (4%)	1 (0%)	48	77
13	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
14	O	215/217 (99%)	203 (94%)	12 (6%)	0	100	100
15	P	206/208 (99%)	199 (97%)	7 (3%)	0	100	100
16	Q	427/430 (99%)	415 (97%)	11 (3%)	1 (0%)	43	72
17	S	68/70 (97%)	63 (93%)	4 (6%)	1 (2%)	8	28
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%)	135 (98%)	3 (2%)	0	100	100
21	W	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
22	Y	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
23	Z	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
24	a	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
25	b	94/126 (75%)	86 (92%)	8 (8%)	0	100	100
26	c	154/156 (99%)	143 (93%)	10 (6%)	1 (1%)	21	51
27	d	173/175 (99%)	171 (99%)	2 (1%)	0	100	100
28	e	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
29	f	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
30	g	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
32	i	345/347 (99%)	331 (96%)	14 (4%)	0	100	100
33	j	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
34	k	96/98 (98%)	95 (99%)	0	1 (1%)	12	39
35	l	604/606 (100%)	580 (96%)	24 (4%)	0	100	100
36	m	173/175 (99%)	160 (92%)	12 (7%)	1 (1%)	21	51
37	n	54/56 (96%)	54 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	o	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
39	p	176/178 (99%)	171 (97%)	4 (2%)	1 (1%)	21	51
40	r	457/459 (100%)	456 (100%)	1 (0%)	0	100	100
41	s	316/318 (99%)	309 (98%)	7 (2%)	0	100	100
42	u	169/171 (99%)	163 (96%)	4 (2%)	2 (1%)	10	34
43	v	122/125 (98%)	118 (97%)	4 (3%)	0	100	100
44	w	318/320 (99%)	305 (96%)	13 (4%)	0	100	100
All	All	8174/8313 (98%)	7886 (96%)	277 (3%)	11 (0%)	49	77

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	S	35	GLU
34	k	24	SER
8	I	41	LEU
42	u	168	PHE
26	c	80	ASP
39	p	174	PRO
7	H	77	ILE
12	M	281	ILE
42	u	152	PRO
16	Q	229	PRO
36	m	24	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/346 (100%)	344 (99%)	2 (1%)	78	93
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	131 (99%)	1 (1%)	73	90
4	E	107/107 (100%)	106 (99%)	1 (1%)	70	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	75/76 (99%)	75 (100%)	0	100	100
6	G	76/81 (94%)	76 (100%)	0	100	100
6	X	78/81 (96%)	77 (99%)	1 (1%)	61	86
7	H	99/99 (100%)	98 (99%)	1 (1%)	68	89
8	I	87/97 (90%)	86 (99%)	1 (1%)	65	88
9	J	296/296 (100%)	296 (100%)	0	100	100
10	K	42/42 (100%)	42 (100%)	0	100	100
11	L	113/113 (100%)	113 (100%)	0	100	100
12	M	580/580 (100%)	576 (99%)	4 (1%)	76	92
13	N	130/130 (100%)	130 (100%)	0	100	100
14	O	183/183 (100%)	181 (99%)	2 (1%)	65	88
15	P	190/190 (100%)	188 (99%)	2 (1%)	65	88
16	Q	370/370 (100%)	369 (100%)	1 (0%)	86	96
17	S	57/58 (98%)	57 (100%)	0	100	100
18	T	79/79 (100%)	78 (99%)	1 (1%)	61	86
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	101 (100%)	0	100	100
21	W	122/123 (99%)	122 (100%)	0	100	100
22	Y	62/62 (100%)	62 (100%)	0	100	100
23	Z	62/62 (100%)	62 (100%)	0	100	100
24	a	121/121 (100%)	121 (100%)	0	100	100
25	b	90/119 (76%)	90 (100%)	0	100	100
26	c	141/141 (100%)	141 (100%)	0	100	100
27	d	155/155 (100%)	155 (100%)	0	100	100
28	e	96/96 (100%)	96 (100%)	0	100	100
29	f	35/45 (78%)	35 (100%)	0	100	100
30	g	108/108 (100%)	108 (100%)	0	100	100
31	h	93/93 (100%)	93 (100%)	0	100	100
32	i	311/311 (100%)	310 (100%)	1 (0%)	86	96
33	j	100/100 (100%)	99 (99%)	1 (1%)	68	89
34	k	85/85 (100%)	84 (99%)	1 (1%)	63	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	l	540/540 (100%)	539 (100%)	1 (0%)	87	96
36	m	129/141 (92%)	129 (100%)	0	100	100
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	113/113 (100%)	113 (100%)	0	100	100
39	p	159/159 (100%)	159 (100%)	0	100	100
40	r	410/410 (100%)	409 (100%)	1 (0%)	87	96
41	s	275/275 (100%)	272 (99%)	3 (1%)	65	88
42	u	153/153 (100%)	152 (99%)	1 (1%)	76	92
43	v	104/111 (94%)	104 (100%)	0	100	100
44	w	282/283 (100%)	282 (100%)	0	100	100
All	All	7160/7240 (99%)	7134 (100%)	26 (0%)	81	94

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASP
1	A	240	THR
3	C	188	LYS
4	E	96	VAL
7	H	104	VAL
8	I	25	GLN
12	M	171	THR
12	M	172	ILE
12	M	173	MET
12	M	688	GLN
14	O	74	HIS
14	O	181	VAL
15	P	107	GLN
15	P	201	ASP
16	Q	143	SER
18	T	46	ASP
6	X	133	ILE
32	i	149	ILE
33	j	31	SER
34	k	21	MET
35	l	119	LYS
40	r	138	ASN
41	s	200	LEU

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Mol	Chain	Res	Type
41	s	202	GLU
41	s	204	GLU
42	u	77	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	ASN
1	A	244	ASN
1	A	418	GLN
1	A	457	HIS
4	E	26	ASN
4	E	48	HIS
4	E	72	HIS
4	E	126	HIS
5	F	48	ASN
5	F	80	ASN
7	H	37	GLN
7	H	76	GLN
7	H	83	GLN
8	I	21	GLN
8	I	47	HIS
9	J	38	HIS
9	J	43	HIS
9	J	79	GLN
9	J	122	HIS
9	J	128	ASN
9	J	154	GLN
9	J	269	ASN
9	J	295	HIS
11	L	71	HIS
11	L	86	ASN
12	M	123	ASN
12	M	142	GLN
12	M	202	ASN
12	M	260	ASN
12	M	278	HIS
12	M	300	GLN
12	M	304	GLN
12	M	336	ASN
12	M	406	ASN
12	M	540	ASN

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Mol	Chain	Res	Type
12	M	604	GLN
12	M	688	GLN
13	N	135	GLN
14	O	41	HIS
14	O	48	ASN
14	O	69	ASN
14	O	90	ASN
14	O	99	ASN
15	P	82	ASN
15	P	107	GLN
15	P	124	ASN
16	Q	285	ASN
17	S	31	ASN
17	S	61	HIS
17	S	68	ASN
18	T	74	GLN
18	T	120	GLN
21	W	76	GLN
21	W	90	ASN
23	Z	21	GLN
25	b	13	GLN
27	d	55	GLN
28	e	86	ASN
29	f	61	GLN
31	h	7	GLN
31	h	34	HIS
31	h	70	GLN
31	h	97	HIS
31	h	98	HIS
32	i	77	ASN
32	i	112	HIS
32	i	134	GLN
32	i	174	GLN
32	i	273	ASN
33	j	26	GLN
34	k	57	ASN
35	l	72	GLN
35	l	135	ASN
35	l	194	ASN
35	l	199	GLN
35	l	348	HIS
35	l	354	GLN

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Mol	Chain	Res	Type
35	l	479	ASN
39	p	12	HIS
39	p	62	GLN
40	r	175	ASN
40	r	255	ASN
40	r	338	HIS
42	u	30	HIS
44	w	188	ASN
44	w	202	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	2.00	1 (10%)	5,13,15	5.94	3 (60%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.75	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	12.11	130.58	119.48
16	Q	118	2MR	CD-NE-CZ	4.28	131.41	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.27	130.68	123.65

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 2 are modelled with single atom and 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	$\# Z > 2$
55	CDL	r	504	-	98,98,99	1.11	8 (8%)	104,110,111	0.86	4 (3%)
48	PLX	j	202	-	51,51,51	1.21	4 (7%)	53,59,59	0.62	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	ADP	w	401	-	28,29,29	3.17	9 (32%)	43,45,45	1.89	8 (18%)
51	NDP	J	401	-	51,52,52	4.24	24 (47%)	71,80,80	2.28	12 (16%)
47	PEE	U	101	-	50,50,50	1.18	6 (12%)	53,55,55	1.00	2 (3%)
47	PEE	B	303	-	50,50,50	1.18	6 (12%)	53,55,55	0.98	2 (3%)
55	CDL	l	702	-	98,98,99	1.11	8 (8%)	104,110,111	0.90	4 (3%)
47	PEE	r	501	-	50,50,50	1.19	6 (12%)	53,55,55	1.03	2 (3%)
53	FES	M	803	12	0,4,4	-	-	-		
47	PEE	l	704	-	49,49,50	1.19	6 (12%)	52,54,55	1.01	2 (3%)
45	SF4	B	302	2	0,12,12	-	-	-		
47	PEE	j	201	-	40,40,50	1.16	5 (12%)	43,45,55	1.05	3 (6%)
45	SF4	M	802	12	0,12,12	-	-	-		
48	PLX	C	302	-	51,51,51	0.60	0	53,59,59	0.80	2 (3%)
46	FMN	A	502	-	33,33,33	1.43	5 (15%)	48,50,50	1.30	8 (16%)
47	PEE	Q	501	-	46,46,50	1.22	6 (13%)	49,51,55	1.00	2 (4%)
47	PEE	s	401	-	46,46,50	1.22	6 (13%)	49,51,55	1.00	2 (4%)
55	CDL	s	402	-	88,88,99	0.98	4 (4%)	94,100,111	1.07	6 (6%)
55	CDL	a	201	-	99,99,99	1.12	8 (8%)	105,111,111	0.87	4 (3%)
48	PLX	a	202	-	51,51,51	1.21	4 (7%)	53,59,59	0.61	1 (1%)
53	FES	O	301	14	0,4,4	-	-	-		
47	PEE	b	201	-	45,45,50	1.24	6 (13%)	48,50,55	1.00	2 (4%)
47	PEE	W	201	-	40,40,50	1.16	5 (12%)	43,45,55	1.03	2 (4%)
45	SF4	M	801	12	0,12,12	-	-	-		
55	CDL	u	201	-	54,54,99	1.24	4 (7%)	60,66,111	1.28	5 (8%)
50	8Q1	X	201	-	32,34,34	2.25	7 (21%)	39,43,43	1.72	10 (25%)
55	CDL	V	202	-	99,99,99	1.12	9 (9%)	105,111,111	0.88	4 (3%)
47	PEE	l	701	-	39,39,50	1.34	6 (15%)	42,44,55	1.10	3 (7%)
45	SF4	A	501	1	0,12,12	-	-	-		
52	UQ	J	402	-	33,33,63	3.51	9 (27%)	42,43,79	2.79	14 (33%)
48	PLX	r	503	-	51,51,51	1.21	5 (9%)	53,59,59	0.55	1 (1%)
52	UQ	s	403	-	38,38,63	3.64	10 (26%)	48,49,79	2.77	17 (35%)
48	PLX	J	403	-	51,51,51	1.20	4 (7%)	53,59,59	0.61	1 (1%)
45	SF4	B	301	2	0,12,12	-	-	-		
55	CDL	m	201	-	94,94,99	1.14	9 (9%)	100,106,111	0.89	4 (4%)
48	PLX	g	201	-	51,51,51	1.21	4 (7%)	53,59,59	0.65	1 (1%)
49	970	C	303	-	33,33,33	4.76	13 (39%)	48,50,50	2.44	20 (41%)
55	CDL	N	201	-	50,50,99	1.29	4 (8%)	56,62,111	1.36	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	CDL	l	703	-	99,99,99	0.93	4 (4%)	105,111,111	1.10	7 (6%)
50	8Q1	G	201	-	32,34,34	2.23	7 (21%)	39,43,43	1.81	10 (25%)
48	PLX	r	502	-	51,51,51	1.21	5 (9%)	53,59,59	0.63	1 (1%)
55	CDL	V	201	-	93,93,99	1.15	9 (9%)	99,105,111	0.87	4 (4%)
45	SF4	C	301	3	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	CDL	r	504	-	-	50/109/109/110	-
48	PLX	j	202	-	-	30/55/55/55	-
57	ADP	w	401	-	-	4/16/32/32	0/3/3/3
51	NDP	J	401	-	-	6/34/77/77	0/5/5/5
47	PEE	U	101	-	-	24/54/54/54	-
47	PEE	B	303	-	-	30/54/54/54	-
55	CDL	l	702	-	-	60/109/109/110	-
47	PEE	r	501	-	-	26/54/54/54	-
53	FES	M	803	12	-	-	0/1/1/1
47	PEE	l	704	-	-	27/53/53/54	-
45	SF4	B	302	2	-	-	0/6/5/5
47	PEE	j	201	-	-	30/44/44/54	-
45	SF4	M	802	12	-	-	0/6/5/5
48	PLX	C	302	-	-	15/55/55/55	-
46	FMN	A	502	-	-	6/18/18/18	0/3/3/3
47	PEE	Q	501	-	-	18/50/50/54	-
47	PEE	s	401	-	-	24/50/50/54	-
55	CDL	s	402	-	-	40/99/99/110	-
55	CDL	a	201	-	-	61/110/110/110	-
48	PLX	a	202	-	-	30/55/55/55	-
53	FES	O	301	14	-	-	0/1/1/1
47	PEE	b	201	-	-	23/49/49/54	-
47	PEE	W	201	-	-	26/44/44/54	-
55	CDL	u	201	-	-	23/65/65/110	-
45	SF4	M	801	12	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	8Q1	X	201	-	-	19/41/41/41	-
55	CDL	V	202	-	-	56/110/110/110	-
47	PEE	l	701	-	-	24/43/43/54	-
52	UQ	J	402	-	-	17/27/51/87	0/1/1/1
45	SF4	A	501	1	-	-	0/6/5/5
48	PLX	r	503	-	-	31/55/55/55	-
52	UQ	s	403	-	-	13/33/57/87	0/1/1/1
48	PLX	J	403	-	-	30/55/55/55	-
45	SF4	B	301	2	-	-	0/6/5/5
55	CDL	m	201	-	-	54/105/105/110	-
48	PLX	g	201	-	-	39/55/55/55	-
49	970	C	303	-	-	4/8/41/41	0/5/5/5
55	CDL	N	201	-	-	23/61/61/110	-
55	CDL	l	703	-	-	39/110/110/110	-
50	8Q1	G	201	-	-	16/41/41/41	-
48	PLX	r	502	-	-	22/55/55/55	-
55	CDL	V	201	-	-	63/104/104/110	-
45	SF4	C	301	3	-	-	0/6/5/5

All (235) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	C	303	970	O16-C17	18.23	1.58	1.37
51	J	401	NDP	C3B-C2B	-12.80	1.25	1.53
49	C	303	970	C14-C23	-12.27	1.41	1.52
51	J	401	NDP	O4D-C4D	10.66	1.68	1.45
51	J	401	NDP	C3D-C4D	-10.13	1.27	1.53
52	s	403	UQ	C18-C19	10.01	1.56	1.33
52	J	402	UQ	C18-C19	9.92	1.55	1.33
52	s	403	UQ	C13-C14	9.64	1.55	1.33
52	J	402	UQ	C13-C14	9.58	1.55	1.33
52	s	403	UQ	C23-C24	9.45	1.54	1.33
52	J	402	UQ	C8-C9	9.32	1.54	1.33
52	s	403	UQ	C8-C9	9.29	1.54	1.33
57	w	401	ADP	C3'-C4'	-9.00	1.30	1.53
51	J	401	NDP	O4B-C4B	-8.19	1.26	1.45
49	C	303	970	O13-C12	7.85	1.49	1.37
50	G	201	8Q1	P24-O27	7.72	1.84	1.60
57	w	401	ADP	O4'-C4'	7.71	1.62	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	X	201	8Q1	P24-O27	7.68	1.84	1.60
52	J	402	UQ	C23-C24	7.49	1.54	1.32
52	s	403	UQ	C28-C29	7.38	1.54	1.32
51	J	401	NDP	C2N-C3N	7.34	1.55	1.35
51	J	401	NDP	C6N-C5N	7.18	1.55	1.33
49	C	303	970	O08-C07	7.10	1.48	1.37
57	w	401	ADP	PA-O3A	6.56	1.66	1.59
51	J	401	NDP	PN-O3	6.55	1.66	1.59
51	J	401	NDP	C6A-N6A	5.68	1.48	1.34
49	C	303	970	C23-C24	-5.49	1.47	1.52
51	J	401	NDP	P2B-O2B	5.46	1.69	1.59
50	X	201	8Q1	C28-C29	5.45	1.61	1.52
51	J	401	NDP	PA-O3	5.44	1.65	1.59
57	w	401	ADP	C6-N6	5.43	1.48	1.34
50	G	201	8Q1	C28-C29	5.42	1.61	1.52
49	C	303	970	C22-C23	-5.19	1.44	1.51
51	J	401	NDP	C3B-C4B	5.19	1.66	1.53
51	J	401	NDP	O4D-C1D	-5.12	1.30	1.42
51	J	401	NDP	C6N-N1N	5.02	1.49	1.37
46	A	502	FMN	C9A-C5A	4.83	1.48	1.41
51	J	401	NDP	O4B-C1B	4.63	1.52	1.42
51	J	401	NDP	C1B-N9A	-4.62	1.33	1.46
57	w	401	ADP	O4'-C1'	-4.57	1.31	1.42
55	N	201	CDL	OB8-CB7	4.35	1.46	1.33
55	s	402	CDL	OA6-CA5	4.32	1.46	1.34
55	l	703	CDL	OA8-CA7	4.31	1.45	1.33
55	u	201	CDL	OA8-CA7	4.29	1.45	1.33
55	s	402	CDL	OA8-CA7	4.26	1.45	1.33
55	N	201	CDL	OA8-CA7	4.24	1.45	1.33
55	l	703	CDL	OB6-CB5	4.21	1.46	1.34
55	l	703	CDL	OB8-CB7	4.18	1.45	1.33
55	N	201	CDL	OA6-CA5	4.18	1.46	1.34
55	u	201	CDL	OB6-CB5	4.16	1.46	1.34
55	u	201	CDL	OB8-CB7	4.15	1.45	1.33
55	l	703	CDL	OA6-CA5	4.14	1.46	1.34
55	s	402	CDL	OB8-CB7	4.13	1.45	1.33
55	s	402	CDL	OB6-CB5	4.12	1.45	1.34
55	u	201	CDL	OA6-CA5	4.06	1.45	1.34
51	J	401	NDP	O2D-C2D	-4.05	1.32	1.43
49	C	303	970	C05-C04	-4.00	1.48	1.54
55	N	201	CDL	OB6-CB5	3.95	1.45	1.34
50	X	201	8Q1	C1-S44	3.86	1.85	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	l	701	PEE	C18-C19	3.82	1.53	1.31
51	J	401	NDP	C7N-N7N	3.81	1.44	1.33
47	b	201	PEE	C18-C19	3.81	1.53	1.31
47	U	101	PEE	C18-C19	3.81	1.53	1.31
47	s	401	PEE	C18-C19	3.81	1.53	1.31
47	r	501	PEE	C18-C19	3.81	1.53	1.31
47	W	201	PEE	C18-C19	3.80	1.53	1.31
47	B	303	PEE	C18-C19	3.80	1.53	1.31
50	G	201	8Q1	C1-S44	3.79	1.85	1.76
47	l	704	PEE	C18-C19	3.79	1.53	1.31
47	j	201	PEE	C18-C19	3.78	1.53	1.31
47	Q	501	PEE	C18-C19	3.78	1.53	1.31
47	r	501	PEE	C39-C38	3.76	1.53	1.31
47	l	701	PEE	C39-C38	3.75	1.53	1.31
47	B	303	PEE	C39-C38	3.74	1.52	1.31
47	s	401	PEE	C39-C38	3.73	1.52	1.31
47	b	201	PEE	C39-C38	3.73	1.52	1.31
47	Q	501	PEE	C39-C38	3.71	1.52	1.31
47	U	101	PEE	C39-C38	3.69	1.52	1.31
47	l	704	PEE	C39-C38	3.68	1.52	1.31
55	m	201	CDL	OA8-CA7	3.52	1.43	1.33
55	V	202	CDL	OA8-CA7	3.46	1.43	1.33
55	a	201	CDL	OA8-CA7	3.46	1.43	1.33
55	l	702	CDL	OA8-CA7	3.44	1.43	1.33
55	V	201	CDL	OA8-CA7	3.44	1.43	1.33
50	X	201	8Q1	O27-C28	-3.42	1.32	1.43
55	r	504	CDL	OA8-CA7	3.40	1.43	1.33
51	J	401	NDP	C8A-N9A	-3.39	1.31	1.37
50	G	201	8Q1	O27-C28	-3.37	1.33	1.43
50	X	201	8Q1	C34-N36	3.37	1.41	1.33
46	A	502	FMN	C8-C7	3.37	1.49	1.40
57	w	401	ADP	C8-N9	-3.33	1.31	1.37
55	m	201	CDL	OA6-CA5	3.29	1.43	1.34
51	J	401	NDP	C5A-N7A	-3.21	1.33	1.39
49	C	303	970	O13-C14	3.18	1.49	1.45
49	C	303	970	O16-C15	3.14	1.52	1.44
57	w	401	ADP	O2'-C2'	-3.09	1.35	1.43
55	V	201	CDL	OA6-CA5	3.08	1.43	1.34
50	G	201	8Q1	C6-C1	3.07	1.53	1.50
50	G	201	8Q1	C34-N36	3.07	1.40	1.33
55	a	201	CDL	OB8-CB7	3.07	1.42	1.33
55	V	201	CDL	OB8-CB7	3.06	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	l	702	CDL	OB8-CB7	3.05	1.42	1.33
55	a	201	CDL	OB6-CB5	3.04	1.42	1.34
55	V	201	CDL	OB6-CB5	3.03	1.42	1.34
55	r	504	CDL	OB8-CB7	3.03	1.42	1.33
55	r	504	CDL	OB6-CB5	3.02	1.42	1.34
55	m	201	CDL	OB6-CB5	3.01	1.42	1.34
55	m	201	CDL	OB8-CB7	3.01	1.42	1.33
55	V	202	CDL	OB8-CB7	3.00	1.42	1.33
55	V	202	CDL	OA6-CA5	2.98	1.42	1.34
57	w	401	ADP	O3'-C3'	2.98	1.50	1.43
55	l	702	CDL	OB6-CB5	2.97	1.42	1.34
55	a	201	CDL	OA6-CA5	2.96	1.42	1.34
55	V	202	CDL	OB6-CB5	2.96	1.42	1.34
55	l	702	CDL	OA6-CA5	2.95	1.42	1.34
50	X	201	8Q1	C6-C1	2.95	1.53	1.50
48	g	201	PLX	O6-C4	-2.94	1.40	1.44
55	r	504	CDL	OA6-CA5	2.90	1.42	1.34
49	C	303	970	O25-C24	-2.84	1.18	1.22
51	J	401	NDP	C7N-C3N	2.81	1.54	1.48
51	J	401	NDP	O3D-C3D	2.80	1.49	1.43
47	l	704	PEE	O2-C2	-2.80	1.40	1.46
47	B	303	PEE	O2-C2	-2.78	1.40	1.46
52	J	402	UQ	C6-C1	2.77	1.54	1.46
48	a	202	PLX	O6-C4	-2.76	1.41	1.44
52	s	403	UQ	C6-C1	2.76	1.54	1.46
48	r	502	PLX	O6-C4	-2.75	1.41	1.44
46	A	502	FMN	C4-N3	-2.73	1.33	1.38
48	r	503	PLX	O6-C4	-2.72	1.41	1.44
50	G	201	8Q1	C39-N41	2.71	1.39	1.33
50	X	201	8Q1	C39-N41	2.70	1.39	1.33
49	C	303	970	C10-C11	2.69	1.44	1.39
47	s	401	PEE	O2-C2	-2.65	1.40	1.46
51	J	401	NDP	O2B-C2B	2.63	1.53	1.44
47	Q	501	PEE	O2-C2	-2.62	1.40	1.46
48	j	202	PLX	O6-C4	-2.61	1.41	1.44
47	l	701	PEE	O2-C2	-2.59	1.40	1.46
47	r	501	PEE	O2-C2	-2.58	1.40	1.46
55	r	504	CDL	OA6-CA4	-2.58	1.40	1.46
47	j	201	PEE	O2-C2	-2.57	1.40	1.46
47	W	201	PEE	O2-C2	-2.57	1.40	1.46
55	a	201	CDL	OA6-CA4	-2.56	1.40	1.46
55	l	702	CDL	OA6-CA4	-2.55	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	U	101	PEE	O2-C2	-2.55	1.40	1.46
55	V	202	CDL	OA6-CA4	-2.53	1.40	1.46
47	b	201	PEE	O2-C2	-2.52	1.40	1.46
47	j	201	PEE	O3-C30	2.48	1.40	1.33
49	C	303	970	C05-C06	-2.48	1.48	1.51
48	j	202	PLX	C7-C6	2.48	1.55	1.50
47	U	101	PEE	O3-C30	2.46	1.40	1.33
47	l	701	PEE	O3-C30	2.46	1.40	1.33
47	s	401	PEE	O3-C30	2.46	1.40	1.33
49	C	303	970	C12-C06	2.45	1.43	1.39
48	J	403	PLX	O6-C4	-2.45	1.41	1.44
47	b	201	PEE	O3-C30	2.44	1.40	1.33
48	r	502	PLX	C7-C6	2.43	1.55	1.50
48	r	503	PLX	C7-C6	2.43	1.55	1.50
48	J	403	PLX	C7-C6	2.41	1.55	1.50
52	s	403	UQ	C7-C8	2.41	1.54	1.50
48	a	202	PLX	C7-C6	2.40	1.55	1.50
47	r	501	PEE	O3-C30	2.38	1.40	1.33
48	g	201	PLX	C7-C6	2.37	1.55	1.50
57	w	401	ADP	C5-N7	-2.37	1.34	1.39
47	l	704	PEE	O3-C30	2.36	1.40	1.33
47	B	303	PEE	O3-C30	2.36	1.40	1.33
55	V	201	CDL	OB6-CB4	-2.34	1.41	1.46
46	A	502	FMN	C5A-N5	-2.34	1.35	1.39
47	Q	501	PEE	O3-C30	2.33	1.40	1.33
47	W	201	PEE	O3-C30	2.32	1.40	1.33
55	V	202	CDL	OB6-CB4	-2.32	1.41	1.46
55	r	504	CDL	PB2-OB2	2.31	1.68	1.59
55	m	201	CDL	OB6-CB4	-2.31	1.41	1.46
55	a	201	CDL	OB6-CB4	-2.31	1.41	1.46
47	r	501	PEE	O2-C10	2.31	1.40	1.34
52	J	402	UQ	C7-C8	2.30	1.54	1.50
55	V	201	CDL	PB2-OB2	2.30	1.68	1.59
55	V	202	CDL	PB2-OB2	2.29	1.68	1.59
55	V	201	CDL	PB2-OB5	2.29	1.68	1.59
47	l	704	PEE	O3-C3	-2.29	1.40	1.45
47	l	701	PEE	O2-C10	2.28	1.40	1.34
55	l	702	CDL	OB6-CB4	-2.28	1.41	1.46
47	U	101	PEE	O2-C10	2.28	1.40	1.34
55	m	201	CDL	PB2-OB2	2.26	1.68	1.59
47	j	201	PEE	O2-C10	2.26	1.40	1.34
47	b	201	PEE	O2-C10	2.26	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	a	201	CDL	PB2-OB2	2.26	1.68	1.59
55	V	201	CDL	OA6-CA4	-2.25	1.41	1.46
47	W	201	PEE	O2-C10	2.25	1.40	1.34
55	r	504	CDL	OB6-CB4	-2.25	1.41	1.46
51	J	401	NDP	O7N-C7N	-2.25	1.19	1.24
47	W	201	PEE	O3-C3	-2.23	1.40	1.45
47	b	201	PEE	O3-C3	-2.23	1.40	1.45
47	r	501	PEE	O3-C3	-2.23	1.40	1.45
55	a	201	CDL	PB2-OB5	2.23	1.68	1.59
55	r	504	CDL	PB2-OB5	2.23	1.68	1.59
55	m	201	CDL	PB2-OB5	2.22	1.68	1.59
55	V	202	CDL	PB2-OB5	2.22	1.68	1.59
47	Q	501	PEE	O2-C10	2.22	1.40	1.34
48	r	502	PLX	P1-O4	2.21	1.68	1.59
55	l	702	CDL	PB2-OB5	2.21	1.68	1.59
55	l	702	CDL	PB2-OB2	2.20	1.68	1.59
48	j	202	PLX	P1-O4	2.20	1.68	1.59
48	a	202	PLX	P1-O4	2.19	1.68	1.59
47	B	303	PEE	O3-C3	-2.19	1.40	1.45
52	s	403	UQ	O4-C4	-2.18	1.18	1.23
47	Q	501	PEE	O3-C3	-2.18	1.40	1.45
48	r	503	PLX	P1-O4	2.18	1.67	1.59
48	g	201	PLX	P1-O4	2.17	1.67	1.59
47	s	401	PEE	O2-C10	2.17	1.40	1.34
47	U	101	PEE	O3-C3	-2.16	1.40	1.45
52	J	402	UQ	O4-C4	-2.15	1.18	1.23
48	J	403	PLX	P1-O4	2.14	1.67	1.59
46	A	502	FMN	C2-N3	-2.14	1.34	1.39
47	l	701	PEE	O3-C3	-2.13	1.40	1.45
48	r	502	PLX	P1-O1	2.13	1.67	1.59
47	l	704	PEE	O2-C10	2.12	1.40	1.34
52	J	402	UQ	O3-CM3	-2.11	1.40	1.45
51	J	401	NDP	C2D-C3D	2.10	1.59	1.53
47	B	303	PEE	O2-C10	2.10	1.40	1.34
48	j	202	PLX	P1-O1	2.10	1.67	1.59
48	a	202	PLX	P1-O1	2.08	1.67	1.59
48	J	403	PLX	P1-O1	2.08	1.67	1.59
48	r	503	PLX	P1-O1	2.08	1.67	1.59
48	g	201	PLX	P1-O1	2.08	1.67	1.59
47	s	401	PEE	O3-C3	-2.06	1.40	1.45
52	s	403	UQ	O3-CM3	-2.06	1.40	1.45
52	s	403	UQ	C21-C19	2.06	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	V	201	CDL	C11-CA5	2.05	1.56	1.50
47	j	201	PEE	O3-C3	-2.04	1.40	1.45
48	r	503	PLX	C1-C2	2.04	1.57	1.51
55	V	202	CDL	C11-CA5	2.02	1.56	1.50
48	r	502	PLX	C25-C24	2.02	1.55	1.50
55	m	201	CDL	OA6-CA4	-2.02	1.41	1.46
55	m	201	CDL	C11-CA5	2.01	1.56	1.50
52	J	402	UQ	C21-C19	2.00	1.55	1.51

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	J	402	UQ	C7-C8-C9	-8.11	112.86	126.83
51	J	401	NDP	C3N-C2N-N1N	-7.99	111.47	123.20
49	C	303	970	O08-C07-C06	-7.86	108.31	112.99
52	s	403	UQ	C7-C8-C9	-7.60	113.74	126.83
51	J	401	NDP	C1D-N1N-C2N	-7.42	108.91	121.14
51	J	401	NDP	C6N-N1N-C2N	-7.11	111.71	119.32
52	J	402	UQ	C17-C18-C19	-6.47	112.82	127.62
52	J	402	UQ	C12-C13-C14	-6.46	112.84	127.62
52	s	403	UQ	C22-C23-C24	-6.27	113.28	127.62
52	s	403	UQ	C12-C13-C14	-6.07	113.73	127.62
52	s	403	UQ	C17-C18-C19	-6.00	113.89	127.62
51	J	401	NDP	C1D-N1N-C6N	-5.92	108.26	120.77
51	J	401	NDP	C5A-C4A-N3A	-5.76	118.79	126.72
49	C	303	970	C15-C14-C23	5.56	115.16	110.65
57	w	401	ADP	C5-C4-N3	-5.47	119.19	126.72
50	G	201	8Q1	C6-C1-S44	4.98	119.33	113.40
49	C	303	970	C05-C04-C02	-4.90	108.05	115.53
50	X	201	8Q1	C6-C1-S44	4.63	118.92	113.40
57	w	401	ADP	N3-C2-N1	-4.57	121.67	128.58
55	l	703	CDL	OA6-CA5-C11	4.48	121.17	111.48
47	r	501	PEE	O2-C10-C11	4.47	121.15	111.48
52	J	402	UQ	C22-C23-C24	-4.46	112.76	127.64
52	s	403	UQ	C10-C9-C8	-4.46	112.17	123.63
52	s	403	UQ	C27-C28-C29	-4.32	113.23	127.64
49	C	303	970	O08-C07-C09	4.32	132.35	123.85
57	w	401	ADP	N3-C4-N9	4.31	134.50	127.17
52	s	403	UQ	C25-C24-C23	-4.24	112.74	123.63
52	J	402	UQ	C10-C9-C8	-4.22	112.79	123.63
47	l	704	PEE	O2-C10-C11	4.22	120.60	111.48
52	J	402	UQ	C20-C19-C18	-4.21	112.82	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	U	101	PEE	O2-C10-C11	4.20	120.57	111.48
52	J	402	UQ	C15-C14-C13	-4.19	112.86	123.63
55	N	201	CDL	OA6-CA5-C11	4.18	120.53	111.48
55	N	201	CDL	OB6-CB5-C51	4.18	120.52	111.48
55	l	703	CDL	OB6-CB5-C51	4.15	120.46	111.48
55	l	702	CDL	OB6-CB5-C51	4.14	120.44	111.48
55	a	201	CDL	OB6-CB5-C51	4.12	120.40	111.48
47	j	201	PEE	O2-C10-C11	4.11	120.38	111.48
51	J	401	NDP	N3A-C4A-N9A	4.09	134.12	127.17
55	m	201	CDL	OB6-CB5-C51	4.08	120.31	111.48
55	s	402	CDL	OB6-CB5-C51	4.06	120.27	111.48
47	W	201	PEE	O2-C10-C11	4.05	120.25	111.48
47	l	701	PEE	O2-C10-C11	4.04	120.22	111.48
47	B	303	PEE	O2-C10-C11	4.03	120.21	111.48
51	J	401	NDP	N3A-C2A-N1A	-4.01	122.52	128.58
55	V	202	CDL	OA6-CA5-C11	4.00	120.13	111.48
47	b	201	PEE	O2-C10-C11	3.98	120.09	111.48
55	u	201	CDL	OB6-CB5-C51	3.97	120.06	111.48
55	V	202	CDL	OB6-CB5-C51	3.96	120.05	111.48
47	s	401	PEE	O2-C10-C11	3.96	120.04	111.48
50	G	201	8Q1	C43-S44-C1	3.94	113.50	101.84
47	Q	501	PEE	O2-C10-C11	3.92	119.95	111.48
55	r	504	CDL	OA6-CA5-C11	3.91	119.95	111.48
55	u	201	CDL	OA6-CA5-C11	3.90	119.93	111.48
52	s	403	UQ	C20-C19-C18	-3.90	113.61	123.63
49	C	303	970	C22-C23-C14	3.89	115.20	109.64
55	l	702	CDL	OA6-CA5-C11	3.88	119.87	111.48
55	s	402	CDL	OA6-CA5-C11	3.87	119.86	111.48
55	a	201	CDL	OA6-CA5-C11	3.87	119.85	111.48
52	s	403	UQ	C21-C19-C18	-3.87	112.49	121.17
52	s	403	UQ	C15-C14-C13	-3.87	113.70	123.63
50	X	201	8Q1	C43-S44-C1	3.85	113.23	101.84
55	V	201	CDL	OA6-CA5-C11	3.83	119.77	111.48
52	s	403	UQ	C11-C9-C8	-3.79	112.66	121.17
52	s	403	UQ	C16-C14-C13	-3.78	112.68	121.17
52	J	402	UQ	C11-C9-C8	-3.78	112.69	121.17
55	V	201	CDL	OB6-CB5-C51	3.76	119.61	111.48
55	r	504	CDL	OB6-CB5-C51	3.73	119.54	111.48
52	J	402	UQ	C16-C14-C13	-3.71	112.83	121.17
52	J	402	UQ	C21-C19-C18	-3.67	112.92	121.17
49	C	303	970	C09-C07-C06	-3.65	119.34	123.21
51	J	401	NDP	C2A-N3A-C4A	3.62	120.68	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	w	401	ADP	C2-N3-C4	3.56	120.53	111.83
57	w	401	ADP	N9-C8-N7	-3.55	108.90	113.94
52	s	403	UQ	C26-C24-C23	-3.54	113.23	121.17
50	G	201	8Q1	O35-C34-N36	-3.51	115.55	122.98
55	m	201	CDL	OA6-CA5-C11	3.40	118.83	111.48
50	X	201	8Q1	O35-C34-N36	-3.36	115.87	122.98
52	J	402	UQ	C25-C24-C23	-3.29	112.78	122.66
52	s	403	UQ	C30-C29-C28	-3.29	112.78	122.66
52	J	402	UQ	C26-C24-C23	-3.27	112.86	122.66
51	J	401	NDP	C4A-C5A-N7A	-3.23	106.89	110.58
50	G	201	8Q1	O2-P24-O27	-3.23	98.25	106.67
57	w	401	ADP	C4-N9-C8	3.22	109.12	105.74
49	C	303	970	O26-C20-C19	3.21	119.75	115.40
57	w	401	ADP	C5-N7-C8	3.19	108.47	103.45
49	C	303	970	C06-C05-C04	3.19	104.25	101.45
49	C	303	970	C07-C06-C12	3.18	121.75	118.72
52	s	403	UQ	C31-C29-C28	-3.12	113.29	122.66
49	C	303	970	O28-C19-C20	3.12	119.63	115.40
55	u	201	CDL	OA8-CA7-C31	3.08	120.50	111.15
51	J	401	NDP	C5A-N7A-C8A	3.04	108.22	103.45
51	J	401	NDP	N9A-C8A-N7A	-3.03	109.64	113.94
52	J	402	UQ	C7-C6-C5	-3.00	119.75	124.89
47	B	303	PEE	O3-C30-C31	2.97	120.90	111.83
47	l	704	PEE	O3-C30-C31	2.97	120.90	111.83
55	s	402	CDL	OA8-CA7-C31	2.97	120.88	111.83
55	l	703	CDL	OA8-CA7-C31	2.96	120.86	111.83
57	w	401	ADP	C4-C5-N7	-2.96	107.20	110.58
55	N	201	CDL	OB8-CB7-C71	2.94	120.81	111.83
55	N	201	CDL	OA8-CA7-C31	2.93	120.77	111.83
50	G	201	8Q1	C32-C34-N36	2.93	122.04	116.48
50	X	201	8Q1	O2-P24-O27	-2.91	99.09	106.67
47	r	501	PEE	O3-C30-C31	2.89	120.64	111.83
50	G	201	8Q1	C37-C38-C39	2.84	117.13	112.39
55	V	201	CDL	OB8-CB7-C71	2.84	120.48	111.83
47	j	201	PEE	O3-C30-C31	2.81	120.39	111.83
55	V	202	CDL	OB8-CB7-C71	2.80	120.36	111.83
55	l	702	CDL	OA8-CA7-C31	2.79	120.34	111.83
47	U	101	PEE	O3-C30-C31	2.79	120.33	111.83
55	u	201	CDL	OB8-CB7-C71	2.77	120.29	111.83
55	l	703	CDL	OB8-CB7-C71	2.76	120.25	111.83
46	A	502	FMN	C4'-C3'-C2'	-2.75	108.99	113.57
50	X	201	8Q1	C32-C34-N36	2.74	121.68	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	J	402	UQ	CM5-C5-C6	-2.73	119.96	124.45
55	a	201	CDL	OB8-CB7-C71	2.73	120.14	111.83
55	N	201	CDL	CB4-OB6-CB5	-2.72	111.28	117.80
55	l	702	CDL	OB8-CB7-C71	2.72	120.13	111.83
55	m	201	CDL	OB8-CB7-C71	2.71	120.11	111.83
47	W	201	PEE	O3-C30-C31	2.70	120.06	111.83
55	m	201	CDL	OA8-CA7-C31	2.70	120.06	111.83
47	b	201	PEE	O3-C30-C31	2.70	120.06	111.83
55	r	504	CDL	OB8-CB7-C71	2.69	120.05	111.83
47	s	401	PEE	O3-C30-C31	2.68	120.00	111.83
47	l	701	PEE	O3-C30-C31	2.67	119.97	111.83
49	C	303	970	C15-O16-C17	-2.64	110.01	115.29
55	s	402	CDL	OB8-CB7-C71	2.64	119.87	111.83
55	V	202	CDL	OA8-CA7-C31	2.63	119.86	111.83
48	g	201	PLX	C1A-N1-C1	2.62	120.31	109.91
55	r	504	CDL	OA8-CA7-C31	2.60	119.77	111.83
55	a	201	CDL	OA8-CA7-C31	2.59	119.72	111.83
46	A	502	FMN	C4A-C10-N1	-2.58	118.26	124.59
47	Q	501	PEE	O3-C30-C31	2.57	119.68	111.83
55	V	201	CDL	OA8-CA7-C31	2.57	119.66	111.83
55	l	703	CDL	CA4-OA6-CA5	-2.54	111.71	117.80
49	C	303	970	O13-C14-C23	2.51	114.94	112.44
50	G	201	8Q1	O4-C1-S44	-2.50	119.51	122.68
48	a	202	PLX	C1A-N1-C1	2.47	119.74	109.91
50	X	201	8Q1	O4-C1-S44	-2.45	119.57	122.68
50	G	201	8Q1	O4-C1-C6	-2.45	121.16	123.98
48	j	202	PLX	C1A-N1-C1	2.43	119.58	109.91
49	C	303	970	C11-C24-C23	2.43	119.19	115.89
49	C	303	970	C27-O26-C20	-2.41	113.97	117.51
50	X	201	8Q1	O1-P24-O2	2.41	116.85	107.80
50	X	201	8Q1	O40-C39-N41	-2.41	118.30	123.03
48	r	502	PLX	C1A-N1-C1	2.41	119.49	109.91
50	G	201	8Q1	O1-P24-O2	2.40	116.80	107.80
46	A	502	FMN	O4-C4-C4A	-2.39	120.24	126.53
46	A	502	FMN	C4-C4A-N5	2.38	121.50	118.21
50	G	201	8Q1	O40-C39-N41	-2.38	118.36	123.03
49	C	303	970	C11-C12-C06	-2.38	119.56	123.22
52	s	403	UQ	C7-C6-C5	-2.33	120.89	124.89
48	J	403	PLX	C1A-N1-C1	2.33	119.17	109.91
47	l	701	PEE	C20-C19-C18	-2.33	112.42	126.42
55	l	703	CDL	CB6-CB4-CB3	-2.32	106.37	111.78
51	J	401	NDP	C4A-N9A-C8A	2.31	108.16	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	s	402	CDL	CA6-CA4-CA3	-2.27	106.48	111.78
49	C	303	970	C05-C06-C12	-2.27	127.41	131.52
49	C	303	970	O26-C20-C21	-2.24	120.22	124.08
49	C	303	970	O28-C19-C18	-2.20	120.28	124.08
48	C	302	PLX	C5-C4-C3	-2.20	106.66	111.78
52	s	403	UQ	CM5-C5-C6	-2.20	120.84	124.45
48	r	503	PLX	C1A-N1-C1	2.19	118.63	109.91
46	A	502	FMN	O2-C2-N1	-2.18	118.18	121.80
55	s	402	CDL	CB4-OB6-CB5	-2.16	112.62	117.80
46	A	502	FMN	C4-N3-C2	-2.15	121.82	125.64
50	X	201	8Q1	C37-C38-C39	2.14	115.97	112.39
50	X	201	8Q1	O4-C1-C6	-2.14	121.51	123.98
47	j	201	PEE	C2-O2-C10	-2.13	112.70	117.80
46	A	502	FMN	C4A-C4-N3	2.10	118.60	113.25
49	C	303	970	C29-O28-C19	-2.08	114.46	117.51
55	l	703	CDL	OA6-CA5-OA7	-2.08	118.84	123.70
48	C	302	PLX	C6-O6-C4	-2.08	111.05	115.20
55	u	201	CDL	CA6-CA4-CA3	-2.08	106.94	111.78
49	C	303	970	O13-C14-C15	-2.07	103.92	106.61
55	N	201	CDL	CA6-CA4-CA3	-2.07	106.97	111.78
55	N	201	CDL	OB6-CB5-OB7	-2.06	118.88	123.70
46	A	502	FMN	C10-N1-C2	2.04	121.27	116.85

There are no chirality outliers.

All (1003) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
47	B	303	PEE	C11-C10-O2-C2
47	B	303	PEE	C4-O4P-P-O3P
47	B	303	PEE	C4-O4P-P-O2P
47	Q	501	PEE	C11-C10-O2-C2
47	Q	501	PEE	O4-C10-O2-C2
47	Q	501	PEE	C4-O4P-P-O1P
47	U	101	PEE	C1-O3P-P-O1P
47	U	101	PEE	C1-O3P-P-O4P
47	W	201	PEE	C1-O3P-P-O2P
47	W	201	PEE	C1-O3P-P-O1P
47	W	201	PEE	C1-O3P-P-O4P
47	W	201	PEE	C4-O4P-P-O2P
47	W	201	PEE	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
47	j	201	PEE	C11-C10-O2-C2
47	j	201	PEE	O4-C10-O2-C2
47	j	201	PEE	C4-O4P-P-O3P
47	j	201	PEE	C4-O4P-P-O2P
47	j	201	PEE	C4-O4P-P-O1P
47	l	701	PEE	C11-C10-O2-C2
47	l	701	PEE	C1-O3P-P-O2P
47	l	701	PEE	C1-O3P-P-O1P
47	l	701	PEE	C1-O3P-P-O4P
47	l	701	PEE	C4-O4P-P-O3P
47	l	701	PEE	C4-O4P-P-O2P
47	l	701	PEE	C4-O4P-P-O1P
47	l	704	PEE	C11-C10-O2-C2
47	l	704	PEE	C4-O4P-P-O3P
47	l	704	PEE	C4-O4P-P-O2P
47	l	704	PEE	C4-O4P-P-O1P
47	r	501	PEE	C11-C10-O2-C2
47	r	501	PEE	C1-O3P-P-O1P
47	r	501	PEE	C1-O3P-P-O4P
48	C	302	PLX	C3-O4-P1-O1
48	C	302	PLX	C3-O4-P1-O3
48	J	403	PLX	O7-C6-C7-C8
48	J	403	PLX	O7-C6-O6-C4
48	J	403	PLX	C3-C4-O6-C6
48	a	202	PLX	O7-C6-O6-C4
48	a	202	PLX	C5-C4-O6-C6
48	a	202	PLX	C3-O4-P1-O3
48	a	202	PLX	C2-O1-P1-O4
48	a	202	PLX	C2-O1-P1-O2
48	a	202	PLX	C2-O1-P1-O3
48	a	202	PLX	O9-C24-C25-C26
48	g	201	PLX	O7-C6-O6-C4
48	g	201	PLX	C3-O4-P1-O1
48	g	201	PLX	C3-O4-P1-O2
48	g	201	PLX	C2-O1-P1-O4
48	g	201	PLX	C2-O1-P1-O2
48	g	201	PLX	C2-O1-P1-O3
48	g	201	PLX	O9-C24-C25-C26
48	j	202	PLX	O7-C6-C7-C8
48	j	202	PLX	C7-C6-O6-C4
48	j	202	PLX	C3-O4-P1-O2
48	j	202	PLX	C2-O1-P1-O4

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Mol	Chain	Res	Type	Atoms
48	j	202	PLX	C2-O1-P1-O2
48	j	202	PLX	O9-C24-O8-C5
48	r	502	PLX	O6-C6-C7-C8
48	r	502	PLX	O9-C24-C25-C26
48	r	503	PLX	O7-C6-O6-C4
48	r	503	PLX	O9-C24-O8-C5
49	C	303	970	C03-C02-C04-C05
49	C	303	970	C03-C02-C04-O08
50	G	201	8Q1	C1-C6-C7-C8
50	G	201	8Q1	O27-C28-C29-C30
50	G	201	8Q1	O27-C28-C29-C31
50	G	201	8Q1	O27-C28-C29-C32
50	G	201	8Q1	C28-C29-C32-C34
50	G	201	8Q1	C30-C29-C32-O33
50	G	201	8Q1	C31-C29-C32-C34
50	G	201	8Q1	C42-C43-S44-C1
50	X	201	8Q1	C28-C29-C32-C34
50	X	201	8Q1	C30-C29-C32-O33
50	X	201	8Q1	C31-C29-C32-C34
50	X	201	8Q1	N36-C37-C38-C39
50	X	201	8Q1	C42-C43-S44-C1
50	X	201	8Q1	C28-O27-P24-O2
50	X	201	8Q1	C28-O27-P24-O1
51	J	401	NDP	C5D-O5D-PN-O3
51	J	401	NDP	C5D-O5D-PN-O1N
51	J	401	NDP	C5D-O5D-PN-O2N
51	J	401	NDP	C2N-C3N-C7N-N7N
52	J	402	UQ	C1-C6-C7-C8
52	J	402	UQ	C5-C6-C7-C8
52	J	402	UQ	C7-C8-C9-C10
52	J	402	UQ	C7-C8-C9-C11
52	s	403	UQ	C7-C8-C9-C10
52	s	403	UQ	C7-C8-C9-C11
55	N	201	CDL	CA2-OA2-PA1-OA3
55	N	201	CDL	CA2-OA2-PA1-OA4
55	N	201	CDL	CA2-OA2-PA1-OA5
55	N	201	CDL	CA6-CA4-OA6-CA5
55	N	201	CDL	C11-CA5-OA6-CA4
55	N	201	CDL	CB3-OB5-PB2-OB2
55	N	201	CDL	CB3-OB5-PB2-OB4
55	V	201	CDL	O1-C1-CA2-OA2
55	V	201	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
55	V	201	CDL	CA2-OA2-PA1-OA5
55	V	201	CDL	CB2-OB2-PB2-OB3
55	V	201	CDL	CB2-OB2-PB2-OB4
55	V	201	CDL	CB2-OB2-PB2-OB5
55	V	201	CDL	CB3-OB5-PB2-OB2
55	V	201	CDL	CB3-OB5-PB2-OB3
55	V	201	CDL	CB3-OB5-PB2-OB4
55	V	202	CDL	CA2-C1-CB2-OB2
55	V	202	CDL	CB2-OB2-PB2-OB3
55	V	202	CDL	CB2-OB2-PB2-OB5
55	V	202	CDL	CB3-OB5-PB2-OB2
55	V	202	CDL	CB3-OB5-PB2-OB3
55	V	202	CDL	CB3-OB5-PB2-OB4
55	V	202	CDL	OB6-CB4-CB6-OB8
55	a	201	CDL	CA2-C1-CB2-OB2
55	a	201	CDL	CA2-OA2-PA1-OA3
55	a	201	CDL	CB2-OB2-PB2-OB3
55	a	201	CDL	CB2-OB2-PB2-OB4
55	a	201	CDL	CB2-OB2-PB2-OB5
55	a	201	CDL	CB3-OB5-PB2-OB2
55	a	201	CDL	CB3-OB5-PB2-OB3
55	a	201	CDL	CB3-OB5-PB2-OB4
55	a	201	CDL	OB7-CB5-OB6-CB4
55	l	702	CDL	O1-C1-CA2-OA2
55	l	702	CDL	CA2-OA2-PA1-OA5
55	l	702	CDL	OA9-CA7-OA8-CA6
55	l	702	CDL	C31-CA7-OA8-CA6
55	l	702	CDL	CB2-OB2-PB2-OB4
55	l	702	CDL	CB2-OB2-PB2-OB5
55	l	702	CDL	CB3-OB5-PB2-OB2
55	l	702	CDL	CB3-OB5-PB2-OB3
55	l	702	CDL	CB3-OB5-PB2-OB4
55	l	703	CDL	CA3-OA5-PA1-OA3
55	l	703	CDL	CB2-OB2-PB2-OB4
55	l	703	CDL	CB2-OB2-PB2-OB5
55	m	201	CDL	O1-C1-CB2-OB2
55	m	201	CDL	CA2-C1-CB2-OB2
55	m	201	CDL	CA2-OA2-PA1-OA3
55	m	201	CDL	CA2-OA2-PA1-OA5
55	m	201	CDL	CA3-OA5-PA1-OA2
55	m	201	CDL	CA3-OA5-PA1-OA3
55	m	201	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
55	m	201	CDL	OA6-CA4-CA6-OA8
55	m	201	CDL	CB2-OB2-PB2-OB3
55	m	201	CDL	CB2-OB2-PB2-OB4
55	m	201	CDL	CB2-OB2-PB2-OB5
55	m	201	CDL	CB3-OB5-PB2-OB2
55	m	201	CDL	CB3-OB5-PB2-OB3
55	m	201	CDL	CB3-OB5-PB2-OB4
55	r	504	CDL	CB2-C1-CA2-OA2
55	r	504	CDL	CA3-OA5-PA1-OA2
55	r	504	CDL	C51-CB5-OB6-CB4
55	s	402	CDL	CA2-OA2-PA1-OA3
55	s	402	CDL	CA2-OA2-PA1-OA4
55	s	402	CDL	CA2-OA2-PA1-OA5
55	s	402	CDL	CB2-OB2-PB2-OB4
55	s	402	CDL	CB2-OB2-PB2-OB5
55	u	201	CDL	CA2-OA2-PA1-OA3
55	u	201	CDL	CA2-OA2-PA1-OA4
55	u	201	CDL	CA2-OA2-PA1-OA5
55	u	201	CDL	CA3-OA5-PA1-OA2
55	u	201	CDL	CB2-OB2-PB2-OB4
55	u	201	CDL	CB2-OB2-PB2-OB5
55	u	201	CDL	CB3-OB5-PB2-OB3
57	w	401	ADP	PA-O3A-PB-O2B
57	w	401	ADP	C5'-O5'-PA-O1A
57	w	401	ADP	C5'-O5'-PA-O2A
57	w	401	ADP	C5'-O5'-PA-O3A
47	B	303	PEE	O4-C10-O2-C2
47	l	701	PEE	O4-C10-O2-C2
47	l	704	PEE	O4-C10-O2-C2
55	N	201	CDL	OA7-CA5-OA6-CA4
55	V	201	CDL	OA7-CA5-OA6-CA4
52	J	402	UQ	C22-C23-C24-C25
55	V	201	CDL	C11-CA5-OA6-CA4
55	a	201	CDL	C51-CB5-OB6-CB4
52	J	402	UQ	C12-C11-C9-C10
52	J	402	UQ	C12-C11-C9-C8
52	s	403	UQ	C18-C19-C21-C22
52	J	402	UQ	C12-C13-C14-C15
47	b	201	PEE	C37-C38-C39-C40
52	J	402	UQ	C17-C18-C19-C21
52	s	403	UQ	C17-C18-C19-C21
52	s	403	UQ	C22-C23-C24-C26

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Mol	Chain	Res	Type	Atoms
47	r	501	PEE	O4-C10-O2-C2
55	r	504	CDL	OB7-CB5-OB6-CB4
55	V	202	CDL	O1-C1-CB2-OB2
55	l	702	CDL	O1-C1-CB2-OB2
55	l	703	CDL	O1-C1-CB2-OB2
55	r	504	CDL	O1-C1-CA2-OA2
55	u	201	CDL	O1-C1-CA2-OA2
47	U	101	PEE	C31-C30-O3-C3
55	V	201	CDL	C31-CA7-OA8-CA6
48	r	502	PLX	C7-C8-C9-C10
51	J	401	NDP	C2D-C1D-N1N-C6N
47	U	101	PEE	O5-C30-O3-C3
52	J	402	UQ	C14-C16-C17-C18
55	l	703	CDL	C71-CB7-OB8-CB6
47	U	101	PEE	C17-C18-C19-C20
55	V	201	CDL	OA9-CA7-OA8-CA6
48	r	502	PLX	C9-C10-C11-C12
48	J	403	PLX	C25-C26-C27-C28
55	V	202	CDL	C37-C38-C39-C40
47	U	101	PEE	C11-C10-O2-C2
47	s	401	PEE	C11-C10-O2-C2
55	l	702	CDL	CA2-C1-CB2-OB2
47	Q	501	PEE	C31-C30-O3-C3
47	W	201	PEE	C31-C30-O3-C3
55	a	201	CDL	C71-CB7-OB8-CB6
55	r	504	CDL	C71-CB7-OB8-CB6
55	s	402	CDL	C31-CA7-OA8-CA6
55	m	201	CDL	C73-C74-C75-C76
48	J	403	PLX	C27-C28-C29-C30
55	V	201	CDL	C62-C63-C64-C65
48	g	201	PLX	C11-C10-C9-C8
47	l	704	PEE	C33-C34-C35-C36
52	J	402	UQ	C15-C14-C16-C17
47	U	101	PEE	C30-C31-C32-C33
55	s	402	CDL	O1-C1-CA2-OA2
55	l	703	CDL	OB9-CB7-OB8-CB6
55	r	504	CDL	OB9-CB7-OB8-CB6
55	s	402	CDL	OA9-CA7-OA8-CA6
48	j	202	PLX	C13-C14-C15-C16
47	l	704	PEE	C40-C41-C42-C43
47	Q	501	PEE	O5-C30-O3-C3
47	l	701	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
47	b	201	PEE	C10-C11-C12-C13
52	s	403	UQ	C22-C23-C24-C25
48	g	201	PLX	C10-C11-C12-C13
55	V	201	CDL	CA7-C31-C32-C33
55	l	702	CDL	C81-C82-C83-C84
47	Q	501	PEE	C11-C12-C13-C14
48	C	302	PLX	C25-C26-C27-C28
48	r	502	PLX	C31-C32-C33-C34
55	l	703	CDL	C17-C18-C19-C20
55	a	201	CDL	CA5-C11-C12-C13
52	s	403	UQ	C27-C28-C29-C31
52	s	403	UQ	C14-C16-C17-C18
48	j	202	PLX	C32-C33-C34-C35
47	W	201	PEE	C10-C11-C12-C13
55	l	702	CDL	CB7-C71-C72-C73
55	V	201	CDL	CB7-C71-C72-C73
55	V	202	CDL	CB7-C71-C72-C73
55	r	504	CDL	CB7-C71-C72-C73
55	s	402	CDL	CB5-C51-C52-C53
47	W	201	PEE	O5-C30-O3-C3
55	a	201	CDL	OB9-CB7-OB8-CB6
47	r	501	PEE	C41-C42-C43-C44
55	l	703	CDL	C41-C42-C43-C44
55	a	201	CDL	O1-C1-CB2-OB2
55	l	702	CDL	C71-CB7-OB8-CB6
47	U	101	PEE	O4-C10-O2-C2
47	s	401	PEE	O4-C10-O2-C2
47	l	701	PEE	C17-C18-C19-C20
55	m	201	CDL	C43-C44-C45-C46
55	V	201	CDL	C71-CB7-OB8-CB6
47	b	201	PEE	C11-C10-O2-C2
55	l	703	CDL	C39-C40-C41-C42
47	l	701	PEE	O5-C30-O3-C3
47	b	201	PEE	O4-C10-O2-C2
55	V	201	CDL	CB2-C1-CA2-OA2
47	b	201	PEE	C31-C30-O3-C3
47	U	101	PEE	C32-C33-C34-C35
48	g	201	PLX	C17-C18-C19-C20
48	g	201	PLX	C2-C1-N1-C1C
48	g	201	PLX	C2-C1-N1-C1B
48	g	201	PLX	C2-C1-N1-C1A
47	l	704	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
55	V	201	CDL	C34-C35-C36-C37
52	s	403	UQ	C23-C24-C26-C27
48	j	202	PLX	O6-C6-C7-C8
55	V	201	CDL	C51-CB5-OB6-CB4
55	V	202	CDL	C51-CB5-OB6-CB4
55	V	202	CDL	C39-C40-C41-C42
55	V	201	CDL	OB7-CB5-OB6-CB4
47	s	401	PEE	C37-C38-C39-C40
55	V	202	CDL	O1-C1-CA2-OA2
55	s	402	CDL	CA5-C11-C12-C13
47	B	303	PEE	C34-C35-C36-C37
55	r	504	CDL	C51-C52-C53-C54
55	a	201	CDL	C34-C35-C36-C37
55	l	702	CDL	C58-C59-C60-C61
55	l	702	CDL	OA6-CA4-CA6-OA8
55	V	201	CDL	OB9-CB7-OB8-CB6
50	G	201	8Q1	C12-C13-C14-C15
47	s	401	PEE	C11-C12-C13-C14
48	J	403	PLX	C31-C32-C33-C34
55	V	202	CDL	C52-C53-C54-C55
55	V	202	CDL	C55-C56-C57-C58
55	m	201	CDL	C17-C18-C19-C20
55	m	201	CDL	C36-C37-C38-C39
55	r	504	CDL	C32-C33-C34-C35
47	l	701	PEE	C37-C38-C39-C40
50	X	201	8Q1	C11-C12-C13-C14
55	V	202	CDL	C14-C15-C16-C17
55	V	202	CDL	C61-C62-C63-C64
55	a	201	CDL	C62-C63-C64-C65
55	l	702	CDL	C59-C60-C61-C62
55	l	702	CDL	OB9-CB7-OB8-CB6
48	r	502	PLX	O7-C6-C7-C8
47	b	201	PEE	C31-C32-C33-C34
48	g	201	PLX	C25-C26-C27-C28
48	r	503	PLX	C28-C29-C30-C31
55	V	201	CDL	C37-C38-C39-C40
55	a	201	CDL	C17-C18-C19-C20
55	a	201	CDL	C76-C77-C78-C79
55	r	504	CDL	C14-C15-C16-C17
55	r	504	CDL	C52-C53-C54-C55
55	r	504	CDL	C80-C81-C82-C83
55	V	202	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
48	J	403	PLX	C26-C27-C28-C29
48	g	201	PLX	C9-C10-C11-C12
48	r	502	PLX	C11-C10-C9-C8
55	m	201	CDL	C56-C57-C58-C59
55	r	504	CDL	C31-C32-C33-C34
55	u	201	CDL	CB5-C51-C52-C53
48	j	202	PLX	C11-C12-C13-C14
48	r	503	PLX	C13-C14-C15-C16
55	V	202	CDL	C17-C18-C19-C20
47	l	704	PEE	C34-C35-C36-C37
48	a	202	PLX	C9-C10-C11-C12
48	a	202	PLX	C28-C29-C30-C31
47	j	201	PEE	C12-C13-C14-C15
48	J	403	PLX	C34-C35-C36-C37
55	V	201	CDL	C59-C60-C61-C62
55	l	702	CDL	C52-C53-C54-C55
55	l	702	CDL	C75-C76-C77-C78
47	b	201	PEE	O5-C30-O3-C3
55	l	702	CDL	CA7-C31-C32-C33
47	l	704	PEE	O5-C30-O3-C3
47	r	501	PEE	C13-C14-C15-C16
48	j	202	PLX	C18-C19-C20-C21
55	V	201	CDL	C56-C57-C58-C59
48	j	202	PLX	C16-C17-C18-C19
55	l	702	CDL	C62-C63-C64-C65
55	l	702	CDL	CB2-C1-CA2-OA2
47	B	303	PEE	C1-C2-C3-O3
47	W	201	PEE	C1-C2-C3-O3
48	g	201	PLX	C3-C4-C5-O8
55	r	504	CDL	C43-C44-C45-C46
47	l	701	PEE	C10-C11-C12-C13
47	B	303	PEE	C11-C12-C13-C14
47	W	201	PEE	C22-C23-C24-C25
47	r	501	PEE	C40-C41-C42-C43
48	g	201	PLX	C7-C8-C9-C10
48	j	202	PLX	C25-C26-C27-C28
48	j	202	PLX	C33-C34-C35-C36
50	G	201	8Q1	C10-C11-C12-C13
55	a	201	CDL	C23-C24-C25-C26
55	r	504	CDL	C73-C74-C75-C76
47	W	201	PEE	C11-C12-C13-C14
47	j	201	PEE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
48	j	202	PLX	C7-C8-C9-C10
55	V	202	CDL	C60-C61-C62-C63
55	l	702	CDL	C35-C36-C37-C38
48	J	403	PLX	C9-C10-C11-C12
48	a	202	PLX	C13-C14-C15-C16
48	j	202	PLX	C14-C15-C16-C17
55	a	201	CDL	C31-C32-C33-C34
47	s	401	PEE	C34-C35-C36-C37
48	g	201	PLX	C32-C33-C34-C35
48	r	503	PLX	C14-C15-C16-C17
48	r	503	PLX	C10-C11-C12-C13
55	V	201	CDL	C55-C56-C57-C58
55	l	702	CDL	C16-C17-C18-C19
47	l	704	PEE	C30-C31-C32-C33
55	N	201	CDL	C51-CB5-OB6-CB4
47	l	704	PEE	C37-C38-C39-C40
55	m	201	CDL	C14-C15-C16-C17
47	B	303	PEE	C31-C32-C33-C34
55	l	702	CDL	C74-C75-C76-C77
48	r	502	PLX	C14-C15-C16-C17
55	V	202	CDL	C82-C83-C84-C85
55	m	201	CDL	C52-C53-C54-C55
47	B	303	PEE	C23-C24-C25-C26
47	j	201	PEE	C14-C15-C16-C17
55	V	201	CDL	C35-C36-C37-C38
55	V	202	CDL	C11-C12-C13-C14
55	m	201	CDL	C71-C72-C73-C74
47	j	201	PEE	C11-C12-C13-C14
48	J	403	PLX	C13-C14-C15-C16
48	a	202	PLX	C33-C34-C35-C36
55	V	202	CDL	C12-C13-C14-C15
55	m	201	CDL	C32-C33-C34-C35
55	r	504	CDL	C12-C13-C14-C15
47	r	501	PEE	C31-C30-O3-C3
55	m	201	CDL	C71-CB7-OB8-CB6
47	r	501	PEE	C12-C13-C14-C15
48	g	201	PLX	C27-C28-C29-C30
55	a	201	CDL	C60-C61-C62-C63
55	l	702	CDL	C31-C32-C33-C34
47	j	201	PEE	C20-C21-C22-C23
48	g	201	PLX	C14-C15-C16-C17
48	r	503	PLX	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
55	V	202	CDL	C75-C76-C77-C78
55	a	201	CDL	C75-C76-C77-C78
47	b	201	PEE	C33-C34-C35-C36
48	a	202	PLX	C25-C26-C27-C28
55	l	703	CDL	C11-C12-C13-C14
47	W	201	PEE	C12-C13-C14-C15
48	J	403	PLX	C28-C29-C30-C31
55	s	402	CDL	O1-C1-CB2-OB2
55	V	201	CDL	C17-C18-C19-C20
55	V	201	CDL	C52-C53-C54-C55
55	V	201	CDL	C74-C75-C76-C77
55	V	201	CDL	C78-C79-C80-C81
55	V	202	CDL	C59-C60-C61-C62
55	l	702	CDL	C56-C57-C58-C59
55	l	702	CDL	C11-CA5-OA6-CA4
55	u	201	CDL	CB7-C71-C72-C73
47	l	704	PEE	C21-C22-C23-C24
55	a	201	CDL	C54-C55-C56-C57
55	s	402	CDL	C12-C13-C14-C15
47	B	303	PEE	C35-C36-C37-C38
47	j	201	PEE	C19-C20-C21-C22
48	g	201	PLX	C30-C31-C32-C33
55	a	201	CDL	C22-C23-C24-C25
55	V	202	CDL	CA7-C31-C32-C33
55	V	201	CDL	C44-C45-C46-C47
55	l	702	CDL	C82-C83-C84-C85
47	B	303	PEE	C17-C18-C19-C20
48	a	202	PLX	C30-C31-C32-C33
55	V	202	CDL	C74-C75-C76-C77
55	a	201	CDL	C32-C33-C34-C35
55	l	702	CDL	C11-C12-C13-C14
55	m	201	CDL	C37-C38-C39-C40
55	a	201	CDL	C35-C36-C37-C38
55	r	504	CDL	C41-C42-C43-C44
55	l	702	CDL	C71-C72-C73-C74
47	l	704	PEE	C42-C43-C44-C45
48	C	302	PLX	O4-C3-C4-O6
48	r	502	PLX	C12-C13-C14-C15
55	V	201	CDL	C38-C39-C40-C41
55	s	402	CDL	C36-C37-C38-C39
47	W	201	PEE	C20-C21-C22-C23
55	V	202	CDL	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
55	m	201	CDL	C82-C83-C84-C85
52	s	403	UQ	C27-C28-C29-C30
55	V	202	CDL	C36-C37-C38-C39
55	m	201	CDL	C19-C20-C21-C22
47	Q	501	PEE	C34-C35-C36-C37
48	g	201	PLX	C28-C29-C30-C31
47	W	201	PEE	C15-C16-C17-C18
47	l	704	PEE	C39-C40-C41-C42
55	V	201	CDL	OB6-CB4-CB6-OB8
55	V	202	CDL	OA6-CA4-CA6-OA8
47	l	701	PEE	C11-C12-C13-C14
48	C	302	PLX	C10-C11-C12-C13
48	a	202	PLX	C10-C11-C12-C13
55	V	202	CDL	C35-C36-C37-C38
55	l	702	CDL	C73-C74-C75-C76
48	g	201	PLX	C18-C19-C20-C21
48	a	202	PLX	C11-C12-C13-C14
48	r	503	PLX	C30-C31-C32-C33
55	m	201	CDL	C20-C21-C22-C23
55	m	201	CDL	C75-C76-C77-C78
48	r	503	PLX	C32-C33-C34-C35
55	V	202	CDL	C15-C16-C17-C18
55	a	201	CDL	C51-C52-C53-C54
47	l	704	PEE	C31-C32-C33-C34
55	a	201	CDL	C71-C72-C73-C74
47	W	201	PEE	C33-C34-C35-C36
47	r	501	PEE	C17-C18-C19-C20
55	m	201	CDL	OB9-CB7-OB8-CB6
55	a	201	CDL	C38-C39-C40-C41
55	a	201	CDL	C82-C83-C84-C85
55	l	702	CDL	C17-C18-C19-C20
55	m	201	CDL	C11-C12-C13-C14
55	m	201	CDL	C79-C80-C81-C82
48	J	403	PLX	C30-C31-C32-C33
55	r	504	CDL	C55-C56-C57-C58
48	g	201	PLX	C16-C17-C18-C19
47	Q	501	PEE	C35-C36-C37-C38
47	r	501	PEE	C39-C40-C41-C42
47	s	401	PEE	C15-C16-C17-C18
47	b	201	PEE	C13-C14-C15-C16
55	l	702	CDL	C37-C38-C39-C40
48	C	302	PLX	O4-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
48	J	403	PLX	O4-C3-C4-C5
55	V	201	CDL	OA5-CA3-CA4-CA6
55	a	201	CDL	OA5-CA3-CA4-CA6
55	a	201	CDL	OB5-CB3-CB4-CB6
55	N	201	CDL	OB7-CB5-OB6-CB4
55	l	702	CDL	OA7-CA5-OA6-CA4
47	W	201	PEE	C13-C14-C15-C16
48	r	503	PLX	C11-C12-C13-C14
50	G	201	8Q1	C11-C12-C13-C14
55	V	201	CDL	C14-C15-C16-C17
55	r	504	CDL	C15-C16-C17-C18
47	s	401	PEE	C32-C33-C34-C35
55	V	201	CDL	C75-C76-C77-C78
47	W	201	PEE	C24-C25-C26-C27
55	s	402	CDL	C78-C79-C80-C81
55	m	201	CDL	C55-C56-C57-C58
55	r	504	CDL	C37-C38-C39-C40
48	r	502	PLX	O8-C24-C25-C26
47	B	303	PEE	C22-C23-C24-C25
55	s	402	CDL	C51-C52-C53-C54
47	b	201	PEE	C22-C23-C24-C25
47	s	401	PEE	C13-C14-C15-C16
55	l	703	CDL	C31-C32-C33-C34
47	r	501	PEE	O5-C30-O3-C3
48	r	502	PLX	C27-C28-C29-C30
47	l	701	PEE	C32-C33-C34-C35
48	J	403	PLX	C11-C12-C13-C14
47	Q	501	PEE	C1-C2-C3-O3
47	b	201	PEE	C1-C2-C3-O3
47	j	201	PEE	C1-C2-C3-O3
52	J	402	UQ	C19-C21-C22-C23
55	V	201	CDL	CA3-CA4-CA6-OA8
55	V	201	CDL	CB3-CB4-CB6-OB8
55	V	202	CDL	CB3-CB4-CB6-OB8
55	m	201	CDL	CB3-CB4-CB6-OB8
47	l	701	PEE	C35-C36-C37-C38
47	s	401	PEE	C19-C20-C21-C22
48	J	403	PLX	C33-C34-C35-C36
47	l	704	PEE	C32-C33-C34-C35
48	J	403	PLX	C16-C17-C18-C19
48	r	502	PLX	C16-C17-C18-C19
47	U	101	PEE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
47	B	303	PEE	C14-C15-C16-C17
50	X	201	8Q1	C28-O27-P24-O3
48	J	403	PLX	C11-C10-C9-C8
48	J	403	PLX	C7-C8-C9-C10
55	l	702	CDL	C18-C19-C20-C21
48	j	202	PLX	C27-C28-C29-C30
55	V	201	CDL	CA6-CA4-OA6-CA5
55	V	201	CDL	C43-C44-C45-C46
47	B	303	PEE	C15-C16-C17-C18
47	j	201	PEE	C15-C16-C17-C18
48	a	202	PLX	C7-C8-C9-C10
48	r	503	PLX	C27-C28-C29-C30
55	V	202	CDL	C38-C39-C40-C41
55	l	702	CDL	C53-C54-C55-C56
55	l	702	CDL	OA5-CA3-CA4-OA6
47	B	303	PEE	C31-C30-O3-C3
55	a	201	CDL	C31-CA7-OA8-CA6
47	s	401	PEE	C33-C34-C35-C36
55	V	201	CDL	C53-C54-C55-C56
47	r	501	PEE	C32-C33-C34-C35
48	g	201	PLX	C13-C14-C15-C16
48	g	201	PLX	C11-C12-C13-C14
47	r	501	PEE	O2-C2-C3-O3
48	g	201	PLX	O6-C4-C5-O8
55	m	201	CDL	OB6-CB4-CB6-OB8
47	j	201	PEE	C24-C25-C26-C27
55	m	201	CDL	C59-C60-C61-C62
48	J	403	PLX	C14-C15-C16-C17
55	a	201	CDL	C52-C53-C54-C55
47	B	303	PEE	C44-C45-C46-C47
48	r	503	PLX	C9-C10-C11-C12
55	l	702	CDL	C34-C35-C36-C37
50	G	201	8Q1	C13-C14-C15-C16
55	l	703	CDL	C73-C74-C75-C76
50	G	201	8Q1	C31-C29-C32-O33
50	X	201	8Q1	C31-C29-C32-O33
55	a	201	CDL	C84-C85-C86-C87
55	r	504	CDL	C17-C18-C19-C20
55	r	504	CDL	C59-C60-C61-C62
47	l	701	PEE	C33-C34-C35-C36
55	l	702	CDL	C24-C25-C26-C27
55	m	201	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
55	s	402	CDL	C72-C73-C74-C75
47	j	201	PEE	C31-C30-O3-C3
55	V	201	CDL	C40-C41-C42-C43
55	a	201	CDL	C61-C62-C63-C64
55	m	201	CDL	C34-C35-C36-C37
55	u	201	CDL	C52-C53-C54-C55
47	B	303	PEE	C21-C22-C23-C24
55	s	402	CDL	C54-C55-C56-C57
47	r	501	PEE	C36-C37-C38-C39
55	V	201	CDL	C51-C52-C53-C54
47	U	101	PEE	C44-C45-C46-C47
55	V	201	CDL	C33-C34-C35-C36
55	r	504	CDL	C21-C22-C23-C24
48	j	202	PLX	C31-C32-C33-C34
48	g	201	PLX	C33-C34-C35-C36
48	r	503	PLX	C16-C17-C18-C19
55	a	201	CDL	C73-C74-C75-C76
55	r	504	CDL	C82-C83-C84-C85
55	s	402	CDL	C80-C81-C82-C83
55	m	201	CDL	C84-C85-C86-C87
55	N	201	CDL	OA5-CA3-CA4-CA6
55	r	504	CDL	OB5-CB3-CB4-CB6
48	g	201	PLX	C12-C13-C14-C15
47	Q	501	PEE	C24-C25-C26-C27
55	V	201	CDL	C22-C23-C24-C25
55	V	201	CDL	C64-C65-C66-C67
55	u	201	CDL	C57-C58-C59-C60
47	s	401	PEE	C44-C45-C46-C47
48	r	503	PLX	C33-C34-C35-C36
55	a	201	CDL	C42-C43-C44-C45
48	a	202	PLX	C14-C15-C16-C17
48	r	503	PLX	C11-C10-C9-C8
47	U	101	PEE	C19-C20-C21-C22
47	l	704	PEE	C15-C16-C17-C18
47	j	201	PEE	C23-C24-C25-C26
47	s	401	PEE	C40-C41-C42-C43
47	s	401	PEE	C1-C2-C3-O3
48	r	503	PLX	C3-C4-C5-O8
55	V	202	CDL	CA3-CA4-CA6-OA8
55	l	702	CDL	CA3-CA4-CA6-OA8
55	m	201	CDL	CA3-CA4-CA6-OA8
47	r	501	PEE	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
48	j	202	PLX	C9-C10-C11-C12
55	s	402	CDL	C14-C15-C16-C17
55	r	504	CDL	C62-C63-C64-C65
55	V	201	CDL	C15-C16-C17-C18
47	W	201	PEE	C21-C22-C23-C24
48	r	502	PLX	C10-C11-C12-C13
48	r	503	PLX	C31-C32-C33-C34
55	N	201	CDL	C11-C12-C13-C14
55	r	504	CDL	C13-C14-C15-C16
47	b	201	PEE	O3P-C1-C2-O2
48	r	503	PLX	O4-C3-C4-O6
55	V	201	CDL	OA5-CA3-CA4-OA6
55	V	202	CDL	OA5-CA3-CA4-OA6
55	a	201	CDL	OB5-CB3-CB4-OB6
48	a	202	PLX	C26-C27-C28-C29
48	a	202	PLX	C27-C28-C29-C30
55	a	201	CDL	C14-C15-C16-C17
50	X	201	8Q1	O4-C1-S44-C43
55	V	201	CDL	C32-C33-C34-C35
48	r	503	PLX	C35-C36-C37-C38
55	V	201	CDL	C73-C74-C75-C76
47	Q	501	PEE	C14-C15-C16-C17
48	r	502	PLX	C25-C26-C27-C28
55	V	201	CDL	C32-C31-CA7-OA8
47	j	201	PEE	O2-C2-C3-O3
48	C	302	PLX	O6-C4-C5-O8
48	j	202	PLX	O6-C4-C5-O8
48	r	503	PLX	O6-C4-C5-O8
55	N	201	CDL	OB6-CB4-CB6-OB8
55	l	703	CDL	C75-C76-C77-C78
47	s	401	PEE	C30-C31-C32-C33
48	j	202	PLX	C17-C18-C19-C20
55	V	201	CDL	C54-C55-C56-C57
47	B	303	PEE	C36-C37-C38-C39
48	a	202	PLX	C34-C35-C36-C37
55	V	202	CDL	C54-C55-C56-C57
55	V	202	CDL	C57-C58-C59-C60
55	a	201	CDL	C15-C16-C17-C18
55	V	202	CDL	CB5-C51-C52-C53
55	N	201	CDL	C51-C52-C53-C54
47	B	303	PEE	O5-C30-O3-C3
47	r	501	PEE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
55	u	201	CDL	C73-C74-C75-C76
52	J	402	UQ	C9-C11-C12-C13
47	U	101	PEE	C38-C39-C40-C41
55	a	201	CDL	OA9-CA7-OA8-CA6
47	B	303	PEE	C20-C21-C22-C23
50	X	201	8Q1	C6-C1-S44-C43
55	u	201	CDL	CB2-C1-CA2-OA2
55	l	702	CDL	C33-C34-C35-C36
55	l	703	CDL	CA5-C11-C12-C13
46	A	502	FMN	C1'-C2'-C3'-O3'
48	g	201	PLX	O4-C3-C4-C5
55	l	702	CDL	OA5-CA3-CA4-CA6
55	s	402	CDL	OA5-CA3-CA4-CA6
47	j	201	PEE	C32-C33-C34-C35
47	B	303	PEE	C38-C39-C40-C41
47	r	501	PEE	C24-C25-C26-C27
55	a	201	CDL	C44-C45-C46-C47
55	s	402	CDL	C32-C33-C34-C35
47	j	201	PEE	C10-C11-C12-C13
47	j	201	PEE	O5-C30-O3-C3
55	l	702	CDL	C38-C39-C40-C41
55	s	402	CDL	CA6-CA4-OA6-CA5
48	r	503	PLX	C18-C19-C20-C21
47	l	704	PEE	C13-C14-C15-C16
55	m	201	CDL	C74-C75-C76-C77
47	j	201	PEE	O3P-C1-C2-O2
47	r	501	PEE	O3P-C1-C2-O2
48	J	403	PLX	O4-C3-C4-O6
48	g	201	PLX	O4-C3-C4-O6
55	V	201	CDL	OB5-CB3-CB4-OB6
55	a	201	CDL	OA5-CA3-CA4-OA6
55	l	703	CDL	OA5-CA3-CA4-OA6
55	r	504	CDL	OB5-CB3-CB4-OB6
55	s	402	CDL	OA5-CA3-CA4-OA6
55	u	201	CDL	OA5-CA3-CA4-OA6
48	j	202	PLX	C30-C31-C32-C33
55	s	402	CDL	C55-C56-C57-C58
48	j	202	PLX	C3-C4-C5-O8
48	r	502	PLX	C3-C4-C5-O8
48	J	403	PLX	C1-C2-O1-P1
50	X	201	8Q1	C30-C29-C32-C34
55	N	201	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
47	b	201	PEE	O2-C2-C3-O3
48	J	403	PLX	O6-C4-C5-O8
48	r	502	PLX	O6-C4-C5-O8
55	V	201	CDL	OA6-CA4-CA6-OA8
55	l	703	CDL	C15-C16-C17-C18
47	Q	501	PEE	C22-C23-C24-C25
55	V	202	CDL	C31-C32-C33-C34
47	r	501	PEE	C21-C22-C23-C24
48	a	202	PLX	C32-C33-C34-C35
55	l	702	CDL	C51-CB5-OB6-CB4
55	m	201	CDL	C31-CA7-OA8-CA6
48	J	403	PLX	N1-C1-C2-O1
55	a	201	CDL	C11-C12-C13-C14
47	s	401	PEE	C39-C40-C41-C42
55	r	504	CDL	C39-C40-C41-C42
48	J	403	PLX	C25-C24-O8-C5
48	a	202	PLX	C25-C24-O8-C5
48	g	201	PLX	C25-C24-O8-C5
47	W	201	PEE	C19-C20-C21-C22
48	C	302	PLX	C15-C16-C17-C18
47	B	303	PEE	O3P-C1-C2-C3
47	b	201	PEE	O3P-C1-C2-C3
47	j	201	PEE	O3P-C1-C2-C3
47	r	501	PEE	O3P-C1-C2-C3
48	r	503	PLX	O4-C3-C4-C5
55	l	703	CDL	OA5-CA3-CA4-CA6
55	l	702	CDL	OB7-CB5-OB6-CB4
48	j	202	PLX	C19-C20-C21-C22
50	X	201	8Q1	O27-C28-C29-C31
55	V	202	CDL	C51-C52-C53-C54
55	l	702	CDL	C54-C55-C56-C57
47	B	303	PEE	C33-C34-C35-C36
47	U	101	PEE	C20-C21-C22-C23
55	r	504	CDL	C1-CB2-OB2-PB2
55	a	201	CDL	C21-C22-C23-C24
55	s	402	CDL	C74-C75-C76-C77
47	B	303	PEE	O3P-C1-C2-O2
47	l	701	PEE	O3P-C1-C2-O2
55	N	201	CDL	OA5-CA3-CA4-OA6
55	l	702	CDL	OB5-CB3-CB4-OB6
47	l	704	PEE	C19-C20-C21-C22
48	j	202	PLX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
48	a	202	PLX	C35-C36-C37-C38
47	W	201	PEE	C11-C10-O2-C2
51	J	401	NDP	C2N-C3N-C7N-O7N
47	j	201	PEE	C33-C34-C35-C36
55	a	201	CDL	C16-C17-C18-C19
55	V	201	CDL	C11-C12-C13-C14
55	r	504	CDL	C74-C75-C76-C77
55	m	201	CDL	OA9-CA7-OA8-CA6
47	B	303	PEE	O2-C2-C3-O3
47	Q	501	PEE	O2-C2-C3-O3
47	W	201	PEE	O2-C2-C3-O3
47	s	401	PEE	O2-C2-C3-O3
55	V	202	CDL	CB2-C1-CA2-OA2
55	l	703	CDL	CA2-C1-CB2-OB2
48	a	202	PLX	C3-C4-C5-O8
47	b	201	PEE	C34-C35-C36-C37
55	V	202	CDL	C78-C79-C80-C81
47	W	201	PEE	O4-C10-O2-C2
55	l	703	CDL	C32-C33-C34-C35
55	l	703	CDL	C56-C57-C58-C59
55	s	402	CDL	C16-C17-C18-C19
46	A	502	FMN	C2'-C1'-N10-C10
47	B	303	PEE	C4-O4P-P-O1P
47	Q	501	PEE	C4-O4P-P-O3P
47	U	101	PEE	C1-O3P-P-O2P
47	W	201	PEE	C4-O4P-P-O3P
47	W	201	PEE	C4-O4P-P-O1P
47	b	201	PEE	C1-O3P-P-O1P
47	j	201	PEE	C1-O3P-P-O2P
47	j	201	PEE	C1-O3P-P-O1P
47	j	201	PEE	C1-O3P-P-O4P
47	r	501	PEE	C1-O3P-P-O2P
48	a	202	PLX	C3-O4-P1-O1
48	a	202	PLX	C3-O4-P1-O2
48	g	201	PLX	C5-C4-O6-C6
48	g	201	PLX	C3-O4-P1-O3
48	j	202	PLX	C2-O1-P1-O3
48	r	502	PLX	C3-C4-O6-C6
48	r	502	PLX	C5-C4-O6-C6
48	r	502	PLX	C3-O4-P1-O2
48	r	502	PLX	C2-O1-P1-O3
48	r	503	PLX	C3-C4-O6-C6

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Mol	Chain	Res	Type	Atoms
48	r	503	PLX	C5-C4-O6-C6
50	G	201	8Q1	C28-C29-C32-O33
50	X	201	8Q1	C28-C29-C32-O33
52	J	402	UQ	C3-C2-O2-CM2
55	V	202	CDL	CB2-OB2-PB2-OB4
55	l	702	CDL	CA2-OA2-PA1-OA3
55	l	702	CDL	CA3-OA5-PA1-OA3
55	l	702	CDL	CB2-OB2-PB2-OB3
55	l	703	CDL	CA2-OA2-PA1-OA3
55	l	703	CDL	CB2-OB2-PB2-OB3
55	r	504	CDL	CA3-OA5-PA1-OA3
55	r	504	CDL	CB2-OB2-PB2-OB3
55	r	504	CDL	CB2-OB2-PB2-OB4
55	r	504	CDL	CB2-OB2-PB2-OB5
55	r	504	CDL	CB3-OB5-PB2-OB2
55	r	504	CDL	CB3-OB5-PB2-OB4
55	u	201	CDL	CA3-OA5-PA1-OA3
47	B	303	PEE	C13-C14-C15-C16
55	V	202	CDL	C76-C77-C78-C79
55	m	201	CDL	CA4-CA3-OA5-PA1
55	u	201	CDL	C51-C52-C53-C54
47	s	401	PEE	C42-C43-C44-C45
55	s	402	CDL	C38-C39-C40-C41
47	s	401	PEE	C20-C21-C22-C23
55	l	703	CDL	C61-C62-C63-C64
47	b	201	PEE	C14-C15-C16-C17
55	a	201	CDL	C58-C59-C60-C61
55	m	201	CDL	CA3-CA4-OA6-CA5
55	l	703	CDL	C64-C65-C66-C67
47	l	701	PEE	O3P-C1-C2-C3
55	V	202	CDL	OA5-CA3-CA4-CA6
55	u	201	CDL	OA5-CA3-CA4-CA6
55	l	703	CDL	C71-C72-C73-C74
55	r	504	CDL	C42-C43-C44-C45
55	s	402	CDL	CB2-C1-CA2-OA2
55	m	201	CDL	OA5-CA3-CA4-OA6
47	b	201	PEE	C30-C31-C32-C33
55	l	703	CDL	C40-C41-C42-C43
48	j	202	PLX	C26-C27-C28-C29
55	s	402	CDL	C31-C32-C33-C34
47	r	501	PEE	C37-C38-C39-C40
55	a	201	CDL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
48	a	202	PLX	C11-C10-C9-C8
47	U	101	PEE	C21-C22-C23-C24
55	a	201	CDL	C53-C54-C55-C56
48	J	403	PLX	C10-C11-C12-C13
47	r	501	PEE	C1-C2-C3-O3
47	l	704	PEE	C22-C23-C24-C25
50	X	201	8Q1	C10-C11-C12-C13
47	Q	501	PEE	C38-C39-C40-C41
47	l	704	PEE	C18-C19-C20-C21
55	l	702	CDL	C32-C33-C34-C35
48	g	201	PLX	C6-C7-C8-C9
55	s	402	CDL	C57-C58-C59-C60
55	l	703	CDL	CB5-C51-C52-C53
48	g	201	PLX	O8-C24-C25-C26
55	V	201	CDL	CA4-CA3-OA5-PA1
52	J	402	UQ	C4-C3-O3-CM3
55	V	202	CDL	C13-C14-C15-C16
47	b	201	PEE	C18-C19-C20-C21
47	s	401	PEE	C17-C18-C19-C20
47	U	101	PEE	C40-C41-C42-C43
48	r	502	PLX	C30-C31-C32-C33
50	X	201	8Q1	C6-C7-C8-C9
55	V	201	CDL	C71-C72-C73-C74
55	l	703	CDL	O1-C1-CA2-OA2
47	s	401	PEE	C12-C13-C14-C15
46	A	502	FMN	O2'-C2'-C3'-O3'
47	b	201	PEE	C16-C17-C18-C19
47	r	501	PEE	C38-C39-C40-C41
55	l	703	CDL	C74-C75-C76-C77
55	r	504	CDL	C36-C37-C38-C39
55	r	504	CDL	C76-C77-C78-C79
48	a	202	PLX	C12-C13-C14-C15
55	r	504	CDL	C72-C73-C74-C75
55	V	201	CDL	C72-C73-C74-C75
55	r	504	CDL	C61-C62-C63-C64
47	l	701	PEE	C39-C40-C41-C42
47	B	303	PEE	C12-C13-C14-C15
48	C	302	PLX	C3-C4-C5-O8
47	U	101	PEE	C42-C43-C44-C45
48	J	403	PLX	C12-C13-C14-C15
55	m	201	CDL	C77-C78-C79-C80
47	l	704	PEE	C3-C2-O2-C10

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	C40-C41-C42-C43
47	Q	501	PEE	C18-C19-C20-C21
55	l	703	CDL	CA7-C31-C32-C33
55	r	504	CDL	CA7-C31-C32-C33
46	A	502	FMN	O2'-C2'-C3'-C4'
47	l	701	PEE	C2-C1-O3P-P
55	r	504	CDL	C11-C12-C13-C14
48	a	202	PLX	O6-C4-C5-O8
55	r	504	CDL	OA6-CA4-CA6-OA8
55	V	202	CDL	C22-C23-C24-C25
55	l	702	CDL	C55-C56-C57-C58
48	a	202	PLX	O6-C6-C7-C8
55	u	201	CDL	O1-C1-CB2-OB2
55	l	703	CDL	C11-CA5-OA6-CA4
47	W	201	PEE	C23-C24-C25-C26
55	m	201	CDL	C33-C34-C35-C36
52	J	402	UQ	C20-C19-C21-C22
48	C	302	PLX	C11-C12-C13-C14
55	s	402	CDL	C59-C60-C61-C62
55	a	201	CDL	C41-C42-C43-C44
47	j	201	PEE	C30-C31-C32-C33
55	V	202	CDL	C64-C65-C66-C67
48	C	302	PLX	O7-C6-C7-C8
48	C	302	PLX	O9-C24-C25-C26
48	g	201	PLX	O7-C6-C7-C8
55	V	202	CDL	C32-C31-CA7-OA8
55	N	201	CDL	O1-C1-CB2-OB2
55	a	201	CDL	C64-C65-C66-C67
55	l	703	CDL	OA7-CA5-OA6-CA4
55	r	504	CDL	C54-C55-C56-C57
55	l	703	CDL	C80-C81-C82-C83
52	s	403	UQ	C6-C7-C8-C9
55	V	202	CDL	C62-C63-C64-C65
55	a	201	CDL	C37-C38-C39-C40
55	a	201	CDL	C13-C14-C15-C16
47	Q	501	PEE	C16-C17-C18-C19
47	j	201	PEE	C18-C19-C20-C21
47	r	501	PEE	C16-C17-C18-C19
47	s	401	PEE	C38-C39-C40-C41
55	V	202	CDL	C81-C82-C83-C84
48	C	302	PLX	C14-C15-C16-C17
48	C	302	PLX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
55	s	402	CDL	C40-C41-C42-C43
47	B	303	PEE	C18-C19-C20-C21
47	l	704	PEE	C41-C42-C43-C44
55	N	201	CDL	OA9-CA7-OA8-CA6
47	b	201	PEE	C2-C3-O3-C30
47	W	201	PEE	C16-C17-C18-C19
55	m	201	CDL	C78-C79-C80-C81
55	l	702	CDL	C19-C20-C21-C22
55	u	201	CDL	C72-C71-CB7-OB8
52	s	403	UQ	C12-C13-C14-C16
47	l	704	PEE	C36-C37-C38-C39
47	l	704	PEE	C2-C1-O3P-P
55	l	702	CDL	CB4-CB3-OB5-PB2
55	u	201	CDL	OB5-CB3-CB4-OB6
55	N	201	CDL	C31-CA7-OA8-CA6
48	J	403	PLX	C3-C4-C5-O8
55	N	201	CDL	CB3-CB4-CB6-OB8
55	V	201	CDL	C32-C31-CA7-OA9
55	m	201	CDL	C53-C54-C55-C56
50	G	201	8Q1	C30-C29-C32-C34
55	V	201	CDL	C39-C40-C41-C42
47	j	201	PEE	C31-C32-C33-C34
55	a	201	CDL	C78-C79-C80-C81
55	N	201	CDL	O1-C1-CA2-OA2
55	l	703	CDL	C51-C52-C53-C54
47	U	101	PEE	C16-C17-C18-C19
47	b	201	PEE	C38-C39-C40-C41
47	j	201	PEE	C16-C17-C18-C19
55	V	201	CDL	OB5-CB3-CB4-CB6
55	l	702	CDL	OB5-CB3-CB4-CB6
48	j	202	PLX	C15-C16-C17-C18
55	l	703	CDL	C52-C53-C54-C55
48	g	201	PLX	C36-C37-C38-C39
55	s	402	CDL	C51-CB5-OB6-CB4
55	l	703	CDL	C52-C51-CB5-OB6
47	Q	501	PEE	C36-C37-C38-C39
55	s	402	CDL	OB7-CB5-OB6-CB4
50	G	201	8Q1	C9-C10-C11-C12
55	u	201	CDL	C1-CB2-OB2-PB2
47	U	101	PEE	C11-C12-C13-C14
48	r	503	PLX	C24-C25-C26-C27
55	m	201	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
55	l	702	CDL	CB5-C51-C52-C53
55	s	402	CDL	C72-C71-CB7-OB8
47	s	401	PEE	C36-C37-C38-C39
55	s	402	CDL	C75-C76-C77-C78
55	s	402	CDL	C15-C16-C17-C18
55	a	201	CDL	C12-C11-CA5-OA6
52	s	403	UQ	C13-C14-C16-C17
55	l	702	CDL	C84-C85-C86-C87
55	m	201	CDL	C51-C52-C53-C54
47	l	701	PEE	O2-C10-C11-C12
55	a	201	CDL	C32-C31-CA7-OA8
48	j	202	PLX	C25-C24-O8-C5
48	r	503	PLX	C2-C1-N1-C1B
55	N	201	CDL	C52-C51-CB5-OB6
47	U	101	PEE	O3-C30-C31-C32
55	r	504	CDL	C72-C71-CB7-OB8
48	r	503	PLX	C12-C13-C14-C15
47	B	303	PEE	C32-C33-C34-C35
55	V	202	CDL	C77-C78-C79-C80
48	r	503	PLX	C7-C8-C9-C10
55	a	201	CDL	C55-C56-C57-C58
49	C	303	970	C01-C02-C04-C05
50	X	201	8Q1	O27-C28-C29-C30
47	l	704	PEE	C1-C2-O2-C10
48	r	503	PLX	C2-C1-N1-C1C
47	U	101	PEE	C14-C15-C16-C17
47	U	101	PEE	C41-C42-C43-C44
55	r	504	CDL	C75-C76-C77-C78
47	s	401	PEE	O3-C30-C31-C32
47	b	201	PEE	C24-C25-C26-C27
49	C	303	970	C01-C02-C04-O08
55	u	201	CDL	C71-C72-C73-C74
52	J	402	UQ	C13-C14-C16-C17
55	V	201	CDL	C57-C58-C59-C60
48	J	403	PLX	O6-C6-C7-C8
48	r	503	PLX	O8-C24-C25-C26
55	V	202	CDL	C24-C25-C26-C27
48	r	502	PLX	C29-C30-C31-C32
55	l	703	CDL	C54-C55-C56-C57
48	C	302	PLX	O9-C24-O8-C5
48	J	403	PLX	O9-C24-O8-C5
55	s	402	CDL	C53-C54-C55-C56

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Mol	Chain	Res	Type	Atoms
55	V	202	CDL	C32-C33-C34-C35
55	N	201	CDL	C72-C71-CB7-OB8
47	l	701	PEE	O4-C10-C11-C12
55	l	703	CDL	C52-C51-CB5-OB7
48	g	201	PLX	C4-C5-O8-C24
48	J	403	PLX	C6-C7-C8-C9
47	U	101	PEE	O5-C30-C31-C32
55	l	703	CDL	C12-C11-CA5-OA6
55	m	201	CDL	C1-CA2-OA2-PA1
48	r	503	PLX	C2-C1-N1-C1A
55	r	504	CDL	C72-C71-CB7-OB9
50	X	201	8Q1	O27-C28-C29-C32
55	a	201	CDL	C12-C11-CA5-OA7
48	j	202	PLX	O4-C3-C4-C5
47	l	701	PEE	O3-C30-C31-C32
55	l	702	CDL	C63-C64-C65-C66
55	s	402	CDL	C60-C61-C62-C63
55	m	201	CDL	C12-C11-CA5-OA6
47	s	401	PEE	O5-C30-C31-C32
55	V	202	CDL	C33-C34-C35-C36
55	a	201	CDL	C56-C57-C58-C59
55	s	402	CDL	C33-C34-C35-C36

There are no ring outliers.

37 monomers are involved in 286 short contacts:

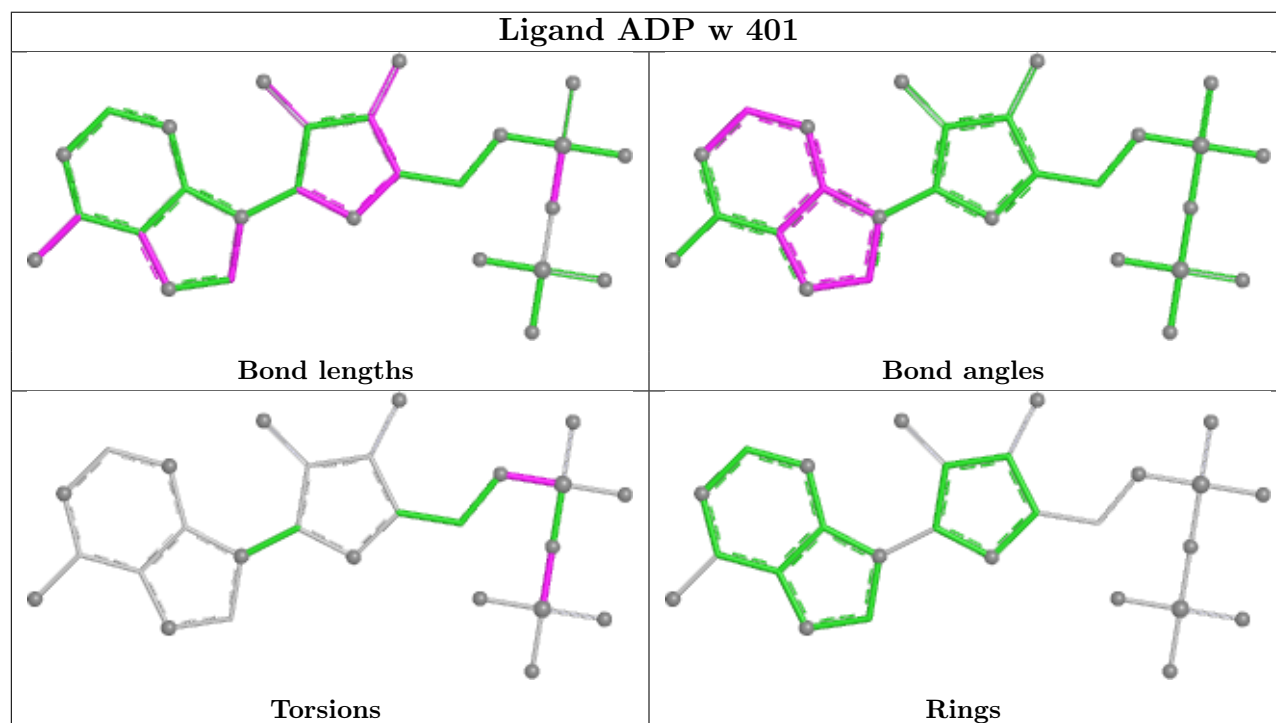
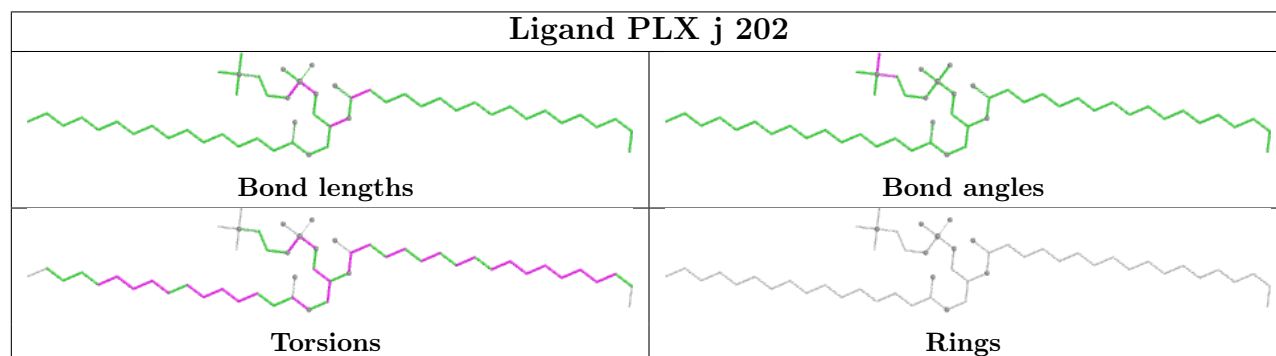
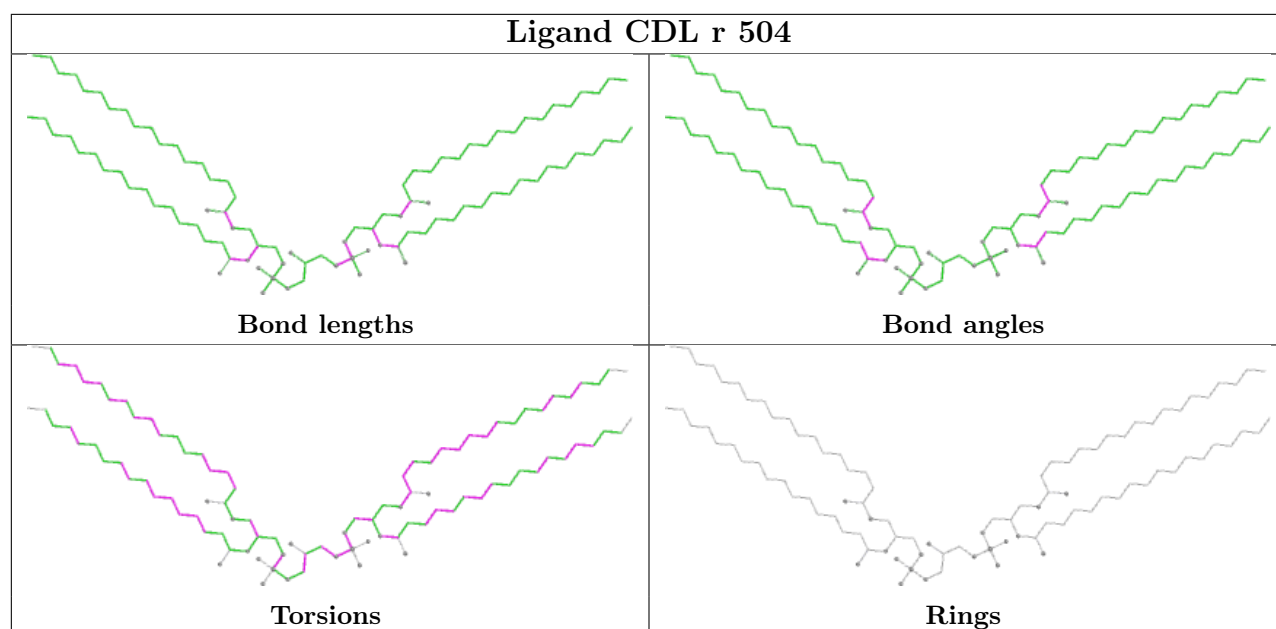
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	r	504	CDL	9	0
48	j	202	PLX	2	0
57	w	401	ADP	2	0
51	J	401	NDP	2	0
47	U	101	PEE	5	0
47	B	303	PEE	3	0
55	l	702	CDL	13	0
47	r	501	PEE	18	0
53	M	803	FES	3	0
47	l	704	PEE	10	0
47	j	201	PEE	4	0
45	M	802	SF4	7	0
48	C	302	PLX	6	0
46	A	502	FMN	6	0
47	Q	501	PEE	23	0

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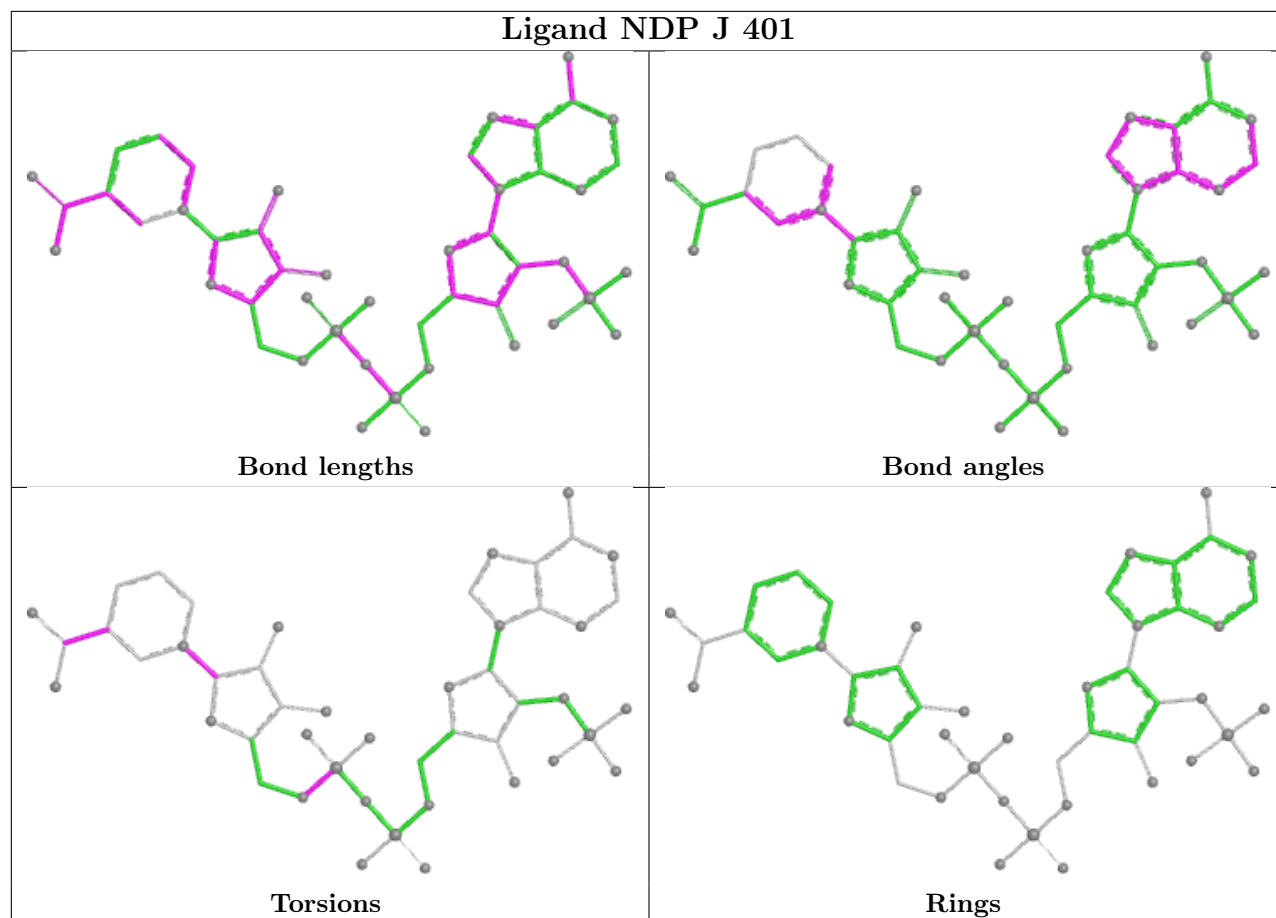
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	s	401	PEE	5	0
55	s	402	CDL	33	0
55	a	201	CDL	8	0
48	a	202	PLX	2	0
53	O	301	FES	3	0
47	b	201	PEE	10	0
47	W	201	PEE	17	0
55	u	201	CDL	8	0
50	X	201	8Q1	5	0
55	V	202	CDL	10	0
45	A	501	SF4	1	0
52	J	402	UQ	11	0
48	r	503	PLX	6	0
52	s	403	UQ	6	0
48	J	403	PLX	4	0
55	m	201	CDL	6	0
48	g	201	PLX	8	0
55	N	201	CDL	18	0
55	l	703	CDL	17	0
48	r	502	PLX	4	0
55	V	201	CDL	6	0
45	C	301	SF4	2	0

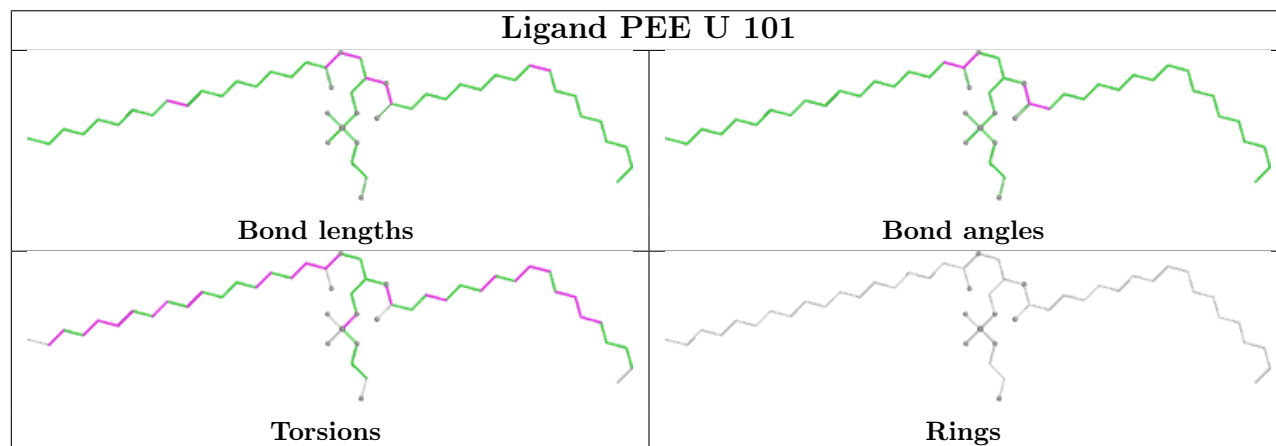
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

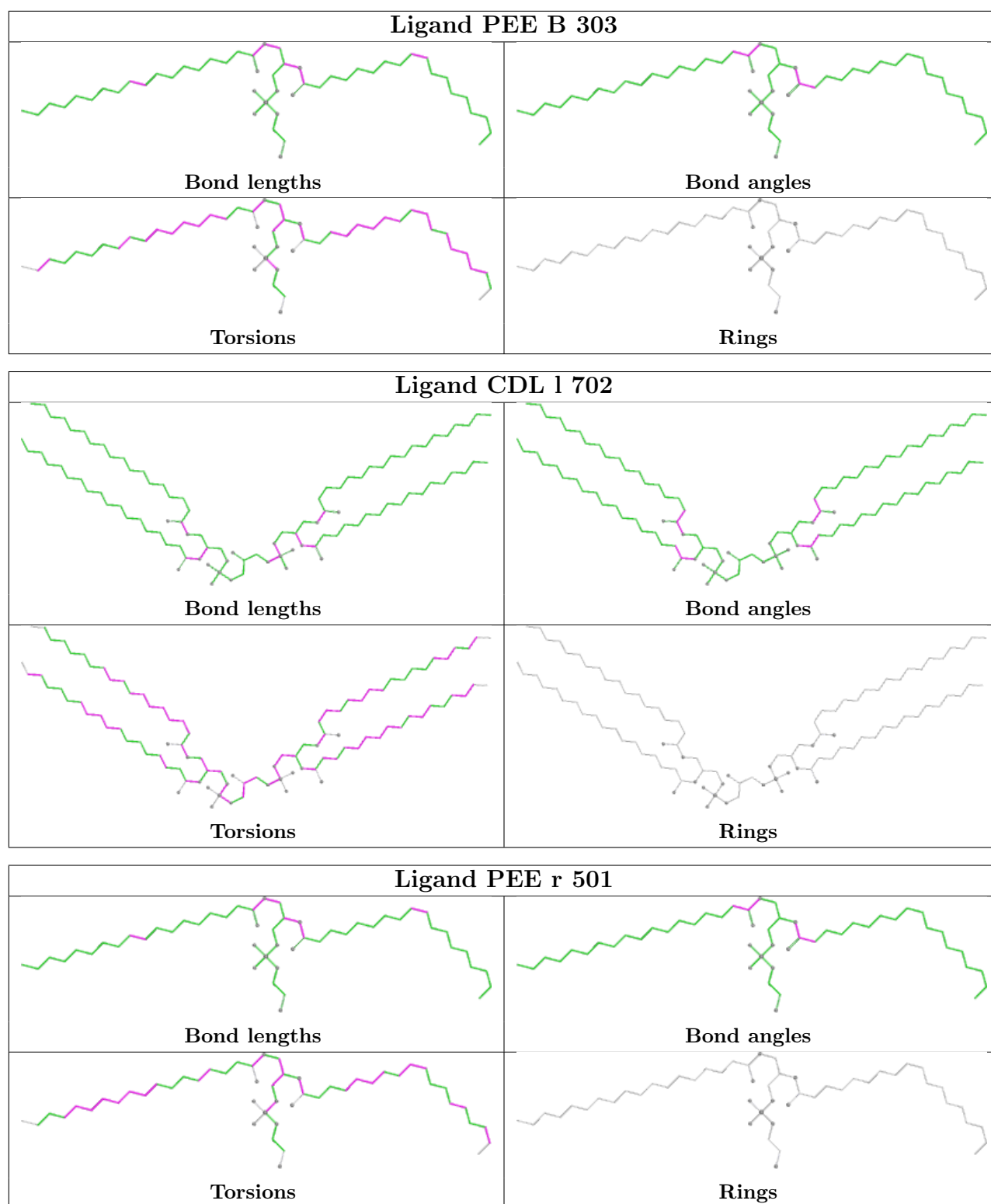


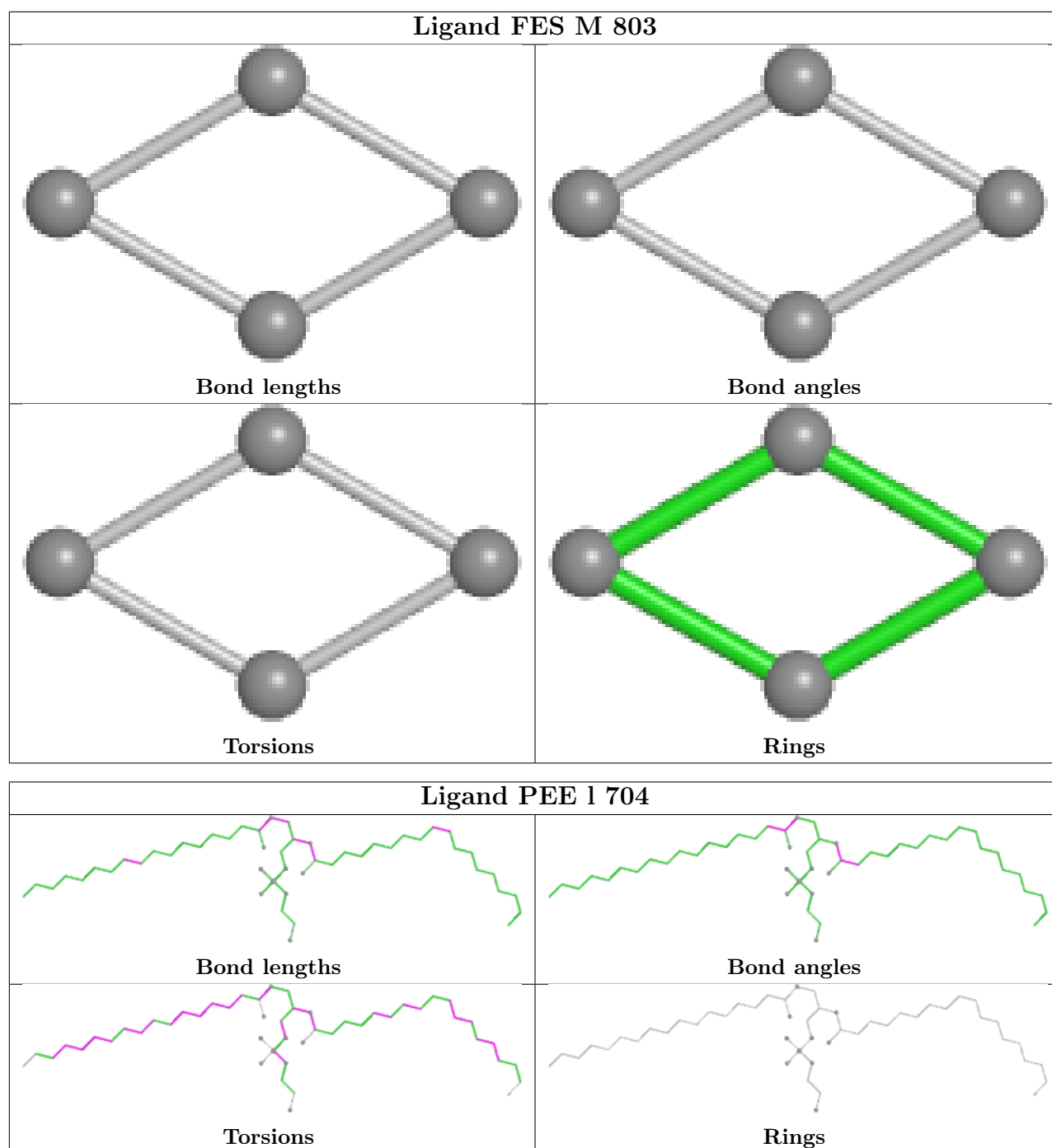
Ligand NDP J 401

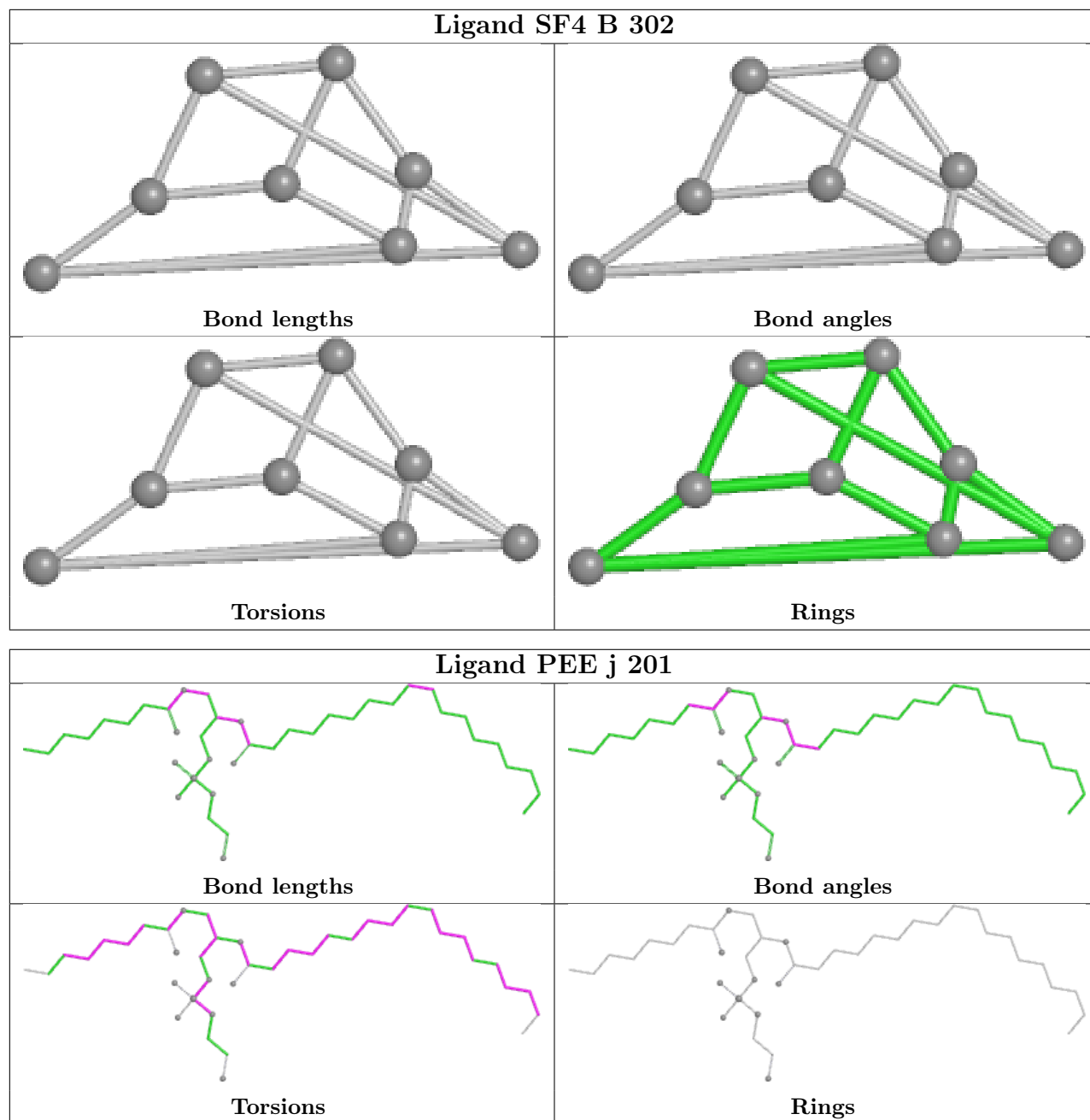


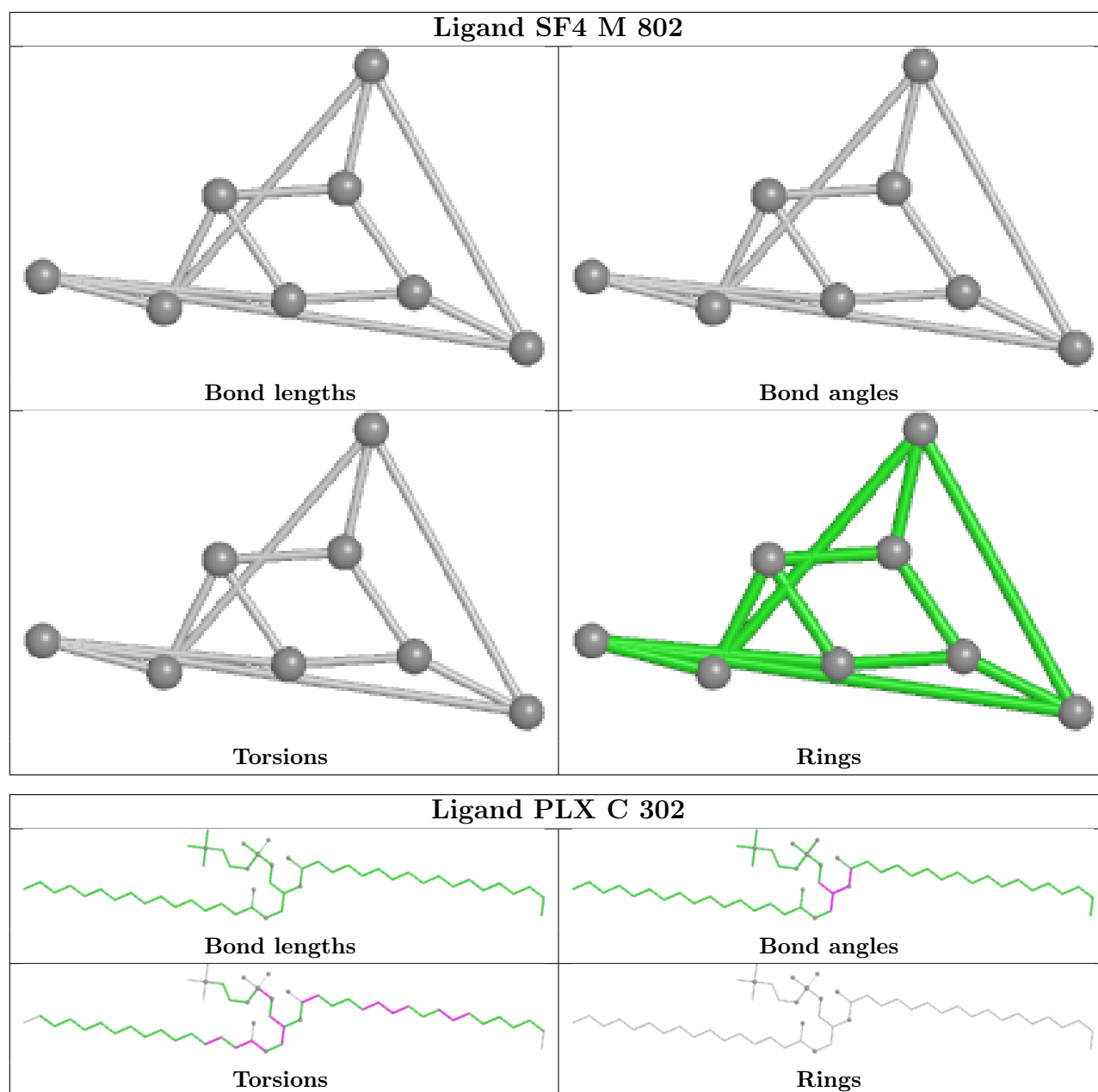
Ligand PEE U 101

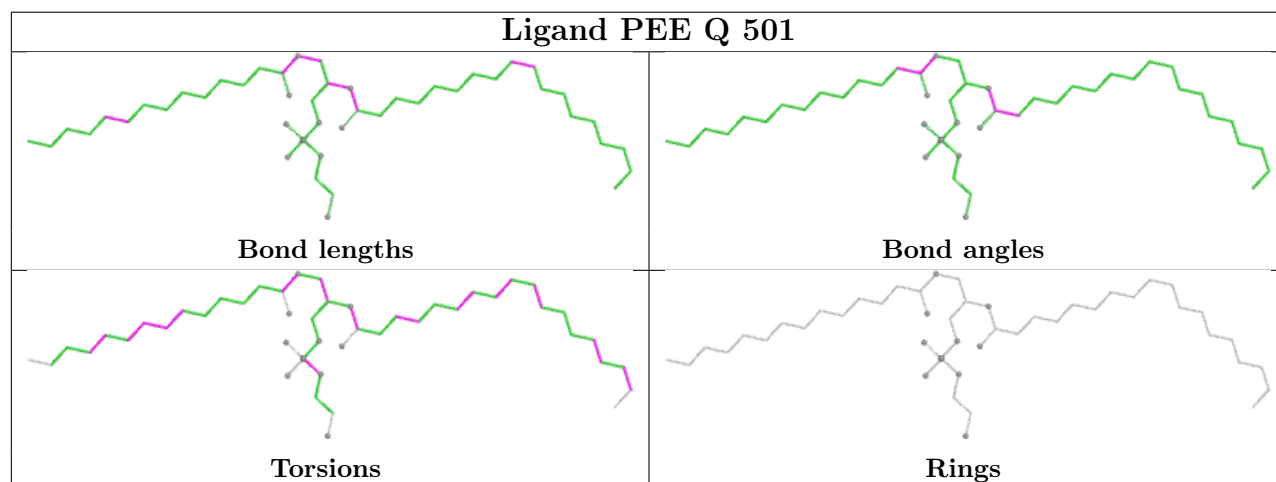
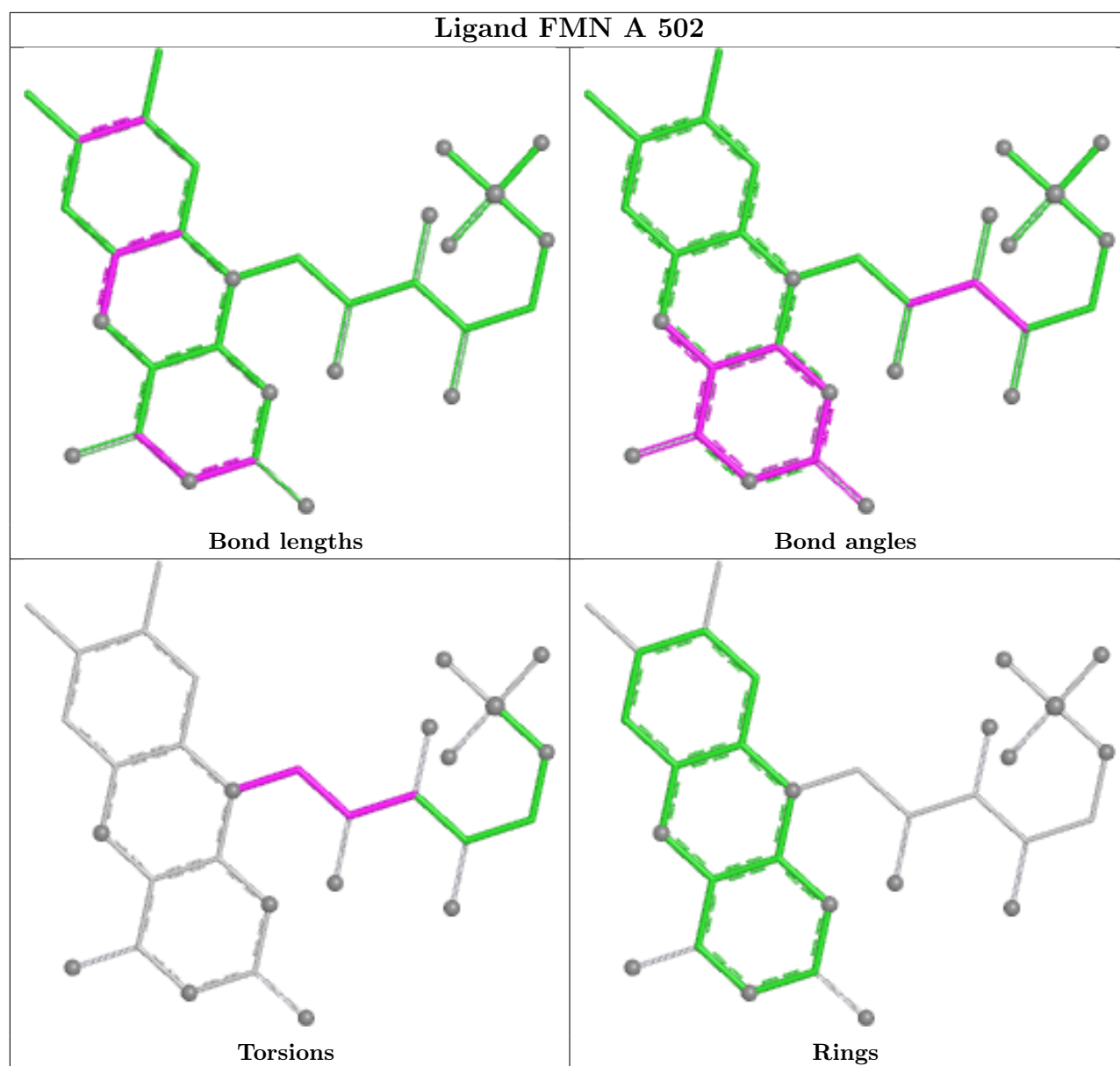


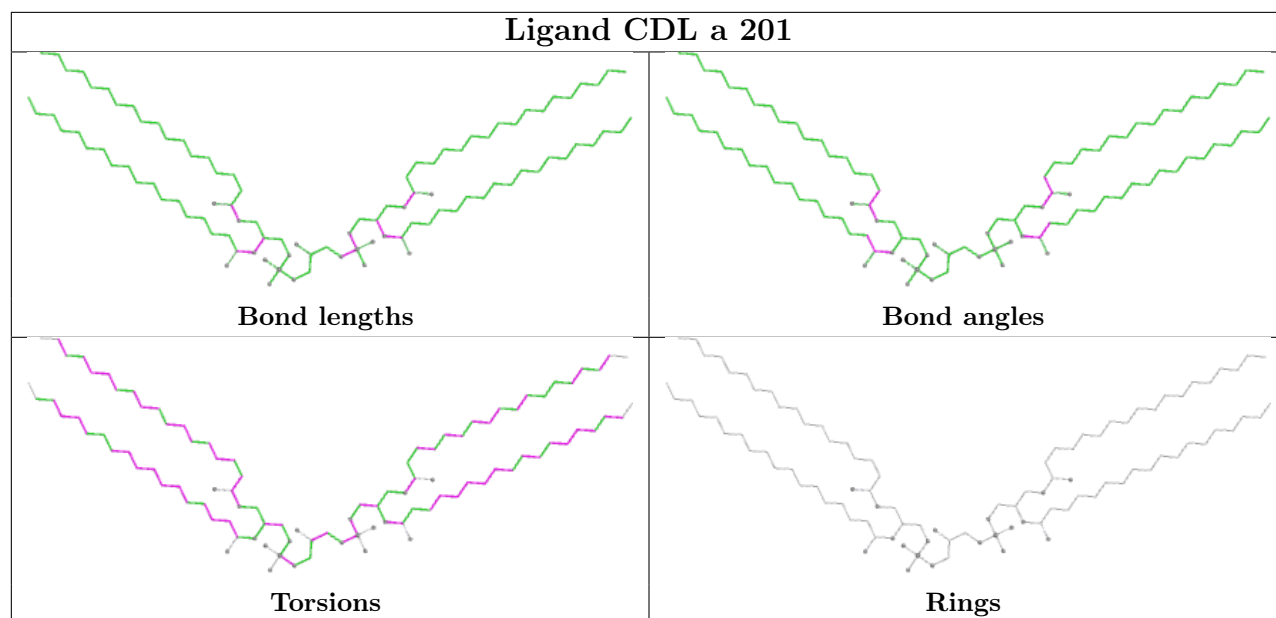
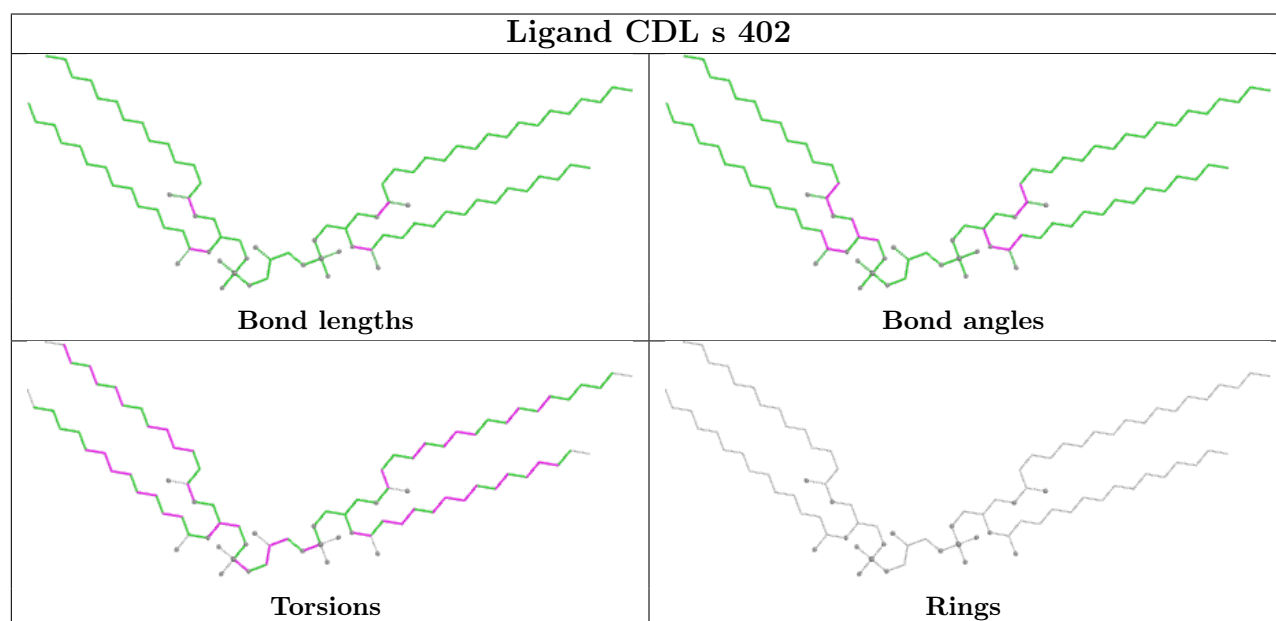
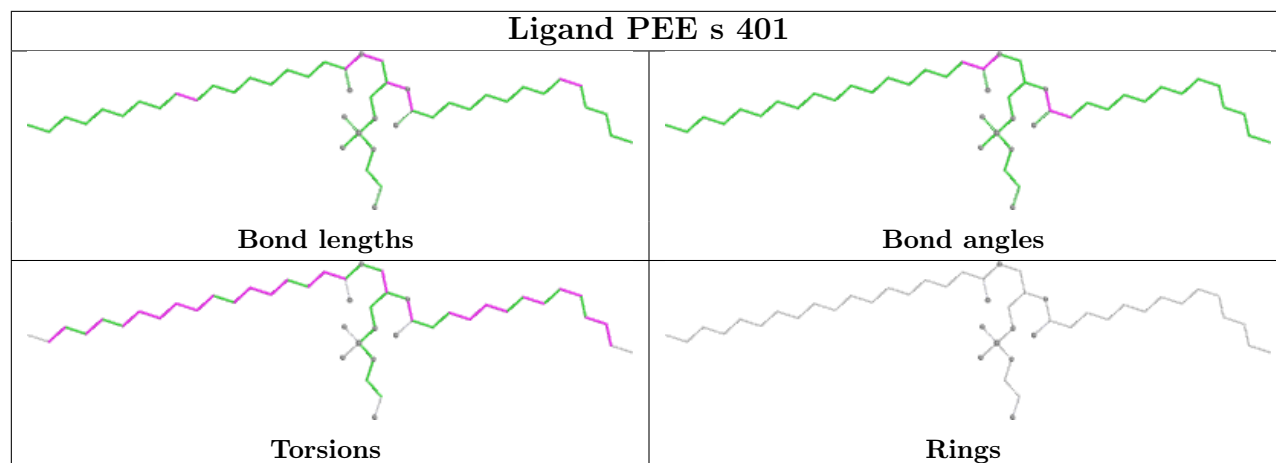


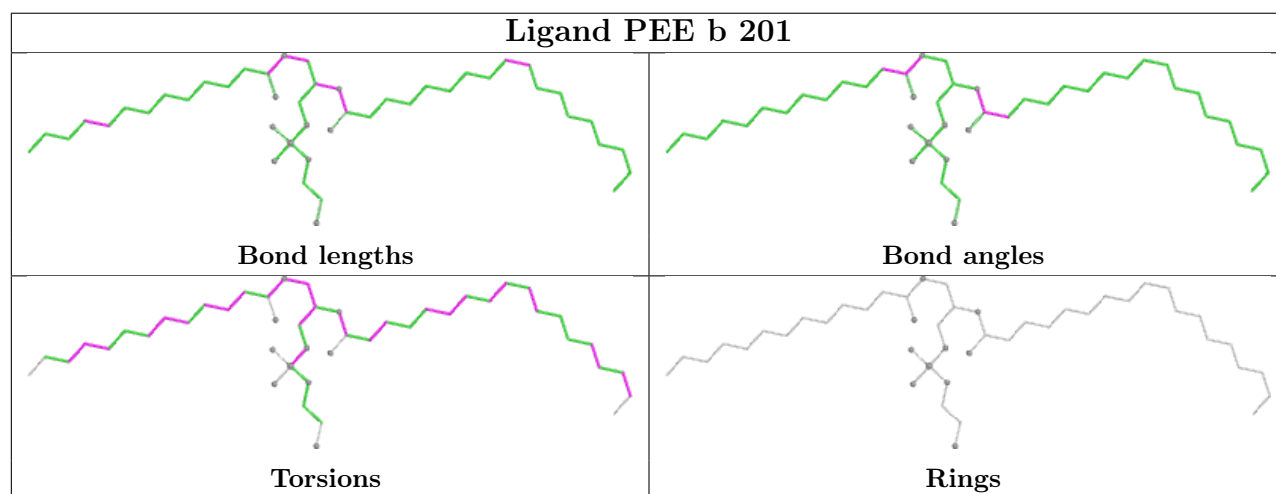
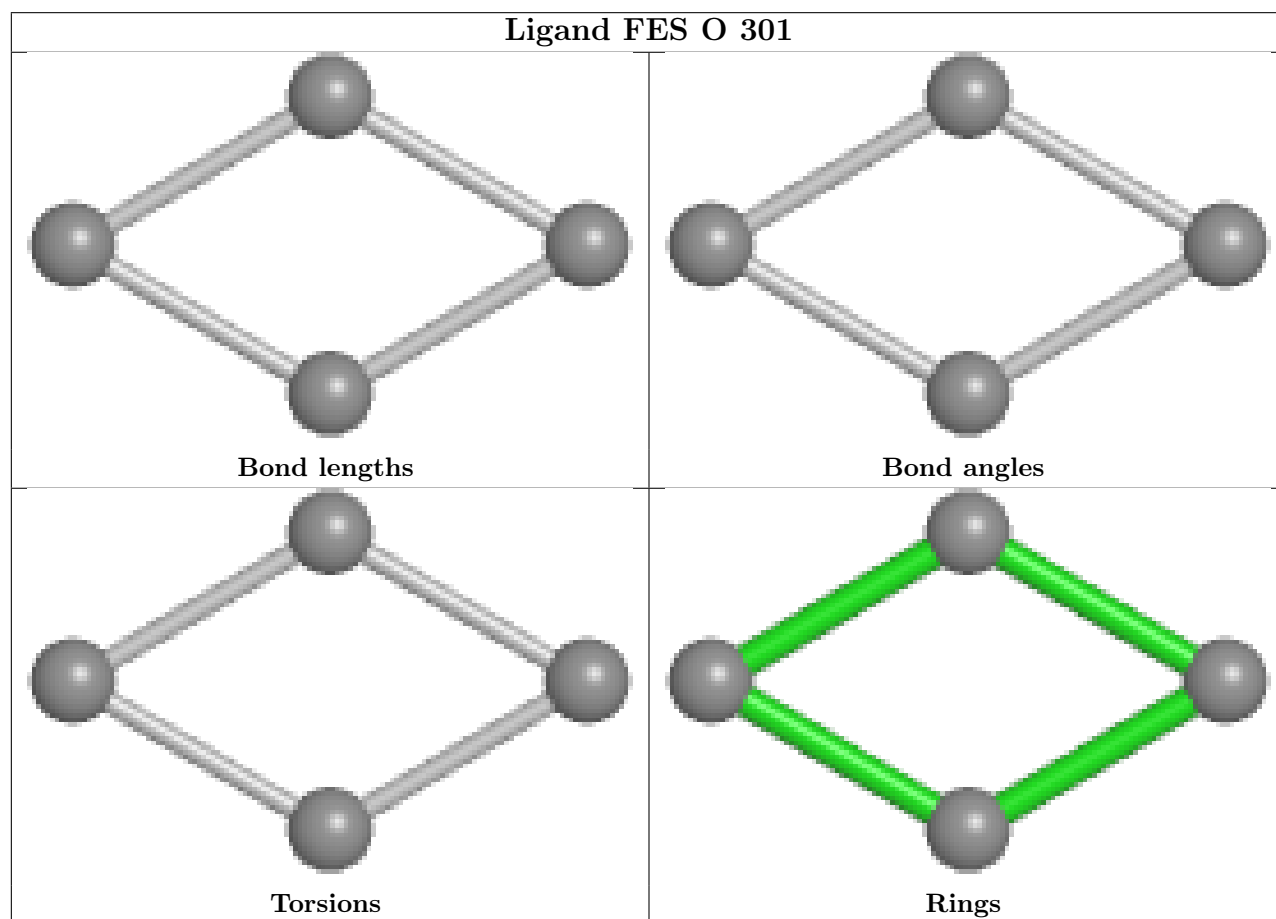
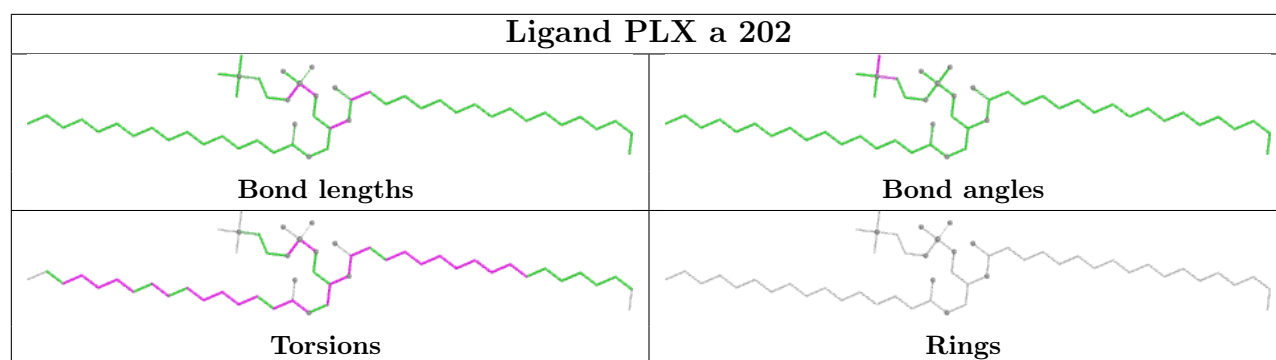


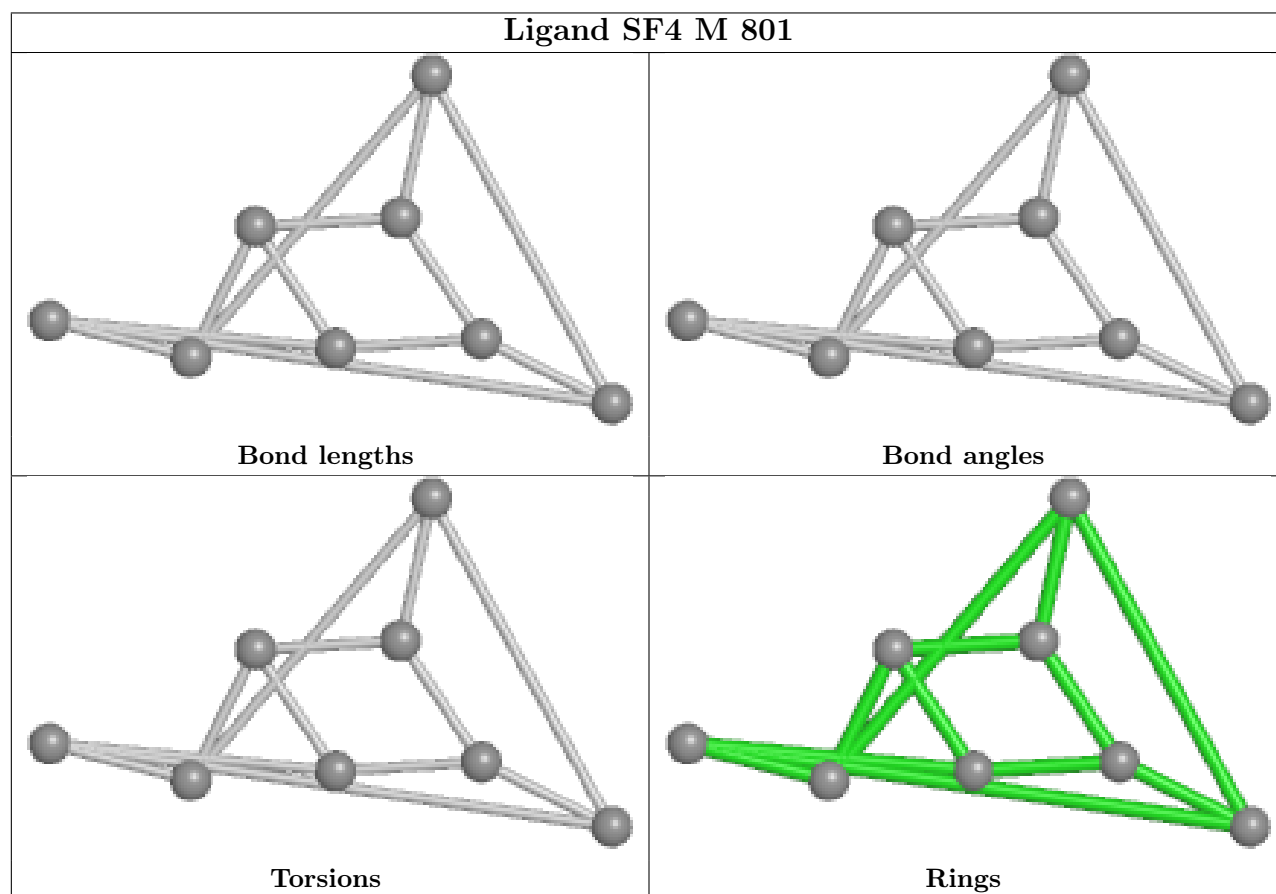
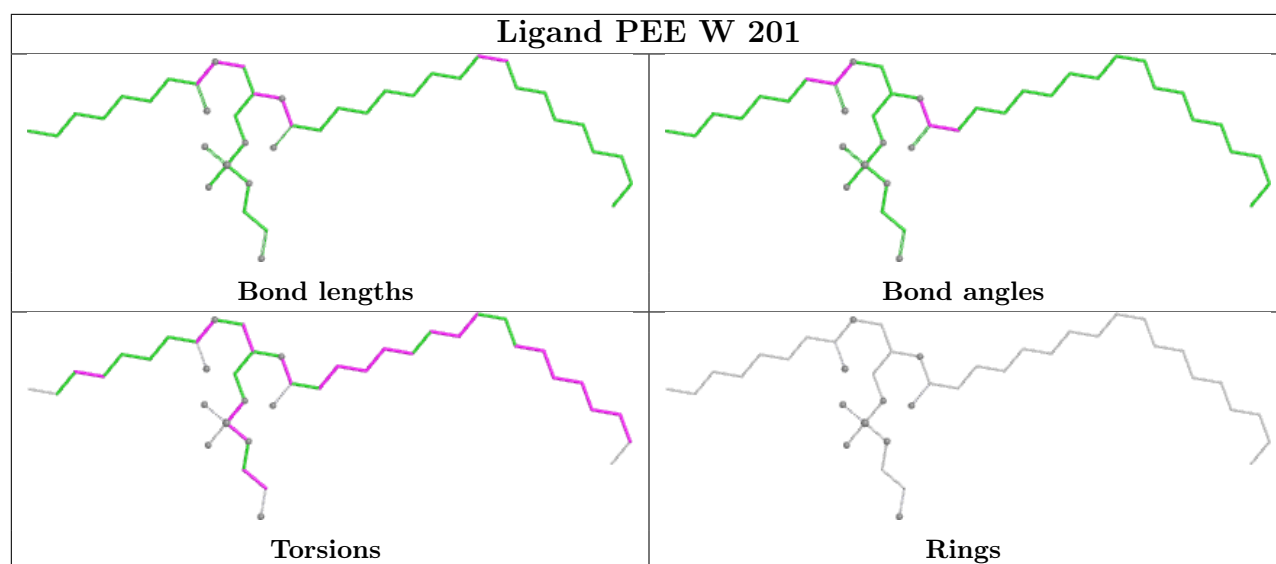


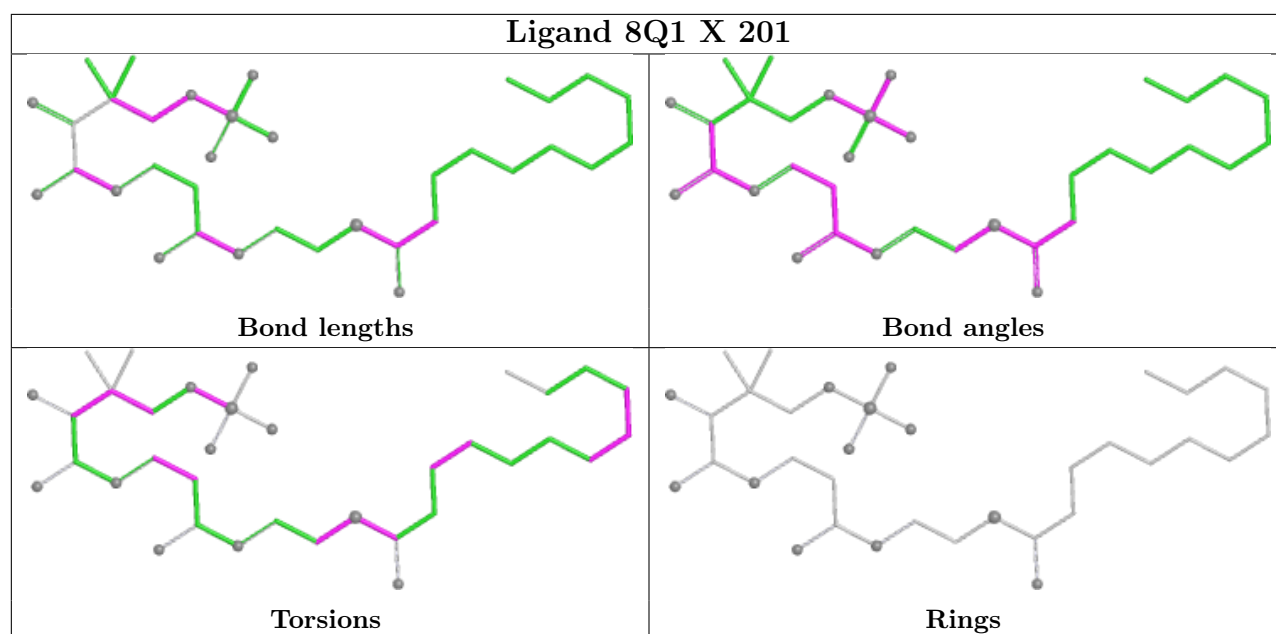
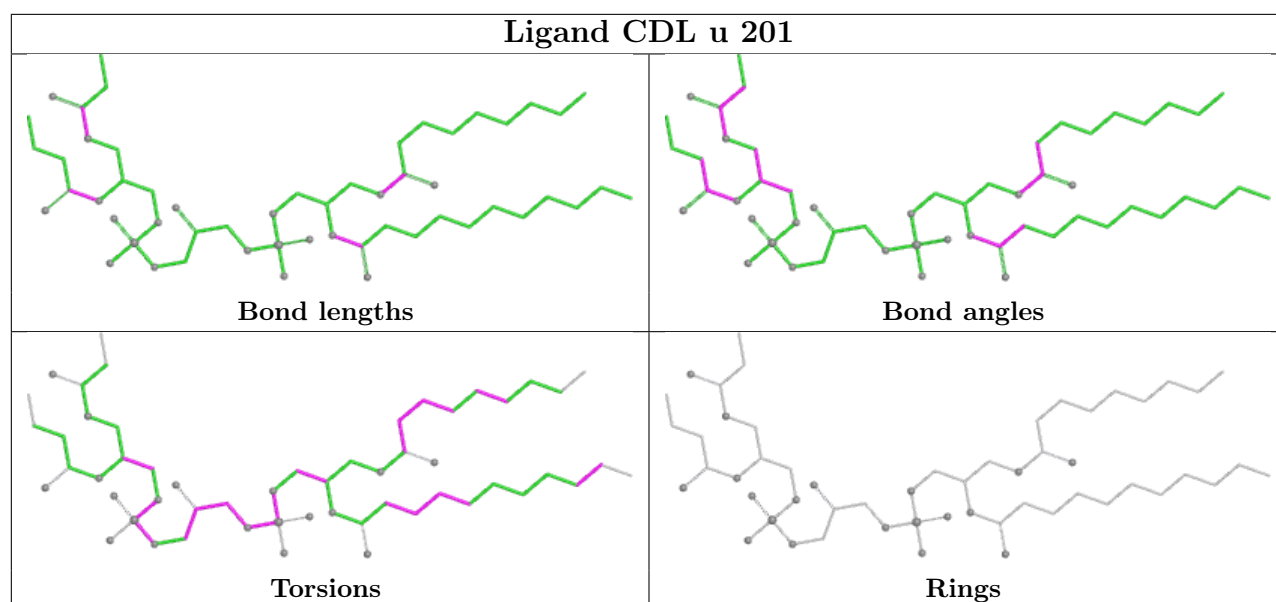


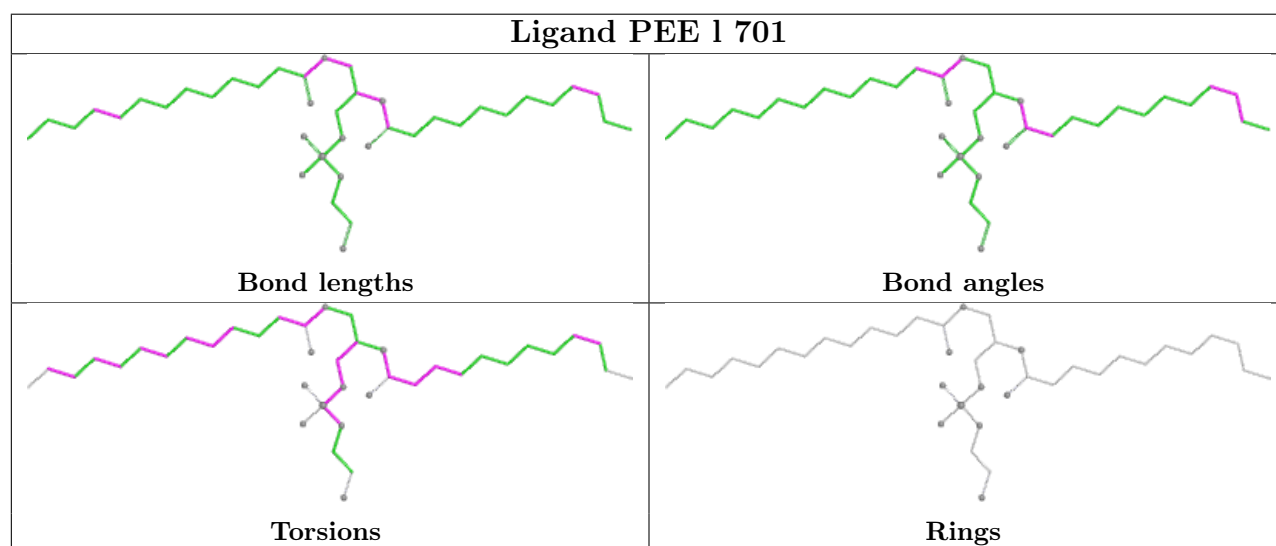
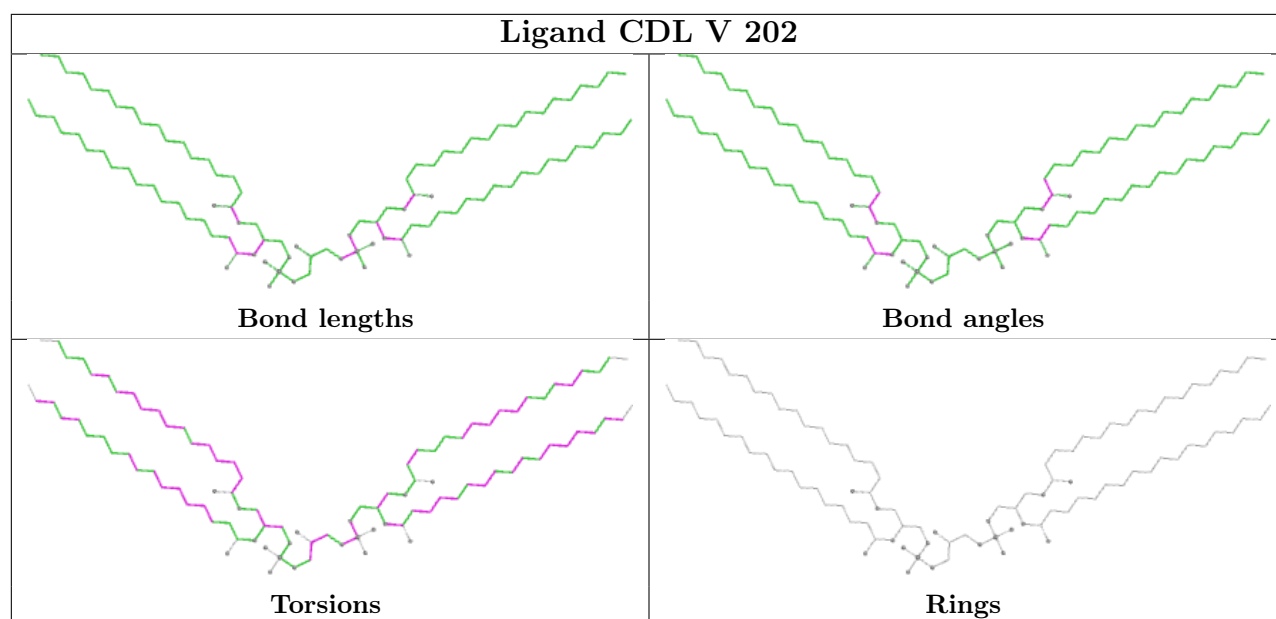


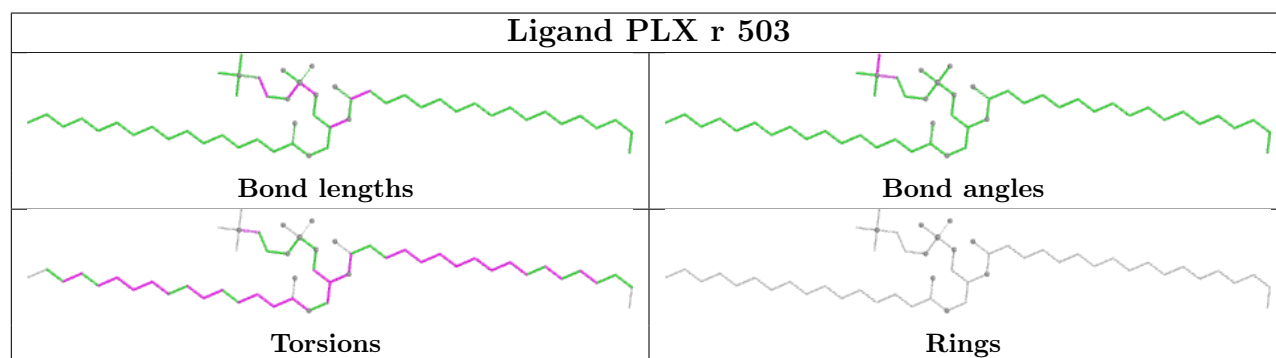
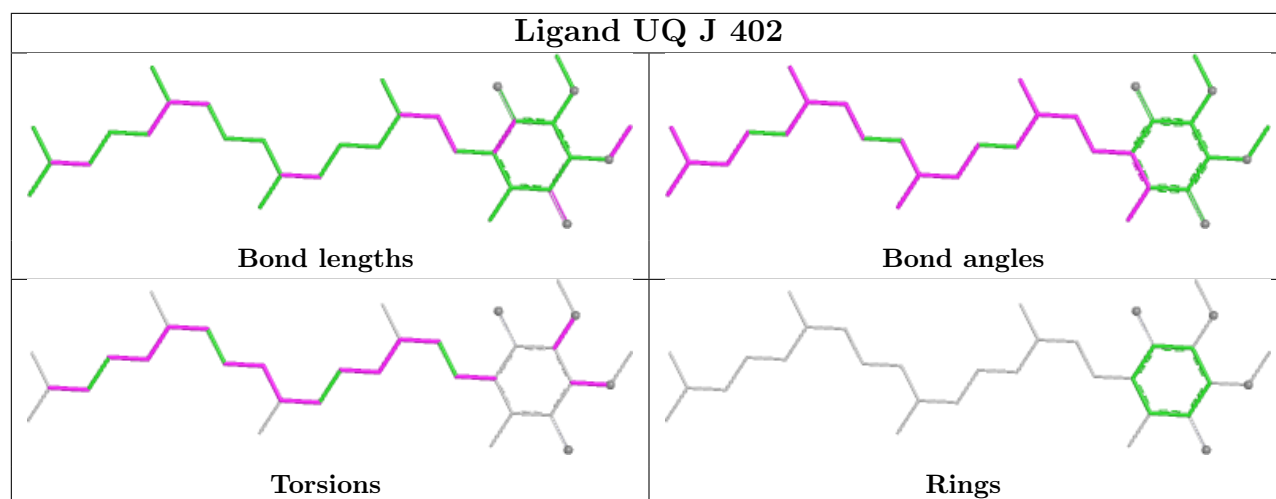
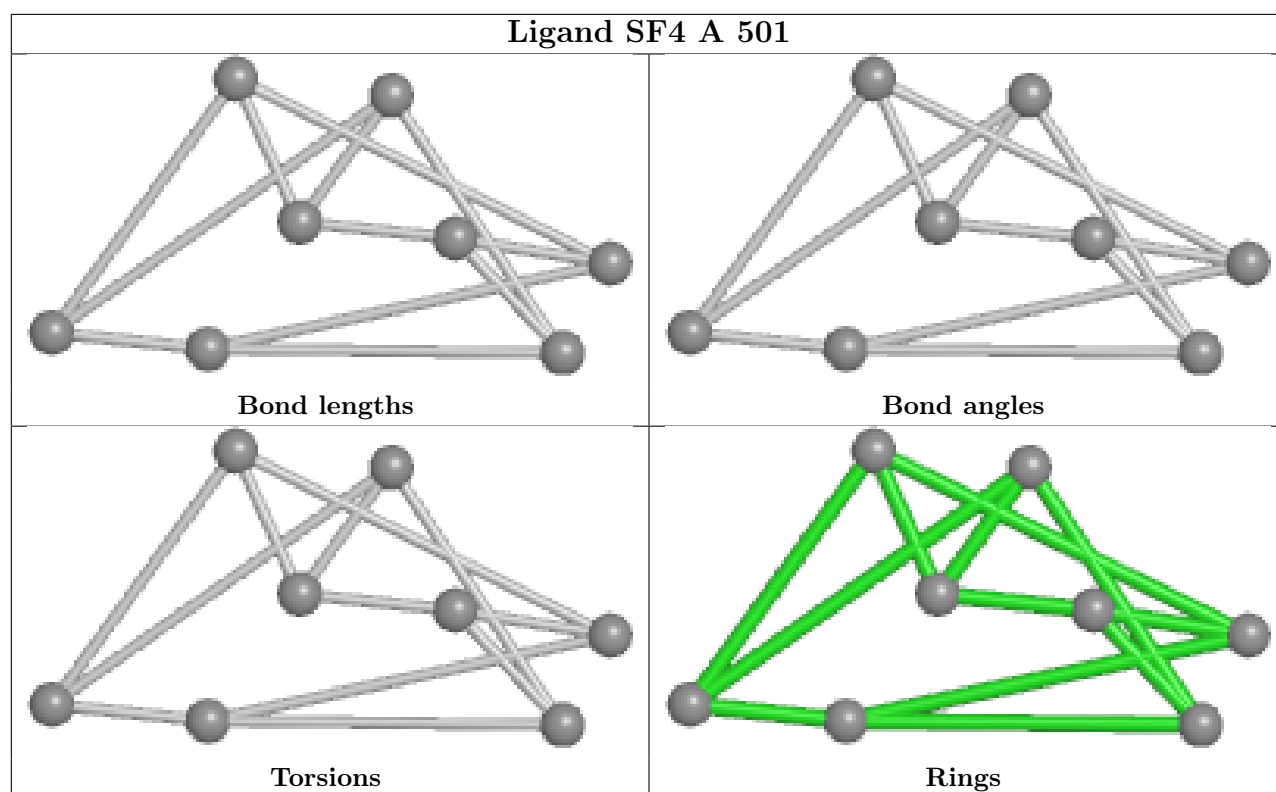


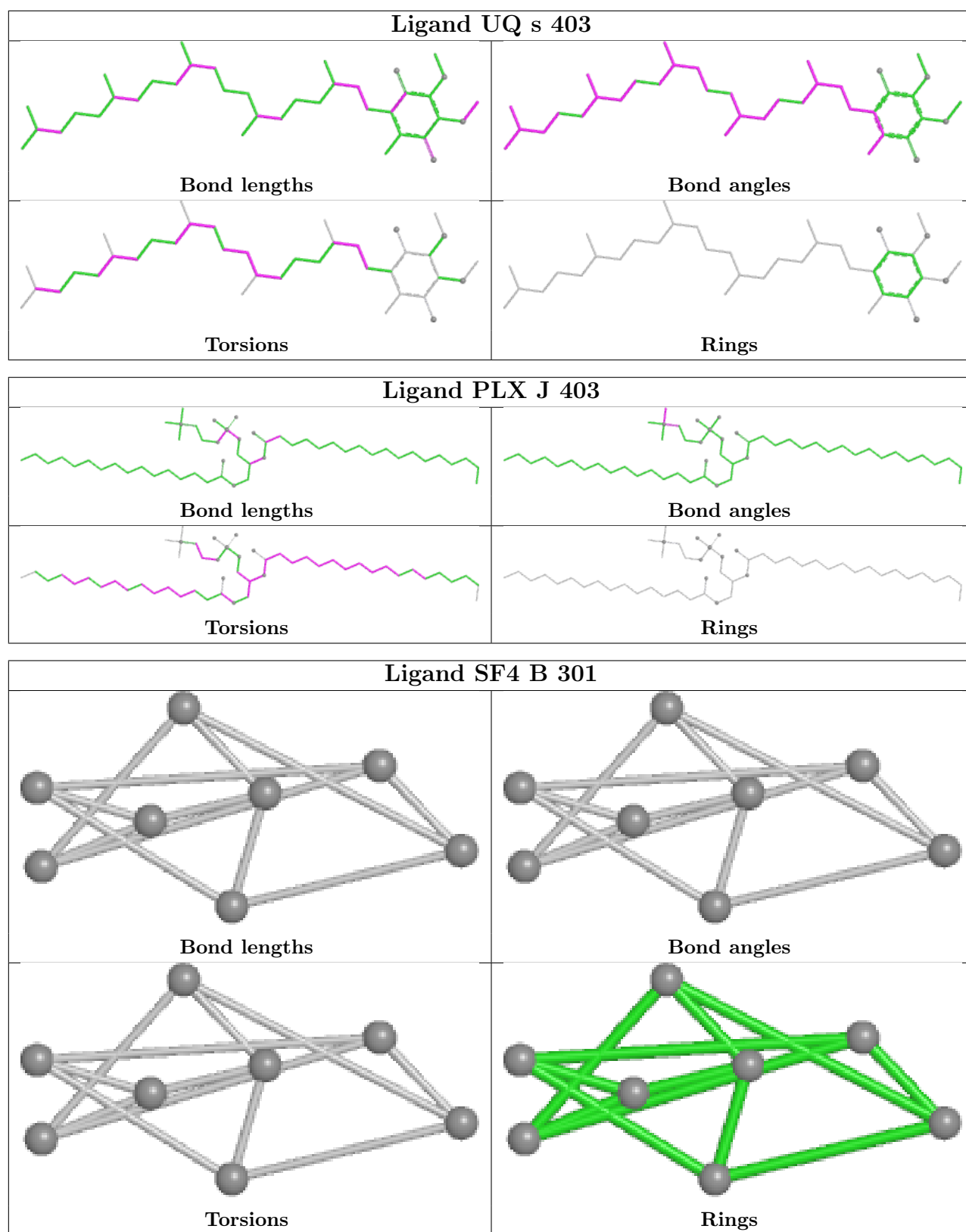


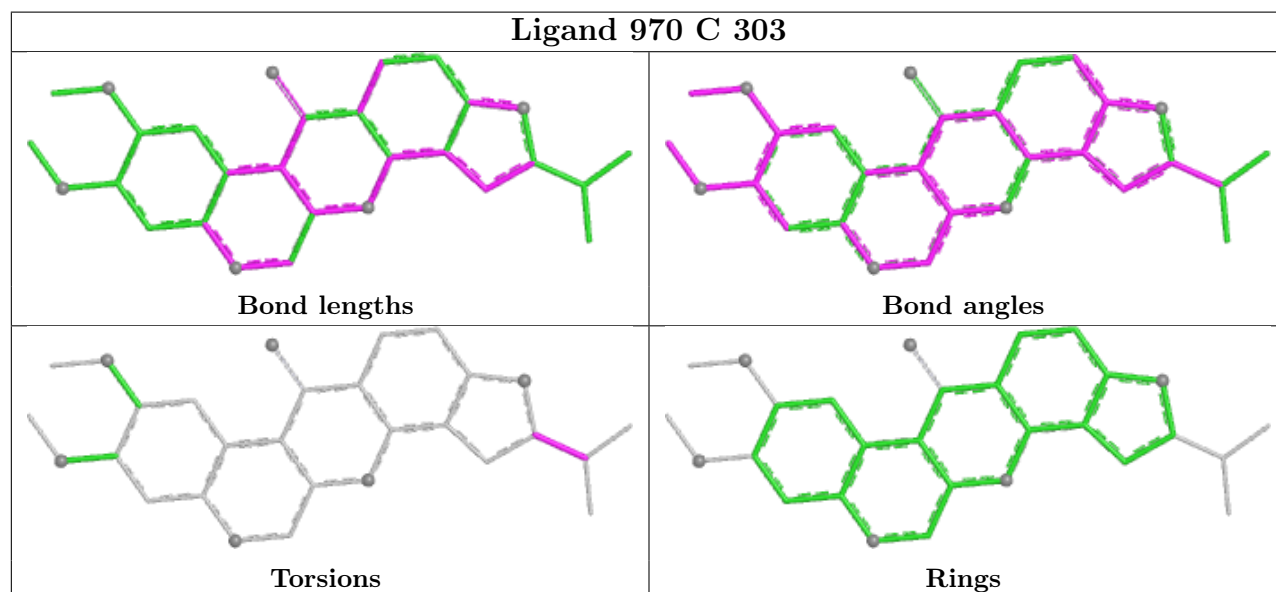
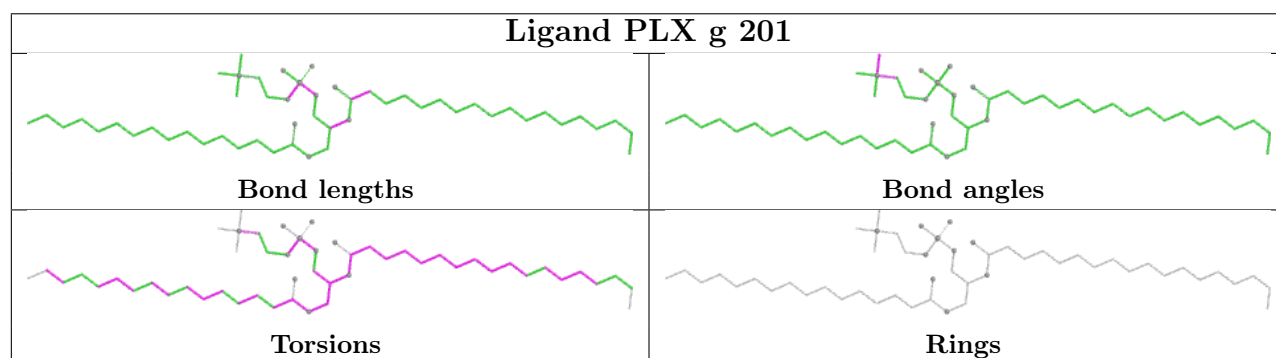
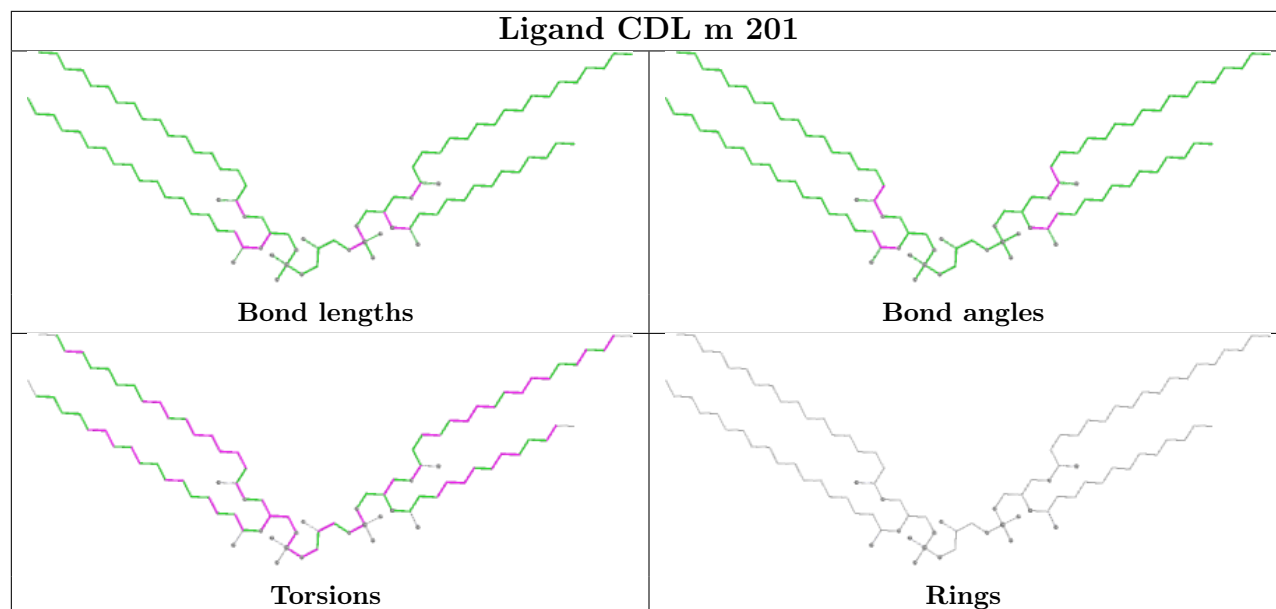


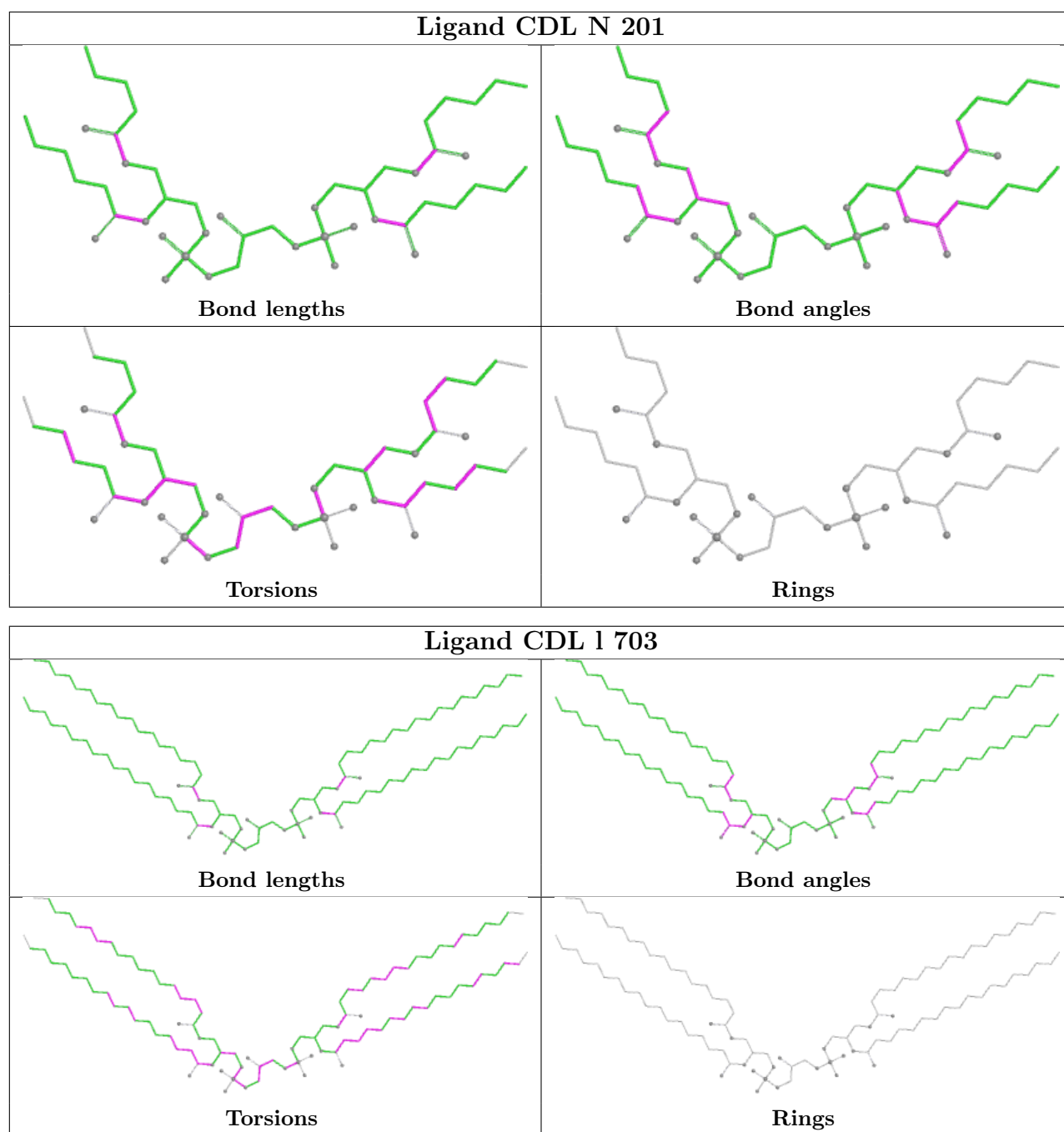


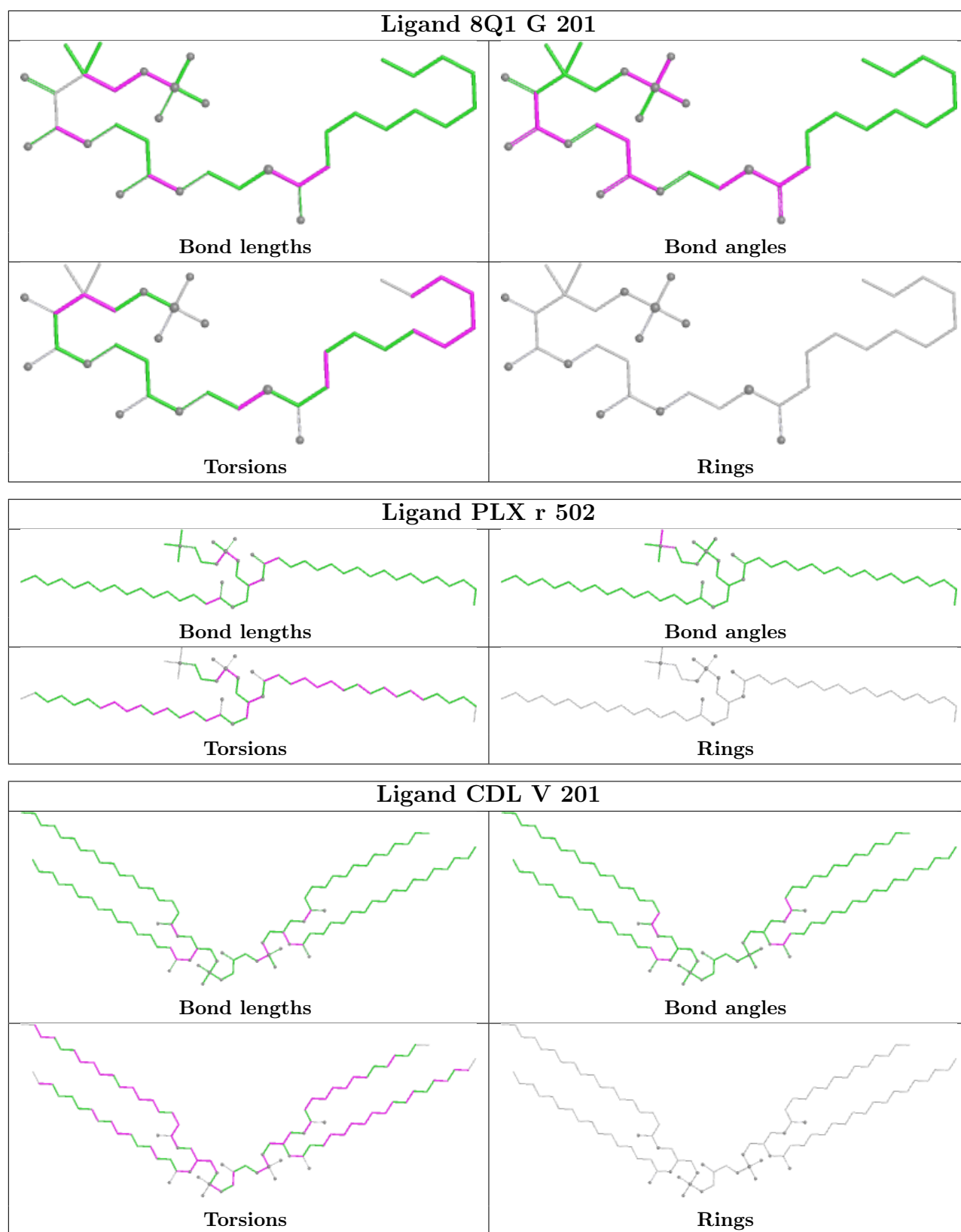


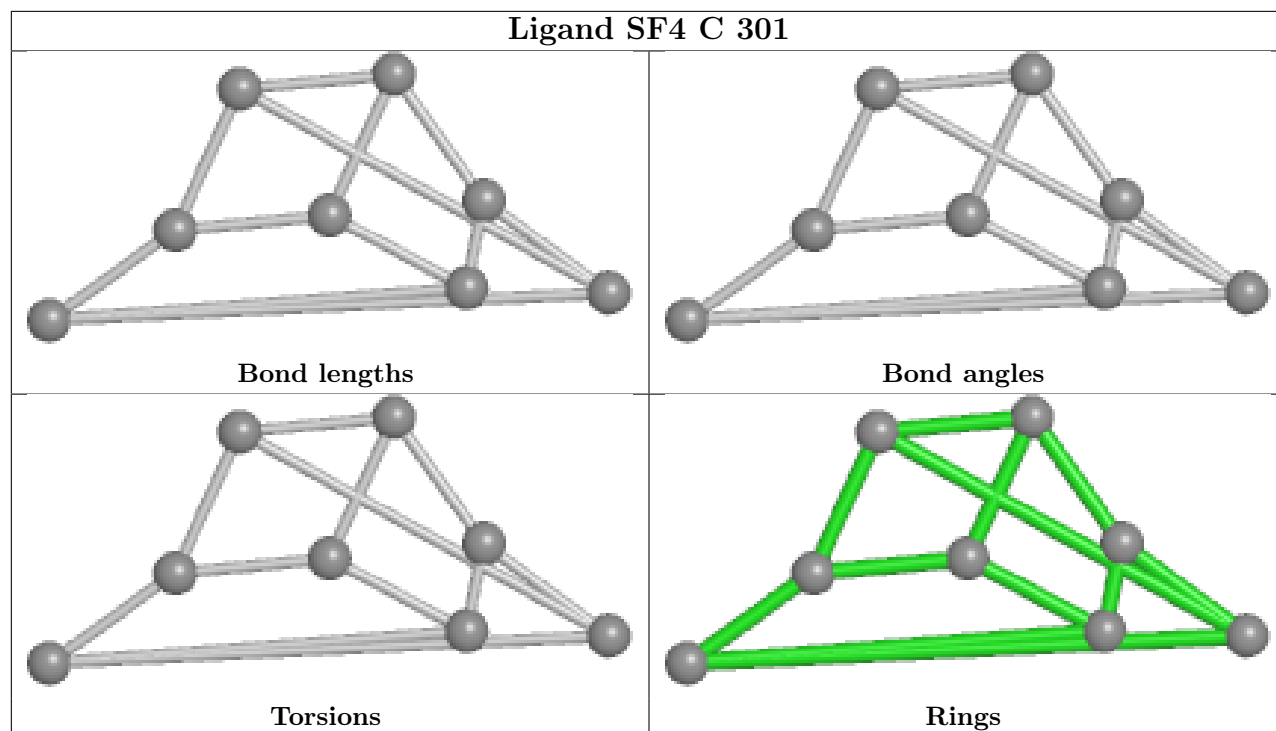












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

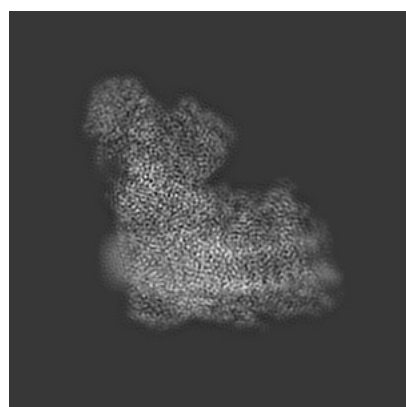
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31649. These allow visual inspection of the internal detail of the map and identification of artifacts.

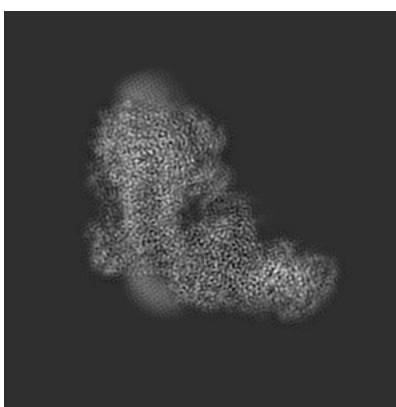
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

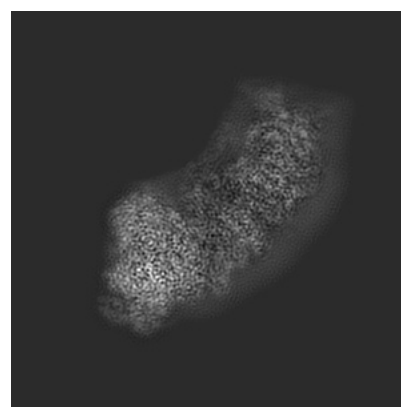
6.1.1 Primary map



X



Y

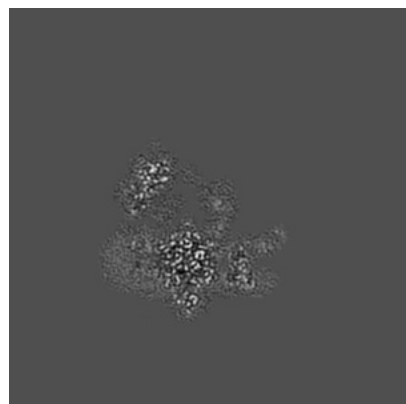


Z

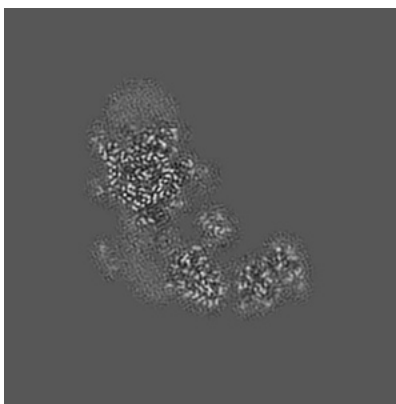
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

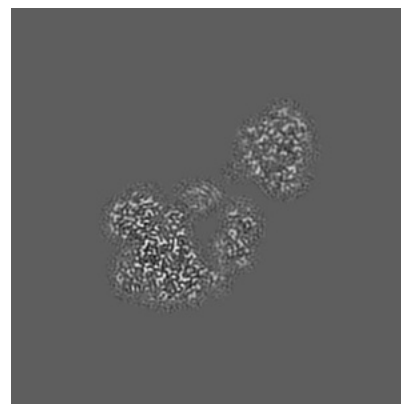
6.2.1 Primary map



X Index: 155



Y Index: 155



Z Index: 155

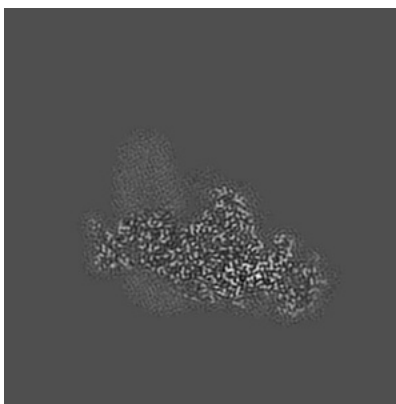
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

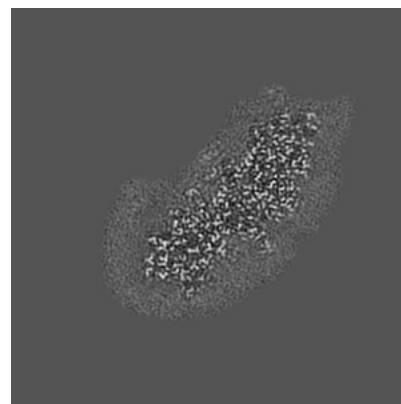
6.3.1 Primary map



X Index: 108



Y Index: 106

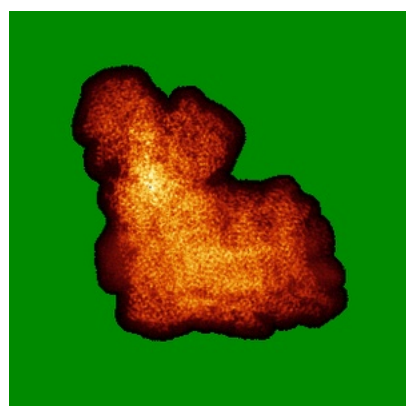


Z Index: 123

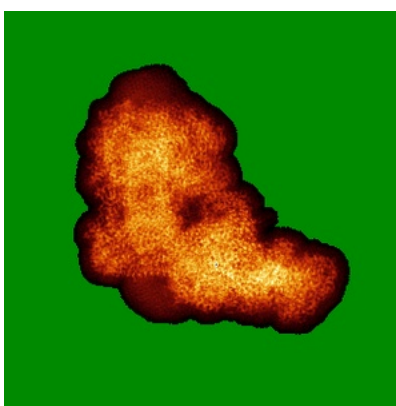
The images above show the largest variance slices of the map in three orthogonal directions.

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

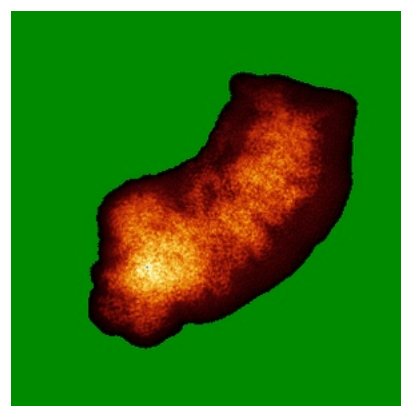
6.4.1 Primary map



X



Y

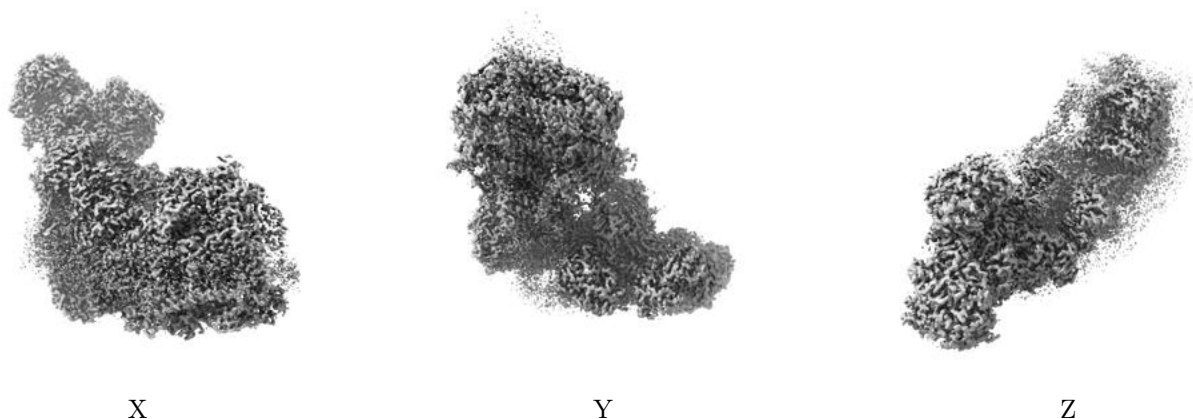


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0257. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

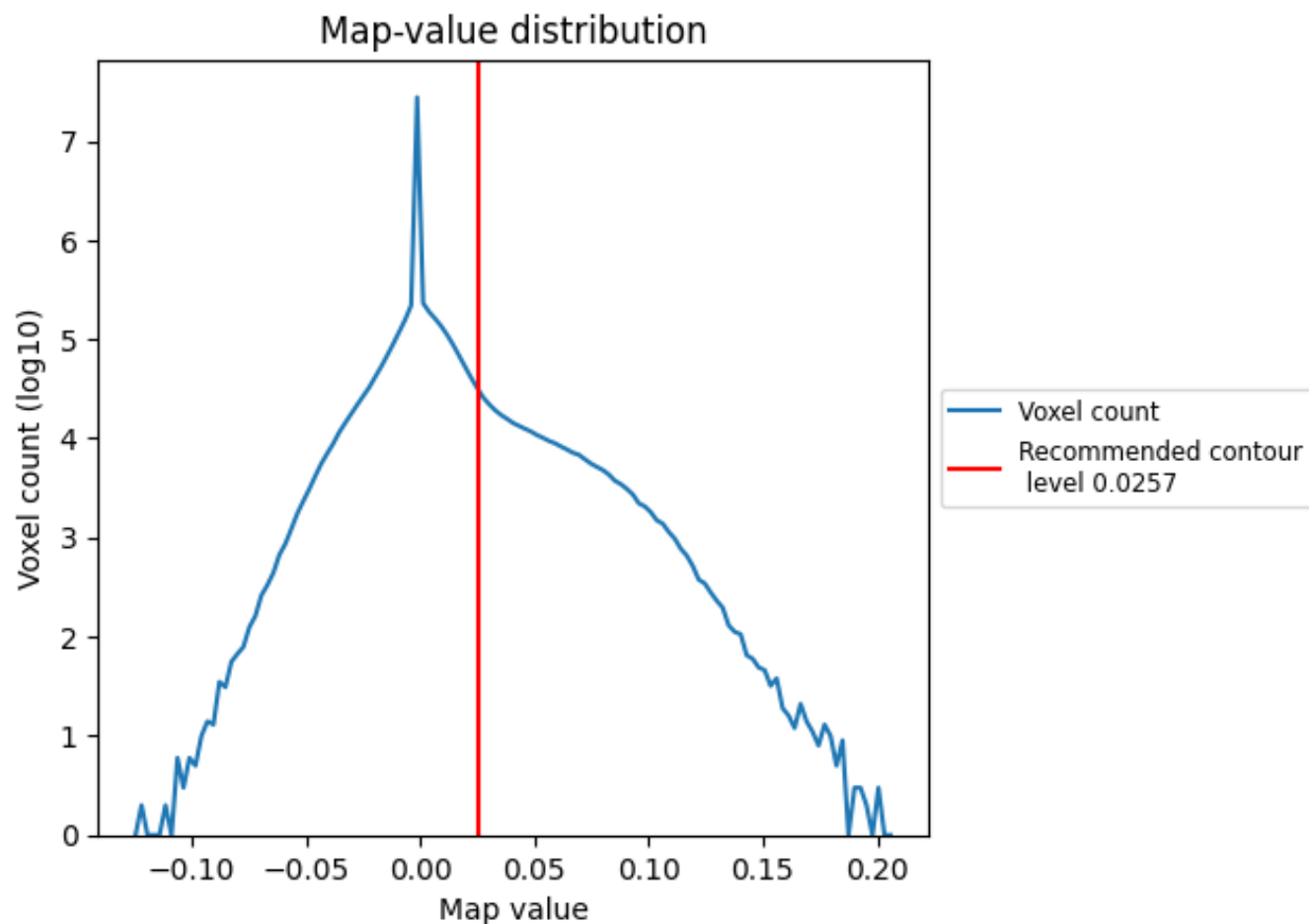
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

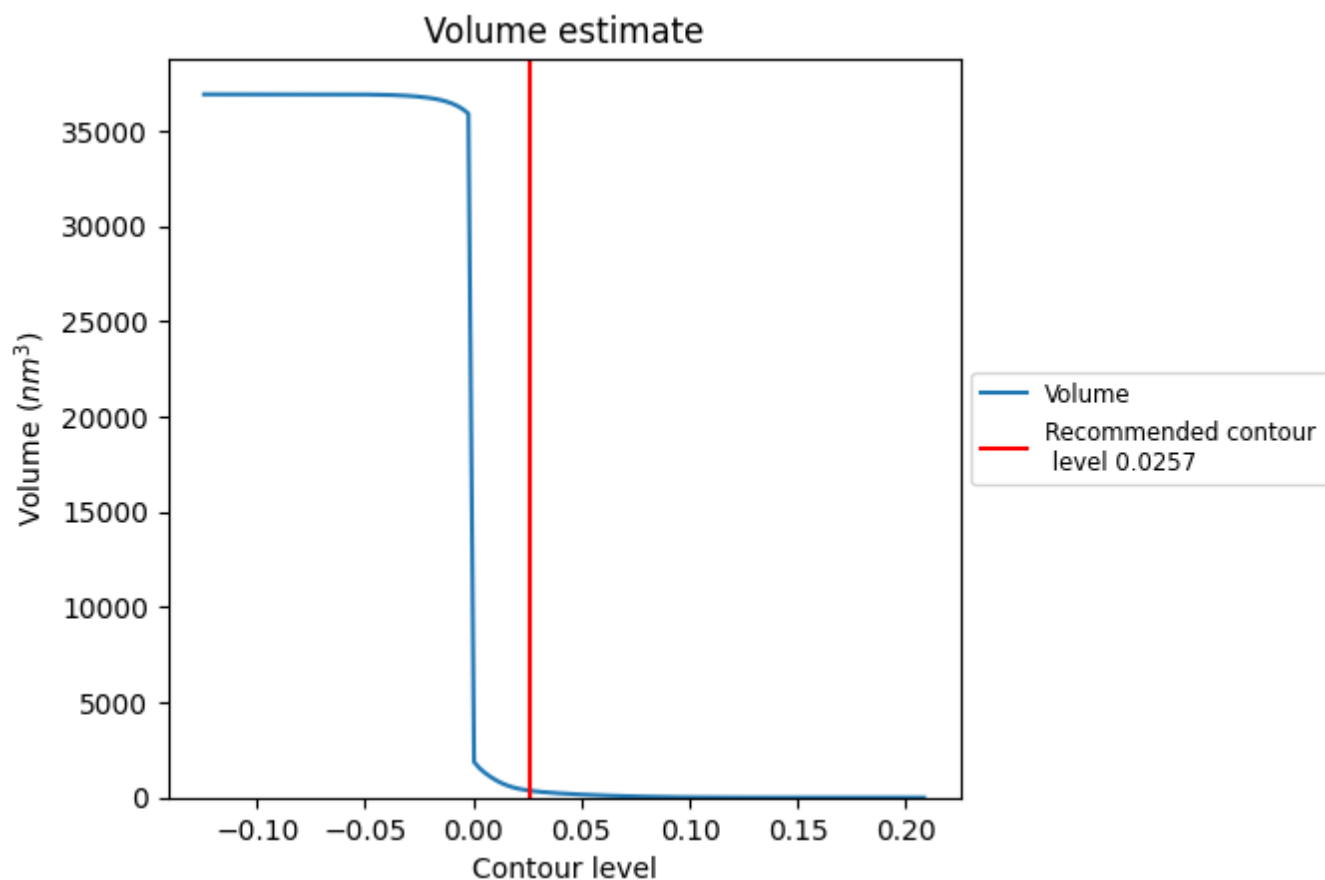
This section contains the results of statistical analysis of the map.

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.

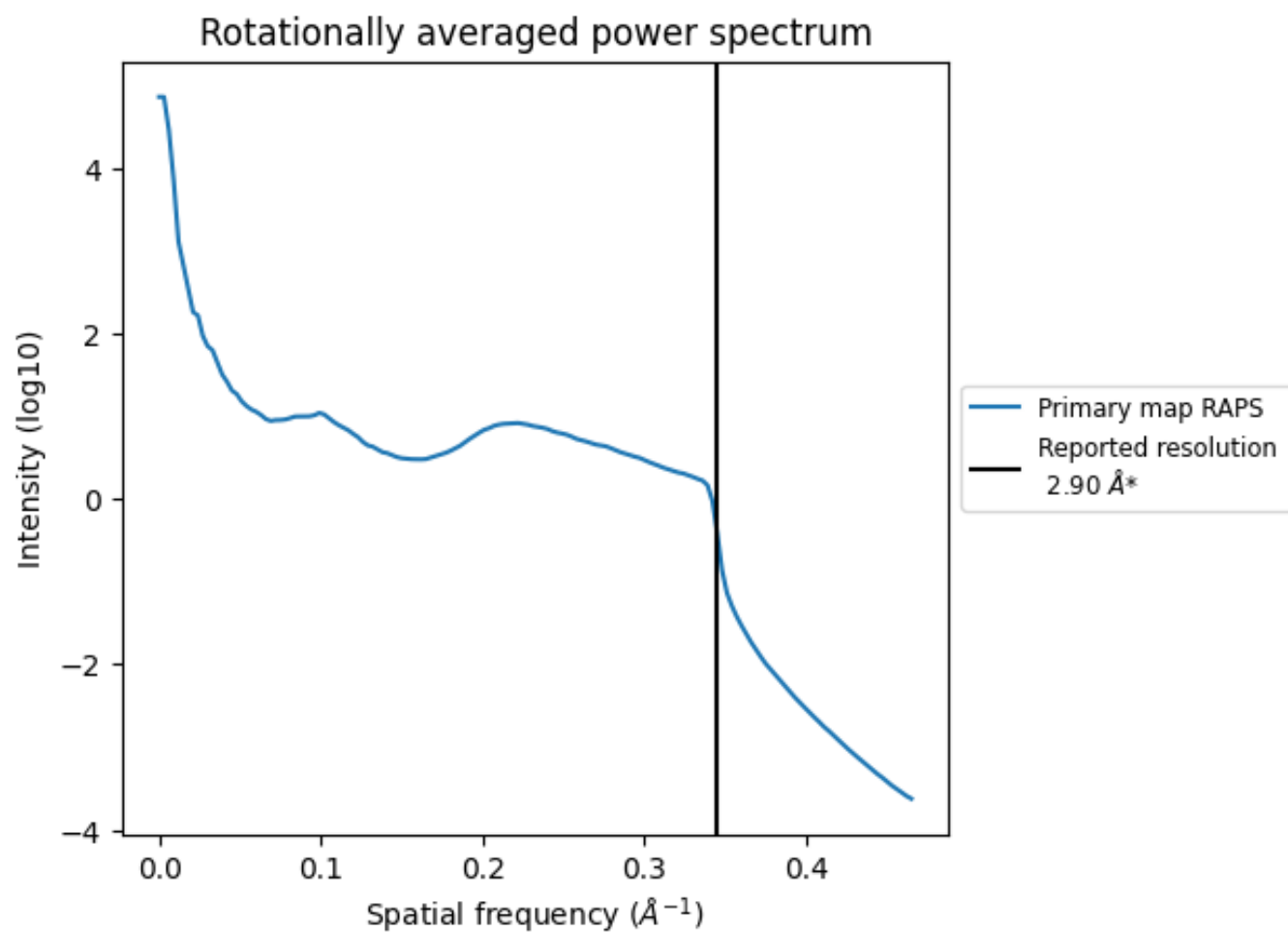
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 370 nm³; this corresponds to an approximate mass of 334 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

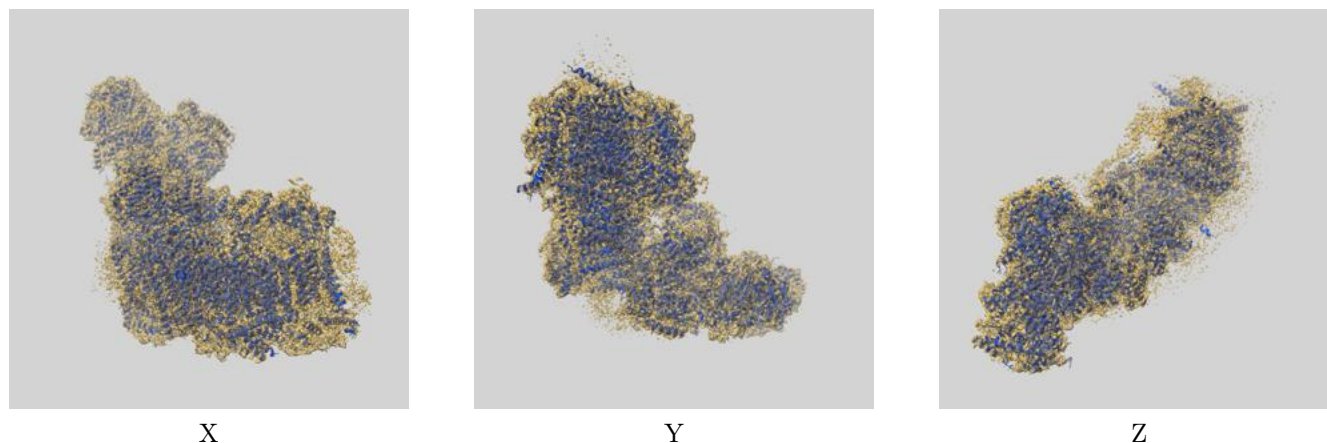
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

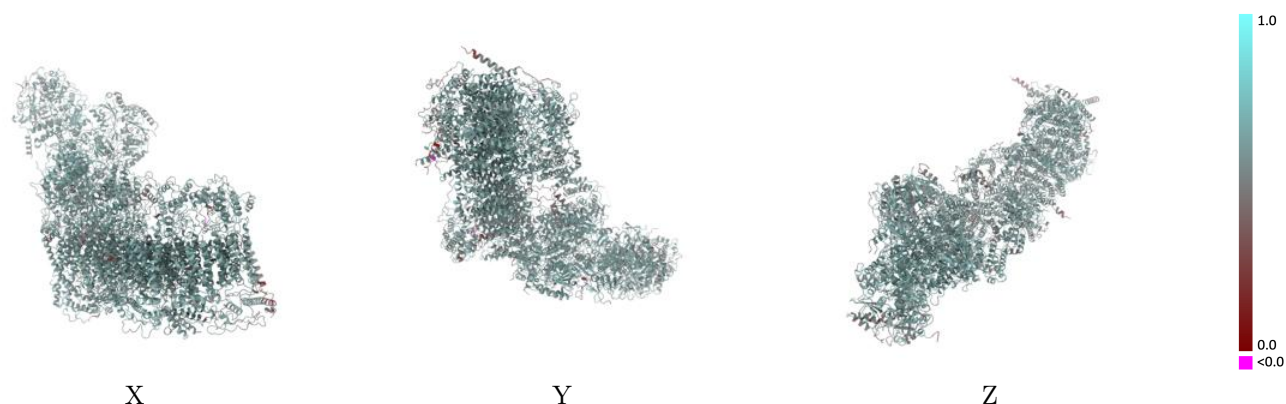
This section contains information regarding the fit between EMDB map EMD-31649 and PDB model 7V31. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0257 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](#)

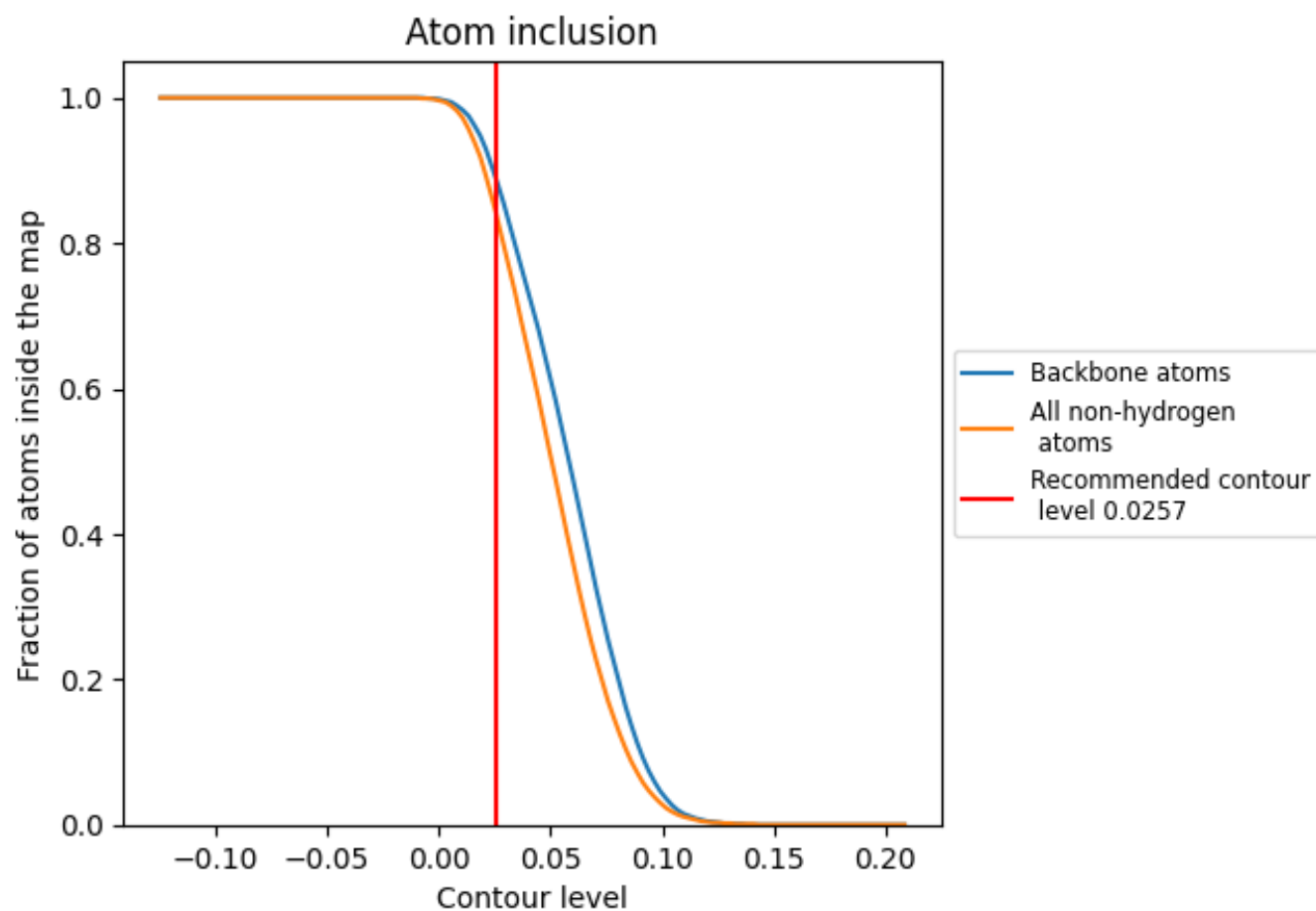


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% 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 (0.0257) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8410	 0.5920
A	 0.8360	 0.5820
B	 0.9380	 0.6330
C	 0.9290	 0.6280
E	 0.8440	 0.5970
F	 0.7310	 0.5350
G	 0.6410	 0.4910
H	 0.8430	 0.5900
I	 0.8070	 0.5760
J	 0.8540	 0.5950
K	 0.6310	 0.5230
L	 0.8580	 0.6080
M	 0.8750	 0.6010
N	 0.7990	 0.5910
O	 0.7780	 0.5600
P	 0.9420	 0.6340
Q	 0.9100	 0.6240
S	 0.8930	 0.6060
T	 0.7640	 0.5790
U	 0.8130	 0.5810
V	 0.7460	 0.5750
W	 0.8500	 0.5880
X	 0.7710	 0.5600
Y	 0.7190	 0.5300
Z	 0.6770	 0.5180
a	 0.8480	 0.6070
b	 0.7440	 0.5470
c	 0.8230	 0.5830
d	 0.7820	 0.5730
e	 0.8010	 0.5790
f	 0.6460	 0.5090
g	 0.8550	 0.6000
h	 0.8360	 0.5820
i	 0.9290	 0.6230
j	 0.8470	 0.6110



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Chain	Atom inclusion	Q-score
k	 0.8930	 0.6160
l	 0.8520	 0.6020
m	 0.7590	 0.5550
n	 0.7110	 0.5450
o	 0.8020	 0.5770
p	 0.8290	 0.5910
r	 0.8880	 0.6160
s	 0.8870	 0.6150
u	 0.8490	 0.5850
v	 0.7290	 0.5270
w	 0.8040	 0.5760