



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 04:24 AM UTC

PDB ID : 7W4C / pdb_00007w4c
EMDB ID : EMD-32300
Title : Active state CI from Q1-NADH dataset, Subclass 1
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-27
Resolution : 2.70 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:

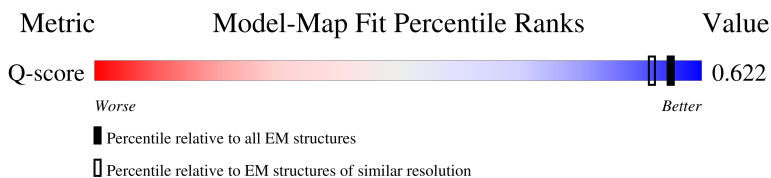
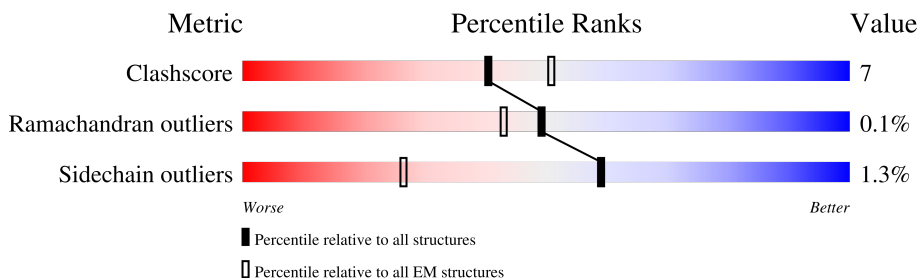
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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 2.70 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	10327 (2.20 - 3.20)

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	 80% 19% .
2	B	176	 89% 10% .
3	C	156	 80% 20%
4	E	115	 86% 12% .

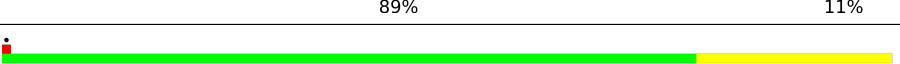
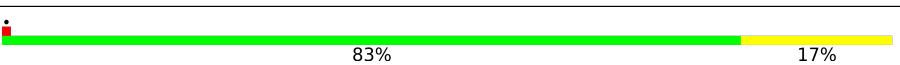
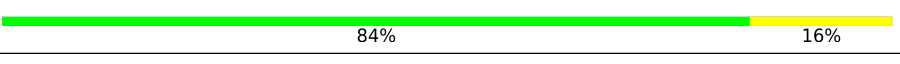
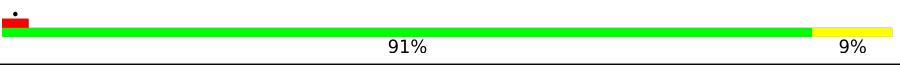
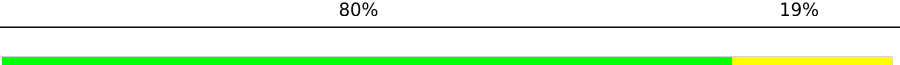
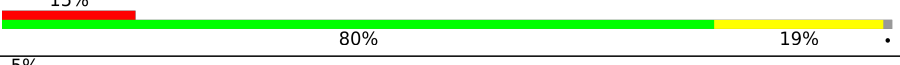
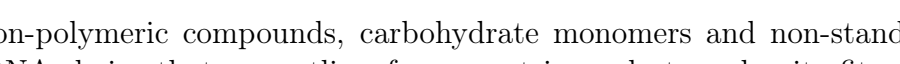
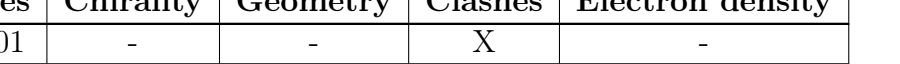
Continued on next page...

Continued from previous page...

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	70	
23	Z	84	
24	a	140	
25	b	126	
26	c	156	
27	d	175	
28	e	107	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	f	49	
30	g	122	
31	h	105	
32	i	347	
33	j	115	
34	k	98	
35	l	606	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	125	
44	w	320	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	A	501	-	-	X	-
53	CDL	l	702	-	-	X	-

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 68216 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
			703	453	104	141	5		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	690	Total	C	N	O	S	0	0
			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
			1657	1054	280	313	10		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a protein called Complex I-AGGG.

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 Complex I-B12.

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 Complex I-SGDH.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	156	Total	C	N	O	S	0	0
			1307	849	213	237	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
			378	246	65	67		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	105	Total	C	N	O	S	0	0
			863	548	161	148	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	S	0	0
			1058	689	182	187			

- 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
			3624	2406	572	608	38		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	318	Total	C	N	O	S	0	0
			2507	1678	385	423	21		

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

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

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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

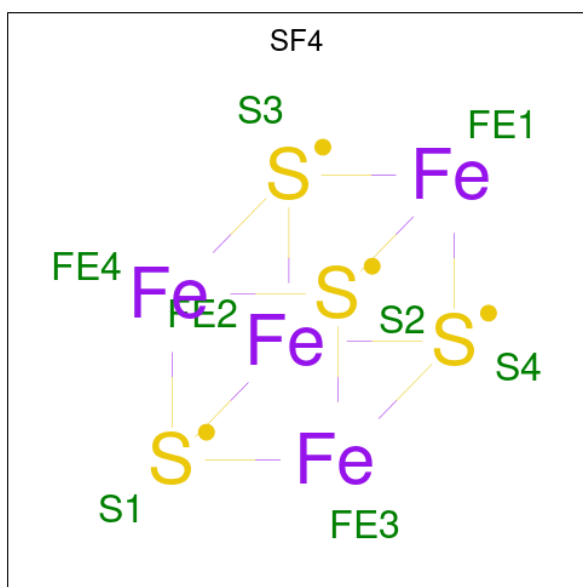
There is a discrepancy between the modelled and reference sequences:

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

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

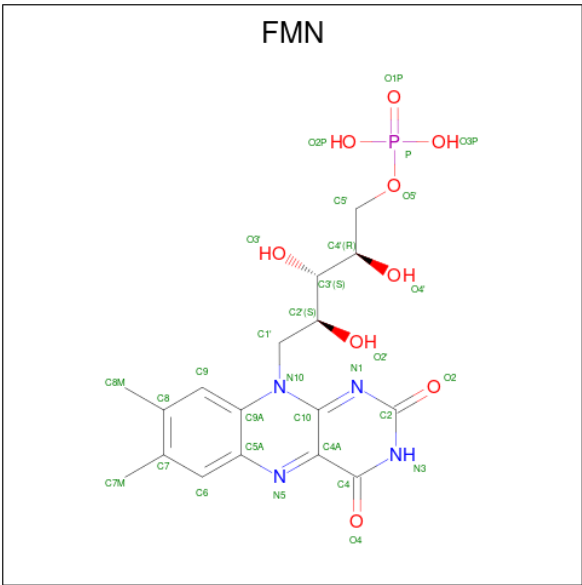
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2582	1643	438	491	10		

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



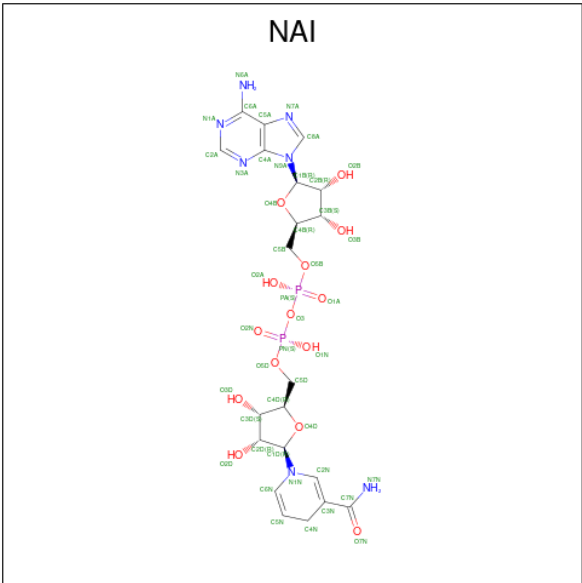
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



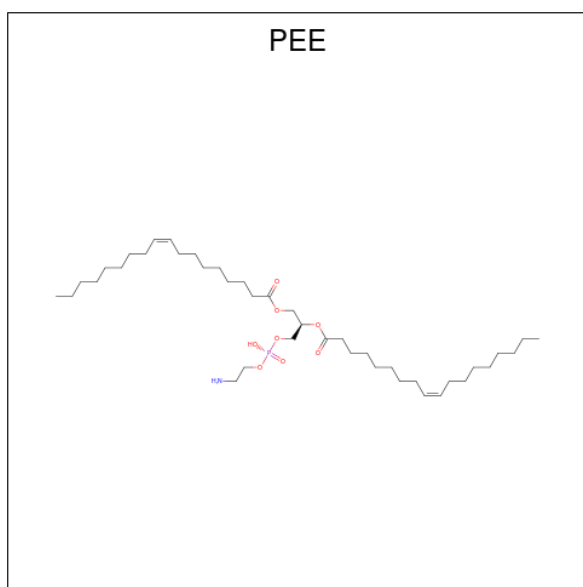
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

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



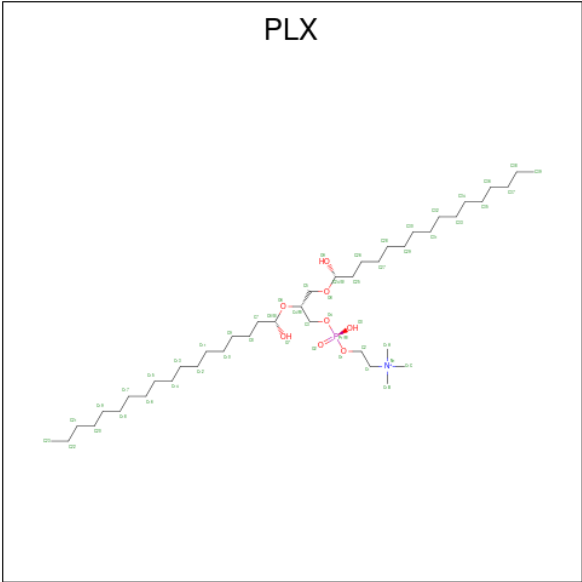
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

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



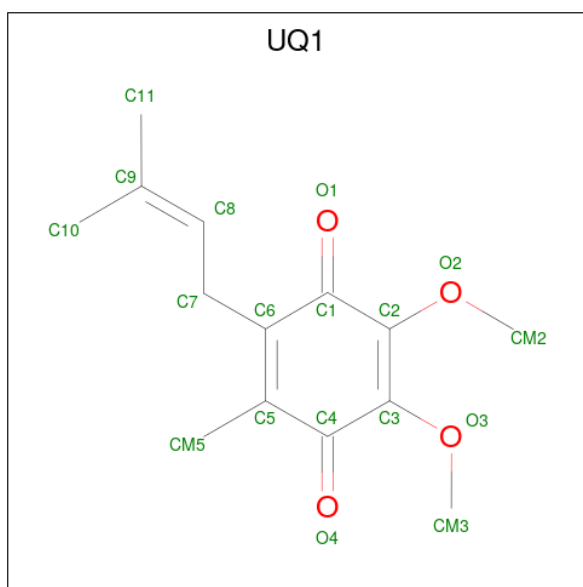
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	V	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	l	1	Total	C	N	O	P	0
			40	30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

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



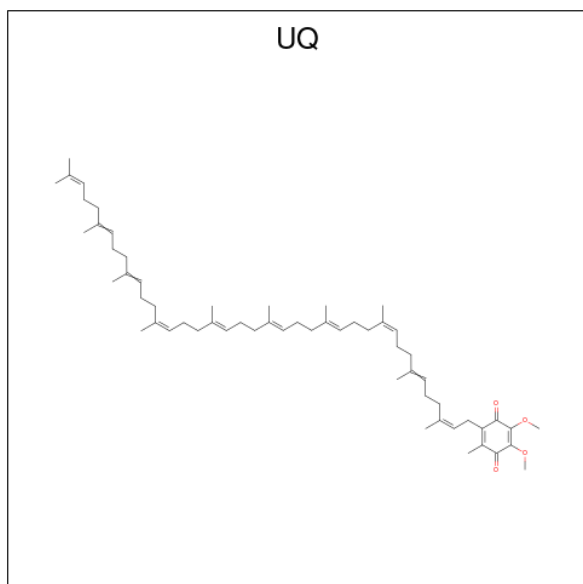
Mol	Chain	Residues	Atoms					AltConf
49	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	J	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	e	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42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

- Molecule 50 is UBIQUINONE-1 (CCD ID: UQ1) (formula: C₁₄H₁₈O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
50	C	1	Total	C	O	0
			18	14	4	
50	Q	1	Total	C	O	0
			18	14	4	

- Molecule 51 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



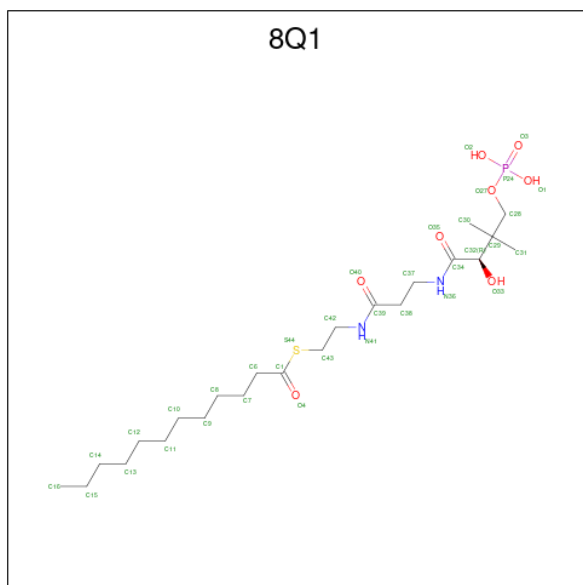
Mol	Chain	Residues	Atoms			AltConf
51	C	1	Total	C	O	0
			38	34	4	

Continued on next page...

Continued from previous page...

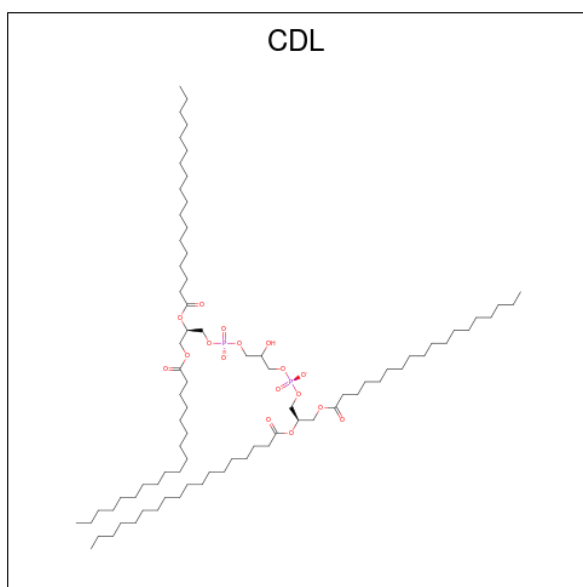
Mol	Chain	Residues	Atoms			AltConf
51	J	1	Total	C	O	0
			33	29	4	

- Molecule 52 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 53 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 54 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).

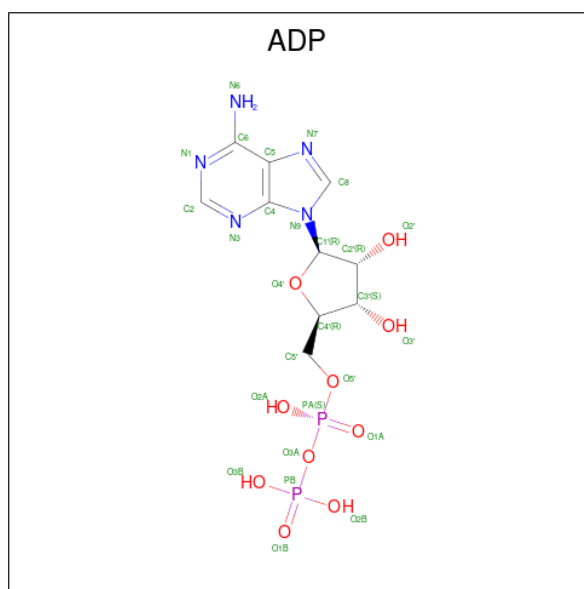
- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

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

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

- Molecule 58 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

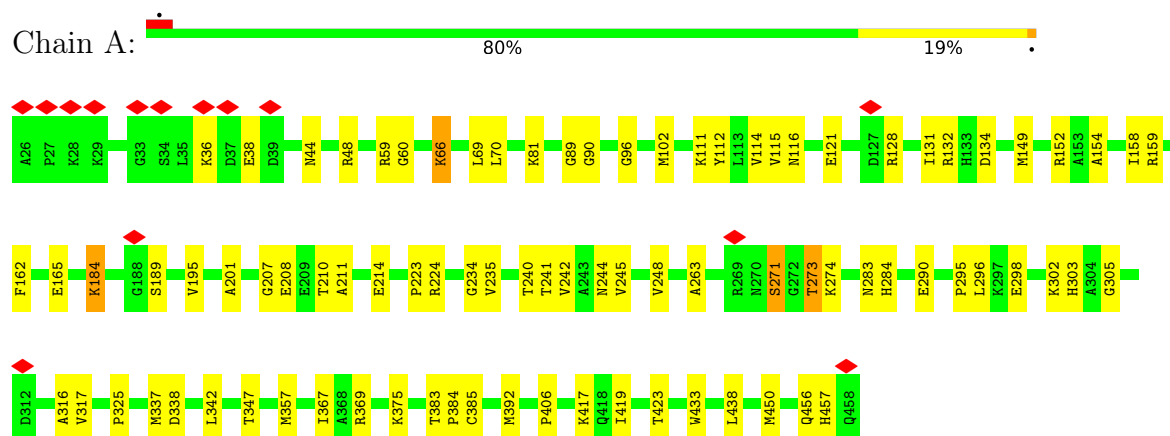


Mol	Chain	Residues	Atoms					AltConf
58	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

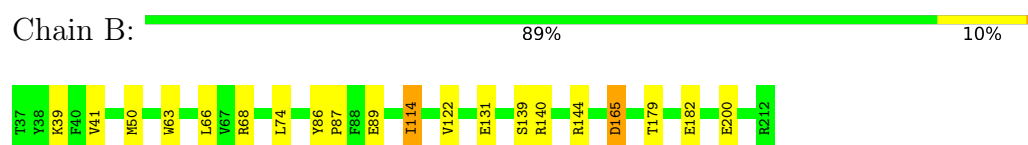
3 Residue-property plots

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

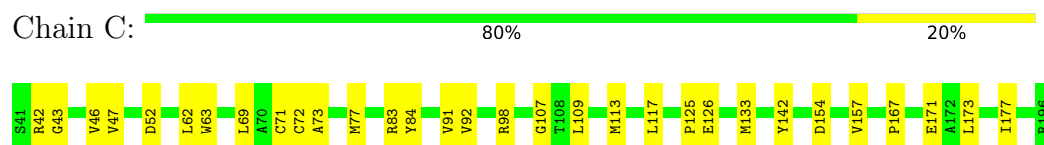
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



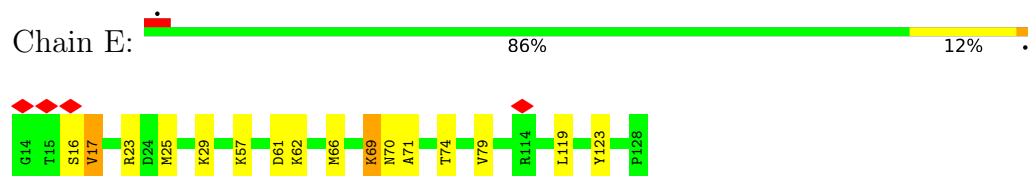
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



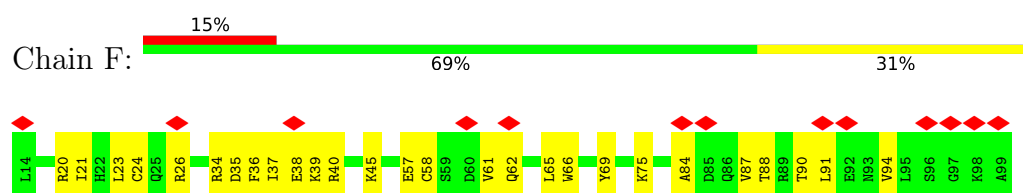
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



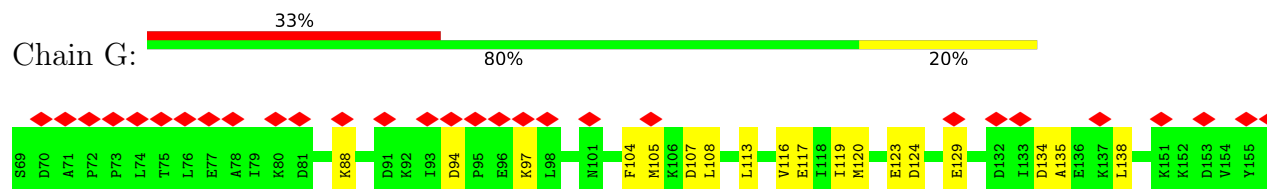
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



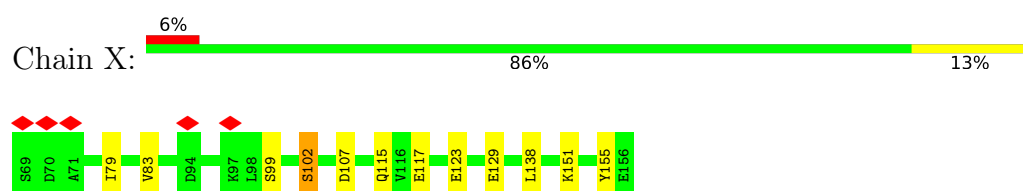
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



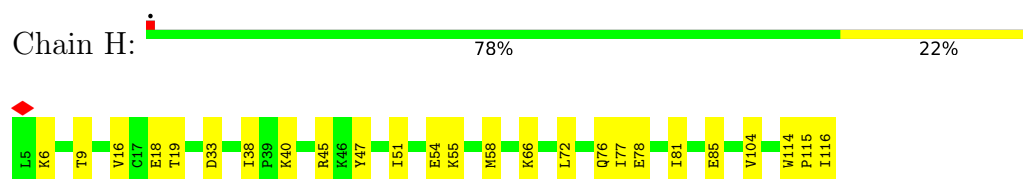
- Molecule 6: Acyl carrier protein



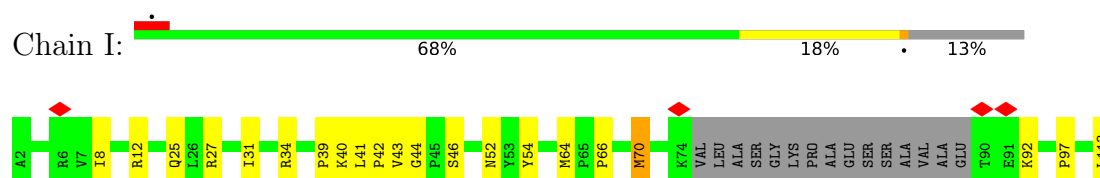
- Molecule 6: Acyl carrier protein



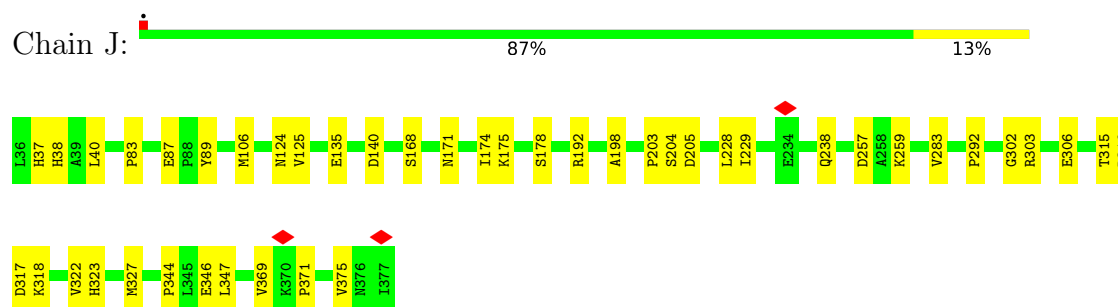
- Molecule 7: Complex I subunit B13



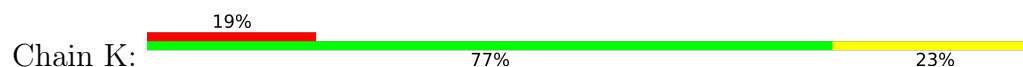
- Molecule 8: Complex I-B14.5a



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

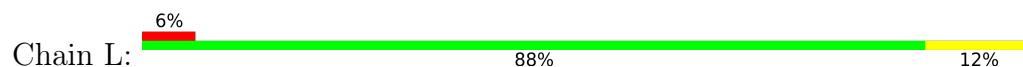


- Molecule 10: Complex I-9kD

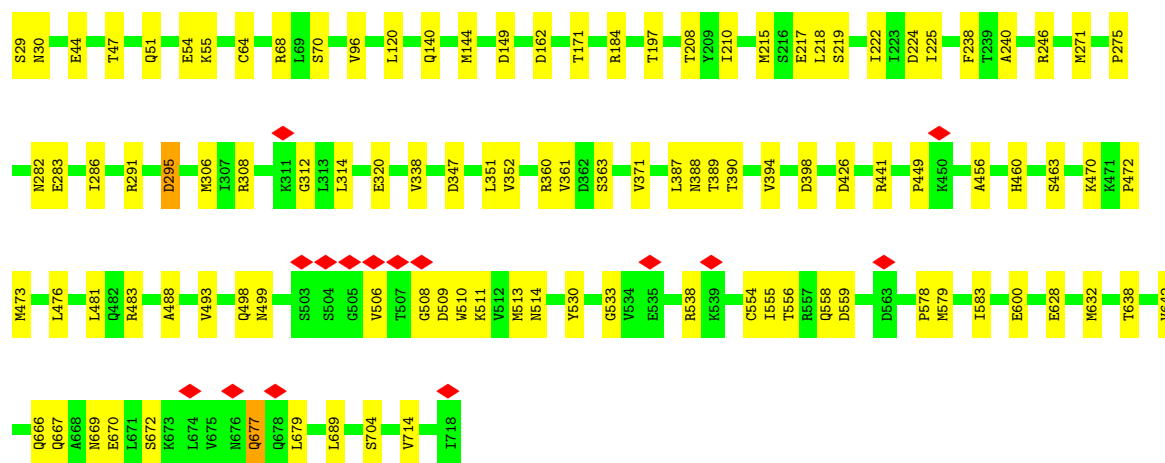
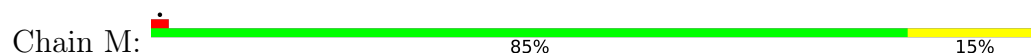




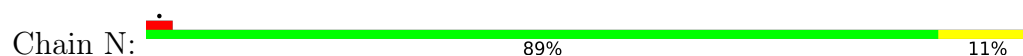
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



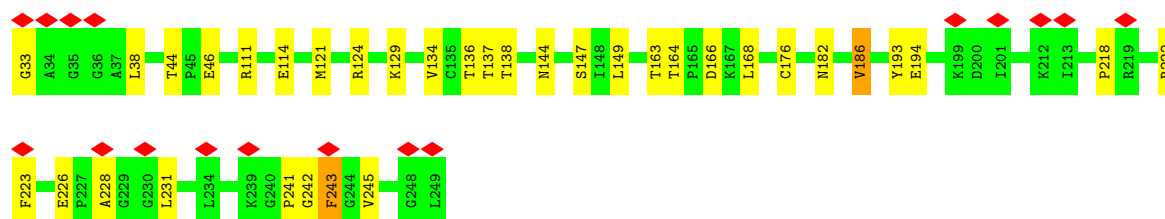
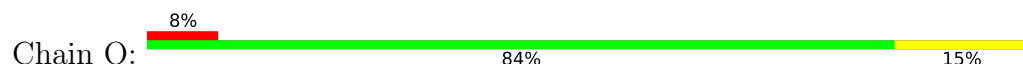
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



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



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



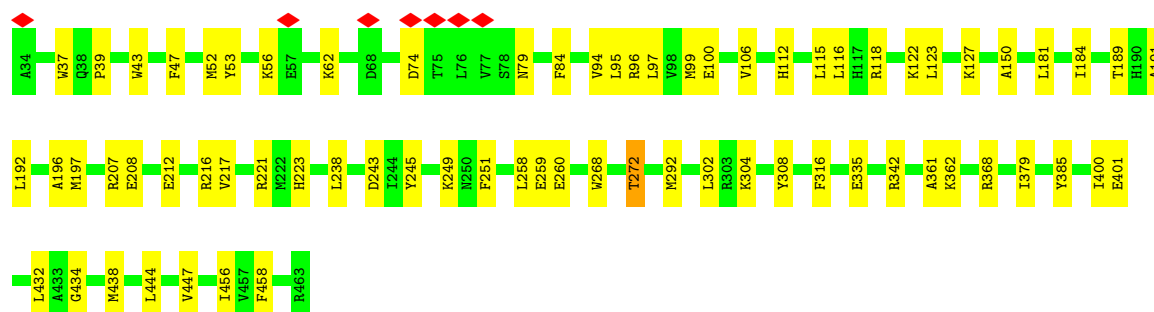
- Molecule 15: Complex I-30kD

Chain P:  87% 13%



- Molecule 16: Complex I-49kD

Chain Q:  83% 16%



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

Chain S:  84% 16%



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

Chain T:  6% 93% 7%



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

Chain U:  5% 83% 16%

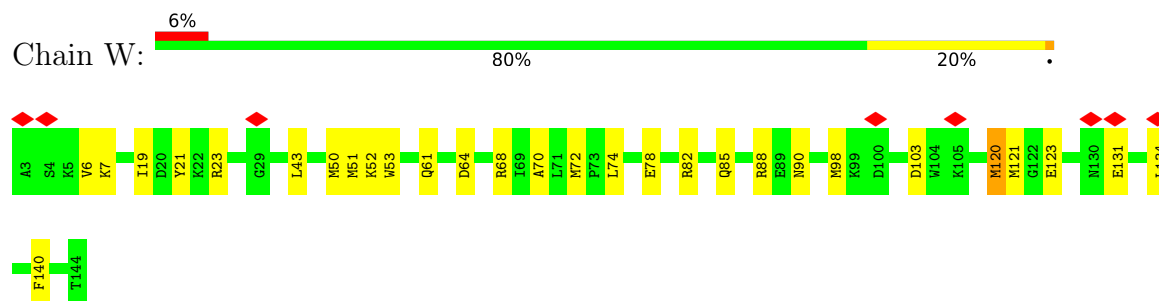


- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

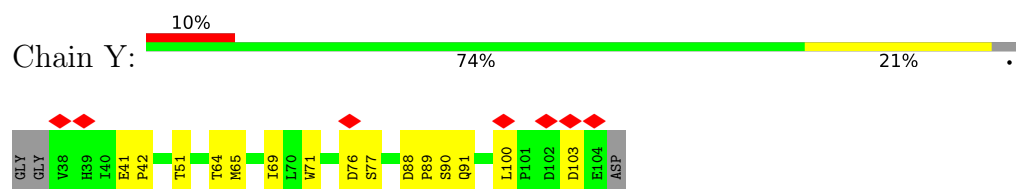
Chain V:  81% 19%



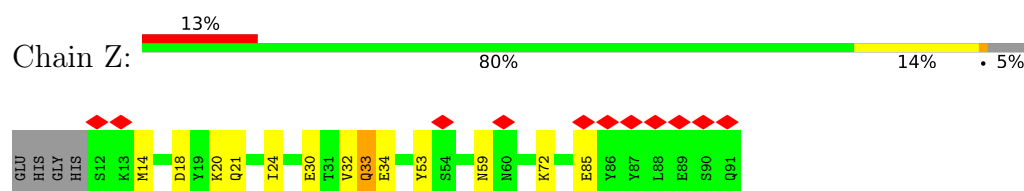
- Molecule 21: Complex I-B16.6



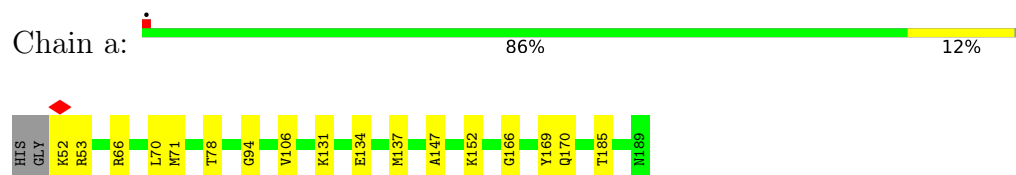
- Molecule 22: Complex I-AGGG



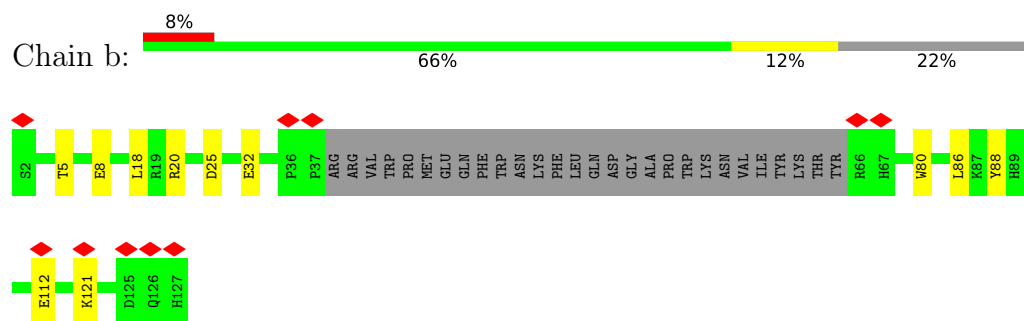
- Molecule 23: Complex I-B12



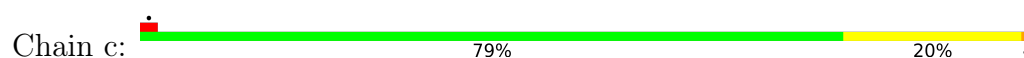
- Molecule 24: Complex I-SGDH

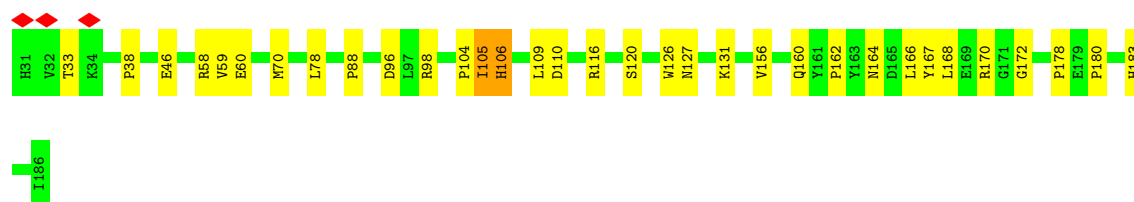


- Molecule 25: Complex I-B17

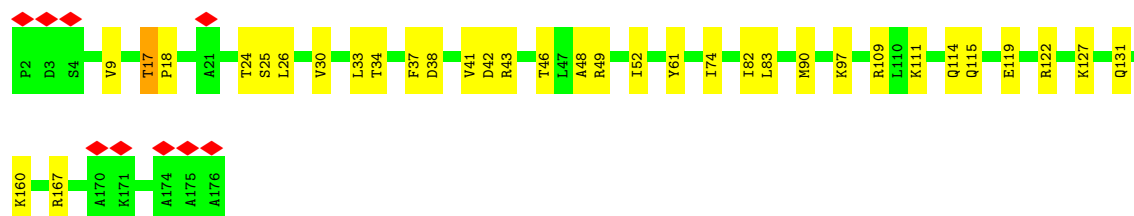
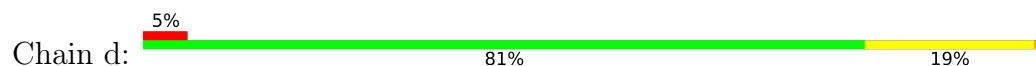


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

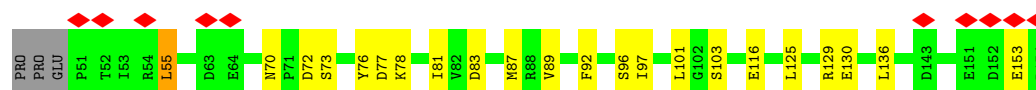
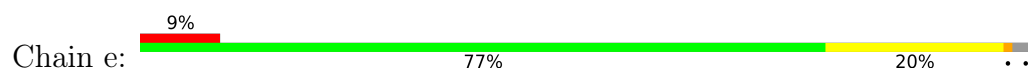




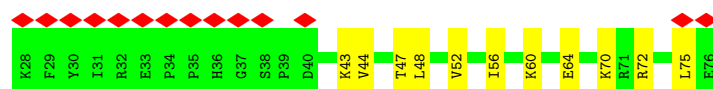
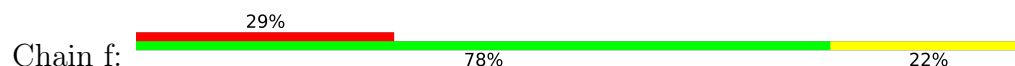
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



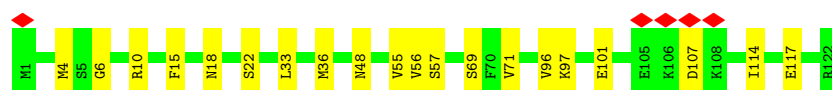
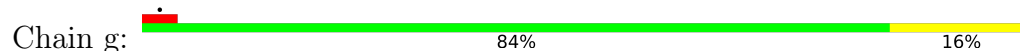
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



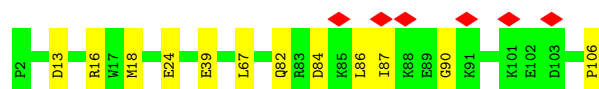
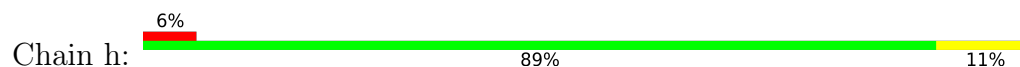
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



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

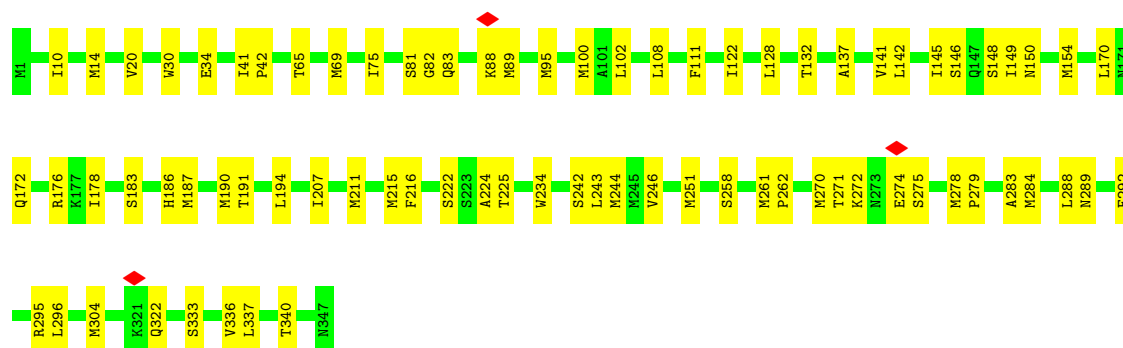


- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain i:  78% 22%



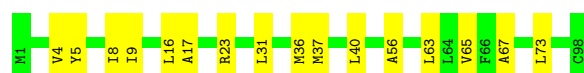
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j:  83% 17%



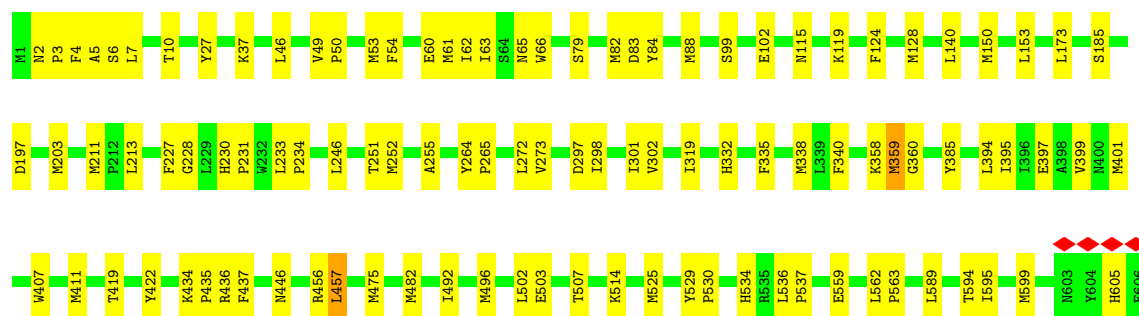
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain k:  84% 16%



- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l:  83% 17%



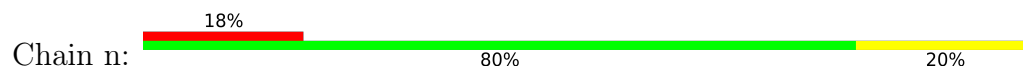
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain m:  15% 82% 17%

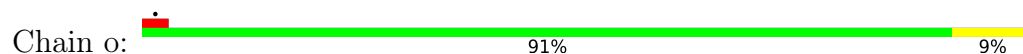




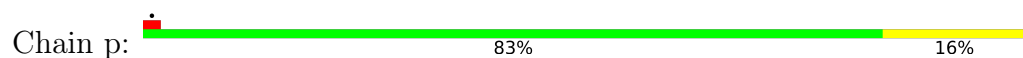
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



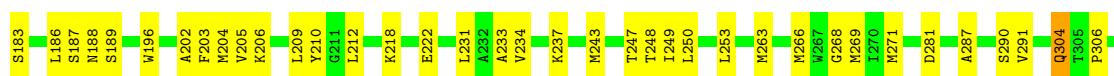
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



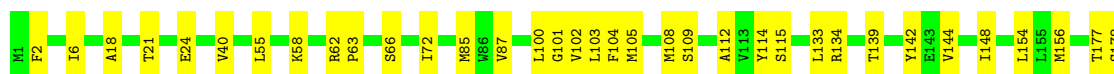
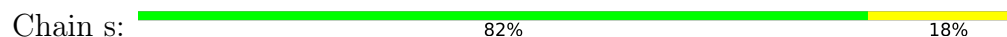
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

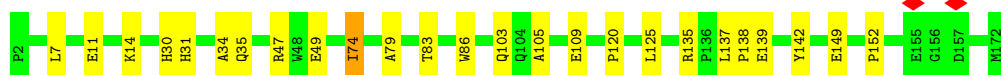


- Molecule 41: NADH-ubiquinone oxidoreductase chain 1



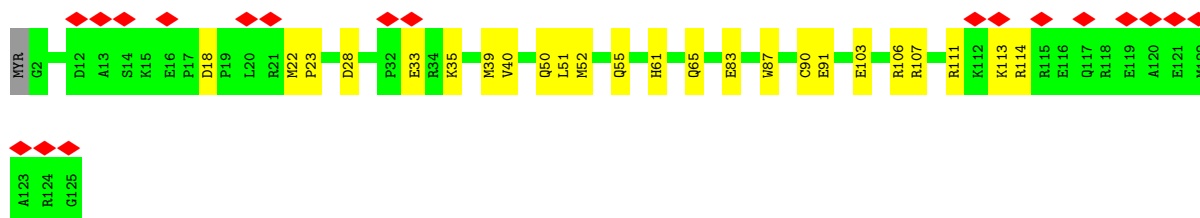
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:  85% 14%



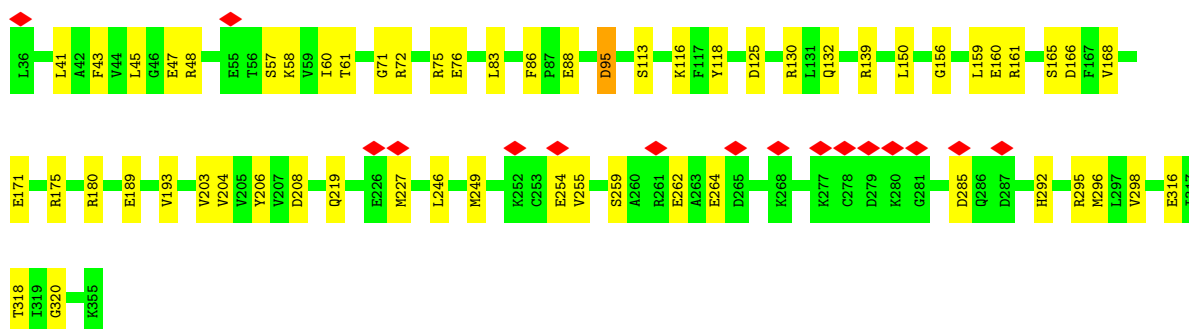
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v:  15% 80% 19%



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

Chain w:  5% 82% 18%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92672	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	0.218	Depositor
Minimum map value	-0.121	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0302	Depositor
Map size (Å)	333.7616, 333.7616, 333.7616	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, SF4, PLX, ADP, NDP, UQ1, UQ, FES, PEE, 2MR, ZN, CDL, 8Q1, MG, NAI

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.12	0/3406	0.31	0/4603
2	B	0.12	0/1443	0.31	0/1952
3	C	0.12	0/1279	0.30	0/1730
4	E	0.16	0/995	0.33	0/1340
5	F	0.14	0/698	0.42	0/940
6	G	0.13	0/705	0.39	0/956
6	X	0.11	0/715	0.32	0/967
7	H	0.15	0/929	0.38	0/1258
8	I	0.15	0/798	0.42	1/1079 (0.1%)
9	J	0.11	0/2828	0.31	0/3834
10	K	0.14	0/377	0.36	0/509
11	L	0.11	0/1039	0.29	0/1403
12	M	0.13	0/5384	0.36	2/7295 (0.0%)
13	N	0.11	0/1245	0.30	0/1694
14	O	0.13	0/1696	0.36	0/2310
15	P	0.13	0/1789	0.33	0/2436
16	Q	0.14	0/3538	0.34	0/4796
17	S	0.14	0/581	0.38	0/781
18	T	0.12	0/755	0.32	0/1018
19	U	0.10	0/664	0.28	0/912
20	V	0.11	0/1042	0.24	0/1411
21	W	0.14	0/1192	0.34	0/1610
22	Y	0.20	0/610	0.46	0/836
23	Z	0.10	0/660	0.29	0/892
24	a	0.14	0/1184	0.29	0/1603
25	b	0.14	0/844	0.36	0/1149
26	c	0.19	0/1363	0.61	3/1865 (0.2%)
27	d	0.14	0/1494	0.30	0/2015
28	e	0.11	0/891	0.31	0/1210
29	f	0.11	0/386	0.26	0/523
30	g	0.12	0/1036	0.30	0/1401
31	h	0.12	0/885	0.34	0/1185

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.15	0/2773	0.36	0/3768
33	j	0.13	0/938	0.31	0/1281
34	k	0.15	0/759	0.35	0/1029
35	l	0.15	0/4947	0.36	0/6728
36	m	0.14	0/1325	0.37	0/1800
37	n	0.11	0/491	0.28	0/663
38	o	0.12	0/1088	0.31	0/1476
39	p	0.15	0/1590	0.39	2/2155 (0.1%)
40	r	0.15	0/3715	0.35	0/5067
41	s	0.15	0/2580	0.38	0/3528
42	u	0.13	0/1436	0.33	0/1938
43	v	0.14	0/1052	0.38	0/1411
44	w	0.13	0/2642	0.34	0/3580
All	All	0.14	0/67787	0.35	8/91937 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	105	ILE	N-CA-C	12.53	123.37	110.72
39	p	133	TRP	N-CA-C	6.11	117.94	111.28
8	I	70	MET	CB-CG-SD	5.86	130.27	112.70
26	c	105	ILE	CA-C-N	5.50	132.05	121.54
26	c	105	ILE	C-N-CA	5.50	132.05	121.54
12	M	282	ASN	CA-C-N	5.20	131.48	121.54
12	M	282	ASN	C-N-CA	5.20	131.48	121.54
39	p	132	SER	N-CA-C	5.14	117.78	111.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3330	0	3292	65	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1412	0	1363	19	0
3	C	1248	0	1254	24	0
4	E	971	0	975	21	0
5	F	687	0	700	19	0
6	G	693	0	671	11	0
6	X	703	0	693	8	0
7	H	910	0	950	18	0
8	I	780	0	808	16	0
9	J	2751	0	2773	26	0
10	K	366	0	338	10	0
11	L	1016	0	1016	9	0
12	M	5296	0	5326	69	0
13	N	1204	0	1162	12	0
14	O	1657	0	1651	35	0
15	P	1738	0	1693	18	0
16	Q	3459	0	3396	49	0
17	S	566	0	561	7	0
18	T	741	0	702	5	0
19	U	643	0	642	13	0
20	V	1021	0	1025	21	0
21	W	1161	0	1144	30	0
22	Y	584	0	529	12	0
23	Z	641	0	620	14	0
24	a	1151	0	1164	16	0
25	b	819	0	835	14	0
26	c	1307	0	1200	31	0
27	d	1461	0	1429	28	0
28	e	867	0	817	18	0
29	f	378	0	356	7	0
30	g	1005	0	999	14	0
31	h	863	0	867	9	0
32	i	2710	0	2874	50	0
33	j	914	0	951	16	0
34	k	748	0	799	13	0
35	l	4816	0	4955	71	0
36	m	1292	0	1261	25	0
37	n	479	0	486	9	0
38	o	1058	0	1068	11	0
39	p	1534	0	1470	23	0
40	r	3624	0	3832	63	0
41	s	2507	0	2604	44	0
42	u	1398	0	1374	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	v	1028	0	982	20	0
44	w	2582	0	2531	34	0
45	A	8	0	0	2	0
45	B	16	0	0	0	0
45	C	8	0	0	1	0
45	M	16	0	0	0	0
46	A	31	0	19	3	0
47	A	44	0	27	5	0
48	B	51	0	82	3	0
48	C	47	0	71	2	0
48	U	51	0	82	4	0
48	V	51	0	82	3	0
48	W	41	0	59	1	0
48	i	47	0	71	2	0
48	l	137	0	205	10	0
48	s	41	0	59	3	0
49	C	52	0	88	2	0
49	J	52	0	88	3	0
49	a	52	0	88	0	0
49	e	52	0	88	10	0
49	g	52	0	88	2	0
49	j	52	0	88	0	0
49	r	52	0	88	5	0
50	C	18	0	18	4	0
50	Q	18	0	18	2	0
51	C	38	0	47	4	0
51	J	33	0	39	1	0
52	G	35	0	0	11	0
52	X	35	0	0	0	0
53	I	51	0	46	0	0
53	V	288	0	435	14	0
53	a	100	0	156	5	0
53	g	100	0	156	6	0
53	l	199	0	307	33	0
53	n	55	0	54	0	0
53	s	89	0	125	4	0
54	J	48	0	25	1	0
55	M	4	0	0	0	0
55	O	4	0	0	0	0
56	M	1	0	0	0	0
57	T	1	0	0	0	0
58	w	27	0	11	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	68216	0	68948	963	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 7.

All (963) 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)
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.26
54:J:401:NDP:O4D	54:J:401:NDP:C4D	1.68	1.13
53:l:702:CDL:H312	53:l:702:CDL:H742	1.31	1.13
53:l:702:CDL:HA62	53:l:702:CDL:H541	1.36	1.08
53:l:702:CDL:H742	53:l:702:CDL:C31	1.92	0.99
49:e:201:PLX:H222	53:l:702:CDL:OB7	1.67	0.93
4:E:70:ASN:HD21	52:G:201:8Q1:C43	1.87	0.86
34:k:37:MET:HE1	34:k:63:LEU:HG	1.56	0.85
1:A:60:GLY:HA2	14:O:241:PRO:HB3	1.59	0.84
13:N:68:MET:HG3	13:N:69:ASN:H	1.42	0.82
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.61	0.82
35:l:5:ALA:HB2	35:l:61:MET:HE1	1.63	0.80
53:l:702:CDL:C66	53:l:702:CDL:H232	2.10	0.80
53:l:702:CDL:H541	53:l:702:CDL:CA6	2.12	0.80
1:A:60:GLY:CA	14:O:241:PRO:HA	2.12	0.78
14:O:242:GLY:O	14:O:245:VAL:HG23	1.83	0.78
34:k:16:LEU:HA	34:k:36:MET:HE2	1.64	0.78
4:E:66:MET:HG3	52:G:201:8Q1:C11	2.14	0.78
4:E:70:ASN:ND2	52:G:201:8Q1:C43	2.47	0.77
53:l:702:CDL:H312	53:l:702:CDL:C74	2.15	0.77
1:A:60:GLY:HA2	14:O:241:PRO:CB	2.14	0.76
26:c:46:GLU:N	26:c:46:GLU:OE2	2.19	0.75
53:l:702:CDL:HA62	53:l:702:CDL:C54	2.14	0.75
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.67	0.75
36:m:72:THR:HG21	41:s:133:LEU:HD21	1.69	0.74
4:E:29:LYS:NZ	52:G:201:8Q1:O35	2.20	0.74
26:c:116:ARG:HG2	48:l:704:PEE:H49	1.70	0.74
36:m:82:VAL:HG11	53:s:402:CDL:HB31	1.68	0.74
37:n:50:ARG:HB2	37:n:53:GLU:HG2	1.70	0.74
8:I:40:LYS:HB3	21:W:7:LYS:H	1.53	0.73
1:A:60:GLY:HA2	14:O:241:PRO:HA	1.70	0.73
1:A:60:GLY:HA2	14:O:241:PRO:CA	2.19	0.72
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.22	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:136:GLU:OE2	39:p:167:TRP:NE1	2.24	0.71
12:M:493:VAL:HG12	12:M:513:MET:HE1	1.72	0.70
22:Y:41:GLU:OE2	22:Y:41:GLU:N	2.23	0.70
12:M:558:GLN:N	12:M:558:GLN:OE1	2.24	0.70
26:c:58:ARG:NH2	26:c:60:GLU:OE1	2.25	0.70
3:C:126:GLU:OE2	33:j:33:LYS:NZ	2.24	0.70
17:S:28:LYS:HG3	17:S:33:GLY:HA2	1.73	0.70
44:w:88:GLU:OE2	44:w:161:ARG:NH1	2.25	0.69
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.24	0.69
16:Q:304:LYS:NZ	16:Q:316:PHE:O	2.26	0.69
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.74	0.69
11:L:109:ASN:ND2	11:L:111:LEU:O	2.25	0.69
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.75	0.69
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.73	0.68
48:i:401:PEE:H37	48:i:401:PEE:H60	1.73	0.68
27:d:30:VAL:O	27:d:34:THR:HG23	1.94	0.68
28:e:129:ARG:NH1	28:e:136:LEU:O	2.24	0.68
32:i:211:MET:HE3	32:i:251:MET:HG2	1.73	0.68
8:I:70:MET:HE3	8:I:70:MET:O	1.94	0.68
16:Q:94:VAL:HG21	16:Q:116:LEU:HB2	1.74	0.68
21:W:121:MET:HG3	36:m:130:THR:HB	1.76	0.68
25:b:112:GLU:N	25:b:112:GLU:OE1	2.24	0.68
3:C:125:PRO:HG2	41:s:58:LYS:HE3	1.75	0.67
14:O:44:THR:HG22	14:O:46:GLU:H	1.60	0.67
26:c:167:TYR:CD2	26:c:178:PRO:HG3	2.29	0.67
1:A:159:ARG:NH2	14:O:176:CYS:O	2.28	0.67
18:T:47:ASP:O	18:T:52:ARG:NH1	2.28	0.67
44:w:264:GLU:OE2	44:w:264:GLU:N	2.28	0.67
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.27	0.66
4:E:23:ARG:HE	11:L:53:ILE:HG22	1.60	0.66
15:P:125:ARG:NH2	15:P:201:ASP:OD1	2.27	0.66
44:w:132:GLN:NE2	44:w:166:ASP:OD1	2.28	0.66
9:J:192:ARG:NH1	9:J:198:ALA:O	2.30	0.65
12:M:68:ARG:NH1	12:M:283:GLU:OE2	2.29	0.65
41:s:195:ARG:HD3	41:s:231:ILE:HD11	1.79	0.65
48:V:202:PEE:H29	48:V:202:PEE:H71	1.79	0.65
1:A:60:GLY:HA3	14:O:241:PRO:HA	1.78	0.65
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.30	0.65
7:H:9:THR:O	7:H:76:GLN:NE2	2.29	0.65
40:r:133:ILE:HD11	40:r:231:LEU:HD11	1.79	0.65
30:g:15:PHE:HB2	49:g:201:PLX:H6	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:65:VAL:HG11	36:m:157:THR:HG23	1.79	0.64
40:r:403:THR:HA	40:r:406:TYR:CE2	2.33	0.64
44:w:125:ASP:O	44:w:130:ARG:NH2	2.31	0.64
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.79	0.64
40:r:74:PRO:O	40:r:78:MET:HG3	1.97	0.64
21:W:61:GLN:HE22	41:s:317:GLN:H	1.43	0.64
24:a:147:ALA:HB2	40:r:173:SER:HB2	1.79	0.64
39:p:136:GLU:OE2	39:p:167:TRP:CD1	2.51	0.64
1:A:385:CYS:HB3	45:A:501:SF4:S2	2.37	0.64
26:c:38:PRO:HD3	38:o:67:ARG:HG2	1.79	0.63
43:v:103:GLU:HA	43:v:106:ARG:HG2	1.80	0.63
5:F:20:ARG:HB2	5:F:66:TRP:HB2	1.80	0.63
53:V:201:CDL:H742	53:V:201:CDL:H361	1.79	0.63
14:O:129:LYS:H	14:O:168:LEU:HA	1.63	0.63
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.79	0.63
3:C:92:VAL:HG11	51:C:305:UQ:H103	1.81	0.63
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.81	0.63
14:O:38:LEU:O	14:O:124:ARG:NH2	2.31	0.63
16:Q:47:PHE:HD1	16:Q:52:MET:HE1	1.63	0.63
35:l:119:LYS:NZ	53:l:702:CDL:OA3	2.26	0.63
5:F:24:CYS:N	5:F:58:CYS:SG	2.72	0.62
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.30	0.62
26:c:78:LEU:HB2	26:c:106:HIS:HD2	1.64	0.62
10:K:105:ARG:NH2	12:M:426:ASP:OD2	2.31	0.62
4:E:25:MET:HE1	4:E:79:VAL:HG21	1.81	0.62
26:c:78:LEU:HB2	26:c:106:HIS:CD2	2.34	0.62
40:r:237:LYS:HD2	40:r:316:MET:HB3	1.81	0.62
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.82	0.62
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.81	0.62
14:O:242:GLY:HA2	14:O:245:VAL:CG2	2.30	0.62
16:Q:192:LEU:HD12	16:Q:197:MET:HA	1.80	0.62
26:c:105:ILE:HG23	26:c:109:LEU:HD22	1.82	0.62
35:l:7:LEU:HD22	35:l:46:LEU:HD11	1.81	0.62
4:E:70:ASN:ND2	52:G:201:8Q1:C42	2.63	0.62
7:H:55:LYS:HE3	15:P:104:THR:HG21	1.81	0.62
32:i:207:ILE:HD13	32:i:262:PRO:HD3	1.80	0.62
12:M:30:ASN:ND2	12:M:44:GLU:OE2	2.32	0.61
42:u:105:ALA:O	42:u:109:GLU:HG2	2.00	0.61
42:u:139:GLU:OE1	42:u:139:GLU:N	2.22	0.61
2:B:200:GLU:HG3	13:N:88:ARG:HB2	1.81	0.61
39:p:28:GLU:OE2	39:p:34:ARG:NH1	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:211:ARG:NH2	15:P:213:ASP:OD2	2.34	0.61
32:i:271:THR:HG22	40:r:169:ASN:HD22	1.64	0.61
53:a:201:CDL:H191	53:a:201:CDL:H752	1.83	0.61
39:p:134:GLU:OE1	39:p:134:GLU:HA	1.99	0.61
1:A:406:PRO:HA	1:A:450:MET:HE1	1.81	0.61
7:H:9:THR:HG23	7:H:16:VAL:HG22	1.82	0.61
16:Q:99:MET:HE1	16:Q:444:LEU:HD21	1.82	0.61
7:H:18:GLU:OE2	7:H:18:GLU:N	2.30	0.60
40:r:204:MET:HG3	40:r:209:LEU:HB2	1.83	0.60
27:d:114:GLN:HG3	35:l:203:MET:HG2	1.84	0.60
31:h:82:GLN:O	31:h:86:LEU:HD12	2.00	0.60
41:s:221:ALA:O	41:s:225:MET:HG3	2.01	0.60
12:M:217:GLU:HG2	12:M:218:LEU:HG	1.83	0.60
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.84	0.60
35:l:150:MET:HE1	53:l:702:CDL:H112	1.82	0.60
21:W:61:GLN:NE2	41:s:317:GLN:OE1	2.35	0.60
9:J:303:ARG:HB2	9:J:316:ARG:HD3	1.83	0.60
26:c:105:ILE:CD1	38:o:65:LEU:HD12	2.31	0.60
1:A:152:ARG:NH2	10:K:99:PRO:O	2.31	0.60
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.84	0.60
14:O:242:GLY:O	14:O:243:PHE:C	2.44	0.59
36:m:77:GLU:OE1	36:m:77:GLU:N	2.35	0.59
53:V:204:CDL:HB62	34:k:23:ARG:HG2	1.83	0.59
14:O:164:THR:HG22	14:O:166:ASP:H	1.66	0.59
5:F:23:LEU:HD13	5:F:37:ILE:HD12	1.85	0.59
11:L:80:PHE:HE1	11:L:100:GLU:HG2	1.68	0.59
5:F:61:VAL:HG23	5:F:62:GLN:H	1.68	0.59
12:M:394:VAL:HG22	12:M:473:MET:HE1	1.84	0.59
16:Q:79:ASN:HB2	16:Q:100:GLU:HG2	1.84	0.59
27:d:97:LYS:NZ	40:r:47:GLU:OE2	2.35	0.59
39:p:128:LEU:HD11	39:p:163:LEU:HD11	1.85	0.59
53:l:702:CDL:H242	48:l:705:PEE:H34	1.85	0.59
35:l:562:LEU:HB3	35:l:563:PRO:HD3	1.85	0.58
42:u:83:THR:HA	42:u:86:TRP:CD1	2.39	0.58
3:C:69:LEU:HB2	3:C:107:GLY:HA3	1.84	0.58
33:j:108:GLN:HB2	36:m:169:MET:HE1	1.84	0.58
44:w:246:LEU:HD22	44:w:255:VAL:HG11	1.84	0.58
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.84	0.58
3:C:77:MET:HE2	50:C:304:UQ1:H113	1.85	0.58
27:d:160:LYS:NZ	30:g:114:ILE:O	2.36	0.58
35:l:228:GLY:HA3	48:l:704:PEE:H38	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:35:ASP:HA	5:F:38:GLU:HG2	1.86	0.58
14:O:134:VAL:HG21	14:O:149:LEU:HD13	1.85	0.58
34:k:37:MET:HE2	34:k:67:ALA:HB2	1.86	0.58
12:M:51:GLN:HA	12:M:54:GLU:HG2	1.84	0.58
27:d:42:ASP:O	27:d:46:THR:OG1	2.20	0.58
32:i:65:THR:O	32:i:69:MET:HG3	2.04	0.58
41:s:85:MET:SD	41:s:108:MET:HB2	2.43	0.58
43:v:33:GLU:N	43:v:33:GLU:OE1	2.36	0.58
2:B:50:MET:HE1	19:U:10:LYS:HG3	1.86	0.58
21:W:88:ARG:NH2	42:u:7:LEU:O	2.36	0.58
22:Y:76:ASP:O	35:l:385:TYR:OH	2.20	0.58
24:a:134:GLU:OE2	37:n:57:TRP:NE1	2.26	0.58
1:A:234:GLY:HA3	1:A:240:THR:HG22	1.85	0.58
38:o:31:LYS:O	38:o:35:GLU:HG3	2.04	0.58
1:A:116:ASN:ND2	1:A:207:GLY:O	2.32	0.57
39:p:35:ASP:OD1	39:p:36:LYS:N	2.37	0.57
12:M:509:ASP:N	12:M:509:ASP:OD1	2.35	0.57
35:l:227:PHE:O	35:l:230:HIS:ND1	2.34	0.57
40:r:218:LYS:O	40:r:222:GLU:HG2	2.04	0.57
11:L:99:MET:HE2	11:L:126:LEU:HD12	1.85	0.57
53:l:702:CDL:H631	53:l:702:CDL:H811	1.86	0.57
12:M:308:ARG:NH1	12:M:312:GLY:O	2.35	0.57
12:M:498:GLN:HB2	12:M:669:ASN:HD21	1.69	0.57
14:O:222:ARG:NH1	14:O:226:GLU:O	2.34	0.57
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.86	0.57
17:S:49:GLU:OE2	17:S:52:ARG:NH1	2.38	0.57
3:C:109:LEU:HD13	3:C:117:LEU:HD13	1.87	0.57
16:Q:249:LYS:HA	21:W:19:ILE:HG23	1.85	0.57
26:c:162:PRO:HB3	43:v:39:MET:HG3	1.86	0.57
1:A:283:ASN:ND2	1:A:305:GLY:O	2.38	0.57
12:M:456:ALA:O	12:M:499:ASN:ND2	2.38	0.57
30:g:56:VAL:HG21	40:r:17:MET:HE1	1.87	0.57
53:g:202:CDL:H241	40:r:97:THR:HG21	1.87	0.57
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.40	0.57
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.87	0.57
5:F:87:VAL:O	5:F:91:LEU:HD12	2.05	0.57
33:j:95:LEU:HD13	41:s:302:MET:HG2	1.87	0.57
31:h:18:MET:HE3	34:k:56:ALA:HA	1.87	0.56
20:V:34:LEU:HD11	53:V:204:CDL:H441	1.87	0.56
27:d:167:ARG:HH21	28:e:153:GLU:HG3	1.69	0.56
40:r:118:PHE:O	40:r:122:PHE:HB3	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:118:TYR:OH	58:w:401:ADP:O2'	2.23	0.56
1:A:134:ASP:N	1:A:134:ASP:OD1	2.37	0.56
4:E:25:MET:O	4:E:29:LYS:HG3	2.05	0.56
35:l:419:THR:HA	35:l:422:TYR:CE2	2.40	0.56
36:m:61:LEU:O	41:s:114:TYR:OH	2.23	0.56
24:a:70:LEU:HD13	28:e:87:MET:HE3	1.87	0.56
1:A:295:PRO:HG2	1:A:298:GLU:HB2	1.88	0.56
32:i:128:LEU:HD12	32:i:216:PHE:HB3	1.87	0.56
12:M:666:GLN:O	12:M:670:GLU:HG3	2.06	0.56
21:W:90:ASN:ND2	21:W:123:GLU:O	2.39	0.56
27:d:24:THR:HG22	27:d:26:LEU:H	1.71	0.56
32:i:183:SER:O	32:i:187:MET:HG2	2.06	0.56
5:F:26:ARG:HB3	5:F:26:ARG:NH1	2.21	0.56
1:A:263:ALA:HA	1:A:271:SER:HB3	1.88	0.56
20:V:81:ARG:NH2	20:V:86:ASP:OD2	2.39	0.56
53:V:201:CDL:H731	53:V:201:CDL:H601	1.88	0.55
24:a:131:LYS:NZ	37:n:32:ASP:OD2	2.32	0.55
26:c:160:GLN:HG2	26:c:183:HIS:ND1	2.20	0.55
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.88	0.55
21:W:74:LEU:O	21:W:78:GLU:HG2	2.04	0.55
35:l:492:ILE:O	35:l:496:MET:HG2	2.06	0.55
37:n:54:GLU:HG3	37:n:55:VAL:HG22	1.87	0.55
4:E:66:MET:HB3	52:G:201:8Q1:C9	2.37	0.55
24:a:152:LYS:HD3	30:g:96:VAL:HG21	1.89	0.55
9:J:174:ILE:HG23	9:J:175:LYS:HG2	1.88	0.55
22:Y:88:ASP:OD1	22:Y:91:GLN:HG2	2.05	0.55
41:s:18:ALA:O	41:s:21:THR:OG1	2.23	0.55
20:V:40:SER:HA	53:V:201:CDL:HB61	1.88	0.55
41:s:306:SER:O	41:s:310:MET:HG3	2.06	0.55
53:a:201:CDL:H751	28:e:103:SER:HB2	1.89	0.55
28:e:55:LEU:HD12	44:w:318:THR:HG22	1.89	0.55
35:l:595:ILE:O	35:l:599:MET:HG2	2.06	0.55
49:e:201:PLX:H21	48:l:705:PEE:H2	1.89	0.55
1:A:89:GLY:O	47:A:503:NAI:H2N	2.08	0.54
1:A:290:GLU:OE2	1:A:303:HIS:NE2	2.39	0.54
9:J:87:GLU:HG3	9:J:89:TYR:H	1.72	0.54
11:L:123:ASN:OD1	12:M:246:ARG:NH2	2.37	0.54
12:M:306:MET:HB2	12:M:583:ILE:HB	1.88	0.54
53:l:702:CDL:H331	53:l:702:CDL:OA9	2.05	0.54
4:E:70:ASN:O	52:G:201:8Q1:N41	2.40	0.54
14:O:186:VAL:HG12	14:O:193:TYR:HB2	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.42	0.54
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.88	0.54
49:e:201:PLX:C22	53:l:702:CDL:OB7	2.48	0.54
30:g:33:LEU:HD22	30:g:71:VAL:HG13	1.90	0.54
1:A:367:ILE:HG13	1:A:438:LEU:HD13	1.88	0.54
12:M:308:ARG:NH2	12:M:578:PRO:O	2.40	0.54
19:U:16:GLU:HG3	48:U:101:PEE:H49	1.88	0.54
53:g:202:CDL:H361	32:i:243:LEU:HD23	1.88	0.54
37:n:18:PRO:O	37:n:22:VAL:HG23	2.08	0.54
8:I:27:ARG:NH2	16:Q:212:GLU:OE2	2.40	0.54
30:g:36:MET:HE1	49:g:201:PLX:H393	1.89	0.54
53:V:204:CDL:H131	35:l:589:LEU:HD21	1.88	0.54
22:Y:89:PRO:HD2	22:Y:90:SER:H	1.73	0.54
20:V:49:PHE:O	20:V:53:VAL:HG23	2.08	0.54
8:I:92:LYS:HA	8:I:92:LYS:HE2	1.89	0.53
27:d:90:MET:HE1	40:r:48:ASN:HB3	1.90	0.53
53:l:703:CDL:H521	53:l:703:CDL:HB61	1.90	0.53
3:C:42:ARG:O	3:C:46:VAL:HG23	2.09	0.53
6:X:123:GLU:HG2	6:X:129:GLU:HA	1.90	0.53
53:l:702:CDL:H581	53:l:702:CDL:H812	1.90	0.53
1:A:48:ARG:HH12	14:O:231:LEU:HD21	1.72	0.53
10:K:91:VAL:O	10:K:94:SER:OG	2.27	0.53
16:Q:268:TRP:O	16:Q:272:THR:OG1	2.22	0.53
1:A:36:LYS:H	1:A:36:LYS:HD3	1.74	0.53
32:i:20:VAL:HG11	32:i:137:ALA:HB1	1.91	0.53
35:l:395:ILE:O	35:l:399:VAL:HG13	2.08	0.53
14:O:134:VAL:HG12	14:O:186:VAL:HG23	1.89	0.53
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.90	0.53
1:A:90:GLY:HA3	47:A:503:NAI:H1D	1.90	0.53
7:H:116:ILE:HD13	11:L:96:LYS:HD2	1.89	0.53
53:g:202:CDL:H142	40:r:94:LEU:HD13	1.91	0.53
53:g:202:CDL:H392	32:i:246:VAL:HG11	1.91	0.53
32:i:337:LEU:O	32:i:340:THR:OG1	2.21	0.53
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.90	0.53
25:b:18:LEU:HD11	39:p:163:LEU:HD22	1.91	0.53
40:r:306:PRO:HB3	40:r:458:LEU:HD12	1.90	0.53
1:A:112:TYR:O	1:A:240:THR:HA	2.09	0.52
9:J:306:GLU:HG2	9:J:315:THR:HG22	1.91	0.52
12:M:140:GLN:HG2	16:Q:379:ILE:HG23	1.91	0.52
14:O:144:ASN:O	14:O:147:SER:OG	2.27	0.52
32:i:215:MET:HE1	32:i:244:MET:HG3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:PRO:O	1:A:347:THR:OG1	2.20	0.52
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.74	0.52
53:l:702:CDL:OA9	53:l:702:CDL:H121	2.10	0.52
36:m:71:THR:HA	36:m:75:ALA:HB3	1.91	0.52
1:A:66:LYS:HD3	1:A:70:LEU:HD23	1.90	0.52
49:e:201:PLX:H202	53:l:702:CDL:C78	2.39	0.52
6:X:115:GLN:NE2	6:X:138:LEU:O	2.42	0.52
53:l:702:CDL:C66	53:l:702:CDL:C23	2.86	0.52
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.25	0.52
9:J:37:HIS:CE1	18:T:49:ASP:HA	2.45	0.52
49:e:201:PLX:H202	53:l:702:CDL:H801	1.91	0.52
40:r:271:MET:HE2	40:r:271:MET:HA	1.91	0.52
41:s:134:ARG:HD3	41:s:200:LEU:HB3	1.91	0.52
9:J:283:VAL:HG22	9:J:369:VAL:HG21	1.91	0.52
26:c:110:ASP:OD1	26:c:110:ASP:N	2.39	0.52
3:C:83:ARG:NH1	16:Q:212:GLU:OE1	2.43	0.52
7:H:19:THR:O	7:H:19:THR:OG1	2.24	0.52
8:I:46:SER:O	8:I:52:ASN:ND2	2.39	0.52
27:d:38:ASP:OD2	27:d:43:ARG:NH2	2.31	0.52
41:s:102:VAL:HG21	41:s:154:LEU:HD11	1.92	0.52
8:I:8:ILE:O	8:I:12:ARG:HG3	2.10	0.51
35:l:394:LEU:HA	35:l:397:GLU:HG2	1.92	0.51
53:l:702:CDL:H742	53:l:702:CDL:H311	1.88	0.51
9:J:178:SER:OG	9:J:317:ASP:OD1	2.23	0.51
12:M:240:ALA:HB2	12:M:271:MET:HE3	1.91	0.51
12:M:275:PRO:HG3	12:M:286:ILE:HG12	1.93	0.51
12:M:449:PRO:HB2	12:M:679:LEU:HD13	1.92	0.51
21:W:82:ARG:NH1	31:h:106:PRO:O	2.42	0.51
24:a:52:LYS:HD3	24:a:53:ARG:H	1.74	0.51
27:d:82:ILE:HG23	27:d:83:LEU:HD22	1.93	0.51
44:w:113:SER:HB3	44:w:116:LYS:HG2	1.92	0.51
4:E:71:ALA:O	52:G:201:8Q1:N36	2.42	0.51
13:N:68:MET:HG3	13:N:69:ASN:N	2.18	0.51
41:s:101:GLY:O	41:s:105:MET:HG2	2.10	0.51
25:b:99:GLU:HG3	35:l:61:MET:HG2	1.91	0.51
32:i:154:MET:HE3	32:i:154:MET:HA	1.92	0.51
1:A:70:LEU:HD21	1:A:189:SER:HA	1.93	0.51
6:G:94:ASP:OD1	6:G:97:LYS:HB3	2.11	0.51
33:j:19:LEU:HD11	48:s:401:PEE:H56	1.93	0.51
35:l:82:MET:HA	35:l:82:MET:HE3	1.93	0.51
35:l:246:LEU:O	35:l:251:THR:OG1	2.28	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:38:ILE:O	7:H:45:ARG:NH1	2.35	0.51
22:Y:42:PRO:HB2	23:Z:14:MET:HE2	1.92	0.51
14:O:111:ARG:NH1	14:O:114:GLU:OE2	2.43	0.51
6:X:79:ILE:O	6:X:83:VAL:HG23	2.10	0.51
26:c:164:ASN:OD1	26:c:180:PRO:HA	2.10	0.51
40:r:339:SER:HB3	40:r:344:LEU:HD22	1.92	0.51
20:V:140:LYS:HE2	32:i:274:GLU:HG2	1.92	0.51
26:c:78:LEU:HD11	26:c:104:PRO:HB2	1.93	0.51
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.93	0.51
43:v:51:LEU:O	43:v:52:MET:HG2	2.11	0.51
21:W:103:ASP:OD1	21:W:103:ASP:N	2.43	0.51
32:i:88:LYS:HG2	32:i:148:SER:HB3	1.92	0.51
1:A:48:ARG:HH21	14:O:223:PHE:HZ	1.57	0.50
12:M:538:ARG:NH1	12:M:559:ASP:OD2	2.44	0.50
41:s:100:LEU:HD13	41:s:103:LEU:HD12	1.93	0.50
3:C:173:LEU:O	3:C:177:ILE:HG12	2.10	0.50
5:F:23:LEU:HD12	5:F:34:ARG:HG2	1.93	0.50
7:H:54:GLU:O	7:H:58:MET:HG3	2.11	0.50
49:e:201:PLX:H282	40:r:446:LEU:HB3	1.93	0.50
30:g:101:GLU:OE2	30:g:101:GLU:N	2.25	0.50
22:Y:51:THR:OG1	35:l:446:ASN:OD1	2.29	0.50
24:a:78:THR:HG21	28:e:96:SER:HA	1.94	0.50
28:e:125:LEU:HD22	28:e:129:ARG:NH2	2.26	0.50
30:g:117:GLU:H	30:g:117:GLU:CD	2.15	0.50
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	1.92	0.50
26:c:70:MET:HE3	26:c:70:MET:HA	1.94	0.50
4:E:16:SER:HA	11:L:52:LEU:HD13	1.93	0.50
12:M:390:THR:HA	12:M:600:GLU:HG2	1.93	0.50
20:V:29:GLY:O	20:V:63:SER:HB3	2.12	0.50
28:e:55:LEU:HD11	44:w:320:GLY:HA2	1.93	0.50
32:i:270:MET:O	32:i:275:SER:HB3	2.11	0.50
37:n:30:ARG:HG3	37:n:30:ARG:HH11	1.77	0.50
40:r:281:ASP:OD1	40:r:340:ARG:HB3	2.12	0.50
14:O:242:GLY:C	14:O:245:VAL:HG23	2.36	0.50
40:r:19:LYS:HG3	40:r:20:HIS:N	2.26	0.50
12:M:389:THR:O	12:M:390:THR:OG1	2.26	0.50
31:h:67:LEU:HD11	32:i:82:GLY:H	1.77	0.50
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.46	0.50
2:B:50:MET:HE2	2:B:50:MET:HA	1.94	0.50
9:J:168:SER:O	9:J:203:PRO:HD2	2.12	0.50
14:O:218:PRO:HD2	14:O:223:PHE:HA	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:208:GLU:OE2	16:Q:221:ARG:NH1	2.36	0.50
48:V:202:PEE:H21	48:V:202:PEE:H49	1.94	0.50
49:e:201:PLX:H202	53:l:702:CDL:C80	2.42	0.50
34:k:23:ARG:HG3	36:m:23:LYS:HE2	1.93	0.50
1:A:369:ARG:NH2	14:O:136:THR:OG1	2.41	0.49
9:J:375:VAL:HG23	9:J:375:VAL:O	2.12	0.49
12:M:140:GLN:O	12:M:144:MET:HG2	2.12	0.49
53:a:201:CDL:H111	48:l:705:PEE:H60	1.92	0.49
28:e:97:ILE:O	28:e:101:LEU:HB2	2.12	0.49
3:C:63:TRP:HH2	51:C:305:UQ:H153	1.77	0.49
15:P:69:LEU:HD13	15:P:96:VAL:HG22	1.94	0.49
20:V:134:GLN:HE22	32:i:274:GLU:HG3	1.76	0.49
24:a:166:GLY:O	24:a:170:GLN:NE2	2.45	0.49
53:a:201:CDL:H781	40:r:446:LEU:HD11	1.94	0.49
4:E:57:LYS:NZ	4:E:61:ASP:OD2	2.43	0.49
49:e:201:PLX:H122	53:l:702:CDL:H632	1.94	0.49
5:F:87:VAL:HA	5:F:90:THR:HG22	1.94	0.49
27:d:119:GLU:HB2	43:v:50:GLN:HB3	1.95	0.49
1:A:273:THR:OG1	1:A:274:LYS:N	2.46	0.49
10:K:87:LEU:O	10:K:91:VAL:HG13	2.13	0.49
12:M:555:ILE:HG23	12:M:559:ASP:HB2	1.95	0.49
34:k:5:TYR:O	34:k:9:ILE:HG13	2.12	0.49
35:l:124:PHE:CE1	35:l:252:MET:HB2	2.47	0.49
1:A:338:ASP:OD1	1:A:338:ASP:N	2.44	0.49
2:B:39:LYS:NZ	16:Q:335:GLU:OE2	2.41	0.49
36:m:34:ILE:HG13	36:m:64:MET:HG3	1.94	0.49
38:o:80:PHE:HE1	38:o:86:THR:HG21	1.76	0.49
6:G:113:LEU:O	6:G:117:GLU:HG3	2.12	0.49
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.95	0.49
53:l:702:CDL:H581	53:l:702:CDL:H841	1.95	0.49
9:J:344:PRO:HG2	9:J:347:LEU:HG	1.95	0.49
39:p:160:GLU:CD	39:p:160:GLU:H	2.20	0.49
12:M:513:MET:HE3	12:M:513:MET:HA	1.95	0.48
22:Y:89:PRO:HB2	43:v:103:GLU:OE1	2.13	0.48
53:g:202:CDL:H232	53:g:202:CDL:H782	1.95	0.48
6:G:135:ALA:HA	6:G:138:LEU:HG	1.95	0.48
15:P:173:MET:HB3	15:P:198:PHE:HB2	1.94	0.48
21:W:50:MET:HE1	21:W:53:TRP:HD1	1.78	0.48
35:l:27:TYR:O	35:l:115:ASN:ND2	2.38	0.48
12:M:488:ALA:HB2	12:M:677:GLN:HG2	1.94	0.48
20:V:120:LEU:HD21	49:r:501:PLX:H341	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:33:LEU:HD13	35:l:49:VAL:HG13	1.95	0.48
42:u:11:GLU:CD	42:u:11:GLU:H	2.21	0.48
44:w:285:ASP:OD1	44:w:285:ASP:O	2.31	0.48
1:A:392:MET:HE2	1:A:419:ILE:HD12	1.95	0.48
1:A:456:GLN:OE1	1:A:457:HIS:ND1	2.46	0.48
19:U:38:TYR:HB2	41:s:310:MET:O	2.13	0.48
20:V:39:TYR:OH	35:l:594:THR:OG1	2.24	0.48
6:X:155:TYR:HA	25:b:20:ARG:HD3	1.95	0.48
26:c:105:ILE:HD12	38:o:65:LEU:HA	1.95	0.48
32:i:122:ILE:O	32:i:176:ARG:NH1	2.43	0.48
35:l:88:MET:HE3	35:l:88:MET:O	2.13	0.48
44:w:189:GLU:O	44:w:193:VAL:HG22	2.14	0.48
12:M:215:MET:HG3	12:M:714:VAL:HG12	1.94	0.48
21:W:70:ALA:HB2	42:u:125:LEU:HD13	1.95	0.48
30:g:107:ASP:OD1	30:g:107:ASP:N	2.46	0.48
2:B:68:ARG:NH2	16:Q:260:GLU:OE1	2.47	0.48
5:F:21:ILE:HG12	5:F:65:LEU:HD12	1.95	0.48
12:M:338:VAL:O	12:M:363:SER:OG	2.29	0.48
8:I:54:TYR:CZ	16:Q:362:LYS:HD2	2.47	0.48
9:J:229:ILE:HB	9:J:323:HIS:HD2	1.79	0.48
43:v:113:LYS:HG3	43:v:114:ARG:N	2.28	0.48
44:w:139:ARG:NH1	44:w:166:ASP:OD2	2.47	0.48
1:A:154:ALA:HB3	1:A:195:VAL:HG12	1.95	0.48
15:P:44:ARG:HB2	15:P:44:ARG:CZ	2.44	0.48
24:a:94:GLY:O	27:d:61:TYR:OH	2.26	0.48
1:A:201:ALA:HA	14:O:121:MET:HE2	1.95	0.48
20:V:141:VAL:HG21	32:i:272:LYS:HB3	1.96	0.48
41:s:62:ARG:NH2	48:s:401:PEE:O1P	2.47	0.48
4:E:69:LYS:HB2	4:E:69:LYS:NZ	2.28	0.47
8:I:64:MET:HE2	15:P:80:CYS:SG	2.54	0.47
16:Q:62:LYS:HE3	16:Q:62:LYS:HA	1.95	0.47
35:l:298:ILE:O	35:l:302:VAL:HG23	2.14	0.47
3:C:73:ALA:HB1	50:C:304:UQ1:H112	1.95	0.47
16:Q:56:LYS:NZ	16:Q:56:LYS:HB3	2.28	0.47
17:S:31:ASN:ND2	17:S:36:LYS:HB2	2.29	0.47
25:b:104:ILE:HD13	27:d:18:PRO:HG3	1.96	0.47
49:e:201:PLX:O2	48:l:705:PEE:N	2.37	0.47
38:o:56:ARG:NH1	40:r:422:HIS:O	2.46	0.47
41:s:55:LEU:HD13	41:s:221:ALA:HB2	1.97	0.47
7:H:66:LYS:HD3	7:H:66:LYS:HA	1.62	0.47
36:m:173:ARG:HG3	36:m:173:ARG:HH11	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:v:52:MET:HB2	43:v:55:GLN:H	1.78	0.47
20:V:141:VAL:O	24:a:169:TYR:OH	2.30	0.47
22:Y:103:ASP:OD1	22:Y:103:ASP:N	2.41	0.47
40:r:1:MET:SD	40:r:111:THR:HG21	2.54	0.47
44:w:204:VAL:HG21	44:w:249:MET:HG2	1.96	0.47
27:d:37:PHE:CD1	35:l:3:PRO:HB3	2.49	0.47
31:h:24:GLU:OE1	36:m:149:TYR:OH	2.31	0.47
32:i:149:ILE:HG13	32:i:150:ASN:N	2.29	0.47
1:A:296:LEU:HD21	1:A:317:VAL:HG11	1.97	0.47
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.49	0.47
33:j:22:PHE:HE1	41:s:62:ARG:HE	1.62	0.47
35:l:503:GLU:O	35:l:507:THR:HG23	2.14	0.47
41:s:112:ALA:O	41:s:115:SER:OG	2.31	0.47
53:s:402:CDL:H191	53:s:402:CDL:H162	1.68	0.47
42:u:149:GLU:OE2	42:u:149:GLU:N	2.41	0.47
44:w:86:PHE:HB2	44:w:159:LEU:HD23	1.97	0.47
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.55	0.47
7:H:18:GLU:H	7:H:18:GLU:CD	2.20	0.47
7:H:47:TYR:O	7:H:51:ILE:HG12	2.15	0.47
9:J:83:PRO:HA	9:J:106:MET:O	2.14	0.47
12:M:64:CYS:O	12:M:184:ARG:NH2	2.35	0.47
12:M:351:LEU:O	12:M:530:TYR:OH	2.33	0.47
12:M:388:ASN:HB3	12:M:511:LYS:HD3	1.95	0.47
12:M:538:ARG:NH2	12:M:554:CYS:O	2.48	0.47
13:N:8:ARG:HA	13:N:11:LEU:HD12	1.96	0.47
18:T:105:GLU:OE2	18:T:105:GLU:HA	2.15	0.47
19:U:28:LEU:O	19:U:32:LEU:HB2	2.14	0.47
48:U:101:PEE:H28	33:j:99:ALA:HB1	1.95	0.47
20:V:85:ASP:HB3	20:V:130:LEU:HD21	1.97	0.47
25:b:121:LYS:HD3	43:v:40:VAL:HA	1.96	0.47
26:c:166:LEU:O	26:c:170:ARG:HG3	2.15	0.47
31:h:84:ASP:HA	31:h:87:ILE:HG12	1.96	0.47
35:l:401:MET:HE2	35:l:482:MET:HG2	1.96	0.47
1:A:114:VAL:HB	1:A:242:VAL:HG22	1.96	0.47
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.49	0.47
16:Q:434:GLY:O	16:Q:438:MET:HG3	2.15	0.47
21:W:134:LEU:HD13	36:m:2:THR:HB	1.97	0.47
34:k:4:VAL:O	34:k:8:ILE:HG12	2.15	0.47
7:H:81:ILE:O	7:H:85:GLU:HG3	2.15	0.47
10:K:107:SER:HB3	10:K:110:HIS:ND1	2.29	0.47
12:M:638:THR:O	12:M:642:VAL:HG23	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:201:ASP:OD1	15:P:201:ASP:N	2.39	0.47
32:i:283:ALA:HB1	40:r:158:LEU:HD13	1.97	0.47
35:l:65:ASN:OD1	35:l:65:ASN:N	2.48	0.47
51:C:305:UQ:H221	51:C:305:UQ:H262	1.57	0.47
49:J:403:PLX:H251	49:J:403:PLX:H282	1.48	0.47
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.50	0.47
24:a:137:MET:HE2	27:d:83:LEU:HD12	1.97	0.47
38:o:117:GLN:OE1	38:o:117:GLN:HA	2.15	0.47
40:r:401:MET:HE2	40:r:401:MET:HB3	1.78	0.47
4:E:70:ASN:HD21	52:G:201:8Q1:C42	2.25	0.46
19:U:53:TYR:HD1	21:W:72:MET:HE3	1.80	0.46
32:i:242:SER:O	32:i:246:VAL:HG23	2.15	0.46
32:i:258:SER:OG	32:i:333:SER:O	2.33	0.46
43:v:65:GLN:HG2	43:v:83:GLU:HG2	1.96	0.46
44:w:57:SER:HB3	44:w:150:LEU:HD11	1.96	0.46
44:w:58:LYS:O	44:w:60:ILE:HG13	2.15	0.46
5:F:45:LYS:HA	5:F:45:LYS:HD2	1.61	0.46
5:F:69:TYR:HE1	5:F:75:LYS:HE2	1.80	0.46
6:G:104:PHE:HD1	6:G:108:LEU:HD12	1.78	0.46
15:P:75:GLN:HB3	15:P:87:PHE:CD1	2.50	0.46
29:f:44:VAL:O	29:f:48:LEU:HD12	2.16	0.46
12:M:371:VAL:HG22	12:M:533:GLY:HA2	1.97	0.46
26:c:167:TYR:CG	26:c:178:PRO:HG3	2.50	0.46
35:l:102:GLU:OE1	35:l:456:ARG:NH2	2.43	0.46
35:l:407:TRP:CE2	35:l:411:MET:HE3	2.50	0.46
43:v:22:MET:HG2	43:v:23:PRO:HA	1.97	0.46
20:V:36:VAL:HG22	53:V:201:CDL:H741	1.97	0.46
25:b:5:THR:OG1	25:b:8:GLU:HG3	2.14	0.46
25:b:25:ASP:OD2	39:p:125:TRP:NE1	2.30	0.46
32:i:261:MET:HB2	32:i:337:LEU:HD12	1.96	0.46
41:s:63:PRO:HB2	41:s:66:SER:HB3	1.97	0.46
41:s:313:SER:O	41:s:313:SER:OG	2.29	0.46
43:v:106:ARG:HG3	43:v:107:ARG:N	2.30	0.46
29:f:48:LEU:O	29:f:52:VAL:HG23	2.16	0.46
38:o:23:TYR:OH	39:p:68:GLU:HG3	2.15	0.46
41:s:104:PHE:O	41:s:108:MET:HG2	2.15	0.46
44:w:61:THR:HG22	44:w:159:LEU:HB2	1.97	0.46
9:J:228:LEU:O	9:J:292:PRO:HA	2.16	0.46
16:Q:96:ARG:HB3	16:Q:112:HIS:HB2	1.97	0.46
53:V:204:CDL:H362	53:V:204:CDL:H392	1.59	0.46
27:d:111:LYS:HD3	35:l:197:ASP:OD2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:81:SER:O	32:i:83:GLN:N	2.46	0.46
35:l:475:MET:HE3	35:l:475:MET:HB2	1.80	0.46
40:r:189:SER:HA	49:r:501:PLX:H1B3	1.98	0.46
43:v:61:HIS:CD2	43:v:61:HIS:H	2.33	0.46
1:A:235:VAL:H	1:A:240:THR:HG21	1.81	0.46
21:W:61:GLN:NE2	41:s:317:GLN:H	2.12	0.46
26:c:167:TYR:CE2	26:c:178:PRO:HG3	2.50	0.46
35:l:213:LEU:HB3	35:l:273:VAL:HG11	1.97	0.46
35:l:358:LYS:HG3	39:p:80:TYR:CE1	2.51	0.46
6:G:123:GLU:OE2	6:G:129:GLU:HA	2.15	0.46
12:M:498:GLN:HB2	12:M:669:ASN:ND2	2.31	0.46
26:c:78:LEU:HD12	26:c:106:HIS:HA	1.96	0.46
49:r:501:PLX:H121	49:r:501:PLX:H92	1.59	0.46
42:u:47:ARG:HD2	42:u:47:ARG:HA	1.80	0.46
12:M:506:VAL:HG12	12:M:508:GLY:H	1.81	0.46
12:M:556:THR:HA	12:M:579:MET:HE1	1.98	0.46
36:m:35:VAL:O	36:m:39:VAL:HG22	2.16	0.46
12:M:667:GLN:OE1	12:M:667:GLN:N	2.47	0.45
22:Y:71:TRP:HH2	23:Z:85:GLU:HG3	1.82	0.45
29:f:72:ARG:NH2	30:g:18:ASN:OD1	2.39	0.45
32:i:222:SER:O	32:i:224:ALA:N	2.49	0.45
35:l:338:MET:HB2	35:l:457:LEU:HB3	1.97	0.45
35:l:407:TRP:CZ2	35:l:411:MET:HE3	2.51	0.45
44:w:72:ARG:O	44:w:76:GLU:HG3	2.15	0.45
12:M:70:SER:O	12:M:184:ARG:NH1	2.48	0.45
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.99	0.45
14:O:137:THR:HG22	14:O:138:THR:H	1.80	0.45
20:V:116:ALA:O	20:V:120:LEU:HG	2.17	0.45
27:d:115:GLN:HG2	35:l:62:ILE:HG12	1.98	0.45
33:j:90:MET:SD	36:m:151:THR:HG23	2.56	0.45
50:C:304:UQ1:HM22	50:Q:501:UQ1:H103	1.98	0.45
5:F:39:LYS:HA	5:F:39:LYS:HD3	1.62	0.45
19:U:30:ILE:HD13	33:j:92:LEU:HD13	1.98	0.45
22:Y:65:MET:O	22:Y:69:ILE:HG13	2.16	0.45
43:v:35:LYS:HE3	43:v:35:LYS:HB3	1.70	0.45
8:I:113:LEU:HD23	8:I:113:LEU:HA	1.82	0.45
12:M:306:MET:HB3	12:M:314:LEU:HD22	1.99	0.45
35:l:319:ILE:HD13	35:l:399:VAL:HG12	1.97	0.45
12:M:47:THR:HG23	12:M:51:GLN:HB2	1.99	0.45
21:W:134:LEU:HD21	36:m:3:MET:SD	2.57	0.45
23:Z:18:ASP:OD2	23:Z:20:LYS:HG2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:38:PRO:HG2	38:o:70:TYR:HD1	1.81	0.45
33:j:80:GLN:HG3	41:s:318:SER:HA	1.99	0.45
53:l:702:CDL:HA62	53:l:702:CDL:C53	2.46	0.45
2:B:74:LEU:HB2	41:s:272:TRP:CZ2	2.52	0.45
5:F:61:VAL:HG23	5:F:62:GLN:N	2.30	0.45
6:G:105:MET:SD	6:G:105:MET:N	2.90	0.45
9:J:323:HIS:O	9:J:323:HIS:ND1	2.49	0.45
16:Q:47:PHE:CD1	16:Q:52:MET:HE1	2.47	0.45
18:T:64:GLU:OE2	18:T:64:GLU:HA	2.17	0.45
19:U:32:LEU:HB3	41:s:310:MET:CE	2.47	0.45
21:W:68:ARG:HD2	36:m:135:PHE:CD2	2.51	0.45
1:A:44:ASN:HD22	1:A:59:ARG:CZ	2.28	0.45
3:C:167:PRO:HD3	16:Q:223:HIS:CD2	2.51	0.45
13:N:68:MET:HG2	13:N:115:PHE:CD2	2.52	0.45
32:i:172:GLN:HB2	32:i:178:ILE:HG13	1.98	0.45
40:r:72:LEU:HB3	40:r:76:MET:HE3	1.99	0.45
49:r:501:PLX:H101	49:r:501:PLX:H72	1.61	0.45
3:C:107:GLY:HA2	45:C:301:SF4:S1	2.57	0.45
12:M:29:SER:OG	12:M:30:ASN:N	2.48	0.45
53:V:201:CDL:H612	53:V:201:CDL:H752	1.98	0.45
29:f:70:LYS:HA	29:f:75:LEU:HD23	1.99	0.45
39:p:98:LYS:HG2	39:p:178:PRO:HG3	1.98	0.45
44:w:295:ARG:HA	44:w:298:VAL:HG22	1.98	0.45
32:i:142:LEU:HB3	32:i:194:LEU:HD21	1.99	0.45
39:p:28:GLU:HB2	39:p:37:TYR:CE1	2.51	0.45
5:F:84:ALA:O	5:F:88:THR:OG1	2.31	0.45
6:G:116:VAL:O	6:G:120:MET:HG3	2.17	0.45
49:J:403:PLX:H6	49:J:403:PLX:H32	1.49	0.45
16:Q:150:ALA:HB2	16:Q:400:ILE:HG12	1.99	0.45
49:e:201:PLX:H371	40:r:447:LEU:HD11	1.99	0.45
32:i:75:ILE:HD12	34:k:40:LEU:HD22	1.99	0.45
32:i:89:MET:HG2	32:i:95:MET:HB2	1.99	0.45
34:k:31:LEU:HD21	36:m:67:VAL:HG11	1.99	0.45
35:l:233:LEU:HB3	35:l:234:PRO:HD3	1.99	0.45
35:l:529:TYR:HB3	35:l:530:PRO:HD3	1.98	0.45
39:p:159:LYS:HG2	39:p:160:GLU:OE1	2.17	0.45
48:C:302:PEE:H31	49:C:303:PLX:H392	1.99	0.44
12:M:472:PRO:O	12:M:510:TRP:NE1	2.35	0.44
14:O:242:GLY:CA	14:O:245:VAL:HG23	2.47	0.44
19:U:58:ARG:NH2	42:u:49:GLU:OE1	2.37	0.44
20:V:138:GLU:O	20:V:140:LYS:NZ	2.44	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:h:39:GLU:OE2	42:u:142:TYR:HB3	2.17	0.44
44:w:219:GLN:OE1	44:w:227:MET:HE3	2.18	0.44
1:A:325:PRO:HG3	1:A:433:TRP:HB3	1.98	0.44
25:b:80:TRP:HD1	27:d:41:VAL:HG13	1.83	0.44
32:i:128:LEU:O	32:i:132:THR:OG1	2.27	0.44
32:i:146:SER:O	32:i:149:ILE:HG22	2.17	0.44
44:w:95:ASP:OD1	44:w:95:ASP:N	2.49	0.44
17:S:50:ARG:O	17:S:54:ILE:HG23	2.17	0.44
19:U:67:PRO:HB3	19:U:72:ASP:HB2	1.98	0.44
41:s:199:ASP:OD1	41:s:199:ASP:N	2.43	0.44
4:E:70:ASN:OD1	52:G:201:8Q1:O4	2.35	0.44
20:V:73:THR:OG1	20:V:93:GLY:HA2	2.17	0.44
21:W:120:MET:HE2	36:m:127:ILE:HA	1.98	0.44
35:l:128:MET:HE1	35:l:255:ALA:HB2	1.99	0.44
40:r:94:LEU:O	40:r:98:MET:HG2	2.17	0.44
40:r:266:MET:HA	40:r:269:MET:HE2	2.00	0.44
43:v:18:ASP:O	43:v:22:MET:HB2	2.18	0.44
5:F:36:PHE:CD2	5:F:87:VAL:HG23	2.53	0.44
53:l:702:CDL:C81	53:l:702:CDL:H611	2.48	0.44
40:r:41:LEU:O	40:r:44:GLN:NE2	2.50	0.44
40:r:210:TYR:CG	40:r:268:GLY:HA3	2.52	0.44
1:A:316:ALA:HB3	1:A:357:MET:HE3	2.00	0.44
48:V:202:PEE:H40	48:V:202:PEE:H79	2.00	0.44
53:V:203:CDL:H792	53:V:203:CDL:H761	1.70	0.44
26:c:96:ASP:N	26:c:96:ASP:OD1	2.51	0.44
26:c:166:LEU:HD12	26:c:170:ARG:NH2	2.32	0.44
31:h:86:LEU:O	31:h:90:GLY:N	2.50	0.44
32:i:30:TRP:O	32:i:34:GLU:HG2	2.18	0.44
35:l:153:LEU:CD1	53:l:702:CDL:H111	2.48	0.44
1:A:210:THR:O	1:A:214:GLU:HG2	2.18	0.44
53:V:204:CDL:H811	34:k:17:ALA:HB2	2.00	0.44
6:X:151:LYS:HA	6:X:151:LYS:HD2	1.59	0.44
35:l:435:PRO:HB3	35:l:437:PHE:CZ	2.52	0.44
44:w:180:ARG:NH1	44:w:316:GLU:OE2	2.50	0.44
7:H:76:GLN:O	7:H:78:GLU:N	2.51	0.44
12:M:441:ARG:HE	12:M:441:ARG:HB2	1.62	0.44
14:O:242:GLY:HA2	14:O:245:VAL:HG23	1.98	0.44
20:V:17:GLU:OE1	20:V:20:ARG:NE	2.51	0.44
21:W:52:LYS:HE2	21:W:52:LYS:HB2	1.62	0.44
35:l:211:MET:HE3	35:l:211:MET:HB2	1.83	0.44
35:l:359:MET:O	35:l:436:ARG:NH2	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:1:MET:HE1	36:m:122:LEU:HA	1.98	0.44
48:B:303:PEE:H55	48:B:303:PEE:H61	1.78	0.44
12:M:47:THR:O	12:M:96:VAL:HG22	2.18	0.44
15:P:43:THR:HA	15:P:47:ILE:HD12	2.00	0.44
15:P:132:LEU:HB2	15:P:141:ILE:HG22	2.00	0.44
53:g:202:CDL:H872	53:g:202:CDL:H841	1.82	0.44
39:p:108:HIS:CD2	39:p:109:PRO:HD2	2.53	0.44
40:r:196:TRP:HB2	40:r:253:LEU:HD23	2.00	0.44
44:w:83:LEU:HD22	44:w:156:GLY:HA3	1.99	0.44
1:A:149:MET:CE	1:A:241:THR:HB	2.48	0.43
4:E:119:LEU:HD11	12:M:628:GLU:HG2	1.99	0.43
49:J:403:PLX:H142	33:j:20:ILE:HG13	1.99	0.43
16:Q:37:TRP:CD2	40:r:140:THR:HB	2.52	0.43
16:Q:292:MET:HE3	16:Q:292:MET:HB3	1.80	0.43
23:Z:32:VAL:HG21	39:p:35:ASP:HB2	2.00	0.43
42:u:79:ALA:O	42:u:83:THR:OG1	2.32	0.43
42:u:103:GLN:OE1	42:u:103:GLN:N	2.50	0.43
1:A:284:HIS:ND1	14:O:228:ALA:HB3	2.33	0.43
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.53	0.43
3:C:62:LEU:O	3:C:91:VAL:HA	2.19	0.43
26:c:58:ARG:NE	38:o:35:GLU:OE2	2.35	0.43
35:l:332:HIS:HA	35:l:335:PHE:CE2	2.54	0.43
40:r:106:LEU:HD13	40:r:234:VAL:HG11	2.00	0.43
43:v:28:ASP:O	43:v:28:ASP:OD1	2.36	0.43
3:C:43:GLY:O	3:C:47:VAL:HG13	2.17	0.43
5:F:40:ARG:HE	5:F:40:ARG:HB3	1.63	0.43
8:I:39:PRO:HB2	8:I:41:LEU:HD13	2.00	0.43
9:J:257:ASP:OD1	9:J:257:ASP:N	2.51	0.43
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.99	0.43
20:V:104:ARG:HD2	20:V:104:ARG:HA	1.84	0.43
53:l:702:CDL:H351	53:l:702:CDL:H392	1.99	0.43
53:l:702:CDL:H651	53:l:702:CDL:H852	1.99	0.43
40:r:370:PRO:HB3	40:r:375:LEU:HD22	1.99	0.43
1:A:337:MET:HE2	1:A:342:LEU:HD11	2.01	0.43
8:I:34:ARG:HA	8:I:34:ARG:HD2	1.90	0.43
53:a:201:CDL:H441	53:a:201:CDL:H411	1.79	0.43
28:e:81:ILE:HD13	28:e:81:ILE:HA	1.86	0.43
40:r:108:MET:HE2	40:r:121:LEU:HD21	1.98	0.43
40:r:248:THR:HG23	40:r:249:ILE:HG23	2.01	0.43
40:r:287:ALA:O	40:r:291:VAL:HG23	2.18	0.43
40:r:329:LEU:HG	40:r:437:MET:HE2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:LYS:HE2	10:K:98:MET:HE1	2.01	0.43
1:A:210:THR:HB	1:A:224:ARG:HG2	2.01	0.43
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.53	0.43
8:I:66:PRO:HB3	15:P:79:SER:HA	2.00	0.43
11:L:78:ARG:NH1	11:L:148:GLU:OE2	2.50	0.43
6:X:117:GLU:OE2	39:p:20:TYR:OH	2.29	0.43
32:i:141:VAL:O	32:i:145:ILE:HG12	2.19	0.43
32:i:186:HIS:O	32:i:190:MET:HE3	2.18	0.43
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.53	0.43
35:l:559:GLU:O	35:l:563:PRO:HD2	2.19	0.43
40:r:203:PHE:HB2	40:r:243:MET:HG3	2.00	0.43
15:P:119:VAL:HG12	15:P:121:THR:HG22	2.01	0.43
23:Z:33:GLN:HA	23:Z:33:GLN:NE2	2.33	0.43
28:e:77:ASP:OD1	28:e:78:LYS:N	2.52	0.43
37:n:30:ARG:HG3	37:n:30:ARG:NH1	2.32	0.43
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.74	0.43
23:Z:18:ASP:O	23:Z:21:GLN:HG2	2.19	0.43
35:l:37:LYS:HB3	35:l:37:LYS:HE3	1.79	0.43
44:w:165:SER:O	44:w:168:VAL:HG22	2.18	0.43
1:A:383:THR:HG21	12:M:120:LEU:HG	2.00	0.43
5:F:90:THR:O	5:F:94:VAL:HG23	2.18	0.43
14:O:231:LEU:HD12	14:O:231:LEU:HA	1.85	0.43
26:c:126:TRP:O	26:c:127:ASN:HB2	2.18	0.43
28:e:92:PHE:O	28:e:96:SER:HB2	2.18	0.43
30:g:4:MET:O	30:g:10:ARG:NH1	2.51	0.43
35:l:525:MET:SD	39:p:77:PRO:HB3	2.59	0.43
10:K:92:GLU:OE2	10:K:92:GLU:HA	2.19	0.43
19:U:27:GLY:O	19:U:31:ILE:HG23	2.19	0.43
21:W:51:MET:HA	41:s:313:SER:HB2	2.01	0.43
30:g:117:GLU:OE1	30:g:117:GLU:N	2.31	0.43
53:l:703:CDL:H362	53:l:703:CDL:H332	1.85	0.43
39:p:107:TRP:HB2	39:p:112:LYS:HE3	2.00	0.43
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.83	0.43
3:C:98:ARG:NH2	33:j:35:SER:O	2.50	0.43
6:G:124:ASP:OD1	6:G:124:ASP:C	2.62	0.43
17:S:45:TRP:CD1	21:W:140:PHE:HB2	2.54	0.43
17:S:66:LEU:HD11	42:u:74:ILE:HG22	2.00	0.43
29:f:43:LYS:O	29:f:47:THR:OG1	2.37	0.43
33:j:19:LEU:HD12	33:j:23:TRP:CD1	2.54	0.43
35:l:297:ASP:O	35:l:301:ILE:HG13	2.19	0.43
40:r:187:SER:OG	40:r:188:ASN:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:375:LEU:O	40:r:375:LEU:HG	2.18	0.43
41:s:72:ILE:HG21	48:s:401:PEE:H18	2.01	0.43
41:s:179:TRP:CG	41:s:180:PRO:HD3	2.54	0.43
42:u:34:ALA:HB2	42:u:120:PRO:HG3	1.99	0.43
1:A:81:LYS:HG2	1:A:96:GLY:HA3	2.00	0.42
1:A:102:MET:HE3	1:A:111:LYS:HB3	2.01	0.42
3:C:52:ASP:HB3	49:C:303:PLX:H251	2.01	0.42
3:C:84:TYR:CE1	3:C:171:GLU:HG3	2.54	0.42
7:H:6:LYS:HE3	7:H:9:THR:HG22	2.01	0.42
48:U:101:PEE:H30	48:U:101:PEE:H35	1.74	0.42
53:V:204:CDL:H131	53:V:204:CDL:H161	1.82	0.42
25:b:80:TRP:CD1	27:d:41:VAL:HG13	2.54	0.42
29:f:52:VAL:O	29:f:56:ILE:HG23	2.19	0.42
32:i:234:TRP:CZ2	32:i:304:MET:HB3	2.54	0.42
35:l:3:PRO:HG2	35:l:53:MET:HE1	2.00	0.42
35:l:54:PHE:CZ	35:l:84:TYR:HB2	2.55	0.42
48:l:705:PEE:H33	48:l:705:PEE:H28	1.79	0.42
41:s:209:SER:HB3	41:s:213:VAL:HA	2.00	0.42
3:C:154:ASP:HA	3:C:157:VAL:O	2.18	0.42
53:V:204:CDL:H432	53:V:204:CDL:H402	1.88	0.42
33:j:97:LEU:HD23	33:j:97:LEU:HA	1.85	0.42
35:l:49:VAL:HB	35:l:50:PRO:HD3	2.01	0.42
1:A:128:ARG:NH2	14:O:194:GLU:OE2	2.49	0.42
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.55	0.42
12:M:162:ASP:O	18:T:104:LYS:NZ	2.50	0.42
12:M:689:LEU:HD23	12:M:689:LEU:HA	1.82	0.42
13:N:144:TYR:HD1	13:N:144:TYR:H	1.67	0.42
19:U:67:PRO:HG3	19:U:74:GLN:C	2.44	0.42
23:Z:24:ILE:HD12	23:Z:30:GLU:HA	2.01	0.42
23:Z:30:GLU:O	23:Z:34:GLU:HG3	2.20	0.42
53:l:702:CDL:H421	40:r:445:LEU:HB3	2.01	0.42
44:w:219:GLN:OE1	44:w:219:GLN:HA	2.19	0.42
46:A:502:FMN:N1	46:A:502:FMN:O3'	2.33	0.42
2:B:41:VAL:HA	8:I:113:LEU:HB2	2.02	0.42
22:Y:89:PRO:HD2	22:Y:90:SER:N	2.35	0.42
26:c:105:ILE:CG2	26:c:109:LEU:HD22	2.48	0.42
35:l:173:LEU:HD12	40:r:405:LEU:HD21	2.01	0.42
48:l:705:PEE:H60	48:l:705:PEE:H55	1.76	0.42
3:C:113:MET:HE3	16:Q:94:VAL:HG12	2.02	0.42
8:I:97:PRO:HD3	15:P:61:PHE:CE1	2.54	0.42
12:M:197:THR:O	14:O:114:GLU:HG2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:432:LEU:HB2	16:Q:456:ILE:HD13	2.02	0.42
21:W:98:MET:HE3	21:W:98:MET:HB3	1.88	0.42
23:Z:33:GLN:CA	23:Z:33:GLN:HE21	2.32	0.42
25:b:88:TYR:CE1	27:d:49:ARG:HG2	2.54	0.42
28:e:76:TYR:HB2	28:e:83:ASP:OD1	2.20	0.42
35:l:60:GLU:HB3	35:l:83:ASP:HA	2.01	0.42
44:w:206:TYR:CD2	44:w:246:LEU:HD11	2.54	0.42
2:B:86:TYR:CE1	3:C:171:GLU:HG2	2.54	0.42
8:I:42:PRO:HD3	21:W:6:VAL:HG13	2.02	0.42
12:M:295:ASP:OD1	12:M:704:SER:OG	2.28	0.42
20:V:2:ALA:HB1	35:l:605:HIS:NE2	2.35	0.42
24:a:70:LEU:HD22	28:e:87:MET:HE1	2.02	0.42
27:d:127:LYS:O	27:d:131:GLN:HG3	2.19	0.42
1:A:115:VAL:HG22	1:A:248:VAL:HG21	2.02	0.42
12:M:347:ASP:OD1	12:M:347:ASP:N	2.46	0.42
13:N:85:GLU:HG2	13:N:86:TRP:H	1.83	0.42
16:Q:245:TYR:O	16:Q:249:LYS:HG2	2.20	0.42
21:W:50:MET:HG2	41:s:156:MET:SD	2.59	0.42
26:c:168:LEU:HA	26:c:172:GLY:HA2	2.02	0.42
35:l:2:ASN:O	35:l:4:PHE:N	2.52	0.42
40:r:122:PHE:CE2	40:r:206:LYS:HE3	2.55	0.42
44:w:254:GLU:CD	44:w:254:GLU:H	2.27	0.42
1:A:131:ILE:HD13	1:A:158:ILE:HD12	2.02	0.42
2:B:131:GLU:HB2	2:B:144:ARG:HB3	2.02	0.42
2:B:179:THR:OG1	2:B:182:GLU:OE2	2.36	0.42
20:V:106:ARG:HA	20:V:106:ARG:NE	2.34	0.42
6:X:107:ASP:OD1	6:X:107:ASP:N	2.53	0.42
27:d:109:ARG:NH1	28:e:130:GLU:OE2	2.38	0.42
32:i:41:ILE:HG13	34:k:73:LEU:HD21	2.00	0.42
32:i:244:MET:HE3	32:i:244:MET:HB2	1.83	0.42
40:r:202:ALA:O	40:r:205:VAL:HG12	2.19	0.42
40:r:370:PRO:CB	40:r:375:LEU:HD22	2.50	0.42
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.50	0.42
42:u:137:LEU:HD12	42:u:138:PRO:HD2	2.01	0.42
8:I:43:VAL:HG23	8:I:44:GLY:H	1.85	0.42
48:i:401:PEE:H14	48:i:401:PEE:H1	1.79	0.42
53:l:703:CDL:H401	53:l:703:CDL:H371	1.75	0.42
40:r:22:MET:HE3	40:r:22:MET:HB3	1.97	0.42
44:w:88:GLU:N	44:w:160:GLU:HG3	2.35	0.42
1:A:38:GLU:H	1:A:38:GLU:CD	2.28	0.42
12:M:476:LEU:HD21	12:M:481:LEU:HD21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:284:MET:HE1	40:r:158:LEU:HB2	2.02	0.42
36:m:16:GLY:HA2	53:s:402:CDL:H791	2.02	0.42
42:u:14:LYS:HB2	42:u:14:LYS:HE2	1.78	0.42
44:w:43:PHE:O	44:w:48:ARG:NH2	2.41	0.42
9:J:171:ASN:HA	9:J:327:MET:SD	2.60	0.41
19:U:28:LEU:HD23	19:U:28:LEU:HA	1.89	0.41
25:b:86:LEU:HD23	25:b:90:VAL:HG21	2.01	0.41
44:w:292:HIS:O	44:w:296:MET:HG2	2.20	0.41
9:J:204:SER:OG	9:J:238:GLN:O	2.39	0.41
10:K:105:ARG:HH22	12:M:426:ASP:CG	2.28	0.41
13:N:85:GLU:HG2	13:N:86:TRP:N	2.35	0.41
23:Z:33:GLN:NE2	23:Z:33:GLN:CA	2.83	0.41
24:a:170:GLN:O	30:g:6:GLY:HA3	2.21	0.41
25:b:112:GLU:OE2	27:d:17:THR:HG22	2.20	0.41
35:l:264:TYR:CG	35:l:265:PRO:HD3	2.55	0.41
40:r:455:LEU:HD23	40:r:455:LEU:HA	1.95	0.41
41:s:198:PHE:CD1	41:s:285:LEU:HD13	2.55	0.41
53:s:402:CDL:H801	53:s:402:CDL:H771	1.84	0.41
1:A:152:ARG:CZ	10:K:101:PRO:HD3	2.50	0.41
9:J:302:GLY:O	9:J:306:GLU:HG3	2.20	0.41
48:W:201:PEE:H46	48:W:201:PEE:H39	1.83	0.41
53:l:702:CDL:H811	53:l:702:CDL:H611	2.02	0.41
40:r:205:VAL:HG23	40:r:212:LEU:HB3	2.02	0.41
40:r:290:SER:HA	40:r:319:HIS:HE2	1.86	0.41
42:u:30:HIS:HB3	42:u:120:PRO:HD2	2.01	0.41
6:G:88:LYS:HB3	6:G:88:LYS:HE2	1.92	0.41
12:M:55:LYS:HE2	12:M:55:LYS:HB2	1.76	0.41
12:M:219:SER:O	12:M:222:ILE:HG12	2.19	0.41
16:Q:53:TYR:OH	32:i:295:ARG:NH2	2.53	0.41
32:i:102:LEU:HD13	32:i:142:LEU:HG	2.03	0.41
35:l:63:ILE:O	35:l:79:SER:HA	2.21	0.41
35:l:230:HIS:N	35:l:231:PRO:HD3	2.35	0.41
40:r:304:GLN:HE21	40:r:304:GLN:HB2	1.66	0.41
44:w:171:GLU:O	44:w:175:ARG:HG2	2.19	0.41
12:M:208:THR:OG1	12:M:210:ILE:O	2.36	0.41
21:W:131:GLU:CD	21:W:131:GLU:H	2.28	0.41
27:d:9:VAL:O	27:d:109:ARG:NH2	2.54	0.41
40:r:186:LEU:HD23	40:r:186:LEU:HA	1.85	0.41
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.56	0.41
40:r:406:TYR:O	40:r:409:TYR:HB3	2.21	0.41
9:J:318:LYS:O	9:J:322:VAL:HG23	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:J:402:UQ:HM53	51:J:402:UQ:H72	1.79	0.41
13:N:85:GLU:HB2	13:N:98:PRO:HB3	2.03	0.41
16:Q:238:LEU:HD23	16:Q:238:LEU:HA	1.81	0.41
16:Q:342:ARG:HD2	21:W:21:TYR:CZ	2.55	0.41
26:c:160:GLN:HG2	26:c:183:HIS:CE1	2.56	0.41
32:i:170:LEU:HD11	32:i:288:LEU:HD22	2.02	0.41
32:i:278:MET:HB3	32:i:279:PRO:HD3	2.03	0.41
40:r:8:THR:HG22	40:r:100:ILE:HG23	2.03	0.41
49:r:501:PLX:H51	49:r:501:PLX:H6	1.38	0.41
44:w:259:SER:OG	44:w:262:GLU:OE1	2.37	0.41
12:M:460:HIS:O	12:M:463:SER:OG	2.26	0.41
15:P:94:ILE:HD13	15:P:94:ILE:HA	1.86	0.41
23:Z:59:ASN:OD1	23:Z:59:ASN:N	2.52	0.41
24:a:66:ARG:HH12	28:e:72:ASP:HB2	1.85	0.41
24:a:106:VAL:HB	37:n:50:ARG:HH21	1.85	0.41
35:l:6:SER:O	35:l:10:THR:OG1	2.29	0.41
37:n:39:ARG:HG3	37:n:57:TRP:CE2	2.56	0.41
40:r:373:ILE:HA	40:r:376:ILE:HD12	2.02	0.41
41:s:139:THR:HA	41:s:142:TYR:CE2	2.56	0.41
1:A:417:LYS:HD3	1:A:417:LYS:HA	1.90	0.41
4:E:17:VAL:HG21	11:L:55:VAL:HG22	2.02	0.41
6:G:107:ASP:OD1	6:G:107:ASP:N	2.53	0.41
9:J:259:LYS:HD3	9:J:259:LYS:HA	1.91	0.41
12:M:470:LYS:HE2	12:M:470:LYS:HB2	1.63	0.41
13:N:42:ASP:HB3	13:N:44:TYR:H	1.84	0.41
15:P:197:PRO:O	16:Q:122:LYS:NZ	2.41	0.41
19:U:52:ASN:HB3	24:a:185:THR:HG22	2.03	0.41
48:U:101:PEE:H67	48:U:101:PEE:H73	1.72	0.41
27:d:48:ALA:O	27:d:52:ILE:HG12	2.21	0.41
35:l:332:HIS:HA	35:l:335:PHE:CZ	2.56	0.41
35:l:534:HIS:CD2	48:l:704:PEE:H13	2.56	0.41
40:r:72:LEU:HD21	40:r:233:ALA:HB3	2.02	0.41
41:s:142:TYR:CZ	41:s:192:GLU:HG2	2.56	0.41
43:v:87:TRP:NE1	43:v:91:GLU:OE2	2.54	0.41
44:w:227:MET:SD	44:w:227:MET:N	2.94	0.41
3:C:126:GLU:HG2	9:J:89:TYR:OH	2.21	0.41
50:C:304:UQ1:HM21	16:Q:189:THR:HG21	2.03	0.41
9:J:124:ASN:OD1	9:J:125:VAL:HG23	2.21	0.41
9:J:135:GLU:HG2	9:J:140:ASP:HA	2.02	0.41
12:M:360:ARG:HG2	12:M:360:ARG:HH11	1.85	0.41
12:M:483:ARG:H	12:M:483:ARG:HG3	1.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:197:PRO:HA	15:P:202:PHE:CG	2.56	0.41
16:Q:74:ASP:OD1	16:Q:74:ASP:N	2.45	0.41
16:Q:123:LEU:O	16:Q:127:LYS:HG2	2.21	0.41
20:V:34:LEU:HD23	20:V:34:LEU:HA	1.93	0.41
53:V:203:CDL:H872	53:V:203:CDL:H841	1.91	0.41
23:Z:32:VAL:HG13	39:p:39:TYR:HB2	2.02	0.41
26:c:162:PRO:CB	43:v:39:MET:HG3	2.51	0.41
31:h:13:ASP:OD1	31:h:16:ARG:HB2	2.21	0.41
32:i:296:LEU:HD12	32:i:296:LEU:HA	1.92	0.41
35:l:66:TRP:CD1	48:l:705:PEE:H16	2.56	0.41
35:l:502:LEU:HD12	35:l:502:LEU:HA	1.90	0.41
38:o:105:PHE:HD2	40:r:263:MET:HE2	1.85	0.41
40:r:121:LEU:O	40:r:125:THR:HG23	2.21	0.41
41:s:109:SER:HB2	41:s:192:GLU:OE1	2.21	0.41
41:s:144:VAL:O	41:s:148:ILE:HG13	2.21	0.41
41:s:204:GLU:HA	41:s:208:VAL:O	2.20	0.41
44:w:71:GLY:O	44:w:75:ARG:HG3	2.21	0.41
1:A:211:ALA:HB2	1:A:223:PRO:HG3	2.02	0.41
48:C:302:PEE:H66	48:C:302:PEE:H32	2.01	0.41
5:F:23:LEU:O	5:F:57:GLU:HA	2.21	0.41
7:H:6:LYS:O	7:H:16:VAL:HG11	2.20	0.41
7:H:58:MET:HE1	7:H:72:LEU:HA	2.03	0.41
12:M:632:MET:HE2	12:M:632:MET:HB3	1.96	0.41
17:S:43:TYR:CZ	21:W:68:ARG:HG3	2.56	0.41
23:Z:53:TYR:CE2	35:l:434:LYS:HG3	2.56	0.41
30:g:48:ASN:HB3	30:g:55:VAL:HA	2.03	0.41
39:p:34:ARG:HD2	39:p:34:ARG:HA	1.81	0.41
41:s:2:PHE:CE2	41:s:6:ILE:HD11	2.55	0.41
41:s:133:LEU:HD13	41:s:133:LEU:HA	1.97	0.41
51:C:305:UQ:H152	51:C:305:UQ:H121	1.85	0.40
4:E:66:MET:CG	52:G:201:8Q1:C11	2.93	0.40
50:Q:501:UQ1:H71	50:Q:501:UQ1:HM51	1.81	0.40
6:X:99:SER:O	6:X:102:SER:OG	2.35	0.40
27:d:74:ILE:HD12	27:d:74:ILE:HA	1.97	0.40
33:j:73:LEU:HD23	33:j:73:LEU:HA	1.81	0.40
39:p:174:PRO:O	39:p:175:ARG:HB2	2.21	0.40
42:u:31:HIS:O	42:u:35:GLN:HG2	2.21	0.40
47:A:503:NAI:H6N	47:A:503:NAI:H2D	1.82	0.40
2:B:63:TRP:HE1	48:B:303:PEE:H13	1.86	0.40
3:C:72:CYS:HB3	3:C:133:MET:SD	2.62	0.40
4:E:62:LYS:O	4:E:66:MET:HG2	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:40:LEU:HD23	9:J:40:LEU:HA	1.88	0.40
12:M:224:ASP:OD2	12:M:291:ARG:NH2	2.51	0.40
22:Y:100:LEU:HB2	43:v:111:ARG:NH2	2.36	0.40
25:b:32:GLU:HB3	39:p:115:TYR:HD1	1.86	0.40
29:f:60:LYS:O	29:f:64:GLU:HG3	2.21	0.40
32:i:10:ILE:O	32:i:14:MET:HG3	2.21	0.40
36:m:95:SER:O	36:m:99:MET:HG2	2.21	0.40
43:v:87:TRP:O	43:v:91:GLU:HG2	2.20	0.40
2:B:39:LYS:HD2	16:Q:335:GLU:HG2	2.03	0.40
48:B:303:PEE:H38	48:B:303:PEE:H43	1.87	0.40
23:Z:72:LYS:HB3	23:Z:72:LYS:HE3	1.89	0.40
1:A:298:GLU:O	1:A:302:LYS:HB2	2.22	0.40
2:B:114:ILE:H	2:B:114:ILE:HG13	1.83	0.40
3:C:113:MET:HE2	16:Q:115:LEU:HB3	2.03	0.40
6:G:119:ILE:HD13	6:G:119:ILE:HA	1.84	0.40
7:H:33:ASP:C	7:H:33:ASP:OD1	2.64	0.40
26:c:127:ASN:O	26:c:131:LYS:HG3	2.20	0.40
28:e:70:ASN:HB3	28:e:73:SER:HB2	2.03	0.40
42:u:83:THR:HA	42:u:86:TRP:NE1	2.36	0.40
1:A:375:LYS:NZ	14:O:33:GLY:O	2.55	0.40
10:K:98:MET:HA	10:K:98:MET:HE3	2.04	0.40
16:Q:259:GLU:OE1	21:W:23:ARG:HD3	2.22	0.40
21:W:50:MET:HA	21:W:50:MET:HE3	2.03	0.40
26:c:88:PRO:HB3	26:c:98:ARG:NH2	2.36	0.40
27:d:122:ARG:HD3	27:d:122:ARG:HA	1.78	0.40
32:i:100:MET:HE3	32:i:111:PHE:CZ	2.56	0.40
33:j:83:ASN:OD1	33:j:83:ASN:N	2.47	0.40
35:l:124:PHE:HE1	35:l:252:MET:HB2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/433 (100%)	417 (97%)	14 (3%)	0	100	100
2	B	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
3	C	154/156 (99%)	147 (96%)	7 (4%)	0	100	100
4	E	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
5	F	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
6	G	86/88 (98%)	82 (95%)	3 (4%)	1 (1%)	10	27
6	X	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
7	H	110/112 (98%)	102 (93%)	7 (6%)	1 (1%)	14	35
8	I	93/112 (83%)	82 (88%)	11 (12%)	0	100	100
9	J	340/342 (99%)	329 (97%)	10 (3%)	1 (0%)	36	60
10	K	41/43 (95%)	41 (100%)	0	0	100	100
11	L	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
12	M	688/690 (100%)	670 (97%)	18 (3%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	203 (94%)	11 (5%)	1 (0%)	24	48
15	P	206/208 (99%)	200 (97%)	6 (3%)	0	100	100
16	Q	427/430 (99%)	414 (97%)	13 (3%)	0	100	100
17	S	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
18	T	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
19	U	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
20	V	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
21	W	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
22	Y	65/70 (93%)	60 (92%)	5 (8%)	0	100	100
23	Z	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
24	a	136/140 (97%)	131 (96%)	5 (4%)	0	100	100
25	b	94/126 (75%)	88 (94%)	6 (6%)	0	100	100
26	c	154/156 (99%)	147 (96%)	6 (4%)	1 (1%)	21	44
27	d	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
28	e	102/107 (95%)	98 (96%)	4 (4%)	0	100	100
29	f	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
30	g	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
31	h	103/105 (98%)	97 (94%)	6 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	i	345/347 (99%)	330 (96%)	15 (4%)	0	100	100
33	j	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
34	k	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
35	l	604/606 (100%)	584 (97%)	20 (3%)	0	100	100
36	m	173/175 (99%)	162 (94%)	11 (6%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
39	p	176/178 (99%)	170 (97%)	5 (3%)	1 (1%)	21	44
40	r	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
41	s	316/318 (99%)	308 (98%)	7 (2%)	1 (0%)	36	60
42	u	169/171 (99%)	164 (97%)	4 (2%)	1 (1%)	21	44
43	v	122/125 (98%)	116 (95%)	6 (5%)	0	100	100
44	w	318/320 (99%)	307 (96%)	11 (4%)	0	100	100
All	All	8175/8326 (98%)	7890 (96%)	277 (3%)	8 (0%)	49	73

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	H	77	ILE
14	O	243	PHE
41	s	208	VAL
9	J	38	HIS
26	c	106	HIS
6	G	134	ASP
39	p	174	PRO
42	u	152	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/346 (100%)	340 (98%)	6 (2%)	53	79
2	B	151/151 (100%)	148 (98%)	3 (2%)	48	76
3	C	132/132 (100%)	130 (98%)	2 (2%)	57	81
4	E	107/107 (100%)	104 (97%)	3 (3%)	38	68
5	F	75/76 (99%)	75 (100%)	0	100	100
6	G	76/81 (94%)	76 (100%)	0	100	100
6	X	79/81 (98%)	78 (99%)	1 (1%)	61	83
7	H	99/99 (100%)	97 (98%)	2 (2%)	48	76
8	I	87/97 (90%)	85 (98%)	2 (2%)	44	73
9	J	296/296 (100%)	295 (100%)	1 (0%)	86	94
10	K	42/42 (100%)	42 (100%)	0	100	100
11	L	113/113 (100%)	111 (98%)	2 (2%)	51	78
12	M	580/580 (100%)	573 (99%)	7 (1%)	63	84
13	N	130/130 (100%)	129 (99%)	1 (1%)	73	88
14	O	180/183 (98%)	178 (99%)	2 (1%)	65	85
15	P	190/190 (100%)	188 (99%)	2 (1%)	65	85
16	Q	370/370 (100%)	366 (99%)	4 (1%)	65	85
17	S	57/58 (98%)	57 (100%)	0	100	100
18	T	79/79 (100%)	78 (99%)	1 (1%)	61	83
19	U	69/69 (100%)	68 (99%)	1 (1%)	59	82
20	V	101/101 (100%)	99 (98%)	2 (2%)	48	76
21	W	121/123 (98%)	118 (98%)	3 (2%)	42	71
22	Y	62/63 (98%)	60 (97%)	2 (3%)	34	64
23	Z	62/65 (95%)	61 (98%)	1 (2%)	55	80
24	a	121/122 (99%)	120 (99%)	1 (1%)	73	88
25	b	90/119 (76%)	89 (99%)	1 (1%)	65	85
26	c	139/141 (99%)	135 (97%)	4 (3%)	37	67
27	d	155/155 (100%)	153 (99%)	2 (1%)	61	83
28	e	96/99 (97%)	94 (98%)	2 (2%)	47	75
29	f	36/45 (80%)	36 (100%)	0	100	100
30	g	108/109 (99%)	104 (96%)	4 (4%)	30	59
31	h	92/93 (99%)	92 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	i	311/311 (100%)	308 (99%)	3 (1%)	68	86
33	j	100/100 (100%)	97 (97%)	3 (3%)	36	66
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	540/540 (100%)	532 (98%)	8 (2%)	57	81
36	m	129/141 (92%)	127 (98%)	2 (2%)	55	80
37	n	53/53 (100%)	52 (98%)	1 (2%)	50	77
38	o	112/113 (99%)	112 (100%)	0	100	100
39	p	159/159 (100%)	158 (99%)	1 (1%)	78	91
40	r	409/410 (100%)	404 (99%)	5 (1%)	63	84
41	s	274/275 (100%)	271 (99%)	3 (1%)	65	85
42	u	153/153 (100%)	152 (99%)	1 (1%)	76	90
43	v	104/111 (94%)	103 (99%)	1 (1%)	68	86
44	w	281/283 (99%)	275 (98%)	6 (2%)	47	75
All	All	7151/7249 (99%)	7055 (99%)	96 (1%)	59	83

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LYS
1	A	69	LEU
1	A	184	LYS
1	A	245	VAL
1	A	271	SER
1	A	273	THR
2	B	114	ILE
2	B	139	SER
2	B	165	ASP
3	C	71	CYS
3	C	142	TYR
4	E	17	VAL
4	E	69	LYS
4	E	74	THR
7	H	40	LYS
7	H	104	VAL
8	I	25	GLN
8	I	31	ILE
9	J	205	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	L	86	ASN
11	L	165	SER
12	M	171	THR
12	M	295	ASP
12	M	352	VAL
12	M	361	VAL
12	M	398	ASP
12	M	672	SER
12	M	677	GLN
13	N	15	SER
14	O	163	THR
14	O	186	VAL
15	P	56	LYS
15	P	77	GLN
16	Q	217	VAL
16	Q	258	LEU
16	Q	272	THR
16	Q	308	TYR
18	T	77	SER
19	U	32	LEU
20	V	80	VAL
20	V	115	CYS
21	W	64	ASP
21	W	85	GLN
21	W	120	MET
6	X	102	SER
22	Y	64	THR
22	Y	77	SER
23	Z	33	GLN
24	a	71	MET
25	b	109	THR
26	c	33	THR
26	c	59	VAL
26	c	120	SER
26	c	156	VAL
27	d	17	THR
27	d	25	SER
28	e	55	LEU
28	e	116	GLU
30	g	22	SER
30	g	57	SER
30	g	69	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	g	97	LYS
32	i	225	THR
32	i	322	GLN
32	i	336	VAL
33	j	1	MET
33	j	87	MET
33	j	105	GLU
35	l	99	SER
35	l	140	LEU
35	l	185	SER
35	l	272	LEU
35	l	340	PHE
35	l	359	MET
35	l	457	LEU
35	l	514	LYS
36	m	82	VAL
36	m	102	CYS
37	n	4	VAL
39	p	110	SER
40	r	122	PHE
40	r	179	ILE
40	r	183	SER
40	r	247	THR
40	r	304	GLN
41	s	40	VAL
41	s	177	THR
41	s	178	SER
42	u	74	ILE
43	v	90	CYS
44	w	41	LEU
44	w	45	LEU
44	w	47	GLU
44	w	95	ASP
44	w	203	VAL
44	w	208	ASP

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

Mol	Chain	Res	Type
1	A	44	ASN
1	A	136	HIS
1	A	164	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	393	ASN
3	C	111	ASN
4	E	70	ASN
4	E	126	HIS
5	F	86	GLN
6	G	115	GLN
8	I	29	GLN
8	I	51	ASN
9	J	128	ASN
9	J	154	GLN
11	L	71	HIS
11	L	85	ASN
12	M	123	ASN
12	M	425	ASN
12	M	453	GLN
12	M	460	HIS
12	M	569	GLN
12	M	604	GLN
13	N	113	HIS
13	N	123	GLN
14	O	90	ASN
14	O	153	GLN
15	P	55	HIS
15	P	63	GLN
15	P	75	GLN
15	P	77	GLN
15	P	180	ASN
15	P	196	HIS
15	P	228	GLN
16	Q	223	HIS
16	Q	313	GLN
17	S	40	HIS
20	V	134	GLN
21	W	61	GLN
21	W	76	GLN
23	Z	21	GLN
23	Z	48	ASN
24	a	181	HIS
25	b	13	GLN
27	d	23	GLN
27	d	107	GLN
28	e	86	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	f	62	HIS
31	h	21	GLN
32	i	77	ASN
32	i	91	ASN
32	i	144	GLN
34	k	92	ASN
35	l	72	GLN
35	l	109	HIS
35	l	136	ASN
35	l	200	GLN
35	l	274	GLN
35	l	296	ASN
36	m	86	ASN
38	o	50	GLN
39	p	12	HIS
40	r	366	ASN
40	r	390	ASN
41	s	194	ASN
41	s	304	HIS
42	u	95	GLN
43	v	85	HIS
44	w	132	GLN
44	w	223	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	2MR	Q	118	16	10,12,13	1.98	1 (10%)	5,13,15	6.00	3 (60%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	2MR	Q	118	16	-	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	5.68	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	12.26	130.72	119.48
16	Q	118	2MR	CD-NE-CZ	4.10	131.07	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.36	130.85	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 47 ligands modelled in this entry, 2 are monoatomic - leaving 45 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$
48	PEE	i	401	-	46,46,50	1.23	6 (13%)	49,51,55	1.04	2 (4%)
53	CDL	s	402	-	88,88,99	1.17	8 (9%)	94,100,111	0.90	4 (4%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
53	CDL	V	204	-	93,93,99	1.14	8 (8%)	99,105,111	0.87	4 (4%)
48	PEE	W	201	-	40,40,50	1.17	5 (12%)	43,45,55	1.01	2 (4%)
53	CDL	a	201	-	99,99,99	1.12	9 (9%)	105,111,111	0.87	4 (3%)
48	PEE	l	701	-	39,39,50	1.34	6 (15%)	42,44,55	1.13	3 (7%)
50	UQ1	C	304	-	18,18,18	2.34	5 (27%)	24,25,25	2.16	7 (29%)
46	FMN	A	502	-	33,33,33	1.05	2 (6%)	48,50,50	1.24	8 (16%)
49	PLX	g	201	-	51,51,51	1.20	4 (7%)	53,59,59	0.64	1 (1%)
49	PLX	a	202	-	51,51,51	1.21	4 (7%)	53,59,59	0.63	1 (1%)
45	SF4	A	501	1	0,12,12	-	-	-	-	-
51	UQ	J	402	-	33,33,63	3.52	9 (27%)	42,43,79	2.76	15 (35%)
48	PEE	V	202	-	50,50,50	1.18	6 (12%)	53,55,55	0.98	2 (3%)
52	8Q1	G	201	-	32,34,34	1.62	6 (18%)	39,43,43	1.76	6 (15%)
45	SF4	C	301	3	0,12,12	-	-	-	-	-
52	8Q1	X	201	-	32,34,34	1.63	6 (18%)	39,43,43	1.56	5 (12%)
48	PEE	l	705	-	45,45,50	1.24	6 (13%)	48,50,55	1.02	2 (4%)
49	PLX	r	501	-	51,51,51	1.21	5 (9%)	53,59,59	0.62	1 (1%)
51	UQ	C	305	-	38,38,63	3.64	10 (26%)	48,49,79	2.77	17 (35%)
55	FES	O	301	14	0,4,4	-	-	-	-	-
48	PEE	l	704	-	50,50,50	1.18	6 (12%)	53,55,55	0.94	2 (3%)
55	FES	M	803	12	0,4,4	-	-	-	-	-
48	PEE	U	101	-	50,50,50	1.18	6 (12%)	53,55,55	0.96	2 (3%)
50	UQ1	Q	501	-	18,18,18	2.29	4 (22%)	24,25,25	1.68	5 (20%)
48	PEE	B	303	-	50,50,50	1.19	6 (12%)	53,55,55	1.01	2 (3%)
48	PEE	s	401	-	40,40,50	1.17	5 (12%)	43,45,55	1.03	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	CDL	l	703	-	99,99,99	1.12	8 (8%)	105,111,111	0.91	5 (4%)
54	NDP	J	401	-	51,52,52	4.29	25 (49%)	71,80,80	2.21	14 (19%)
49	PLX	j	201	-	51,51,51	1.21	4 (7%)	53,59,59	0.65	1 (1%)
45	SF4	B	302	2	0,12,12	-	-	-	-	-
53	CDL	V	203	-	99,99,99	1.11	8 (8%)	105,111,111	0.89	4 (3%)
49	PLX	e	201	-	51,51,51	1.21	5 (9%)	53,59,59	0.54	1 (1%)
58	ADP	w	401	-	28,29,29	3.17	9 (32%)	43,45,45	1.89	8 (18%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
53	CDL	l	702	-	98,98,99	0.92	4 (4%)	104,110,111	1.09	8 (7%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-
53	CDL	V	201	-	93,93,99	1.14	9 (9%)	99,105,111	0.87	4 (4%)
47	NAI	A	503	-	47,48,48	4.02	22 (46%)	64,73,73	1.67	11 (17%)
48	PEE	C	302	-	46,46,50	1.23	6 (13%)	49,51,55	0.99	2 (4%)
53	CDL	I	201	-	50,50,99	1.44	8 (16%)	56,62,111	1.15	4 (7%)
53	CDL	g	202	-	99,99,99	1.12	8 (8%)	105,111,111	0.87	4 (3%)
53	CDL	n	101	-	54,54,99	1.38	8 (14%)	60,66,111	1.10	4 (6%)
49	PLX	J	403	-	51,51,51	1.20	4 (7%)	53,59,59	0.62	1 (1%)
49	PLX	C	303	-	51,51,51	1.21	5 (9%)	53,59,59	0.62	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PEE	i	401	-	-	19/50/50/54	-
53	CDL	s	402	-	-	48/99/99/110	-
53	CDL	V	204	-	-	51/104/104/110	-
45	SF4	M	802	12	-	-	0/6/5/5
48	PEE	W	201	-	-	18/44/44/54	-
53	CDL	a	201	-	-	57/110/110/110	-
48	PEE	l	701	-	-	16/43/43/54	-
50	UQ1	C	304	-	-	4/9/33/33	0/1/1/1
46	FMN	A	502	-	-	7/18/18/18	0/3/3/3
49	PLX	g	201	-	-	30/55/55/55	-
49	PLX	a	202	-	-	30/55/55/55	-
45	SF4	A	501	1	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	UQ	J	402	-	-	10/27/51/87	0/1/1/1
48	PEE	V	202	-	-	25/54/54/54	-
52	8Q1	G	201	-	-	12/41/41/41	-
45	SF4	C	301	3	-	-	0/6/5/5
52	8Q1	X	201	-	-	10/41/41/41	-
48	PEE	l	705	-	-	15/49/49/54	-
49	PLX	r	501	-	-	32/55/55/55	-
51	UQ	C	305	-	-	11/33/57/87	0/1/1/1
55	FES	O	301	14	-	-	0/1/1/1
48	PEE	l	704	-	-	29/54/54/54	-
55	FES	M	803	12	-	-	0/1/1/1
48	PEE	U	101	-	-	22/54/54/54	-
50	UQ1	Q	501	-	-	1/9/33/33	0/1/1/1
48	PEE	B	303	-	-	25/54/54/54	-
48	PEE	s	401	-	-	24/44/44/54	-
53	CDL	l	703	-	-	65/110/110/110	-
54	NDP	J	401	-	-	7/34/77/77	0/5/5/5
49	PLX	j	201	-	-	22/55/55/55	-
45	SF4	B	302	2	-	-	0/6/5/5
53	CDL	V	203	-	-	53/110/110/110	-
49	PLX	e	201	-	-	32/55/55/55	-
58	ADP	w	401	-	-	5/16/32/32	0/3/3/3
45	SF4	B	301	2	-	-	0/6/5/5
53	CDL	l	702	-	-	41/109/109/110	-
45	SF4	M	801	12	-	-	0/6/5/5
53	CDL	V	201	-	-	57/104/104/110	-
48	PEE	C	302	-	-	28/50/50/54	-
47	NAI	A	503	-	-	3/29/72/72	0/5/5/5
53	CDL	I	201	-	-	26/61/61/110	-
53	CDL	g	202	-	-	58/110/110/110	-
53	CDL	n	101	-	-	25/65/65/110	-
49	PLX	J	403	-	-	32/55/55/55	-
49	PLX	C	303	-	-	23/55/55/55	-

All (265) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	J	401	NDP	C3B-C2B	-13.24	1.24	1.53
54	J	401	NDP	O4D-C4D	10.70	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.30	1.26	1.53
51	C	305	UQ	C18-C19	9.98	1.56	1.33
54	J	401	NDP	C3D-C4D	-9.94	1.27	1.53
51	J	402	UQ	C18-C19	9.88	1.55	1.33
51	C	305	UQ	C13-C14	9.58	1.55	1.33
51	J	402	UQ	C13-C14	9.55	1.55	1.33
51	C	305	UQ	C23-C24	9.50	1.54	1.33
51	J	402	UQ	C8-C9	9.39	1.54	1.33
47	A	503	NAI	O4B-C1B	9.34	1.63	1.42
51	C	305	UQ	C8-C9	9.33	1.54	1.33
58	w	401	ADP	C3'-C4'	-8.99	1.30	1.53
47	A	503	NAI	O4B-C4B	-8.30	1.26	1.45
54	J	401	NDP	O4B-C4B	-7.91	1.27	1.45
58	w	401	ADP	O4'-C4'	7.76	1.62	1.45
47	A	503	NAI	C2D-C1D	-7.71	1.29	1.53
51	J	402	UQ	C23-C24	7.51	1.54	1.32
54	J	401	NDP	C2N-C3N	7.48	1.55	1.35
47	A	503	NAI	C2B-C1B	-7.40	1.30	1.53
51	C	305	UQ	C28-C29	7.35	1.54	1.32
54	J	401	NDP	C6N-C5N	7.26	1.55	1.33
50	C	304	UQ1	C8-C9	7.06	1.53	1.32
47	A	503	NAI	O4D-C4D	6.93	1.60	1.45
50	Q	501	UQ1	C8-C9	6.93	1.53	1.32
54	J	401	NDP	PN-O3	6.53	1.66	1.59
47	A	503	NAI	PA-O3	6.46	1.66	1.59
58	w	401	ADP	PA-O3A	6.45	1.66	1.59
47	A	503	NAI	C2D-C3D	6.04	1.69	1.53
54	J	401	NDP	P2B-O2B	5.92	1.69	1.59
54	J	401	NDP	C6A-N6A	5.78	1.49	1.34
47	A	503	NAI	PN-O3	5.69	1.65	1.59
54	J	401	NDP	PA-O3	5.66	1.65	1.59
47	A	503	NAI	O4D-C1D	5.55	1.54	1.42
54	J	401	NDP	C3B-C4B	5.46	1.66	1.53
58	w	401	ADP	C6-N6	5.43	1.48	1.34
47	A	503	NAI	C7N-N7N	5.32	1.48	1.33
47	A	503	NAI	C4N-C3N	-5.27	1.40	1.50
52	X	201	8Q1	C39-N41	5.18	1.45	1.33
52	G	201	8Q1	C39-N41	5.12	1.45	1.33
52	X	201	8Q1	C34-N36	5.12	1.45	1.33
54	J	401	NDP	O4D-C1D	-5.06	1.30	1.42
47	A	503	NAI	C6A-N6A	5.05	1.47	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	J	401	NDP	C6N-N1N	5.05	1.49	1.37
52	G	201	8Q1	C34-N36	4.94	1.45	1.33
54	J	401	NDP	O4B-C1B	4.75	1.53	1.42
54	J	401	NDP	C1B-N9A	-4.59	1.33	1.46
58	w	401	ADP	O4'-C1'	-4.52	1.31	1.42
47	A	503	NAI	O2B-C2B	4.33	1.53	1.43
53	l	702	CDL	OB8-CB7	4.26	1.45	1.33
53	l	702	CDL	OA8-CA7	4.21	1.45	1.33
53	l	702	CDL	OB6-CB5	4.05	1.45	1.34
53	l	702	CDL	OA6-CA5	3.99	1.45	1.34
54	J	401	NDP	O2D-C2D	-3.95	1.33	1.43
54	J	401	NDP	C7N-N7N	3.86	1.44	1.33
48	l	704	PEE	C18-C19	3.84	1.53	1.31
48	C	302	PEE	C18-C19	3.83	1.53	1.31
48	l	701	PEE	C18-C19	3.83	1.53	1.31
48	V	202	PEE	C18-C19	3.82	1.53	1.31
48	U	101	PEE	C18-C19	3.81	1.53	1.31
48	l	705	PEE	C18-C19	3.81	1.53	1.31
48	W	201	PEE	C18-C19	3.81	1.53	1.31
48	B	303	PEE	C18-C19	3.81	1.53	1.31
48	s	401	PEE	C18-C19	3.80	1.53	1.31
48	i	401	PEE	C18-C19	3.80	1.53	1.31
48	U	101	PEE	C39-C38	3.76	1.53	1.31
48	B	303	PEE	C39-C38	3.75	1.53	1.31
48	V	202	PEE	C39-C38	3.73	1.52	1.31
48	l	701	PEE	C39-C38	3.73	1.52	1.31
48	C	302	PEE	C39-C38	3.73	1.52	1.31
48	l	704	PEE	C39-C38	3.72	1.52	1.31
48	l	705	PEE	C39-C38	3.72	1.52	1.31
48	i	401	PEE	C39-C38	3.71	1.52	1.31
47	A	503	NAI	C7N-C3N	3.61	1.56	1.48
53	l	703	CDL	OA8-CA7	3.49	1.43	1.33
53	I	201	CDL	OA8-CA7	3.48	1.43	1.33
53	n	101	CDL	OA8-CA7	3.47	1.43	1.33
53	a	201	CDL	OA8-CA7	3.46	1.43	1.33
53	V	203	CDL	OA8-CA7	3.45	1.43	1.33
53	V	204	CDL	OA8-CA7	3.45	1.43	1.33
53	s	402	CDL	OA8-CA7	3.44	1.43	1.33
53	V	201	CDL	OA8-CA7	3.44	1.43	1.33
53	g	202	CDL	OA8-CA7	3.42	1.43	1.33
58	w	401	ADP	C8-N9	-3.37	1.31	1.37
47	A	503	NAI	C4N-C5N	-3.35	1.40	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	A	502	FMN	C4A-N5	3.35	1.38	1.30
53	V	204	CDL	OA6-CA5	3.26	1.43	1.34
58	w	401	ADP	O2'-C2'	-3.19	1.35	1.43
54	J	401	NDP	C8A-N9A	-3.15	1.32	1.37
53	V	201	CDL	OA6-CA5	3.11	1.43	1.34
54	J	401	NDP	C5A-N7A	-3.09	1.33	1.39
53	I	201	CDL	OB8-CB7	3.08	1.42	1.33
53	g	202	CDL	OB6-CB5	3.08	1.43	1.34
53	s	402	CDL	OB6-CB5	3.08	1.43	1.34
53	a	201	CDL	OB6-CB5	3.06	1.42	1.34
53	V	204	CDL	OB6-CB5	3.05	1.42	1.34
53	l	703	CDL	OB8-CB7	3.05	1.42	1.33
53	V	201	CDL	OB6-CB5	3.05	1.42	1.34
53	a	201	CDL	OB8-CB7	3.04	1.42	1.33
53	I	201	CDL	OB6-CB5	3.02	1.42	1.34
53	n	101	CDL	OB6-CB5	3.02	1.42	1.34
53	g	202	CDL	OB8-CB7	3.01	1.42	1.33
53	V	203	CDL	OB6-CB5	3.01	1.42	1.34
53	s	402	CDL	OB8-CB7	3.00	1.42	1.33
54	J	401	NDP	C7N-C3N	3.00	1.55	1.48
53	V	204	CDL	OB8-CB7	3.00	1.42	1.33
53	s	402	CDL	OA6-CA5	2.99	1.42	1.34
53	l	703	CDL	OB6-CB5	2.99	1.42	1.34
53	V	201	CDL	OB8-CB7	2.98	1.42	1.33
53	V	203	CDL	OB8-CB7	2.98	1.42	1.33
53	g	202	CDL	OA6-CA5	2.97	1.42	1.34
58	w	401	ADP	O3'-C3'	2.97	1.50	1.43
53	a	201	CDL	OA6-CA5	2.96	1.42	1.34
53	n	101	CDL	OB8-CB7	2.96	1.42	1.33
53	l	703	CDL	OA6-CA5	2.96	1.42	1.34
54	J	401	NDP	O3D-C3D	2.95	1.50	1.43
53	V	203	CDL	OA6-CA5	2.94	1.42	1.34
53	n	101	CDL	OA6-CA5	2.94	1.42	1.34
53	I	201	CDL	OA6-CA5	2.94	1.42	1.34
49	g	201	PLX	O6-C4	-2.89	1.40	1.44
51	J	402	UQ	C6-C1	2.86	1.54	1.46
49	C	303	PLX	O6-C4	-2.82	1.41	1.44
49	j	201	PLX	O6-C4	-2.79	1.41	1.44
49	a	202	PLX	O6-C4	-2.79	1.41	1.44
51	C	305	UQ	C6-C1	2.73	1.54	1.46
50	C	304	UQ1	C6-C1	2.72	1.54	1.46
47	A	503	NAI	C8A-N9A	-2.71	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	e	201	PLX	O6-C4	-2.66	1.41	1.44
48	B	303	PEE	O2-C2	-2.61	1.40	1.46
48	C	302	PEE	O2-C2	-2.60	1.40	1.46
48	W	201	PEE	O2-C2	-2.60	1.40	1.46
53	I	201	CDL	OA6-CA4	-2.59	1.40	1.46
53	n	101	CDL	OA6-CA4	-2.58	1.40	1.46
53	g	202	CDL	OA6-CA4	-2.57	1.40	1.46
48	i	401	PEE	O2-C2	-2.57	1.40	1.46
53	s	402	CDL	OA6-CA4	-2.56	1.40	1.46
53	a	201	CDL	OA6-CA4	-2.56	1.40	1.46
53	V	203	CDL	OA6-CA4	-2.55	1.40	1.46
48	V	202	PEE	O2-C2	-2.54	1.40	1.46
48	l	701	PEE	O2-C2	-2.54	1.40	1.46
48	U	101	PEE	O2-C2	-2.53	1.40	1.46
46	A	502	FMN	C10-N1	2.52	1.38	1.33
54	J	401	NDP	O2B-C2B	2.51	1.52	1.44
47	A	503	NAI	PN-O5D	2.50	1.69	1.59
48	l	704	PEE	O2-C2	-2.50	1.40	1.46
48	l	701	PEE	O3-C30	2.50	1.40	1.33
48	l	705	PEE	O2-C2	-2.50	1.40	1.46
48	l	705	PEE	O3-C30	2.48	1.40	1.33
48	s	401	PEE	O3-C30	2.48	1.40	1.33
52	X	201	8Q1	C1-S44	2.48	1.82	1.76
53	l	703	CDL	OA6-CA4	-2.48	1.40	1.46
48	s	401	PEE	O2-C2	-2.48	1.40	1.46
49	j	201	PLX	C7-C6	2.47	1.55	1.50
48	i	401	PEE	O3-C30	2.47	1.40	1.33
49	r	501	PLX	O6-C4	-2.45	1.41	1.44
48	U	101	PEE	O3-C30	2.45	1.40	1.33
48	B	303	PEE	O3-C30	2.44	1.40	1.33
48	V	202	PEE	O3-C30	2.44	1.40	1.33
47	A	503	NAI	C6N-C5N	2.44	1.40	1.33
52	G	201	8Q1	O40-C39	-2.44	1.18	1.23
58	w	401	ADP	C5-N7	-2.42	1.34	1.39
48	W	201	PEE	O3-C30	2.42	1.40	1.33
50	Q	501	UQ1	C6-C1	2.42	1.53	1.46
52	G	201	8Q1	O35-C34	-2.41	1.18	1.23
48	C	302	PEE	O3-C30	2.40	1.40	1.33
48	l	704	PEE	O3-C30	2.40	1.40	1.33
49	r	501	PLX	C7-C6	2.39	1.55	1.50
49	e	201	PLX	C7-C6	2.38	1.55	1.50
49	J	403	PLX	C7-C6	2.38	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	l	703	CDL	OB6-CB4	-2.38	1.41	1.46
51	C	305	UQ	C7-C8	2.38	1.54	1.50
53	V	203	CDL	OB6-CB4	-2.38	1.41	1.46
50	C	304	UQ1	O2-CM2	-2.37	1.40	1.45
54	J	401	NDP	C2D-C3D	2.37	1.59	1.53
47	A	503	NAI	C5B-C4B	2.36	1.58	1.51
49	a	202	PLX	C7-C6	2.35	1.55	1.50
48	B	303	PEE	O2-C10	2.34	1.40	1.34
49	C	303	PLX	C7-C6	2.34	1.55	1.50
53	a	201	CDL	OB6-CB4	-2.34	1.41	1.46
48	i	401	PEE	O2-C10	2.33	1.40	1.34
49	g	201	PLX	C7-C6	2.33	1.55	1.50
49	J	403	PLX	O6-C4	-2.33	1.41	1.44
52	X	201	8Q1	C6-C1	2.32	1.53	1.50
47	A	503	NAI	O3B-C3B	-2.32	1.37	1.43
48	l	705	PEE	O2-C10	2.32	1.40	1.34
53	V	201	CDL	PB2-OB2	2.31	1.68	1.59
53	I	201	CDL	OB6-CB4	-2.31	1.41	1.46
53	n	101	CDL	OB6-CB4	-2.30	1.41	1.46
48	l	701	PEE	O2-C10	2.30	1.40	1.34
48	l	704	PEE	O2-C10	2.30	1.40	1.34
52	G	201	8Q1	C1-S44	2.30	1.81	1.76
53	s	402	CDL	OB6-CB4	-2.29	1.41	1.46
53	V	204	CDL	OB6-CB4	-2.29	1.41	1.46
48	s	401	PEE	O2-C10	2.29	1.40	1.34
53	V	203	CDL	PB2-OB2	2.29	1.68	1.59
53	V	201	CDL	OA6-CA4	-2.29	1.41	1.46
53	g	202	CDL	PB2-OB2	2.29	1.68	1.59
53	s	402	CDL	PB2-OB2	2.29	1.68	1.59
51	J	402	UQ	C7-C8	2.29	1.54	1.50
53	n	101	CDL	PB2-OB2	2.29	1.68	1.59
48	W	201	PEE	O2-C10	2.28	1.40	1.34
53	V	201	CDL	OB6-CB4	-2.28	1.41	1.46
52	X	201	8Q1	O40-C39	-2.28	1.18	1.23
48	C	302	PEE	O2-C10	2.27	1.40	1.34
48	V	202	PEE	O2-C10	2.27	1.40	1.34
53	a	201	CDL	PB2-OB2	2.27	1.68	1.59
53	g	202	CDL	OB6-CB4	-2.26	1.41	1.46
48	U	101	PEE	O2-C10	2.25	1.40	1.34
52	X	201	8Q1	O35-C34	-2.25	1.19	1.23
53	l	703	CDL	PB2-OB2	2.25	1.68	1.59
49	r	501	PLX	P1-O4	2.25	1.68	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	V	204	CDL	PB2-OB2	2.25	1.68	1.59
53	l	703	CDL	PB2-OB5	2.25	1.68	1.59
53	a	201	CDL	PB2-OB5	2.25	1.68	1.59
53	I	201	CDL	PB2-OB2	2.24	1.68	1.59
50	Q	501	UQ1	O2-CM2	-2.24	1.40	1.45
53	g	202	CDL	PB2-OB5	2.23	1.68	1.59
53	I	201	CDL	PB2-OB5	2.21	1.68	1.59
53	V	203	CDL	PB2-OB5	2.21	1.68	1.59
53	s	402	CDL	PB2-OB5	2.20	1.68	1.59
53	V	204	CDL	PB2-OB5	2.20	1.68	1.59
53	V	201	CDL	PB2-OB5	2.19	1.68	1.59
49	a	202	PLX	P1-O4	2.19	1.68	1.59
48	B	303	PEE	O3-C3	-2.18	1.40	1.45
53	n	101	CDL	PB2-OB5	2.18	1.67	1.59
52	G	201	8Q1	C6-C1	2.18	1.53	1.50
49	j	201	PLX	P1-O4	2.18	1.67	1.59
49	J	403	PLX	P1-O4	2.17	1.67	1.59
48	l	701	PEE	O3-C3	-2.17	1.40	1.45
54	J	401	NDP	PA-O5B	2.16	1.67	1.59
49	g	201	PLX	P1-O4	2.15	1.67	1.59
50	C	304	UQ1	O3-CM3	-2.15	1.40	1.45
50	Q	501	UQ1	O3-CM3	-2.15	1.40	1.45
51	J	402	UQ	O4-C4	-2.15	1.18	1.23
48	l	704	PEE	O3-C3	-2.15	1.40	1.45
49	e	201	PLX	P1-O4	2.15	1.67	1.59
54	J	401	NDP	O7N-C7N	-2.15	1.19	1.24
48	V	202	PEE	O3-C3	-2.14	1.40	1.45
53	V	204	CDL	OA6-CA4	-2.14	1.41	1.46
49	r	501	PLX	P1-O1	2.13	1.67	1.59
48	C	302	PEE	O3-C3	-2.13	1.40	1.45
49	C	303	PLX	P1-O4	2.13	1.67	1.59
48	W	201	PEE	O3-C3	-2.13	1.40	1.45
48	i	401	PEE	O3-C3	-2.12	1.40	1.45
51	C	305	UQ	O3-CM3	-2.11	1.40	1.45
51	C	305	UQ	O4-C4	-2.10	1.18	1.23
49	a	202	PLX	P1-O1	2.09	1.67	1.59
48	s	401	PEE	O3-C3	-2.09	1.40	1.45
48	U	101	PEE	O3-C3	-2.08	1.40	1.45
49	e	201	PLX	P1-O1	2.08	1.67	1.59
51	J	402	UQ	O3-CM3	-2.07	1.40	1.45
51	J	402	UQ	C21-C19	2.06	1.55	1.51
49	j	201	PLX	P1-O1	2.06	1.67	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	l	705	PEE	O3-C3	-2.06	1.40	1.45
49	J	403	PLX	P1-O1	2.06	1.67	1.59
47	A	503	NAI	C5A-N7A	-2.05	1.35	1.39
49	g	201	PLX	P1-O1	2.05	1.67	1.59
51	C	305	UQ	C21-C19	2.05	1.55	1.51
49	e	201	PLX	C1-C2	2.05	1.57	1.51
49	r	501	PLX	C25-C24	2.04	1.55	1.50
49	C	303	PLX	P1-O1	2.04	1.67	1.59
49	C	303	PLX	C25-C24	2.03	1.55	1.50
50	C	304	UQ1	O1-C1	-2.01	1.18	1.23
53	V	201	CDL	C11-CA5	2.01	1.56	1.50
53	a	201	CDL	C11-CA5	2.00	1.56	1.50

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	J	402	UQ	C7-C8-C9	-8.06	112.95	126.83
51	C	305	UQ	C7-C8-C9	-7.60	113.73	126.83
54	J	401	NDP	C3N-C2N-N1N	-7.57	112.10	123.20
54	J	401	NDP	C1D-N1N-C2N	-7.30	109.11	121.14
52	G	201	8Q1	C6-C1-S44	6.95	121.68	113.40
51	C	305	UQ	C17-C18-C19	-6.32	113.16	127.62
54	J	401	NDP	C6N-N1N-C2N	-6.28	112.59	119.32
51	J	402	UQ	C12-C13-C14	-6.21	113.40	127.62
51	J	402	UQ	C17-C18-C19	-6.19	113.45	127.62
51	C	305	UQ	C12-C13-C14	-6.18	113.48	127.62
51	C	305	UQ	C22-C23-C24	-5.95	114.00	127.62
54	J	401	NDP	C1D-N1N-C6N	-5.62	108.89	120.77
54	J	401	NDP	C5A-C4A-N3A	-5.60	119.01	126.72
58	w	401	ADP	C5-C4-N3	-5.39	119.29	126.72
50	C	304	UQ1	C7-C6-C1	5.37	124.75	118.52
47	A	503	NAI	C5A-C4A-N3A	-5.35	119.35	126.72
52	X	201	8Q1	C6-C1-S44	5.28	119.70	113.40
50	Q	501	UQ1	C7-C8-C9	-4.98	113.15	127.25
50	C	304	UQ1	C7-C6-C5	-4.71	116.82	124.89
58	w	401	ADP	N3-C2-N1	-4.62	121.59	128.58
51	J	402	UQ	C20-C19-C18	-4.47	112.14	123.63
51	J	402	UQ	C22-C23-C24	-4.44	112.84	127.64
47	A	503	NAI	N3A-C2A-N1A	-4.42	121.89	128.58
51	C	305	UQ	C10-C9-C8	-4.42	112.28	123.63
51	C	305	UQ	C27-C28-C29	-4.39	113.01	127.64
53	l	702	CDL	OA6-CA5-C11	4.32	120.83	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	C	305	UQ	C25-C24-C23	-4.30	112.57	123.63
58	w	401	ADP	N3-C4-N9	4.30	134.47	127.17
48	i	401	PEE	O2-C10-C11	4.25	120.67	111.48
51	J	402	UQ	C15-C14-C13	-4.21	112.81	123.63
51	J	402	UQ	C10-C9-C8	-4.21	112.82	123.63
53	l	702	CDL	OB6-CB5-C51	4.15	120.46	111.48
48	l	701	PEE	O2-C10-C11	4.14	120.44	111.48
48	V	202	PEE	O2-C10-C11	4.14	120.43	111.48
52	G	201	8Q1	O4-C1-C6	-4.13	119.21	123.98
48	s	401	PEE	O2-C10-C11	4.13	120.42	111.48
51	J	402	UQ	C16-C14-C13	-4.12	111.92	121.17
53	a	201	CDL	OB6-CB5-C51	4.12	120.39	111.48
50	C	304	UQ1	C7-C8-C9	-4.11	115.61	127.25
53	l	703	CDL	OA6-CA5-C11	4.11	120.37	111.48
48	l	705	PEE	O2-C10-C11	4.08	120.30	111.48
53	V	201	CDL	OB6-CB5-C51	4.04	120.22	111.48
48	B	303	PEE	O2-C10-C11	4.03	120.20	111.48
54	J	401	NDP	N3A-C4A-N9A	3.99	133.95	127.17
53	g	202	CDL	OB6-CB5-C51	3.98	120.10	111.48
53	V	203	CDL	OA6-CA5-C11	3.98	120.08	111.48
53	V	204	CDL	OB6-CB5-C51	3.97	120.08	111.48
51	C	305	UQ	C20-C19-C18	-3.95	113.47	123.63
48	U	101	PEE	O2-C10-C11	3.94	120.01	111.48
53	s	402	CDL	OB6-CB5-C51	3.94	120.01	111.48
53	I	201	CDL	OB6-CB5-C51	3.94	120.00	111.48
53	n	101	CDL	OB6-CB5-C51	3.94	120.00	111.48
48	W	201	PEE	O2-C10-C11	3.93	119.99	111.48
53	V	203	CDL	OB6-CB5-C51	3.93	119.97	111.48
54	J	401	NDP	N3A-C2A-N1A	-3.92	122.64	128.58
53	I	201	CDL	OA6-CA5-C11	3.91	119.94	111.48
51	J	402	UQ	C21-C19-C18	-3.90	112.40	121.17
53	l	703	CDL	OB6-CB5-C51	3.90	119.92	111.48
53	n	101	CDL	OA6-CA5-C11	3.88	119.88	111.48
48	C	302	PEE	O2-C10-C11	3.88	119.87	111.48
53	g	202	CDL	OA6-CA5-C11	3.87	119.85	111.48
47	A	503	NAI	N3A-C4A-N9A	3.83	133.67	127.17
51	C	305	UQ	C15-C14-C13	-3.80	113.88	123.63
53	V	201	CDL	OA6-CA5-C11	3.78	119.66	111.48
53	a	201	CDL	OA6-CA5-C11	3.75	119.60	111.48
53	s	402	CDL	OA6-CA5-C11	3.72	119.52	111.48
51	C	305	UQ	C11-C9-C8	-3.72	112.83	121.17
51	C	305	UQ	C16-C14-C13	-3.68	112.90	121.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	A	503	NAI	C2A-N3A-C4A	3.66	120.78	111.83
48	l	704	PEE	O2-C10-C11	3.61	119.28	111.48
51	C	305	UQ	C21-C19-C18	-3.58	113.13	121.17
52	X	201	8Q1	C37-C38-C39	3.58	118.35	112.39
58	w	401	ADP	C2-N3-C4	3.57	120.55	111.83
54	J	401	NDP	C2A-N3A-C4A	3.54	120.47	111.83
58	w	401	ADP	N9-C8-N7	-3.50	108.97	113.94
52	X	201	8Q1	O4-C1-C6	-3.40	120.06	123.98
51	C	305	UQ	C26-C24-C23	-3.32	113.72	121.17
47	A	503	NAI	C4A-C5A-N7A	-3.31	106.79	110.58
51	J	402	UQ	C25-C24-C23	-3.29	112.77	122.66
47	A	503	NAI	C5A-N7A-C8A	3.27	108.59	103.45
53	V	204	CDL	OA6-CA5-C11	3.27	118.55	111.48
46	A	502	FMN	C4-N3-C2	-3.26	119.85	125.64
47	A	503	NAI	N9A-C8A-N7A	-3.25	109.32	113.94
51	J	402	UQ	C26-C24-C23	-3.25	112.91	122.66
58	w	401	ADP	C4-N9-C8	3.22	109.12	105.74
52	G	201	8Q1	C37-C38-C39	3.22	117.76	112.39
51	C	305	UQ	C31-C29-C28	-3.22	112.99	122.66
51	C	305	UQ	C30-C29-C28	-3.19	113.10	122.66
51	J	402	UQ	C11-C9-C8	-3.17	114.06	121.17
51	J	402	UQ	C7-C6-C5	-3.13	119.52	124.89
58	w	401	ADP	C5-N7-C8	3.13	108.36	103.45
54	J	401	NDP	C4A-C5A-N7A	-3.12	107.01	110.58
50	Q	501	UQ1	C10-C9-C8	-3.09	113.38	122.66
47	A	503	NAI	C3D-C2D-C1D	3.03	107.19	101.46
54	J	401	NDP	N9A-C8A-N7A	-3.02	109.65	113.94
50	Q	501	UQ1	C11-C9-C8	-3.01	113.62	122.66
54	J	401	NDP	C5A-N7A-C8A	2.98	108.13	103.45
53	l	702	CDL	OB8-CB7-C71	2.96	120.85	111.83
48	B	303	PEE	O3-C30-C31	2.93	120.76	111.83
53	l	702	CDL	OA8-CA7-C31	2.91	120.72	111.83
53	l	702	CDL	CA4-OA6-CA5	-2.89	110.88	117.80
50	C	304	UQ1	C10-C9-C8	-2.88	114.00	122.66
53	V	203	CDL	OB8-CB7-C71	2.88	120.61	111.83
53	n	101	CDL	OA8-CA7-C31	2.87	119.87	111.15
58	w	401	ADP	C4-C5-N7	-2.87	107.30	110.58
48	l	704	PEE	O3-C30-C31	2.84	120.48	111.83
53	l	703	CDL	OB8-CB7-C71	2.83	120.46	111.83
53	V	204	CDL	OA8-CA7-C31	2.81	120.42	111.83
52	G	201	8Q1	O4-C1-S44	-2.81	119.11	122.68
53	I	201	CDL	OB8-CB7-C71	2.81	120.39	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	a	201	CDL	OB8-CB7-C71	2.79	120.33	111.83
53	s	402	CDL	OA8-CA7-C31	2.78	120.32	111.83
53	I	201	CDL	OA8-CA7-C31	2.78	120.30	111.83
53	l	703	CDL	OA8-CA7-C31	2.78	120.30	111.83
47	A	503	NAI	C2D-C3D-C4D	2.77	107.96	102.61
48	i	401	PEE	O3-C30-C31	2.76	120.26	111.83
52	X	201	8Q1	C43-S44-C1	2.75	109.98	101.84
47	A	503	NAI	C4D-O4D-C1D	-2.75	103.39	109.47
53	V	204	CDL	OB8-CB7-C71	2.75	120.21	111.83
53	g	202	CDL	OB8-CB7-C71	2.73	120.17	111.83
53	n	101	CDL	OB8-CB7-C71	2.71	120.10	111.83
46	A	502	FMN	C4A-C4-N3	2.68	120.08	113.25
53	g	202	CDL	OA8-CA7-C31	2.68	120.00	111.83
48	V	202	PEE	O3-C30-C31	2.66	119.95	111.83
48	s	401	PEE	O3-C30-C31	2.66	119.94	111.83
53	V	203	CDL	OA8-CA7-C31	2.66	119.94	111.83
48	W	201	PEE	O3-C30-C31	2.66	119.93	111.83
48	l	705	PEE	O3-C30-C31	2.65	119.90	111.83
53	s	402	CDL	OB8-CB7-C71	2.65	119.90	111.83
53	V	201	CDL	OB8-CB7-C71	2.64	119.90	111.83
50	Q	501	UQ1	C7-C6-C5	-2.64	120.36	124.89
51	J	402	UQ	CM5-C5-C6	-2.64	120.12	124.45
53	a	201	CDL	OA8-CA7-C31	2.63	119.86	111.83
48	l	701	PEE	O3-C30-C31	2.62	119.84	111.83
48	C	302	PEE	O3-C30-C31	2.60	119.77	111.83
50	C	304	UQ1	C6-C5-C4	2.60	121.22	119.17
48	U	101	PEE	O3-C30-C31	2.60	119.76	111.83
50	C	304	UQ1	C11-C9-C8	-2.57	114.94	122.66
49	r	501	PLX	C1A-N1-C1	2.55	120.04	109.91
49	j	201	PLX	C1A-N1-C1	2.54	119.99	109.91
49	g	201	PLX	C1A-N1-C1	2.52	119.94	109.91
53	V	201	CDL	OA8-CA7-C31	2.52	119.52	111.83
46	A	502	FMN	O4-C4-C4A	-2.52	119.89	126.53
47	A	503	NAI	C4A-N9A-C8A	2.46	108.32	105.74
52	G	201	8Q1	C43-S44-C1	2.44	109.06	101.84
49	a	202	PLX	C1A-N1-C1	2.44	119.61	109.91
50	Q	501	UQ1	CM5-C5-C6	-2.44	120.45	124.45
51	C	305	UQ	C7-C6-C5	-2.43	120.72	124.89
46	A	502	FMN	C5A-C9A-N10	2.43	120.16	117.97
54	J	401	NDP	C2B-C1B-N9A	-2.42	109.77	113.75
46	A	502	FMN	C4A-C10-N10	2.41	119.94	116.48
50	C	304	UQ1	CM5-C5-C6	-2.40	120.51	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	C	303	PLX	C1A-N1-C1	2.35	119.27	109.91
48	l	701	PEE	C20-C19-C18	-2.34	112.35	126.42
49	J	403	PLX	C1A-N1-C1	2.31	119.09	109.91
54	J	401	NDP	C4A-N9A-C8A	2.31	108.16	105.74
46	A	502	FMN	C9A-C5A-N5	-2.23	120.08	122.45
53	l	702	CDL	CB4-OB6-CB5	-2.21	112.51	117.80
49	e	201	PLX	C1A-N1-C1	2.19	118.62	109.91
46	A	502	FMN	C10-C4A-N5	-2.19	120.34	124.81
52	G	201	8Q1	C38-C39-N41	2.18	120.32	116.34
46	A	502	FMN	C4A-C10-N1	-2.18	119.25	124.59
51	C	305	UQ	CM5-C5-C6	-2.16	120.90	124.45
52	X	201	8Q1	C38-C39-N41	2.11	120.19	116.34
54	J	401	NDP	P2B-O2B-C2B	-2.09	117.86	123.43
53	l	703	CDL	CB4-OB6-CB5	-2.06	112.88	117.80
53	l	702	CDL	OA8-CA7-OA9	-2.05	118.50	123.63
51	J	402	UQ	C7-C6-C1	2.04	120.88	118.52
53	l	702	CDL	OA6-CA5-OA7	-2.01	119.01	123.70

There are no chirality outliers.

All (973) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C3'-C4'-C5'-O5'
46	A	502	FMN	O4'-C4'-C5'-O5'
46	A	502	FMN	C5'-O5'-P-O1P
46	A	502	FMN	C5'-O5'-P-O2P
47	A	503	NAI	PN-O3-PA-O5B
48	B	303	PEE	C1-O3P-P-O1P
48	B	303	PEE	C1-O3P-P-O4P
48	C	302	PEE	C4-O4P-P-O3P
48	C	302	PEE	C4-O4P-P-O1P
48	U	101	PEE	C4-O4P-P-O3P
48	U	101	PEE	C4-O4P-P-O2P
48	V	202	PEE	C1-O3P-P-O1P
48	V	202	PEE	C4-O4P-P-O3P
48	V	202	PEE	C4-O4P-P-O2P
48	V	202	PEE	C5-C4-O4P-P
48	i	401	PEE	C11-C10-O2-C2
48	i	401	PEE	O4-C10-O2-C2
48	i	401	PEE	C4-O4P-P-O3P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	i	401	PEE	C4-O4P-P-O2P
48	i	401	PEE	C4-O4P-P-O1P
48	l	701	PEE	C1-O3P-P-O4P
48	l	704	PEE	C11-C10-O2-C2
48	l	704	PEE	C4-O4P-P-O3P
48	l	704	PEE	C4-O4P-P-O2P
48	l	705	PEE	C11-C10-O2-C2
48	l	705	PEE	O4-C10-O2-C2
48	l	705	PEE	O4P-C4-C5-N
48	s	401	PEE	C11-C10-O2-C2
48	s	401	PEE	C1-O3P-P-O2P
48	s	401	PEE	C1-O3P-P-O4P
48	s	401	PEE	C4-O4P-P-O2P
48	s	401	PEE	O4P-C4-C5-N
49	C	303	PLX	O7-C6-C7-C8
49	C	303	PLX	O6-C6-C7-C8
49	C	303	PLX	O6-C4-C5-O8
49	J	403	PLX	O7-C6-O6-C4
49	J	403	PLX	C3-C4-O6-C6
49	J	403	PLX	C2-O1-P1-O4
49	J	403	PLX	C2-O1-P1-O2
49	a	202	PLX	O7-C6-O6-C4
49	a	202	PLX	C3-O4-P1-O2
49	a	202	PLX	C3-O4-P1-O3
49	a	202	PLX	C2-O1-P1-O2
49	a	202	PLX	N1-C1-C2-O1
49	a	202	PLX	O9-C24-O8-C5
49	a	202	PLX	O9-C24-C25-C26
49	g	201	PLX	C3-O4-P1-O1
49	g	201	PLX	C3-O4-P1-O2
49	g	201	PLX	C3-O4-P1-O3
49	g	201	PLX	C2-O1-P1-O4
49	g	201	PLX	C2-O1-P1-O2
49	g	201	PLX	C2-O1-P1-O3
49	j	201	PLX	O7-C6-C7-C8
49	j	201	PLX	O9-C24-O8-C5
49	r	501	PLX	C5-C4-O6-C6
49	r	501	PLX	C2-O1-P1-O2
49	r	501	PLX	O9-C24-C25-C26
50	C	304	UQ1	C1-C6-C7-C8
50	C	304	UQ1	C5-C6-C7-C8
51	C	305	UQ	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
51	C	305	UQ	C7-C8-C9-C11
51	C	305	UQ	C12-C13-C14-C16
51	J	402	UQ	C7-C8-C9-C10
51	J	402	UQ	C12-C13-C14-C15
51	J	402	UQ	C17-C18-C19-C21
52	G	201	8Q1	O27-C28-C29-C30
52	G	201	8Q1	O27-C28-C29-C31
52	G	201	8Q1	C28-C29-C32-C34
52	G	201	8Q1	C28-C29-C32-O33
52	G	201	8Q1	C30-C29-C32-C34
52	G	201	8Q1	C30-C29-C32-O33
52	G	201	8Q1	C31-C29-C32-C34
52	G	201	8Q1	C31-C29-C32-O33
52	G	201	8Q1	C28-O27-P24-O3
52	G	201	8Q1	C28-O27-P24-O2
52	G	201	8Q1	C28-O27-P24-O1
52	X	201	8Q1	C1-C6-C7-C8
52	X	201	8Q1	C28-O27-P24-O3
52	X	201	8Q1	C28-O27-P24-O2
52	X	201	8Q1	C28-O27-P24-O1
53	I	201	CDL	CA2-OA2-PA1-OA4
53	I	201	CDL	CA2-OA2-PA1-OA5
53	I	201	CDL	CB2-OB2-PB2-OB3
53	I	201	CDL	CB2-OB2-PB2-OB5
53	I	201	CDL	CB3-OB5-PB2-OB2
53	I	201	CDL	CB3-OB5-PB2-OB3
53	I	201	CDL	CB3-OB5-PB2-OB4
53	V	201	CDL	CB2-C1-CA2-OA2
53	V	201	CDL	CA2-C1-CB2-OB2
53	V	201	CDL	CA3-OA5-PA1-OA4
53	V	201	CDL	C1-CB2-OB2-PB2
53	V	201	CDL	CB2-OB2-PB2-OB3
53	V	201	CDL	CB2-OB2-PB2-OB4
53	V	201	CDL	CB2-OB2-PB2-OB5
53	V	201	CDL	CB3-OB5-PB2-OB2
53	V	203	CDL	CA2-C1-CB2-OB2
53	V	203	CDL	CB3-OB5-PB2-OB2
53	V	203	CDL	OB5-CB3-CB4-OB6
53	V	203	CDL	OB6-CB4-CB6-OB8
53	V	204	CDL	CA2-OA2-PA1-OA3
53	V	204	CDL	CA2-OA2-PA1-OA5
53	V	204	CDL	CA3-OA5-PA1-OA2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	V	204	CDL	CA3-OA5-PA1-OA3
53	V	204	CDL	CA3-OA5-PA1-OA4
53	V	204	CDL	CB2-OB2-PB2-OB3
53	V	204	CDL	CB2-OB2-PB2-OB4
53	V	204	CDL	CB2-OB2-PB2-OB5
53	a	201	CDL	CB2-C1-CA2-OA2
53	a	201	CDL	CA2-C1-CB2-OB2
53	a	201	CDL	CA2-OA2-PA1-OA3
53	a	201	CDL	CB2-OB2-PB2-OB3
53	a	201	CDL	CB2-OB2-PB2-OB4
53	a	201	CDL	CB2-OB2-PB2-OB5
53	a	201	CDL	CB3-OB5-PB2-OB2
53	a	201	CDL	CB3-OB5-PB2-OB3
53	a	201	CDL	CB3-OB5-PB2-OB4
53	a	201	CDL	OB7-CB5-OB6-CB4
53	g	202	CDL	O1-C1-CA2-OA2
53	g	202	CDL	CA2-OA2-PA1-OA3
53	g	202	CDL	CA2-OA2-PA1-OA5
53	g	202	CDL	CA3-OA5-PA1-OA2
53	g	202	CDL	CA3-OA5-PA1-OA3
53	g	202	CDL	CB3-OB5-PB2-OB2
53	g	202	CDL	CB3-OB5-PB2-OB3
53	g	202	CDL	OB7-CB5-OB6-CB4
53	g	202	CDL	C51-CB5-OB6-CB4
53	l	702	CDL	CA2-OA2-PA1-OA3
53	l	702	CDL	CA3-OA5-PA1-OA3
53	l	702	CDL	CB2-OB2-PB2-OB3
53	l	702	CDL	CB2-OB2-PB2-OB4
53	l	702	CDL	CB2-OB2-PB2-OB5
53	l	702	CDL	CB3-OB5-PB2-OB2
53	l	702	CDL	CB3-OB5-PB2-OB4
53	l	703	CDL	CA2-C1-CB2-OB2
53	l	703	CDL	CA3-OA5-PA1-OA2
53	l	703	CDL	CA3-OA5-PA1-OA3
53	l	703	CDL	CA3-OA5-PA1-OA4
53	l	703	CDL	OA6-CA4-CA6-OA8
53	l	703	CDL	CB2-OB2-PB2-OB3
53	l	703	CDL	CB2-OB2-PB2-OB4
53	l	703	CDL	CB2-OB2-PB2-OB5
53	l	703	CDL	CB3-OB5-PB2-OB2
53	l	703	CDL	CB3-OB5-PB2-OB3
53	l	703	CDL	CB3-OB5-PB2-OB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	n	101	CDL	O1-C1-CA2-OA2
53	n	101	CDL	CB2-C1-CA2-OA2
53	n	101	CDL	CB2-OB2-PB2-OB4
53	n	101	CDL	CB2-OB2-PB2-OB5
53	s	402	CDL	CA2-C1-CB2-OB2
53	s	402	CDL	OA5-CA3-CA4-OA6
53	s	402	CDL	OA9-CA7-OA8-CA6
53	s	402	CDL	C31-CA7-OA8-CA6
58	w	401	ADP	C5'-O5'-PA-O2A
48	i	401	PEE	O5-C30-O3-C3
50	C	304	UQ1	C7-C8-C9-C10
48	i	401	PEE	C31-C30-O3-C3
48	U	101	PEE	O5-C30-O3-C3
48	l	701	PEE	O5-C30-O3-C3
48	l	704	PEE	O4-C10-O2-C2
48	s	401	PEE	O4-C10-O2-C2
48	l	701	PEE	C31-C30-O3-C3
53	l	703	CDL	C71-CB7-OB8-CB6
53	a	201	CDL	C51-CB5-OB6-CB4
51	J	402	UQ	C15-C14-C16-C17
51	C	305	UQ	C18-C19-C21-C22
51	J	402	UQ	C18-C19-C21-C22
48	U	101	PEE	C31-C30-O3-C3
51	C	305	UQ	C22-C23-C24-C25
48	B	303	PEE	C17-C18-C19-C20
48	U	101	PEE	C37-C38-C39-C40
51	C	305	UQ	C17-C18-C19-C21
53	l	703	CDL	OB9-CB7-OB8-CB6
49	g	201	PLX	C2-C1-N1-C1A
53	I	201	CDL	O1-C1-CA2-OA2
53	V	203	CDL	O1-C1-CB2-OB2
53	V	204	CDL	O1-C1-CB2-OB2
53	a	201	CDL	O1-C1-CA2-OA2
53	l	703	CDL	O1-C1-CA2-OA2
53	l	703	CDL	O1-C1-CB2-OB2
53	V	201	CDL	C11-CA5-OA6-CA4
51	C	305	UQ	C14-C16-C17-C18
51	C	305	UQ	C27-C28-C29-C31
51	J	402	UQ	C22-C23-C24-C26
53	l	702	CDL	C31-CA7-OA8-CA6
48	U	101	PEE	C17-C18-C19-C20
48	V	202	PEE	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	l	701	PEE	C17-C18-C19-C20
51	C	305	UQ	C22-C23-C24-C26
49	j	201	PLX	C13-C14-C15-C16
48	C	302	PEE	C11-C10-O2-C2
53	l	702	CDL	OA9-CA7-OA8-CA6
53	V	201	CDL	OA7-CA5-OA6-CA4
53	V	204	CDL	C71-CB7-OB8-CB6
53	V	201	CDL	C11-C12-C13-C14
48	B	303	PEE	C11-C12-C13-C14
49	r	501	PLX	C11-C12-C13-C14
49	r	501	PLX	C9-C10-C11-C12
49	g	201	PLX	C2-C1-N1-C1B
49	J	403	PLX	C25-C26-C27-C28
51	J	402	UQ	C12-C11-C9-C8
53	l	703	CDL	C37-C38-C39-C40
53	V	201	CDL	O1-C1-CB2-OB2
53	a	201	CDL	O1-C1-CB2-OB2
53	s	402	CDL	O1-C1-CA2-OA2
53	V	204	CDL	CA7-C31-C32-C33
49	r	501	PLX	C7-C8-C9-C10
50	Q	501	UQ1	C7-C8-C9-C11
48	l	704	PEE	O3P-C1-C2-O2
53	I	201	CDL	OA5-CA3-CA4-OA6
53	V	203	CDL	C51-CB5-OB6-CB4
48	W	201	PEE	C31-C30-O3-C3
48	B	303	PEE	C37-C38-C39-C40
49	C	303	PLX	C25-C26-C27-C28
51	J	402	UQ	C20-C19-C21-C22
53	l	702	CDL	CB5-C51-C52-C53
53	l	703	CDL	CB5-C51-C52-C53
53	g	202	CDL	C74-C75-C76-C77
53	V	203	CDL	CA5-C11-C12-C13
53	V	204	CDL	OB9-CB7-OB8-CB6
53	s	402	CDL	C14-C15-C16-C17
48	l	705	PEE	C21-C22-C23-C24
49	C	303	PLX	C27-C28-C29-C30
53	V	204	CDL	C36-C37-C38-C39
48	B	303	PEE	C23-C24-C25-C26
53	V	201	CDL	O1-C1-CA2-OA2
53	V	203	CDL	O1-C1-CA2-OA2
53	l	702	CDL	O1-C1-CB2-OB2
53	s	402	CDL	O1-C1-CB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	s	401	PEE	C31-C30-O3-C3
53	g	202	CDL	CB5-C51-C52-C53
53	s	402	CDL	CA7-C31-C32-C33
53	s	402	CDL	CB7-C71-C72-C73
48	C	302	PEE	O4-C10-O2-C2
48	l	705	PEE	C37-C38-C39-C40
53	V	204	CDL	CA5-C11-C12-C13
53	V	204	CDL	C43-C44-C45-C46
48	W	201	PEE	O5-C30-O3-C3
53	s	402	CDL	C33-C34-C35-C36
53	V	203	CDL	OB7-CB5-OB6-CB4
53	g	202	CDL	CB2-C1-CA2-OA2
53	l	703	CDL	CB2-C1-CA2-OA2
48	B	303	PEE	C31-C30-O3-C3
53	V	201	CDL	C31-CA7-OA8-CA6
53	V	204	CDL	C53-C54-C55-C56
53	l	703	CDL	C33-C34-C35-C36
53	V	203	CDL	C39-C40-C41-C42
53	a	201	CDL	C34-C35-C36-C37
53	I	201	CDL	CB7-C71-C72-C73
49	J	403	PLX	O8-C24-C25-C26
49	e	201	PLX	O8-C24-C25-C26
53	s	402	CDL	C51-CB5-OB6-CB4
53	a	201	CDL	CB5-C51-C52-C53
53	V	201	CDL	C62-C63-C64-C65
48	l	705	PEE	C34-C35-C36-C37
49	J	403	PLX	C34-C35-C36-C37
53	n	101	CDL	CB7-C71-C72-C73
53	s	402	CDL	OB7-CB5-OB6-CB4
53	l	703	CDL	C51-CB5-OB6-CB4
53	n	101	CDL	C75-C76-C77-C78
54	J	401	NDP	C2D-C1D-N1N-C6N
48	l	704	PEE	C21-C22-C23-C24
49	j	201	PLX	C33-C34-C35-C36
49	r	501	PLX	C11-C10-C9-C8
49	r	501	PLX	C28-C29-C30-C31
53	V	203	CDL	C14-C15-C16-C17
53	s	402	CDL	C82-C83-C84-C85
49	C	303	PLX	C14-C15-C16-C17
49	e	201	PLX	C25-C26-C27-C28
53	V	204	CDL	C11-C12-C13-C14
53	V	204	CDL	C71-C72-C73-C74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	l	703	CDL	C73-C74-C75-C76
53	n	101	CDL	C52-C53-C54-C55
53	s	402	CDL	C71-C72-C73-C74
49	g	201	PLX	C27-C28-C29-C30
49	g	201	PLX	C28-C29-C30-C31
53	a	201	CDL	C51-C52-C53-C54
53	g	202	CDL	C75-C76-C77-C78
53	n	101	CDL	C54-C55-C56-C57
53	s	402	CDL	C59-C60-C61-C62
48	s	401	PEE	O5-C30-O3-C3
49	J	403	PLX	O9-C24-C25-C26
49	e	201	PLX	O9-C24-C25-C26
49	r	501	PLX	O7-C6-C7-C8
49	J	403	PLX	C33-C34-C35-C36
49	j	201	PLX	C7-C8-C9-C10
49	j	201	PLX	C25-C26-C27-C28
53	l	703	CDL	C32-C33-C34-C35
48	l	705	PEE	C13-C14-C15-C16
48	s	401	PEE	C12-C13-C14-C15
53	V	203	CDL	C17-C18-C19-C20
53	V	204	CDL	C75-C76-C77-C78
53	a	201	CDL	C60-C61-C62-C63
53	s	402	CDL	C51-C52-C53-C54
53	n	101	CDL	CB5-C51-C52-C53
48	l	701	PEE	C32-C33-C34-C35
49	J	403	PLX	C31-C32-C33-C34
53	g	202	CDL	C41-C42-C43-C44
49	a	202	PLX	C7-C8-C9-C10
49	a	202	PLX	C25-C26-C27-C28
53	l	703	CDL	C75-C76-C77-C78
49	j	201	PLX	C14-C15-C16-C17
53	a	201	CDL	C35-C36-C37-C38
53	V	201	CDL	C55-C56-C57-C58
53	s	402	CDL	C32-C33-C34-C35
53	g	202	CDL	CA7-C31-C32-C33
53	s	402	CDL	CB5-C51-C52-C53
49	J	403	PLX	C7-C8-C9-C10
49	g	201	PLX	C11-C10-C9-C8
53	l	702	CDL	C71-C72-C73-C74
53	n	101	CDL	C56-C57-C58-C59
48	B	303	PEE	O5-C30-O3-C3
53	V	204	CDL	C54-C55-C56-C57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	V	201	CDL	OA9-CA7-OA8-CA6
49	r	501	PLX	C27-C28-C29-C30
53	g	202	CDL	C34-C35-C36-C37
53	s	402	CDL	C35-C36-C37-C38
53	l	702	CDL	CA2-C1-CB2-OB2
53	V	203	CDL	C31-CA7-OA8-CA6
49	C	303	PLX	C10-C11-C12-C13
49	C	303	PLX	C28-C29-C30-C31
49	J	403	PLX	C27-C28-C29-C30
49	e	201	PLX	C14-C15-C16-C17
52	X	201	8Q1	C9-C10-C11-C12
53	V	203	CDL	C75-C76-C77-C78
53	V	204	CDL	C73-C74-C75-C76
53	g	202	CDL	C33-C34-C35-C36
53	g	202	CDL	C43-C44-C45-C46
48	l	701	PEE	C10-C11-C12-C13
49	C	303	PLX	C11-C12-C13-C14
49	J	403	PLX	C13-C14-C15-C16
49	a	202	PLX	C14-C15-C16-C17
53	V	203	CDL	C12-C13-C14-C15
53	V	204	CDL	C37-C38-C39-C40
53	a	201	CDL	C54-C55-C56-C57
53	a	201	CDL	C62-C63-C64-C65
53	g	202	CDL	C57-C58-C59-C60
53	l	702	CDL	C58-C59-C60-C61
53	n	101	CDL	C73-C74-C75-C76
48	U	101	PEE	C22-C23-C24-C25
49	e	201	PLX	C13-C14-C15-C16
49	e	201	PLX	C10-C11-C12-C13
53	l	702	CDL	C56-C57-C58-C59
48	V	202	PEE	C31-C32-C33-C34
49	j	201	PLX	C10-C11-C12-C13
53	V	203	CDL	C76-C77-C78-C79
49	g	201	PLX	C2-C1-N1-C1C
53	g	202	CDL	C83-C84-C85-C86
53	l	703	CDL	C14-C15-C16-C17
48	B	303	PEE	C35-C36-C37-C38
48	i	401	PEE	C19-C20-C21-C22
49	a	202	PLX	C9-C10-C11-C12
52	X	201	8Q1	C11-C10-C9-C8
53	s	402	CDL	C75-C76-C77-C78
49	C	303	PLX	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	a	201	CDL	CB7-C71-C72-C73
48	C	302	PEE	C32-C33-C34-C35
48	i	401	PEE	C21-C22-C23-C24
49	J	403	PLX	C10-C11-C12-C13
49	g	201	PLX	C9-C10-C11-C12
53	V	201	CDL	C31-C32-C33-C34
53	V	201	CDL	C52-C53-C54-C55
53	n	101	CDL	C71-C72-C73-C74
49	g	201	PLX	C14-C15-C16-C17
53	V	204	CDL	C15-C16-C17-C18
51	C	305	UQ	C23-C24-C26-C27
51	J	402	UQ	C13-C14-C16-C17
48	V	202	PEE	C20-C21-C22-C23
49	j	201	PLX	C12-C13-C14-C15
53	V	203	CDL	C59-C60-C61-C62
53	g	202	CDL	C71-C72-C73-C74
53	s	402	CDL	C73-C74-C75-C76
53	g	202	CDL	CA5-C11-C12-C13
49	g	201	PLX	C17-C18-C19-C20
53	s	402	CDL	C52-C53-C54-C55
53	a	201	CDL	C11-C12-C13-C14
53	l	703	CDL	C72-C73-C74-C75
53	s	402	CDL	C37-C38-C39-C40
49	a	202	PLX	C12-C13-C14-C15
49	a	202	PLX	C27-C28-C29-C30
53	a	201	CDL	C32-C33-C34-C35
49	g	201	PLX	C25-C26-C27-C28
53	n	101	CDL	C51-C52-C53-C54
53	I	201	CDL	CA7-C31-C32-C33
53	V	201	CDL	C73-C74-C75-C76
49	e	201	PLX	C30-C31-C32-C33
49	r	501	PLX	C31-C32-C33-C34
48	B	303	PEE	C11-C10-O2-C2
48	l	701	PEE	C11-C10-O2-C2
53	I	201	CDL	C51-CB5-OB6-CB4
53	V	201	CDL	C51-CB5-OB6-CB4
53	l	703	CDL	C11-CA5-OA6-CA4
53	s	402	CDL	C11-CA5-OA6-CA4
53	l	703	CDL	OB7-CB5-OB6-CB4
53	s	402	CDL	OA7-CA5-OA6-CA4
48	B	303	PEE	C34-C35-C36-C37
53	V	201	CDL	C37-C38-C39-C40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	a	201	CDL	C21-C22-C23-C24
48	i	401	PEE	C35-C36-C37-C38
48	l	705	PEE	C15-C16-C17-C18
49	J	403	PLX	C11-C10-C9-C8
49	J	403	PLX	C28-C29-C30-C31
48	V	202	PEE	C14-C15-C16-C17
48	W	201	PEE	C23-C24-C25-C26
49	r	501	PLX	C13-C14-C15-C16
54	J	401	NDP	O4D-C4D-C5D-O5D
49	a	202	PLX	C15-C16-C17-C18
49	g	201	PLX	C32-C33-C34-C35
53	s	402	CDL	C17-C18-C19-C20
53	V	203	CDL	OA9-CA7-OA8-CA6
48	W	201	PEE	C21-C22-C23-C24
53	V	203	CDL	C36-C37-C38-C39
53	a	201	CDL	C52-C53-C54-C55
53	l	702	CDL	C51-C52-C53-C54
53	l	703	CDL	C71-C72-C73-C74
49	J	403	PLX	C19-C20-C21-C22
49	e	201	PLX	C11-C10-C9-C8
53	V	204	CDL	C78-C79-C80-C81
49	j	201	PLX	C27-C28-C29-C30
53	V	201	CDL	CA7-C31-C32-C33
53	n	101	CDL	C55-C56-C57-C58
48	B	303	PEE	O4-C10-O2-C2
53	V	201	CDL	OB5-CB3-CB4-OB6
53	V	204	CDL	OA5-CA3-CA4-OA6
53	g	202	CDL	C62-C63-C64-C65
53	l	703	CDL	C55-C56-C57-C58
48	V	202	PEE	C11-C10-O2-C2
53	V	204	CDL	C14-C15-C16-C17
53	V	204	CDL	C32-C33-C34-C35
53	a	201	CDL	C17-C18-C19-C20
53	V	201	CDL	CB7-C71-C72-C73
48	s	401	PEE	C21-C22-C23-C24
48	V	202	PEE	C19-C20-C21-C22
53	V	204	CDL	OB6-CB4-CB6-OB8
49	e	201	PLX	C19-C20-C21-C22
53	V	201	CDL	C75-C76-C77-C78
53	a	201	CDL	C23-C24-C25-C26
49	g	201	PLX	C10-C11-C12-C13
53	V	204	CDL	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	V	204	CDL	C52-C53-C54-C55
48	i	401	PEE	C12-C13-C14-C15
53	a	201	CDL	C22-C23-C24-C25
48	U	101	PEE	C14-C15-C16-C17
53	l	703	CDL	C62-C63-C64-C65
53	V	203	CDL	C13-C14-C15-C16
53	V	203	CDL	CB2-C1-CA2-OA2
53	V	204	CDL	CA2-C1-CB2-OB2
53	V	201	CDL	C56-C57-C58-C59
53	g	202	CDL	C56-C57-C58-C59
48	U	101	PEE	C23-C24-C25-C26
53	l	702	CDL	C36-C37-C38-C39
49	a	202	PLX	C31-C32-C33-C34
53	V	201	CDL	C71-C72-C73-C74
53	V	201	CDL	C53-C54-C55-C56
53	V	201	CDL	C44-C45-C46-C47
48	U	101	PEE	C13-C14-C15-C16
53	s	402	CDL	C36-C37-C38-C39
48	U	101	PEE	C31-C32-C33-C34
49	r	501	PLX	C16-C17-C18-C19
49	r	501	PLX	C12-C13-C14-C15
49	r	501	PLX	C33-C34-C35-C36
48	B	303	PEE	C38-C39-C40-C41
49	e	201	PLX	C7-C8-C9-C10
53	g	202	CDL	C60-C61-C62-C63
48	l	704	PEE	O3P-C1-C2-C3
49	J	403	PLX	O4-C3-C4-C5
53	I	201	CDL	OA5-CA3-CA4-CA6
53	I	201	CDL	OB5-CB3-CB4-CB6
53	V	204	CDL	OA5-CA3-CA4-CA6
53	n	101	CDL	OA5-CA3-CA4-CA6
53	s	402	CDL	OA5-CA3-CA4-CA6
48	l	701	PEE	O4-C10-O2-C2
53	V	203	CDL	C32-C33-C34-C35
53	V	204	CDL	C82-C83-C84-C85
49	j	201	PLX	O6-C6-C7-C8
49	r	501	PLX	O6-C6-C7-C8
53	V	201	CDL	C57-C58-C59-C60
53	V	204	CDL	C21-C22-C23-C24
48	C	302	PEE	C31-C30-O3-C3
48	l	704	PEE	C31-C30-O3-C3
53	l	703	CDL	C61-C62-C63-C64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	l	703	CDL	C77-C78-C79-C80
48	W	201	PEE	C1-C2-C3-O3
53	V	204	CDL	CB3-CB4-CB6-OB8
53	l	703	CDL	CA3-CA4-CA6-OA8
53	s	402	CDL	C16-C17-C18-C19
48	W	201	PEE	C19-C20-C21-C22
48	l	704	PEE	C15-C16-C17-C18
48	U	101	PEE	C40-C41-C42-C43
49	C	303	PLX	C9-C10-C11-C12
53	l	703	CDL	C39-C40-C41-C42
48	l	704	PEE	C11-C12-C13-C14
53	a	201	CDL	C71-CB7-OB8-CB6
48	W	201	PEE	C13-C14-C15-C16
53	V	203	CDL	C37-C38-C39-C40
53	V	203	CDL	C40-C41-C42-C43
53	g	202	CDL	C37-C38-C39-C40
53	V	203	CDL	C54-C55-C56-C57
48	C	302	PEE	C13-C14-C15-C16
49	a	202	PLX	C34-C35-C36-C37
53	V	203	CDL	C42-C43-C44-C45
53	l	703	CDL	C21-C22-C23-C24
48	V	202	PEE	C36-C37-C38-C39
53	g	202	CDL	C84-C85-C86-C87
53	V	201	CDL	OB7-CB5-OB6-CB4
48	l	701	PEE	C33-C34-C35-C36
53	a	201	CDL	C53-C54-C55-C56
49	r	501	PLX	C30-C31-C32-C33
53	V	201	CDL	C14-C15-C16-C17
49	a	202	PLX	C11-C12-C13-C14
53	a	201	CDL	C42-C43-C44-C45
48	C	302	PEE	C15-C16-C17-C18
48	W	201	PEE	C15-C16-C17-C18
48	B	303	PEE	C20-C21-C22-C23
48	U	101	PEE	C11-C12-C13-C14
48	V	202	PEE	C23-C24-C25-C26
49	a	202	PLX	C28-C29-C30-C31
49	C	303	PLX	C13-C14-C15-C16
53	g	202	CDL	C11-C12-C13-C14
48	W	201	PEE	C17-C18-C19-C20
48	U	101	PEE	C34-C35-C36-C37
53	V	204	CDL	C13-C14-C15-C16
53	l	702	CDL	C11-CA5-OA6-CA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	V	202	PEE	C40-C41-C42-C43
49	j	201	PLX	C11-C12-C13-C14
53	g	202	CDL	C14-C15-C16-C17
49	C	303	PLX	C35-C36-C37-C38
49	r	501	PLX	O6-C4-C5-O8
48	W	201	PEE	C24-C25-C26-C27
49	e	201	PLX	C26-C27-C28-C29
53	l	703	CDL	C41-C42-C43-C44
48	l	704	PEE	C10-C11-C12-C13
49	e	201	PLX	C12-C13-C14-C15
53	l	703	CDL	C35-C36-C37-C38
53	a	201	CDL	C44-C45-C46-C47
53	g	202	CDL	C64-C65-C66-C67
53	g	202	CDL	C32-C33-C34-C35
53	g	202	CDL	C63-C64-C65-C66
48	C	302	PEE	C39-C40-C41-C42
53	n	101	CDL	C74-C75-C76-C77
48	U	101	PEE	C11-C10-O2-C2
48	l	704	PEE	C42-C43-C44-C45
53	V	204	CDL	C34-C35-C36-C37
49	g	201	PLX	C7-C8-C9-C10
48	C	302	PEE	C11-C12-C13-C14
48	W	201	PEE	C22-C23-C24-C25
53	a	201	CDL	C14-C15-C16-C17
53	g	202	CDL	C59-C60-C61-C62
53	g	202	CDL	C13-C14-C15-C16
53	n	101	CDL	C72-C73-C74-C75
48	V	202	PEE	C41-C42-C43-C44
53	s	402	CDL	C54-C55-C56-C57
49	e	201	PLX	C27-C28-C29-C30
53	g	202	CDL	C17-C18-C19-C20
53	V	201	CDL	OB5-CB3-CB4-CB6
53	l	703	CDL	OB5-CB3-CB4-CB6
48	V	202	PEE	C12-C13-C14-C15
48	W	201	PEE	C12-C13-C14-C15
48	s	401	PEE	C13-C14-C15-C16
49	e	201	PLX	C16-C17-C18-C19
53	V	204	CDL	C84-C85-C86-C87
53	g	202	CDL	C72-C71-CB7-OB8
49	e	201	PLX	C36-C37-C38-C39
49	J	403	PLX	C14-C15-C16-C17
53	V	203	CDL	C64-C65-C66-C67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	l	705	PEE	C18-C19-C20-C21
48	C	302	PEE	O5-C30-O3-C3
53	a	201	CDL	OB9-CB7-OB8-CB6
48	V	202	PEE	C13-C14-C15-C16
48	l	704	PEE	O5-C30-O3-C3
49	r	501	PLX	C25-C26-C27-C28
49	J	403	PLX	C30-C31-C32-C33
53	V	204	CDL	C55-C56-C57-C58
53	V	201	CDL	C64-C65-C66-C67
53	l	703	CDL	C40-C41-C42-C43
48	l	704	PEE	C1-C2-C3-O3
48	l	705	PEE	C1-C2-C3-O3
48	s	401	PEE	C1-C2-C3-O3
49	J	403	PLX	C3-C4-C5-O8
49	a	202	PLX	C3-C4-C5-O8
49	e	201	PLX	C3-C4-C5-O8
53	V	203	CDL	CB3-CB4-CB6-OB8
48	i	401	PEE	C24-C25-C26-C27
53	g	202	CDL	C77-C78-C79-C80
49	g	201	PLX	C12-C13-C14-C15
49	r	501	PLX	C14-C15-C16-C17
53	a	201	CDL	C82-C83-C84-C85
49	e	201	PLX	C33-C34-C35-C36
48	V	202	PEE	O4-C10-O2-C2
53	I	201	CDL	OB7-CB5-OB6-CB4
53	l	703	CDL	OA7-CA5-OA6-CA4
53	a	201	CDL	CA5-C11-C12-C13
53	V	203	CDL	OA5-CA3-CA4-OA6
49	C	303	PLX	C7-C8-C9-C10
49	a	202	PLX	C29-C30-C31-C32
53	n	101	CDL	C53-C54-C55-C56
48	C	302	PEE	C42-C43-C44-C45
49	e	201	PLX	C28-C29-C30-C31
52	X	201	8Q1	C10-C11-C12-C13
53	V	203	CDL	C74-C75-C76-C77
48	W	201	PEE	O2-C2-C3-O3
53	s	402	CDL	OB6-CB4-CB6-OB8
53	I	201	CDL	C11-C12-C13-C14
53	V	201	CDL	C74-C75-C76-C77
48	V	202	PEE	C11-C12-C13-C14
49	C	303	PLX	C11-C10-C9-C8
48	B	303	PEE	C40-C41-C42-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	U	101	PEE	C12-C13-C14-C15
49	g	201	PLX	C13-C14-C15-C16
53	V	204	CDL	C17-C18-C19-C20
53	g	202	CDL	C52-C53-C54-C55
49	r	501	PLX	O8-C24-C25-C26
48	B	303	PEE	C14-C15-C16-C17
49	j	201	PLX	C30-C31-C32-C33
48	l	704	PEE	C32-C33-C34-C35
48	s	401	PEE	C11-C12-C13-C14
53	V	203	CDL	C24-C25-C26-C27
51	J	402	UQ	C14-C16-C17-C18
48	U	101	PEE	C38-C39-C40-C41
48	i	401	PEE	C18-C19-C20-C21
49	a	202	PLX	C13-C14-C15-C16
53	g	202	CDL	C44-C45-C46-C47
48	l	704	PEE	C24-C25-C26-C27
49	e	201	PLX	C24-C25-C26-C27
53	I	201	CDL	CB2-C1-CA2-OA2
53	V	201	CDL	C54-C55-C56-C57
53	V	203	CDL	C60-C61-C62-C63
53	g	202	CDL	C16-C17-C18-C19
49	e	201	PLX	C11-C12-C13-C14
53	V	203	CDL	OB5-CB3-CB4-CB6
49	a	202	PLX	C16-C17-C18-C19
48	B	303	PEE	C10-C11-C12-C13
48	l	704	PEE	C33-C34-C35-C36
46	A	502	FMN	C5'-O5'-P-O3P
48	C	302	PEE	C37-C38-C39-C40
48	C	302	PEE	C20-C21-C22-C23
48	U	101	PEE	O4-C10-O2-C2
53	V	204	CDL	C20-C21-C22-C23
53	V	201	CDL	CA6-CA4-OA6-CA5
53	V	204	CDL	CA6-CA4-OA6-CA5
48	l	704	PEE	C19-C20-C21-C22
53	V	203	CDL	C53-C54-C55-C56
53	s	402	CDL	C11-C12-C13-C14
53	V	204	CDL	C81-C82-C83-C84
53	l	702	CDL	OA7-CA5-OA6-CA4
49	r	501	PLX	C18-C19-C20-C21
49	C	303	PLX	C3-C4-C5-O8
53	V	201	CDL	CA3-CA4-CA6-OA8
53	s	402	CDL	CB3-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	j	201	PLX	C31-C32-C33-C34
48	l	704	PEE	O2-C2-C3-O3
48	l	705	PEE	O2-C2-C3-O3
48	s	401	PEE	O2-C2-C3-O3
49	J	403	PLX	O6-C4-C5-O8
49	j	201	PLX	O6-C4-C5-O8
53	l	703	CDL	OB6-CB4-CB6-OB8
48	C	302	PEE	C34-C35-C36-C37
49	C	303	PLX	C31-C32-C33-C34
49	J	403	PLX	C35-C36-C37-C38
49	a	202	PLX	C35-C36-C37-C38
49	j	201	PLX	C7-C6-O6-C4
53	g	202	CDL	C39-C40-C41-C42
49	J	403	PLX	C29-C30-C31-C32
48	C	302	PEE	C44-C45-C46-C47
53	V	204	CDL	C31-C32-C33-C34
48	V	202	PEE	C21-C22-C23-C24
49	C	303	PLX	N1-C1-C2-O1
49	J	403	PLX	N1-C1-C2-O1
53	g	202	CDL	C35-C36-C37-C38
48	C	302	PEE	C35-C36-C37-C38
48	s	401	PEE	C23-C24-C25-C26
53	s	402	CDL	C55-C56-C57-C58
49	e	201	PLX	C29-C30-C31-C32
53	V	201	CDL	C51-C52-C53-C54
49	C	303	PLX	C25-C24-O8-C5
49	J	403	PLX	C25-C24-O8-C5
49	a	202	PLX	C25-C24-O8-C5
53	l	703	CDL	C51-C52-C53-C54
48	V	202	PEE	C33-C34-C35-C36
53	a	201	CDL	C31-C32-C33-C34
53	V	201	CDL	OA5-CA3-CA4-CA6
53	V	203	CDL	OA5-CA3-CA4-CA6
49	e	201	PLX	C31-C32-C33-C34
53	g	202	CDL	C15-C16-C17-C18
48	s	401	PEE	C24-C25-C26-C27
49	a	202	PLX	C30-C31-C32-C33
53	a	201	CDL	C64-C65-C66-C67
48	B	303	PEE	C41-C42-C43-C44
53	V	203	CDL	C83-C84-C85-C86
53	V	201	CDL	C32-C33-C34-C35
53	g	202	CDL	C1-CB2-OB2-PB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	l	702	CDL	C35-C36-C37-C38
52	X	201	8Q1	C42-C43-S44-C1
53	V	203	CDL	C35-C36-C37-C38
53	I	201	CDL	C51-C52-C53-C54
49	J	403	PLX	O4-C3-C4-O6
53	I	201	CDL	OB5-CB3-CB4-OB6
53	l	703	CDL	OB5-CB3-CB4-OB6
53	n	101	CDL	OA5-CA3-CA4-OA6
48	U	101	PEE	C19-C20-C21-C22
53	l	702	CDL	C54-C55-C56-C57
53	l	703	CDL	C82-C83-C84-C85
52	X	201	8Q1	C13-C14-C15-C16
54	J	401	NDP	O4D-C1D-N1N-C6N
49	e	201	PLX	C15-C16-C17-C18
48	C	302	PEE	O2-C2-C3-O3
49	a	202	PLX	O6-C4-C5-O8
49	e	201	PLX	O6-C4-C5-O8
53	V	201	CDL	OA6-CA4-CA6-OA8
48	C	302	PEE	C1-C2-C3-O3
49	j	201	PLX	C3-C4-C5-O8
49	r	501	PLX	C3-C4-C5-O8
49	J	403	PLX	C12-C13-C14-C15
53	V	201	CDL	C19-C20-C21-C22
48	l	705	PEE	C38-C39-C40-C41
49	g	201	PLX	C33-C34-C35-C36
48	C	302	PEE	C1-O3P-P-O2P
48	C	302	PEE	C1-O3P-P-O4P
48	C	302	PEE	C4-O4P-P-O2P
48	V	202	PEE	C1-O3P-P-O4P
48	W	201	PEE	C4-O4P-P-O3P
48	W	201	PEE	C4-O4P-P-O2P
48	W	201	PEE	C4-O4P-P-O1P
48	i	401	PEE	C1-O3P-P-O2P
48	i	401	PEE	C1-O3P-P-O1P
48	i	401	PEE	C1-O3P-P-O4P
48	l	704	PEE	C1-O3P-P-O1P
48	s	401	PEE	C4-O4P-P-O3P
48	s	401	PEE	C4-O4P-P-O1P
49	C	303	PLX	C2-O1-P1-O3
49	J	403	PLX	C2-O1-P1-O3
49	a	202	PLX	C3-O4-P1-O1
49	e	201	PLX	C3-O4-P1-O1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	e	201	PLX	C3-O4-P1-O2
49	e	201	PLX	C3-O4-P1-O3
49	e	201	PLX	C2-O1-P1-O4
49	r	501	PLX	C3-O4-P1-O1
49	r	501	PLX	C3-O4-P1-O2
49	r	501	PLX	C3-O4-P1-O3
49	r	501	PLX	C2-O1-P1-O4
49	r	501	PLX	C2-O1-P1-O3
53	I	201	CDL	CB2-OB2-PB2-OB4
53	V	201	CDL	CA3-OA5-PA1-OA2
53	V	201	CDL	CA3-OA5-PA1-OA3
53	V	201	CDL	CB3-OB5-PB2-OB4
53	V	203	CDL	CA3-OA5-PA1-OA2
53	V	203	CDL	CA3-OA5-PA1-OA3
53	V	203	CDL	CA3-OA5-PA1-OA4
53	g	202	CDL	CA2-OA2-PA1-OA4
53	g	202	CDL	CB2-OB2-PB2-OB3
53	g	202	CDL	CB2-OB2-PB2-OB4
53	g	202	CDL	CB2-OB2-PB2-OB5
53	g	202	CDL	CB3-OB5-PB2-OB4
53	l	702	CDL	CA3-OA5-PA1-OA2
53	l	702	CDL	CA3-OA5-PA1-OA4
53	s	402	CDL	CA2-OA2-PA1-OA3
53	s	402	CDL	CB2-OB2-PB2-OB3
58	w	401	ADP	C5'-O5'-PA-O1A
58	w	401	ADP	C5'-O5'-PA-O3A
53	l	703	CDL	C18-C19-C20-C21
53	V	201	CDL	CA4-CA3-OA5-PA1
53	V	203	CDL	C1-CB2-OB2-PB2
53	l	702	CDL	CA4-CA3-OA5-PA1
53	V	203	CDL	CA7-C31-C32-C33
53	l	703	CDL	C32-C31-CA7-OA8
49	J	403	PLX	C24-C25-C26-C27
48	l	705	PEE	C23-C24-C25-C26
53	V	201	CDL	C58-C59-C60-C61
53	l	702	CDL	C34-C35-C36-C37
48	l	704	PEE	C3-C2-O2-C10
53	s	402	CDL	CA3-CA4-OA6-CA5
53	V	201	CDL	C43-C44-C45-C46
53	V	203	CDL	C31-C32-C33-C34
53	a	201	CDL	C72-C73-C74-C75
53	l	702	CDL	C82-C83-C84-C85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	l	703	CDL	C12-C13-C14-C15
53	s	402	CDL	CB2-C1-CA2-OA2
53	a	201	CDL	C71-C72-C73-C74
48	C	302	PEE	C12-C13-C14-C15
53	V	204	CDL	C72-C73-C74-C75
48	l	701	PEE	C18-C19-C20-C21
48	B	303	PEE	C13-C14-C15-C16
48	l	704	PEE	C40-C41-C42-C43
53	l	702	CDL	C53-C54-C55-C56
48	B	303	PEE	C15-C16-C17-C18
53	V	204	CDL	C39-C40-C41-C42
48	l	705	PEE	C11-C12-C13-C14
53	l	702	CDL	CA5-C11-C12-C13
53	s	402	CDL	C15-C16-C17-C18
48	B	303	PEE	C44-C45-C46-C47
52	X	201	8Q1	C7-C8-C9-C10
49	g	201	PLX	C36-C37-C38-C39
48	l	701	PEE	C31-C32-C33-C34
48	V	202	PEE	C15-C16-C17-C18
53	a	201	CDL	C41-C42-C43-C44
49	a	202	PLX	O8-C24-C25-C26
49	g	201	PLX	O6-C6-C7-C8
49	g	201	PLX	O8-C24-C25-C26
53	l	703	CDL	C15-C16-C17-C18
48	V	202	PEE	C24-C25-C26-C27
53	s	402	CDL	C12-C13-C14-C15
48	U	101	PEE	C21-C22-C23-C24
53	s	402	CDL	OB9-CB7-OB8-CB6
53	s	402	CDL	C71-CB7-OB8-CB6
48	B	303	PEE	O3P-C1-C2-O2
53	V	201	CDL	OA5-CA3-CA4-OA6
53	l	702	CDL	OA5-CA3-CA4-OA6
48	i	401	PEE	C16-C17-C18-C19
48	i	401	PEE	C38-C39-C40-C41
48	l	704	PEE	C38-C39-C40-C41
48	C	302	PEE	C41-C42-C43-C44
48	U	101	PEE	C41-C42-C43-C44
53	V	201	CDL	C35-C36-C37-C38
49	J	403	PLX	C17-C18-C19-C20
48	l	701	PEE	C38-C39-C40-C41
48	B	303	PEE	O2-C2-C3-O3
48	l	701	PEE	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	I	201	CDL	C71-C72-C73-C74
53	l	703	CDL	C64-C65-C66-C67
53	V	203	CDL	C61-C62-C63-C64
53	a	201	CDL	C57-C58-C59-C60
53	n	101	CDL	CA5-C11-C12-C13
53	V	204	CDL	C42-C43-C44-C45
49	j	201	PLX	C28-C29-C30-C31
48	V	202	PEE	C38-C39-C40-C41
53	l	702	CDL	C39-C40-C41-C42
48	l	705	PEE	C2-C1-O3P-P
53	V	201	CDL	C33-C34-C35-C36
48	C	302	PEE	C19-C20-C21-C22
53	l	702	CDL	C16-C17-C18-C19
49	g	201	PLX	C18-C19-C20-C21
53	l	702	CDL	C55-C56-C57-C58
49	g	201	PLX	C30-C31-C32-C33
53	a	201	CDL	C58-C59-C60-C61
53	l	702	CDL	C63-C64-C65-C66
53	s	402	CDL	CA6-CA4-OA6-CA5
53	l	703	CDL	CB7-C71-C72-C73
49	C	303	PLX	C19-C20-C21-C22
49	g	201	PLX	C20-C21-C22-C23
49	r	501	PLX	C34-C35-C36-C37
53	a	201	CDL	C33-C34-C35-C36
49	r	501	PLX	C4-C3-O4-P1
53	V	204	CDL	CA4-CA3-OA5-PA1
53	l	702	CDL	C21-C22-C23-C24
53	a	201	CDL	C20-C21-C22-C23
49	C	303	PLX	C16-C17-C18-C19
47	A	503	NAI	O4D-C1D-N1N-C2N
54	J	401	NDP	C3D-C4D-C5D-O5D
48	l	704	PEE	C20-C21-C22-C23
48	W	201	PEE	C20-C21-C22-C23
53	s	402	CDL	C78-C79-C80-C81
49	j	201	PLX	C15-C16-C17-C18
47	A	503	NAI	C2D-C1D-N1N-C2N
53	g	202	CDL	C73-C74-C75-C76
51	C	305	UQ	C12-C11-C9-C10
54	J	401	NDP	C2B-O2B-P2B-O1X
53	s	402	CDL	C84-C85-C86-C87
53	V	201	CDL	C80-C81-C82-C83
53	a	201	CDL	C24-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	e	201	PLX	C35-C36-C37-C38
53	l	703	CDL	C56-C57-C58-C59
53	l	702	CDL	C75-C76-C77-C78
53	l	703	CDL	C36-C37-C38-C39
49	J	403	PLX	C26-C27-C28-C29
53	l	702	CDL	C76-C77-C78-C79
53	l	703	CDL	CB3-CB4-CB6-OB8
48	W	201	PEE	C16-C17-C18-C19
49	C	303	PLX	O9-C24-C25-C26
53	V	203	CDL	C77-C78-C79-C80
53	V	203	CDL	C33-C34-C35-C36
53	a	201	CDL	C43-C44-C45-C46
49	e	201	PLX	C2-C1-N1-C1B
53	V	203	CDL	C43-C44-C45-C46
53	g	202	CDL	C72-C71-CB7-OB9
53	a	201	CDL	OB5-CB3-CB4-CB6
53	g	202	CDL	OA6-CA4-CA6-OA8
53	n	101	CDL	OA6-CA4-CA6-OA8
48	s	401	PEE	C18-C19-C20-C21
53	l	702	CDL	C18-C19-C20-C21
53	n	101	CDL	C1-CB2-OB2-PB2
48	s	401	PEE	C15-C16-C17-C18
53	V	203	CDL	C72-C73-C74-C75
48	V	202	PEE	C16-C17-C18-C19
49	e	201	PLX	C2-C1-N1-C1C
48	C	302	PEE	C18-C19-C20-C21
53	a	201	CDL	OB5-CB3-CB4-OB6
53	g	202	CDL	OB9-CB7-OB8-CB6
53	g	202	CDL	C55-C56-C57-C58
53	l	702	CDL	C37-C38-C39-C40
48	l	701	PEE	C16-C17-C18-C19
53	l	703	CDL	C57-C58-C59-C60
49	a	202	PLX	O6-C6-C7-C8
48	l	704	PEE	C13-C14-C15-C16
53	g	202	CDL	C58-C59-C60-C61
53	a	201	CDL	C32-C31-CA7-OA8
53	I	201	CDL	C52-C53-C54-C55
48	l	704	PEE	C16-C17-C18-C19
48	s	401	PEE	C16-C17-C18-C19
49	r	501	PLX	C35-C36-C37-C38
53	V	203	CDL	C52-C51-CB5-OB6
53	a	201	CDL	C12-C11-CA5-OA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	s	402	CDL	C72-C71-CB7-OB8
48	B	303	PEE	O3P-C1-C2-C3
53	a	201	CDL	C38-C39-C40-C41
53	l	703	CDL	C79-C80-C81-C82
49	e	201	PLX	C2-C1-N1-C1A
48	s	401	PEE	O3-C30-C31-C32
53	I	201	CDL	C72-C71-CB7-OB8
49	a	202	PLX	C10-C11-C12-C13
53	V	204	CDL	C58-C59-C60-C61
58	w	401	ADP	O4'-C4'-C5'-O5'
53	a	201	CDL	C81-C82-C83-C84
53	l	703	CDL	C31-C32-C33-C34
58	w	401	ADP	PB-O3A-PA-O2A
48	l	704	PEE	C30-C31-C32-C33
48	l	701	PEE	C36-C37-C38-C39
48	l	704	PEE	C36-C37-C38-C39
53	V	203	CDL	C55-C56-C57-C58
53	l	703	CDL	C78-C79-C80-C81
53	a	201	CDL	C36-C37-C38-C39
53	g	202	CDL	C71-CB7-OB8-CB6
49	j	201	PLX	C29-C30-C31-C32
48	s	401	PEE	C22-C23-C24-C25
53	l	702	CDL	C72-C71-CB7-OB8
53	n	101	CDL	C52-C51-CB5-OB6
53	V	201	CDL	C12-C13-C14-C15
53	l	703	CDL	C43-C44-C45-C46
49	j	201	PLX	C24-C25-C26-C27
54	J	401	NDP	C2B-O2B-P2B-O2X
54	J	401	NDP	C2B-O2B-P2B-O3X
48	i	401	PEE	C22-C23-C24-C25
53	V	201	CDL	C32-C31-CA7-OA8
53	l	703	CDL	C72-C71-CB7-OB8
48	l	704	PEE	C43-C44-C45-C46
49	j	201	PLX	C25-C24-O8-C5
53	l	703	CDL	C38-C39-C40-C41
53	V	204	CDL	OA7-CA5-OA6-CA4
48	C	302	PEE	O3-C30-C31-C32
48	l	701	PEE	C11-C12-C13-C14
53	l	703	CDL	C76-C77-C78-C79
53	a	201	CDL	C40-C41-C42-C43
53	s	402	CDL	C56-C57-C58-C59
53	l	703	CDL	CA5-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	V	201	CDL	C22-C23-C24-C25
53	l	702	CDL	CA6-CA4-OA6-CA5
53	V	203	CDL	C52-C51-CB5-OB7
53	a	201	CDL	C32-C31-CA7-OA9
50	C	304	UQ1	C6-C7-C8-C9
53	l	703	CDL	OA5-CA3-CA4-OA6
53	V	203	CDL	C63-C64-C65-C66
53	s	402	CDL	C34-C35-C36-C37
53	a	201	CDL	C12-C11-CA5-OA7
53	I	201	CDL	C52-C51-CB5-OB6
49	g	201	PLX	O9-C24-O8-C5
49	r	501	PLX	O9-C24-O8-C5
53	g	202	CDL	C52-C51-CB5-OB6
48	C	302	PEE	O5-C30-C31-C32
53	I	201	CDL	C72-C71-CB7-OB9
53	l	703	CDL	C72-C71-CB7-OB9
49	g	201	PLX	C15-C16-C17-C18
53	l	703	CDL	C11-C12-C13-C14
53	V	203	CDL	C32-C31-CA7-OA8
53	n	101	CDL	C12-C11-CA5-OA6
53	V	204	CDL	C44-C45-C46-C47
53	l	702	CDL	C72-C71-CB7-OB9
52	G	201	8Q1	O27-C28-C29-C32
48	U	101	PEE	O2-C10-C11-C12
48	s	401	PEE	C10-C11-C12-C13
48	B	303	PEE	O3-C30-C31-C32
53	g	202	CDL	C52-C51-CB5-OB7
53	n	101	CDL	C52-C51-CB5-OB7
53	I	201	CDL	C52-C51-CB5-OB7

There are no ring outliers.

33 monomers are involved in 135 short contacts:

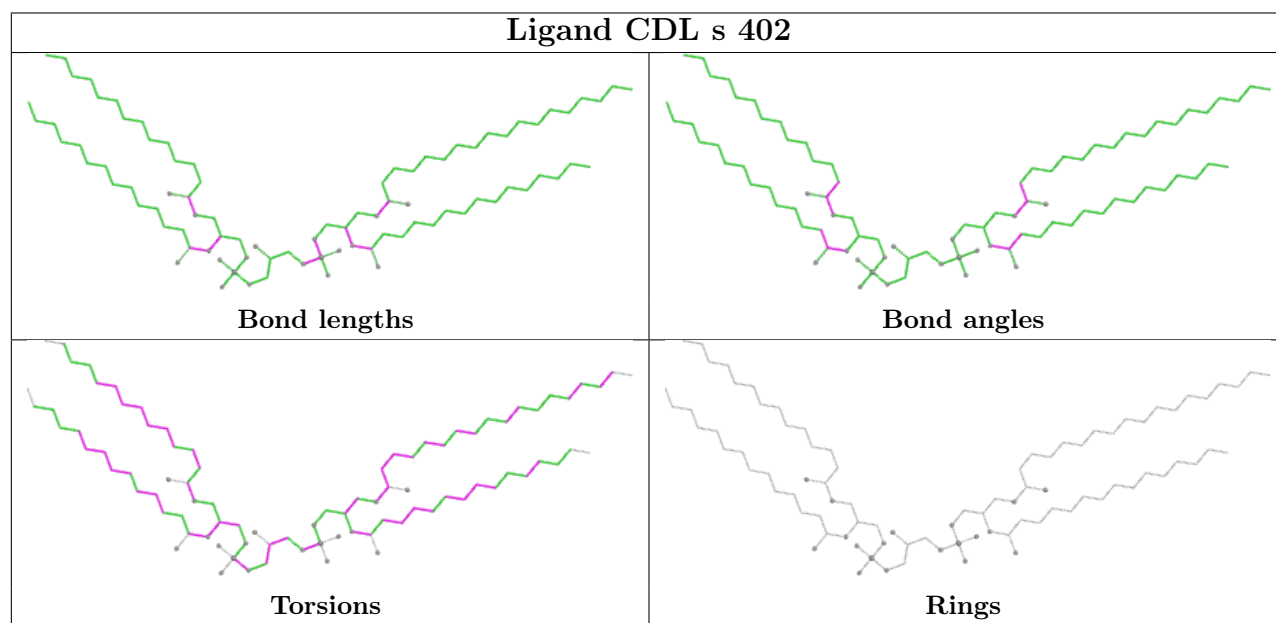
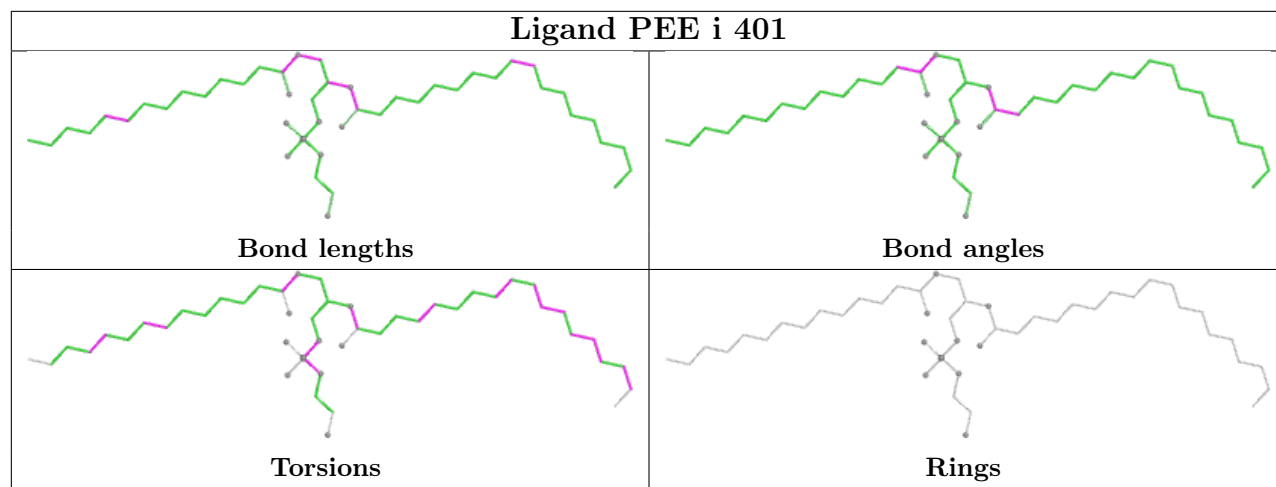
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	i	401	PEE	2	0
53	s	402	CDL	4	0
53	V	204	CDL	7	0
48	W	201	PEE	1	0
53	a	201	CDL	5	0
50	C	304	UQ1	4	0
46	A	502	FMN	3	0
49	g	201	PLX	2	0

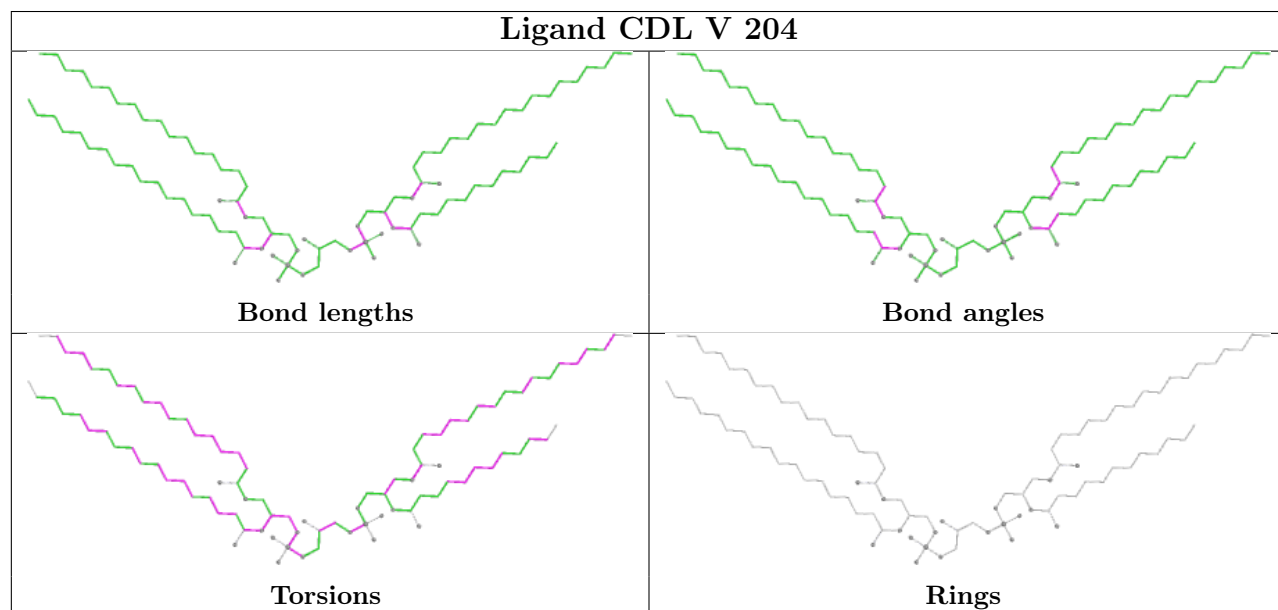
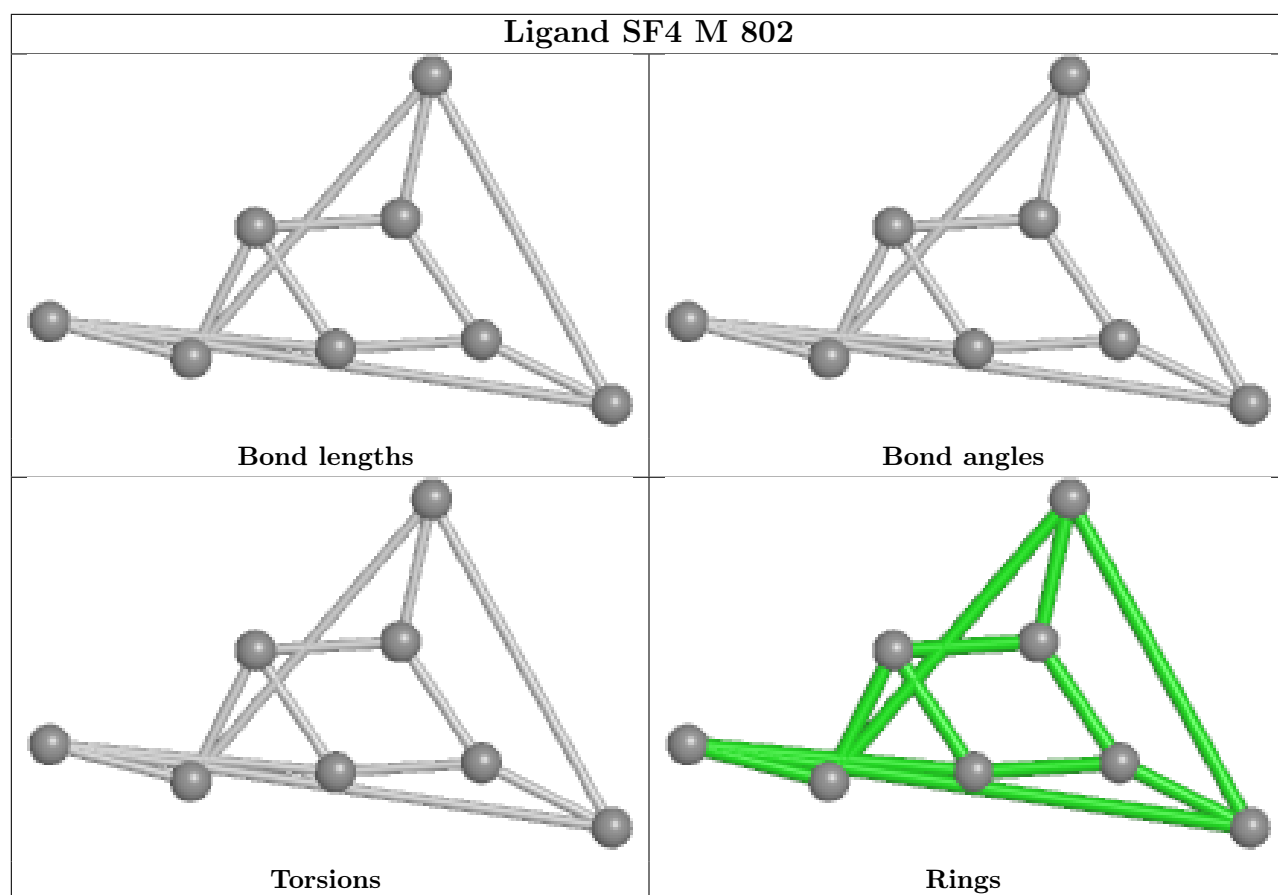
Continued on next page...

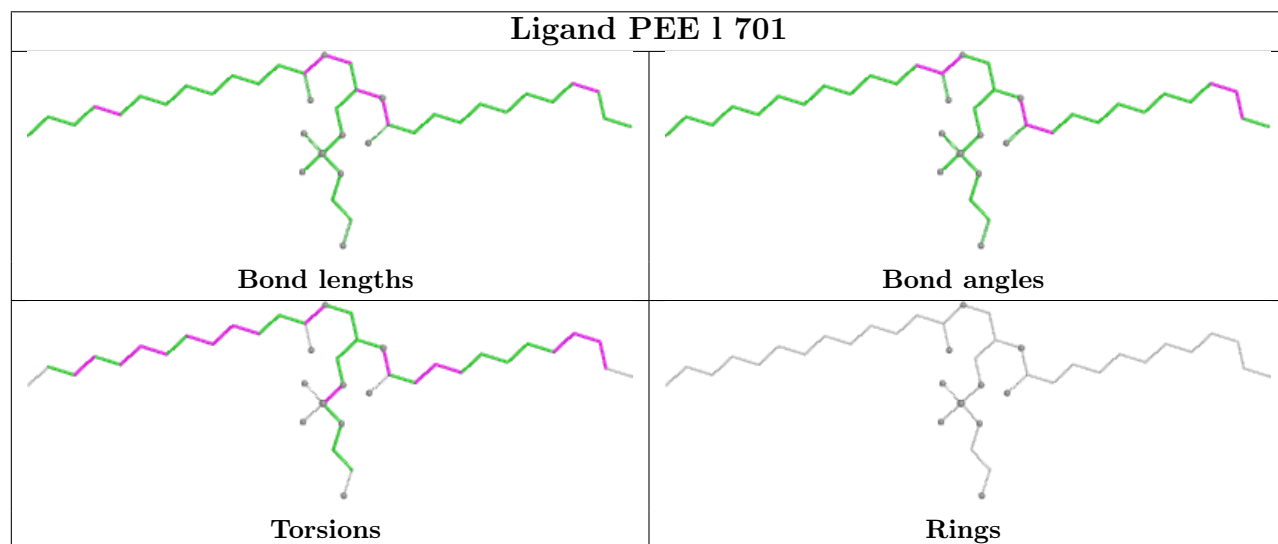
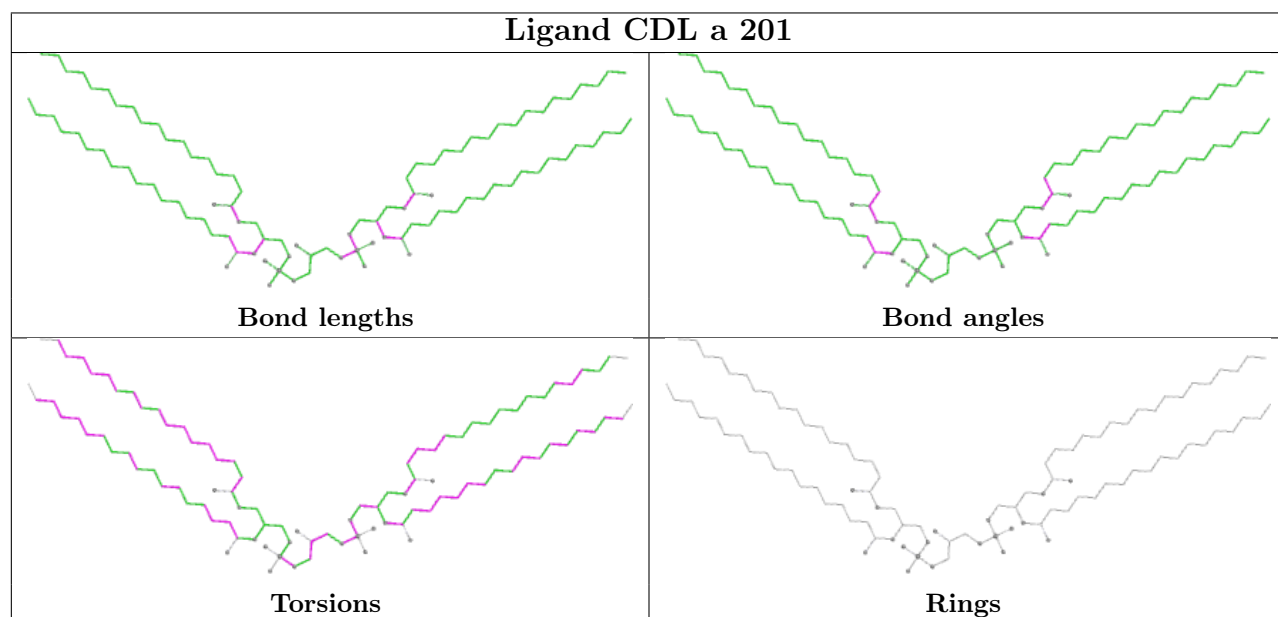
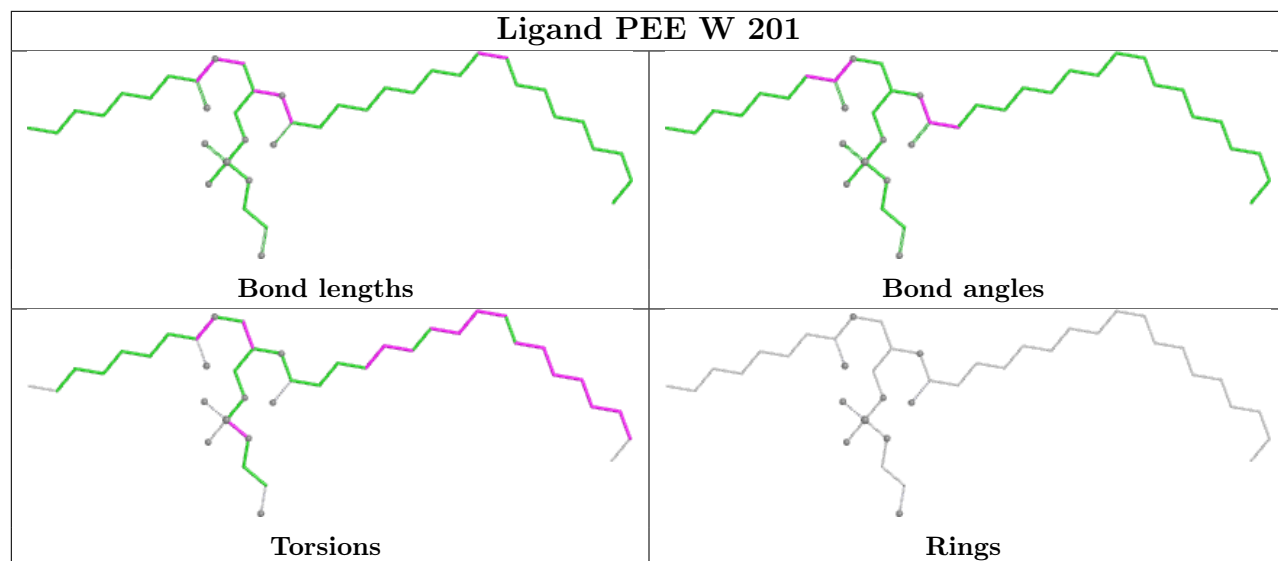
Continued from previous page...

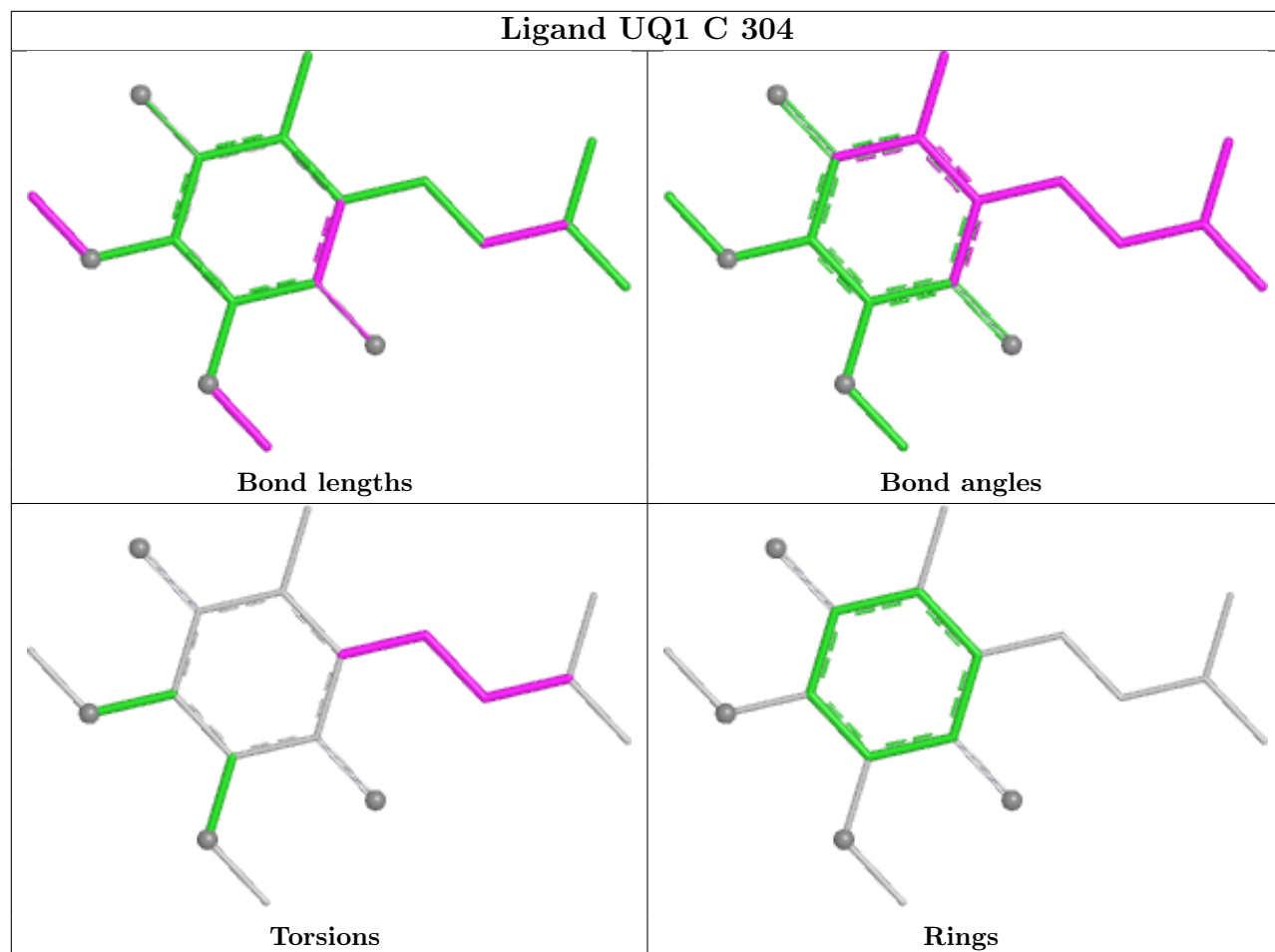
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	A	501	SF4	2	0
51	J	402	UQ	1	0
48	V	202	PEE	3	0
52	G	201	8Q1	11	0
45	C	301	SF4	1	0
48	l	705	PEE	7	0
49	r	501	PLX	5	0
51	C	305	UQ	4	0
48	l	704	PEE	3	0
48	U	101	PEE	4	0
50	Q	501	UQ1	2	0
48	B	303	PEE	3	0
48	s	401	PEE	3	0
53	l	703	CDL	3	0
54	J	401	NDP	1	0
53	V	203	CDL	2	0
49	e	201	PLX	10	0
58	w	401	ADP	1	0
53	l	702	CDL	30	0
53	V	201	CDL	5	0
47	A	503	NAI	5	0
48	C	302	PEE	2	0
53	g	202	CDL	6	0
49	J	403	PLX	3	0
49	C	303	PLX	2	0

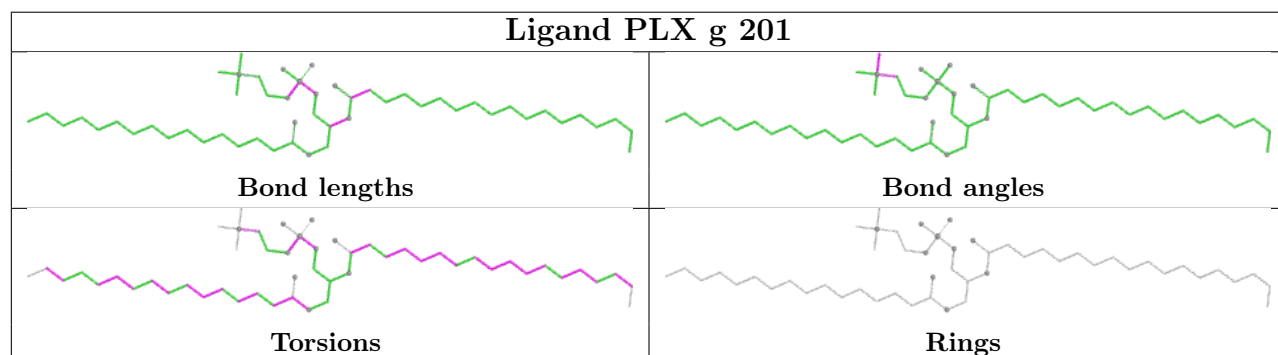
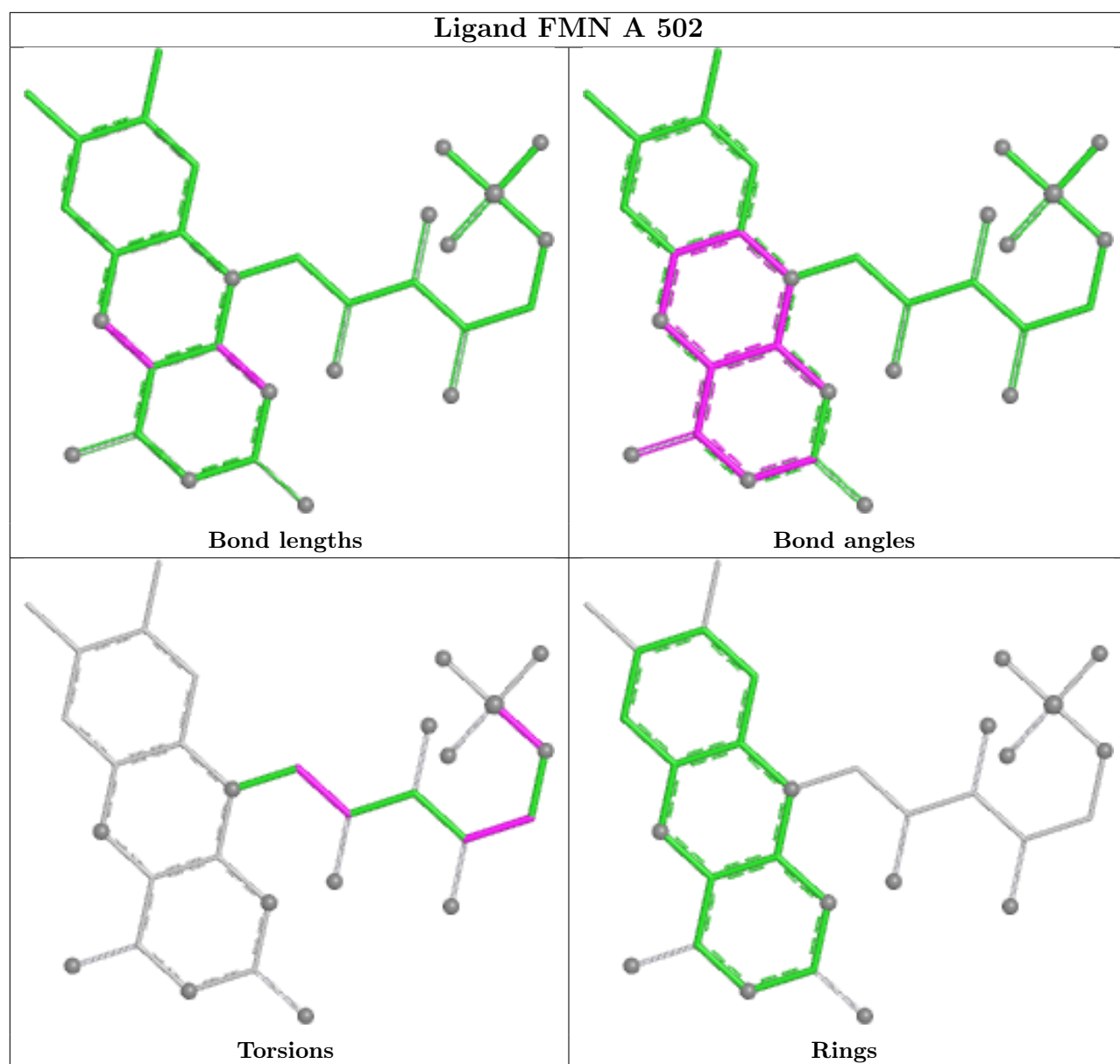
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



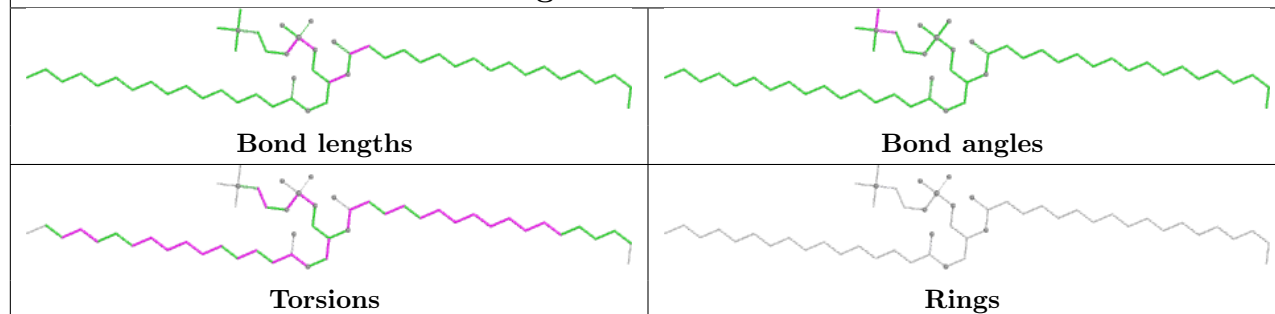




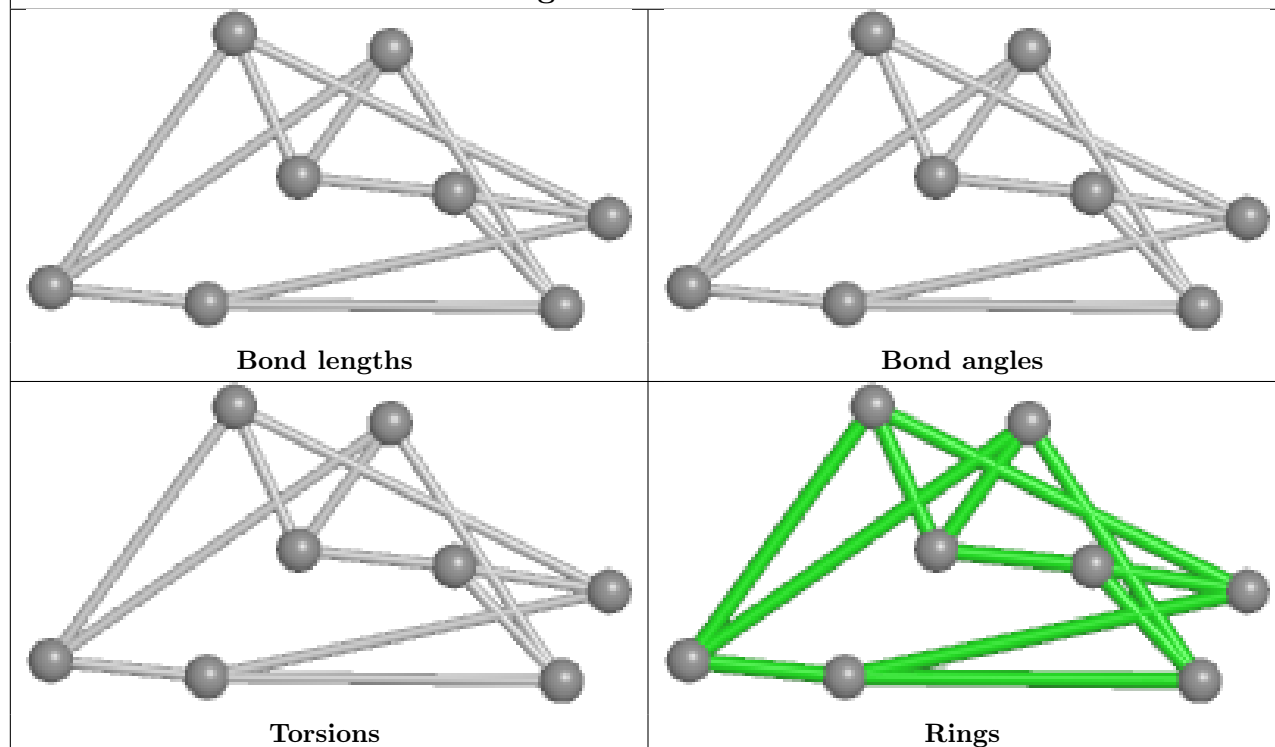




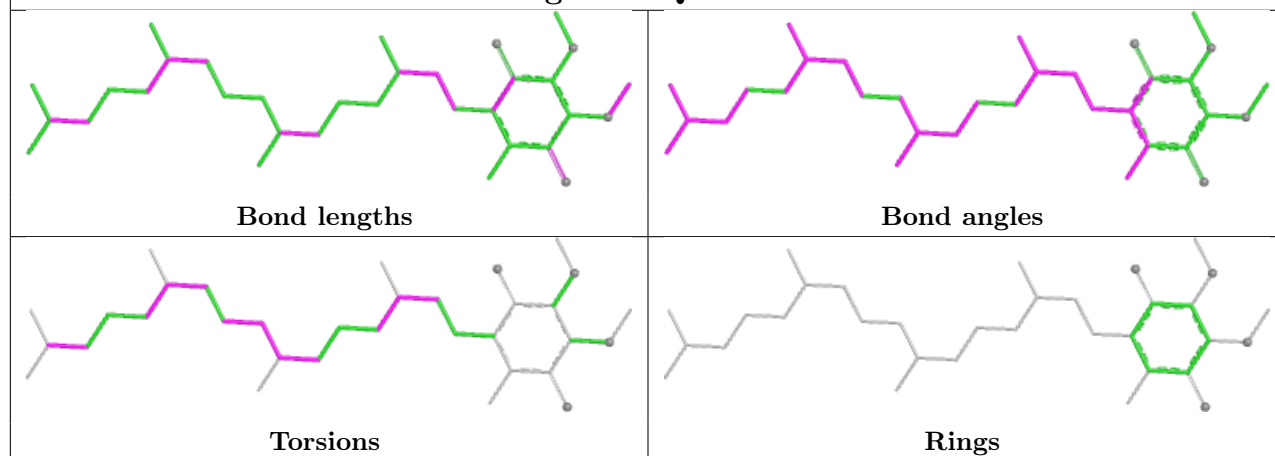
Ligand PLX a 202

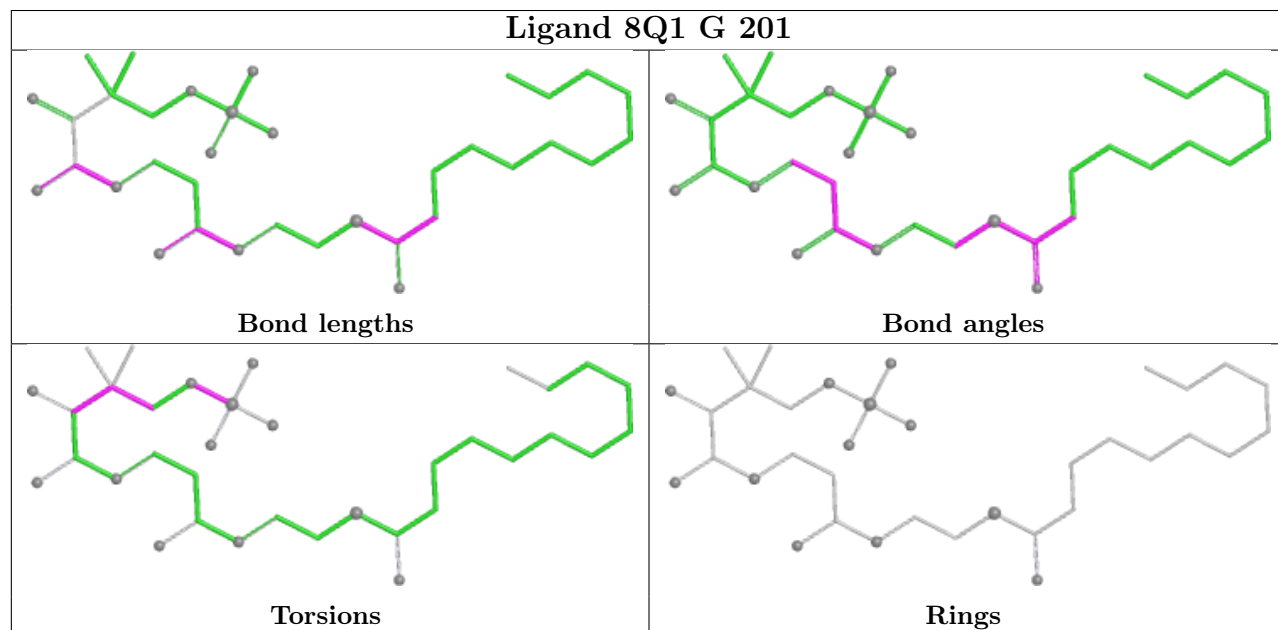
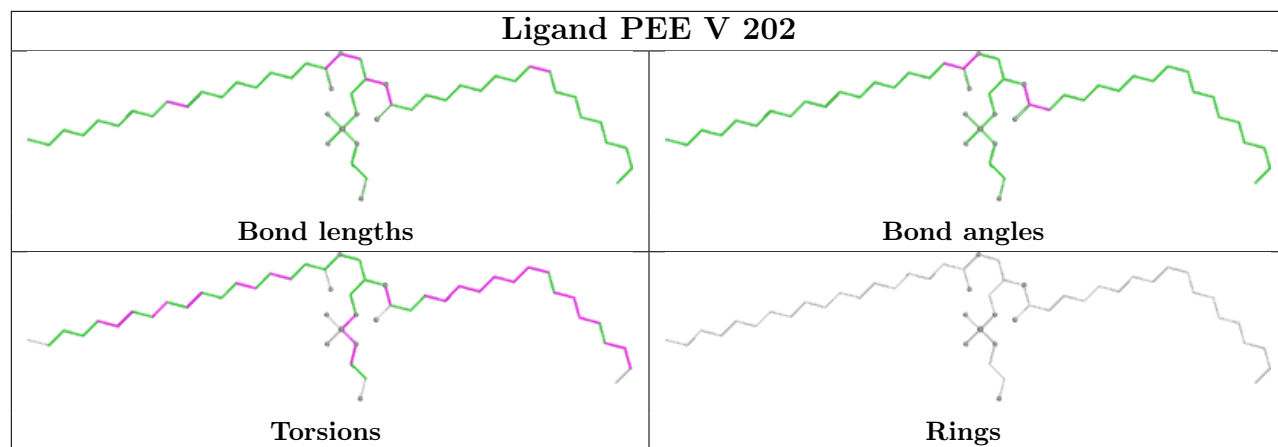


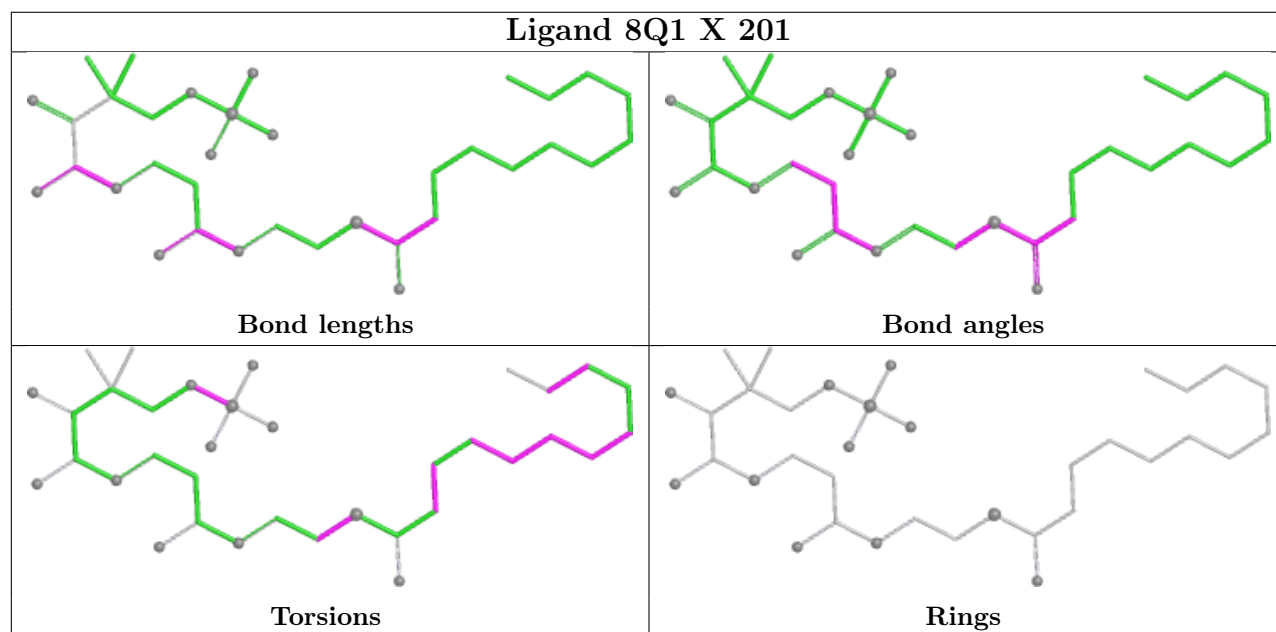
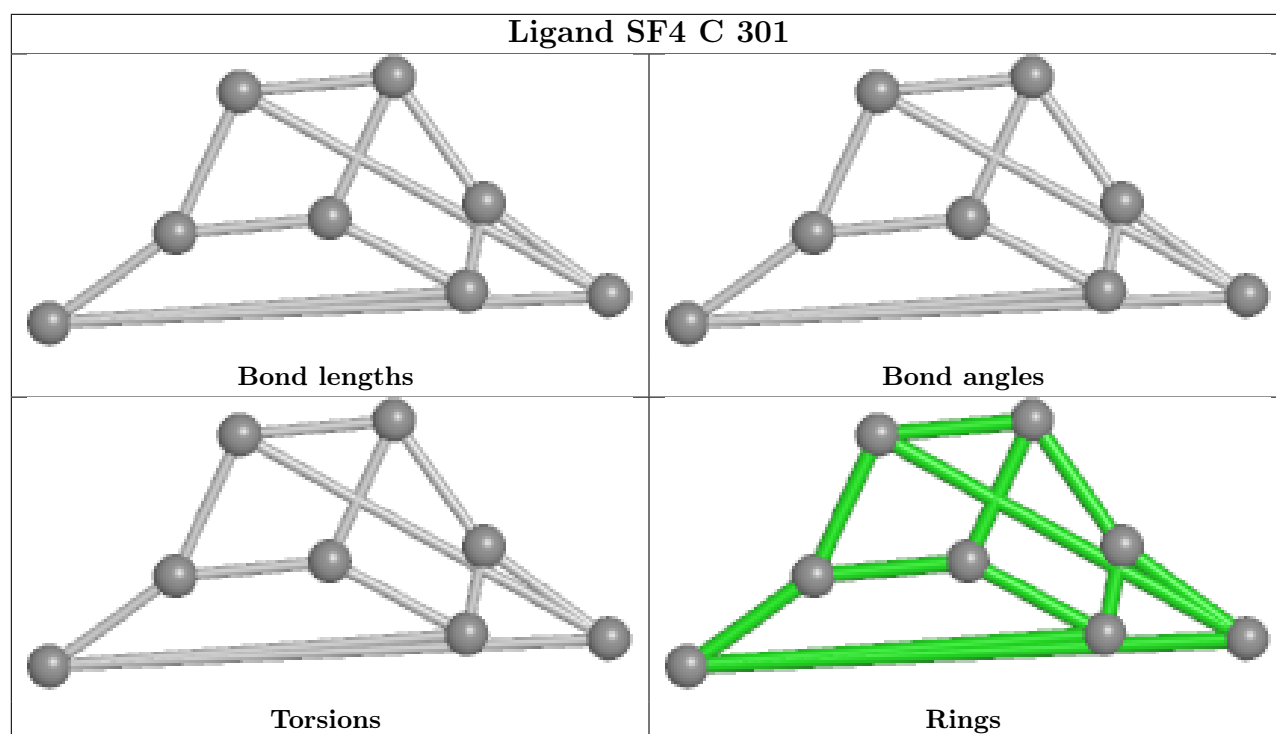
Ligand SF4 A 501

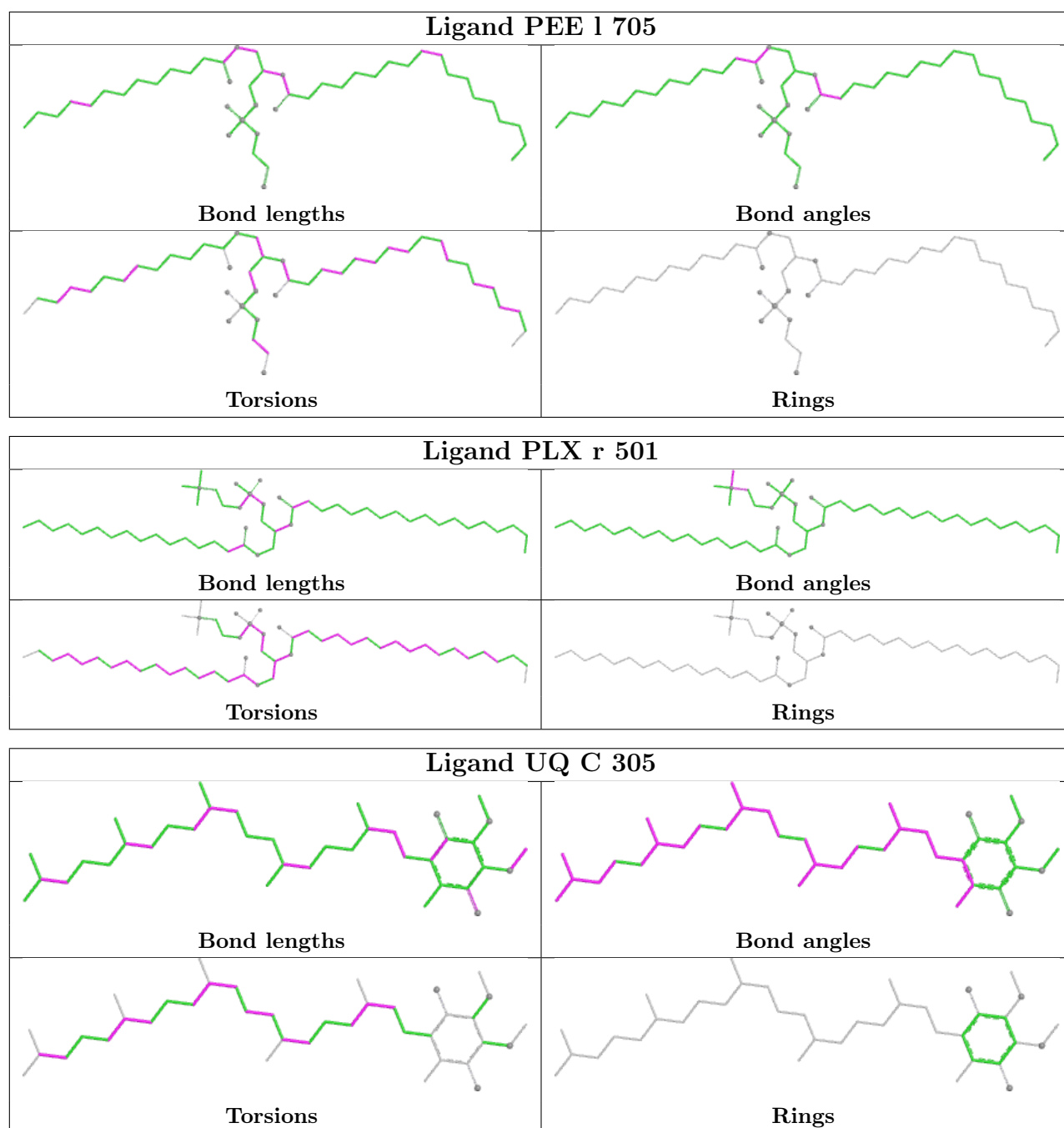


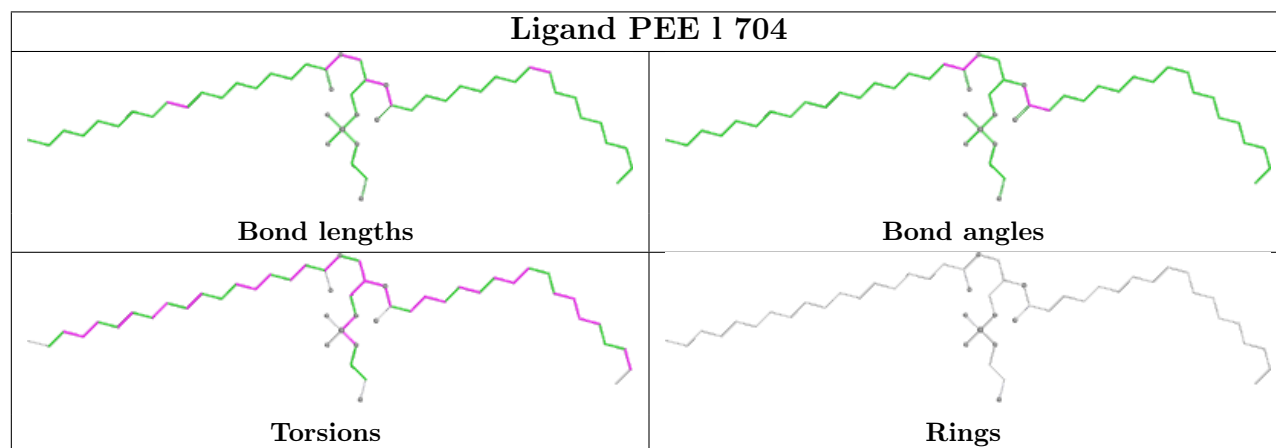
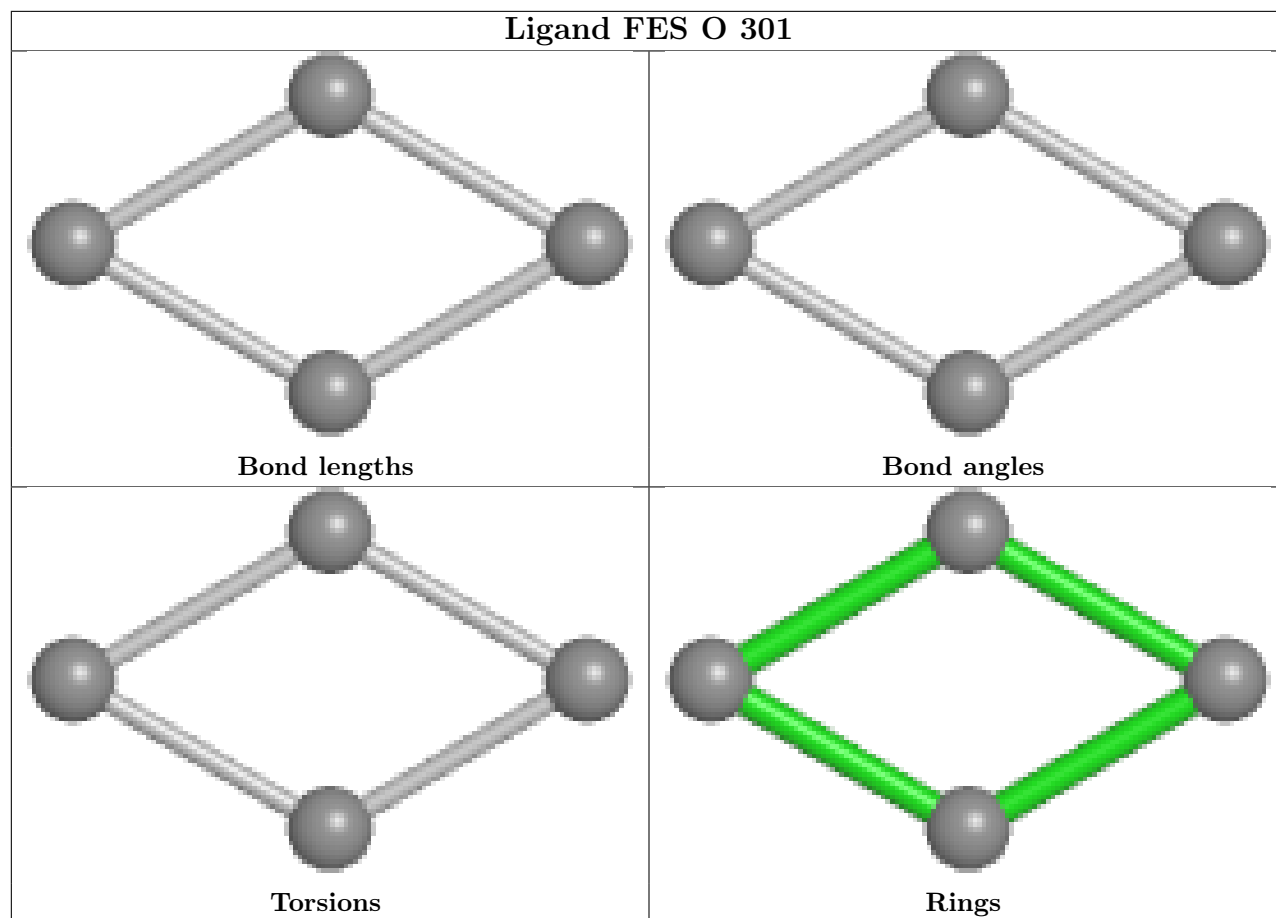
Ligand ULQ J 402

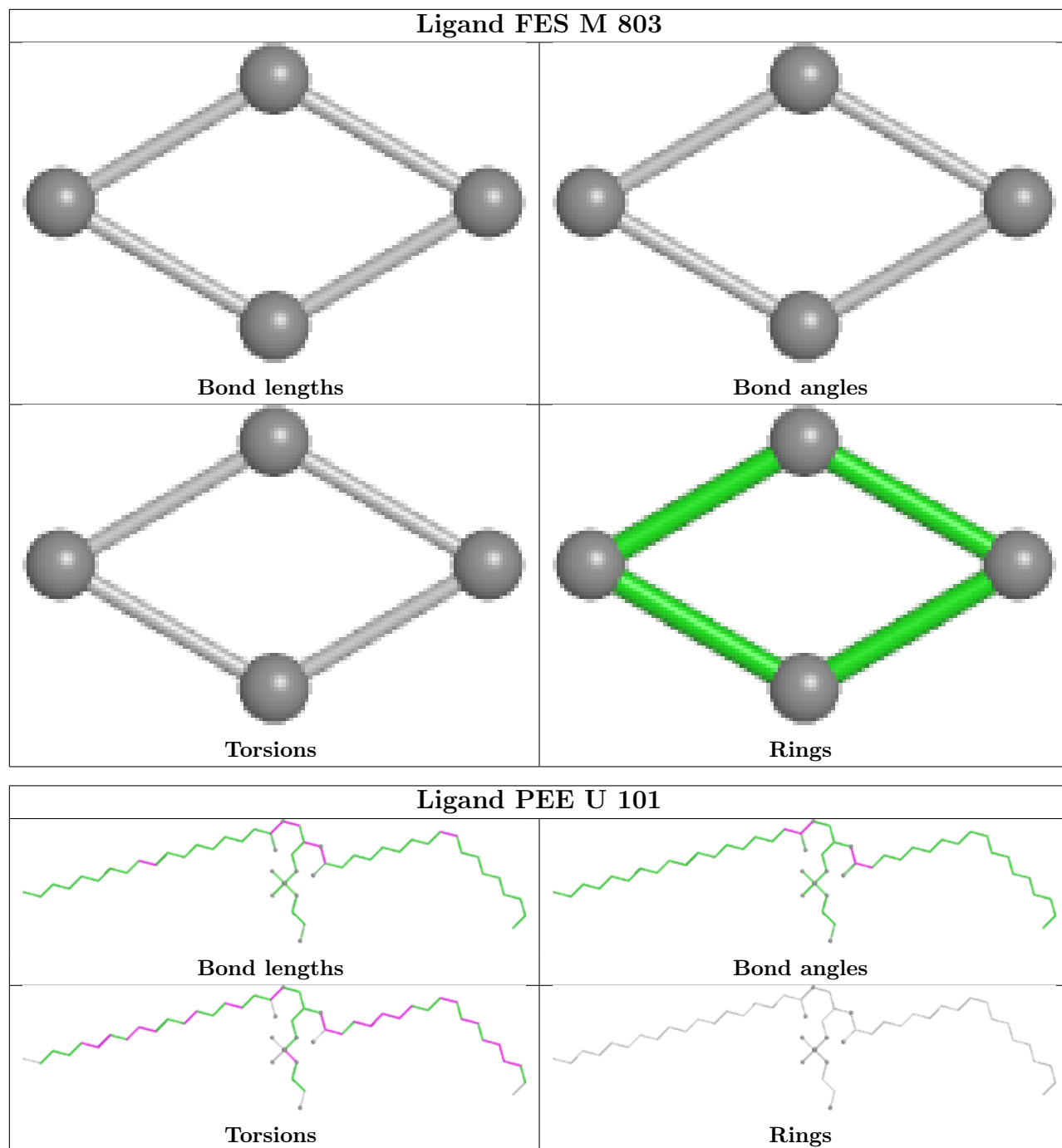




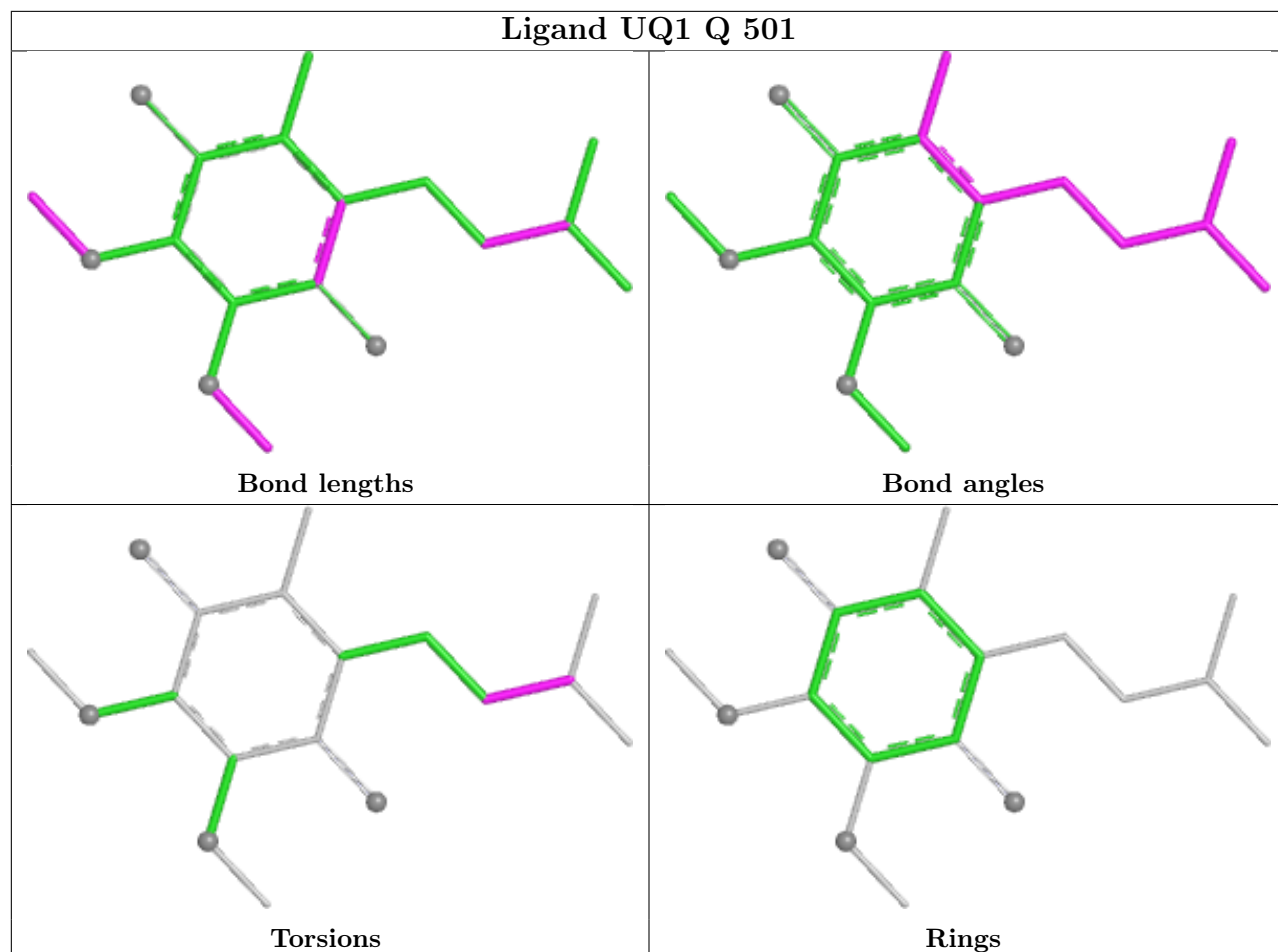




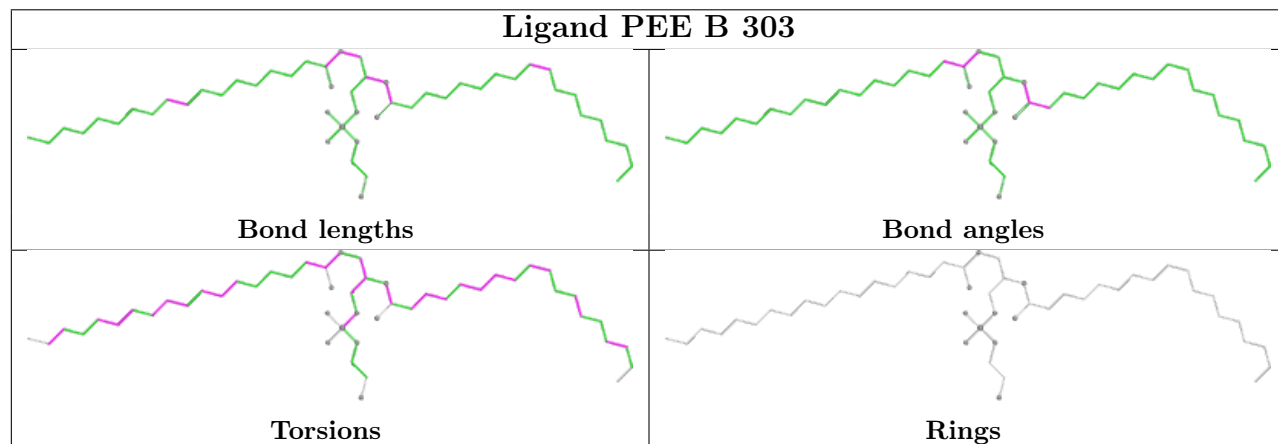


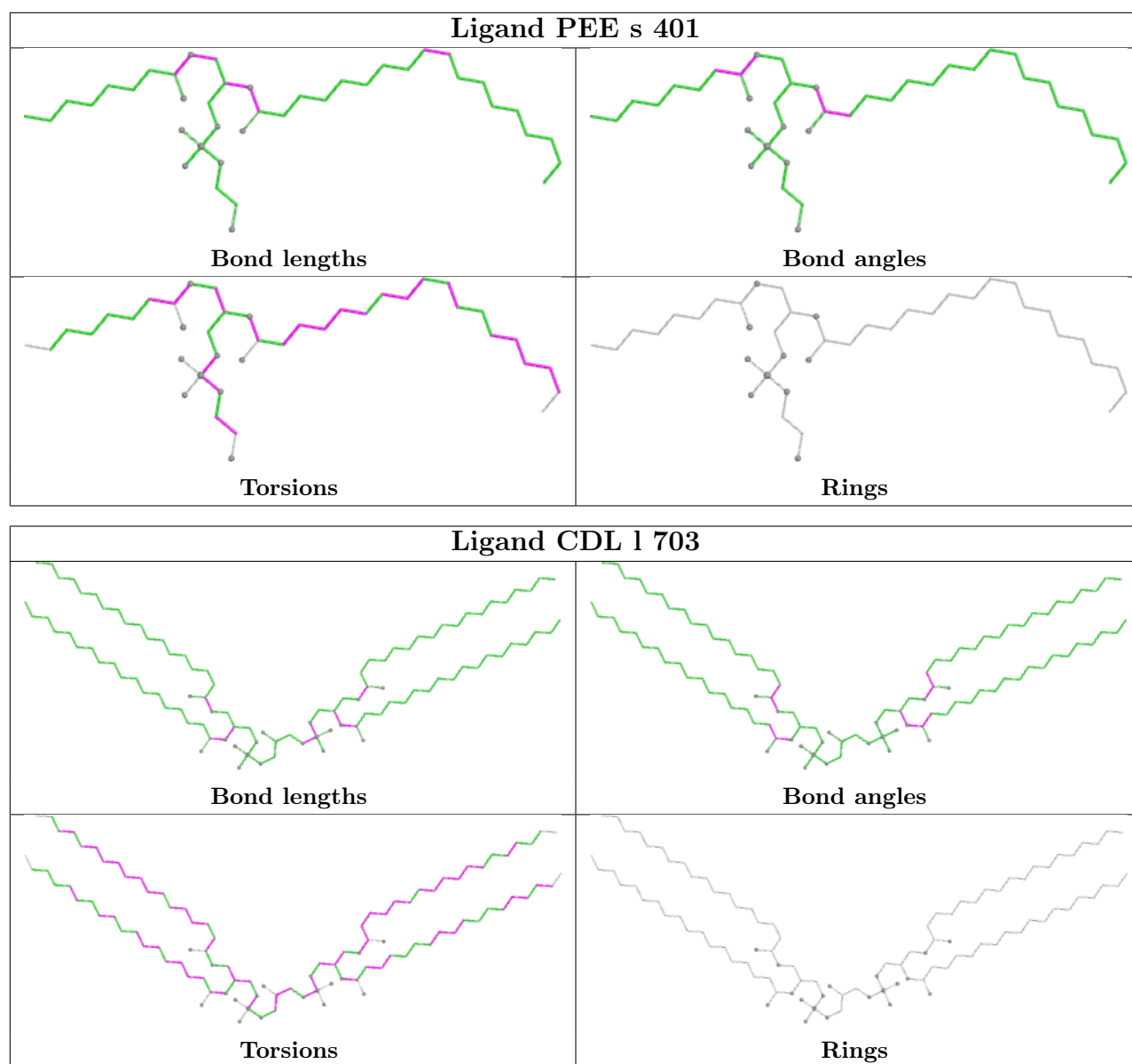


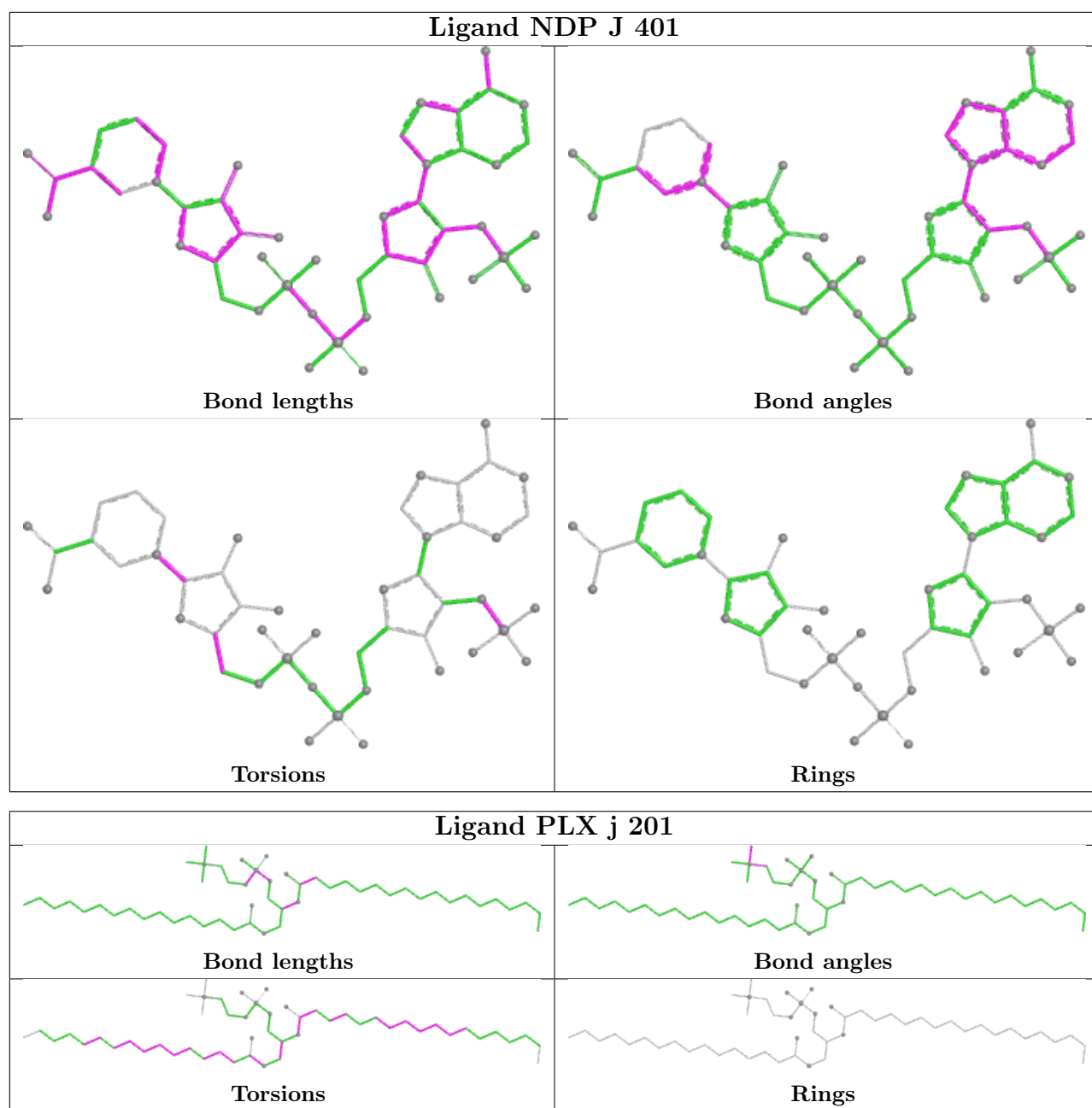
Ligand UQ1 Q 501

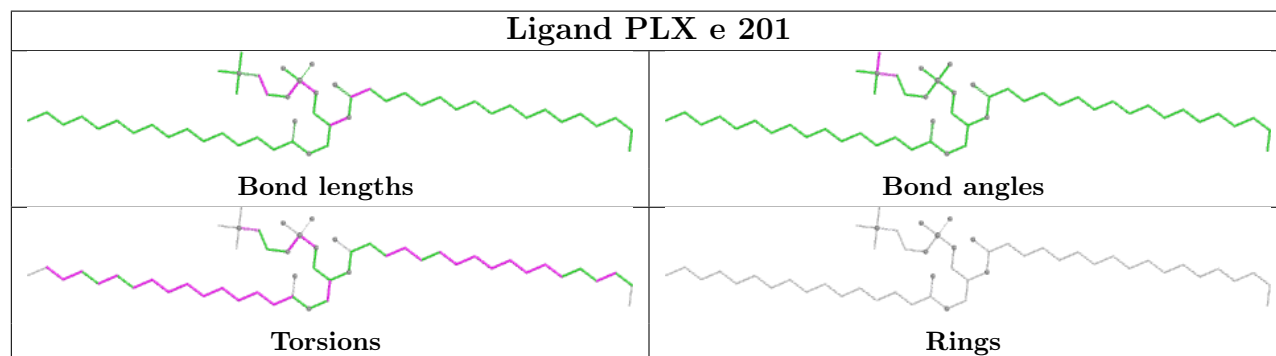
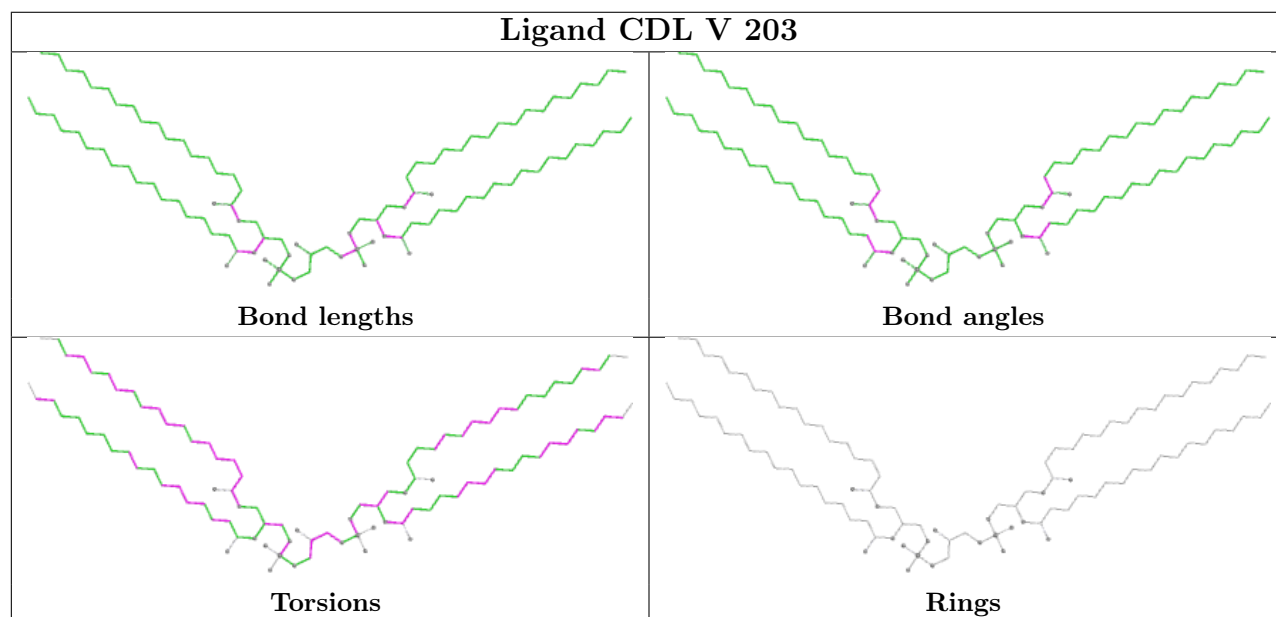
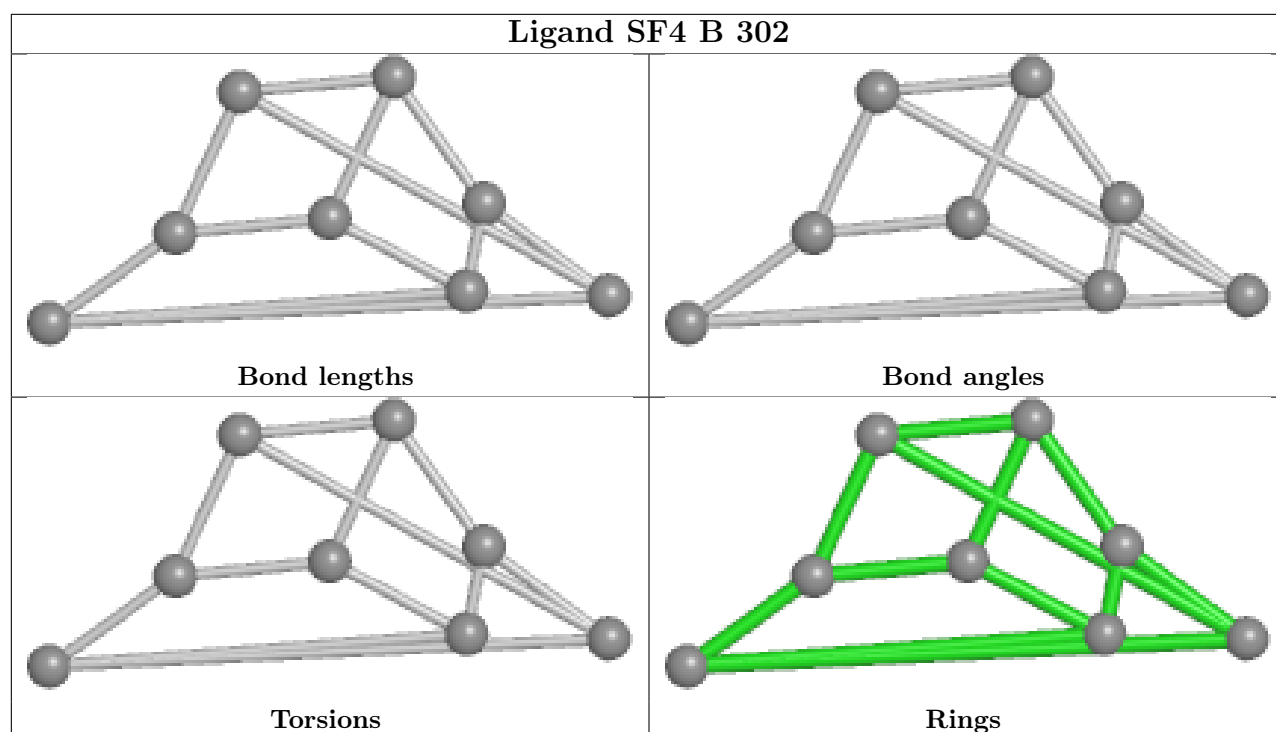


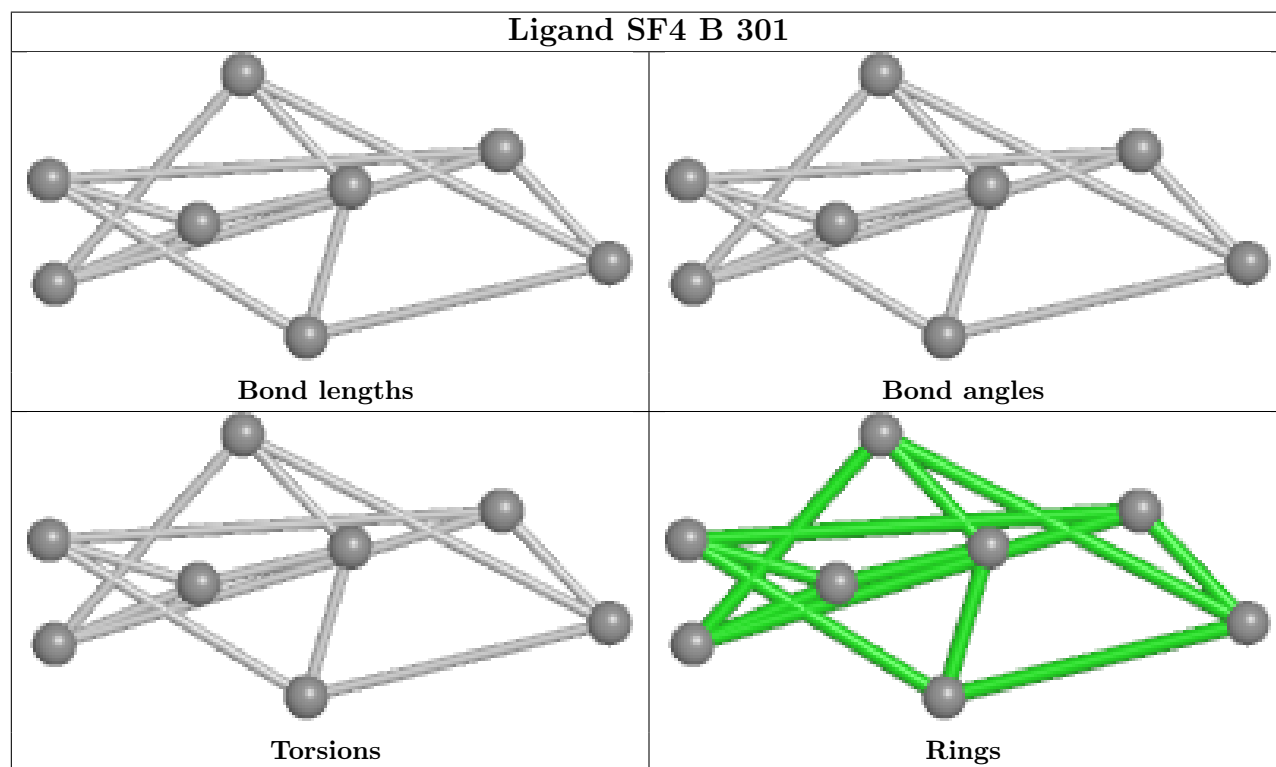
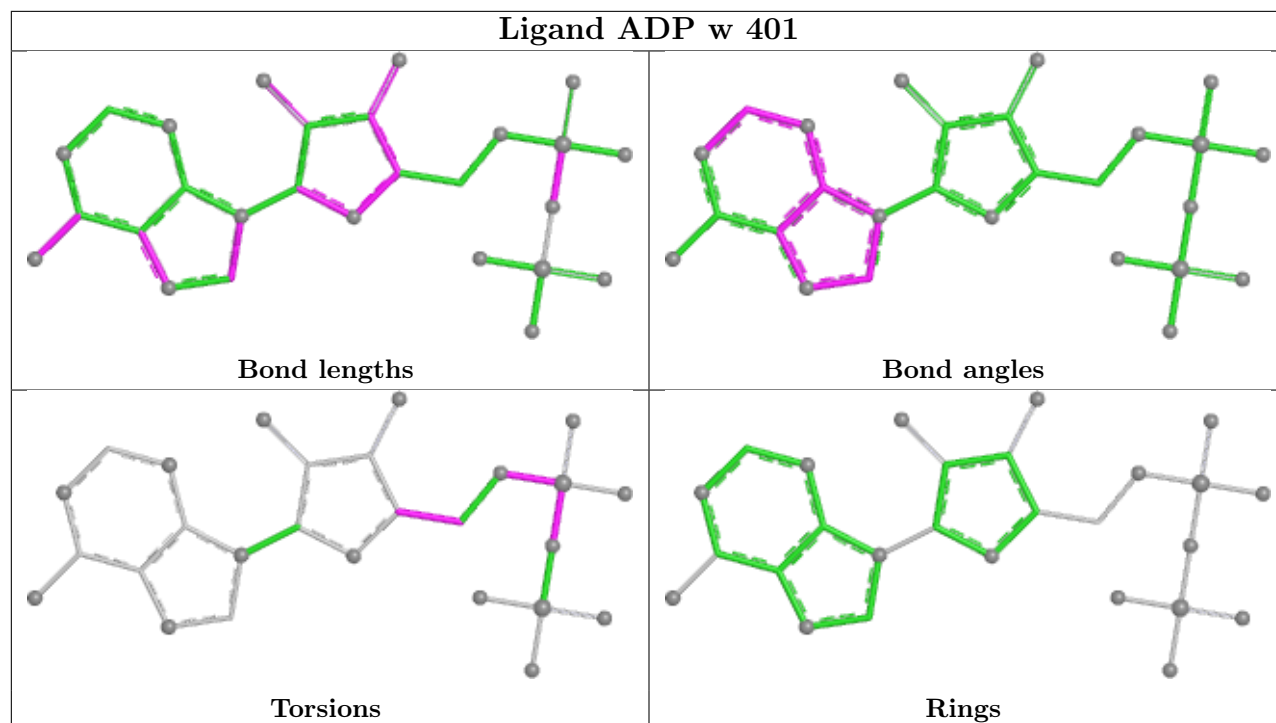
Ligand PEE B 303

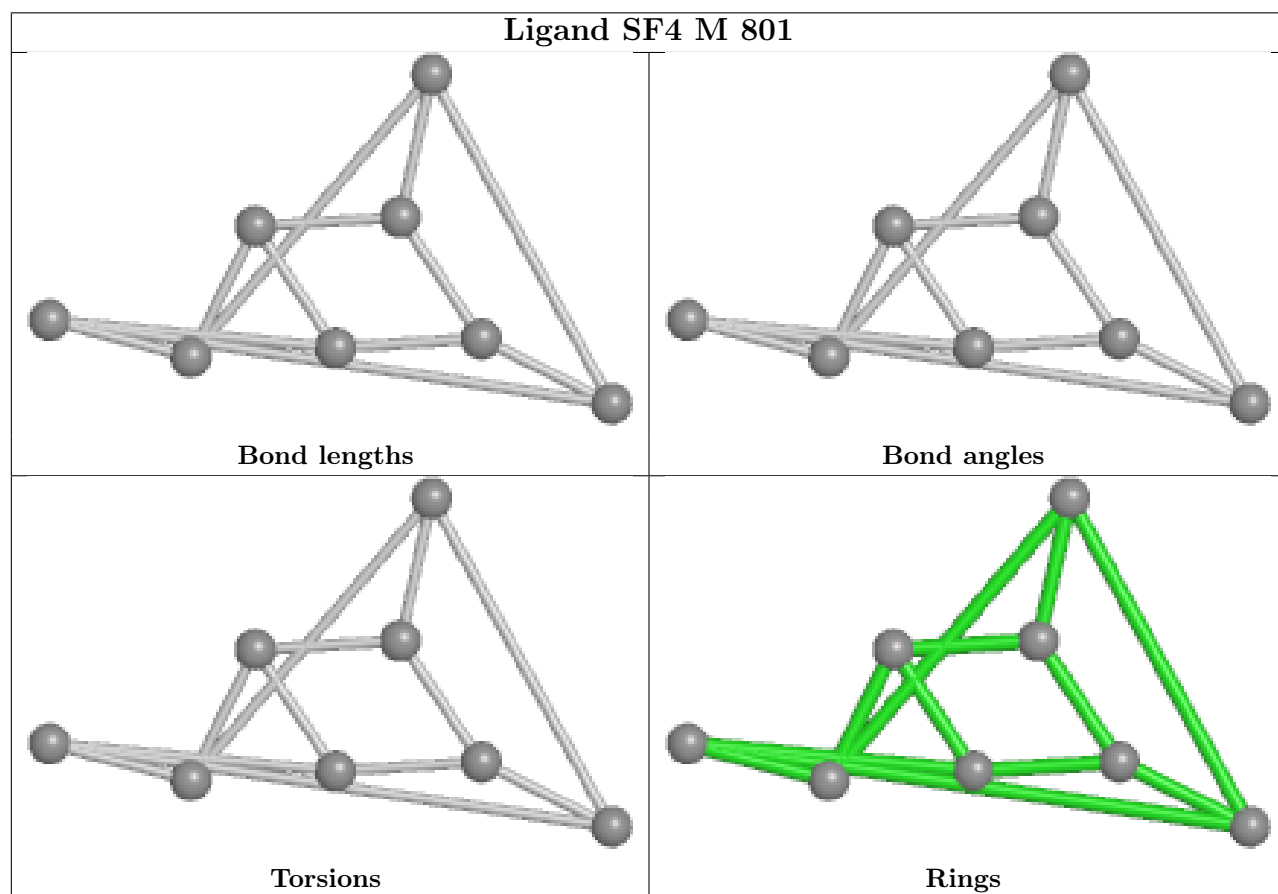
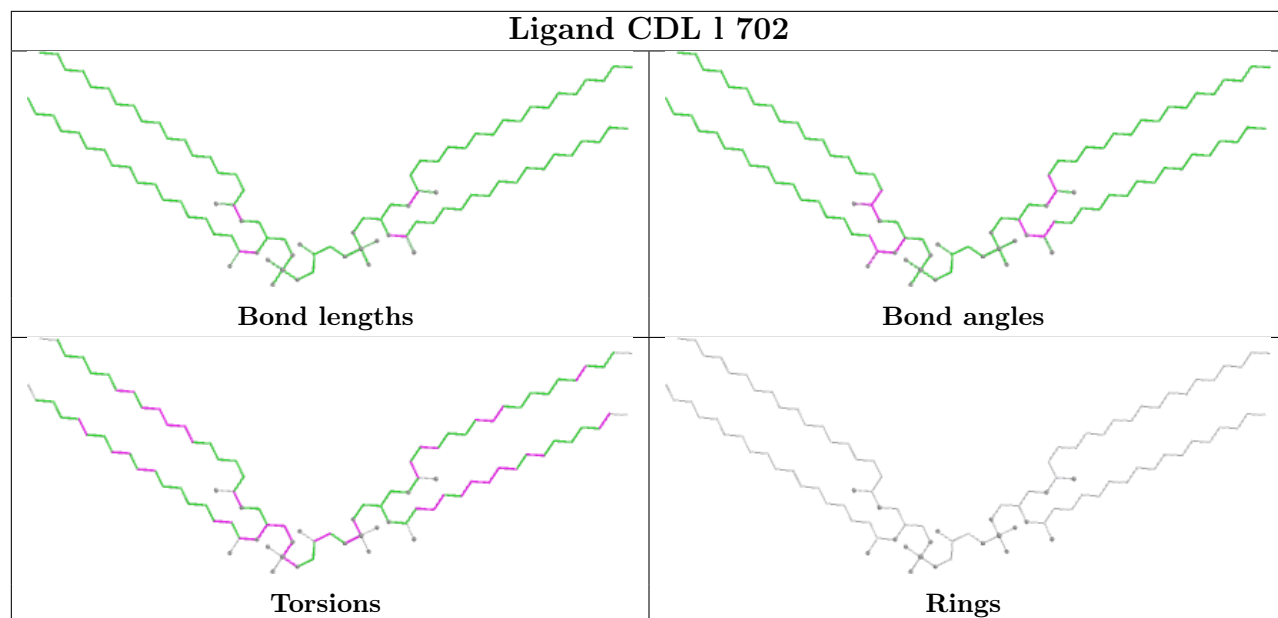


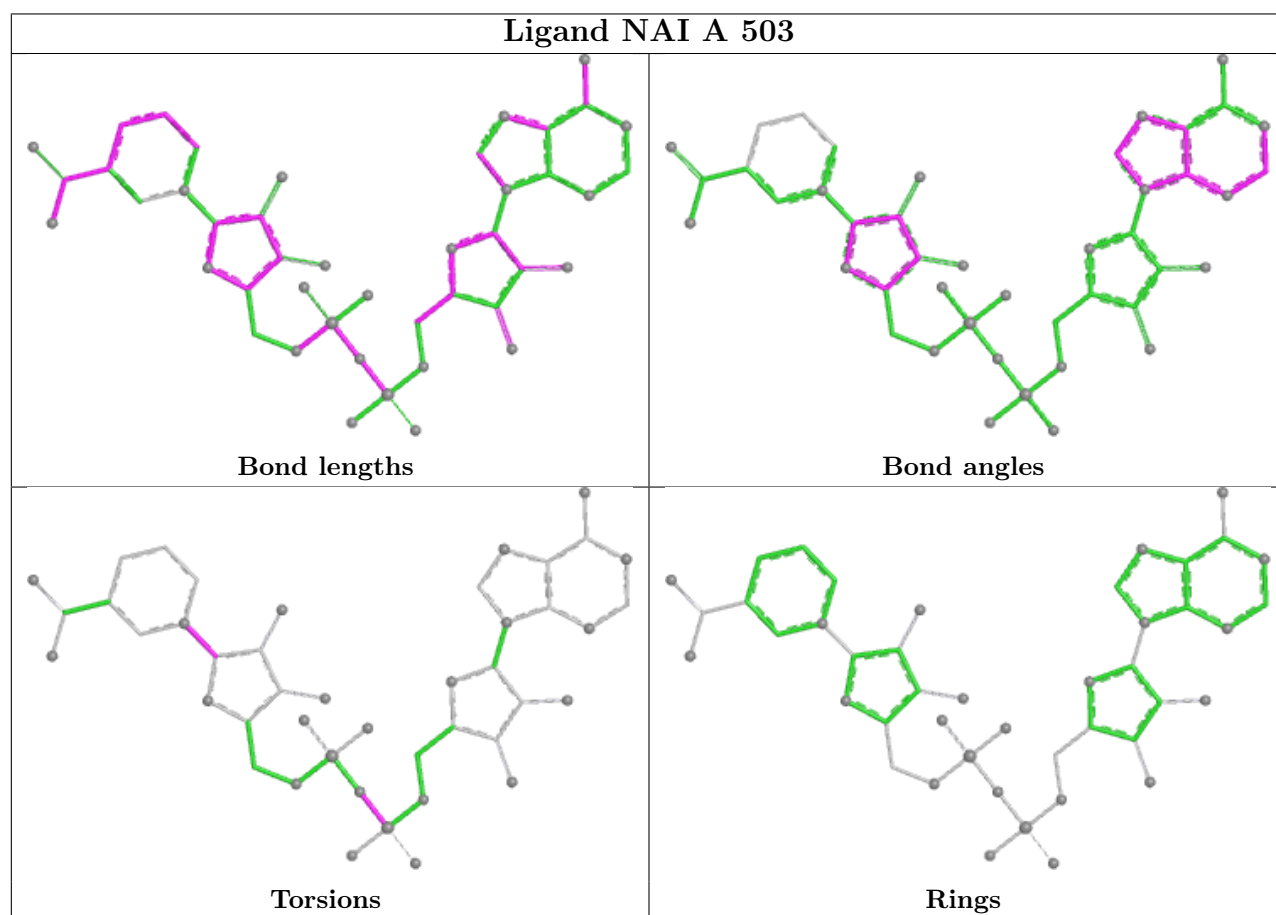
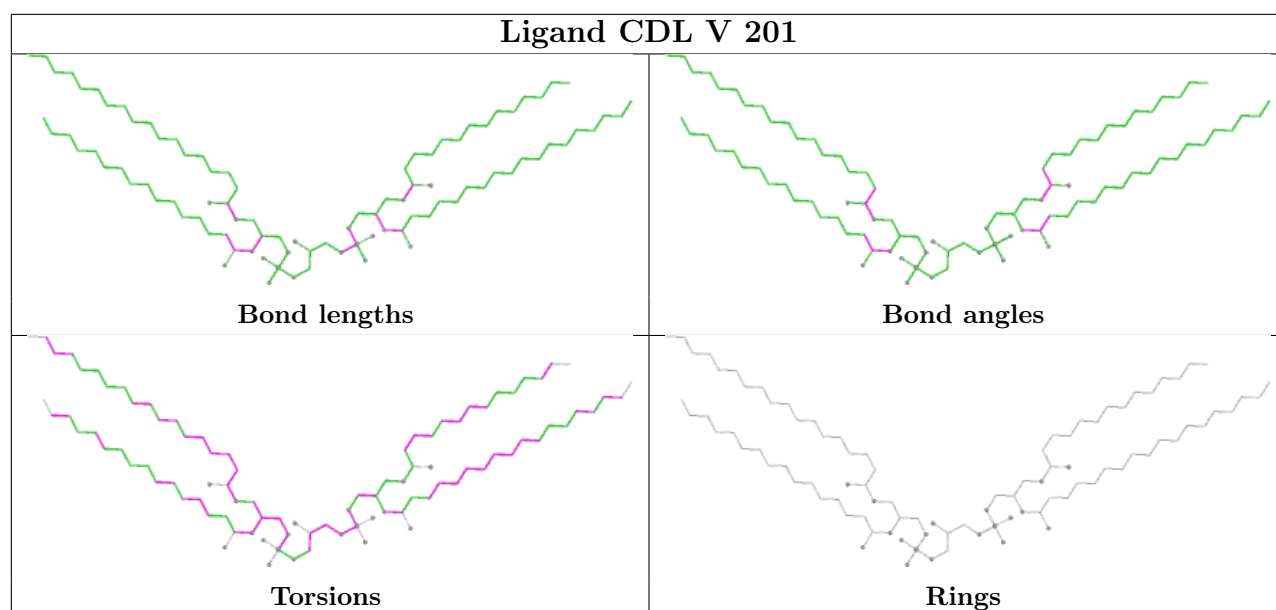


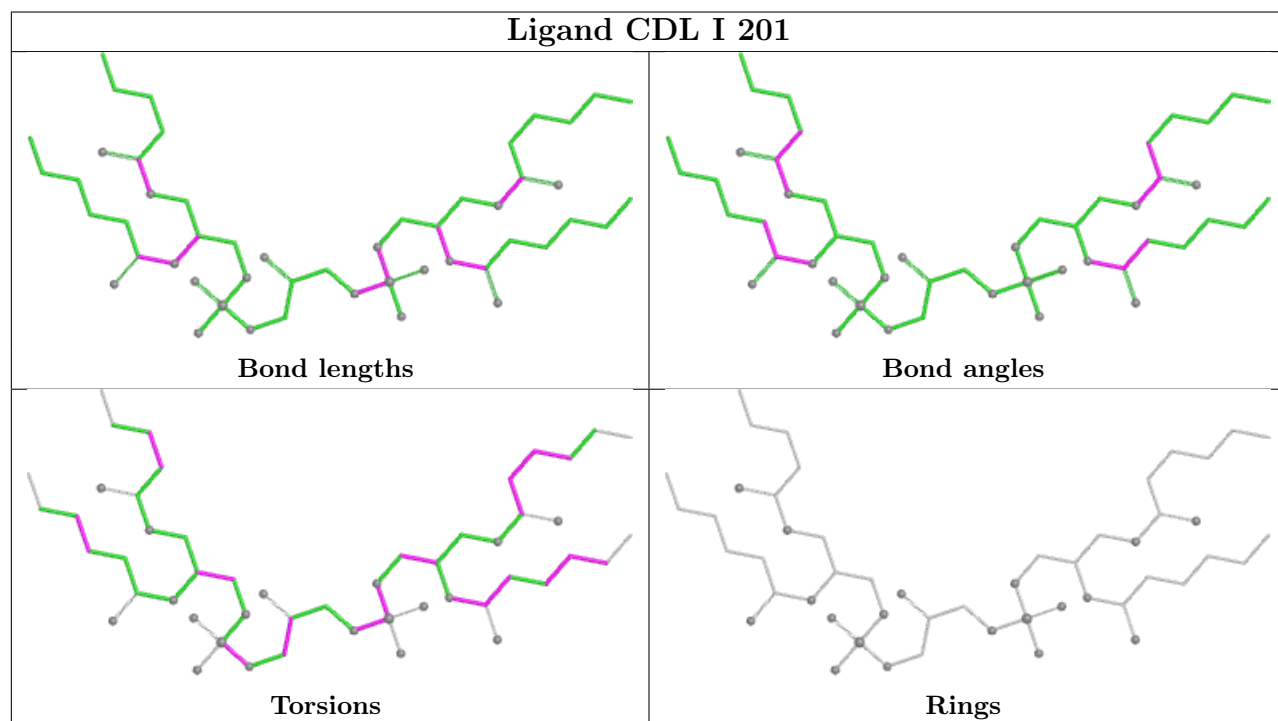
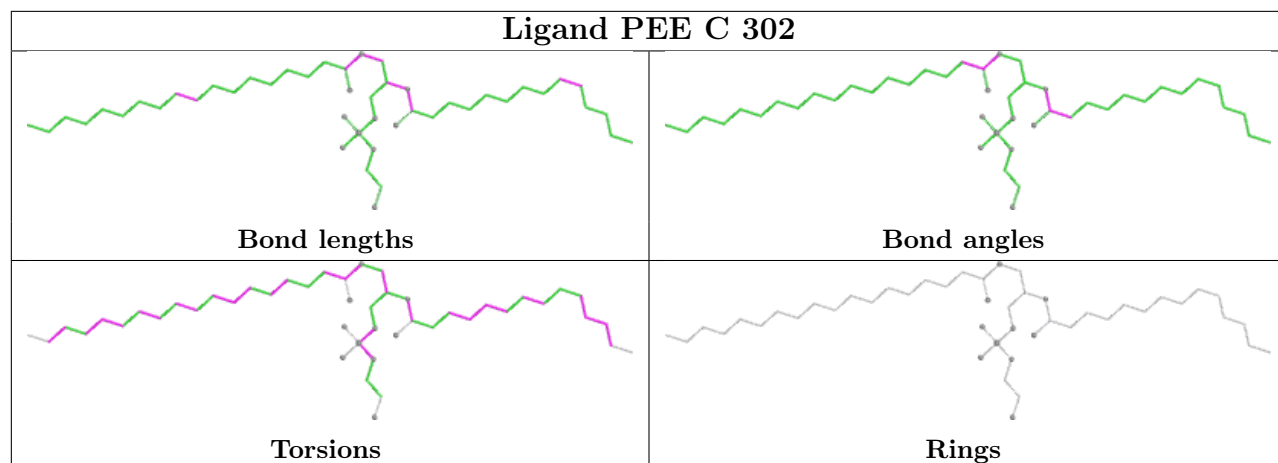


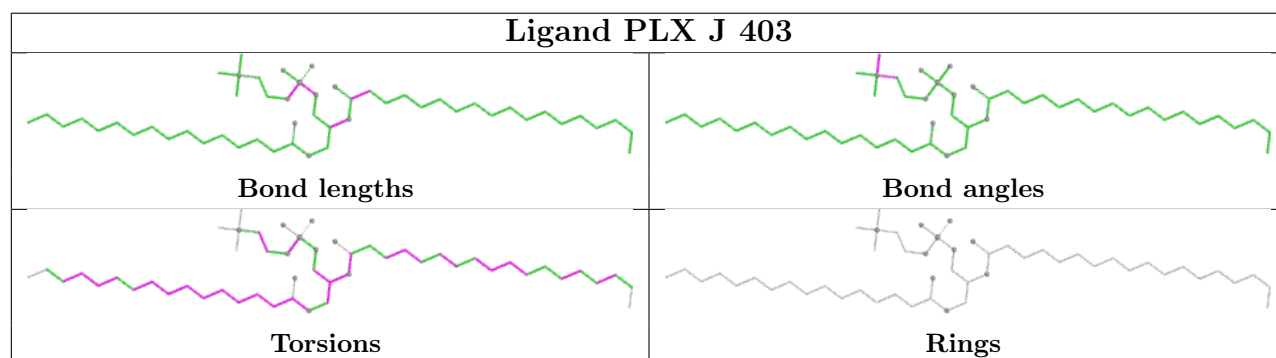
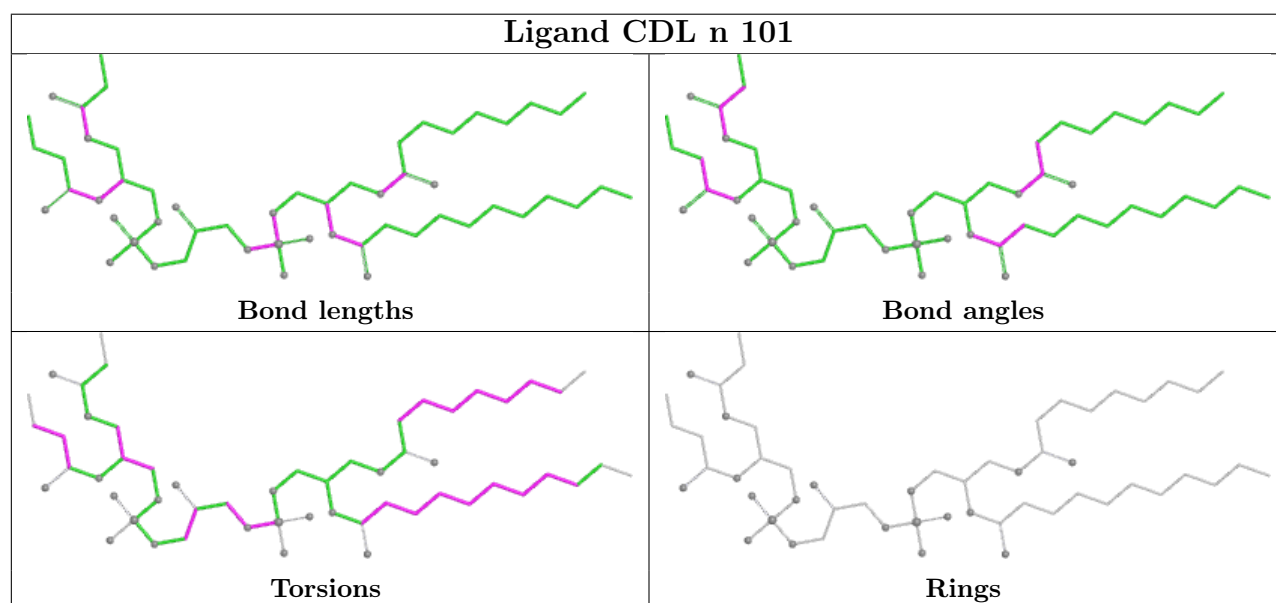
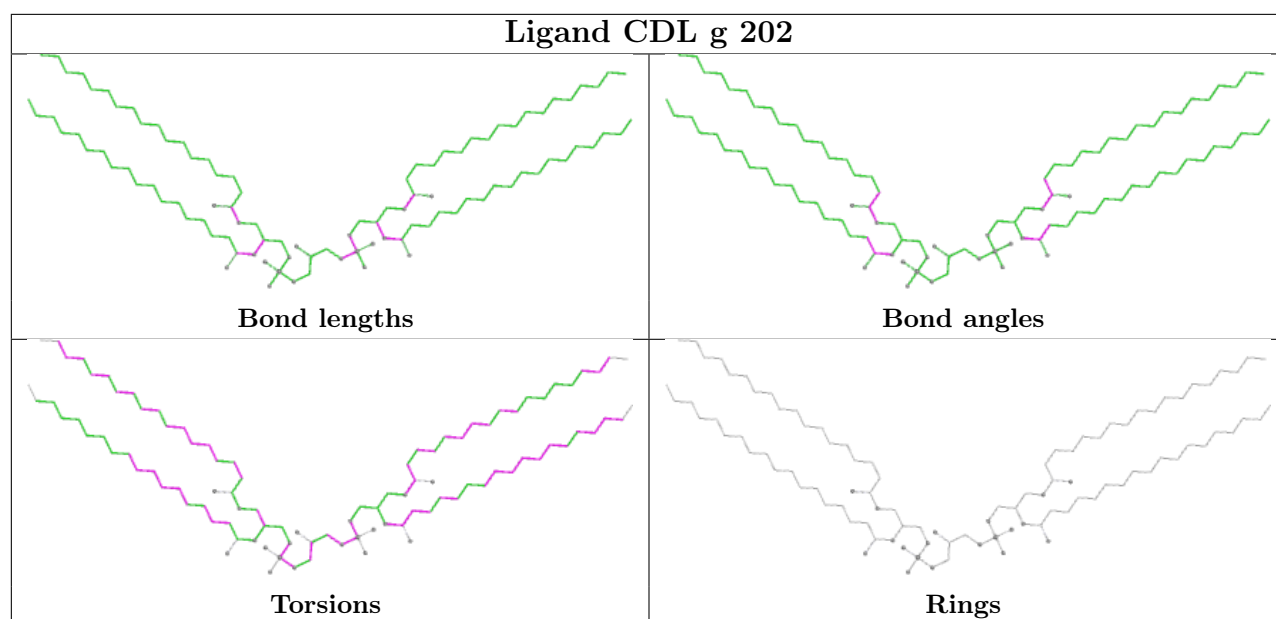


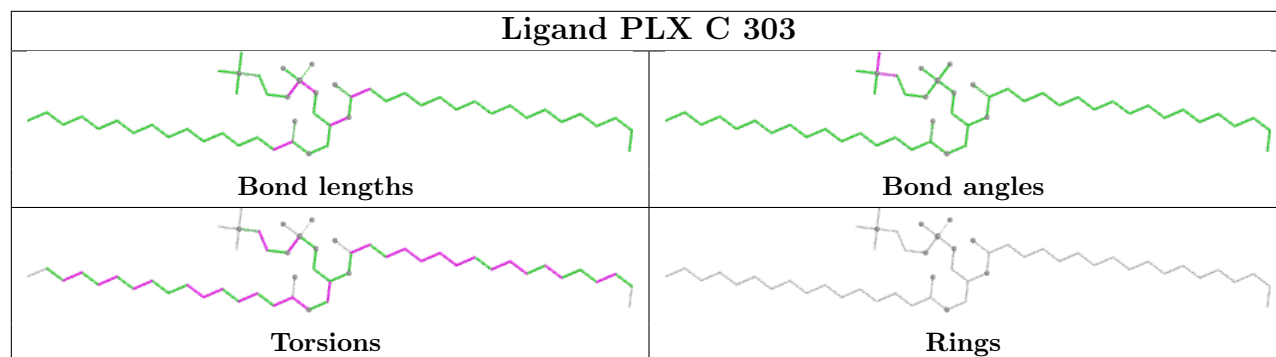












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

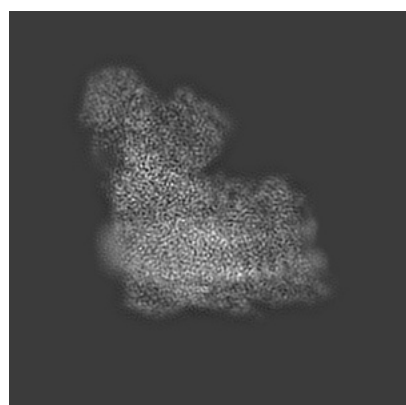
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32300. These allow visual inspection of the internal detail of the map and identification of artifacts.

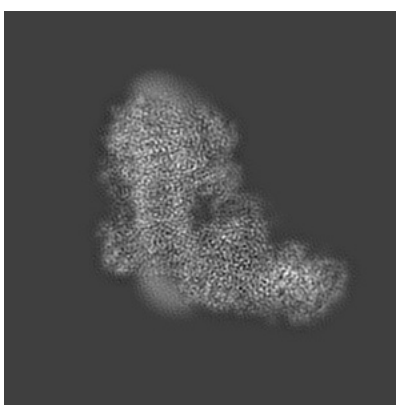
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

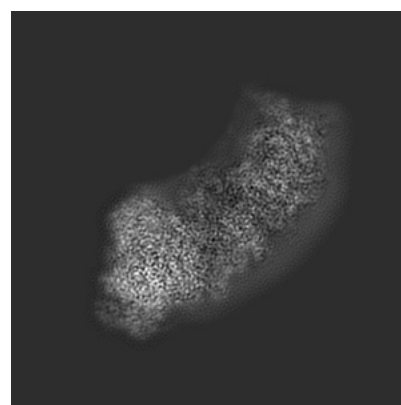
6.1.1 Primary map



X



Y

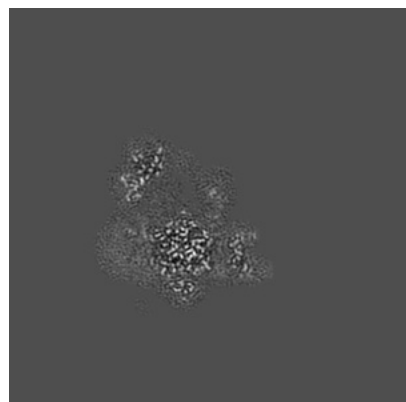


Z

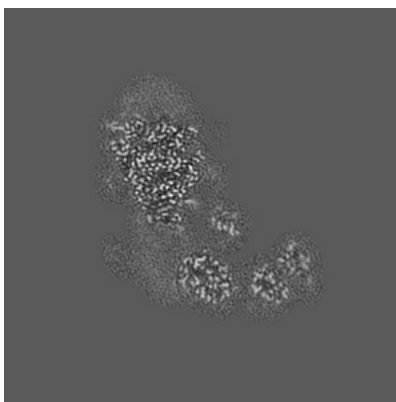
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

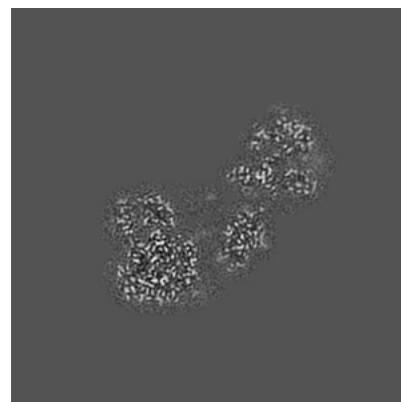
6.2.1 Primary map



X Index: 152



Y Index: 152

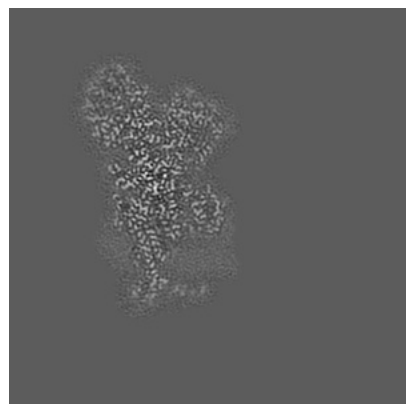


Z Index: 152

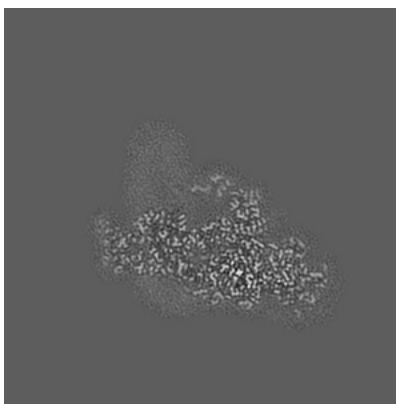
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

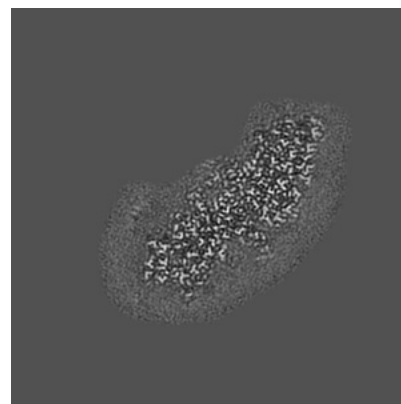
6.3.1 Primary map



X Index: 105



Y Index: 105

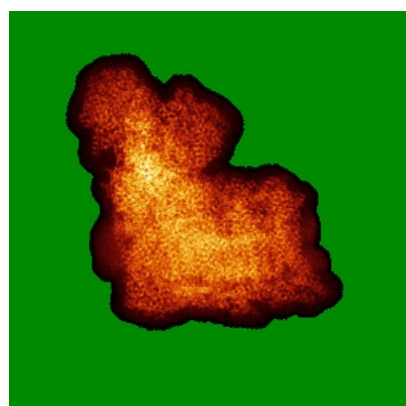


Z Index: 129

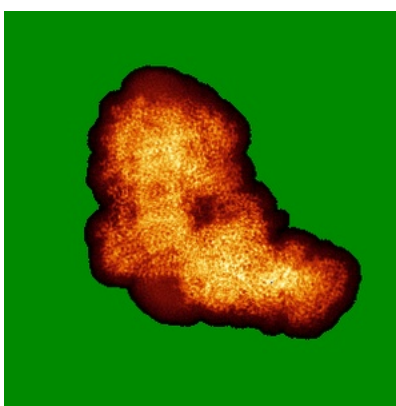
The images above show the largest variance slices of the map in three orthogonal directions.

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

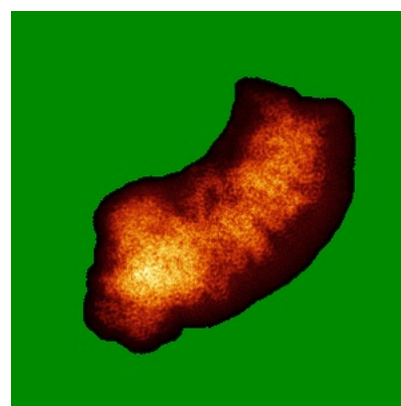
6.4.1 Primary map



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 0.0302. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

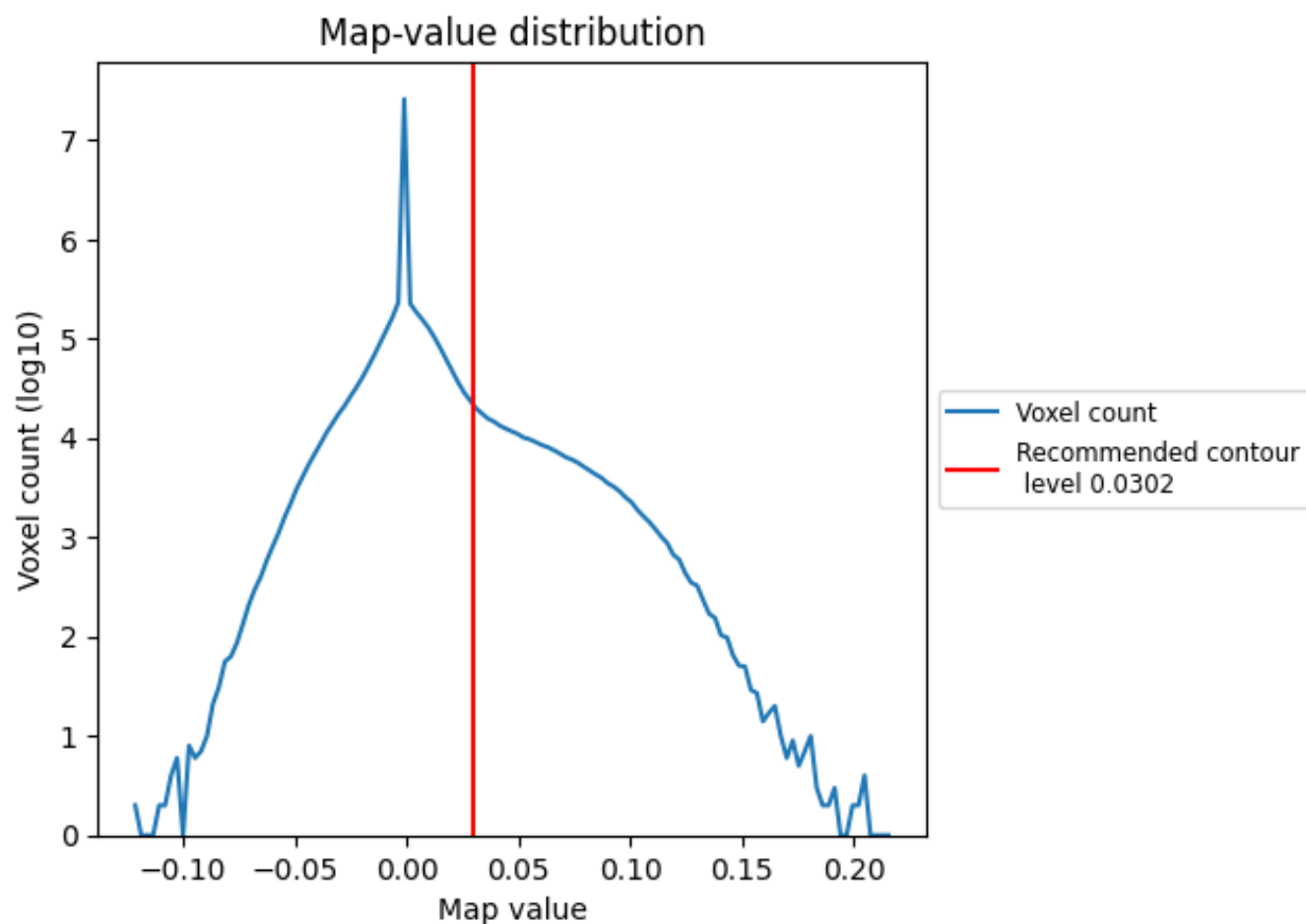
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

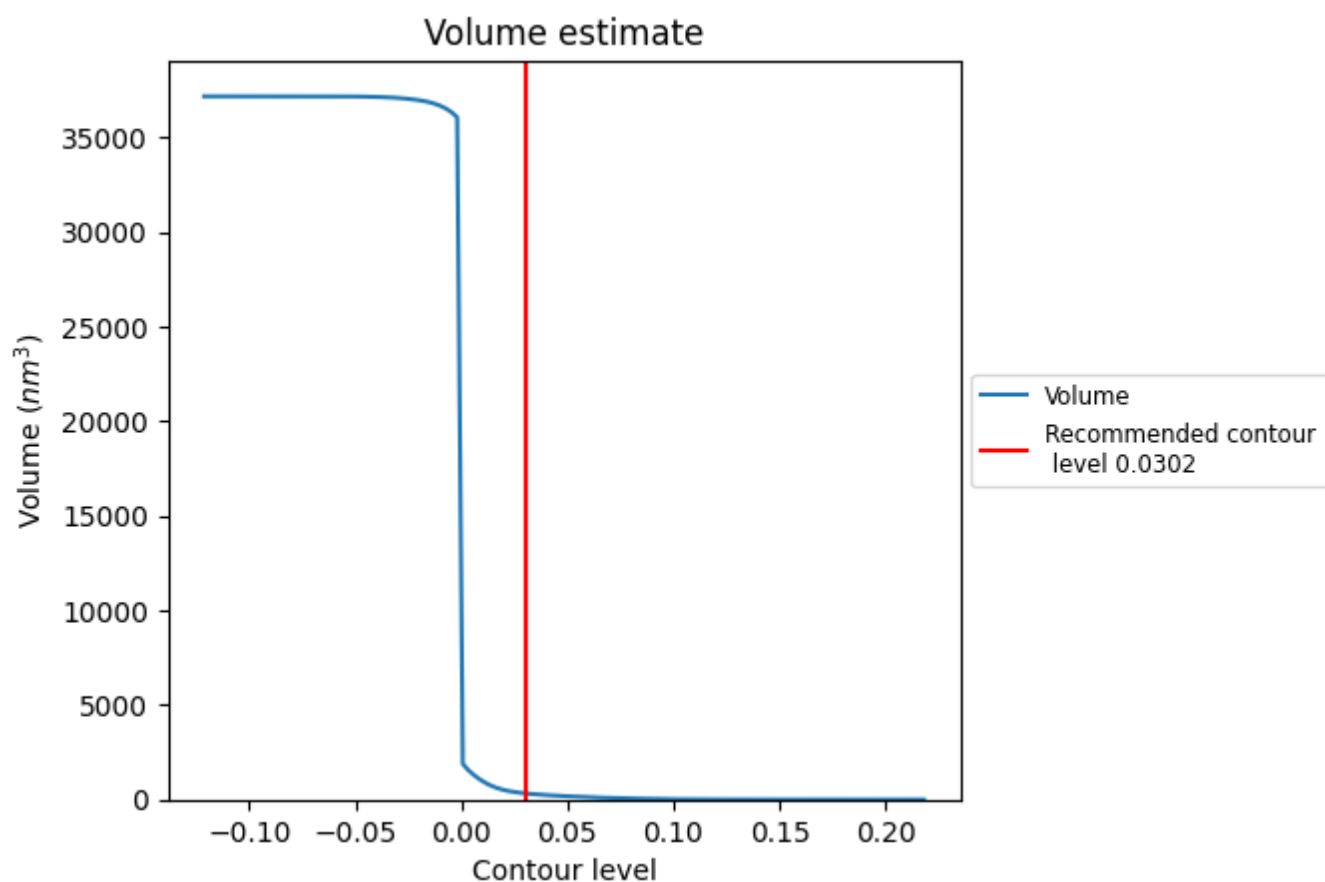
This section contains the results of statistical analysis of the map.

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.

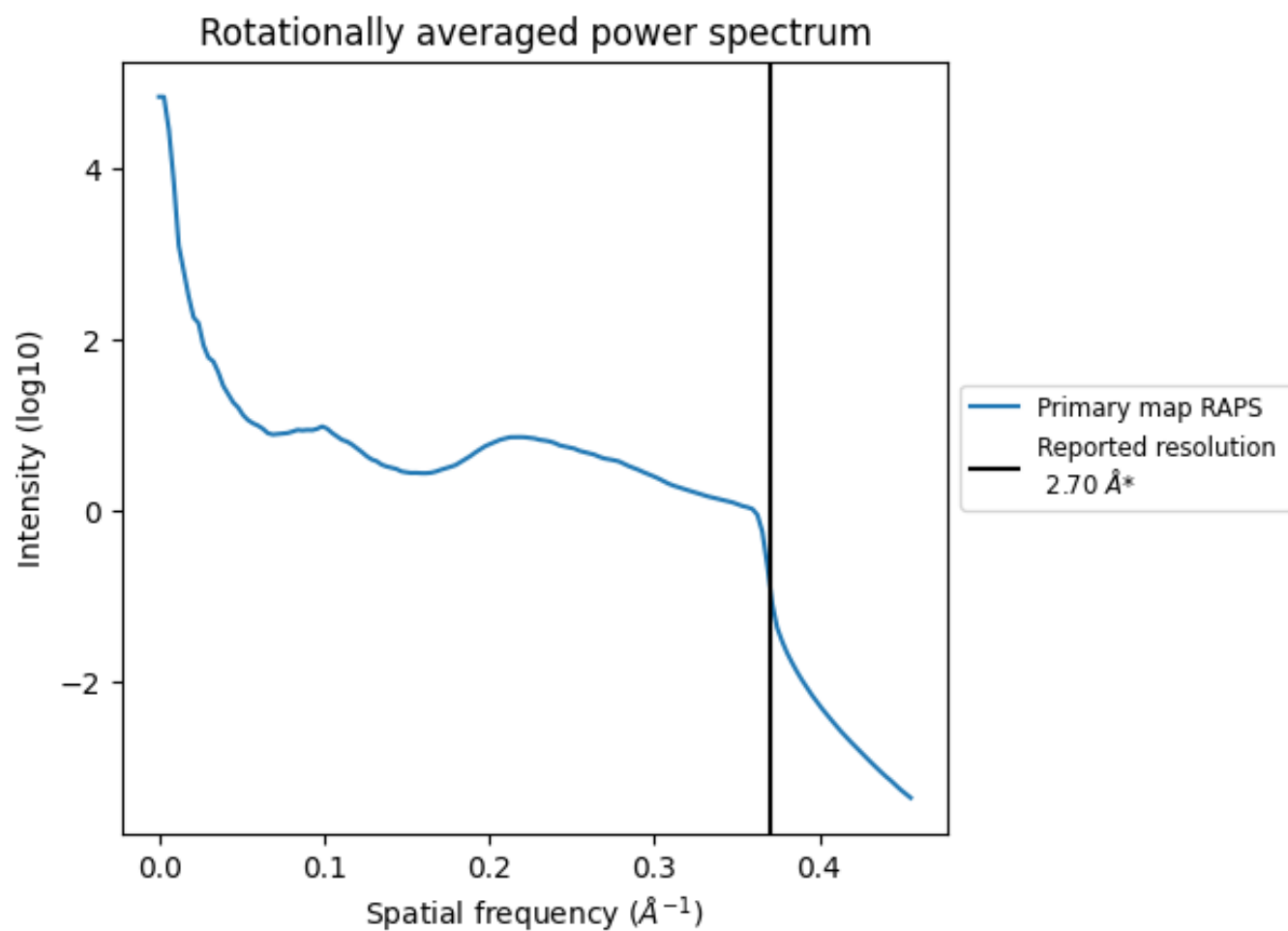
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 325 nm³; this corresponds to an approximate mass of 294 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 0.370 Å⁻¹

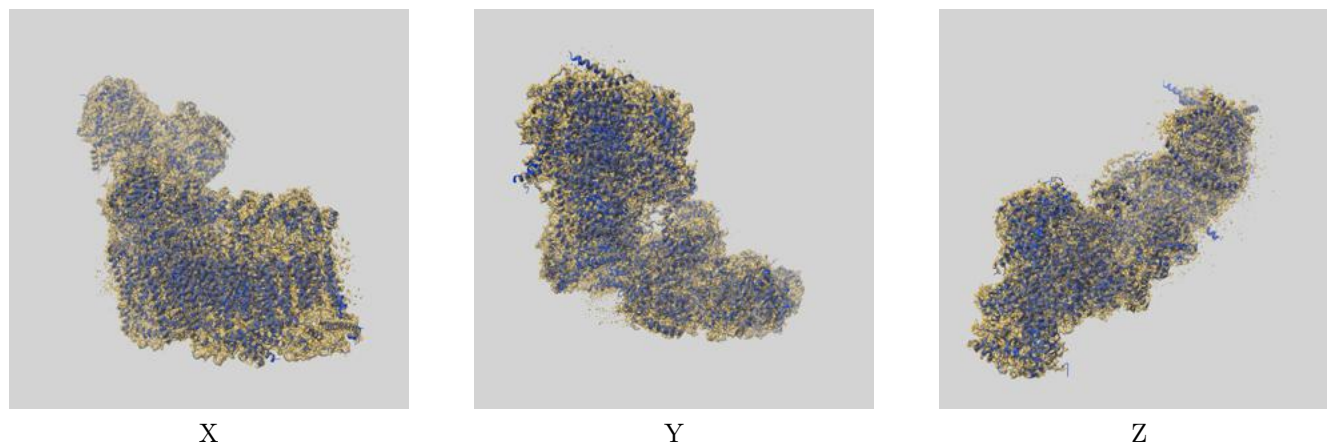
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

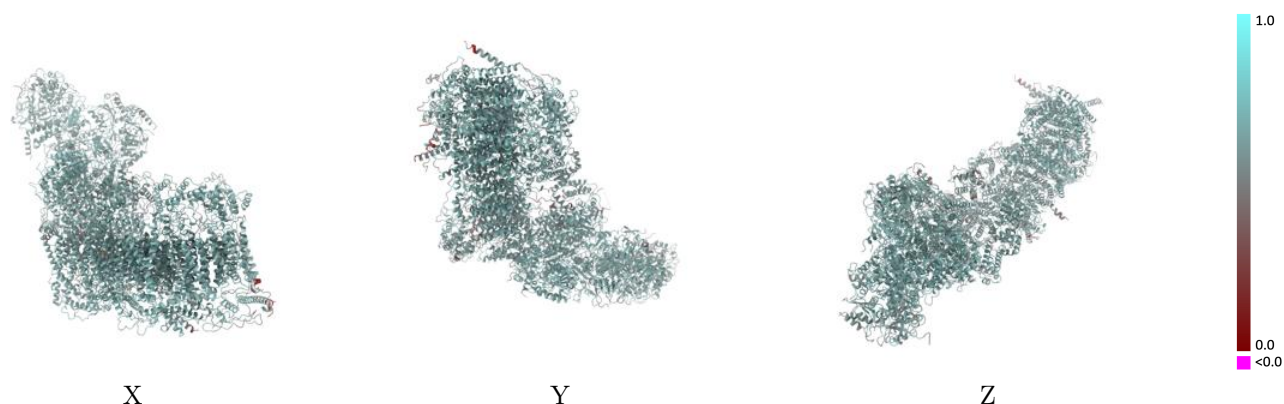
This section contains information regarding the fit between EMDB map EMD-32300 and PDB model 7W4C. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



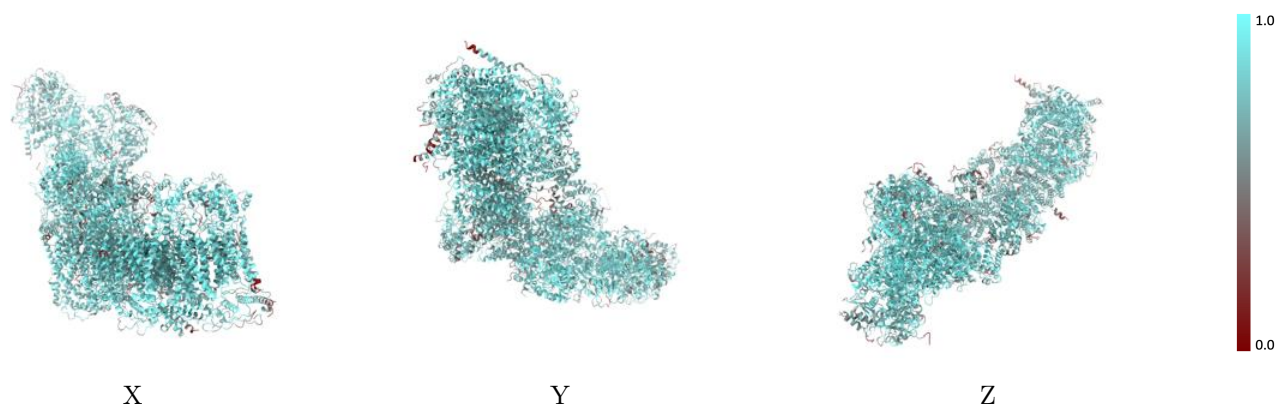
The images above show the 3D surface view of the map at the recommended contour level 0.0302 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



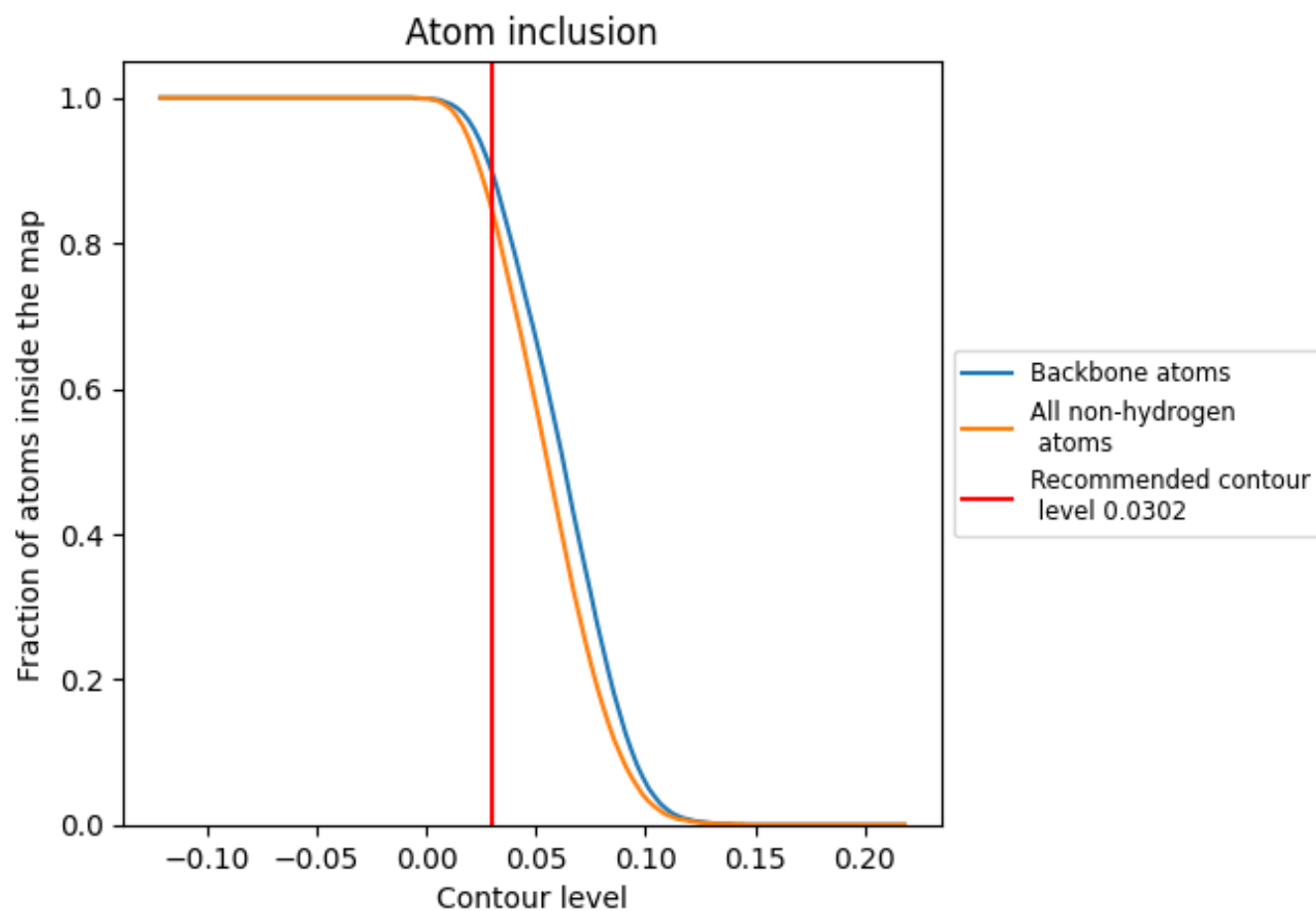
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0302).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% 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 (0.0302) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8430	 0.6220
A	 0.7930	 0.6020
B	 0.9360	 0.6590
C	 0.9140	 0.6520
E	 0.8590	 0.6270
F	 0.6660	 0.5550
G	 0.5610	 0.5230
H	 0.8220	 0.6090
I	 0.8050	 0.6060
J	 0.8600	 0.6310
K	 0.6990	 0.5790
L	 0.8590	 0.6420
M	 0.8580	 0.6250
N	 0.8630	 0.6370
O	 0.7460	 0.5850
P	 0.9330	 0.6580
Q	 0.9320	 0.6550
S	 0.9090	 0.6370
T	 0.8350	 0.6340
U	 0.7940	 0.6100
V	 0.6980	 0.5990
W	 0.8280	 0.6130
X	 0.7750	 0.5990
Y	 0.7260	 0.5610
Z	 0.6820	 0.5540
a	 0.8390	 0.6350
b	 0.7750	 0.5870
c	 0.8390	 0.6220
d	 0.8000	 0.6120
e	 0.7690	 0.6000
f	 0.6270	 0.5450
g	 0.8190	 0.6220
h	 0.8270	 0.6110
i	 0.9380	 0.6510
j	 0.8610	 0.6350



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	 0.9350	 0.6490
l	 0.8750	 0.6330
m	 0.7900	 0.5920
n	 0.6980	 0.5830
o	 0.8540	 0.6300
p	 0.8340	 0.6220
r	 0.9370	 0.6480
s	 0.9080	 0.6460
u	 0.8320	 0.6180
v	 0.7120	 0.5680
w	 0.8080	 0.6040