



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:57 AM UTC

PDB ID : 7W0H / pdb_00007w0h
EMDB ID : EMD-32242
Title : Deactive state CI from Q10 dataset, Subclass 2
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-18
Resolution : 3.40 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

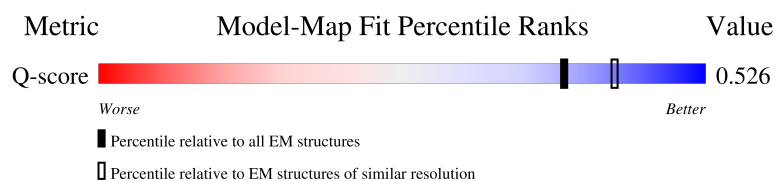
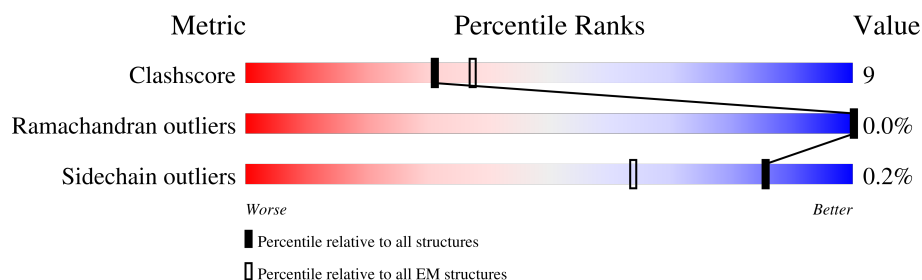
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	431	 78% 22%
2	B	176	 84% 16%
3	C	156	 72% 27% .
4	E	115	 82% 18%

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	341	
10	K	42	
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	42	
30	g	121	
31	h	105	
32	i	347	
33	j	113	
34	k	98	
35	l	603	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	124	
44	w	320	

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	B	302	-	-	X	-
45	SF4	C	301	-	-	X	-

2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 66850 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	431	Total	C	N	O	S	0	0
			3318	2095	591	612	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
			1244	792	227	211	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
			691	434	129	126	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
			678	438	102	133	5		
6	X	88	Total	C	N	O	S	0	0
			699	450	103	141	5		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	297	Total	C	N	O	S	0	0
			2356	1513	421	414	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	42	Total	C	N	O	S	0	0
			355	219	67	68	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
			5290	3317	920	1014	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	144	Total	C	N	O	S	0	0
			1204	770	218	212	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	217	Total	C	N	O	S	0	0
			1671	1065	281	315	10		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	419	Total	C	N	O	S	0	0
			3377	2162	578	613	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
			567	364	104	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
			1167	752	200	206	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	70	Total	C	N	O	S	0	0
			597	392	98	106	1		

- Molecule 23 is a protein called Complex I-B12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	84	Total	C	N	O	S	0	0
			674	437	116	120	1		

- Molecule 24 is a protein called Complex I-SGDH.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	140	Total	C	N	O	S	0	0
			1165	762	199	201	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	103	Total	C	N	O	S	0	0
			875	571	158	145	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
			1299	843	211	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	107	Total	C	N	O	S	0	0
			890	568	145	173	4		

- Molecule 29 is a protein called Complex I-KFYI.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	42	Total	C	N	O	0	0
			344	227	58	59		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	99	Total	C	N	O	S	0	0
			797	544	117	131	5		

- 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	603	Total	C	N	O	S	0	0
			4785	3173	741	820	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	129	Total	C	N	O	S	0	0
			951	637	138	168	8		

- 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
			1062	691	182	189			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	178	Total	C	N	O	S	0	0
			1529	979	277	265	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	459	Total	C	N	O	S	0	0
			3631	2412	572	609	38		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	303	Total	C	N	O	S	0	0
			2394	1607	369	397	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		

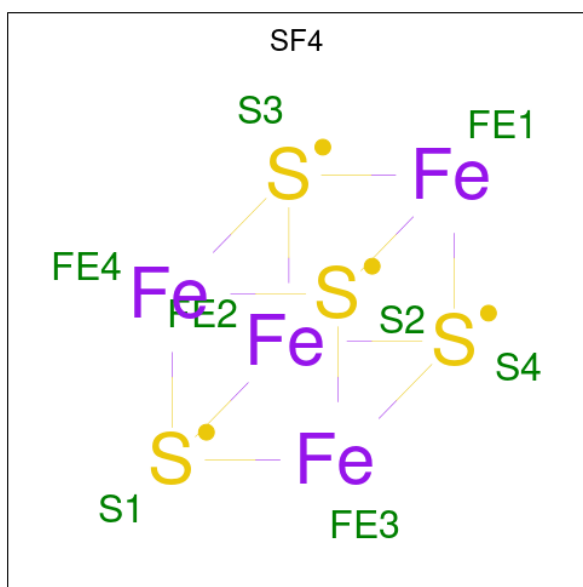
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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

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

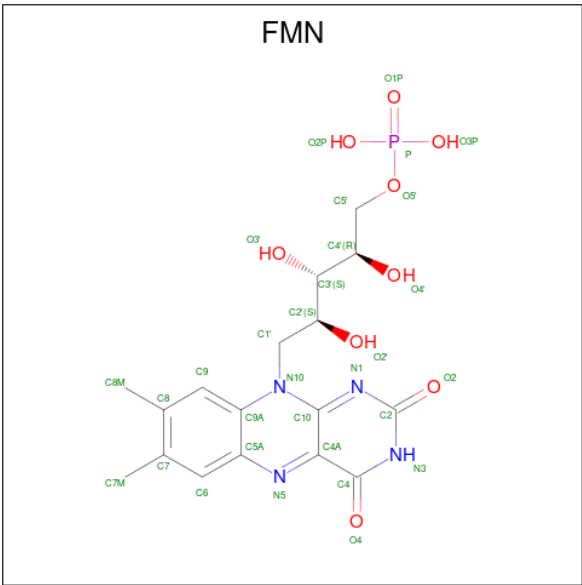
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2581	1645	437	489	10		

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



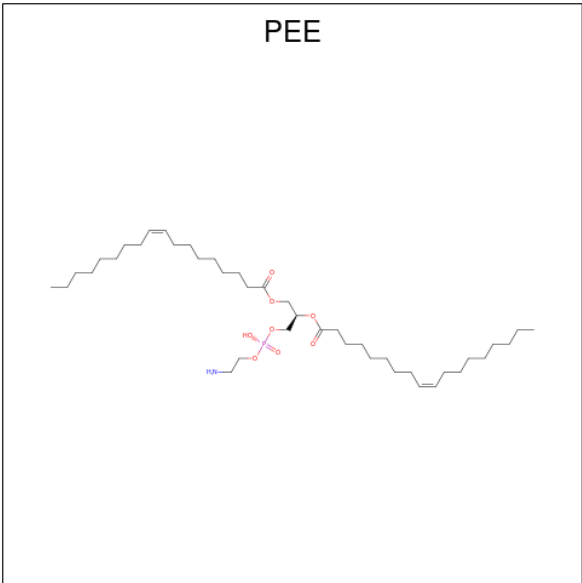
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

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



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

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



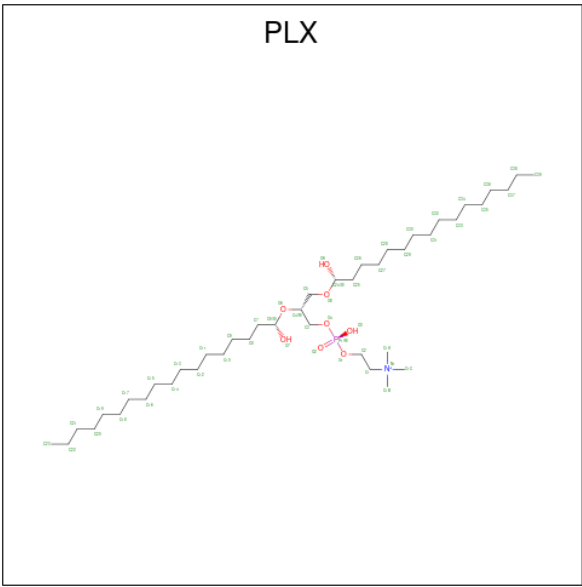
Mol	Chain	Residues	Atoms					AltConf
47	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
47	Q	1	Total	C	N	O	P	0
			51	41	1	8	1	

Continued on next page...

Continued from previous page...

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

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



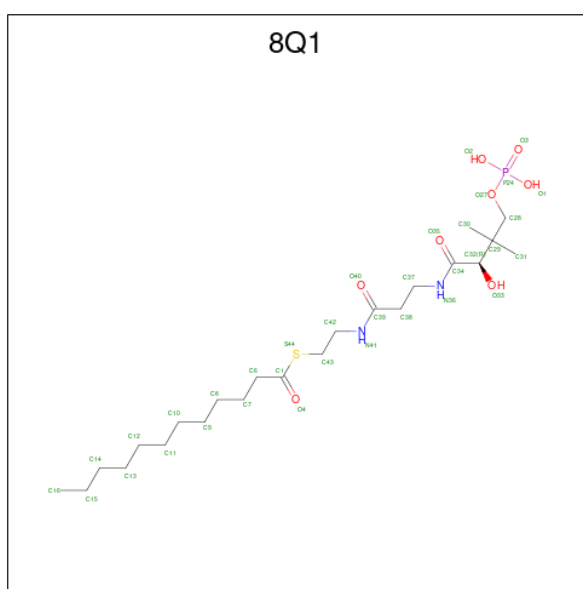
Mol	Chain	Residues	Atoms					AltConf
48	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	g	1	Total	C	N	O	P	0
			52	42	1	8	1	

Continued on next page...

Continued from previous page...

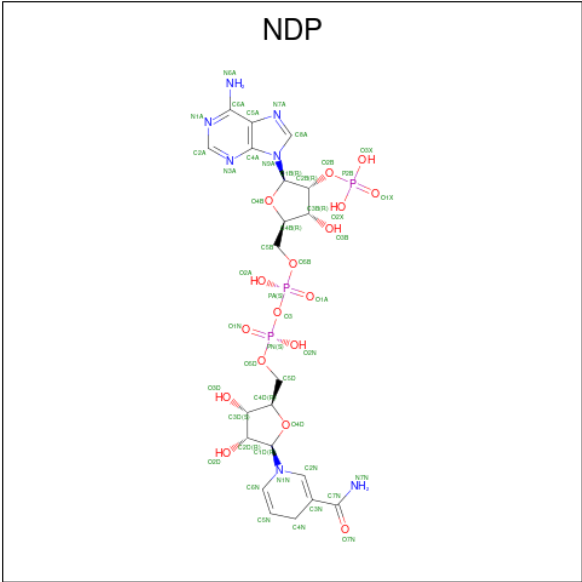
Mol	Chain	Residues	Atoms					AltConf
48	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 49 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



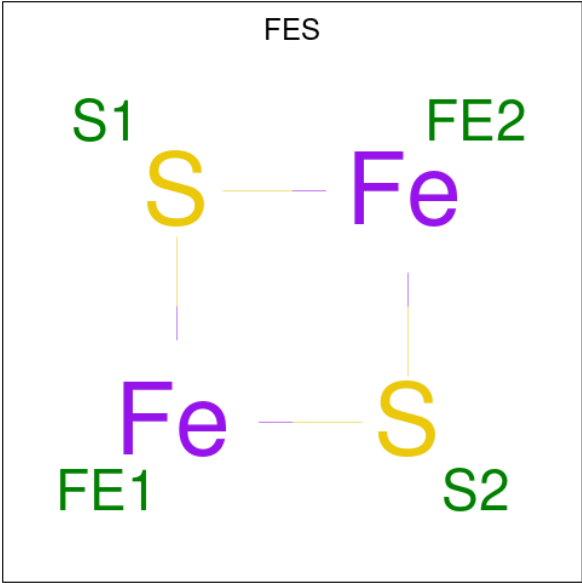
Mol	Chain	Residues	Atoms						AltConf
49	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
49	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 50 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 51 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).

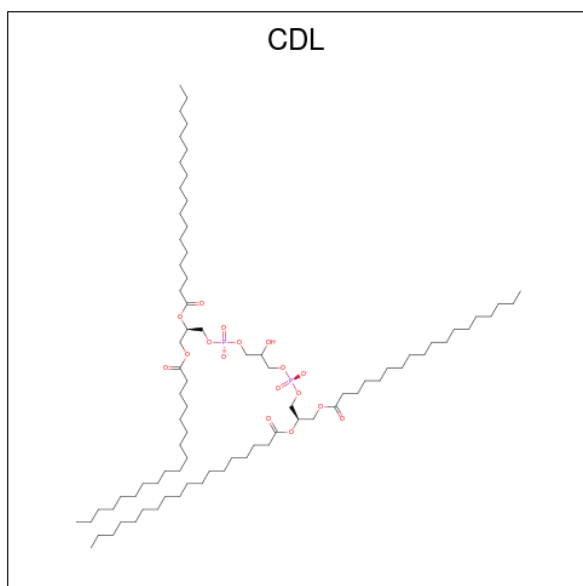


Mol	Chain	Residues	Atoms			AltConf
51	M	1	Total	Fe	S	0
			4	2	2	
51	O	1	Total	Fe	S	0
			4	2	2	

- Molecule 52 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 53 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).

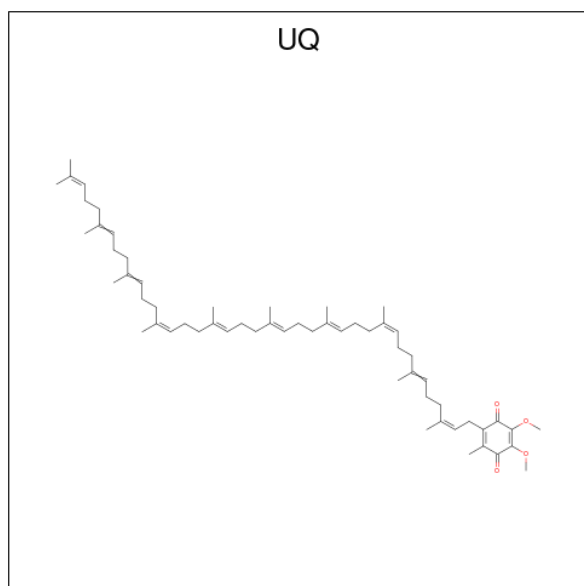


Mol	Chain	Residues	Atoms				AltConf
53	N	1	Total	C	O	P	0
			51	32	17	2	
53	V	1	Total	C	O	P	0
			94	75	17	2	
53	a	1	Total	C	O	P	0
			91	72	17	2	
53	i	1	Total	C	O	P	0
			66	47	17	2	
53	l	1	Total	C	O	P	0
			100	81	17	2	
53	o	1	Total	C	O	P	0
			68	49	17	2	
53	r	1	Total	C	O	P	0
			99	80	17	2	
53	r	1	Total	C	O	P	0
			95	76	17	2	
53	u	1	Total	C	O	P	0
			78	59	17	2	

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

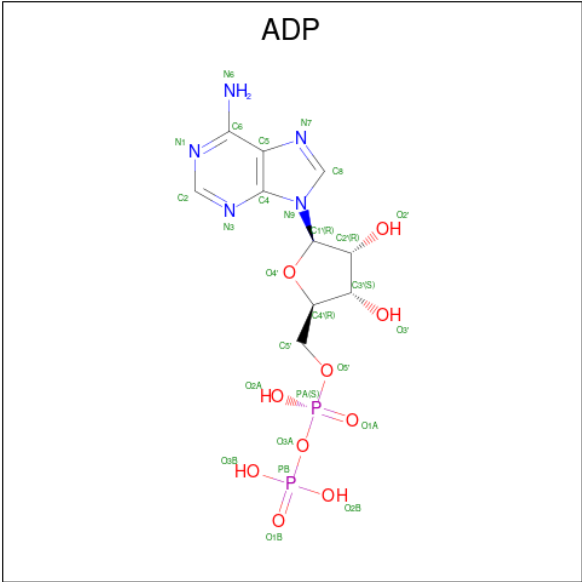
Mol	Chain	Residues	Atoms		AltConf
54	T	1	Total	Zn	0
			1	1	

- Molecule 55 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
55	s	1	Total	C	O	0
			28	24	4	

- Molecule 56 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

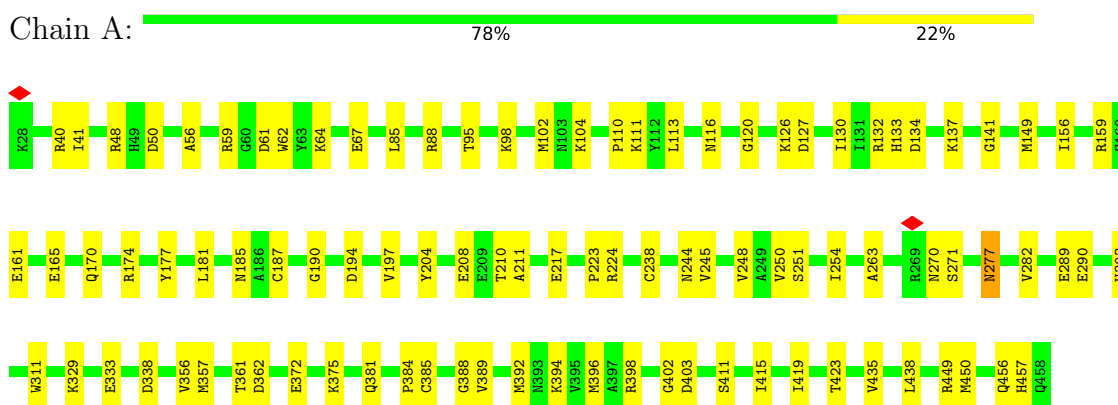


Mol	Chain	Residues	Atoms					AltConf
56	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

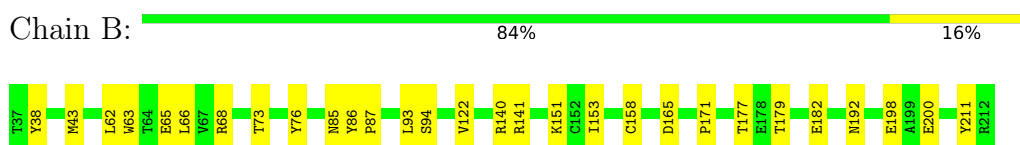
3 Residue-property plots

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

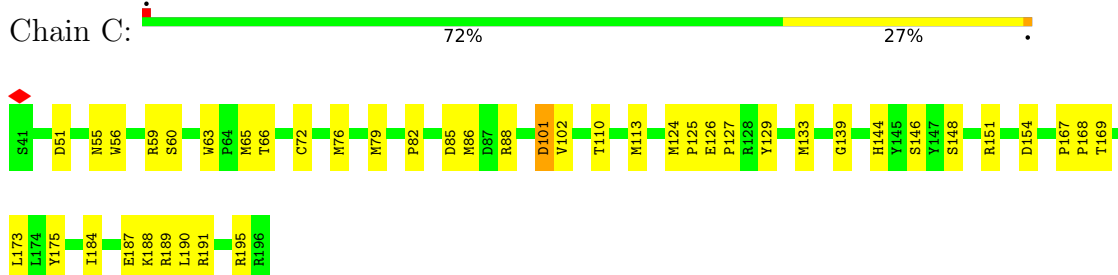
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



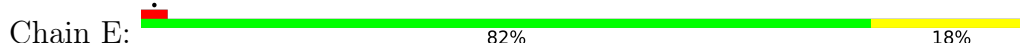
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



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

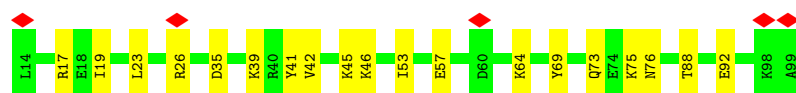
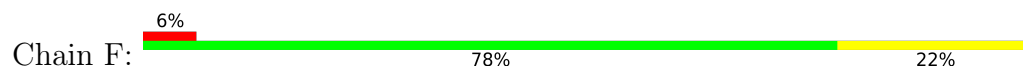


- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

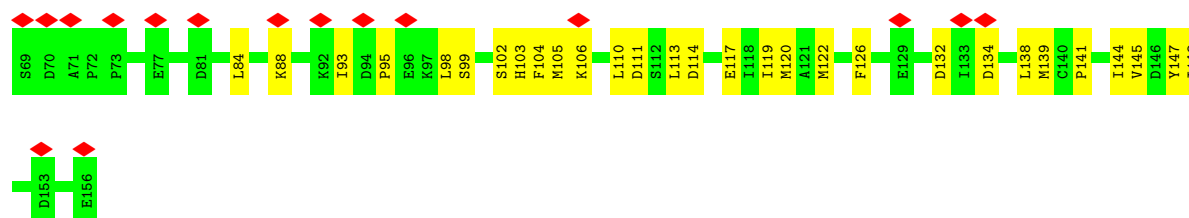




- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



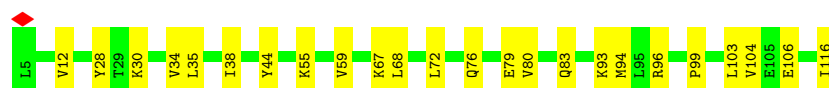
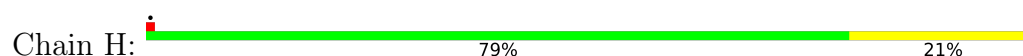
- Molecule 6: Acyl carrier protein



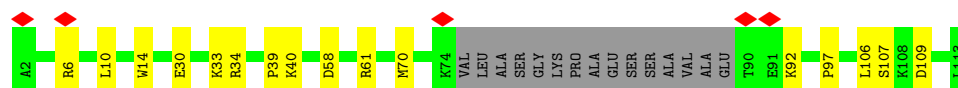
- Molecule 6: Acyl carrier protein



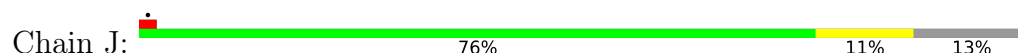
- Molecule 7: Complex I subunit B13

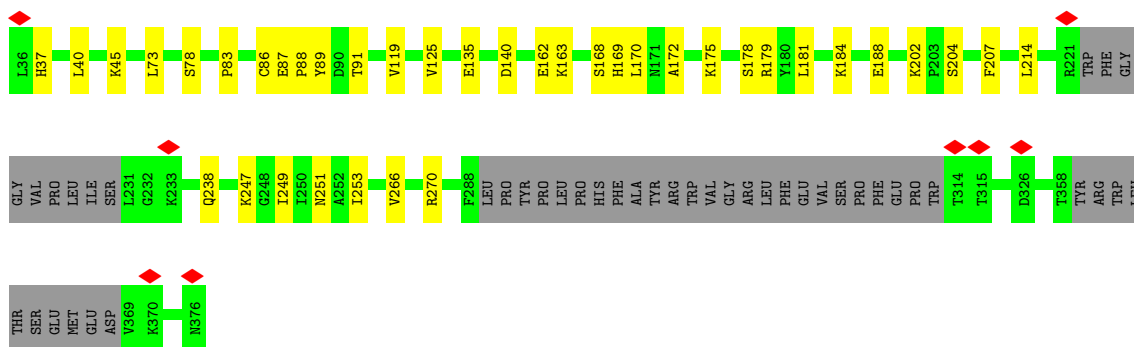


- Molecule 8: Complex I-B14.5a

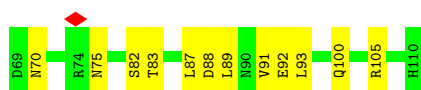


- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

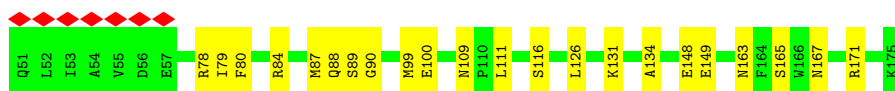
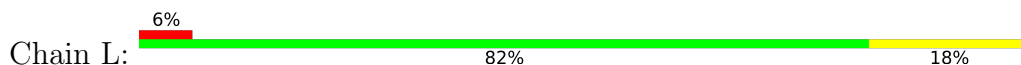




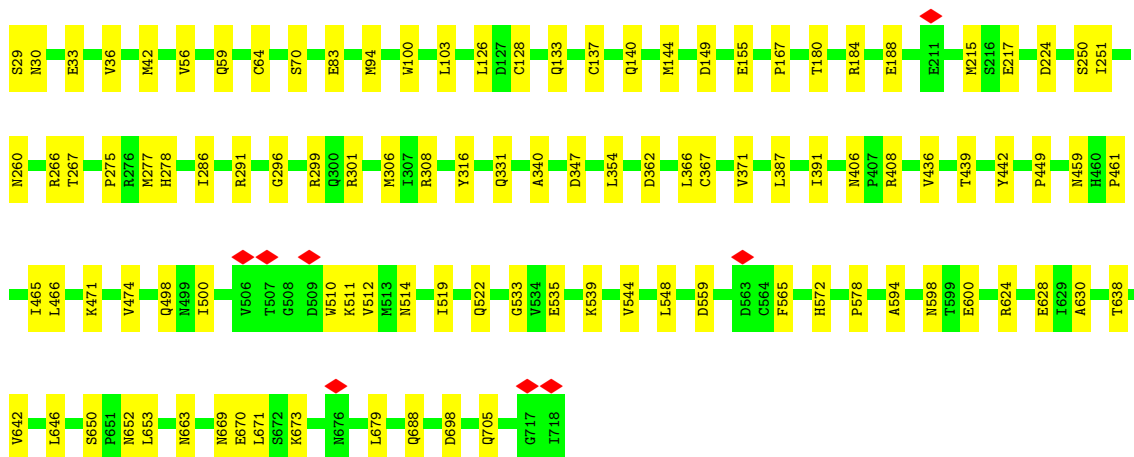
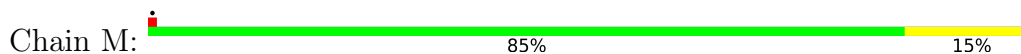
- Molecule 10: Complex I-9kD



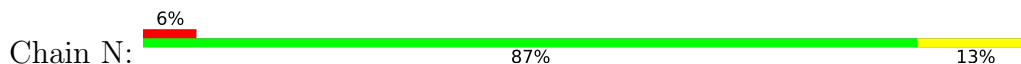
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



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

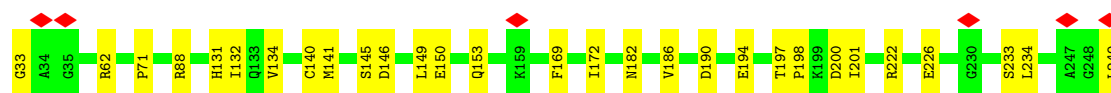
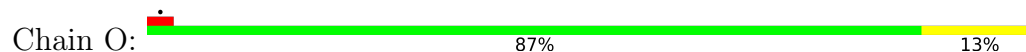


- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

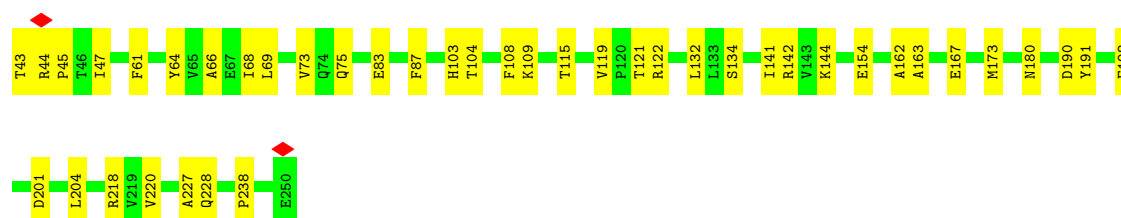
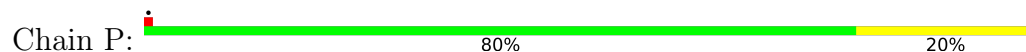




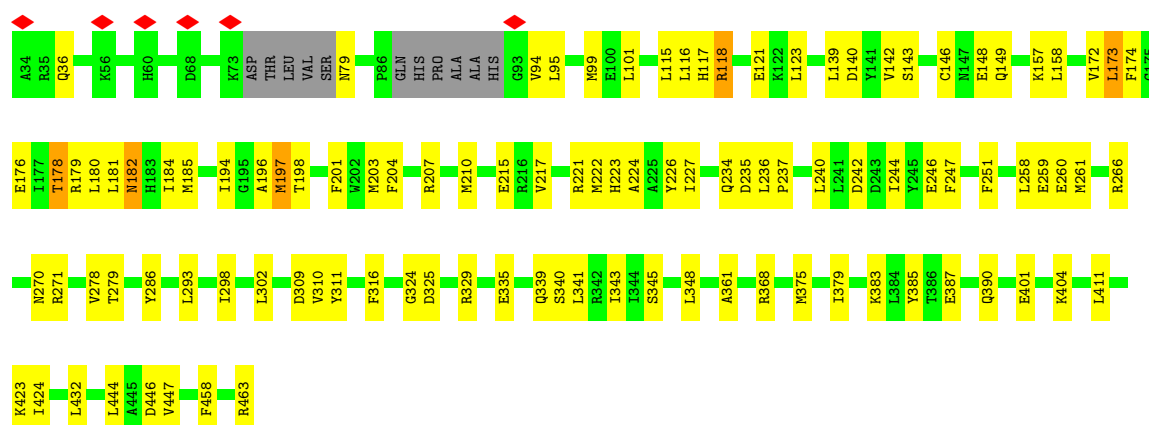
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



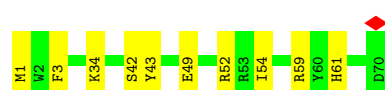
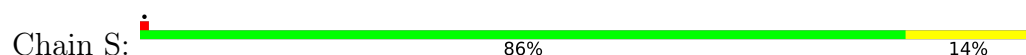
- Molecule 15: Complex I-30kD



- Molecule 16: Complex I-49kD

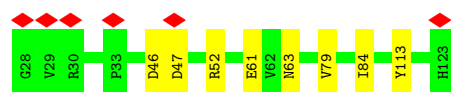


- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

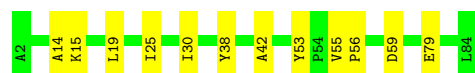
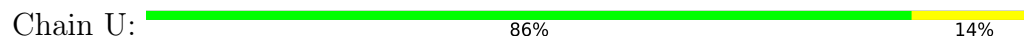


- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

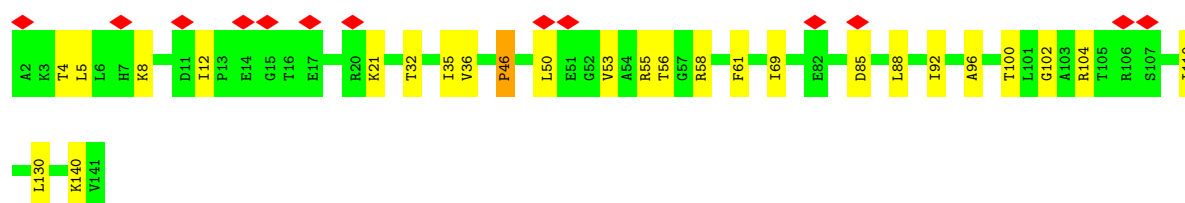
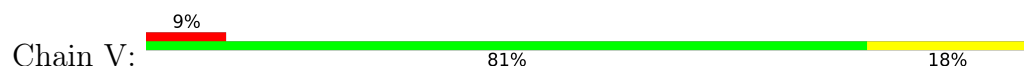




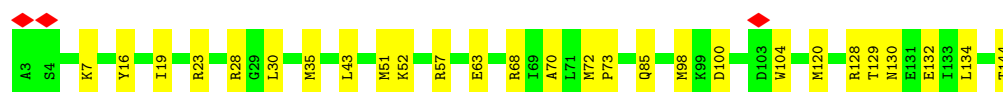
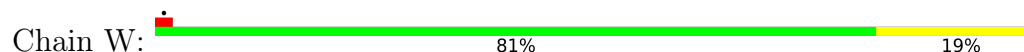
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



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



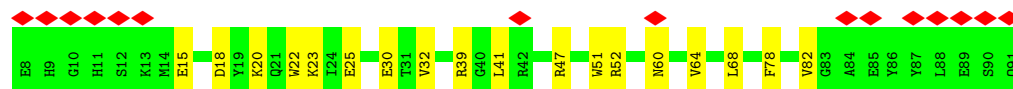
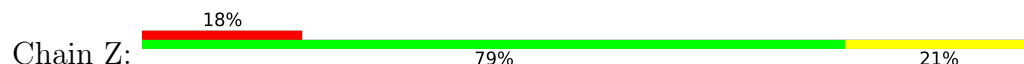
- Molecule 21: Complex I-B16.6



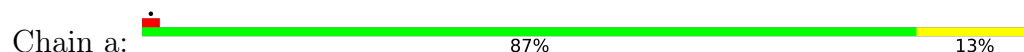
- Molecule 22: Complex I-AGGG



- Molecule 23: Complex I-B12

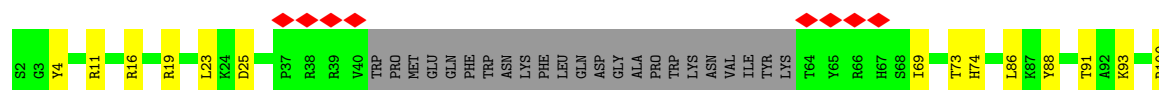


- Molecule 24: Complex I-SGDH





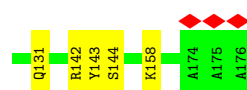
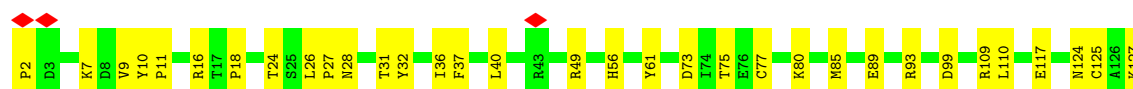
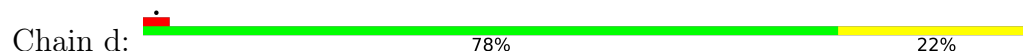
- Molecule 25: Complex I-B17



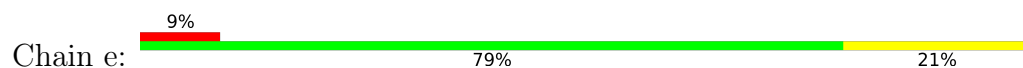
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



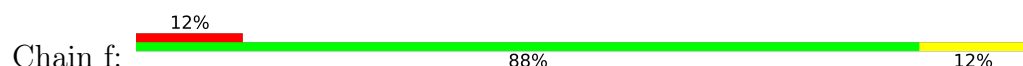
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



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

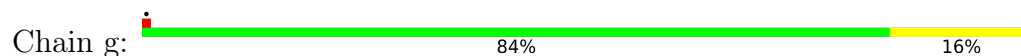


- Molecule 29: Complex I-KFYI

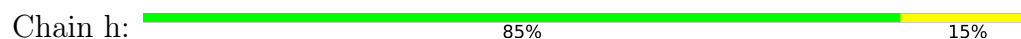




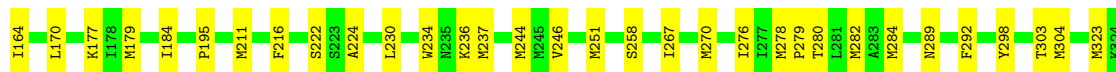
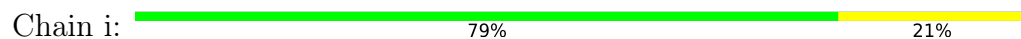
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



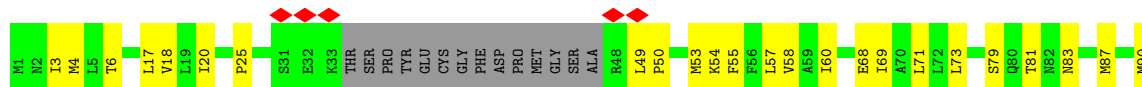
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



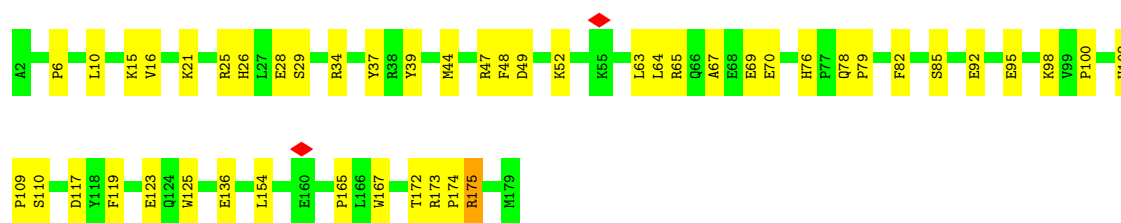
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3



- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

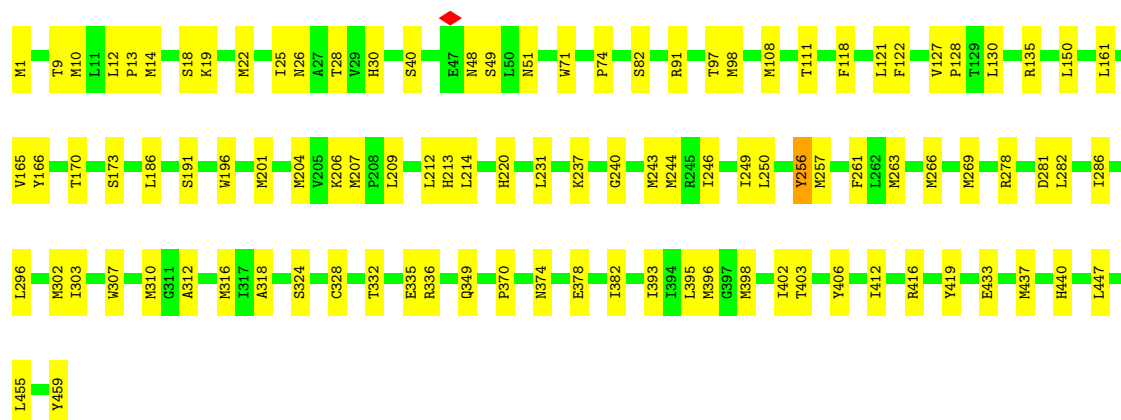






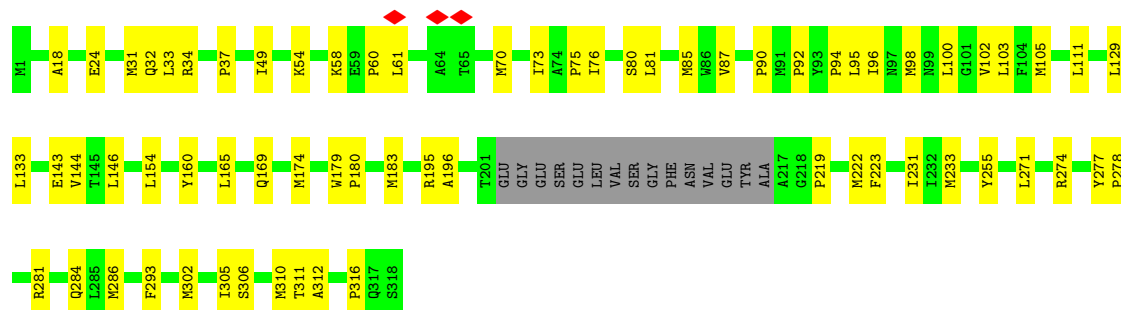
• Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r: 78% 22%



• Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s: 74% 21% 5%



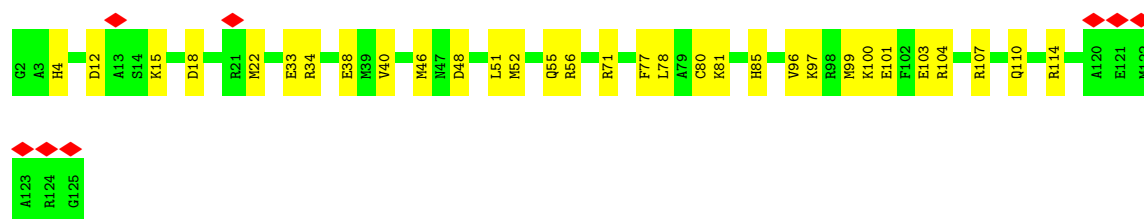
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u: 82% 18%

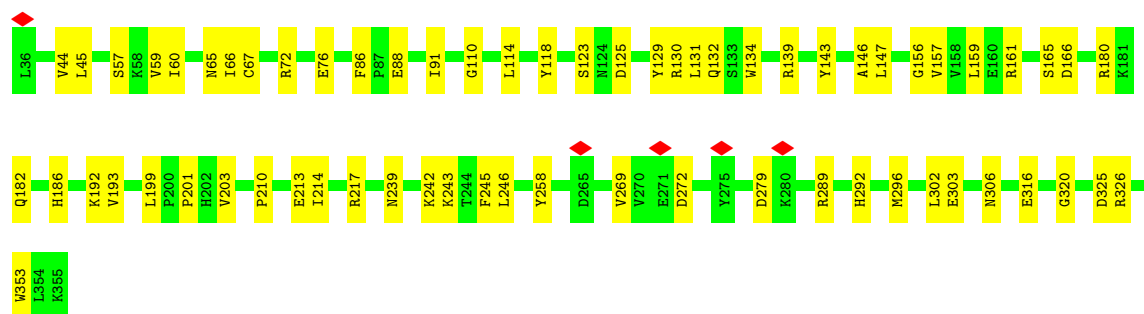
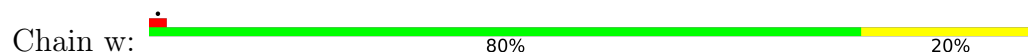


• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v: 6% 75% 25%



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94040	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	0.209	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0187	Depositor
Map size ($\text{\AA}$)	354.48602, 354.48602, 354.48602	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0/3393	0.28	0/4584
2	B	0.14	0/1443	0.30	0/1952
3	C	0.16	0/1275	0.40	2/1725 (0.1%)
4	E	0.13	0/995	0.31	0/1340
5	F	0.16	0/702	0.47	0/945
6	G	0.18	0/689	0.52	0/935
6	X	0.12	0/711	0.37	0/963
7	H	0.13	0/929	0.32	0/1258
8	I	0.14	0/798	0.37	0/1079
9	J	0.11	0/2408	0.28	0/3250
10	K	0.14	0/365	0.37	0/493
11	L	0.12	0/1039	0.29	0/1403
12	M	0.13	0/5378	0.29	0/7288
13	N	0.11	0/1245	0.29	0/1694
14	O	0.12	0/1711	0.31	0/2328
15	P	0.13	0/1789	0.31	0/2436
16	Q	0.17	0/3451	0.35	1/4672 (0.0%)
17	S	0.13	0/582	0.31	0/783
18	T	0.10	0/755	0.23	0/1018
19	U	0.12	0/664	0.28	0/912
20	V	0.15	0/1042	0.32	0/1411
21	W	0.13	0/1198	0.27	0/1617
22	Y	0.21	0/623	0.53	1/853 (0.1%)
23	Z	0.12	0/695	0.34	0/939
24	a	0.13	0/1199	0.31	0/1623
25	b	0.16	0/902	0.37	0/1227
26	c	0.15	0/1355	0.36	0/1857
27	d	0.13	0/1494	0.31	0/2015
28	e	0.13	0/916	0.34	0/1246
29	f	0.10	0/353	0.26	0/477
30	g	0.12	0/1031	0.28	0/1394
31	h	0.12	0/889	0.29	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.15	0/2773	0.32	0/3768
33	j	0.16	0/816	0.38	0/1113
34	k	0.16	0/759	0.32	0/1029
35	l	0.14	0/4914	0.34	0/6683
36	m	0.17	0/973	0.40	0/1320
37	n	0.11	0/491	0.28	0/663
38	o	0.14	0/1092	0.33	0/1481
39	p	0.15	0/1584	0.37	0/2147
40	r	0.15	0/3723	0.32	0/5078
41	s	0.15	0/2464	0.34	0/3369
42	u	0.12	0/1436	0.30	0/1938
43	v	0.14	0/1052	0.34	0/1411
44	w	0.13	0/2641	0.32	0/3577
All	All	0.14	0/66737	0.33	4/90484 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Y	80	VAL	N-CA-C	6.36	117.14	110.72
3	C	124	MET	CA-C-N	5.98	125.89	119.85
3	C	124	MET	C-N-CA	5.98	125.89	119.85
16	Q	224	ALA	N-CA-C	5.77	117.57	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	126	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3318	0	3280	68	0
2	B	1412	0	1363	30	0
3	C	1244	0	1250	48	0
4	E	971	0	975	17	0
5	F	691	0	704	15	0
6	G	678	0	655	27	0
6	X	699	0	682	26	0
7	H	910	0	950	17	0
8	I	780	0	808	12	0
9	J	2356	0	2400	28	0
10	K	355	0	329	11	0
11	L	1016	0	1016	15	0
12	M	5290	0	5315	69	0
13	N	1204	0	1162	18	0
14	O	1671	0	1673	23	0
15	P	1738	0	1693	31	0
16	Q	3377	0	3320	98	0
17	S	567	0	565	7	0
18	T	741	0	702	6	0
19	U	643	0	642	11	0
20	V	1021	0	1027	16	0
21	W	1167	0	1155	29	0
22	Y	597	0	537	29	0
23	Z	674	0	643	13	0
24	a	1165	0	1174	19	0
25	b	875	0	895	20	0
26	c	1299	0	1178	30	0
27	d	1461	0	1429	31	0
28	e	890	0	837	16	0
29	f	344	0	347	3	0
30	g	1000	0	994	18	0
31	h	867	0	871	15	0
32	i	2710	0	2874	53	0
33	j	797	0	851	29	0
34	k	748	0	799	24	0
35	l	4785	0	4933	122	0
36	m	951	0	962	32	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	n	479	0	486	9	0
38	o	1062	0	1072	15	0
39	p	1529	0	1465	37	0
40	r	3631	0	3839	82	0
41	s	2394	0	2508	63	0
42	u	1398	0	1378	23	0
43	v	1028	0	980	28	0
44	w	2581	0	2540	43	0
45	A	8	0	0	1	0
45	B	16	0	0	2	0
45	C	8	0	0	2	0
45	M	16	0	0	0	0
46	A	31	0	19	3	0
47	C	47	0	71	2	0
47	Q	51	0	82	4	0
47	U	51	0	82	0	0
47	W	41	0	59	2	0
47	b	46	0	69	1	0
47	i	47	0	71	3	0
47	l	86	0	123	5	0
47	r	51	0	82	3	0
48	C	52	0	88	4	0
48	a	52	0	88	2	0
48	g	52	0	88	4	0
48	j	52	0	88	3	0
48	r	104	0	176	6	0
49	G	35	0	0	0	0
49	X	35	0	0	3	0
50	J	48	0	25	2	0
51	M	4	0	0	0	0
51	O	4	0	0	0	0
52	M	1	0	0	0	0
53	N	51	0	46	3	0
53	V	94	0	138	3	0
53	a	91	0	132	2	0
53	i	66	0	76	2	0
53	l	100	0	156	3	0
53	o	68	0	83	5	0
53	r	194	0	294	20	0
53	u	78	0	103	8	0
54	T	1	0	0	0	0
55	s	28	0	31	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	w	27	0	11	2	0
All	All	66850	0	67539	1181	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 9.

All (1181) 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)
16:Q:181:LEU:HD23	16:Q:210:MET:SD	1.81	1.19
50:J:401:NDP:O4D	50:J:401:NDP:C4D	1.68	1.18
16:Q:181:LEU:CD2	16:Q:210:MET:SD	2.35	1.14
22:Y:71:TRP:CE2	22:Y:75:HIS:CE1	2.42	1.06
3:C:167:PRO:HG3	16:Q:222:MET:CE	1.89	1.03
3:C:167:PRO:HG3	16:Q:222:MET:HE2	1.40	1.03
16:Q:181:LEU:HD21	16:Q:210:MET:CB	1.89	1.01
22:Y:71:TRP:CZ2	22:Y:75:HIS:CE1	2.50	0.99
16:Q:172:VAL:HG21	16:Q:310:VAL:HG22	1.43	0.98
39:p:174:PRO:O	39:p:175:ARG:HB2	1.63	0.95
22:Y:71:TRP:CZ2	22:Y:75:HIS:HE1	1.85	0.94
22:Y:71:TRP:CE2	22:Y:75:HIS:HE1	1.87	0.93
16:Q:181:LEU:HD21	16:Q:210:MET:SD	2.11	0.90
16:Q:181:LEU:HD21	16:Q:210:MET:HB3	1.62	0.81
53:r:504:CDL:H621	53:r:504:CDL:H432	1.67	0.77
33:j:18:VAL:HG22	41:s:222:MET:HG3	1.67	0.77
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.66	0.76
1:A:396:MET:HE1	1:A:438:LEU:HD23	1.70	0.73
6:X:123:GLU:HG2	6:X:129:GLU:HA	1.69	0.72
21:W:51:MET:HE2	41:s:311:THR:HB	1.70	0.72
9:J:247:LYS:O	9:J:251:ASN:ND2	2.21	0.71
40:r:108:MET:HB3	40:r:121:LEU:HD13	1.72	0.71
8:I:14:TRP:O	21:W:28:ARG:NH2	2.21	0.71
26:c:108:ASP:OD1	40:r:278:ARG:NH2	2.23	0.71
35:l:375:ILE:HD12	35:l:458:LEU:HD11	1.73	0.71
44:w:67:CYS:HB3	44:w:214:ILE:HD11	1.73	0.70
40:r:191:SER:HB3	47:r:501:PEE:H3	1.72	0.70
32:i:149:ILE:HD11	32:i:195:PRO:HG3	1.74	0.70
15:P:64:TYR:HH	15:P:103:HIS:HE2	1.38	0.70
43:v:38:GLU:N	43:v:38:GLU:OE2	2.25	0.70
44:w:292:HIS:CE1	44:w:296:MET:HE1	2.26	0.70
6:G:144:ILE:O	6:G:148:ILE:HD12	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:102:VAL:HG23	3:C:129:TYR:O	1.91	0.69
1:A:113:LEU:HD13	1:A:149:MET:HE1	1.75	0.69
30:g:110:THR:HG22	30:g:112:GLY:H	1.57	0.69
4:E:37:ARG:NH1	6:G:132:ASP:OD2	2.26	0.68
16:Q:181:LEU:HD21	16:Q:210:MET:HB2	1.74	0.68
41:s:169:GLN:HE21	41:s:174:MET:HE2	1.59	0.68
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.27	0.67
32:i:43:VAL:HG11	32:i:129:LEU:HD23	1.76	0.67
43:v:52:MET:HB2	43:v:55:GLN:HB2	1.77	0.67
45:C:301:SF4:S4	16:Q:223:HIS:CD2	2.88	0.67
32:i:267:ILE:HG12	32:i:279:PRO:HB3	1.76	0.67
25:b:11:ARG:NH2	39:p:165:PRO:O	2.26	0.67
26:c:119:THR:HG22	38:o:11:LEU:HA	1.76	0.67
33:j:60:ILE:HG21	36:m:168:ILE:HG21	1.75	0.67
41:s:195:ARG:HD3	41:s:231:ILE:HD11	1.77	0.67
3:C:187:GLU:OE1	3:C:189:ARG:NH1	2.28	0.67
16:Q:101:LEU:HD11	16:Q:444:LEU:HD13	1.77	0.67
36:m:57:PHE:HE1	41:s:111:LEU:HD11	1.58	0.67
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.27	0.66
34:k:22:TYR:HB3	35:l:585:LYS:HG2	1.77	0.66
5:F:19:ILE:HG13	5:F:53:ILE:HG23	1.76	0.66
47:i:402:PEE:H37	47:i:402:PEE:H60	1.77	0.66
41:s:102:VAL:HG21	41:s:154:LEU:HD11	1.77	0.66
1:A:398:ARG:HG2	1:A:403:ASP:HB3	1.78	0.66
40:r:263:MET:HA	40:r:263:MET:HE3	1.78	0.66
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.29	0.66
44:w:139:ARG:NH1	44:w:166:ASP:OD2	2.29	0.66
27:d:26:LEU:HD12	27:d:27:PRO:HD2	1.78	0.65
34:k:98:CYS:HB2	35:l:580:GLN:HB2	1.78	0.65
16:Q:173:LEU:O	16:Q:173:LEU:HD12	1.96	0.65
21:W:85:GLN:OE1	31:h:105:ARG:NH1	2.28	0.65
35:l:558:LEU:HB3	40:r:214:LEU:HD21	1.77	0.65
45:C:301:SF4:S4	16:Q:223:HIS:NE2	2.69	0.65
1:A:41:ILE:HG21	1:A:250:VAL:HG12	1.78	0.65
16:Q:139:LEU:HD11	16:Q:424:ILE:HD13	1.79	0.65
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.78	0.65
3:C:101:ASP:OD1	41:s:58:LYS:NZ	2.24	0.64
24:a:170:GLN:OE1	42:u:151:ASN:ND2	2.30	0.64
18:T:47:ASP:O	18:T:52:ARG:NH2	2.31	0.64
38:o:5:LYS:NZ	39:p:69:GLU:OE1	2.30	0.64
12:M:406:ASN:ND2	12:M:688:GLN:O	2.29	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:211:MET:HE3	32:i:251:MET:HG3	1.78	0.64
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.27	0.64
14:O:134:VAL:HG21	14:O:149:LEU:HD13	1.79	0.63
14:O:182:ASN:OD1	14:O:222:ARG:NH2	2.31	0.63
27:d:24:THR:HG23	27:d:26:LEU:H	1.63	0.63
1:A:50:ASP:O	1:A:59:ARG:NH2	2.31	0.63
33:j:79:SER:HA	33:j:87:MET:HE2	1.79	0.63
35:l:419:THR:HA	35:l:422:TYR:CE2	2.34	0.63
2:B:177:THR:HG21	2:B:182:GLU:HB2	1.80	0.63
1:A:362:ASP:OD1	1:A:449:ARG:NH2	2.32	0.63
1:A:396:MET:HE3	1:A:435:VAL:HG22	1.81	0.63
27:d:11:PRO:HD2	27:d:109:ARG:HD2	1.81	0.63
2:B:171:PRO:HG2	2:B:200:GLU:OE1	1.99	0.62
16:Q:176:GLU:OE1	16:Q:176:GLU:HA	1.98	0.62
32:i:84:TRP:HH2	34:k:59:MET:HE2	1.63	0.62
44:w:146:ALA:HB1	44:w:157:VAL:HG21	1.80	0.62
1:A:357:MET:HB3	1:A:361:THR:HG21	1.81	0.62
39:p:98:LYS:HB3	39:p:174:PRO:HG2	1.81	0.62
7:H:93:LYS:HD2	7:H:96:ARG:HH12	1.64	0.62
35:l:338:MET:HE2	35:l:458:LEU:HA	1.80	0.62
6:X:118:ILE:O	6:X:122:MET:HG2	1.99	0.62
39:p:29:SER:HB3	39:p:76:HIS:HD2	1.65	0.62
33:j:17:LEU:HD23	41:s:222:MET:HE1	1.79	0.62
6:X:114:ASP:O	6:X:118:ILE:HD12	2.00	0.62
22:Y:65:MET:HE1	35:l:378:LEU:HD13	1.82	0.62
22:Y:83:HIS:CE1	43:v:85:HIS:HE1	2.17	0.62
31:h:97:HIS:HA	31:h:102:GLU:HB3	1.81	0.62
40:r:328:CYS:O	40:r:332:THR:HG23	2.00	0.61
30:g:32:ARG:HB3	32:i:339:MET:HE1	1.80	0.61
48:a:202:PLX:H102	40:r:40:SER:HB3	1.82	0.61
12:M:128:CYS:SG	12:M:140:GLN:NE2	2.72	0.61
17:S:49:GLU:OE2	17:S:52:ARG:NH1	2.33	0.61
26:c:129:MET:HG2	35:l:528:TYR:CG	2.35	0.61
40:r:378:GLU:O	40:r:382:ILE:HG12	2.01	0.61
22:Y:94:ASP:HB3	22:Y:99:ILE:HB	1.82	0.61
5:F:42:VAL:O	5:F:46:LYS:HG2	2.00	0.61
3:C:59:ARG:NH1	48:C:303:PLX:O3	2.28	0.61
35:l:60:GLU:OE1	35:l:83:ASP:HA	2.00	0.61
12:M:598:ASN:ND2	12:M:600:GLU:OE2	2.33	0.61
25:b:108:ASP:OD2	43:v:71:ARG:NH2	2.34	0.61
40:r:328:CYS:HB3	40:r:437:MET:HE1	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:573:MET:HE2	47:l:701:PEE:H21	1.82	0.61
16:Q:181:LEU:HD21	16:Q:210:MET:CG	2.31	0.60
1:A:251:SER:HA	1:A:254:ILE:HD12	1.82	0.60
1:A:98:LYS:NZ	46:A:502:FMN:O3P	2.33	0.60
26:c:84:GLN:O	26:c:98:ARG:NH1	2.30	0.60
39:p:10:LEU:O	39:p:15:LYS:NZ	2.35	0.60
35:l:237:MET:HE2	35:l:303:ALA:HB2	1.82	0.60
11:L:80:PHE:HE1	11:L:100:GLU:HG2	1.67	0.60
48:r:503:PLX:H222	53:r:504:CDL:H521	1.84	0.60
32:i:155:LEU:HD12	32:i:278:MET:HE2	1.84	0.60
14:O:134:VAL:HG12	14:O:186:VAL:HG22	1.83	0.60
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.30	0.60
27:d:110:LEU:HD11	35:l:203:MET:HG2	1.83	0.60
32:i:159:MET:HE1	32:i:282:MET:HG2	1.82	0.60
43:v:51:LEU:O	43:v:52:MET:HG2	2.02	0.60
12:M:471:LYS:HB3	12:M:510:TRP:CE2	2.37	0.60
16:Q:446:ASP:OD1	41:s:281:ARG:NH1	2.35	0.60
21:W:57:ARG:HB3	41:s:316:PRO:HG3	1.83	0.60
32:i:298:TYR:O	32:i:303:THR:OG1	2.20	0.60
3:C:190:LEU:HD11	47:C:302:PEE:H19	1.84	0.59
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.84	0.59
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.83	0.59
53:u:201:CDL:H251	53:u:201:CDL:H792	1.82	0.59
2:B:73:THR:HG22	41:s:31:MET:HG2	1.83	0.59
35:l:407:TRP:O	35:l:411:MET:HG2	2.02	0.59
42:u:83:THR:HA	42:u:86:TRP:CD1	2.38	0.59
34:k:17:ALA:O	34:k:21:MET:HG2	2.02	0.59
12:M:308:ARG:NH2	12:M:578:PRO:O	2.35	0.59
35:l:393:ASP:O	35:l:397:GLU:HG3	2.02	0.59
20:V:4:THR:O	20:V:8:LYS:HG3	2.02	0.59
24:a:134:GLU:OE1	37:n:57:TRP:NE1	2.27	0.59
27:d:144:SER:O	27:d:158:LYS:NZ	2.30	0.59
40:r:256:TYR:OH	48:r:502:PLX:H82	2.03	0.59
48:C:303:PLX:H272	48:C:303:PLX:H91	1.85	0.59
25:b:88:TYR:CE2	27:d:49:ARG:HG2	2.38	0.59
31:h:2:PRO:HA	32:i:140:SER:HB2	1.84	0.59
34:k:32:CYS:O	34:k:36:MET:HG3	2.03	0.59
22:Y:92:TRP:O	43:v:107:ARG:NH2	2.31	0.59
35:l:552:LEU:HD21	38:o:90:GLY:HA2	1.84	0.59
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.42	0.58
21:W:70:ALA:HB2	42:u:125:LEU:HD13	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:122:THR:O	38:o:6:TYR:HE2	1.86	0.58
53:r:505:CDL:H742	53:r:505:CDL:H271	1.84	0.58
12:M:217:GLU:H	12:M:217:GLU:CD	2.11	0.58
32:i:280:THR:O	32:i:284:MET:HG2	2.03	0.58
40:r:403:THR:HA	40:r:406:TYR:CE2	2.39	0.58
35:l:10:THR:O	35:l:14:ILE:HG22	2.02	0.58
12:M:624:ARG:NH1	12:M:628:GLU:OE1	2.32	0.58
12:M:698:ASP:OD1	12:M:698:ASP:N	2.36	0.58
47:l:701:PEE:H58	47:l:701:PEE:H23	1.85	0.58
53:u:201:CDL:H161	53:u:201:CDL:HB31	1.85	0.58
24:a:136:THR:OG1	40:r:51:ASN:ND2	2.32	0.58
28:e:77:ASP:OD1	28:e:78:LYS:N	2.36	0.58
35:l:417:SER:HB2	35:l:493:VAL:HG22	1.86	0.58
44:w:242:LYS:HA	44:w:246:LEU:HD12	1.85	0.58
49:X:201:8Q1:N36	49:X:201:8Q1:O40	2.35	0.58
5:F:88:THR:O	5:F:92:GLU:HG2	2.04	0.58
21:W:128:ARG:NH1	31:h:102:GLU:OE2	2.35	0.58
36:m:45:LEU:HD23	36:m:50:SER:HA	1.85	0.58
6:X:79:ILE:O	6:X:83:VAL:HG23	2.03	0.57
24:a:147:ALA:HB2	40:r:173:SER:HB2	1.86	0.57
4:E:64:ARG:NH2	6:G:114:ASP:OD1	2.36	0.57
14:O:182:ASN:ND2	14:O:194:GLU:OE1	2.29	0.57
17:S:54:ILE:HD12	42:u:19:LYS:HA	1.86	0.57
43:v:46:MET:HG2	43:v:56:ARG:HG2	1.86	0.57
44:w:91:ILE:HD11	44:w:131:LEU:HD12	1.86	0.57
26:c:84:GLN:HA	26:c:114:ARG:HG2	1.86	0.57
26:c:110:ASP:OD1	40:r:278:ARG:NE	2.33	0.57
12:M:306:MET:HE1	13:N:139:PRO:HG3	1.86	0.57
27:d:2:PRO:O	27:d:7:LYS:NZ	2.34	0.57
40:r:204:MET:HE1	40:r:302:MET:HE3	1.86	0.57
6:G:113:LEU:O	6:G:117:GLU:HG3	2.05	0.57
20:V:5:LEU:HA	20:V:8:LYS:HD3	1.86	0.57
3:C:167:PRO:HD3	16:Q:223:HIS:CD2	2.39	0.57
35:l:1:MET:HE2	35:l:2:ASN:HB2	1.86	0.57
40:r:324:SER:OG	40:r:440:HIS:NE2	2.33	0.57
41:s:222:MET:HE3	41:s:222:MET:HA	1.85	0.57
7:H:94:MET:SD	7:H:99:PRO:HG3	2.45	0.57
12:M:94:MET:HE2	12:M:100:TRP:HH2	1.70	0.57
27:d:16:ARG:NH2	43:v:48:ASP:OD2	2.36	0.57
35:l:55:MET:HE2	35:l:471:ASN:HB3	1.86	0.57
16:Q:180:LEU:HB3	16:Q:210:MET:HE1	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.40	0.57
3:C:154:ASP:OD1	3:C:154:ASP:N	2.38	0.57
11:L:165:SER:O	11:L:171:ARG:NH1	2.38	0.57
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.87	0.57
32:i:87:THR:HG22	32:i:88:LYS:H	1.70	0.57
41:s:100:LEU:HD23	41:s:103:LEU:HD22	1.87	0.57
1:A:185:ASN:HB3	1:A:190:GLY:H	1.70	0.56
11:L:131:LYS:NZ	11:L:149:GLU:OE2	2.31	0.56
15:P:66:ALA:HA	15:P:73:VAL:HG11	1.86	0.56
35:l:359:MET:O	35:l:436:ARG:NH2	2.38	0.56
5:F:57:GLU:OE2	5:F:57:GLU:N	2.38	0.56
14:O:146:ASP:O	14:O:150:GLU:HG2	2.05	0.56
33:j:91:ALA:HB1	41:s:305:ILE:HD13	1.87	0.56
35:l:72:GLN:NE2	40:r:459:TYR:O	2.37	0.56
16:Q:121:GLU:OE2	16:Q:463:ARG:NH1	2.35	0.56
35:l:142:ILE:HG12	40:r:370:PRO:HB2	1.87	0.56
41:s:18:ALA:HB2	55:s:401:UQ:H152	1.86	0.56
44:w:125:ASP:O	44:w:130:ARG:NH2	2.39	0.56
1:A:375:LYS:NZ	14:O:33:GLY:O	2.38	0.56
13:N:44:TYR:HH	13:N:113:HIS:H	1.53	0.56
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.37	0.56
26:c:57:MET:HE3	26:c:104:PRO:HG3	1.88	0.56
48:j:201:PLX:H381	48:j:201:PLX:H322	1.86	0.56
3:C:167:PRO:HD3	16:Q:223:HIS:HD2	1.71	0.56
6:G:88:LYS:HE3	6:G:95:PRO:HB3	1.87	0.56
7:H:12:VAL:HG12	16:Q:279:THR:HA	1.86	0.56
12:M:471:LYS:HB3	12:M:510:TRP:CZ2	2.40	0.56
24:a:160:MET:HE2	24:a:167:PRO:HD2	1.88	0.56
33:j:92:LEU:HD22	41:s:302:MET:HG2	1.87	0.56
1:A:411:SER:O	1:A:415:ILE:HG13	2.05	0.56
12:M:36:VAL:HB	12:M:56:VAL:HG21	1.88	0.56
16:Q:335:GLU:OE2	16:Q:339:GLN:NE2	2.37	0.56
16:Q:375:MET:HE3	16:Q:379:ILE:HG13	1.87	0.56
35:l:7:LEU:O	35:l:11:THR:HG23	2.05	0.56
35:l:391:SER:O	35:l:395:ILE:HG12	2.06	0.56
35:l:558:LEU:HD11	53:o:201:CDL:H852	1.86	0.56
1:A:133:HIS:CD2	10:K:75:ASN:HD22	2.23	0.56
9:J:238:GLN:HG2	9:J:266:VAL:HB	1.88	0.56
26:c:186:ILE:HD13	43:v:100:LYS:HB3	1.88	0.56
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.87	0.56
2:B:68:ARG:NH1	16:Q:260:GLU:OE2	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:196:ALA:HB3	41:s:274:ARG:HG2	1.88	0.55
1:A:130:ILE:HD11	1:A:245:VAL:HG12	1.89	0.55
43:v:12:ASP:OD1	43:v:15:LYS:N	2.39	0.55
2:B:85:ASN:OD1	3:C:88:ARG:NH2	2.40	0.55
26:c:153:TYR:HB3	35:l:403:TYR:HD1	1.72	0.55
32:i:95:MET:HE2	32:i:149:ILE:HG22	1.87	0.55
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.87	0.55
5:F:73:GLN:N	5:F:73:GLN:OE1	2.40	0.55
12:M:217:GLU:OE1	12:M:217:GLU:N	2.30	0.55
6:G:138:LEU:HD11	6:G:147:TYR:CD2	2.41	0.55
27:d:32:TYR:O	27:d:36:ILE:HG22	2.06	0.55
39:p:16:VAL:HG22	39:p:64:LEU:HD13	1.89	0.55
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.72	0.55
2:B:192:ASN:ND2	18:T:61:GLU:OE2	2.38	0.55
25:b:100:ARG:HB2	35:l:60:GLU:HB2	1.89	0.55
32:i:347:ASN:N	32:i:347:ASN:OD1	2.39	0.55
20:V:69:ILE:HG13	20:V:100:THR:HG21	1.89	0.55
28:e:85:TRP:O	28:e:89:VAL:HG13	2.07	0.55
1:A:210:THR:HB	1:A:224:ARG:HG2	1.89	0.55
9:J:168:SER:OG	9:J:188:GLU:OE2	2.21	0.55
35:l:366:MET:O	35:l:370:THR:HG22	2.07	0.55
43:v:33:GLU:OE1	43:v:33:GLU:N	2.28	0.55
12:M:449:PRO:HB2	12:M:679:LEU:HD13	1.89	0.55
35:l:488:MET:O	35:l:492:ILE:HG13	2.07	0.54
6:G:84:LEU:O	6:G:88:LYS:HG2	2.08	0.54
30:g:2:THR:HG21	30:g:4:MET:HE2	1.88	0.54
32:i:10:ILE:HG21	53:i:401:CDL:H532	1.89	0.54
44:w:258:TYR:HE2	44:w:269:VAL:HG13	1.71	0.54
6:X:153:ASP:OD1	25:b:19:ARG:NH2	2.37	0.54
25:b:104:ILE:HD13	27:d:18:PRO:HG3	1.89	0.54
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.42	0.54
47:W:201:PEE:H19	33:j:4:MET:HE3	1.89	0.54
6:G:93:ILE:HD11	6:G:110:LEU:HD11	1.88	0.54
23:Z:64:VAL:O	23:Z:68:LEU:HD12	2.08	0.54
41:s:286:MET:HA	41:s:286:MET:HE2	1.89	0.54
19:U:56:PRO:HG2	42:u:45:LEU:HB2	1.90	0.54
40:r:161:LEU:O	40:r:165:VAL:HG22	2.07	0.54
44:w:118:TYR:OH	56:w:401:ADP:O2'	2.26	0.54
29:f:52:VAL:O	29:f:56:ILE:HG12	2.08	0.54
34:k:8:ILE:HG21	34:k:43:MET:HB2	1.90	0.54
9:J:162:GLU:HG3	9:J:163:LYS:HG3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.90	0.54
11:L:90:GLY:HA3	15:P:238:PRO:HB2	1.89	0.54
20:V:53:VAL:HA	20:V:56:THR:HG22	1.90	0.54
22:Y:87:PRO:HG2	43:v:96:VAL:HG22	1.89	0.54
24:a:82:VAL:HG11	28:e:104:THR:HG21	1.89	0.54
33:j:25:PRO:HB2	41:s:60:PRO:HD3	1.89	0.54
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.24	0.53
1:A:456:GLN:OE1	1:A:457:HIS:ND1	2.36	0.53
16:Q:387:GLU:OE2	16:Q:390:GLN:NE2	2.40	0.53
32:i:177:LYS:NZ	34:k:97:GLN:O	2.28	0.53
40:r:1:MET:SD	40:r:111:THR:HG21	2.47	0.53
1:A:290:GLU:OE1	1:A:303:HIS:NE2	2.41	0.53
1:A:372:GLU:OE2	14:O:33:GLY:N	2.40	0.53
13:N:85:GLU:CD	13:N:85:GLU:H	2.16	0.53
53:r:504:CDL:H541	53:r:504:CDL:HA61	1.89	0.53
1:A:116:ASN:OD1	46:A:502:FMN:O3'	2.27	0.53
4:E:68:MET:HE3	4:E:68:MET:HA	1.91	0.53
7:H:35:LEU:HA	7:H:38:ILE:HD12	1.90	0.53
10:K:105:ARG:NH1	11:L:167:ASN:O	2.40	0.53
16:Q:148:GLU:HB3	16:Q:227:ILE:HB	1.90	0.53
22:Y:93:THR:OG1	22:Y:96:GLU:OE1	2.24	0.53
27:d:109:ARG:NH2	27:d:131:GLN:OE1	2.42	0.53
4:E:40:TYR:HB3	6:G:120:MET:HE1	1.91	0.53
8:I:40:LYS:HB3	21:W:7:LYS:H	1.74	0.53
53:N:201:CDL:H742	53:N:201:CDL:H531	1.89	0.53
47:Q:501:PEE:H38	19:U:25:ILE:HG12	1.91	0.53
19:U:79:GLU:OE1	19:U:79:GLU:N	2.41	0.53
21:W:134:LEU:HD11	36:m:1:MET:SD	2.49	0.53
35:l:293:ILE:HG13	35:l:418:LEU:HD22	1.89	0.53
16:Q:345:SER:HB2	21:W:19:ILE:HD12	1.91	0.53
2:B:66:LEU:HD13	47:Q:501:PEE:H59	1.91	0.53
26:c:82:SER:OG	26:c:83:GLN:N	2.42	0.53
1:A:211:ALA:HB2	1:A:223:PRO:HG3	1.91	0.53
2:B:94:SER:OG	16:Q:215:GLU:OE2	2.24	0.53
14:O:88:ARG:NH2	14:O:190:ASP:OD2	2.42	0.53
4:E:62:LYS:O	4:E:66:MET:HG2	2.07	0.53
16:Q:79:ASN:HA	16:Q:101:LEU:O	2.08	0.53
26:c:85:GLU:OE1	26:c:120:SER:HA	2.09	0.53
41:s:306:SER:O	41:s:310:MET:HG3	2.08	0.53
1:A:282:VAL:HG13	1:A:356:VAL:HG21	1.90	0.53
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:146:SER:OG	16:Q:118:2MR:O	2.21	0.53
13:N:85:GLU:OE1	13:N:85:GLU:N	2.39	0.53
6:X:119:ILE:HG21	6:X:135:ALA:HB1	1.90	0.53
35:l:362:LEU:HD22	35:l:366:MET:HE2	1.91	0.53
6:G:126:PHE:CE2	6:G:148:ILE:HG12	2.44	0.52
11:L:78:ARG:NH1	11:L:148:GLU:OE2	2.36	0.52
44:w:129:TYR:OH	44:w:186:HIS:ND1	2.35	0.52
3:C:184:ILE:O	3:C:187:GLU:HG2	2.10	0.52
6:G:105:MET:HE2	6:G:105:MET:N	2.23	0.52
23:Z:15:GLU:N	23:Z:15:GLU:OE1	2.43	0.52
2:B:151:LYS:NZ	15:P:228:GLN:OE1	2.41	0.52
20:V:32:THR:O	20:V:36:VAL:HG12	2.10	0.52
26:c:184:TYR:HA	43:v:34:ARG:HH12	1.74	0.52
41:s:24:GLU:OE1	41:s:274:ARG:NH2	2.42	0.52
3:C:167:PRO:CG	16:Q:222:MET:HE2	2.26	0.52
25:b:11:ARG:HE	39:p:154:LEU:HB2	1.73	0.52
9:J:125:VAL:HG22	9:J:163:LYS:HB2	1.90	0.52
19:U:42:ALA:HB2	41:s:312:ALA:HA	1.92	0.52
24:a:127:ASP:O	28:e:112:TYR:OH	2.26	0.52
33:j:73:LEU:O	41:s:160:TYR:OH	2.26	0.52
47:r:501:PEE:H74	47:r:501:PEE:H34	1.92	0.52
25:b:88:TYR:CD2	27:d:49:ARG:HG2	2.45	0.52
46:A:502:FMN:O4'	46:A:502:FMN:O2'	2.19	0.52
22:Y:83:HIS:CE1	43:v:85:HIS:CE1	2.98	0.52
34:k:22:TYR:O	35:l:585:LYS:NZ	2.30	0.52
40:r:22:MET:O	40:r:26:ASN:ND2	2.43	0.52
3:C:175:TYR:HE1	13:N:78:ASP:HB2	1.75	0.52
9:J:135:GLU:OE2	9:J:179:ARG:NH2	2.43	0.52
6:X:155:TYR:CE1	25:b:23:LEU:HB3	2.45	0.52
43:v:18:ASP:O	43:v:22:MET:HG3	2.10	0.52
43:v:110:GLN:O	43:v:114:ARG:HG3	2.10	0.52
15:P:68:ILE:HG22	15:P:69:LEU:HG	1.92	0.51
6:X:94:ASP:OD1	6:X:94:ASP:N	2.42	0.51
40:r:336:ARG:NH2	40:r:433:GLU:OE1	2.43	0.51
36:m:41:CYS:SG	36:m:57:PHE:HD2	2.33	0.51
40:r:282:LEU:O	40:r:286:ILE:HD12	2.10	0.51
7:H:30:LYS:O	7:H:34:VAL:HG12	2.11	0.51
13:N:136:GLU:OE1	13:N:136:GLU:N	2.41	0.51
2:B:179:THR:OG1	2:B:182:GLU:OE2	2.29	0.51
8:I:6:ARG:O	8:I:10:LEU:HG	2.10	0.51
15:P:44:ARG:HB3	15:P:45:PRO:HD2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:554:ASP:OD1	40:r:213:HIS:NE2	2.43	0.51
2:B:62:LEU:HD12	21:W:35:MET:HE3	1.92	0.51
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.92	0.51
11:L:99:MET:HE2	11:L:126:LEU:HD13	1.92	0.51
14:O:132:ILE:HD11	14:O:169:PHE:HD1	1.75	0.51
39:p:119:PHE:O	39:p:123:GLU:HG2	2.11	0.51
44:w:60:ILE:HG12	44:w:203:VAL:HB	1.93	0.51
3:C:127:PRO:HA	9:J:89:TYR:OH	2.11	0.51
9:J:204:SER:OG	9:J:238:GLN:O	2.28	0.51
12:M:70:SER:O	12:M:184:ARG:NH1	2.44	0.51
35:l:83:ASP:OD2	35:l:262:ARG:NH1	2.43	0.51
35:l:78:LEU:HD11	53:r:504:CDL:H251	1.92	0.51
40:r:13:PRO:HB3	53:r:505:CDL:H582	1.92	0.51
41:s:165:LEU:O	41:s:169:GLN:HG3	2.11	0.51
1:A:64:LYS:HG2	1:A:67:GLU:HB2	1.93	0.51
1:A:338:ASP:OD1	1:A:338:ASP:N	2.40	0.51
9:J:249:ILE:O	9:J:253:ILE:HG12	2.10	0.51
26:c:96:ASP:OD1	26:c:97:LEU:N	2.43	0.51
1:A:159:ARG:HD3	1:A:161:GLU:HB2	1.92	0.51
22:Y:71:TRP:CH2	22:Y:75:HIS:HE1	2.26	0.51
3:C:88:ARG:HA	41:s:37:PRO:HA	1.93	0.51
16:Q:172:VAL:HG21	16:Q:310:VAL:CG2	2.29	0.51
16:Q:173:LEU:HD12	16:Q:173:LEU:C	2.36	0.51
22:Y:62:SER:OG	35:l:371:THR:OG1	2.29	0.51
23:Z:25:GLU:HA	23:Z:30:GLU:OE2	2.10	0.51
27:d:99:ASP:OD2	27:d:143:TYR:OH	2.25	0.51
3:C:188:LYS:HD2	3:C:191:ARG:HD2	1.92	0.50
12:M:299:ARG:HD2	12:M:705:GLN:HE21	1.76	0.50
21:W:68:ARG:HD2	36:m:135:PHE:HD2	1.77	0.50
26:c:149:ILE:HG22	26:c:150:TYR:CD1	2.45	0.50
11:L:84:ARG:NH1	11:L:88:GLN:O	2.44	0.50
12:M:512:VAL:O	12:M:514:ASN:ND2	2.44	0.50
27:d:36:ILE:O	27:d:40:LEU:HD23	2.11	0.50
30:g:12:PRO:HB3	31:h:5:ASP:HB3	1.92	0.50
12:M:250:SER:OG	12:M:251:ILE:N	2.44	0.50
12:M:296:GLY:O	12:M:572:HIS:NE2	2.36	0.50
16:Q:146:CYS:SG	16:Q:178:THR:CG2	3.00	0.50
25:b:74:HIS:NE2	35:l:35:TYR:OH	2.28	0.50
32:i:38:LEU:HD12	34:k:73:LEU:HD22	1.93	0.50
40:r:12:LEU:HB2	40:r:13:PRO:HD3	1.94	0.50
1:A:102:MET:HG2	1:A:111:LYS:HE2	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:55:ARG:O	20:V:58:ARG:HG2	2.11	0.50
40:r:433:GLU:O	40:r:437:MET:HG2	2.10	0.50
44:w:65:ASN:OD1	44:w:66:ILE:N	2.41	0.50
4:E:101:THR:O	4:E:105:ARG:HG3	2.12	0.50
20:V:50:LEU:O	20:V:53:VAL:HG12	2.12	0.50
20:V:102:GLY:HA2	20:V:110:ILE:HG23	1.92	0.50
9:J:238:GLN:OE1	9:J:270:ARG:NH1	2.45	0.50
12:M:340:ALA:HB3	12:M:366:LEU:HD23	1.93	0.50
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.92	0.50
35:l:534:HIS:CD2	47:l:703:PEE:H13	2.47	0.50
1:A:277:ASN:N	1:A:277:ASN:ND2	2.60	0.50
30:g:109:LYS:HE3	30:g:114:ILE:HG12	1.93	0.50
33:j:17:LEU:HA	33:j:20:ILE:HG12	1.94	0.50
35:l:298:ILE:O	35:l:302:VAL:HG23	2.12	0.50
12:M:266:ARG:HD2	12:M:267:THR:HG23	1.93	0.50
15:P:69:LEU:O	15:P:73:VAL:HG12	2.12	0.50
15:P:190:ASP:OD1	15:P:191:TYR:N	2.45	0.50
26:c:38:PRO:HB2	38:o:75:ASN:HD22	1.76	0.50
32:i:72:MET:HG3	32:i:97:MET:HE3	1.93	0.50
35:l:418:LEU:HD23	53:l:702:CDL:H562	1.93	0.50
38:o:22:GLU:OE2	38:o:22:GLU:N	2.33	0.50
41:s:75:PRO:HG3	41:s:223:PHE:HE1	1.76	0.50
1:A:394:LYS:HB3	12:M:155:GLU:HG2	1.94	0.50
17:S:59:ARG:HG3	17:S:59:ARG:HH11	1.77	0.50
1:A:217:GLU:OE1	11:L:171:ARG:NH2	2.45	0.49
3:C:113:MET:HE1	16:Q:94:VAL:HG21	1.93	0.49
3:C:167:PRO:HG3	16:Q:222:MET:HE3	1.88	0.49
35:l:327:LEU:O	35:l:331:MET:HG2	2.12	0.49
39:p:26:HIS:CD2	39:p:79:PRO:HB3	2.47	0.49
41:s:85:MET:HE3	41:s:233:MET:HE2	1.94	0.49
16:Q:235:ASP:OD1	16:Q:236:LEU:N	2.44	0.49
21:W:98:MET:HE1	31:h:82:GLN:HB3	1.94	0.49
35:l:107:TYR:HD2	35:l:108:MET:HG2	1.77	0.49
42:u:16:GLN:OE1	42:u:16:GLN:N	2.33	0.49
31:h:105:ARG:NH2	42:u:17:GLU:OE2	2.45	0.49
35:l:190:LEU:HD11	40:r:307:TRP:CH2	2.47	0.49
35:l:250:SER:HB2	35:l:333:ALA:HA	1.94	0.49
1:A:40:ARG:NH1	1:A:289:GLU:O	2.46	0.49
4:E:24:ASP:OD1	4:E:26:ASN:N	2.44	0.49
49:X:201:8Q1:O27	49:X:201:8Q1:O33	2.31	0.49
24:a:96:ALA:HB2	27:d:61:TYR:CE1	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:12:THR:HG21	36:m:163:ILE:HG21	1.94	0.49
36:m:25:SER:O	36:m:27:ILE:N	2.45	0.49
40:r:312:ALA:O	40:r:316:MET:HG3	2.12	0.49
43:v:97:LYS:O	43:v:101:GLU:HG2	2.12	0.49
3:C:169:THR:HG22	16:Q:221:ARG:HD3	1.94	0.49
47:W:201:PEE:H51	36:m:45:LEU:HD13	1.94	0.49
33:j:90:MET:HE1	48:j:201:PLX:H281	1.94	0.49
17:S:43:TYR:CZ	21:W:68:ARG:HG3	2.47	0.49
6:X:123:GLU:OE2	39:p:21:LYS:NZ	2.33	0.49
24:a:96:ALA:HB2	27:d:61:TYR:HE1	1.78	0.49
26:c:100:ASN:N	26:c:103:GLU:OE2	2.33	0.49
40:r:204:MET:HG3	40:r:209:LEU:HB2	1.93	0.49
21:W:63:GLU:OE2	42:u:119:ARG:NH2	2.46	0.49
22:Y:83:HIS:O	22:Y:83:HIS:ND1	2.44	0.49
25:b:69:ILE:O	25:b:73:THR:HG22	2.13	0.49
36:m:1:MET:HE1	36:m:5:ILE:HG22	1.95	0.49
53:N:201:CDL:H512	53:N:201:CDL:H722	1.94	0.49
34:k:23:ARG:HD3	36:m:23:LYS:HB2	1.95	0.49
35:l:482:MET:HE3	35:l:486:MET:HG2	1.95	0.49
39:p:117:ASP:OD1	39:p:117:ASP:N	2.46	0.49
41:s:87:VAL:HG12	41:s:95:LEU:HD23	1.95	0.49
10:K:82:SER:OG	10:K:83:THR:N	2.46	0.49
28:e:97:ILE:O	28:e:101:LEU:HB2	2.13	0.49
33:j:95:LEU:HD13	41:s:302:MET:HG3	1.95	0.49
38:o:102:TYR:HB2	40:r:263:MET:HG3	1.94	0.49
39:p:172:THR:HG23	39:p:172:THR:O	2.13	0.49
40:r:18:SER:OG	40:r:26:ASN:ND2	2.46	0.49
4:E:98:LYS:HB3	4:E:102:HIS:HB2	1.94	0.49
5:F:35:ASP:O	5:F:39:LYS:HG2	2.13	0.49
16:Q:176:GLU:OE2	16:Q:311:TYR:OH	2.26	0.49
39:p:92:GLU:HB3	39:p:95:GLU:HG3	1.95	0.49
3:C:51:ASP:HB2	3:C:190:LEU:HB2	1.94	0.48
9:J:170:LEU:HA	9:J:202:LYS:HB3	1.94	0.48
12:M:408:ARG:HD2	12:M:439:THR:HG23	1.94	0.48
14:O:131:HIS:NE2	14:O:172:ILE:HD12	2.28	0.48
16:Q:242:ASP:O	16:Q:246:GLU:HG2	2.13	0.48
1:A:134:ASP:OD2	1:A:137:LYS:HE2	2.13	0.48
9:J:125:VAL:HG11	9:J:253:ILE:HD12	1.94	0.48
9:J:163:LYS:NZ	9:J:253:ILE:O	2.43	0.48
16:Q:203:MET:HE2	16:Q:258:LEU:HD22	1.94	0.48
32:i:236:LYS:HG2	32:i:237:MET:HG3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:428:PHE:HD1	35:l:432:LEU:HD12	1.78	0.48
44:w:57:SER:O	44:w:156:GLY:HA3	2.12	0.48
1:A:277:ASN:N	1:A:277:ASN:HD22	2.11	0.48
13:N:3:LEU:O	13:N:6:VAL:HG22	2.13	0.48
22:Y:83:HIS:O	22:Y:84:PHE:CD1	2.66	0.48
35:l:159:HIS:ND1	40:r:349:GLN:OE1	2.47	0.48
48:r:503:PLX:H121	48:r:503:PLX:H152	1.54	0.48
4:E:64:ARG:NH1	6:G:117:GLU:OE1	2.46	0.48
5:F:23:LEU:O	5:F:57:GLU:HA	2.13	0.48
16:Q:179:ARG:HD2	16:Q:340:SER:OG	2.14	0.48
30:g:36:MET:HE1	48:g:201:PLX:H382	1.95	0.48
6:G:111:ASP:OD1	6:G:113:LEU:N	2.45	0.48
23:Z:20:LYS:O	23:Z:23:LYS:NZ	2.46	0.48
34:k:23:ARG:HG2	36:m:23:LYS:HE3	1.94	0.48
4:E:70:ASN:HD22	4:E:82:LEU:HD13	1.78	0.48
12:M:29:SER:OG	12:M:30:ASN:N	2.43	0.48
13:N:68:MET:SD	13:N:81:MET:HE3	2.53	0.48
31:h:17:TRP:CZ3	31:h:18:MET:HE2	2.48	0.48
35:l:482:MET:HE2	35:l:487:LYS:HA	1.96	0.48
40:r:130:LEU:HD22	40:r:150:LEU:HD13	1.95	0.48
44:w:123:SER:OG	44:w:125:ASP:OD1	2.23	0.48
1:A:110:PRO:O	1:A:238:CYS:HB3	2.14	0.48
6:G:110:LEU:HB3	6:G:114:ASP:HB2	1.96	0.48
21:W:52:LYS:HD2	21:W:52:LYS:HA	1.65	0.48
32:i:95:MET:HE1	32:i:145:ILE:HD12	1.96	0.48
35:l:119:LYS:NZ	53:r:504:CDL:OA3	2.46	0.48
37:n:27:LEU:HD21	53:u:201:CDL:H112	1.94	0.48
2:B:192:ASN:OD1	18:T:63:ASN:ND2	2.41	0.48
3:C:85:ASP:O	3:C:88:ARG:HG2	2.14	0.48
20:V:85:ASP:HB2	20:V:130:LEU:HD21	1.96	0.48
26:c:117:VAL:HG21	35:l:539:TYR:HB2	1.95	0.48
30:g:12:PRO:HG3	31:h:8:LYS:HD2	1.95	0.48
35:l:227:PHE:O	35:l:230:HIS:ND1	2.45	0.48
39:p:100:PRO:HG3	40:r:419:TYR:CE2	2.48	0.48
40:r:237:LYS:HD2	40:r:316:MET:HB3	1.96	0.48
42:u:106:LYS:O	42:u:109:GLU:HG3	2.13	0.48
15:P:43:THR:HG23	15:P:47:ILE:HB	1.94	0.48
16:Q:259:GLU:OE2	21:W:23:ARG:NH2	2.39	0.48
35:l:310:LEU:HA	35:l:313:MET:HE2	1.95	0.48
15:P:115:THR:HB	16:Q:423:LYS:HE3	1.96	0.48
16:Q:140:ASP:OD2	16:Q:143:SER:OG	2.31	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:46:ASP:N	18:T:46:ASP:OD1	2.41	0.48
29:f:73:ASN:HB3	29:f:75:LEU:HD23	1.96	0.48
34:k:37:MET:HG3	34:k:67:ALA:HB1	1.96	0.48
3:C:133:MET:SD	3:C:173:LEU:HD22	2.54	0.47
15:P:163:ALA:O	15:P:167:GLU:HG3	2.13	0.47
16:Q:99:MET:HE1	16:Q:447:VAL:HG21	1.96	0.47
25:b:121:LYS:HD3	43:v:40:VAL:HA	1.95	0.47
3:C:188:LYS:N	9:J:87:GLU:OE1	2.46	0.47
12:M:511:LYS:HG2	12:M:663:ASN:ND2	2.29	0.47
15:P:75:GLN:HB3	15:P:87:PHE:CD1	2.49	0.47
15:P:154:GLU:OE2	15:P:180:ASN:ND2	2.36	0.47
6:X:87:LEU:HD21	6:X:118:ILE:HG21	1.96	0.47
27:d:37:PHE:CE2	35:l:3:PRO:HB3	2.49	0.47
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.48	0.47
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.96	0.47
35:l:562:LEU:HB3	35:l:563:PRO:HD3	1.96	0.47
38:o:9:SER:OG	38:o:10:ARG:N	2.47	0.47
48:r:502:PLX:H301	48:r:502:PLX:H331	1.65	0.47
43:v:81:LYS:HE2	43:v:81:LYS:HB2	1.63	0.47
6:G:139:MET:HE2	6:G:139:MET:HA	1.96	0.47
16:Q:196:ALA:O	16:Q:197:MET:HG2	2.14	0.47
20:V:96:ALA:O	20:V:100:THR:HG23	2.15	0.47
35:l:176:ARG:HD2	35:l:176:ARG:HA	1.76	0.47
15:P:173:MET:HB3	15:P:198:PHE:HB2	1.95	0.47
19:U:30:ILE:HD11	33:j:96:ILE:HD11	1.96	0.47
32:i:276:ILE:HG21	47:r:501:PEE:H14	1.96	0.47
35:l:249:SER:HB3	35:l:340:PHE:CE2	2.49	0.47
53:r:505:CDL:H401	53:r:505:CDL:H211	1.97	0.47
7:H:83:GLN:HE21	15:P:104:THR:HA	1.80	0.47
11:L:79:ILE:HD13	11:L:134:ALA:HB1	1.97	0.47
12:M:83:GLU:HG3	12:M:103:LEU:HD11	1.95	0.47
24:a:132:ASN:ND2	40:r:49:SER:O	2.39	0.47
35:l:401:MET:SD	35:l:482:MET:HG2	2.54	0.47
16:Q:182:ASN:C	16:Q:182:ASN:ND2	2.73	0.47
1:A:62:TRP:CD2	1:A:181:LEU:HD13	2.50	0.47
1:A:185:ASN:C	1:A:187:CYS:H	2.22	0.47
2:B:93:LEU:O	8:I:34:ARG:NH2	2.46	0.47
9:J:207:PHE:HB2	9:J:214:LEU:HD13	1.96	0.47
53:V:201:CDL:H441	53:V:201:CDL:H191	1.96	0.47
28:e:143:ASP:OD2	28:e:145:ASN:ND2	2.48	0.47
32:i:11:MET:O	32:i:15:SER:OG	2.27	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:44:PHE:HB2	35:l:94:LEU:HB3	1.96	0.47
35:l:559:GLU:O	35:l:563:PRO:HD2	2.14	0.47
35:l:566:THR:O	35:l:570:GLN:HG2	2.14	0.47
37:n:34:LYS:NZ	37:n:34:LYS:HB2	2.30	0.47
38:o:3:PHE:CE2	39:p:70:GLU:HG3	2.50	0.47
3:C:66:THR:HG21	3:C:76:MET:HE2	1.97	0.47
18:T:79:VAL:HG21	18:T:84:ILE:HD13	1.95	0.47
53:a:201:CDL:H191	53:a:201:CDL:H732	1.97	0.47
27:d:73:ASP:OD1	27:d:75:THR:OG1	2.30	0.47
34:k:25:HIS:O	34:k:28:SER:N	2.40	0.47
35:l:15:LEU:HD11	35:l:94:LEU:HD21	1.96	0.47
38:o:103:TYR:O	38:o:107:THR:HG23	2.15	0.47
1:A:170:GLN:HE21	10:K:93:LEU:HD12	1.80	0.47
4:E:31:ARG:O	4:E:34:GLU:HG2	2.15	0.47
7:H:76:GLN:O	7:H:79:GLU:HG2	2.14	0.47
15:P:75:GLN:HB3	15:P:87:PHE:HD1	1.80	0.47
16:Q:142:VAL:HG11	16:Q:185:MET:HG2	1.96	0.47
16:Q:324:GLY:O	16:Q:329:ARG:NH2	2.47	0.47
34:k:60:PRO:O	34:k:63:LEU:HB3	2.15	0.47
39:p:29:SER:HB3	39:p:76:HIS:CD2	2.47	0.47
14:O:149:LEU:O	14:O:153:GLN:HG3	2.15	0.47
47:b:201:PEE:H33	53:r:504:CDL:H241	1.96	0.47
30:g:106:LYS:HZ3	30:g:108:LYS:HA	1.80	0.47
35:l:292:ALA:HB2	35:l:304:PHE:HB3	1.95	0.47
53:l:702:CDL:H382	53:l:702:CDL:H351	1.72	0.47
38:o:113:GLU:OE1	38:o:117:GLN:NE2	2.48	0.47
41:s:96:ILE:HG22	41:s:98:MET:HG3	1.96	0.47
42:u:121:ASP:N	42:u:124:GLU:OE1	2.43	0.47
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	1.96	0.46
31:h:7:GLN:O	31:h:11:GLY:N	2.45	0.46
32:i:270:MET:HE1	32:i:282:MET:HE2	1.96	0.46
41:s:81:LEU:O	41:s:85:MET:HB2	2.15	0.46
1:A:126:LYS:O	1:A:130:ILE:HG23	2.15	0.46
1:A:270:ASN:ND2	1:A:338:ASP:HB2	2.30	0.46
2:B:198:GLU:HG2	13:N:108:TYR:HE1	1.80	0.46
5:F:17:ARG:NH1	12:M:362:ASP:OD1	2.48	0.46
6:X:135:ALA:HA	6:X:138:LEU:HD12	1.96	0.46
40:r:310:MET:HG2	40:r:455:LEU:O	2.15	0.46
3:C:66:THR:HG21	3:C:76:MET:HG3	1.97	0.46
8:I:70:MET:HE3	8:I:70:MET:O	2.15	0.46
27:d:142:ARG:HB3	27:d:143:TYR:CD1	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:90:ILE:HD13	35:l:129:MET:SD	2.55	0.46
40:r:243:MET:HA	40:r:246:ILE:HG22	1.96	0.46
2:B:76:TYR:HE1	41:s:33:LEU:HD13	1.80	0.46
12:M:64:CYS:O	12:M:184:ARG:NH2	2.33	0.46
12:M:535:GLU:OE1	12:M:535:GLU:HA	2.15	0.46
28:e:76:TYR:HB2	28:e:83:ASP:OD1	2.16	0.46
30:g:36:MET:HE2	32:i:339:MET:HE2	1.97	0.46
33:j:73:LEU:HD13	36:m:55:MET:HE1	1.96	0.46
35:l:127:THR:HG21	35:l:146:GLY:HA3	1.98	0.46
36:m:124:ASP:OD1	36:m:124:ASP:N	2.46	0.46
40:r:14:MET:SD	40:r:26:ASN:HB3	2.56	0.46
53:r:504:CDL:H611	53:r:504:CDL:H581	1.68	0.46
12:M:646:LEU:HD22	12:M:653:LEU:HD12	1.98	0.46
15:P:109:LYS:HD3	15:P:109:LYS:HA	1.68	0.46
32:i:236:LYS:HE2	44:w:302:LEU:HD11	1.98	0.46
35:l:161:ARG:HA	39:p:92:GLU:HB2	1.97	0.46
39:p:28:GLU:HB2	39:p:37:TYR:CE1	2.51	0.46
40:r:48:ASN:OD1	40:r:48:ASN:N	2.47	0.46
42:u:38:LYS:HB3	42:u:39:PRO:HD3	1.97	0.46
1:A:104:LYS:HE3	1:A:104:LYS:HB2	1.80	0.46
2:B:158:CYS:HB3	45:B:302:SF4:S2	2.55	0.46
10:K:89:LEU:O	10:K:93:LEU:HG	2.15	0.46
17:S:42:SER:O	17:S:42:SER:OG	2.33	0.46
22:Y:93:THR:HG1	22:Y:96:GLU:CD	2.22	0.46
24:a:108:GLU:N	24:a:111:GLU:OE2	2.43	0.46
33:j:90:MET:SD	36:m:151:THR:HG23	2.56	0.46
40:r:98:MET:HG3	40:r:128:PRO:HB3	1.96	0.46
13:N:14:VAL:HG23	13:N:23:TYR:CG	2.51	0.46
20:V:35:ILE:HG21	53:V:201:CDL:H781	1.97	0.46
22:Y:80:VAL:HG23	35:l:385:TYR:OH	2.16	0.46
22:Y:92:TRP:CE2	43:v:100:LYS:HE3	2.51	0.46
33:j:69:ILE:HD11	41:s:144:VAL:HG13	1.96	0.46
40:r:318:ALA:HB1	40:r:374:ASN:OD1	2.16	0.46
53:r:505:CDL:H241	53:r:505:CDL:H812	1.97	0.46
3:C:144:HIS:O	3:C:151:ARG:NH1	2.48	0.46
15:P:119:VAL:HB	15:P:122:ARG:HD2	1.98	0.46
16:Q:36:GLN:NE2	40:r:135:ARG:O	2.46	0.46
34:k:23:ARG:HG3	34:k:24:SER:H	1.81	0.46
35:l:150:MET:HE1	53:r:504:CDL:H112	1.97	0.46
40:r:382:ILE:HD12	40:r:396:MET:HB3	1.98	0.46
1:A:48:ARG:NH1	10:K:70:ASN:O	2.40	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:TRP:O	3:C:60:SER:HB2	2.15	0.46
12:M:544:VAL:HG23	12:M:565:PHE:HB3	1.98	0.46
16:Q:293:LEU:HD22	16:Q:298:ILE:HD12	1.98	0.46
25:b:19:ARG:NE	39:p:173:ARG:HH21	2.14	0.46
35:l:332:HIS:HA	35:l:335:PHE:CZ	2.51	0.46
40:r:240:GLY:O	40:r:244:MET:HG3	2.16	0.46
8:I:58:ASP:OD2	8:I:61:ARG:HB2	2.16	0.46
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.98	0.46
16:Q:174:PHE:CE1	16:Q:217:VAL:HG11	2.51	0.46
16:Q:179:ARG:NH2	16:Q:401:GLU:O	2.44	0.46
16:Q:261:MET:HE3	16:Q:261:MET:HB3	1.82	0.46
47:Q:501:PEE:H22	41:s:180:PRO:HB3	1.97	0.46
20:V:88:LEU:O	20:V:92:ILE:HG12	2.16	0.46
33:j:3:ILE:HA	33:j:6:THR:HG22	1.98	0.46
40:r:14:MET:HE2	40:r:30:HIS:ND1	2.31	0.46
3:C:82:PRO:HG3	16:Q:201:PHE:HB3	1.98	0.45
15:P:87:PHE:CE2	15:P:144:LYS:HE3	2.51	0.45
21:W:120:MET:SD	31:h:69:ARG:HD2	2.56	0.45
34:k:22:TYR:HE2	35:l:588:PHE:CD2	2.34	0.45
10:K:87:LEU:HB3	14:O:62:ARG:HG2	1.98	0.45
13:N:132:LYS:NZ	13:N:135:GLN:OE1	2.46	0.45
6:X:137:LYS:HD3	25:b:4:TYR:CE1	2.51	0.45
32:i:118:VAL:O	32:i:122:ILE:HG12	2.17	0.45
53:i:401:CDL:H142	53:i:401:CDL:H171	1.69	0.45
35:l:200:GLN:HG3	35:l:204:LEU:HD23	1.97	0.45
36:m:51:PHE:CD1	36:m:143:ILE:HD13	2.51	0.45
3:C:79:MET:HE2	3:C:86:MET:CB	2.46	0.45
6:G:148:ILE:HD12	6:G:148:ILE:H	1.81	0.45
9:J:172:ALA:HA	9:J:181:LEU:HB3	1.99	0.45
12:M:461:PRO:O	12:M:465:ILE:HG23	2.16	0.45
16:Q:237:PRO:HD2	16:Q:240:LEU:HD22	1.98	0.45
30:g:109:LYS:HB3	30:g:114:ILE:HD11	1.98	0.45
48:g:201:PLX:H131	48:g:201:PLX:H102	1.40	0.45
32:i:112:HIS:CE1	32:i:164:ILE:HG21	2.50	0.45
33:j:49:LEU:N	33:j:50:PRO:HD2	2.31	0.45
36:m:173:ARG:HG3	36:m:173:ARG:HH11	1.81	0.45
44:w:86:PHE:HB2	44:w:159:LEU:HD23	1.97	0.45
3:C:110:THR:OG1	16:Q:115:LEU:O	2.28	0.45
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.52	0.45
16:Q:242:ASP:OD1	21:W:16:TYR:OH	2.29	0.45
23:Z:32:VAL:HG13	39:p:39:TYR:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:452:ASN:HA	35:l:455:LYS:HG2	1.98	0.45
38:o:82:PRO:HB2	53:o:201:CDL:HB61	1.99	0.45
39:p:100:PRO:HG3	40:r:419:TYR:CZ	2.50	0.45
48:C:303:PLX:H31	13:N:75:TRP:CD2	2.51	0.45
12:M:331:GLN:NE2	12:M:630:ALA:O	2.47	0.45
25:b:25:ASP:OD2	39:p:125:TRP:NE1	2.38	0.45
35:l:237:MET:SD	35:l:237:MET:N	2.89	0.45
5:F:64:LYS:NZ	5:F:76:ASN:OD1	2.32	0.45
47:Q:501:PEE:H13	41:s:293:PHE:HE1	1.81	0.45
25:b:86:LEU:O	25:b:91:THR:HG22	2.16	0.45
40:r:266:MET:HE3	40:r:395:LEU:HD12	1.98	0.45
2:B:153:ILE:HG12	45:B:302:SF4:S3	2.57	0.45
3:C:133:MET:HG2	3:C:168:PRO:HG2	1.98	0.45
14:O:197:THR:OG1	14:O:200:ASP:OD2	2.32	0.45
22:Y:78:ASP:HB3	22:Y:83:HIS:HD2	1.82	0.45
27:d:125:CYS:HB2	35:l:203:MET:HE1	1.99	0.45
34:k:14:ILE:HD13	36:m:18:VAL:HG22	1.98	0.45
35:l:83:ASP:OD1	35:l:85:PHE:N	2.49	0.45
40:r:166:TYR:O	40:r:170:THR:HG23	2.17	0.45
40:r:281:ASP:OD1	40:r:282:LEU:N	2.49	0.45
53:u:201:CDL:H171	53:u:201:CDL:H201	1.80	0.45
43:v:77:PHE:CE1	43:v:78:LEU:HD23	2.52	0.45
12:M:126:LEU:O	18:T:113:TYR:OH	2.26	0.45
16:Q:158:LEU:HD12	16:Q:411:LEU:HD23	1.97	0.45
16:Q:215:GLU:C	16:Q:215:GLU:CD	2.85	0.45
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.98	0.45
21:W:98:MET:HG3	21:W:104:TRP:CE2	2.51	0.45
35:l:296:ASN:HD22	35:l:357:ARG:CZ	2.30	0.45
53:o:201:CDL:H752	53:o:201:CDL:H721	1.58	0.45
3:C:82:PRO:HB3	41:s:33:LEU:O	2.17	0.45
12:M:260:ASN:HD21	12:M:278:HIS:CD2	2.35	0.45
15:P:108:PHE:HA	15:P:134:SER:HB2	1.99	0.45
16:Q:180:LEU:CB	16:Q:210:MET:HE1	2.47	0.45
16:Q:244:ILE:HG22	16:Q:348:LEU:HD11	1.98	0.45
6:X:146:ASP:OD2	25:b:16:ARG:NH1	2.50	0.45
26:c:58:ARG:HB2	26:c:61:ASP:HB2	1.98	0.45
30:g:51:ARG:HB2	30:g:53:ARG:HG3	1.99	0.45
35:l:184:LEU:HB2	40:r:393:ILE:HG12	1.99	0.45
39:p:76:HIS:O	39:p:78:GLN:N	2.50	0.45
42:u:18:VAL:HG12	42:u:20:VAL:HG22	1.99	0.45
2:B:43:MET:HA	2:B:43:MET:HE2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:105:MET:HE3	6:G:139:MET:SD	2.57	0.45
12:M:367:CYS:HB3	12:M:533:GLY:O	2.17	0.45
16:Q:181:LEU:CD2	16:Q:210:MET:HB2	2.47	0.45
32:i:128:LEU:HD12	32:i:216:PHE:HB3	1.99	0.45
40:r:256:TYR:O	40:r:256:TYR:CD1	2.70	0.45
41:s:92:PRO:HB3	41:s:255:TYR:CD2	2.52	0.45
44:w:239:ASN:HB2	44:w:243:LYS:HZ2	1.82	0.45
1:A:392:MET:HE3	1:A:435:VAL:HG21	1.99	0.44
10:K:100:GLN:HB3	14:O:71:PRO:HA	1.99	0.44
12:M:519:ILE:HG13	12:M:522:GLN:HB2	2.00	0.44
21:W:98:MET:HG3	21:W:104:TRP:CD1	2.52	0.44
24:a:52:LYS:HE2	24:a:52:LYS:HA	1.97	0.44
26:c:93:ASP:OD1	38:o:44:LYS:NZ	2.39	0.44
41:s:179:TRP:O	41:s:183:MET:HG3	2.18	0.44
42:u:83:THR:HA	42:u:86:TRP:NE1	2.31	0.44
10:K:88:ASP:O	10:K:91:VAL:HG12	2.17	0.44
12:M:260:ASN:HD21	12:M:278:HIS:HD2	1.66	0.44
12:M:277:MET:HE3	12:M:277:MET:HB3	1.88	0.44
12:M:466:LEU:HD11	12:M:500:ILE:HD11	1.99	0.44
13:N:44:TYR:OH	13:N:113:HIS:N	2.34	0.44
21:W:129:THR:HG22	21:W:132:GLU:HG2	1.98	0.44
6:X:69:SER:OG	6:X:70:ASP:N	2.49	0.44
32:i:112:HIS:HB2	32:i:184:ILE:HD13	1.98	0.44
47:i:402:PEE:H42	47:i:402:PEE:H35	1.79	0.44
41:s:76:ILE:O	41:s:80:SER:OG	2.24	0.44
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.99	0.44
3:C:191:ARG:HD3	3:C:195:ARG:NH2	2.32	0.44
6:G:105:MET:HE3	6:G:139:MET:HE1	1.99	0.44
12:M:371:VAL:HG12	12:M:533:GLY:HA2	1.98	0.44
32:i:62:THR:HG21	32:i:114:TRP:CD1	2.52	0.44
32:i:246:VAL:HG11	53:r:505:CDL:H392	1.98	0.44
44:w:59:VAL:HG13	44:w:201:PRO:HA	1.99	0.44
3:C:101:ASP:OD2	41:s:54:LYS:HD2	2.18	0.44
7:H:44:TYR:CD2	7:H:94:MET:HG2	2.52	0.44
12:M:459:ASN:N	12:M:459:ASN:OD1	2.51	0.44
19:U:55:VAL:HG21	24:a:183:PRO:HG3	1.99	0.44
49:X:201:8Q1:C30	39:p:52:LYS:HG3	2.47	0.44
34:k:11:ALA:HB1	36:m:17:PHE:CD2	2.53	0.44
53:u:201:CDL:H521	53:u:201:CDL:H551	1.59	0.44
4:E:110:THR:HG21	15:P:220:VAL:HG11	1.99	0.44
19:U:38:TYR:HB2	41:s:310:MET:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:n:52:ASN:OD1	37:n:52:ASN:N	2.49	0.44
44:w:279:ASP:OD1	44:w:279:ASP:N	2.48	0.44
1:A:277:ASN:HD22	1:A:277:ASN:H	1.66	0.44
9:J:140:ASP:OD1	9:J:140:ASP:N	2.36	0.44
12:M:33:GLU:HB2	12:M:42:MET:HE1	2.00	0.44
17:S:34:LYS:NZ	17:S:61:HIS:O	2.49	0.44
25:b:93:LYS:HD3	25:b:93:LYS:N	2.32	0.44
26:c:62:TYR:OH	26:c:74:ASP:OD1	2.26	0.44
33:j:101:SER:OG	36:m:165:VAL:HG21	2.18	0.44
3:C:85:ASP:OD2	41:s:34:ARG:HD2	2.18	0.44
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.52	0.44
16:Q:325:ASP:OD1	16:Q:325:ASP:N	2.49	0.44
53:V:201:CDL:H322	53:V:201:CDL:H352	1.40	0.44
35:l:7:LEU:HD22	35:l:46:LEU:HD11	1.99	0.44
36:m:25:SER:O	36:m:28:TYR:N	2.49	0.44
40:r:82:SER:OG	40:r:335:GLU:OE1	2.33	0.44
44:w:88:GLU:OE2	44:w:161:ARG:NH1	2.51	0.44
1:A:116:ASN:HD22	1:A:116:ASN:HA	1.71	0.44
5:F:26:ARG:HA	5:F:26:ARG:NE	2.33	0.44
32:i:96:THR:O	32:i:100:MET:HG2	2.17	0.44
33:j:55:PHE:O	33:j:58:VAL:HG12	2.17	0.44
36:m:51:PHE:HD2	41:s:100:LEU:HD21	1.83	0.44
39:p:108:HIS:ND1	39:p:110:SER:HB3	2.32	0.44
6:X:115:GLN:HA	6:X:118:ILE:HD12	2.00	0.44
22:Y:97:LEU:O	43:v:104:ARG:HG3	2.18	0.44
31:h:76:LEU:HD23	31:h:76:LEU:HA	1.88	0.44
53:r:504:CDL:H551	53:r:504:CDL:H582	1.81	0.44
4:E:24:ASP:OD1	4:E:24:ASP:C	2.61	0.43
9:J:87:GLU:HG3	9:J:89:TYR:H	1.83	0.43
12:M:275:PRO:HB3	12:M:286:ILE:HG23	1.99	0.43
12:M:669:ASN:O	12:M:673:LYS:HG3	2.18	0.43
13:N:78:ASP:OD1	13:N:78:ASP:N	2.51	0.43
21:W:144:THR:HB	41:s:96:ILE:HG23	1.98	0.43
53:o:201:CDL:H841	53:o:201:CDL:H872	1.77	0.43
53:r:505:CDL:H792	53:r:505:CDL:H761	1.90	0.43
43:v:15:LYS:HZ2	43:v:110:GLN:HE22	1.66	0.43
44:w:72:ARG:O	44:w:76:GLU:HG3	2.18	0.43
2:B:200:GLU:HG3	13:N:88:ARG:HB2	2.00	0.43
16:Q:194:ILE:HG22	41:s:278:PRO:HB3	2.00	0.43
6:X:91:ASP:HB3	23:Z:47:ARG:HH12	1.82	0.43
6:X:138:LEU:HD23	6:X:143:GLU:HG3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:174:TYR:CD2	35:l:232:TRP:HB3	2.53	0.43
40:r:447:LEU:HD11	48:r:503:PLX:H371	2.00	0.43
44:w:114:LEU:HD21	56:w:401:ADP:H1'	2.00	0.43
11:L:116:SER:OG	15:P:227:ALA:O	2.28	0.43
12:M:638:THR:O	12:M:642:VAL:HG23	2.18	0.43
17:S:1:MET:HB2	17:S:3:PHE:CZ	2.52	0.43
23:Z:78:PHE:O	23:Z:82:VAL:HG23	2.18	0.43
27:d:117:GLU:HG3	27:d:124:ASN:HB2	2.00	0.43
30:g:7:ARG:NH1	30:g:91:ASP:OD1	2.51	0.43
32:i:278:MET:HB2	32:i:279:PRO:HD3	2.00	0.43
35:l:154:LEU:HD13	35:l:243:VAL:HG22	1.99	0.43
35:l:214:ILE:HG12	35:l:276:MET:HE1	2.00	0.43
35:l:331:MET:HB3	35:l:387:THR:HG22	1.99	0.43
40:r:19:LYS:HB3	40:r:19:LYS:HE2	1.71	0.43
44:w:88:GLU:OE2	44:w:139:ARG:NH2	2.47	0.43
1:A:329:LYS:O	1:A:333:GLU:HG2	2.18	0.43
5:F:26:ARG:HH11	5:F:26:ARG:HG2	1.82	0.43
6:G:111:ASP:OD1	6:G:111:ASP:C	2.62	0.43
6:G:134:ASP:OD1	6:G:134:ASP:C	2.61	0.43
15:P:204:LEU:HD11	16:Q:123:LEU:HD23	2.01	0.43
16:Q:210:MET:HE3	16:Q:247:PHE:HZ	1.83	0.43
26:c:160:GLN:HB3	26:c:183:HIS:CD2	2.54	0.43
27:d:142:ARG:NE	28:e:138:GLU:O	2.51	0.43
48:j:201:PLX:H372	48:j:201:PLX:H342	1.87	0.43
35:l:233:LEU:HB3	35:l:234:PRO:HD3	1.99	0.43
39:p:82:PHE:HB2	39:p:85:SER:OG	2.18	0.43
7:H:76:GLN:O	7:H:79:GLU:N	2.51	0.43
14:O:141:MET:HE2	14:O:141:MET:HB3	1.94	0.43
22:Y:72:ARG:HB3	35:l:385:TYR:CD2	2.53	0.43
26:c:140:MET:HE1	35:l:286:LEU:HD23	2.00	0.43
29:f:47:THR:HG23	30:g:65:LEU:HD22	2.00	0.43
48:g:201:PLX:H1C3	48:g:201:PLX:H22	1.71	0.43
32:i:13:VAL:HG13	32:i:36:ASN:ND2	2.33	0.43
41:s:219:PRO:HA	41:s:222:MET:HG2	2.00	0.43
33:j:109:LYS:HA	33:j:109:LYS:HD3	1.91	0.43
35:l:221:ALA:HA	35:l:226:GLN:HG2	2.01	0.43
38:o:101:TRP:HB3	40:r:263:MET:HE2	2.00	0.43
43:v:103:GLU:OE2	43:v:103:GLU:HA	2.17	0.43
44:w:110:GLY:HA2	44:w:134:TRP:CD2	2.54	0.43
44:w:180:ARG:NH1	44:w:316:GLU:OE2	2.49	0.43
6:G:119:ILE:O	6:G:122:MET:HB2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:33:LYS:HD2	8:I:33:LYS:N	2.33	0.43
21:W:73:PRO:HG2	42:u:40:ASN:HB3	2.01	0.43
22:Y:87:PRO:HD2	43:v:99:MET:HE1	2.01	0.43
23:Z:18:ASP:OD1	23:Z:18:ASP:C	2.61	0.43
27:d:77:CYS:SG	27:d:85:MET:HG3	2.58	0.43
30:g:87:LEU:HD23	30:g:87:LEU:HA	1.87	0.43
31:h:7:GLN:HG2	31:h:14:LEU:HD12	2.00	0.43
32:i:211:MET:HE3	32:i:251:MET:HA	2.01	0.43
53:o:201:CDL:H582	53:o:201:CDL:H742	2.00	0.43
44:w:165:SER:HB3	44:w:245:PHE:CE1	2.53	0.43
1:A:165:GLU:H	1:A:165:GLU:CD	2.25	0.43
53:N:201:CDL:H511	53:N:201:CDL:H542	1.90	0.43
6:X:133:ILE:HD11	39:p:6:PRO:HA	2.01	0.43
33:j:81:THR:C	33:j:83:ASN:H	2.27	0.43
34:k:7:ASN:HD22	36:m:10:SER:HB2	1.84	0.43
35:l:260:LEU:HD22	35:l:267:MET:HE3	2.00	0.43
53:l:702:CDL:H622	53:l:702:CDL:H591	1.52	0.43
36:m:3:MET:O	36:m:3:MET:HG3	2.19	0.43
40:r:118:PHE:O	40:r:122:PHE:HB3	2.19	0.43
42:u:55:ARG:HA	42:u:55:ARG:HD3	1.84	0.43
44:w:180:ARG:NH2	44:w:182:GLN:OE1	2.51	0.43
2:B:141:ARG:HA	2:B:141:ARG:HD3	1.80	0.43
3:C:148:SER:OG	16:Q:117:HIS:O	2.32	0.43
6:G:99:SER:H	6:G:102:SER:HB3	1.83	0.43
12:M:391:ILE:HG13	12:M:600:GLU:CD	2.44	0.43
16:Q:184:ILE:HG12	16:Q:203:MET:HE3	2.01	0.43
6:X:105:MET:HE1	6:X:112:SER:HA	2.01	0.43
39:p:64:LEU:HA	39:p:67:ALA:HB3	2.01	0.43
40:r:207:MET:SD	40:r:240:GLY:N	2.92	0.43
1:A:223:PRO:O	1:A:381:GLN:NE2	2.52	0.43
2:B:66:LEU:HB3	41:s:277:TYR:OH	2.18	0.43
2:B:140:ARG:O	2:B:141:ARG:NH1	2.41	0.43
16:Q:182:ASN:OD1	16:Q:404:LYS:NZ	2.50	0.43
25:b:106:PRO:HG2	25:b:120:MET:SD	2.59	0.43
35:l:294:THR:O	35:l:294:THR:OG1	2.36	0.43
44:w:147:LEU:HD23	44:w:147:LEU:HA	1.89	0.43
1:A:141:GLY:HA3	1:A:248:VAL:O	2.19	0.42
7:H:103:LEU:HD23	7:H:104:VAL:N	2.34	0.42
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.48	0.42
12:M:650:SER:OG	12:M:652:ASN:OD1	2.27	0.42
28:e:119:ARG:O	28:e:123:GLU:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:g:201:PLX:H311	48:g:201:PLX:H341	1.67	0.42
35:l:88:MET:HE2	35:l:468:ILE:HD13	2.01	0.42
35:l:346:ILE:HD11	35:l:431:PHE:CZ	2.54	0.42
9:J:168:SER:O	9:J:202:LYS:HA	2.19	0.42
10:K:92:GLU:C	10:K:92:GLU:OE1	2.62	0.42
12:M:306:MET:HE3	12:M:316:TYR:CE1	2.54	0.42
20:V:61:PHE:HD2	20:V:104:ARG:HH21	1.66	0.42
27:d:28:ASN:HD21	27:d:31:THR:HG23	1.84	0.42
33:j:54:LYS:HD3	33:j:113:TRP:HA	2.00	0.42
33:j:68:GLU:HG2	36:m:161:LEU:HD13	2.00	0.42
33:j:95:LEU:HB3	41:s:302:MET:HE2	2.01	0.42
37:n:50:ARG:HB2	37:n:53:GLU:HB3	2.00	0.42
41:s:129:LEU:O	41:s:133:LEU:HG	2.19	0.42
9:J:169:HIS:H	9:J:184:LYS:HE3	1.85	0.42
14:O:198:PRO:HA	14:O:201:ILE:HG22	2.01	0.42
30:g:47:ASP:O	30:g:51:ARG:HG2	2.20	0.42
32:i:222:SER:O	32:i:224:ALA:N	2.53	0.42
35:l:83:ASP:OD1	35:l:83:ASP:C	2.62	0.42
35:l:338:MET:HE3	35:l:461:SER:HB3	2.01	0.42
43:v:15:LYS:NZ	43:v:110:GLN:HE22	2.16	0.42
1:A:244:ASN:OD1	1:A:245:VAL:N	2.49	0.42
2:B:38:TYR:CZ	8:I:106:LEU:HD13	2.54	0.42
12:M:301:ARG:HD2	12:M:301:ARG:HA	1.73	0.42
14:O:140:CYS:O	14:O:145:SER:HB2	2.19	0.42
14:O:234:LEU:HD13	14:O:234:LEU:HA	1.87	0.42
19:U:14:ALA:O	19:U:15:LYS:HG2	2.19	0.42
26:c:179:GLU:OE2	26:c:179:GLU:N	2.52	0.42
26:c:184:TYR:HA	43:v:34:ARG:NH1	2.34	0.42
28:e:57:GLU:OE1	44:w:320:GLY:HA3	2.19	0.42
33:j:94:LEU:HD12	36:m:147:TYR:HE1	1.85	0.42
53:r:504:CDL:H312	53:r:504:CDL:H761	2.00	0.42
53:r:504:CDL:H572	53:r:504:CDL:H871	2.00	0.42
44:w:132:GLN:NE2	44:w:166:ASP:OD1	2.52	0.42
1:A:385:CYS:O	1:A:389:VAL:HB	2.20	0.42
1:A:388:GLY:HA3	1:A:419:ILE:HD11	2.01	0.42
3:C:125:PRO:HG3	41:s:61:LEU:HD11	2.01	0.42
3:C:139:GLY:O	3:C:144:HIS:ND1	2.45	0.42
7:H:106:GLU:OE2	7:H:106:GLU:HA	2.20	0.42
9:J:83:PRO:HG3	9:J:119:VAL:HG11	2.02	0.42
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.83	0.42
22:Y:43:ARG:HH21	22:Y:49:GLN:HG2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:167:TYR:CD2	26:c:178:PRO:HG3	2.54	0.42
27:d:9:VAL:HG13	27:d:10:TYR:CD2	2.54	0.42
34:k:81:VAL:O	34:k:84:THR:HG22	2.19	0.42
37:n:7:ILE:O	37:n:11:HIS:N	2.52	0.42
40:r:127:VAL:HB	40:r:128:PRO:HD3	2.00	0.42
40:r:412:ILE:HA	40:r:416:ARG:HG2	2.02	0.42
41:s:70:MET:HA	41:s:73:ILE:HB	2.01	0.42
3:C:65:MET:O	3:C:65:MET:HG3	2.20	0.42
3:C:79:MET:HE2	3:C:86:MET:HB3	2.02	0.42
3:C:113:MET:HE2	16:Q:94:VAL:HG11	2.02	0.42
4:E:109:GLU:OE1	15:P:218:ARG:NH2	2.36	0.42
8:I:92:LYS:HD2	8:I:92:LYS:HA	1.91	0.42
11:L:163:ASN:O	11:L:171:ARG:HA	2.19	0.42
12:M:559:ASP:OD1	12:M:559:ASP:N	2.35	0.42
16:Q:270:ASN:HB3	41:s:284:GLN:NE2	2.34	0.42
26:c:155:PRO:HG3	43:v:4:HIS:CE1	2.54	0.42
32:i:179:MET:HE3	32:i:179:MET:HB3	1.92	0.42
48:r:502:PLX:H1C3	48:r:502:PLX:H22	1.74	0.42
41:s:143:GLU:HA	41:s:146:LEU:HB2	2.01	0.42
53:u:201:CDL:H712	53:u:201:CDL:H741	1.46	0.42
1:A:402:GLY:HA2	1:A:450:MET:HG2	2.02	0.42
7:H:59:VAL:HG23	7:H:68:LEU:HD21	2.01	0.42
12:M:498:GLN:HB2	12:M:669:ASN:ND2	2.35	0.42
13:N:68:MET:HG2	13:N:69:ASN:H	1.85	0.42
16:Q:226:TYR:OH	16:Q:234:GLN:O	2.30	0.42
21:W:30:LEU:HD12	21:W:30:LEU:HA	1.82	0.42
26:c:149:ILE:O	26:c:151:PRO:HD3	2.19	0.42
32:i:234:TRP:CH2	32:i:304:MET:HE3	2.54	0.42
39:p:63:LEU:C	39:p:65:ARG:H	2.26	0.42
44:w:143:TYR:OH	44:w:199:LEU:O	2.30	0.42
44:w:239:ASN:HB2	44:w:243:LYS:NZ	2.34	0.42
1:A:85:LEU:HD23	1:A:95:THR:HG21	2.02	0.42
8:I:97:PRO:HD3	15:P:61:PHE:CE1	2.55	0.42
9:J:73:LEU:O	9:J:78:SER:OG	2.34	0.42
16:Q:174:PHE:CZ	16:Q:217:VAL:HG11	2.55	0.42
27:d:127:LYS:HE3	27:d:127:LYS:HB3	1.82	0.42
28:e:90:VAL:HG22	40:r:28:THR:HG21	2.02	0.42
32:i:170:LEU:HD13	47:i:402:PEE:H48	2.02	0.42
32:i:258:SER:HB2	32:i:336:VAL:HG12	2.02	0.42
33:j:53:MET:HE2	33:j:53:MET:HB2	1.89	0.42
36:m:25:SER:HB3	36:m:28:TYR:HD2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:186:LEU:HD13	40:r:249:ILE:O	2.19	0.42
41:s:195:ARG:HD3	41:s:231:ILE:CD1	2.49	0.42
47:C:302:PEE:H26	47:C:302:PEE:H20	1.78	0.42
48:C:303:PLX:H141	41:s:49:ILE:HG21	2.02	0.42
6:G:103:HIS:ND1	6:G:106:LYS:HG2	2.35	0.42
7:H:72:LEU:HD13	7:H:80:VAL:HG11	2.01	0.42
12:M:144:MET:HG3	16:Q:383:LYS:HG3	2.00	0.42
16:Q:271:ARG:HD2	16:Q:271:ARG:HA	1.80	0.42
6:X:87:LEU:HD23	6:X:87:LEU:HA	1.74	0.42
32:i:45:MET:HE2	32:i:45:MET:HB3	1.90	0.42
34:k:61:ILE:HD11	36:m:51:PHE:HE1	1.85	0.42
35:l:24:SER:OG	35:l:25:ASN:N	2.52	0.42
35:l:226:GLN:OE1	35:l:284:THR:HG21	2.20	0.42
35:l:336:LYS:HA	35:l:336:LYS:HD3	1.81	0.42
1:A:174:ARG:HB2	10:K:93:LEU:HD21	2.02	0.42
5:F:69:TYR:HE2	5:F:75:LYS:HG2	1.85	0.42
16:Q:116:LEU:O	16:Q:118:2MR:HD3	2.19	0.42
6:X:77:GLU:OE1	6:X:77:GLU:N	2.43	0.42
24:a:78:THR:OG1	28:e:96:SER:HB3	2.20	0.42
26:c:149:ILE:HD13	26:c:149:ILE:HA	1.83	0.42
28:e:58:ASP:OD2	44:w:326:ARG:NE	2.50	0.42
32:i:13:VAL:HG13	32:i:36:ASN:HD21	1.85	0.42
40:r:257:MET:O	40:r:257:MET:HG3	2.20	0.42
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.55	0.41
3:C:51:ASP:OD1	3:C:55:ASN:ND2	2.53	0.41
27:d:80:LYS:HA	27:d:80:LYS:HD3	1.79	0.41
35:l:144:TRP:CE2	35:l:223:LYS:HD2	2.55	0.41
35:l:268:GLU:H	35:l:268:GLU:HG3	1.60	0.41
39:p:108:HIS:CD2	39:p:109:PRO:HD2	2.55	0.41
1:A:156:ILE:HB	1:A:197:VAL:HG22	2.02	0.41
7:H:116:ILE:HG13	15:P:121:THR:HG21	2.02	0.41
20:V:46:PRO:HB3	20:V:55:ARG:NH2	2.35	0.41
21:W:130:ASN:HD22	21:W:130:ASN:C	2.27	0.41
24:a:95:GLU:OE2	27:d:56:HIS:ND1	2.44	0.41
25:b:86:LEU:HD11	35:l:9:LEU:HD12	2.01	0.41
27:d:127:LYS:HG2	27:d:131:GLN:HE21	1.85	0.41
30:g:108:LYS:HA	30:g:108:LYS:HD3	1.68	0.41
32:i:54:GLU:O	32:i:57:THR:HG22	2.20	0.41
35:l:174:TYR:CD1	35:l:229:LEU:HB3	2.54	0.41
40:r:71:TRP:O	40:r:74:PRO:HD2	2.20	0.41
44:w:192:LYS:HG3	44:w:193:VAL:N	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:TRP:HE1	1:A:333:GLU:CD	2.28	0.41
5:F:41:TYR:CD1	5:F:41:TYR:C	2.98	0.41
7:H:28:TYR:OH	7:H:55:LYS:HD3	2.19	0.41
11:L:89:SER:O	12:M:59:GLN:NE2	2.51	0.41
12:M:167:PRO:HD2	12:M:215:MET:HE1	2.02	0.41
12:M:474:VAL:O	12:M:514:ASN:HB2	2.20	0.41
21:W:51:MET:HE3	21:W:51:MET:HB2	1.92	0.41
23:Z:52:ARG:HD2	39:p:34:ARG:HG3	2.01	0.41
32:i:340:THR:N	32:i:341:PRO:HD2	2.35	0.41
35:l:428:PHE:CD1	35:l:432:LEU:HD12	2.55	0.41
35:l:551:SER:HA	35:l:555:LEU:HB2	2.02	0.41
40:r:122:PHE:HE1	40:r:206:LYS:HD2	1.85	0.41
42:u:152:PRO:C	42:u:153:GLU:HG3	2.46	0.41
44:w:210:PRO:O	44:w:214:ILE:HG22	2.20	0.41
1:A:64:LYS:HD2	14:O:249:LEU:HD23	2.02	0.41
9:J:37:HIS:O	9:J:40:LEU:HG	2.20	0.41
15:P:119:VAL:HG12	15:P:121:THR:HG22	2.02	0.41
16:Q:95:LEU:HD22	16:Q:458:PHE:HZ	1.84	0.41
22:Y:71:TRP:CD2	22:Y:75:HIS:CE1	3.03	0.41
24:a:137:MET:HE3	24:a:137:MET:HB3	1.83	0.41
30:g:106:LYS:HD3	30:g:106:LYS:C	2.46	0.41
35:l:6:SER:O	35:l:10:THR:OG1	2.20	0.41
40:r:269:MET:HE1	40:r:296:LEU:HD13	2.02	0.41
41:s:169:GLN:HE21	41:s:174:MET:HB2	1.85	0.41
55:s:401:UQ:H202	55:s:401:UQ:H171	1.86	0.41
1:A:56:ALA:HB1	1:A:61:ASP:HB2	2.01	0.41
3:C:175:TYR:CE1	13:N:78:ASP:HB2	2.56	0.41
7:H:67:LYS:HB3	7:H:67:LYS:HE3	1.98	0.41
9:J:86:CYS:HB3	50:J:401:NDP:O1X	2.20	0.41
9:J:178:SER:HB3	9:J:181:LEU:HD12	2.01	0.41
14:O:132:ILE:HD11	14:O:169:PHE:CD1	2.55	0.41
16:Q:316:PHE:CG	16:Q:343:ILE:HD11	2.55	0.41
16:Q:432:LEU:HD12	16:Q:432:LEU:HA	1.95	0.41
20:V:12:ILE:HB	20:V:21:LYS:HD3	2.01	0.41
23:Z:60:ASN:OD1	23:Z:60:ASN:N	2.47	0.41
53:a:201:CDL:H211	53:a:201:CDL:H182	1.77	0.41
33:j:71:LEU:HD23	33:j:71:LEU:HA	1.83	0.41
35:l:338:MET:CE	35:l:458:LEU:HA	2.49	0.41
6:G:95:PRO:HA	6:G:98:LEU:HD22	2.03	0.41
31:h:16:ARG:HH11	31:h:16:ARG:HG2	1.85	0.41
33:j:57:LEU:HD23	33:j:57:LEU:HA	1.90	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:49:VAL:HB	35:l:50:PRO:HD3	2.02	0.41
35:l:173:LEU:HD13	47:l:703:PEE:H15	2.01	0.41
35:l:261:ILE:HG13	35:l:317:ILE:HD11	2.03	0.41
35:l:332:HIS:CD2	35:l:336:LYS:HB2	2.56	0.41
4:E:18:LYS:HA	4:E:19:PRO:HD3	1.95	0.41
16:Q:251:PHE:HB3	16:Q:341:LEU:HD11	2.03	0.41
23:Z:39:ARG:HG3	23:Z:41:LEU:HD12	2.03	0.41
26:c:55:TYR:OH	26:c:74:ASP:O	2.22	0.41
35:l:190:LEU:HB2	35:l:196:TRP:NE1	2.34	0.41
37:n:14:HIS:NE2	40:r:26:ASN:OD1	2.53	0.41
39:p:44:MET:O	39:p:48:PHE:HB2	2.20	0.41
40:r:10:MET:HE1	53:r:505:CDL:H632	2.02	0.41
40:r:201:MET:HE1	40:r:212:LEU:HD11	2.03	0.41
40:r:303:ILE:HD13	40:r:303:ILE:HA	1.89	0.41
40:r:398:MET:O	40:r:402:ILE:HG13	2.20	0.41
8:I:107:SER:C	8:I:109:ASP:H	2.29	0.41
16:Q:198:THR:HG23	41:s:32:GLN:HG2	2.02	0.41
6:X:83:VAL:HG13	6:X:122:MET:HE1	2.02	0.41
22:Y:47:PHE:HZ	35:l:364:LYS:HB3	1.86	0.41
48:a:202:PLX:H81	40:r:40:SER:HB3	2.02	0.41
28:e:109:LEU:HD23	28:e:109:LEU:HA	1.92	0.41
30:g:13:LEU:O	31:h:9:ARG:NH1	2.54	0.41
41:s:49:ILE:H	41:s:49:ILE:HG12	1.67	0.41
44:w:258:TYR:OH	44:w:272:ASP:OD2	2.36	0.41
1:A:177:TYR:OH	1:A:194:ASP:OD1	2.24	0.41
2:B:65:GLU:OE2	16:Q:266:ARG:NH2	2.51	0.41
3:C:63:TRP:H	3:C:101:ASP:HB2	1.85	0.41
5:F:42:VAL:HG21	12:M:670:GLU:HG2	2.02	0.41
7:H:94:MET:HE2	7:H:94:MET:HB2	1.69	0.41
11:L:109:ASN:ND2	11:L:111:LEU:O	2.50	0.41
16:Q:335:GLU:O	16:Q:339:GLN:HG2	2.21	0.41
19:U:53:TYR:HB2	21:W:72:MET:SD	2.60	0.41
6:X:124:ASP:OD1	39:p:25:ARG:NH1	2.54	0.41
22:Y:73:PHE:CD1	22:Y:73:PHE:C	2.98	0.41
32:i:61:LEU:HD13	34:k:22:TYR:OH	2.20	0.41
32:i:230:LEU:HD11	32:i:244:MET:CE	2.50	0.41
32:i:323:MET:H	32:i:323:MET:HG2	1.61	0.41
35:l:5:ALA:HB2	35:l:61:MET:SD	2.60	0.41
35:l:79:SER:OG	35:l:135:ASN:ND2	2.47	0.41
35:l:172:ILE:O	35:l:176:ARG:HG2	2.20	0.41
35:l:237:MET:HB3	35:l:299:LYS:HE2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:n:47:ARG:NH2	37:n:53:GLU:OE1	2.37	0.41
38:o:19:ASP:HA	38:o:20:PRO:HD3	1.93	0.41
40:r:9:THR:HG21	53:u:201:CDL:H242	2.02	0.41
53:r:504:CDL:H792	53:r:504:CDL:H762	1.90	0.41
42:u:40:ASN:O	42:u:44:MET:HG2	2.20	0.41
44:w:44:VAL:HG12	44:w:45:LEU:HD23	2.03	0.41
1:A:40:ARG:NE	14:O:233:SER:OG	2.54	0.41
1:A:88:ARG:HA	1:A:88:ARG:HD3	1.89	0.41
4:E:37:ARG:HD2	6:G:120:MET:SD	2.60	0.41
6:X:100:VAL:HG13	6:X:101:ASN:OD1	2.20	0.41
22:Y:80:VAL:HG12	22:Y:81:LEU:HD23	2.03	0.41
28:e:73:SER:O	28:e:74:HIS:HB2	2.21	0.41
32:i:98:MET:HE2	32:i:98:MET:HB2	1.96	0.41
47:l:701:PEE:H13	47:l:701:PEE:H49	2.03	0.41
39:p:44:MET:HA	39:p:47:ARG:HG2	2.03	0.41
40:r:97:THR:HG21	53:r:505:CDL:H242	2.03	0.41
42:u:16:GLN:H	42:u:16:GLN:CD	2.24	0.41
42:u:158:LEU:HD23	42:u:158:LEU:HA	1.88	0.41
44:w:303:GLU:HA	44:w:306:ASN:HB2	2.03	0.41
1:A:263:ALA:HA	1:A:271:SER:HB2	2.03	0.40
3:C:55:ASN:ND2	3:C:187:GLU:O	2.55	0.40
6:G:141:PRO:O	6:G:145:VAL:HG23	2.21	0.40
9:J:88:PRO:O	9:J:91:THR:HG22	2.21	0.40
12:M:133:GLN:O	12:M:137:CYS:HB2	2.21	0.40
12:M:180:THR:O	12:M:184:ARG:NE	2.47	0.40
12:M:354:LEU:HD22	12:M:548:LEU:HD22	2.03	0.40
12:M:539:LYS:HB2	12:M:539:LYS:HE2	1.87	0.40
20:V:140:LYS:HE2	20:V:140:LYS:HB3	1.60	0.40
27:d:28:ASN:OD1	27:d:28:ASN:C	2.64	0.40
34:k:20:LEU:HD13	35:l:592:LEU:HB2	2.03	0.40
35:l:234:PRO:O	35:l:237:MET:HG2	2.21	0.40
35:l:253:VAL:HB	35:l:310:LEU:HD11	2.02	0.40
37:n:17:VAL:HB	37:n:18:PRO:HD3	2.02	0.40
41:s:105:MET:HE1	41:s:233:MET:SD	2.61	0.40
53:u:201:CDL:H132	53:u:201:CDL:H762	2.03	0.40
6:G:104:PHE:HB2	6:G:105:MET:HE2	2.03	0.40
21:W:128:ARG:HB3	21:W:132:GLU:OE2	2.21	0.40
22:Y:71:TRP:CD2	22:Y:75:HIS:HE1	2.36	0.40
24:a:136:THR:HG21	40:r:48:ASN:HD22	1.86	0.40
32:i:72:MET:HG2	34:k:12:PHE:CE2	2.56	0.40
35:l:292:ALA:HB2	35:l:304:PHE:CB	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:467:ILE:O	35:l:471:ASN:HB2	2.22	0.40
40:r:220:HIS:CE1	40:r:231:LEU:HB3	2.56	0.40
41:s:90:PRO:HB3	41:s:94:PRO:HD3	2.03	0.40
44:w:125:ASP:OD1	44:w:125:ASP:N	2.55	0.40
5:F:45:LYS:HB3	12:M:671:LEU:HD21	2.02	0.40
9:J:175:LYS:HD3	9:J:175:LYS:HA	1.74	0.40
12:M:436:VAL:O	12:M:442:TYR:OH	2.28	0.40
13:N:11:LEU:O	13:N:14:VAL:HG12	2.21	0.40
14:O:226:GLU:OE1	14:O:226:GLU:N	2.48	0.40
15:P:201:ASP:OD1	15:P:201:ASP:N	2.40	0.40
16:Q:95:LEU:HD13	16:Q:458:PHE:CE2	2.57	0.40
19:U:19:LEU:HD23	19:U:19:LEU:HA	1.92	0.40
22:Y:45:ARG:HD3	23:Z:51:TRP:CD1	2.56	0.40
24:a:154:LEU:HD23	24:a:154:LEU:HA	1.90	0.40
32:i:325:LEU:O	32:i:329:MET:HG2	2.21	0.40
36:m:17:PHE:HA	36:m:20:PHE:CE1	2.56	0.40
36:m:173:ARG:HD3	44:w:289:ARG:NH2	2.36	0.40
39:p:49:ASP:OD1	39:p:49:ASP:C	2.63	0.40
3:C:72:CYS:HB3	3:C:133:MET:CE	2.52	0.40
4:E:127:ASP:OD2	9:J:45:LYS:NZ	2.55	0.40
11:L:87:MET:HE3	11:L:87:MET:HB3	1.88	0.40
12:M:184:ARG:O	12:M:188:GLU:HG3	2.21	0.40
15:P:162:ALA:HB2	16:Q:286:TYR:C	2.47	0.40
27:d:89:GLU:O	27:d:93:ARG:HG2	2.21	0.40
35:l:152:PHE:CD1	35:l:168:ALA:HB1	2.55	0.40
36:m:1:MET:SD	36:m:2:THR:N	2.94	0.40
40:r:91:ARG:HH22	44:w:325:ASP:CG	2.30	0.40
44:w:353:TRP:CD1	44:w:353:TRP:H	2.39	0.40
1:A:120:GLY:HA3	1:A:204:TYR:HD1	1.87	0.40
1:A:126:LYS:NZ	1:A:127:ASP:OD1	2.55	0.40
2:B:76:TYR:CE1	41:s:33:LEU:HD13	2.55	0.40
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.56	0.40
12:M:224:ASP:OD2	12:M:291:ARG:NH2	2.35	0.40
16:Q:157:LYS:HE3	16:Q:157:LYS:HB2	1.92	0.40
16:Q:278:VAL:HG12	16:Q:329:ARG:HH21	1.87	0.40
19:U:59:ASP:OD1	42:u:130:LYS:HD2	2.21	0.40
6:X:111:ASP:OD1	6:X:112:SER:N	2.53	0.40
24:a:136:THR:HG21	40:r:48:ASN:ND2	2.36	0.40
39:p:136:GLU:OE2	39:p:167:TRP:NE1	2.53	0.40
40:r:204:MET:HE3	40:r:261:PHE:CD1	2.57	0.40
42:u:41:LYS:HA	42:u:41:LYS:HD3	1.78	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:213:GLU:OE1	44:w:217:ARG:HD2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	418 (97%)	11 (3%)	0	100	100
2	B	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
3	C	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
4	E	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
5	F	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
6	G	86/88 (98%)	80 (93%)	6 (7%)	0	100	100
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
8	I	93/112 (83%)	83 (89%)	10 (11%)	0	100	100
9	J	289/341 (85%)	279 (96%)	10 (4%)	0	100	100
10	K	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
11	L	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
12	M	688/690 (100%)	670 (97%)	18 (3%)	0	100	100
13	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
14	O	215/217 (99%)	208 (97%)	7 (3%)	0	100	100
15	P	206/208 (99%)	195 (95%)	11 (5%)	0	100	100
16	Q	412/430 (96%)	395 (96%)	17 (4%)	0	100	100
17	S	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
18	T	94/96 (98%)	93 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	U	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
20	V	138/140 (99%)	130 (94%)	7 (5%)	1 (1%)	18	47
21	W	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
22	Y	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
23	Z	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
24	a	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
25	b	99/126 (79%)	97 (98%)	2 (2%)	0	100	100
26	c	154/156 (99%)	143 (93%)	11 (7%)	0	100	100
27	d	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
28	e	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
29	f	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
30	g	119/121 (98%)	113 (95%)	6 (5%)	0	100	100
31	h	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
32	i	345/347 (99%)	331 (96%)	14 (4%)	0	100	100
33	j	95/113 (84%)	90 (95%)	5 (5%)	0	100	100
34	k	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
35	l	601/603 (100%)	576 (96%)	25 (4%)	0	100	100
36	m	125/175 (71%)	112 (90%)	13 (10%)	0	100	100
37	n	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
38	o	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
39	p	176/178 (99%)	167 (95%)	8 (4%)	1 (1%)	21	50
40	r	457/459 (100%)	441 (96%)	16 (4%)	0	100	100
41	s	299/318 (94%)	285 (95%)	14 (5%)	0	100	100
42	u	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
43	v	122/124 (98%)	118 (97%)	4 (3%)	0	100	100
44	w	318/320 (99%)	302 (95%)	16 (5%)	0	100	100
All	All	8029/8308 (97%)	7708 (96%)	319 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
39	p	175	ARG
20	V	46	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	345/345 (100%)	344 (100%)	1 (0%)	86	84
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	131/132 (99%)	130 (99%)	1 (1%)	73	77
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	76/76 (100%)	76 (100%)	0	100	100
6	G	72/81 (89%)	72 (100%)	0	100	100
6	X	78/81 (96%)	78 (100%)	0	100	100
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	86 (99%)	1 (1%)	65	74
9	J	254/295 (86%)	254 (100%)	0	100	100
10	K	41/41 (100%)	41 (100%)	0	100	100
11	L	113/113 (100%)	113 (100%)	0	100	100
12	M	579/580 (100%)	579 (100%)	0	100	100
13	N	130/130 (100%)	130 (100%)	0	100	100
14	O	183/183 (100%)	183 (100%)	0	100	100
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	361/370 (98%)	357 (99%)	4 (1%)	65	74
17	S	58/58 (100%)	58 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	101 (100%)	0	100	100
21	W	122/123 (99%)	121 (99%)	1 (1%)	73	77
22	Y	62/63 (98%)	62 (100%)	0	100	100
23	Z	65/65 (100%)	65 (100%)	0	100	100
24	a	122/122 (100%)	122 (100%)	0	100	100
25	b	97/119 (82%)	97 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	c	137/141 (97%)	135 (98%)	2 (2%)	57	69
27	d	155/155 (100%)	155 (100%)	0	100	100
28	e	99/99 (100%)	99 (100%)	0	100	100
29	f	36/38 (95%)	36 (100%)	0	100	100
30	g	108/108 (100%)	108 (100%)	0	100	100
31	h	93/93 (100%)	93 (100%)	0	100	100
32	i	311/311 (100%)	311 (100%)	0	100	100
33	j	87/99 (88%)	87 (100%)	0	100	100
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	537/537 (100%)	536 (100%)	1 (0%)	87	85
36	m	99/141 (70%)	99 (100%)	0	100	100
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	113/113 (100%)	113 (100%)	0	100	100
39	p	158/159 (99%)	158 (100%)	0	100	100
40	r	410/410 (100%)	409 (100%)	1 (0%)	87	85
41	s	263/275 (96%)	263 (100%)	0	100	100
42	u	153/153 (100%)	152 (99%)	1 (1%)	76	78
43	v	104/111 (94%)	103 (99%)	1 (1%)	68	75
44	w	281/283 (99%)	281 (100%)	0	100	100
All	All	7054/7234 (98%)	7040 (100%)	14 (0%)	85	85

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	ASN
3	C	101	ASP
8	I	30	GLU
16	Q	173	LEU
16	Q	178	THR
16	Q	182	ASN
16	Q	197	MET
21	W	100	ASP
26	c	122	THR
26	c	124	VAL
35	l	338	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	r	256	TYR
42	u	90	ASP
43	v	80	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	164	ASN
1	A	270	ASN
1	A	277	ASN
1	A	393	ASN
2	B	59	GLN
5	F	25	GLN
5	F	31	GLN
5	F	48	ASN
8	I	25	GLN
9	J	122	HIS
9	J	215	ASN
10	K	75	ASN
10	K	78	HIS
12	M	142	GLN
12	M	260	ASN
12	M	482	GLN
12	M	604	GLN
12	M	663	ASN
12	M	676	ASN
12	M	678	GLN
13	N	13	GLN
13	N	69	ASN
14	O	153	GLN
14	O	246	GLN
15	P	181	HIS
15	P	196	HIS
16	Q	183	HIS
16	Q	233	HIS
16	Q	234	GLN
16	Q	250	ASN
17	S	58	ASN
18	T	120	GLN
6	X	142	GLN
22	Y	46	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	Y	54	GLN
22	Y	75	HIS
22	Y	83	HIS
27	d	161	GLN
28	e	86	ASN
28	e	145	ASN
29	f	61	GLN
31	h	27	HIS
32	i	63	GLN
32	i	120	GLN
32	i	152	ASN
32	i	309	ASN
32	i	310	ASN
32	i	316	GLN
34	k	50	ASN
34	k	57	ASN
35	l	56	HIS
35	l	135	ASN
35	l	194	ASN
35	l	199	GLN
35	l	210	ASN
35	l	270	ASN
35	l	323	HIS
35	l	400	ASN
35	l	518	GLN
37	n	3	ASN
40	r	20	HIS
40	r	51	ASN
40	r	81	GLN
40	r	220	HIS
40	r	251	ASN
41	s	47	GLN
41	s	157	ASN
41	s	169	GLN
41	s	235	ASN
41	s	317	GLN
42	u	30	HIS
42	u	77	HIS
43	v	85	HIS
43	v	110	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	2MR	Q	118	16	10,12,13	1.94	1 (10%)	5,13,15	6.15	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	5.54	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	12.58	131.01	119.48
16	Q	118	2MR	CD-NE-CZ	4.44	131.71	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.14	130.40	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	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Q	118	2MR	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 2 are monoatomic - leaving 38 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
48	PLX	C	303	-	51,51,51	1.21	4 (7%)	53,59,59	0.64	1 (1%)
53	CDL	u	201	-	77,77,99	1.22	9 (11%)	83,89,111	0.96	4 (4%)
47	PEE	Q	501	-	50,50,50	1.18	6 (12%)	53,55,55	0.98	2 (3%)
48	PLX	a	202	-	51,51,51	1.21	4 (7%)	53,59,59	0.63	1 (1%)
48	PLX	g	201	-	51,51,51	1.21	4 (7%)	53,59,59	0.62	1 (1%)
50	NDP	J	401	-	51,52,52	4.28	25 (49%)	71,80,80	2.23	16 (22%)
48	PLX	r	502	-	51,51,51	1.20	4 (7%)	53,59,59	0.62	1 (1%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
53	CDL	r	505	-	94,94,99	1.14	9 (9%)	100,106,111	0.88	4 (4%)
48	PLX	j	201	-	51,51,51	1.21	4 (7%)	53,59,59	0.62	1 (1%)
47	PEE	C	302	-	46,46,50	1.23	6 (13%)	49,51,55	0.98	2 (4%)
48	PLX	r	503	-	51,51,51	1.20	4 (7%)	53,59,59	0.61	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	SF4	M	802	12	0,12,12	-	-	-		
53	CDL	i	401	-	65,65,99	1.30	8 (12%)	71,77,111	1.03	4 (5%)
51	FES	M	803	12	0,4,4	-	-	-		
49	8Q1	X	201	-	32,34,34	1.62	6 (18%)	39,43,43	1.58	7 (17%)
45	SF4	C	301	3,16	0,12,12	-	-	-		
47	PEE	W	201	-	40,40,50	1.17	5 (12%)	43,45,55	1.01	2 (4%)
47	PEE	U	101	-	50,50,50	1.18	6 (12%)	53,55,55	0.97	2 (3%)
51	FES	O	301	14	0,4,4	-	-	-		
55	UQ	s	401	-	28,28,63	3.34	7 (25%)	36,37,79	2.73	12 (33%)
45	SF4	M	801	12	0,12,12	-	-	-		
46	FMN	A	502	-	33,33,33	1.07	2 (6%)	48,50,50	1.20	7 (14%)
47	PEE	i	402	-	46,46,50	1.22	6 (13%)	49,51,55	1.01	2 (4%)
49	8Q1	G	201	-	32,34,34	1.63	6 (18%)	39,43,43	1.59	7 (17%)
53	CDL	a	201	-	90,90,99	1.15	8 (8%)	96,102,111	0.95	4 (4%)
53	CDL	r	504	-	98,98,99	1.11	8 (8%)	104,110,111	0.90	4 (3%)
45	SF4	A	501	1	0,12,12	-	-	-		
45	SF4	B	302	2	0,12,12	-	-	-		
53	CDL	N	201	-	50,50,99	1.43	9 (18%)	56,62,111	1.16	4 (7%)
47	PEE	r	501	-	50,50,50	1.18	6 (12%)	53,55,55	0.99	2 (3%)
47	PEE	l	701	-	39,39,50	1.34	6 (15%)	42,44,55	1.12	3 (7%)
53	CDL	V	201	-	93,93,99	1.14	9 (9%)	99,105,111	0.86	4 (4%)
56	ADP	w	401	-	28,29,29	3.17	9 (32%)	43,45,45	1.92	9 (20%)
53	CDL	o	201	-	67,67,99	1.28	9 (13%)	73,79,111	1.04	4 (5%)
53	CDL	l	702	-	99,99,99	1.12	9 (9%)	105,111,111	0.85	4 (3%)
47	PEE	l	703	-	45,45,50	1.24	6 (13%)	48,50,55	0.99	2 (4%)
47	PEE	b	201	-	45,45,50	1.24	6 (13%)	48,50,55	1.00	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PLX	C	303	-	-	27/55/55/55	-
53	CDL	u	201	-	-	39/88/88/110	-
47	PEE	Q	501	-	-	25/54/54/54	-
48	PLX	a	202	-	-	24/55/55/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PLX	g	201	-	-	29/55/55/55	-
50	NDP	J	401	-	-	4/34/77/77	0/5/5/5
48	PLX	r	502	-	-	21/55/55/55	-
53	CDL	r	505	-	-	59/105/105/110	-
45	SF4	B	301	2	-	-	0/6/5/5
48	PLX	j	201	-	-	34/55/55/55	-
47	PEE	C	302	-	-	20/50/50/54	-
48	PLX	r	503	-	-	35/55/55/55	-
53	CDL	i	401	-	-	39/76/76/110	-
45	SF4	M	802	12	-	-	0/6/5/5
51	FES	M	803	12	-	-	0/1/1/1
49	8Q1	X	201	-	-	17/41/41/41	-
47	PEE	W	201	-	-	18/44/44/54	-
45	SF4	C	301	3,16	-	-	0/6/5/5
47	PEE	U	101	-	-	26/54/54/54	-
51	FES	O	301	14	-	-	0/1/1/1
55	UQ	s	401	-	-	10/21/45/87	0/1/1/1
46	FMN	A	502	-	-	5/18/18/18	0/3/3/3
49	8Q1	G	201	-	-	14/41/41/41	-
47	PEE	i	402	-	-	22/50/50/54	-
45	SF4	M	801	12	-	-	0/6/5/5
53	CDL	a	201	-	-	46/101/101/110	-
53	CDL	r	504	-	-	48/109/109/110	-
45	SF4	A	501	1	-	-	0/6/5/5
45	SF4	B	302	2	-	-	0/6/5/5
53	CDL	N	201	-	-	35/61/61/110	-
47	PEE	r	501	-	-	27/54/54/54	-
47	PEE	l	701	-	-	28/43/43/54	-
53	CDL	V	201	-	-	52/104/104/110	-
56	ADP	w	401	-	-	4/16/32/32	0/3/3/3
53	CDL	o	201	-	-	47/78/78/110	-
53	CDL	l	702	-	-	58/110/110/110	-
47	PEE	l	703	-	-	20/49/49/54	-
47	PEE	b	201	-	-	24/49/49/54	-

All (210) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	J	401	NDP	C3B-C2B	-13.15	1.24	1.53
50	J	401	NDP	O4D-C4D	10.74	1.68	1.45
50	J	401	NDP	C3D-C4D	-9.92	1.27	1.53
55	s	401	UQ	C13-C14	9.70	1.55	1.33
55	s	401	UQ	C8-C9	9.28	1.54	1.33
56	w	401	ADP	C3'-C4'	-8.92	1.30	1.53
50	J	401	NDP	O4B-C4B	-7.91	1.27	1.45
55	s	401	UQ	C18-C19	7.89	1.56	1.32
56	w	401	ADP	O4'-C4'	7.76	1.62	1.45
50	J	401	NDP	C2N-C3N	7.48	1.55	1.35
50	J	401	NDP	C6N-C5N	7.28	1.55	1.33
50	J	401	NDP	PN-O3	6.56	1.66	1.59
56	w	401	ADP	PA-O3A	6.51	1.66	1.59
50	J	401	NDP	P2B-O2B	5.94	1.69	1.59
50	J	401	NDP	C6A-N6A	5.76	1.48	1.34
50	J	401	NDP	PA-O3	5.55	1.65	1.59
56	w	401	ADP	C6-N6	5.44	1.48	1.34
50	J	401	NDP	C3B-C4B	5.40	1.66	1.53
49	X	201	8Q1	C39-N41	5.18	1.45	1.33
49	G	201	8Q1	C39-N41	5.13	1.45	1.33
49	G	201	8Q1	C34-N36	5.09	1.45	1.33
49	X	201	8Q1	C34-N36	5.03	1.45	1.33
50	J	401	NDP	O4D-C1D	-5.02	1.30	1.42
50	J	401	NDP	C6N-N1N	5.01	1.49	1.37
50	J	401	NDP	O4B-C1B	4.71	1.52	1.42
50	J	401	NDP	C1B-N9A	-4.55	1.33	1.46
56	w	401	ADP	O4'-C1'	-4.54	1.31	1.42
50	J	401	NDP	O2D-C2D	-3.97	1.33	1.43
50	J	401	NDP	C7N-N7N	3.87	1.44	1.33
47	l	701	PEE	C18-C19	3.84	1.53	1.31
47	W	201	PEE	C18-C19	3.83	1.53	1.31
47	C	302	PEE	C18-C19	3.82	1.53	1.31
47	l	703	PEE	C18-C19	3.82	1.53	1.31
47	r	501	PEE	C18-C19	3.81	1.53	1.31
47	Q	501	PEE	C18-C19	3.81	1.53	1.31
47	b	201	PEE	C18-C19	3.80	1.53	1.31
47	i	402	PEE	C18-C19	3.80	1.53	1.31
47	U	101	PEE	C18-C19	3.78	1.53	1.31
47	l	701	PEE	C39-C38	3.75	1.53	1.31
47	r	501	PEE	C39-C38	3.75	1.53	1.31
47	b	201	PEE	C39-C38	3.74	1.52	1.31
47	C	302	PEE	C39-C38	3.73	1.52	1.31
47	i	402	PEE	C39-C38	3.73	1.52	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	U	101	PEE	C39-C38	3.72	1.52	1.31
47	l	703	PEE	C39-C38	3.71	1.52	1.31
47	Q	501	PEE	C39-C38	3.70	1.52	1.31
53	o	201	CDL	OA8-CA7	3.48	1.43	1.33
53	N	201	CDL	OA8-CA7	3.48	1.43	1.33
53	V	201	CDL	OA8-CA7	3.46	1.43	1.33
53	r	504	CDL	OA8-CA7	3.44	1.43	1.33
53	l	702	CDL	OA8-CA7	3.44	1.43	1.33
53	u	201	CDL	OA8-CA7	3.44	1.43	1.33
53	i	401	CDL	OA8-CA7	3.42	1.43	1.33
46	A	502	FMN	C4A-N5	3.40	1.38	1.30
53	a	201	CDL	OA8-CA7	3.39	1.43	1.33
53	r	505	CDL	OA8-CA7	3.39	1.43	1.33
56	w	401	ADP	C8-N9	-3.36	1.31	1.37
56	w	401	ADP	O2'-C2'	-3.19	1.35	1.43
50	J	401	NDP	C8A-N9A	-3.17	1.32	1.37
53	V	201	CDL	OA6-CA5	3.09	1.43	1.34
50	J	401	NDP	C5A-N7A	-3.06	1.33	1.39
53	r	505	CDL	OB6-CB5	3.06	1.42	1.34
53	N	201	CDL	OA6-CA5	3.03	1.42	1.34
53	N	201	CDL	OB6-CB5	3.03	1.42	1.34
53	l	702	CDL	OB6-CB5	3.03	1.42	1.34
53	r	504	CDL	OB6-CB5	3.03	1.42	1.34
53	N	201	CDL	OB8-CB7	3.03	1.42	1.33
53	i	401	CDL	OB6-CB5	3.02	1.42	1.34
53	i	401	CDL	OB8-CB7	3.02	1.42	1.33
53	u	201	CDL	OB8-CB7	3.01	1.42	1.33
50	J	401	NDP	C7N-C3N	3.00	1.55	1.48
53	o	201	CDL	OB8-CB7	3.00	1.42	1.33
53	r	505	CDL	OB8-CB7	2.99	1.42	1.33
53	o	201	CDL	OB6-CB5	2.99	1.42	1.34
53	r	504	CDL	OB8-CB7	2.99	1.42	1.33
53	V	201	CDL	OB6-CB5	2.98	1.42	1.34
53	V	201	CDL	OB8-CB7	2.98	1.42	1.33
53	a	201	CDL	OA6-CA5	2.97	1.42	1.34
53	l	702	CDL	OB8-CB7	2.97	1.42	1.33
53	l	702	CDL	OA6-CA5	2.97	1.42	1.34
53	a	201	CDL	OB8-CB7	2.97	1.42	1.33
53	o	201	CDL	OA6-CA5	2.97	1.42	1.34
53	i	401	CDL	OA6-CA5	2.96	1.42	1.34
50	J	401	NDP	O3D-C3D	2.96	1.50	1.43
56	w	401	ADP	O3'-C3'	2.96	1.50	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	a	201	CDL	OB6-CB5	2.96	1.42	1.34
53	u	201	CDL	OB6-CB5	2.95	1.42	1.34
53	r	505	CDL	OA6-CA5	2.94	1.42	1.34
48	a	202	PLX	O6-C4	-2.92	1.40	1.44
53	u	201	CDL	OA6-CA5	2.92	1.42	1.34
53	r	504	CDL	OA6-CA5	2.89	1.42	1.34
55	s	401	UQ	C6-C1	2.89	1.54	1.46
48	g	201	PLX	O6-C4	-2.87	1.40	1.44
48	C	303	PLX	O6-C4	-2.86	1.40	1.44
48	r	503	PLX	O6-C4	-2.84	1.41	1.44
48	j	201	PLX	O6-C4	-2.69	1.41	1.44
53	u	201	CDL	OA6-CA4	-2.64	1.40	1.46
53	r	504	CDL	OA6-CA4	-2.63	1.40	1.46
53	r	505	CDL	OA6-CA4	-2.59	1.40	1.46
47	C	302	PEE	O2-C2	-2.58	1.40	1.46
47	l	703	PEE	O2-C2	-2.57	1.40	1.46
47	Q	501	PEE	O2-C2	-2.57	1.40	1.46
47	i	402	PEE	O2-C2	-2.57	1.40	1.46
53	i	401	CDL	OA6-CA4	-2.56	1.40	1.46
50	J	401	NDP	O2B-C2B	2.56	1.52	1.44
47	U	101	PEE	O2-C2	-2.56	1.40	1.46
53	a	201	CDL	OA6-CA4	-2.55	1.40	1.46
53	o	201	CDL	OA6-CA4	-2.53	1.40	1.46
47	r	501	PEE	O2-C2	-2.52	1.40	1.46
47	W	201	PEE	O2-C2	-2.52	1.40	1.46
46	A	502	FMN	C10-N1	2.50	1.38	1.33
47	b	201	PEE	O3-C30	2.50	1.40	1.33
47	b	201	PEE	O2-C2	-2.49	1.40	1.46
47	l	701	PEE	O2-C2	-2.48	1.40	1.46
53	l	702	CDL	OA6-CA4	-2.48	1.40	1.46
47	Q	501	PEE	O3-C30	2.48	1.40	1.33
47	l	701	PEE	O3-C30	2.47	1.40	1.33
47	U	101	PEE	O3-C30	2.47	1.40	1.33
47	i	402	PEE	O3-C30	2.46	1.40	1.33
47	r	501	PEE	O3-C30	2.45	1.40	1.33
48	r	502	PLX	O6-C4	-2.44	1.41	1.44
48	j	201	PLX	C7-C6	2.43	1.55	1.50
49	G	201	8Q1	C1-S44	2.43	1.82	1.76
48	r	502	PLX	C7-C6	2.43	1.55	1.50
47	C	302	PEE	O3-C30	2.43	1.40	1.33
47	l	703	PEE	O3-C30	2.42	1.40	1.33
49	X	201	8Q1	C1-S44	2.40	1.81	1.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	C	303	PLX	C7-C6	2.38	1.55	1.50
48	r	503	PLX	C7-C6	2.37	1.55	1.50
50	J	401	NDP	C2D-C3D	2.37	1.59	1.53
48	g	201	PLX	C7-C6	2.37	1.55	1.50
49	X	201	8Q1	O35-C34	-2.35	1.18	1.23
53	V	201	CDL	OB6-CB4	-2.35	1.41	1.46
47	l	701	PEE	O2-C10	2.34	1.40	1.34
56	w	401	ADP	C5-N7	-2.34	1.34	1.39
47	W	201	PEE	O2-C10	2.34	1.40	1.34
53	a	201	CDL	OB6-CB4	-2.34	1.41	1.46
49	G	201	8Q1	O35-C34	-2.34	1.18	1.23
47	W	201	PEE	O3-C30	2.34	1.40	1.33
48	a	202	PLX	C7-C6	2.33	1.55	1.50
53	o	201	CDL	OB6-CB4	-2.33	1.41	1.46
53	l	702	CDL	OB6-CB4	-2.32	1.41	1.46
53	u	201	CDL	OB6-CB4	-2.31	1.41	1.46
53	i	401	CDL	OB6-CB4	-2.31	1.41	1.46
47	l	703	PEE	O2-C10	2.31	1.40	1.34
53	r	504	CDL	OB6-CB4	-2.28	1.41	1.46
49	G	201	8Q1	O40-C39	-2.28	1.18	1.23
53	u	201	CDL	PB2-OB2	2.27	1.68	1.59
53	N	201	CDL	OA6-CA4	-2.27	1.41	1.46
53	o	201	CDL	PB2-OB2	2.27	1.68	1.59
47	Q	501	PEE	O2-C10	2.27	1.40	1.34
47	b	201	PEE	O2-C10	2.27	1.40	1.34
53	l	702	CDL	PB2-OB2	2.27	1.68	1.59
53	i	401	CDL	PB2-OB2	2.27	1.68	1.59
47	U	101	PEE	O2-C10	2.27	1.40	1.34
53	V	201	CDL	OA6-CA4	-2.26	1.41	1.46
47	i	402	PEE	O2-C10	2.26	1.40	1.34
53	N	201	CDL	OB6-CB4	-2.26	1.41	1.46
53	V	201	CDL	PB2-OB2	2.26	1.68	1.59
53	i	401	CDL	PB2-OB5	2.25	1.68	1.59
47	C	302	PEE	O2-C10	2.25	1.40	1.34
53	r	505	CDL	PB2-OB2	2.25	1.68	1.59
53	N	201	CDL	PB2-OB5	2.24	1.68	1.59
53	a	201	CDL	PB2-OB2	2.24	1.68	1.59
53	r	505	CDL	PB2-OB5	2.23	1.68	1.59
47	r	501	PEE	O2-C10	2.23	1.40	1.34
53	r	505	CDL	OB6-CB4	-2.23	1.41	1.46
49	G	201	8Q1	C6-C1	2.23	1.53	1.50
49	X	201	8Q1	O40-C39	-2.23	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	N	201	CDL	PB2-OB2	2.22	1.68	1.59
53	o	201	CDL	PB2-OB5	2.22	1.68	1.59
47	W	201	PEE	O3-C3	-2.22	1.40	1.45
49	X	201	8Q1	C6-C1	2.21	1.53	1.50
53	r	504	CDL	PB2-OB2	2.21	1.68	1.59
53	u	201	CDL	PB2-OB5	2.21	1.68	1.59
53	r	504	CDL	PB2-OB5	2.21	1.68	1.59
48	j	201	PLX	P1-O4	2.21	1.68	1.59
48	r	502	PLX	P1-O4	2.21	1.68	1.59
55	s	401	UQ	O4-C4	-2.20	1.18	1.23
50	J	401	NDP	PA-O5B	2.20	1.68	1.59
53	V	201	CDL	PB2-OB5	2.19	1.68	1.59
47	l	703	PEE	O3-C3	-2.19	1.40	1.45
47	U	101	PEE	O3-C3	-2.18	1.40	1.45
53	l	702	CDL	PB2-OB5	2.18	1.67	1.59
48	C	303	PLX	P1-O4	2.17	1.67	1.59
53	a	201	CDL	PB2-OB5	2.16	1.67	1.59
48	a	202	PLX	P1-O4	2.16	1.67	1.59
48	r	503	PLX	P1-O4	2.15	1.67	1.59
55	s	401	UQ	C7-C8	2.14	1.53	1.50
48	g	201	PLX	P1-O4	2.13	1.67	1.59
47	C	302	PEE	O3-C3	-2.13	1.40	1.45
47	l	701	PEE	O3-C3	-2.13	1.40	1.45
47	i	402	PEE	O3-C3	-2.11	1.40	1.45
47	Q	501	PEE	O3-C3	-2.10	1.40	1.45
50	J	401	NDP	O7N-C7N	-2.09	1.19	1.24
47	r	501	PEE	O3-C3	-2.08	1.40	1.45
55	s	401	UQ	O3-CM3	-2.08	1.40	1.45
53	N	201	CDL	C11-CA5	2.08	1.56	1.50
48	C	303	PLX	P1-O1	2.08	1.67	1.59
48	j	201	PLX	P1-O1	2.07	1.67	1.59
48	a	202	PLX	P1-O1	2.07	1.67	1.59
48	r	502	PLX	P1-O1	2.06	1.67	1.59
47	b	201	PEE	O3-C3	-2.06	1.40	1.45
53	V	201	CDL	C11-CA5	2.05	1.56	1.50
48	r	503	PLX	P1-O1	2.05	1.67	1.59
53	l	702	CDL	C11-CA5	2.04	1.56	1.50
53	o	201	CDL	C11-CA5	2.03	1.56	1.50
48	g	201	PLX	P1-O1	2.02	1.67	1.59
53	r	505	CDL	C11-CA5	2.01	1.56	1.50
53	u	201	CDL	C11-CA5	2.01	1.56	1.50

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	s	401	UQ	C7-C8-C9	-9.25	110.89	126.83
50	J	401	NDP	C3N-C2N-N1N	-7.35	112.41	123.20
50	J	401	NDP	C1D-N1N-C2N	-7.14	109.38	121.14
50	J	401	NDP	C6N-N1N-C2N	-6.87	111.97	119.32
55	s	401	UQ	C12-C13-C14	-6.10	113.66	127.62
49	X	201	8Q1	C6-C1-S44	5.90	120.43	113.40
49	G	201	8Q1	C6-C1-S44	5.73	120.23	113.40
50	J	401	NDP	C5A-C4A-N3A	-5.64	118.94	126.72
50	J	401	NDP	C1D-N1N-C6N	-5.50	109.15	120.77
56	w	401	ADP	C5-C4-N3	-5.44	119.23	126.72
56	w	401	ADP	N3-C2-N1	-4.55	121.69	128.58
53	a	201	CDL	OA6-CA5-C11	4.26	120.71	111.48
56	w	401	ADP	N3-C4-N9	4.21	134.34	127.17
55	s	401	UQ	C15-C14-C13	-4.21	112.83	123.63
50	J	401	NDP	N3A-C2A-N1A	-4.15	122.30	128.58
47	l	701	PEE	O2-C10-C11	4.10	120.36	111.48
55	s	401	UQ	C10-C9-C8	-4.08	113.14	123.63
53	a	201	CDL	OB6-CB5-C51	4.08	120.31	111.48
53	r	504	CDL	OB6-CB5-C51	4.08	120.31	111.48
47	Q	501	PEE	O2-C10-C11	4.08	120.30	111.48
55	s	401	UQ	C17-C18-C19	-4.08	114.05	127.64
53	r	505	CDL	OB6-CB5-C51	4.07	120.28	111.48
53	u	201	CDL	OB6-CB5-C51	4.05	120.25	111.48
53	i	401	CDL	OA6-CA5-C11	4.05	120.24	111.48
53	l	702	CDL	OA6-CA5-C11	4.02	120.17	111.48
53	o	201	CDL	OA6-CA5-C11	4.01	120.15	111.48
53	N	201	CDL	OB6-CB5-C51	4.00	120.14	111.48
47	r	501	PEE	O2-C10-C11	4.00	120.14	111.48
47	W	201	PEE	O2-C10-C11	4.00	120.14	111.48
50	J	401	NDP	N3A-C4A-N9A	4.00	133.97	127.17
53	o	201	CDL	OB6-CB5-C51	3.98	120.08	111.48
47	U	101	PEE	O2-C10-C11	3.97	120.06	111.48
47	b	201	PEE	O2-C10-C11	3.92	119.97	111.48
53	r	504	CDL	OA6-CA5-C11	3.91	119.93	111.48
53	i	401	CDL	OB6-CB5-C51	3.90	119.92	111.48
53	N	201	CDL	OA6-CA5-C11	3.89	119.90	111.48
55	s	401	UQ	C11-C9-C8	-3.89	112.44	121.17
47	i	402	PEE	O2-C10-C11	3.88	119.88	111.48
47	C	302	PEE	O2-C10-C11	3.87	119.85	111.48
53	u	201	CDL	OA6-CA5-C11	3.84	119.78	111.48
53	l	702	CDL	OB6-CB5-C51	3.80	119.70	111.48
47	l	703	PEE	O2-C10-C11	3.80	119.70	111.48
53	r	505	CDL	OA6-CA5-C11	3.79	119.67	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	V	201	CDL	OA6-CA5-C11	3.74	119.57	111.48
55	s	401	UQ	C7-C6-C5	-3.71	118.53	124.89
53	V	201	CDL	OB6-CB5-C51	3.70	119.50	111.48
50	J	401	NDP	C2A-N3A-C4A	3.63	120.70	111.83
55	s	401	UQ	C16-C14-C13	-3.60	113.08	121.17
56	w	401	ADP	C2-N3-C4	3.56	120.54	111.83
49	X	201	8Q1	O4-C1-C6	-3.52	119.92	123.98
49	G	201	8Q1	O4-C1-C6	-3.51	119.94	123.98
56	w	401	ADP	N9-C8-N7	-3.50	108.98	113.94
55	s	401	UQ	C21-C19-C18	-3.26	112.88	122.66
49	G	201	8Q1	C37-C38-C39	3.22	117.76	112.39
56	w	401	ADP	C5-N7-C8	3.20	108.49	103.45
46	A	502	FMN	C4-N3-C2	-3.19	119.97	125.64
50	J	401	NDP	C4A-C5A-N7A	-3.18	106.94	110.58
56	w	401	ADP	C4-N9-C8	3.13	109.03	105.74
50	J	401	NDP	N9A-C8A-N7A	-3.10	109.53	113.94
56	w	401	ADP	C4-C5-N7	-3.07	107.08	110.58
50	J	401	NDP	C5A-N7A-C8A	3.03	108.21	103.45
55	s	401	UQ	C20-C19-C18	-3.01	113.63	122.66
55	s	401	UQ	C7-C6-C1	2.99	121.99	118.52
53	V	201	CDL	OB8-CB7-C71	2.86	120.56	111.83
47	r	501	PEE	O3-C30-C31	2.84	120.48	111.83
47	Q	501	PEE	O3-C30-C31	2.82	120.43	111.83
53	i	401	CDL	OB8-CB7-C71	2.78	120.30	111.83
53	u	201	CDL	OB8-CB7-C71	2.77	120.28	111.83
47	i	402	PEE	O3-C30-C31	2.75	120.23	111.83
53	N	201	CDL	OB8-CB7-C71	2.75	120.23	111.83
53	o	201	CDL	OA8-CA7-C31	2.75	120.21	111.83
47	b	201	PEE	O3-C30-C31	2.74	120.20	111.83
53	a	201	CDL	OB8-CB7-C71	2.74	120.19	111.83
53	N	201	CDL	OA8-CA7-C31	2.73	120.17	111.83
53	r	504	CDL	OA8-CA7-C31	2.73	120.15	111.83
53	o	201	CDL	OB8-CB7-C71	2.73	120.14	111.83
47	l	703	PEE	O3-C30-C31	2.72	120.14	111.83
53	r	504	CDL	OB8-CB7-C71	2.71	120.10	111.83
47	U	101	PEE	O3-C30-C31	2.71	120.09	111.83
55	s	401	UQ	CM5-C5-C6	-2.71	120.00	124.45
53	a	201	CDL	OA8-CA7-C31	2.69	120.05	111.83
53	r	505	CDL	OB8-CB7-C71	2.67	119.97	111.83
47	l	701	PEE	O3-C30-C31	2.66	119.95	111.83
53	l	702	CDL	OB8-CB7-C71	2.66	119.95	111.83
53	i	401	CDL	OA8-CA7-C31	2.66	119.94	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	l	702	CDL	OA8-CA7-C31	2.65	119.93	111.83
53	u	201	CDL	OA8-CA7-C31	2.63	119.86	111.83
47	C	302	PEE	O3-C30-C31	2.62	119.81	111.83
53	r	505	CDL	OA8-CA7-C31	2.62	119.81	111.83
46	A	502	FMN	C4A-C4-N3	2.60	119.88	113.25
53	V	201	CDL	OA8-CA7-C31	2.59	119.72	111.83
48	r	503	PLX	C1A-N1-C1	2.56	120.07	109.91
47	W	201	PEE	O3-C30-C31	2.53	119.54	111.83
48	j	201	PLX	C1A-N1-C1	2.52	119.94	109.91
48	r	502	PLX	C1A-N1-C1	2.50	119.85	109.91
49	G	201	8Q1	C43-S44-C1	2.49	109.20	101.84
46	A	502	FMN	C4A-C10-N10	2.47	120.02	116.48
46	A	502	FMN	O4-C4-C4A	-2.45	120.07	126.53
56	w	401	ADP	C4'-O4'-C1'	-2.44	104.08	109.47
48	a	202	PLX	C1A-N1-C1	2.42	119.53	109.91
48	g	201	PLX	C1A-N1-C1	2.42	119.52	109.91
49	X	201	8Q1	O4-C1-S44	-2.39	119.64	122.68
50	J	401	NDP	C4A-N9A-C8A	2.37	108.22	105.74
49	X	201	8Q1	C37-C38-C39	2.33	116.27	112.39
47	l	701	PEE	C20-C19-C18	-2.32	112.44	126.42
48	C	303	PLX	C1A-N1-C1	2.32	119.14	109.91
49	X	201	8Q1	C43-S44-C1	2.31	108.67	101.84
49	G	201	8Q1	C38-C39-N41	2.28	120.49	116.34
50	J	401	NDP	C2B-C3B-C4B	2.28	106.89	101.99
46	A	502	FMN	C5A-C9A-N10	2.26	120.02	117.97
46	A	502	FMN	C10-C4A-N5	-2.24	120.23	124.81
49	G	201	8Q1	O4-C1-S44	-2.24	119.84	122.68
49	X	201	8Q1	C38-C39-N41	2.23	120.41	116.34
46	A	502	FMN	C9A-C5A-N5	-2.19	120.13	122.45
50	J	401	NDP	C2B-C1B-N9A	-2.12	110.27	113.75
49	X	201	8Q1	O27-C28-C29	-2.10	107.17	110.55
50	J	401	NDP	C2D-C3D-C4D	2.09	106.65	102.61
49	G	201	8Q1	C32-C34-N36	2.05	120.38	116.48
50	J	401	NDP	P2B-O2B-C2B	-2.05	117.96	123.43

There are no chirality outliers.

All (857) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C1'-C2'-C3'-O3'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
47	U	101	PEE	C1-O3P-P-O1P
47	U	101	PEE	C1-O3P-P-O4P
47	U	101	PEE	C4-O4P-P-O3P
47	U	101	PEE	C4-O4P-P-O2P
47	b	201	PEE	C1-O3P-P-O1P
47	i	402	PEE	C11-C10-O2-C2
47	l	701	PEE	O2-C2-C3-O3
47	l	701	PEE	C1-O3P-P-O2P
47	l	701	PEE	C1-O3P-P-O1P
47	l	701	PEE	C1-O3P-P-O4P
47	l	701	PEE	C4-O4P-P-O3P
47	l	701	PEE	C4-O4P-P-O1P
47	l	703	PEE	O3P-C1-C2-O2
47	r	501	PEE	C4-O4P-P-O3P
47	r	501	PEE	C4-O4P-P-O2P
47	r	501	PEE	C4-O4P-P-O1P
48	C	303	PLX	O7-C6-O6-C4
48	C	303	PLX	N1-C1-C2-O1
48	a	202	PLX	C3-O4-P1-O1
48	a	202	PLX	C3-O4-P1-O3
48	g	201	PLX	C3-O4-P1-O1
48	g	201	PLX	C3-O4-P1-O3
48	g	201	PLX	C25-C24-O8-C5
48	j	201	PLX	O7-C6-C7-C8
48	j	201	PLX	O7-C6-O6-C4
48	j	201	PLX	C3-O4-P1-O1
48	j	201	PLX	C3-O4-P1-O3
48	j	201	PLX	O9-C24-C25-C26
48	r	502	PLX	O7-C6-O6-C4
48	r	502	PLX	C5-C4-O6-C6
48	r	502	PLX	O9-C24-C25-C26
48	r	503	PLX	O7-C6-O6-C4
48	r	503	PLX	C3-O4-P1-O1
48	r	503	PLX	C3-O4-P1-O2
48	r	503	PLX	C3-O4-P1-O3
48	r	503	PLX	C2-O1-P1-O4
48	r	503	PLX	C2-O1-P1-O2
48	r	503	PLX	C2-O1-P1-O3
48	r	503	PLX	C25-C24-O8-C5
48	r	503	PLX	O9-C24-C25-C26
49	G	201	8Q1	O4-C1-S44-C43
49	G	201	8Q1	C6-C1-S44-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	G	201	8Q1	O27-C28-C29-C30
49	G	201	8Q1	O27-C28-C29-C31
49	G	201	8Q1	O27-C28-C29-C32
49	G	201	8Q1	C42-C43-S44-C1
49	G	201	8Q1	C28-O27-P24-O3
49	G	201	8Q1	C28-O27-P24-O2
49	G	201	8Q1	C28-O27-P24-O1
49	X	201	8Q1	C1-C6-C7-C8
49	X	201	8Q1	C28-C29-C32-C34
49	X	201	8Q1	C28-C29-C32-O33
49	X	201	8Q1	C30-C29-C32-C34
49	X	201	8Q1	C30-C29-C32-O33
49	X	201	8Q1	C31-C29-C32-C34
49	X	201	8Q1	C31-C29-C32-O33
49	X	201	8Q1	N36-C37-C38-C39
49	X	201	8Q1	C42-C43-S44-C1
49	X	201	8Q1	C28-O27-P24-O3
49	X	201	8Q1	C28-O27-P24-O2
49	X	201	8Q1	C28-O27-P24-O1
53	N	201	CDL	O1-C1-CB2-OB2
53	N	201	CDL	CA2-C1-CB2-OB2
53	N	201	CDL	CA2-OA2-PA1-OA4
53	N	201	CDL	CA2-OA2-PA1-OA5
53	N	201	CDL	CA3-OA5-PA1-OA2
53	N	201	CDL	CA3-OA5-PA1-OA3
53	N	201	CDL	CA3-OA5-PA1-OA4
53	N	201	CDL	C11-CA5-OA6-CA4
53	N	201	CDL	CB2-OB2-PB2-OB3
53	N	201	CDL	CB2-OB2-PB2-OB4
53	N	201	CDL	CB2-OB2-PB2-OB5
53	N	201	CDL	CB3-OB5-PB2-OB3
53	V	201	CDL	CB2-C1-CA2-OA2
53	V	201	CDL	CA2-C1-CB2-OB2
53	V	201	CDL	CA2-OA2-PA1-OA4
53	V	201	CDL	CA2-OA2-PA1-OA5
53	V	201	CDL	CA3-OA5-PA1-OA2
53	V	201	CDL	CA3-OA5-PA1-OA4
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	201	CDL	CB3-OB5-PB2-OB3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	V	201	CDL	CB3-OB5-PB2-OB4
53	a	201	CDL	CA2-C1-CB2-OB2
53	a	201	CDL	CA2-OA2-PA1-OA3
53	a	201	CDL	CA2-OA2-PA1-OA4
53	a	201	CDL	CA2-OA2-PA1-OA5
53	a	201	CDL	CA3-OA5-PA1-OA2
53	a	201	CDL	CB2-OB2-PB2-OB3
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	i	401	CDL	CB3-OB5-PB2-OB2
53	i	401	CDL	CB3-OB5-PB2-OB3
53	l	702	CDL	CA2-C1-CB2-OB2
53	l	702	CDL	CA3-OA5-PA1-OA2
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	OB6-CB4-CB6-OB8
53	o	201	CDL	CB2-C1-CA2-OA2
53	o	201	CDL	CA2-C1-CB2-OB2
53	o	201	CDL	CA2-OA2-PA1-OA4
53	o	201	CDL	CA2-OA2-PA1-OA5
53	o	201	CDL	OA6-CA4-CA6-OA8
53	o	201	CDL	CB2-OB2-PB2-OB3
53	o	201	CDL	CB3-OB5-PB2-OB2
53	o	201	CDL	CB3-OB5-PB2-OB3
53	o	201	CDL	CB3-OB5-PB2-OB4
53	o	201	CDL	OB6-CB4-CB6-OB8
53	r	504	CDL	CA2-C1-CB2-OB2
53	r	504	CDL	CA2-OA2-PA1-OA3
53	r	504	CDL	CA2-OA2-PA1-OA5
53	r	504	CDL	CB2-OB2-PB2-OB3
53	r	504	CDL	CB2-OB2-PB2-OB4
53	r	504	CDL	CB2-OB2-PB2-OB5
53	r	504	CDL	CB3-OB5-PB2-OB2
53	r	504	CDL	CB3-OB5-PB2-OB3
53	r	505	CDL	CB2-C1-CA2-OA2
53	r	505	CDL	CA2-OA2-PA1-OA3
53	r	505	CDL	CA2-OA2-PA1-OA4
53	r	505	CDL	CA2-OA2-PA1-OA5
53	r	505	CDL	CA3-OA5-PA1-OA2
53	r	505	CDL	CA3-OA5-PA1-OA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	r	505	CDL	CB2-OB2-PB2-OB3
53	r	505	CDL	CB3-OB5-PB2-OB2
53	r	505	CDL	CB3-OB5-PB2-OB3
53	r	505	CDL	CB3-OB5-PB2-OB4
53	u	201	CDL	O1-C1-CA2-OA2
53	u	201	CDL	CA2-OA2-PA1-OA4
53	u	201	CDL	CA2-OA2-PA1-OA5
53	u	201	CDL	CB2-OB2-PB2-OB3
53	u	201	CDL	CB2-OB2-PB2-OB5
53	u	201	CDL	CB3-OB5-PB2-OB2
53	u	201	CDL	CB3-OB5-PB2-OB3
55	s	401	UQ	C7-C8-C9-C11
55	s	401	UQ	C12-C13-C14-C16
56	w	401	ADP	C5'-O5'-PA-O1A
56	w	401	ADP	C5'-O5'-PA-O2A
56	w	401	ADP	C5'-O5'-PA-O3A
53	r	504	CDL	C31-CA7-OA8-CA6
53	i	401	CDL	OA9-CA7-OA8-CA6
53	r	504	CDL	OA9-CA7-OA8-CA6
47	i	402	PEE	O4-C10-O2-C2
47	l	703	PEE	O4-C10-O2-C2
53	N	201	CDL	OA7-CA5-OA6-CA4
47	l	703	PEE	C11-C10-O2-C2
53	i	401	CDL	C31-CA7-OA8-CA6
47	Q	501	PEE	C37-C38-C39-C40
47	U	101	PEE	C17-C18-C19-C20
47	l	701	PEE	C17-C18-C19-C20
47	b	201	PEE	O5-C30-O3-C3
47	l	703	PEE	O5-C30-O3-C3
55	s	401	UQ	C17-C18-C19-C21
53	N	201	CDL	O1-C1-CA2-OA2
53	V	201	CDL	O1-C1-CA2-OA2
53	l	702	CDL	O1-C1-CA2-OA2
53	l	702	CDL	O1-C1-CB2-OB2
53	o	201	CDL	O1-C1-CA2-OA2
53	r	504	CDL	O1-C1-CA2-OA2
53	r	504	CDL	O1-C1-CB2-OB2
47	l	703	PEE	C31-C30-O3-C3
53	l	702	CDL	C71-CB7-OB8-CB6
53	V	201	CDL	C11-CA5-OA6-CA4
47	b	201	PEE	C31-C30-O3-C3
53	u	201	CDL	C52-C53-C54-C55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
55	s	401	UQ	C12-C11-C9-C8
55	s	401	UQ	C9-C11-C12-C13
53	l	702	CDL	OB9-CB7-OB8-CB6
53	l	702	CDL	C75-C76-C77-C78
47	W	201	PEE	C31-C30-O3-C3
53	r	505	CDL	C71-CB7-OB8-CB6
47	b	201	PEE	C37-C38-C39-C40
53	u	201	CDL	C71-C72-C73-C74
48	g	201	PLX	C10-C11-C12-C13
53	N	201	CDL	C11-C12-C13-C14
53	V	201	CDL	C11-C12-C13-C14
53	V	201	CDL	C32-C33-C34-C35
47	Q	501	PEE	C11-C10-O2-C2
48	a	202	PLX	C33-C34-C35-C36
48	r	503	PLX	C12-C13-C14-C15
53	r	505	CDL	OB9-CB7-OB8-CB6
53	u	201	CDL	CB2-C1-CA2-OA2
53	u	201	CDL	CA2-C1-CB2-OB2
47	l	701	PEE	C31-C30-O3-C3
53	V	201	CDL	C31-CA7-OA8-CA6
53	r	504	CDL	C71-CB7-OB8-CB6
53	V	201	CDL	C62-C63-C64-C65
48	j	201	PLX	C28-C29-C30-C31
48	r	502	PLX	C9-C10-C11-C12
53	l	702	CDL	C59-C60-C61-C62
53	o	201	CDL	C32-C33-C34-C35
53	u	201	CDL	C75-C76-C77-C78
53	V	201	CDL	C59-C60-C61-C62
53	l	702	CDL	C11-C12-C13-C14
53	r	504	CDL	C55-C56-C57-C58
53	V	201	CDL	O1-C1-CB2-OB2
53	u	201	CDL	O1-C1-CB2-OB2
48	r	502	PLX	C30-C31-C32-C33
53	r	505	CDL	C74-C75-C76-C77
47	l	701	PEE	O5-C30-O3-C3
53	r	504	CDL	OB9-CB7-OB8-CB6
53	i	401	CDL	OB6-CB4-CB6-OB8
53	l	702	CDL	OA6-CA4-CA6-OA8
53	N	201	CDL	C31-CA7-OA8-CA6
47	l	703	PEE	C33-C34-C35-C36
53	l	702	CDL	C35-C36-C37-C38
53	a	201	CDL	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	V	201	CDL	CB7-C71-C72-C73
53	r	505	CDL	CA5-C11-C12-C13
47	U	101	PEE	C31-C30-O3-C3
53	o	201	CDL	C71-CB7-OB8-CB6
47	l	701	PEE	C30-C31-C32-C33
47	r	501	PEE	C10-C11-C12-C13
53	r	504	CDL	CB7-C71-C72-C73
53	V	201	CDL	OA7-CA5-OA6-CA4
48	r	502	PLX	C11-C12-C13-C14
53	r	505	CDL	C76-C77-C78-C79
48	r	503	PLX	C2-C1-N1-C1A
47	l	703	PEE	C30-C31-C32-C33
53	N	201	CDL	CB7-C71-C72-C73
53	a	201	CDL	CA5-C11-C12-C13
53	i	401	CDL	CA7-C31-C32-C33
53	i	401	CDL	CB7-C71-C72-C73
53	l	702	CDL	CB7-C71-C72-C73
53	r	505	CDL	CA7-C31-C32-C33
53	V	201	CDL	OA9-CA7-OA8-CA6
47	i	402	PEE	C30-C31-C32-C33
53	a	201	CDL	CA7-C31-C32-C33
53	i	401	CDL	CA5-C11-C12-C13
53	l	702	CDL	CB5-C51-C52-C53
53	o	201	CDL	CB7-C71-C72-C73
53	u	201	CDL	CB5-C51-C52-C53
47	U	101	PEE	C34-C35-C36-C37
48	g	201	PLX	C12-C13-C14-C15
48	g	201	PLX	C31-C32-C33-C34
53	a	201	CDL	O1-C1-CA2-OA2
53	a	201	CDL	O1-C1-CB2-OB2
53	i	401	CDL	O1-C1-CA2-OA2
53	o	201	CDL	O1-C1-CB2-OB2
53	r	505	CDL	O1-C1-CA2-OA2
53	u	201	CDL	CB7-C71-C72-C73
47	Q	501	PEE	O4-C10-O2-C2
47	Q	501	PEE	C17-C18-C19-C20
47	W	201	PEE	O5-C30-O3-C3
47	U	101	PEE	C11-C10-O2-C2
53	o	201	CDL	C51-CB5-OB6-CB4
53	i	401	CDL	C14-C15-C16-C17
47	U	101	PEE	O5-C30-O3-C3
53	N	201	CDL	OA9-CA7-OA8-CA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
50	J	401	NDP	C2D-C1D-N1N-C6N
47	U	101	PEE	O4-C10-O2-C2
53	o	201	CDL	OB7-CB5-OB6-CB4
53	a	201	CDL	CB2-C1-CA2-OA2
53	i	401	CDL	CB2-C1-CA2-OA2
53	r	504	CDL	CB2-C1-CA2-OA2
53	V	201	CDL	C71-CB7-OB8-CB6
48	j	201	PLX	C15-C16-C17-C18
47	l	701	PEE	C11-C12-C13-C14
53	o	201	CDL	C72-C73-C74-C75
48	r	503	PLX	C2-C1-N1-C1C
48	g	201	PLX	O8-C24-C25-C26
47	C	302	PEE	C11-C10-O2-C2
47	b	201	PEE	C11-C10-O2-C2
53	r	505	CDL	C51-CB5-OB6-CB4
47	b	201	PEE	O4-C10-O2-C2
53	r	505	CDL	OB7-CB5-OB6-CB4
53	r	504	CDL	C58-C59-C60-C61
53	o	201	CDL	OB9-CB7-OB8-CB6
53	N	201	CDL	CA6-CA4-OA6-CA5
47	U	101	PEE	C32-C33-C34-C35
48	a	202	PLX	C29-C30-C31-C32
53	u	201	CDL	C17-C18-C19-C20
47	C	302	PEE	O4-C10-O2-C2
53	V	201	CDL	C51-CB5-OB6-CB4
47	b	201	PEE	C10-C11-C12-C13
53	a	201	CDL	C71-CB7-OB8-CB6
48	a	202	PLX	C28-C29-C30-C31
53	V	201	CDL	C31-C32-C33-C34
53	r	504	CDL	C52-C53-C54-C55
47	r	501	PEE	C21-C22-C23-C24
48	r	502	PLX	C27-C28-C29-C30
53	r	505	CDL	C12-C13-C14-C15
53	r	505	CDL	C35-C36-C37-C38
48	C	303	PLX	C25-C26-C27-C28
48	r	503	PLX	C10-C11-C12-C13
53	a	201	CDL	C73-C74-C75-C76
53	l	702	CDL	C37-C38-C39-C40
53	l	702	CDL	C74-C75-C76-C77
53	r	504	CDL	C59-C60-C61-C62
53	r	505	CDL	C56-C57-C58-C59
53	r	505	CDL	C59-C60-C61-C62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	g	201	PLX	O9-C24-C25-C26
47	b	201	PEE	C13-C14-C15-C16
53	o	201	CDL	C71-C72-C73-C74
53	o	201	CDL	C73-C74-C75-C76
53	r	504	CDL	C74-C75-C76-C77
53	u	201	CDL	C55-C56-C57-C58
48	a	202	PLX	C7-C8-C9-C10
53	l	702	CDL	C71-C72-C73-C74
53	N	201	CDL	CA7-C31-C32-C33
53	V	201	CDL	C52-C53-C54-C55
53	a	201	CDL	C21-C22-C23-C24
47	Q	501	PEE	C35-C36-C37-C38
53	a	201	CDL	C37-C38-C39-C40
53	i	401	CDL	C52-C53-C54-C55
47	b	201	PEE	C31-C32-C33-C34
53	u	201	CDL	C13-C14-C15-C16
53	V	201	CDL	C33-C34-C35-C36
53	r	504	CDL	C20-C21-C22-C23
53	N	201	CDL	C71-CB7-OB8-CB6
47	Q	501	PEE	C33-C34-C35-C36
53	l	702	CDL	C39-C40-C41-C42
53	r	504	CDL	C75-C76-C77-C78
53	V	201	CDL	C74-C75-C76-C77
53	o	201	CDL	C55-C56-C57-C58
47	i	402	PEE	C11-C12-C13-C14
48	r	503	PLX	C13-C14-C15-C16
53	V	201	CDL	OB9-CB7-OB8-CB6
48	r	503	PLX	C25-C26-C27-C28
53	V	201	CDL	OB7-CB5-OB6-CB4
48	r	502	PLX	C7-C8-C9-C10
53	r	504	CDL	C82-C83-C84-C85
53	r	505	CDL	C71-C72-C73-C74
53	u	201	CDL	C11-C12-C13-C14
53	l	702	CDL	CB2-C1-CA2-OA2
47	C	302	PEE	C13-C14-C15-C16
48	r	502	PLX	C31-C32-C33-C34
53	r	504	CDL	C56-C57-C58-C59
47	Q	501	PEE	C12-C13-C14-C15
47	b	201	PEE	C33-C34-C35-C36
48	g	201	PLX	C27-C28-C29-C30
53	a	201	CDL	C75-C76-C77-C78
53	r	504	CDL	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	r	504	CDL	C35-C36-C37-C38
48	r	502	PLX	C13-C14-C15-C16
53	l	702	CDL	C58-C59-C60-C61
48	g	201	PLX	C33-C34-C35-C36
47	r	501	PEE	C13-C14-C15-C16
48	g	201	PLX	C11-C10-C9-C8
48	j	201	PLX	C12-C13-C14-C15
53	r	505	CDL	C32-C33-C34-C35
47	r	501	PEE	C11-C10-O2-C2
46	A	502	FMN	O2'-C2'-C3'-C4'
47	i	402	PEE	C19-C20-C21-C22
53	o	201	CDL	C75-C76-C77-C78
53	o	201	CDL	C83-C84-C85-C86
53	i	401	CDL	CB5-C51-C52-C53
53	r	505	CDL	CB5-C51-C52-C53
53	i	401	CDL	C33-C34-C35-C36
53	l	702	CDL	C73-C74-C75-C76
53	r	505	CDL	C43-C44-C45-C46
53	N	201	CDL	OB9-CB7-OB8-CB6
53	a	201	CDL	OB9-CB7-OB8-CB6
48	j	201	PLX	C7-C8-C9-C10
53	l	702	CDL	C55-C56-C57-C58
48	C	303	PLX	C14-C15-C16-C17
48	r	503	PLX	C14-C15-C16-C17
48	r	503	PLX	C27-C28-C29-C30
53	r	504	CDL	C11-C12-C13-C14
53	r	505	CDL	C73-C74-C75-C76
47	U	101	PEE	C41-C42-C43-C44
48	g	201	PLX	C9-C10-C11-C12
48	j	201	PLX	C10-C11-C12-C13
48	C	303	PLX	C27-C28-C29-C30
48	g	201	PLX	C28-C29-C30-C31
53	r	504	CDL	C73-C74-C75-C76
53	r	505	CDL	C37-C38-C39-C40
47	l	701	PEE	C32-C33-C34-C35
48	g	201	PLX	C25-C26-C27-C28
47	Q	501	PEE	C11-C12-C13-C14
48	C	303	PLX	C9-C10-C11-C12
48	a	202	PLX	C14-C15-C16-C17
48	g	201	PLX	C35-C36-C37-C38
47	b	201	PEE	C22-C23-C24-C25
53	r	504	CDL	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	r	505	CDL	C72-C73-C74-C75
47	W	201	PEE	C11-C10-O2-C2
47	l	701	PEE	C11-C10-O2-C2
53	u	201	CDL	C11-CA5-OA6-CA4
53	u	201	CDL	C59-C60-C61-C62
47	l	701	PEE	O4-C10-O2-C2
47	r	501	PEE	O4-C10-O2-C2
48	j	201	PLX	C14-C15-C16-C17
53	r	505	CDL	C41-C42-C43-C44
47	C	302	PEE	C19-C20-C21-C22
53	o	201	CDL	CA7-C31-C32-C33
47	i	402	PEE	C37-C38-C39-C40
47	W	201	PEE	C22-C23-C24-C25
48	r	503	PLX	C2-C1-N1-C1B
48	C	303	PLX	C13-C14-C15-C16
48	r	502	PLX	C14-C15-C16-C17
53	l	702	CDL	C41-C42-C43-C44
47	l	701	PEE	O3P-C1-C2-O2
48	a	202	PLX	O4-C3-C4-O6
53	l	702	CDL	C43-C44-C45-C46
48	j	201	PLX	C27-C28-C29-C30
53	a	201	CDL	C43-C44-C45-C46
48	r	503	PLX	C28-C29-C30-C31
53	V	201	CDL	C58-C59-C60-C61
47	r	501	PEE	C11-C12-C13-C14
47	Q	501	PEE	C39-C40-C41-C42
47	i	402	PEE	C35-C36-C37-C38
48	r	502	PLX	C15-C16-C17-C18
48	r	503	PLX	C31-C32-C33-C34
48	C	303	PLX	C16-C17-C18-C19
53	l	702	CDL	C14-C15-C16-C17
47	U	101	PEE	C36-C37-C38-C39
47	r	501	PEE	C36-C37-C38-C39
53	a	201	CDL	C52-C53-C54-C55
53	r	505	CDL	CB4-CB3-OB5-PB2
48	a	202	PLX	C9-C10-C11-C12
47	W	201	PEE	C23-C24-C25-C26
48	j	201	PLX	C25-C26-C27-C28
53	r	505	CDL	C57-C58-C59-C60
47	l	703	PEE	C11-C12-C13-C14
53	V	201	CDL	C55-C56-C57-C58
53	u	201	CDL	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
47	i	402	PEE	C21-C22-C23-C24
48	r	503	PLX	C29-C30-C31-C32
53	o	201	CDL	C82-C83-C84-C85
48	r	503	PLX	C33-C34-C35-C36
47	l	701	PEE	O3P-C1-C2-C3
53	N	201	CDL	OB5-CB3-CB4-CB6
53	i	401	CDL	OA5-CA3-CA4-CA6
53	i	401	CDL	OB5-CB3-CB4-CB6
47	W	201	PEE	O4-C10-O2-C2
53	u	201	CDL	OA7-CA5-OA6-CA4
53	V	201	CDL	C54-C55-C56-C57
53	i	401	CDL	C32-C33-C34-C35
48	r	503	PLX	C30-C31-C32-C33
53	r	504	CDL	C42-C43-C44-C45
48	C	303	PLX	C18-C19-C20-C21
48	r	503	PLX	C26-C27-C28-C29
53	o	201	CDL	C84-C85-C86-C87
48	j	201	PLX	C26-C27-C28-C29
53	i	401	CDL	C71-C72-C73-C74
53	r	505	CDL	C75-C76-C77-C78
53	i	401	CDL	C71-CB7-OB8-CB6
53	V	201	CDL	C40-C41-C42-C43
53	l	702	CDL	C60-C61-C62-C63
47	r	501	PEE	C17-C18-C19-C20
48	C	303	PLX	C17-C18-C19-C20
53	u	201	CDL	C53-C54-C55-C56
47	W	201	PEE	C1-C2-C3-O3
47	b	201	PEE	C1-C2-C3-O3
47	i	402	PEE	C1-C2-C3-O3
47	l	701	PEE	C1-C2-C3-O3
48	r	503	PLX	C3-C4-C5-O8
53	V	201	CDL	CA3-CA4-CA6-OA8
53	i	401	CDL	CB3-CB4-CB6-OB8
53	l	702	CDL	CA3-CA4-CA6-OA8
53	l	702	CDL	CB3-CB4-CB6-OB8
53	o	201	CDL	CB3-CB4-CB6-OB8
53	r	505	CDL	CB3-CB4-CB6-OB8
53	u	201	CDL	CA3-CA4-CA6-OA8
48	C	303	PLX	C26-C27-C28-C29
48	r	503	PLX	C15-C16-C17-C18
53	i	401	CDL	C37-C38-C39-C40
47	Q	501	PEE	C31-C30-O3-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	a	202	PLX	C11-C12-C13-C14
53	r	505	CDL	C17-C18-C19-C20
47	U	101	PEE	C31-C32-C33-C34
53	r	505	CDL	C52-C53-C54-C55
47	Q	501	PEE	C21-C22-C23-C24
47	b	201	PEE	C23-C24-C25-C26
48	a	202	PLX	C11-C10-C9-C8
53	a	201	CDL	C14-C15-C16-C17
53	r	504	CDL	C71-C72-C73-C74
47	l	701	PEE	C35-C36-C37-C38
53	l	702	CDL	CA7-C31-C32-C33
53	i	401	CDL	OB9-CB7-OB8-CB6
48	C	303	PLX	O4-C3-C4-O6
53	N	201	CDL	C51-C52-C53-C54
53	a	201	CDL	C76-C77-C78-C79
48	r	502	PLX	C16-C17-C18-C19
53	r	504	CDL	C34-C35-C36-C37
47	b	201	PEE	C32-C33-C34-C35
53	r	504	CDL	C39-C40-C41-C42
53	r	505	CDL	OB6-CB4-CB6-OB8
53	l	702	CDL	C64-C65-C66-C67
47	l	703	PEE	C19-C20-C21-C22
53	u	201	CDL	CA5-C11-C12-C13
49	X	201	8Q1	C29-C32-C34-O35
48	C	303	PLX	C33-C34-C35-C36
48	g	201	PLX	C14-C15-C16-C17
53	a	201	CDL	C32-C33-C34-C35
53	r	505	CDL	C14-C15-C16-C17
53	r	505	CDL	C60-C61-C62-C63
47	i	402	PEE	C18-C19-C20-C21
48	r	503	PLX	C16-C17-C18-C19
53	u	201	CDL	C60-C61-C62-C63
47	C	302	PEE	C42-C43-C44-C45
53	l	702	CDL	C56-C57-C58-C59
53	r	505	CDL	C20-C21-C22-C23
47	Q	501	PEE	C44-C45-C46-C47
49	G	201	8Q1	C13-C14-C15-C16
48	r	502	PLX	C33-C34-C35-C36
48	r	503	PLX	C7-C8-C9-C10
53	V	201	CDL	C14-C15-C16-C17
53	i	401	CDL	C11-C12-C13-C14
53	o	201	CDL	C52-C53-C54-C55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	a	202	PLX	O4-C3-C4-C5
48	j	201	PLX	O4-C3-C4-C5
53	a	201	CDL	OB5-CB3-CB4-CB6
53	r	505	CDL	C31-C32-C33-C34
48	r	503	PLX	C35-C36-C37-C38
53	a	201	CDL	C60-C61-C62-C63
53	N	201	CDL	C71-C72-C73-C74
48	j	201	PLX	C33-C34-C35-C36
47	W	201	PEE	O3-C30-C31-C32
53	a	201	CDL	C71-C72-C73-C74
47	Q	501	PEE	O5-C30-O3-C3
47	U	101	PEE	C30-C31-C32-C33
47	l	703	PEE	C31-C32-C33-C34
48	g	201	PLX	C11-C12-C13-C14
53	r	504	CDL	C76-C77-C78-C79
53	l	702	CDL	C52-C53-C54-C55
48	g	201	PLX	C36-C37-C38-C39
47	C	302	PEE	C1-C2-C3-O3
48	j	201	PLX	C3-C4-C5-O8
48	r	502	PLX	C3-C4-C5-O8
49	X	201	8Q1	O33-C32-C34-N36
53	N	201	CDL	CA3-CA4-CA6-OA8
53	i	401	CDL	CA3-CA4-CA6-OA8
53	o	201	CDL	CA3-CA4-CA6-OA8
47	l	703	PEE	C14-C15-C16-C17
47	b	201	PEE	C11-C12-C13-C14
48	C	303	PLX	C15-C16-C17-C18
48	C	303	PLX	C11-C12-C13-C14
48	a	202	PLX	C30-C31-C32-C33
53	l	702	CDL	C53-C54-C55-C56
48	g	201	PLX	C13-C14-C15-C16
53	r	505	CDL	CB7-C71-C72-C73
48	j	201	PLX	O4-C3-C4-O6
53	V	201	CDL	OB5-CB3-CB4-OB6
53	a	201	CDL	OA5-CA3-CA4-OA6
48	j	201	PLX	C13-C14-C15-C16
53	V	201	CDL	C75-C76-C77-C78
49	X	201	8Q1	O4-C1-S44-C43
48	C	303	PLX	C28-C29-C30-C31
47	l	701	PEE	C13-C14-C15-C16
47	i	402	PEE	C24-C25-C26-C27
53	r	505	CDL	C54-C55-C56-C57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
47	C	302	PEE	O2-C2-C3-O3
47	W	201	PEE	O2-C2-C3-O3
47	b	201	PEE	O2-C2-C3-O3
48	r	502	PLX	O6-C4-C5-O8
48	r	503	PLX	O6-C4-C5-O8
53	r	505	CDL	OA6-CA4-CA6-OA8
48	j	201	PLX	C9-C10-C11-C12
53	r	504	CDL	C40-C41-C42-C43
48	r	503	PLX	O8-C24-C25-C26
53	V	201	CDL	C57-C58-C59-C60
53	a	201	CDL	C53-C54-C55-C56
53	o	201	CDL	C54-C55-C56-C57
53	N	201	CDL	C31-C32-C33-C34
53	r	504	CDL	CA7-C31-C32-C33
47	Q	501	PEE	C40-C41-C42-C43
53	i	401	CDL	C75-C76-C77-C78
48	r	502	PLX	C28-C29-C30-C31
48	C	303	PLX	C31-C32-C33-C34
53	i	401	CDL	C73-C74-C75-C76
48	g	201	PLX	C16-C17-C18-C19
53	r	505	CDL	C78-C79-C80-C81
53	i	401	CDL	C74-C75-C76-C77
49	X	201	8Q1	C6-C1-S44-C43
47	U	101	PEE	C40-C41-C42-C43
53	l	702	CDL	C54-C55-C56-C57
53	N	201	CDL	CB2-C1-CA2-OA2
48	r	503	PLX	C18-C19-C20-C21
53	o	201	CDL	C32-C31-CA7-OA8
53	r	505	CDL	C55-C56-C57-C58
47	Q	501	PEE	O3P-C1-C2-C3
47	b	201	PEE	O3P-C1-C2-C3
47	i	402	PEE	O3P-C1-C2-C3
47	l	703	PEE	O3P-C1-C2-C3
48	C	303	PLX	O4-C3-C4-C5
53	a	201	CDL	OA5-CA3-CA4-CA6
53	a	201	CDL	C15-C16-C17-C18
53	o	201	CDL	C33-C34-C35-C36
47	i	402	PEE	C14-C15-C16-C17
47	Q	501	PEE	C34-C35-C36-C37
53	i	401	CDL	C35-C36-C37-C38
55	s	401	UQ	C5-C6-C7-C8
53	l	702	CDL	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	r	502	PLX	C12-C13-C14-C15
53	r	504	CDL	C23-C24-C25-C26
53	V	201	CDL	CA6-CA4-OA6-CA5
47	b	201	PEE	C16-C17-C18-C19
47	C	302	PEE	C39-C40-C41-C42
47	b	201	PEE	C15-C16-C17-C18
48	a	202	PLX	C13-C14-C15-C16
48	g	201	PLX	C29-C30-C31-C32
53	u	201	CDL	C54-C55-C56-C57
48	g	201	PLX	O4-C3-C4-O6
53	V	201	CDL	OA5-CA3-CA4-OA6
53	i	401	CDL	OB5-CB3-CB4-OB6
53	o	201	CDL	OA5-CA3-CA4-OA6
47	r	501	PEE	C1-C2-C3-O3
47	Q	501	PEE	C32-C33-C34-C35
47	r	501	PEE	C12-C13-C14-C15
55	s	401	UQ	C1-C6-C7-C8
47	C	302	PEE	C37-C38-C39-C40
47	C	302	PEE	C14-C15-C16-C17
53	a	201	CDL	C11-C12-C13-C14
53	r	505	CDL	C39-C40-C41-C42
48	j	201	PLX	O6-C4-C5-O8
53	i	401	CDL	OA6-CA4-CA6-OA8
53	u	201	CDL	OA6-CA4-CA6-OA8
53	u	201	CDL	C72-C73-C74-C75
47	U	101	PEE	C12-C13-C14-C15
48	a	202	PLX	C10-C11-C12-C13
53	a	201	CDL	C17-C18-C19-C20
53	r	504	CDL	C36-C37-C38-C39
48	j	201	PLX	C7-C6-O6-C4
48	C	303	PLX	C7-C8-C9-C10
48	j	201	PLX	C31-C32-C33-C34
50	J	401	NDP	O4D-C1D-N1N-C6N
48	r	503	PLX	C9-C10-C11-C12
48	r	503	PLX	C11-C12-C13-C14
53	l	702	CDL	C32-C33-C34-C35
48	C	303	PLX	O9-C24-C25-C26
48	a	202	PLX	C25-C24-O8-C5
48	j	201	PLX	C25-C24-O8-C5
48	a	202	PLX	C19-C20-C21-C22
47	r	501	PEE	O3P-C1-C2-C3
48	g	201	PLX	O4-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	a	202	PLX	C25-C26-C27-C28
46	A	502	FMN	O2'-C2'-C3'-O3'
48	C	303	PLX	C11-C10-C9-C8
53	a	201	CDL	C31-CA7-OA8-CA6
53	r	504	CDL	C61-C62-C63-C64
47	C	302	PEE	C18-C19-C20-C21
47	W	201	PEE	C16-C17-C18-C19
47	l	703	PEE	C16-C17-C18-C19
47	W	201	PEE	C13-C14-C15-C16
53	r	504	CDL	C81-C82-C83-C84
48	j	201	PLX	O6-C6-C7-C8
47	Q	501	PEE	O3P-C1-C2-O2
47	b	201	PEE	O3P-C1-C2-O2
47	i	402	PEE	O3P-C1-C2-O2
47	r	501	PEE	O3P-C1-C2-O2
53	N	201	CDL	OB5-CB3-CB4-OB6
53	a	201	CDL	OB5-CB3-CB4-OB6
53	i	401	CDL	OA5-CA3-CA4-OA6
53	l	702	CDL	OA5-CA3-CA4-OA6
53	o	201	CDL	C56-C57-C58-C59
47	l	701	PEE	C38-C39-C40-C41
47	l	703	PEE	C36-C37-C38-C39
48	C	303	PLX	C29-C30-C31-C32
47	r	501	PEE	O2-C2-C3-O3
53	N	201	CDL	OA6-CA4-CA6-OA8
53	r	505	CDL	CA3-CA4-CA6-OA8
47	b	201	PEE	C34-C35-C36-C37
53	a	201	CDL	OA9-CA7-OA8-CA6
53	u	201	CDL	C57-C58-C59-C60
47	l	701	PEE	C33-C34-C35-C36
47	r	501	PEE	C20-C21-C22-C23
47	C	302	PEE	C1-O3P-P-O2P
47	U	101	PEE	C1-O3P-P-O2P
47	U	101	PEE	C4-O4P-P-O1P
47	W	201	PEE	C4-O4P-P-O1P
47	l	701	PEE	C4-O4P-P-O2P
47	r	501	PEE	C1-O3P-P-O2P
48	C	303	PLX	C3-C4-O6-C6
48	C	303	PLX	C5-C4-O6-C6
48	a	202	PLX	C3-O4-P1-O2
48	j	201	PLX	C2-O1-P1-O3
48	r	502	PLX	C2-O1-P1-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	N	201	CDL	CB3-OB5-PB2-OB2
53	N	201	CDL	CB3-OB5-PB2-OB4
53	a	201	CDL	CB2-OB2-PB2-OB4
53	i	401	CDL	CA2-OA2-PA1-OA5
53	i	401	CDL	CB3-OB5-PB2-OB4
53	l	702	CDL	CB3-OB5-PB2-OB2
53	l	702	CDL	CB3-OB5-PB2-OB3
53	l	702	CDL	CB3-OB5-PB2-OB4
53	o	201	CDL	CA3-OA5-PA1-OA3
53	o	201	CDL	CB2-OB2-PB2-OB4
53	o	201	CDL	CB2-OB2-PB2-OB5
53	r	504	CDL	CA3-OA5-PA1-OA3
53	r	504	CDL	CB3-OB5-PB2-OB4
53	r	505	CDL	CA3-OA5-PA1-OA3
53	u	201	CDL	CB2-OB2-PB2-OB4
53	u	201	CDL	CB3-OB5-PB2-OB4
47	Q	501	PEE	C20-C21-C22-C23
55	s	401	UQ	C13-C14-C16-C17
47	W	201	PEE	C12-C13-C14-C15
53	l	702	CDL	C51-C52-C53-C54
48	j	201	PLX	C19-C20-C21-C22
53	a	201	CDL	C39-C40-C41-C42
48	a	202	PLX	C35-C36-C37-C38
48	C	303	PLX	C19-C20-C21-C22
47	Q	501	PEE	C10-C11-C12-C13
49	G	201	8Q1	C9-C10-C11-C12
53	l	702	CDL	OA5-CA3-CA4-CA6
47	C	302	PEE	C16-C17-C18-C19
47	W	201	PEE	O3P-C1-C2-O2
53	o	201	CDL	OB5-CB3-CB4-OB6
53	r	505	CDL	C42-C43-C44-C45
53	r	505	CDL	C44-C45-C46-C47
53	i	401	CDL	C15-C16-C17-C18
53	l	702	CDL	C40-C41-C42-C43
47	i	402	PEE	O2-C2-C3-O3
47	l	701	PEE	C18-C19-C20-C21
48	a	202	PLX	C26-C27-C28-C29
48	g	201	PLX	C15-C16-C17-C18
53	V	201	CDL	C71-C72-C73-C74
47	C	302	PEE	C32-C33-C34-C35
53	r	504	CDL	C60-C61-C62-C63
53	r	505	CDL	C64-C65-C66-C67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	j	201	PLX	C2-C1-N1-C1A
53	V	201	CDL	C34-C35-C36-C37
53	o	201	CDL	CB4-CB3-OB5-PB2
49	G	201	8Q1	N41-C42-C43-S44
47	l	701	PEE	C10-C11-C12-C13
47	Q	501	PEE	C23-C24-C25-C26
53	l	702	CDL	OB5-CB3-CB4-OB6
47	r	501	PEE	C38-C39-C40-C41
48	g	201	PLX	C32-C33-C34-C35
53	i	401	CDL	C11-CA5-OA6-CA4
47	Q	501	PEE	C13-C14-C15-C16
47	l	703	PEE	C22-C23-C24-C25
53	r	504	CDL	C54-C55-C56-C57
53	l	702	CDL	C72-C73-C74-C75
48	j	201	PLX	C11-C12-C13-C14
49	X	201	8Q1	C29-C32-C34-N36
47	U	101	PEE	C38-C39-C40-C41
48	j	201	PLX	C34-C35-C36-C37
49	G	201	8Q1	C6-C7-C8-C9
47	C	302	PEE	C33-C34-C35-C36
47	W	201	PEE	C33-C34-C35-C36
53	i	401	CDL	OA7-CA5-OA6-CA4
47	b	201	PEE	C38-C39-C40-C41
53	r	505	CDL	C33-C34-C35-C36
47	U	101	PEE	C22-C23-C24-C25
53	r	504	CDL	C16-C17-C18-C19
47	i	402	PEE	C2-C1-O3P-P
53	V	201	CDL	CA4-CA3-OA5-PA1
47	Q	501	PEE	C24-C25-C26-C27
47	Q	501	PEE	C22-C23-C24-C25
47	W	201	PEE	O3P-C1-C2-C3
53	V	201	CDL	OB5-CB3-CB4-CB6
53	l	702	CDL	OB5-CB3-CB4-CB6
53	o	201	CDL	OA5-CA3-CA4-CA6
53	V	201	CDL	C35-C36-C37-C38
47	i	402	PEE	C22-C23-C24-C25
47	i	402	PEE	C31-C32-C33-C34
47	l	703	PEE	C13-C14-C15-C16
50	J	401	NDP	C2N-C3N-C7N-N7N
47	r	501	PEE	C23-C24-C25-C26
53	r	505	CDL	C23-C24-C25-C26
53	a	201	CDL	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	l	702	CDL	C31-C32-C33-C34
53	a	201	CDL	C59-C60-C61-C62
48	j	201	PLX	O8-C24-C25-C26
47	l	703	PEE	C23-C24-C25-C26
47	W	201	PEE	O5-C30-C31-C32
48	a	202	PLX	C6-C7-C8-C9
53	a	201	CDL	C19-C20-C21-C22
48	a	202	PLX	O9-C24-C25-C26
49	G	201	8Q1	N36-C37-C38-C39
47	l	701	PEE	C16-C17-C18-C19
53	l	702	CDL	C33-C34-C35-C36
47	U	101	PEE	C19-C20-C21-C22
47	l	701	PEE	C15-C16-C17-C18
53	V	201	CDL	OA5-CA3-CA4-CA6
53	o	201	CDL	OB5-CB3-CB4-CB6
53	V	201	CDL	OA6-CA4-CA6-OA8
53	V	201	CDL	OB6-CB4-CB6-OB8
47	W	201	PEE	C18-C19-C20-C21
53	i	401	CDL	CA4-CA3-OA5-PA1
47	r	501	PEE	C41-C42-C43-C44
53	o	201	CDL	C74-C75-C76-C77
53	o	201	CDL	C57-C58-C59-C60
48	j	201	PLX	C4-C5-O8-C24
47	b	201	PEE	C18-C19-C20-C21
47	i	402	PEE	C16-C17-C18-C19
47	i	402	PEE	C38-C39-C40-C41
47	r	501	PEE	C14-C15-C16-C17
53	u	201	CDL	C22-C23-C24-C25
53	V	201	CDL	C44-C45-C46-C47
47	C	302	PEE	C38-C39-C40-C41
53	i	401	CDL	C34-C35-C36-C37
47	U	101	PEE	C37-C38-C39-C40
47	i	402	PEE	C36-C37-C38-C39
53	a	201	CDL	C18-C19-C20-C21
48	j	201	PLX	C2-C1-N1-C1C
55	s	401	UQ	C14-C16-C17-C18
48	C	303	PLX	C36-C37-C38-C39
48	g	201	PLX	O6-C6-C7-C8
53	l	702	CDL	C34-C35-C36-C37
48	r	502	PLX	C25-C26-C27-C28
47	i	402	PEE	C32-C33-C34-C35
47	U	101	PEE	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
47	l	703	PEE	C38-C39-C40-C41
47	r	501	PEE	C18-C19-C20-C21
53	N	201	CDL	OB7-CB5-OB6-CB4
47	b	201	PEE	C30-C31-C32-C33
47	U	101	PEE	O2-C10-C11-C12
53	i	401	CDL	C13-C14-C15-C16
53	o	201	CDL	C32-C31-CA7-OA9
53	l	702	CDL	C12-C11-CA5-OA6
47	Q	501	PEE	C18-C19-C20-C21
47	r	501	PEE	C16-C17-C18-C19
53	l	702	CDL	C82-C83-C84-C85
53	N	201	CDL	C51-CB5-OB6-CB4
53	a	201	CDL	C38-C39-C40-C41
53	l	702	CDL	C80-C81-C82-C83
48	j	201	PLX	C2-C1-N1-C1B
53	l	702	CDL	C63-C64-C65-C66
47	C	302	PEE	O3-C30-C31-C32
48	g	201	PLX	C30-C31-C32-C33
53	r	505	CDL	C11-C12-C13-C14
53	a	201	CDL	CB5-C51-C52-C53
47	C	302	PEE	O5-C30-O3-C3
53	u	201	CDL	C72-C71-CB7-OB8
53	r	504	CDL	OB6-CB4-CB6-OB8
48	a	202	PLX	C12-C13-C14-C15
53	r	505	CDL	C51-C52-C53-C54
47	l	703	PEE	C37-C38-C39-C40
47	r	501	PEE	C39-C40-C41-C42
47	l	701	PEE	C12-C13-C14-C15
47	l	701	PEE	O3-C30-C31-C32
47	r	501	PEE	O5-C30-O3-C3
48	g	201	PLX	C6-C7-C8-C9
47	U	101	PEE	O4-C10-C11-C12
53	u	201	CDL	C72-C71-CB7-OB9
53	l	702	CDL	C12-C11-CA5-OA7
53	V	201	CDL	C64-C65-C66-C67
47	C	302	PEE	C31-C30-O3-C3
47	r	501	PEE	C31-C30-O3-C3
55	s	401	UQ	C17-C18-C19-C20
53	o	201	CDL	C80-C81-C82-C83
53	u	201	CDL	C56-C57-C58-C59
48	g	201	PLX	O9-C24-O8-C5
48	r	502	PLX	O9-C24-O8-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	r	503	PLX	O9-C24-O8-C5
50	J	401	NDP	C2N-C3N-C7N-O7N
53	N	201	CDL	C72-C71-CB7-OB8
47	l	703	PEE	C2-C1-O3P-P
53	u	201	CDL	OB7-CB5-OB6-CB4
48	C	303	PLX	C24-C25-C26-C27
47	C	302	PEE	O5-C30-C31-C32
53	o	201	CDL	C52-C51-CB5-OB6
53	r	505	CDL	C52-C51-CB5-OB6
53	r	505	CDL	C13-C14-C15-C16
53	r	504	CDL	C72-C71-CB7-OB8
53	u	201	CDL	C51-CB5-OB6-CB4
56	w	401	ADP	PB-O3A-PA-O2A
53	l	702	CDL	C52-C51-CB5-OB6

There are no ring outliers.

31 monomers are involved in 100 short contacts:

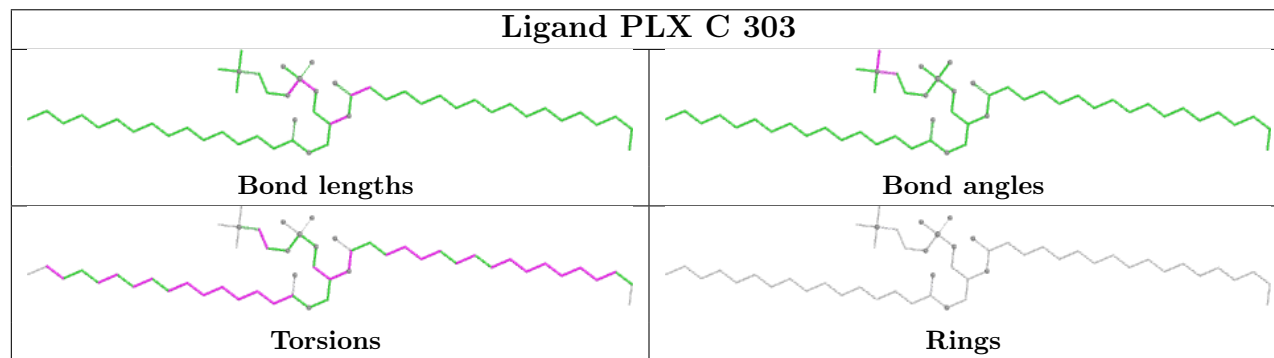
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	C	303	PLX	4	0
53	u	201	CDL	8	0
47	Q	501	PEE	4	0
48	a	202	PLX	2	0
48	g	201	PLX	4	0
50	J	401	NDP	2	0
48	r	502	PLX	3	0
53	r	505	CDL	8	0
48	j	201	PLX	3	0
47	C	302	PEE	2	0
48	r	503	PLX	3	0
53	i	401	CDL	2	0
49	X	201	8Q1	3	0
45	C	301	SF4	2	0
47	W	201	PEE	2	0
55	s	401	UQ	2	0
46	A	502	FMN	3	0
47	i	402	PEE	3	0
53	a	201	CDL	2	0
53	r	504	CDL	12	0
45	A	501	SF4	1	0
45	B	302	SF4	2	0
53	N	201	CDL	3	0

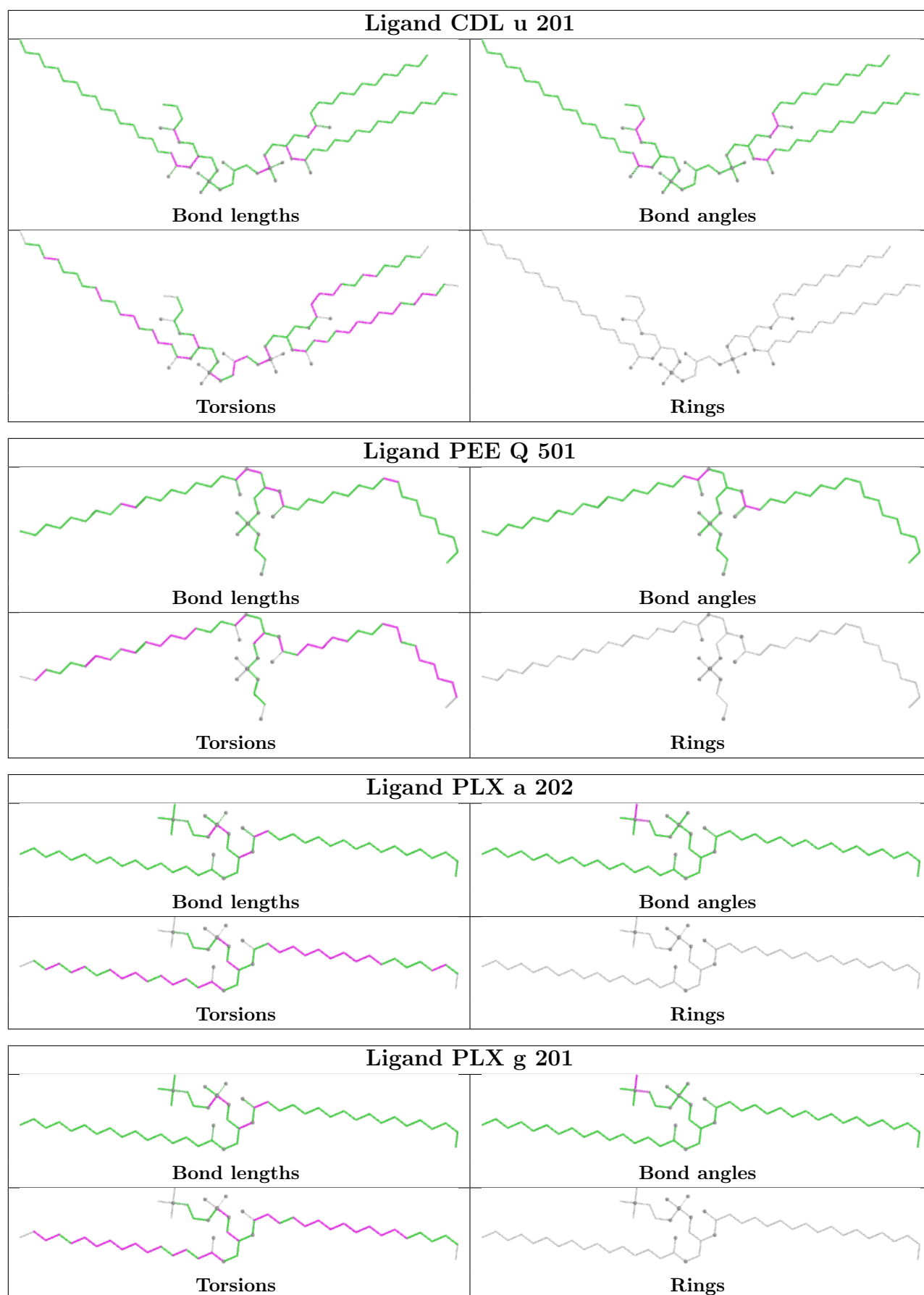
Continued on next page...

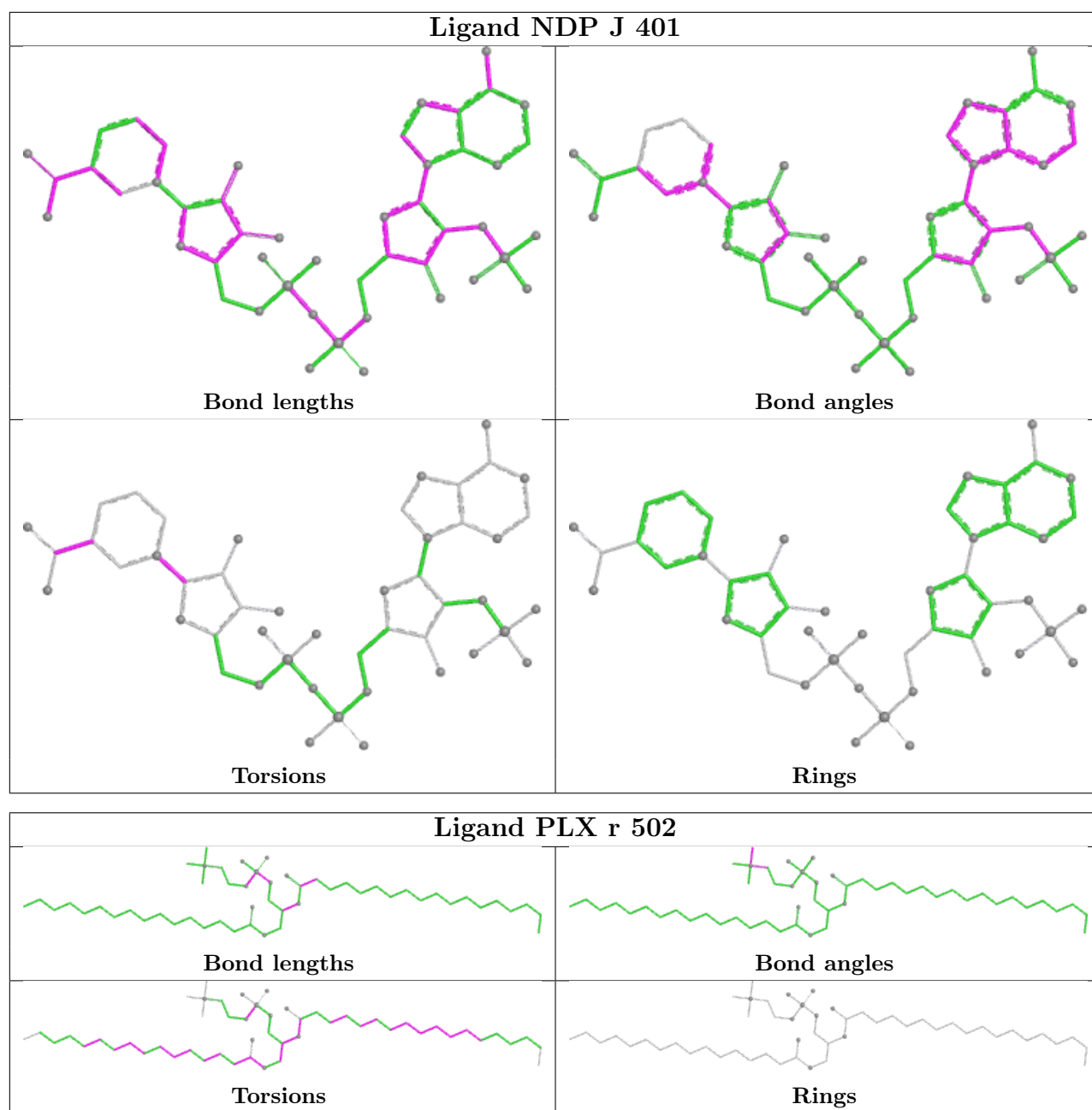
Continued from previous page...

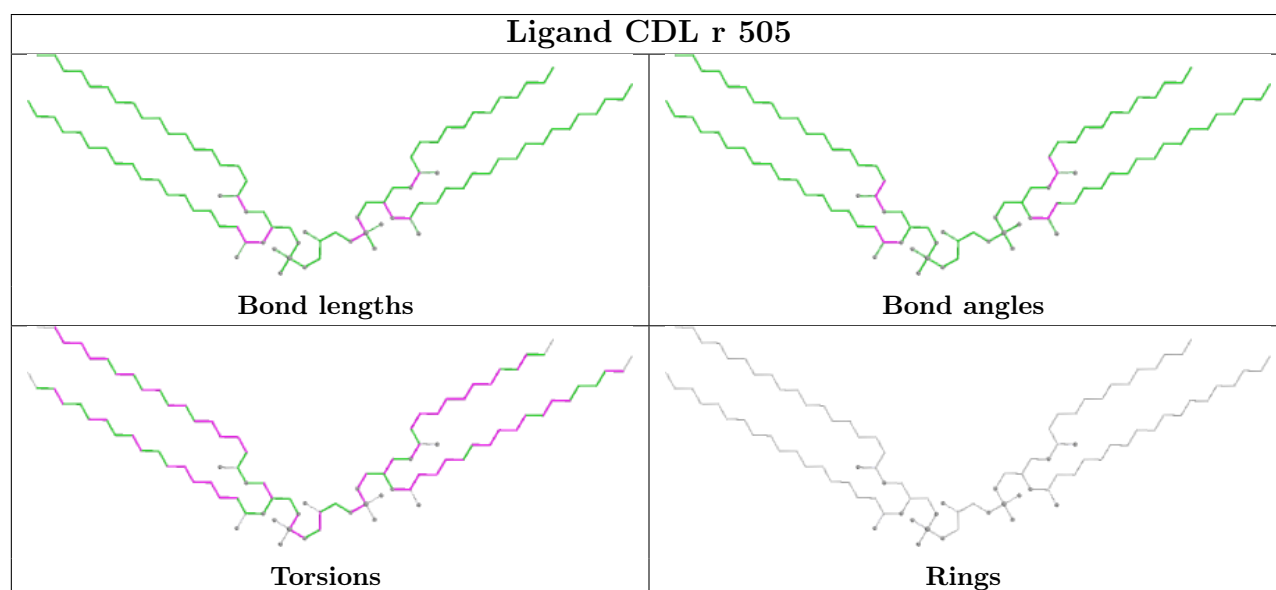
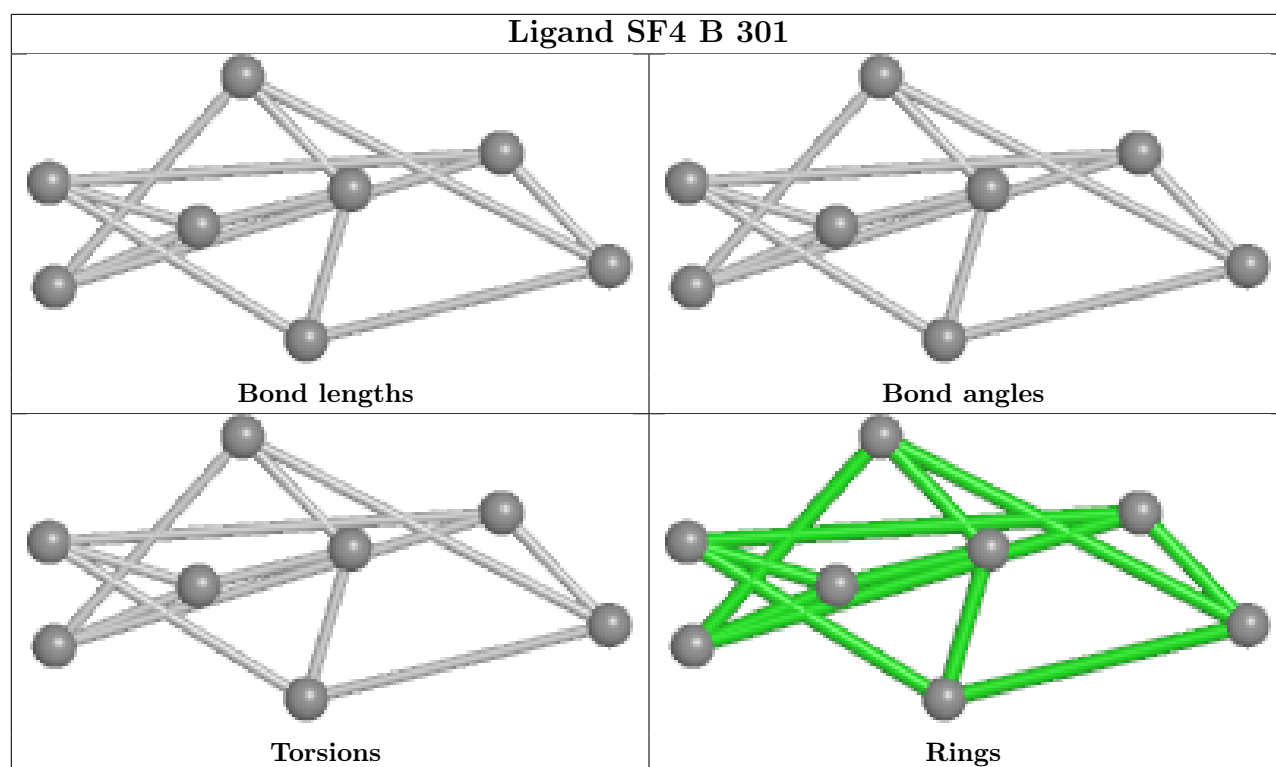
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	r	501	PEE	3	0
47	l	701	PEE	3	0
53	V	201	CDL	3	0
56	w	401	ADP	2	0
53	o	201	CDL	5	0
53	l	702	CDL	3	0
47	l	703	PEE	2	0
47	b	201	PEE	1	0

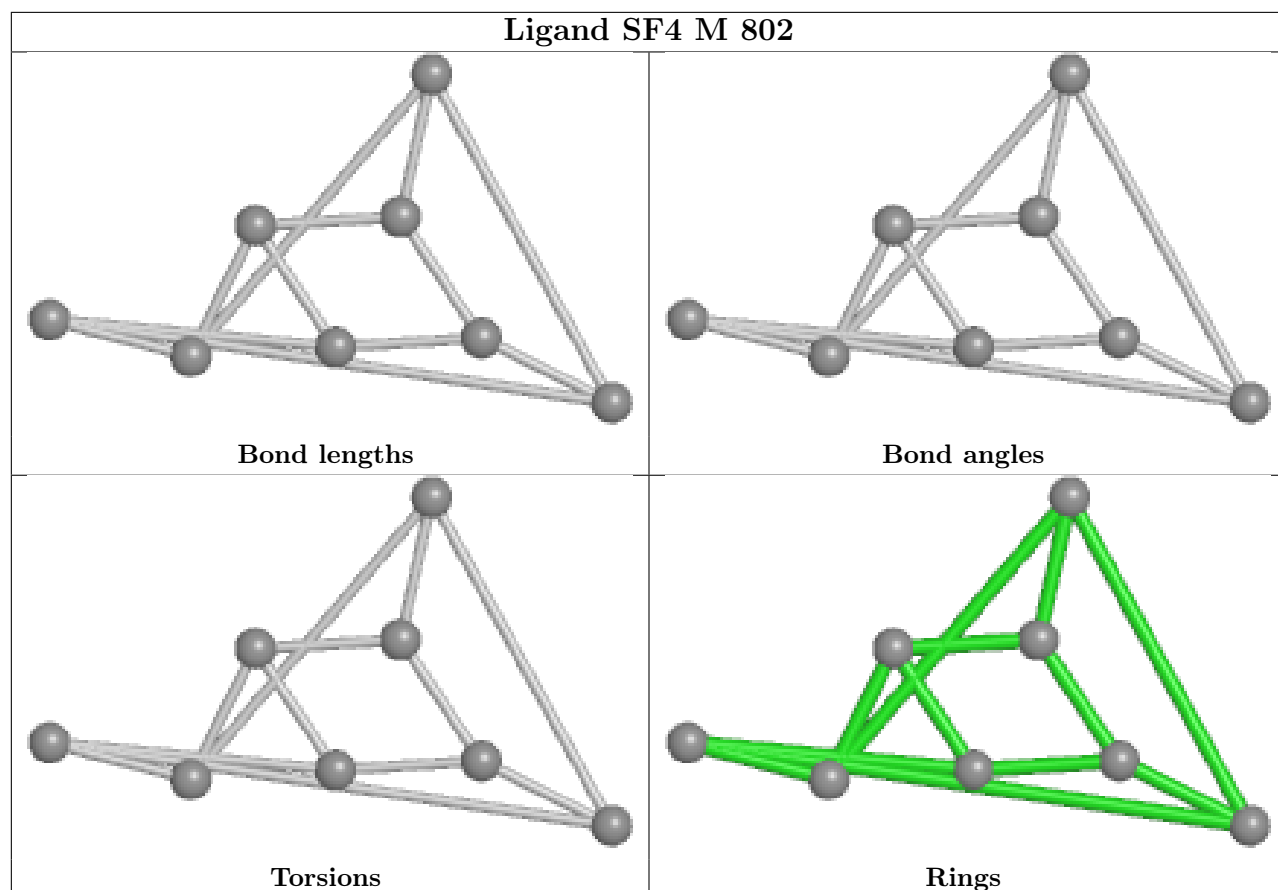
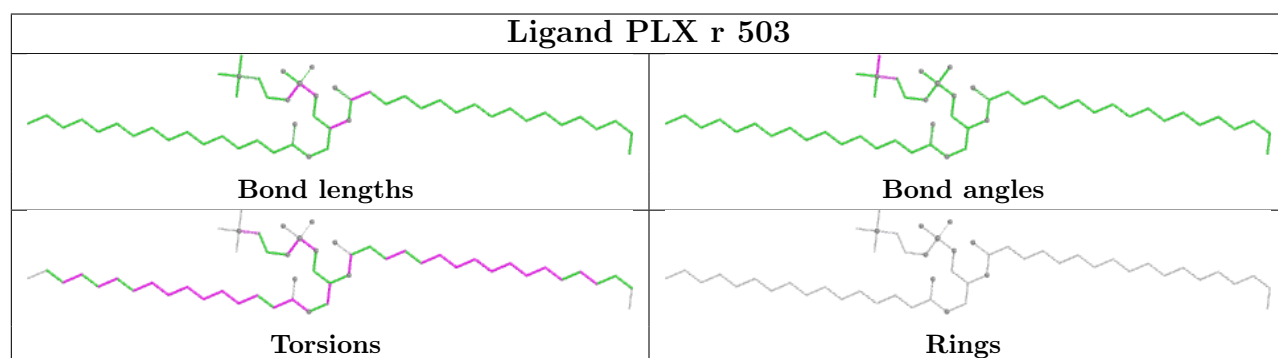
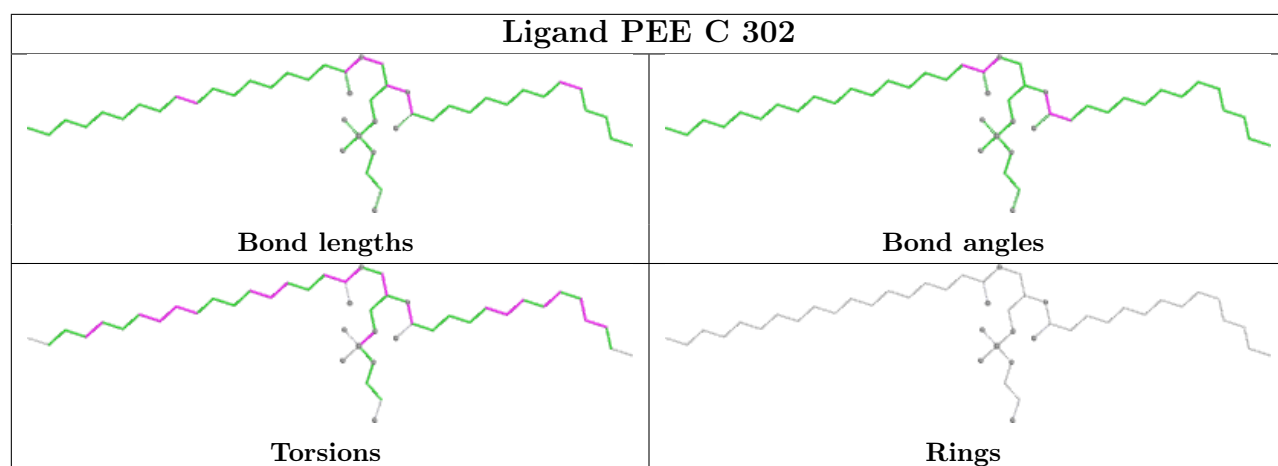
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

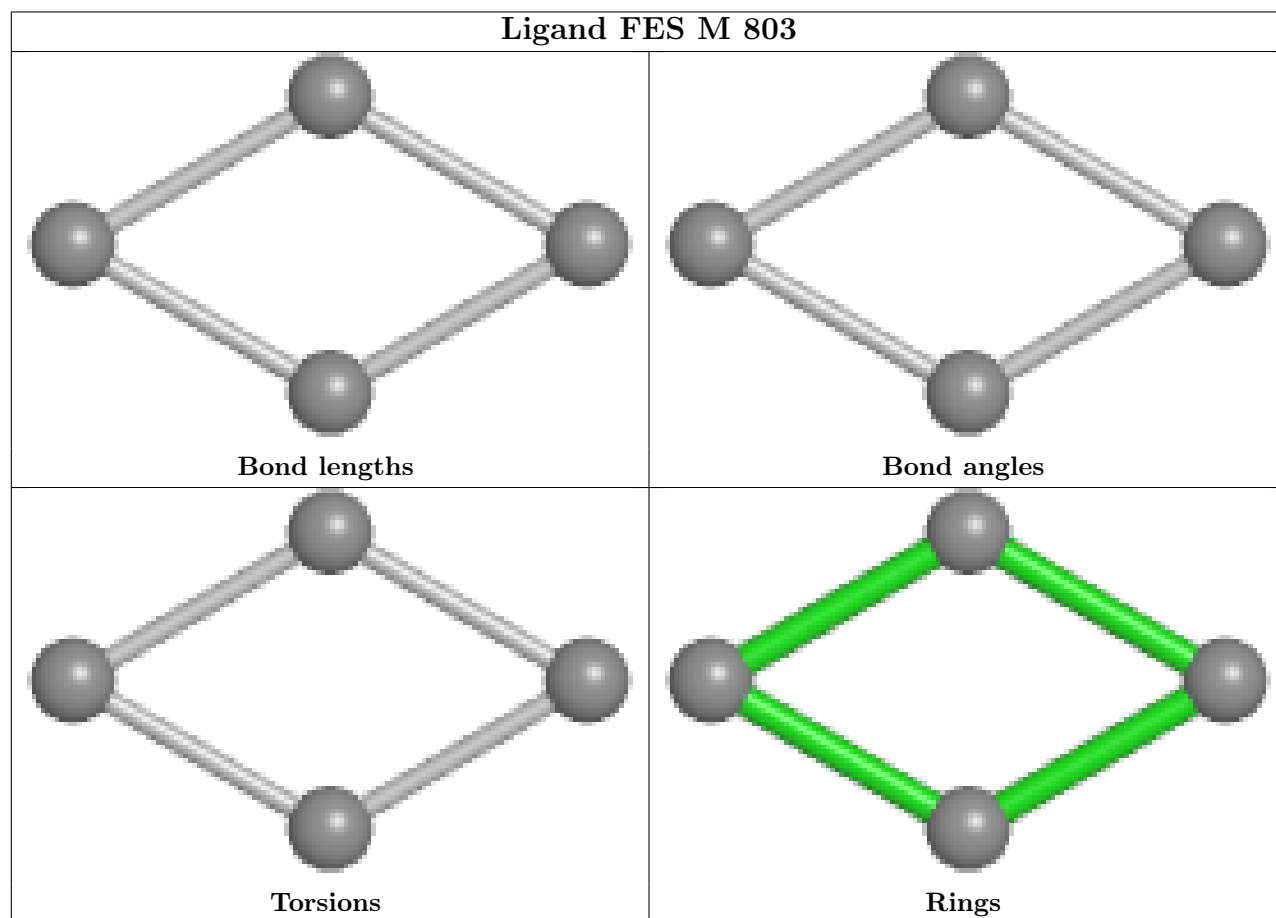
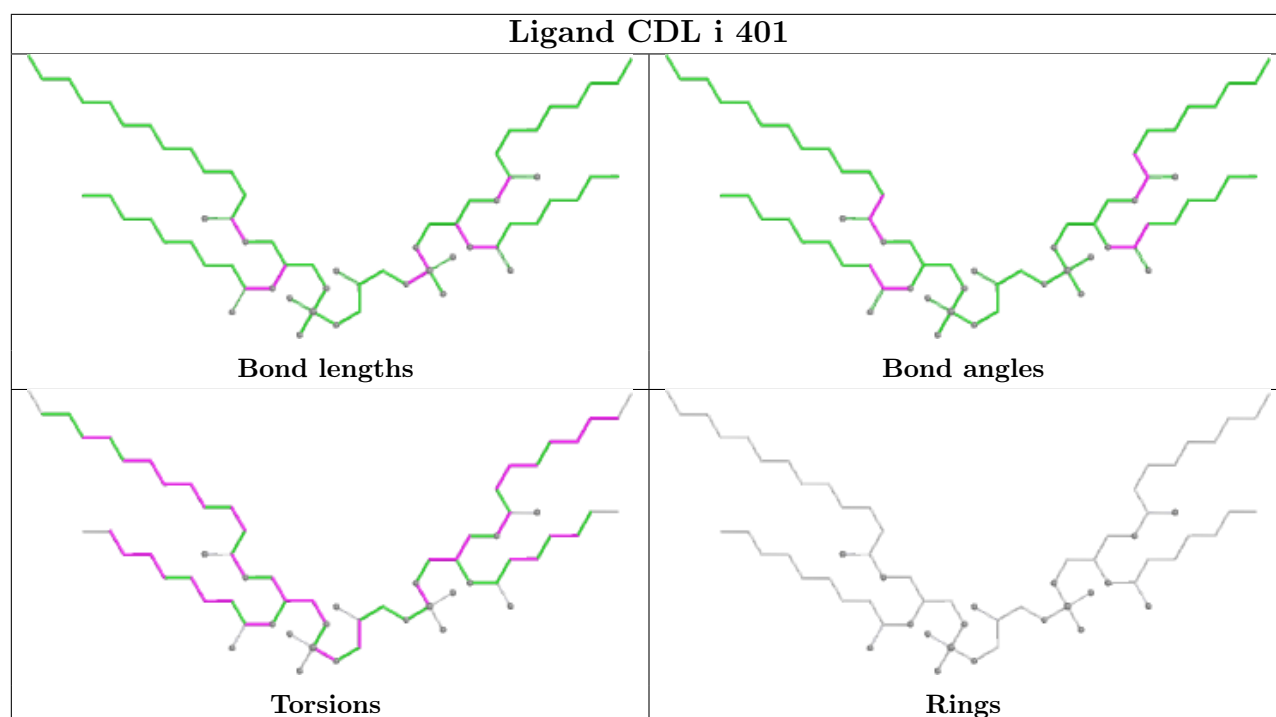


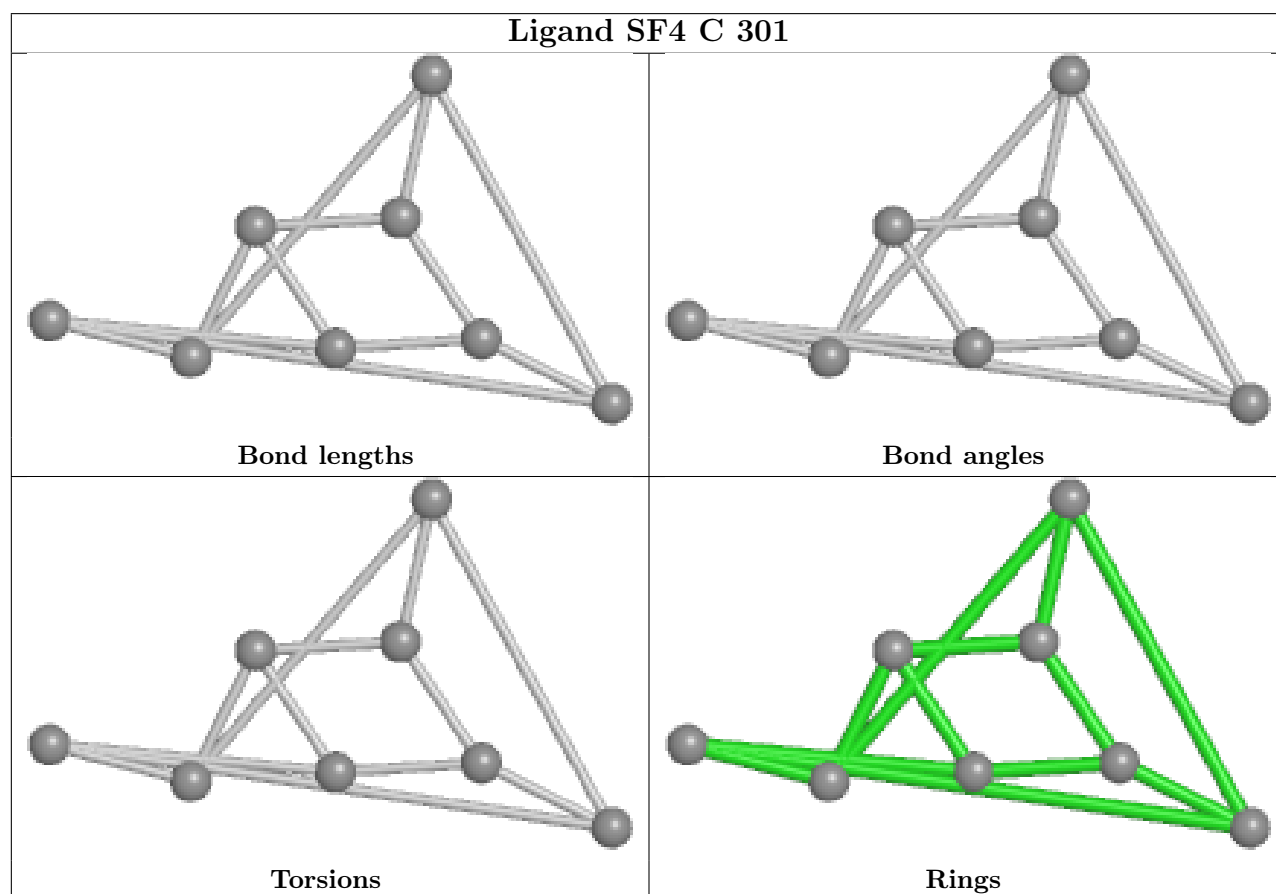
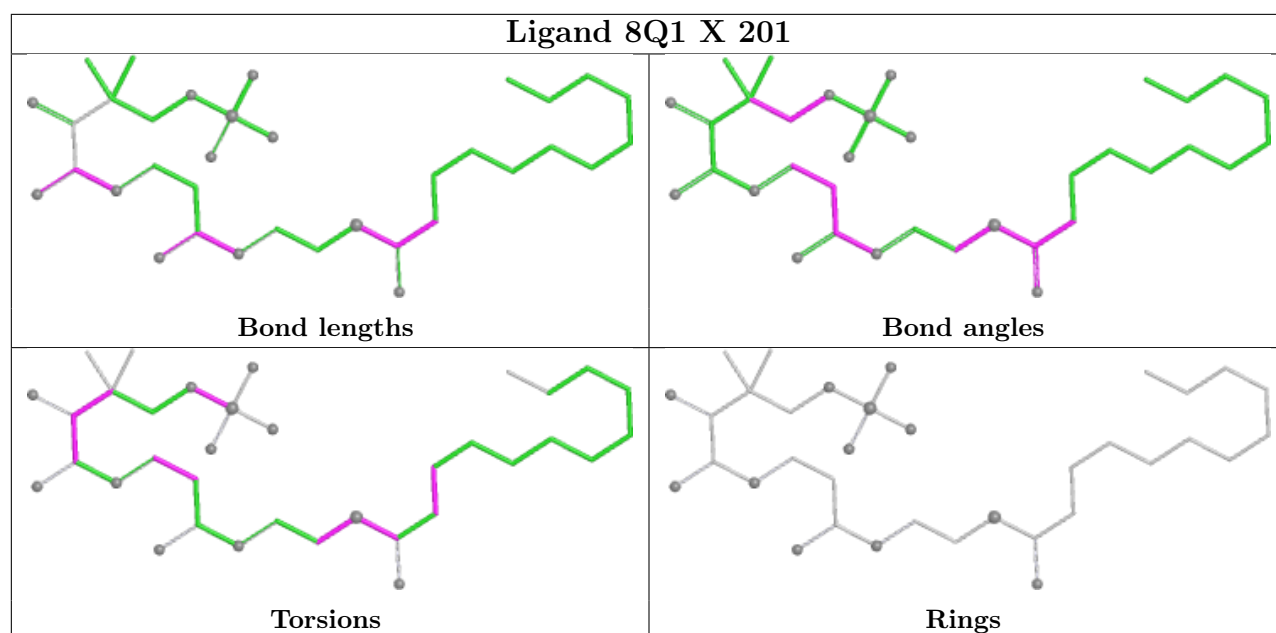


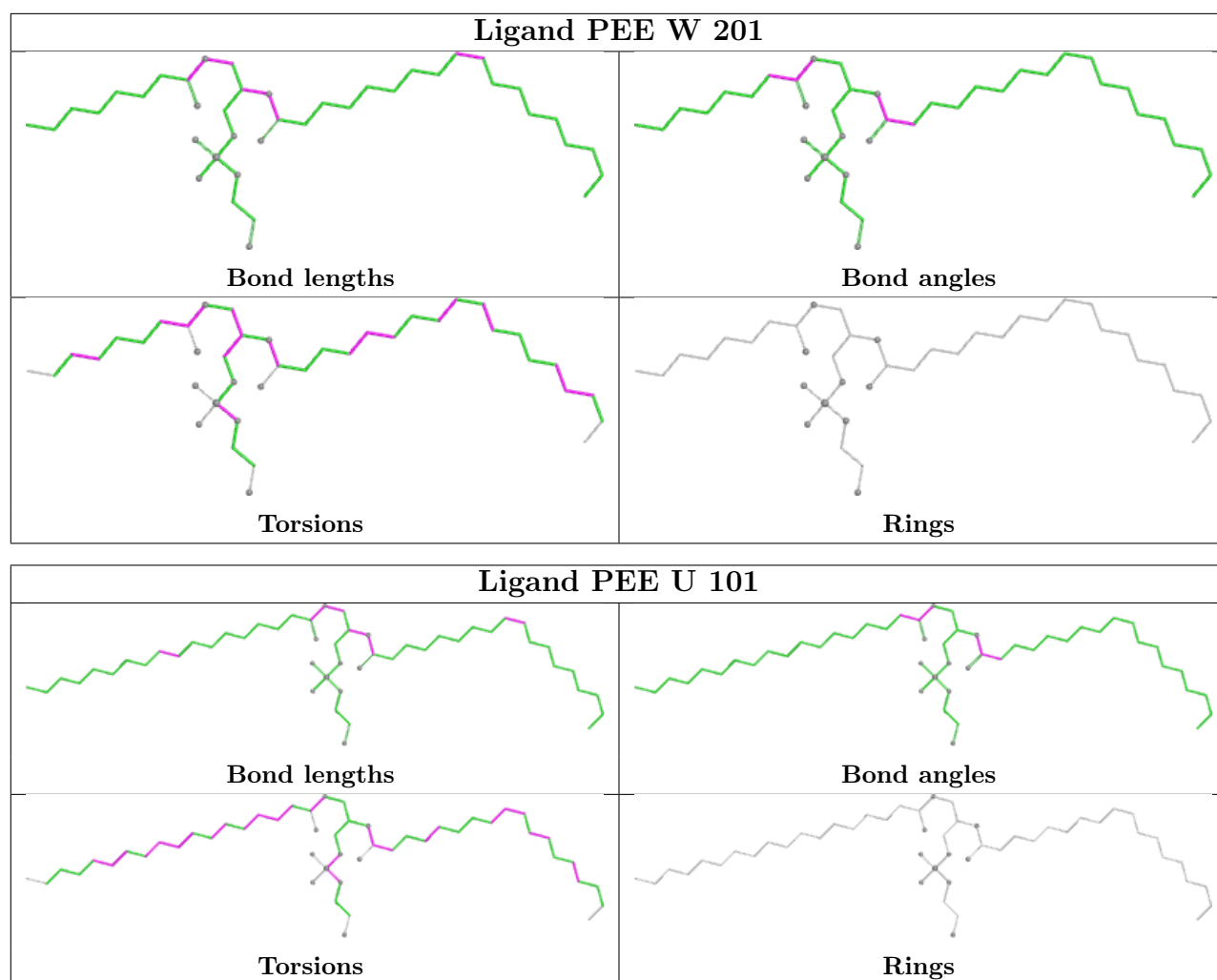


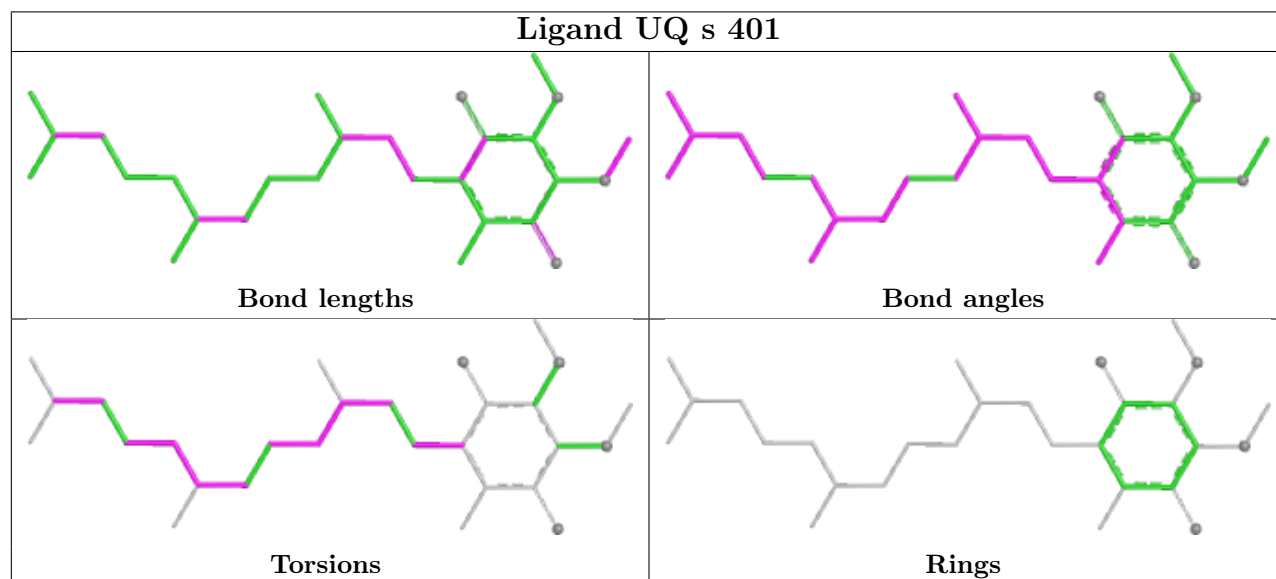
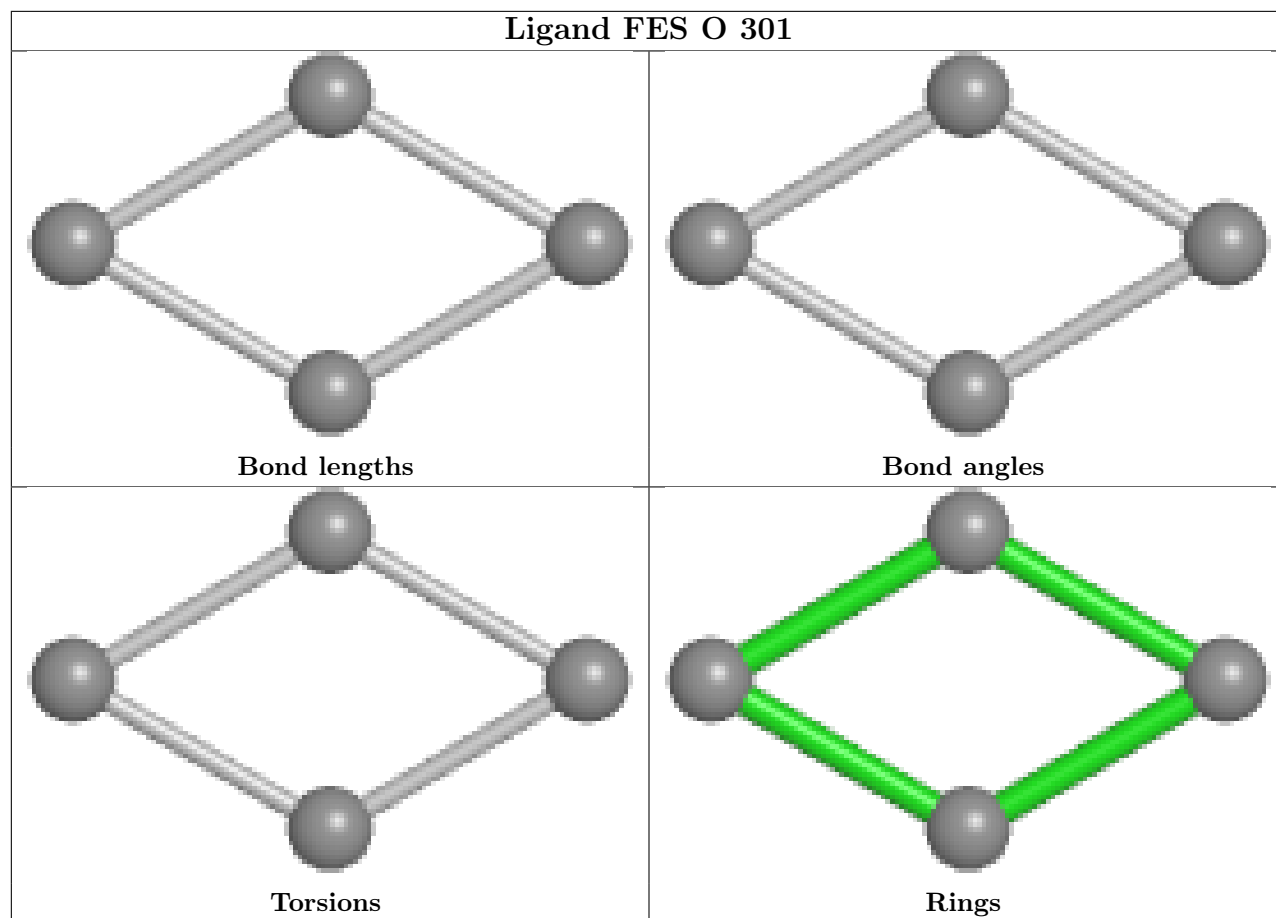


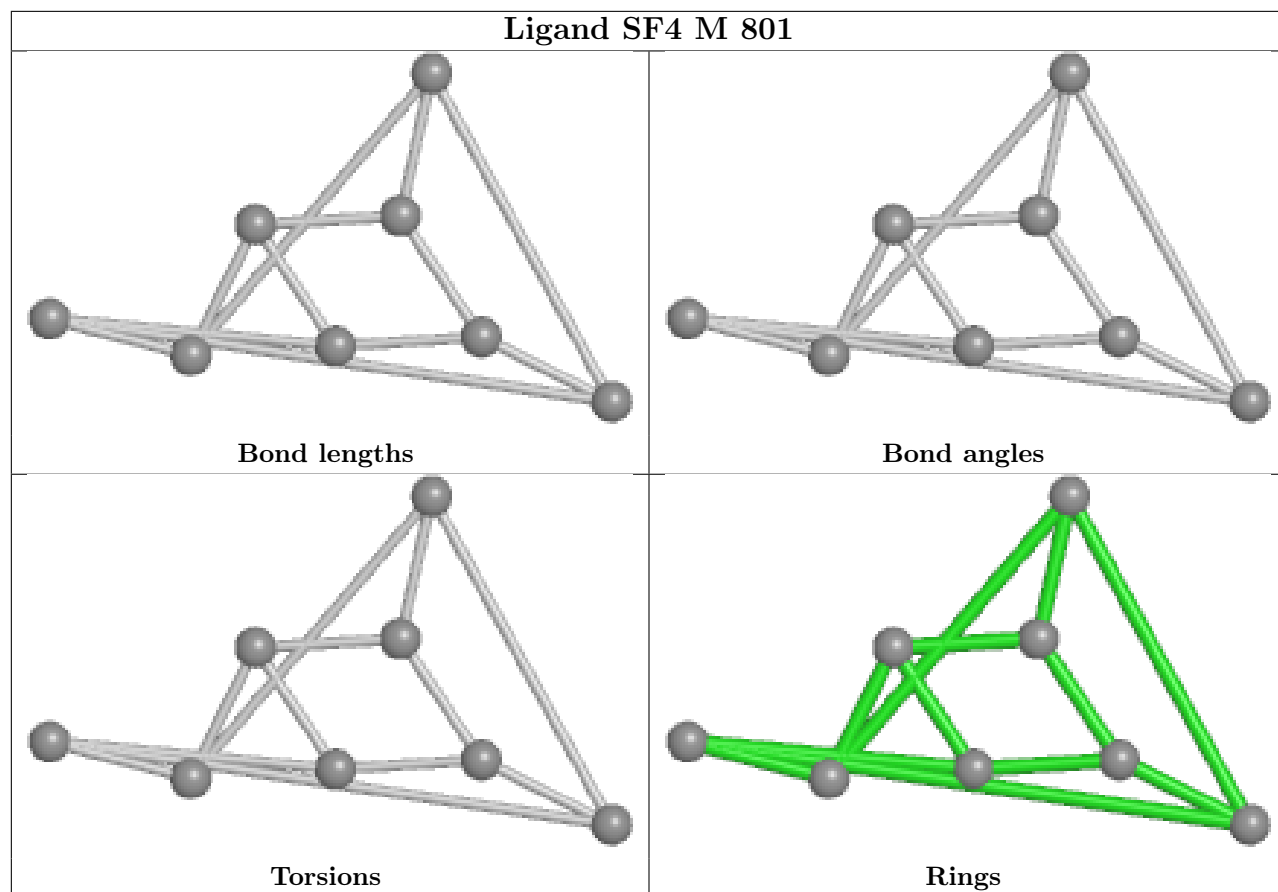


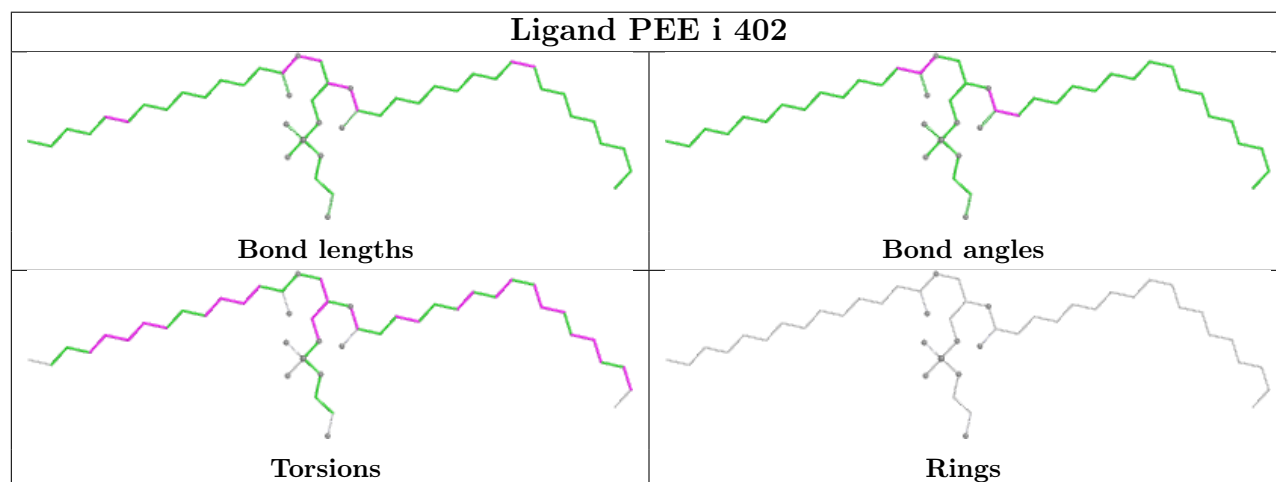
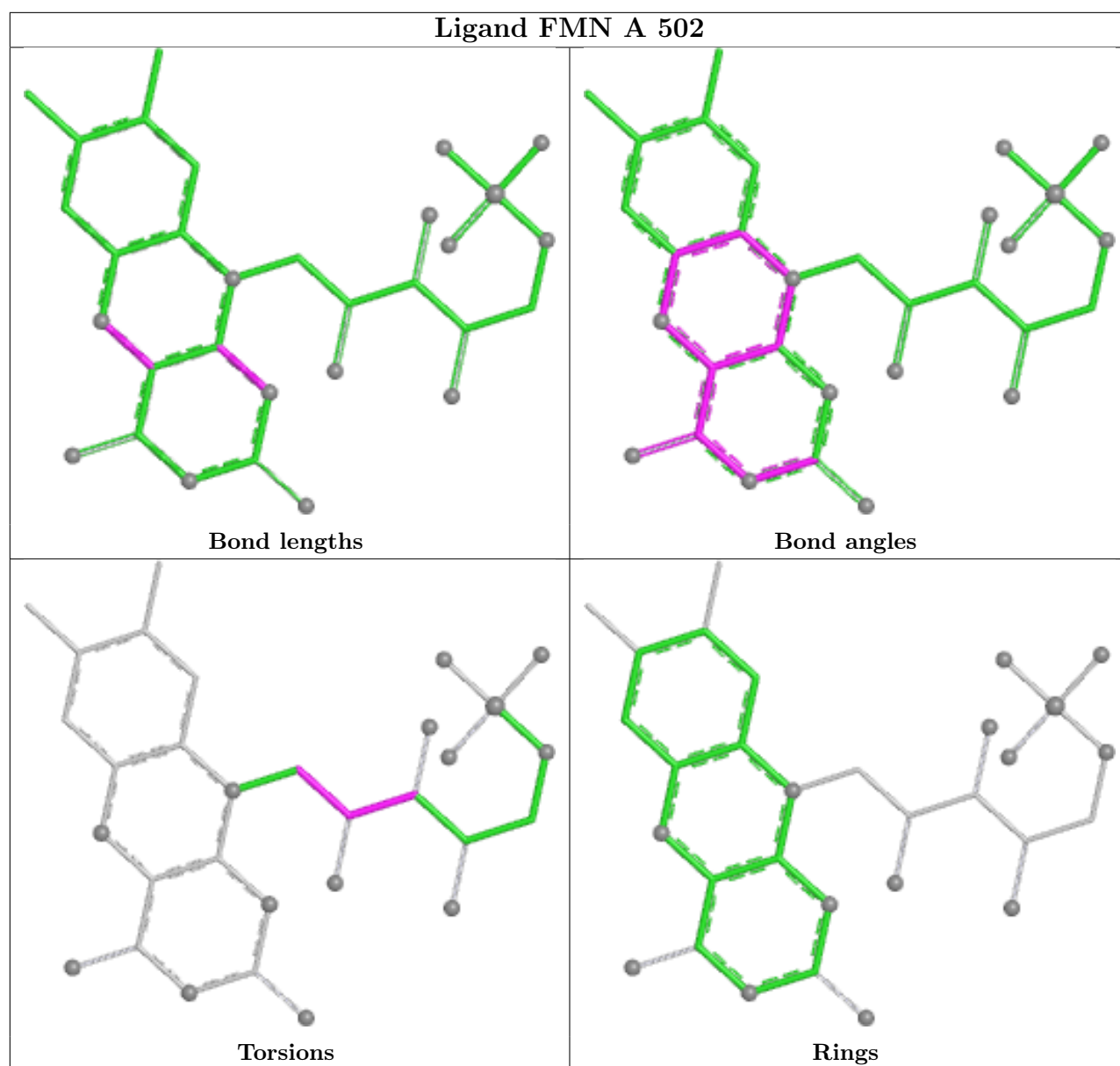


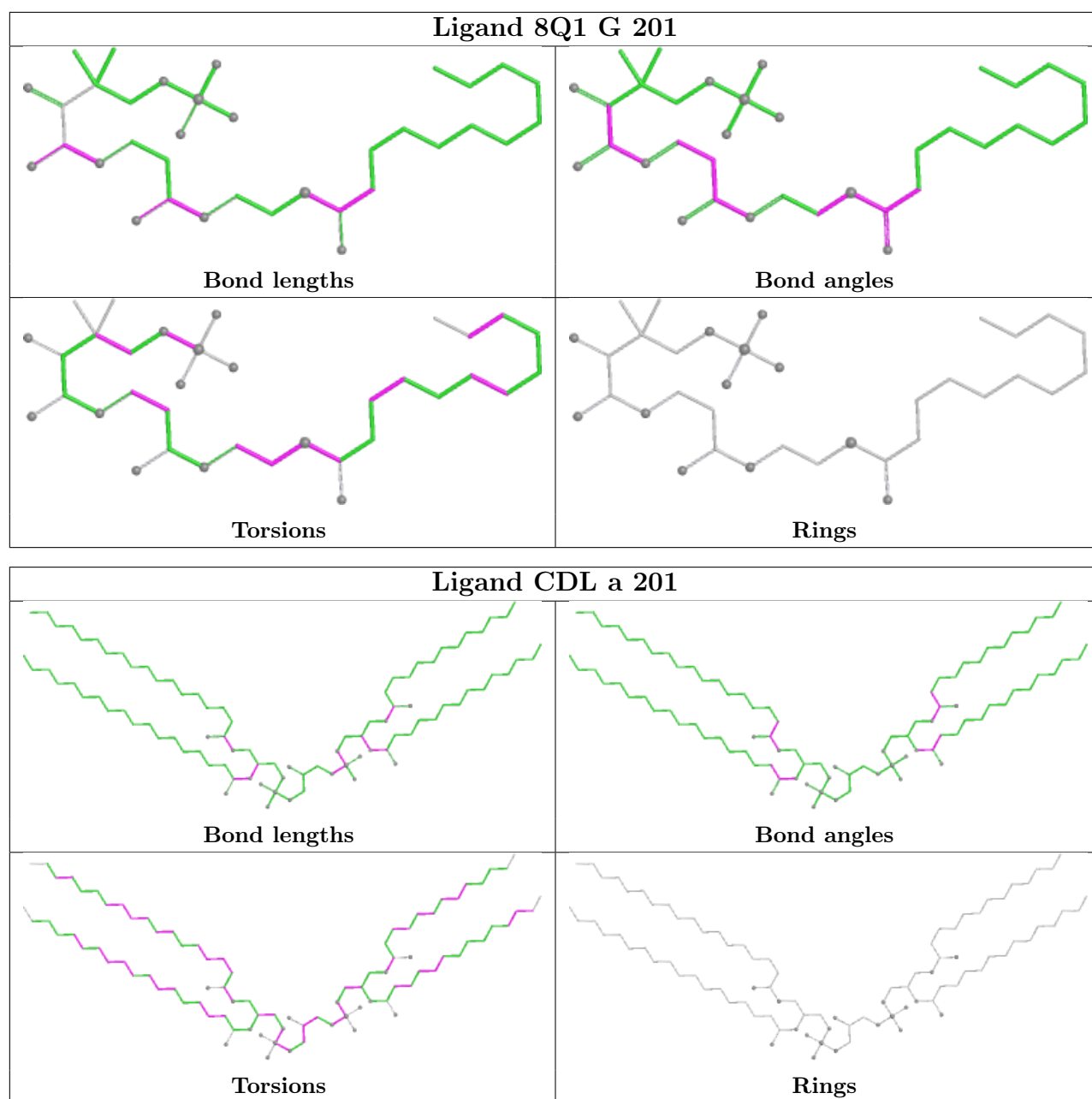


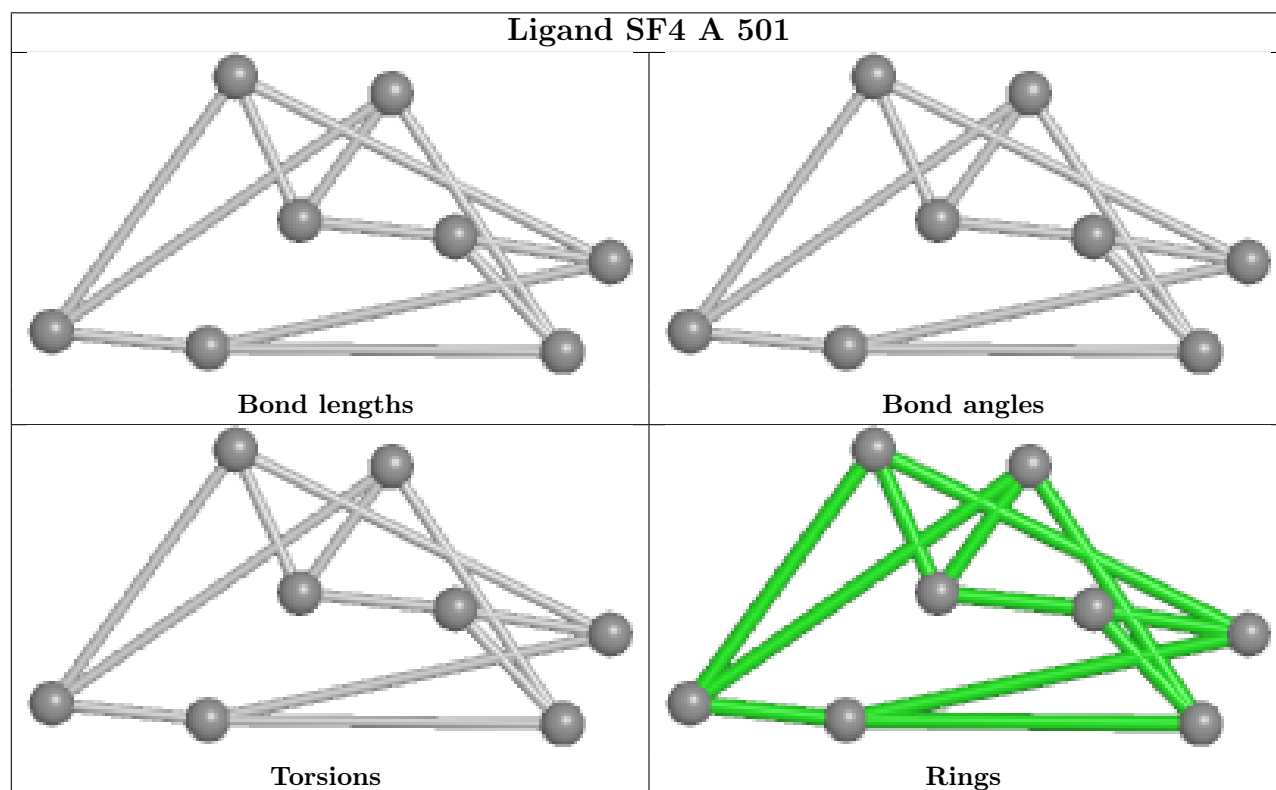
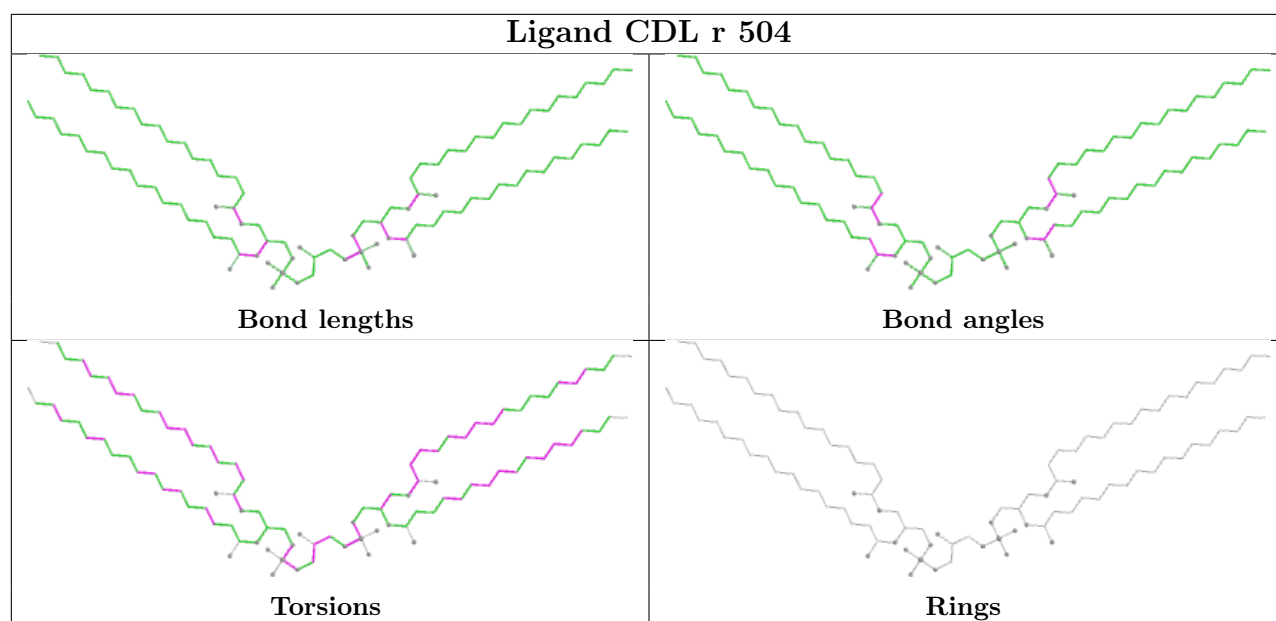


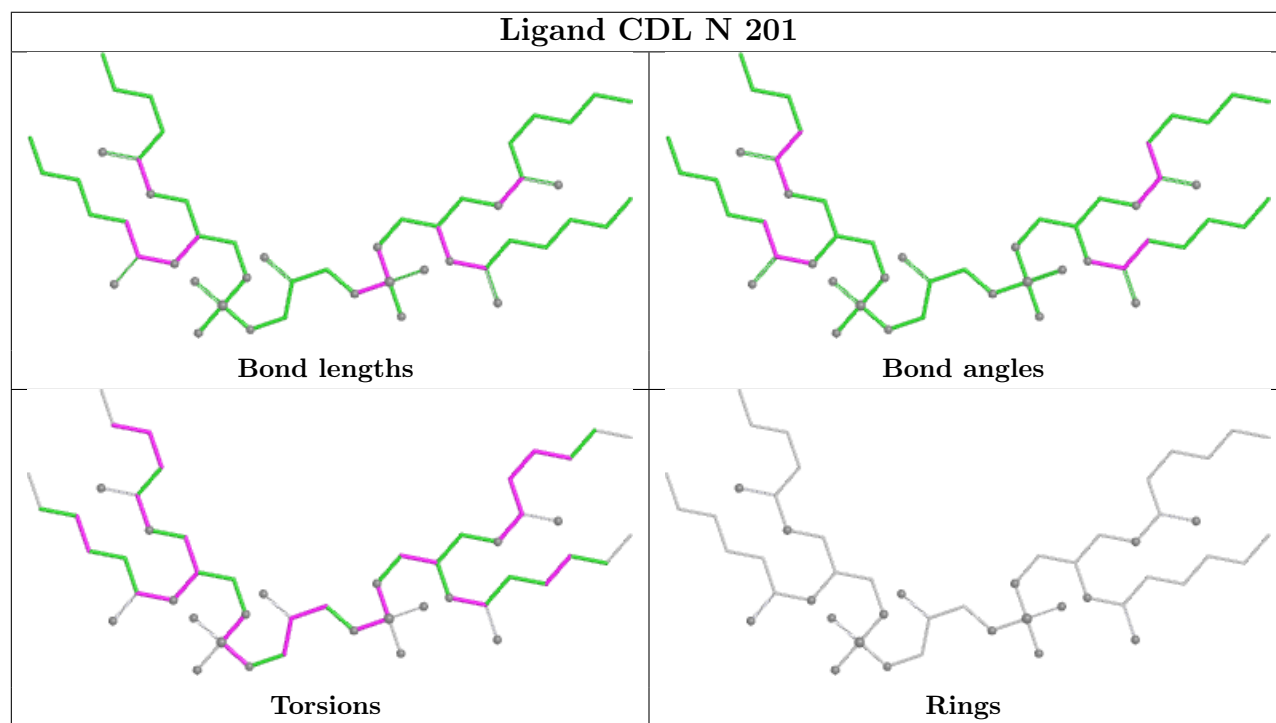
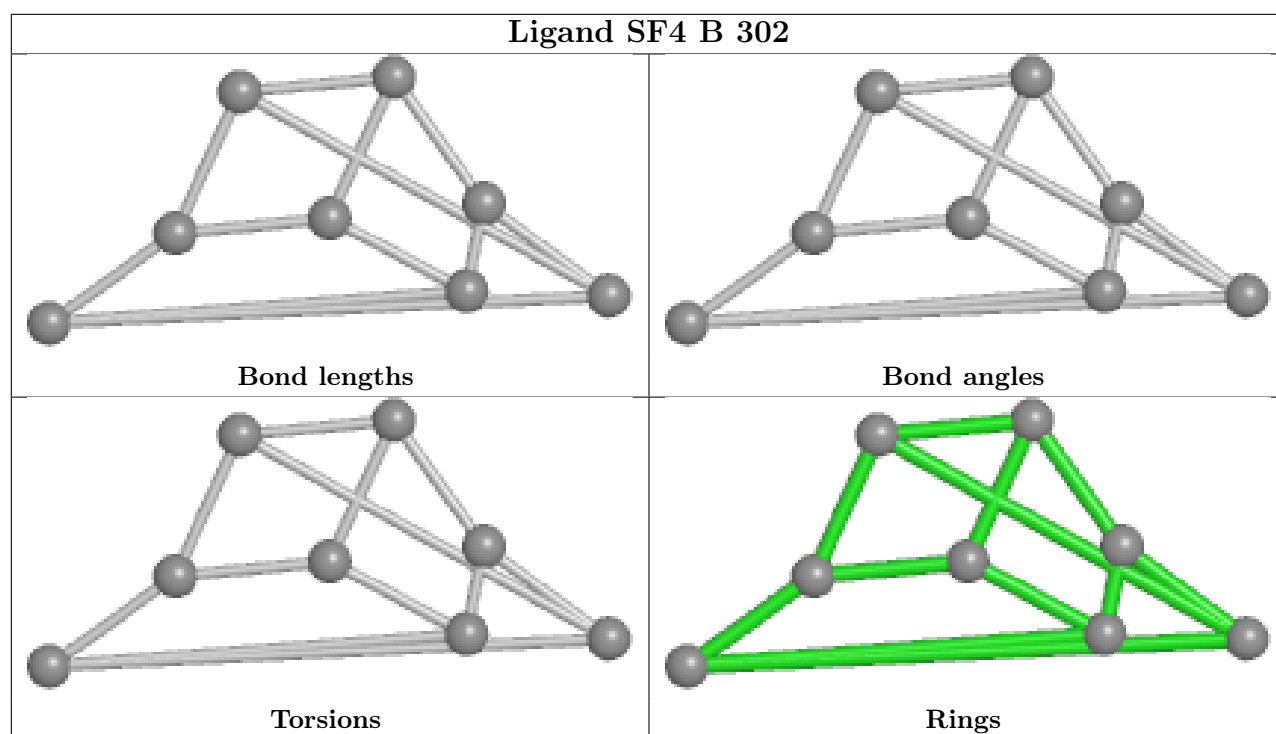


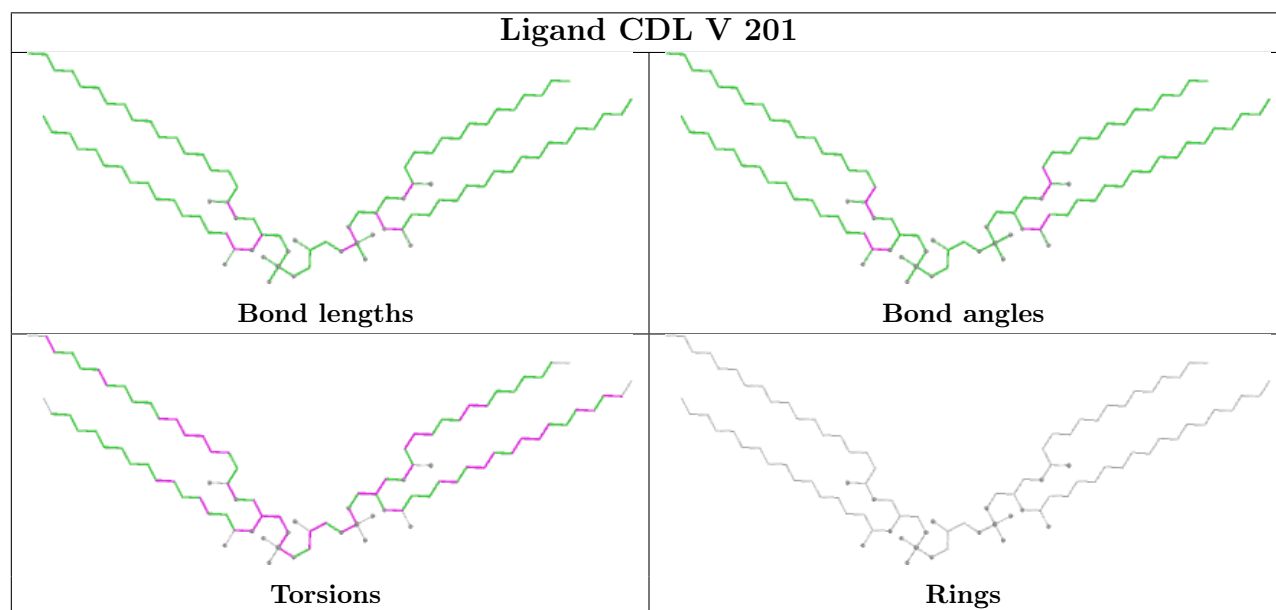
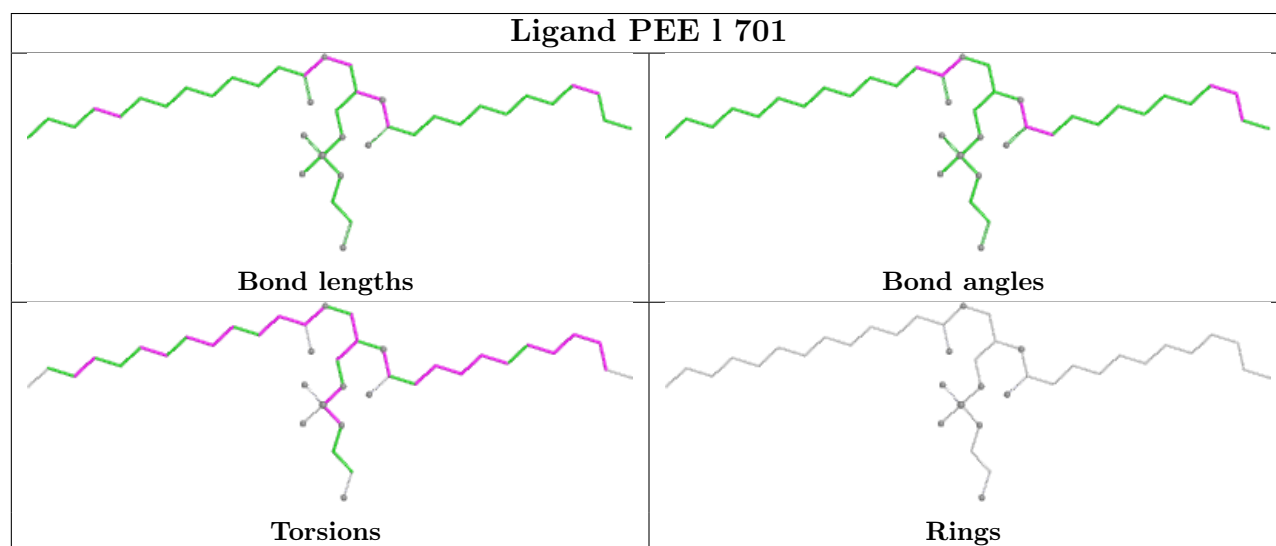
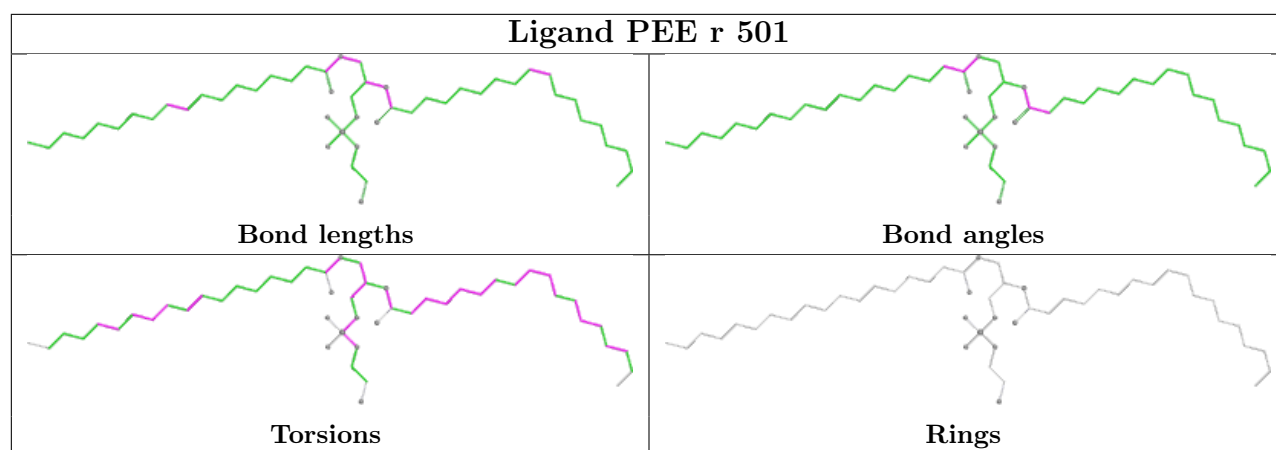


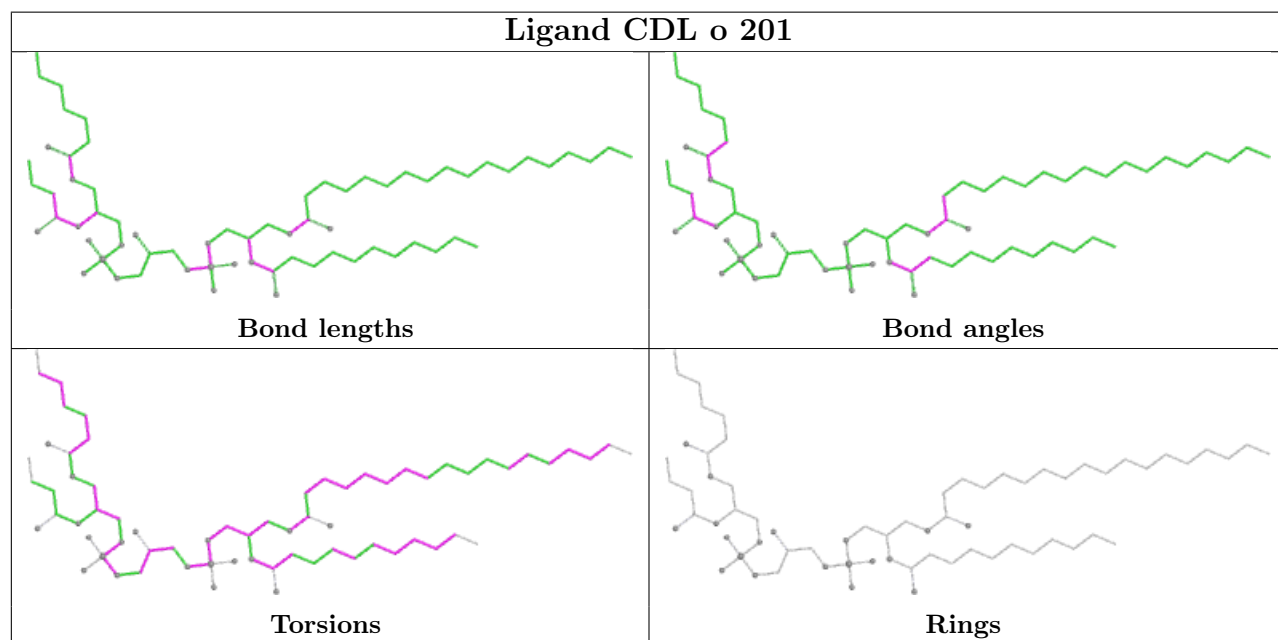
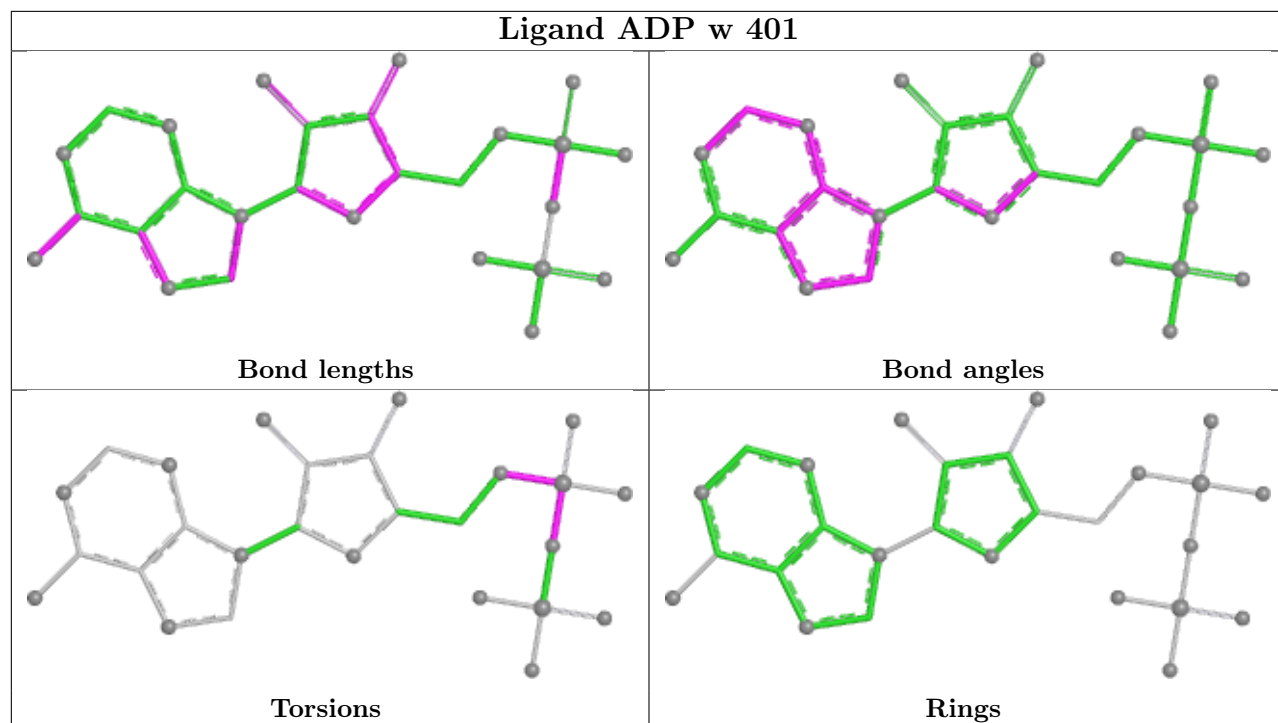


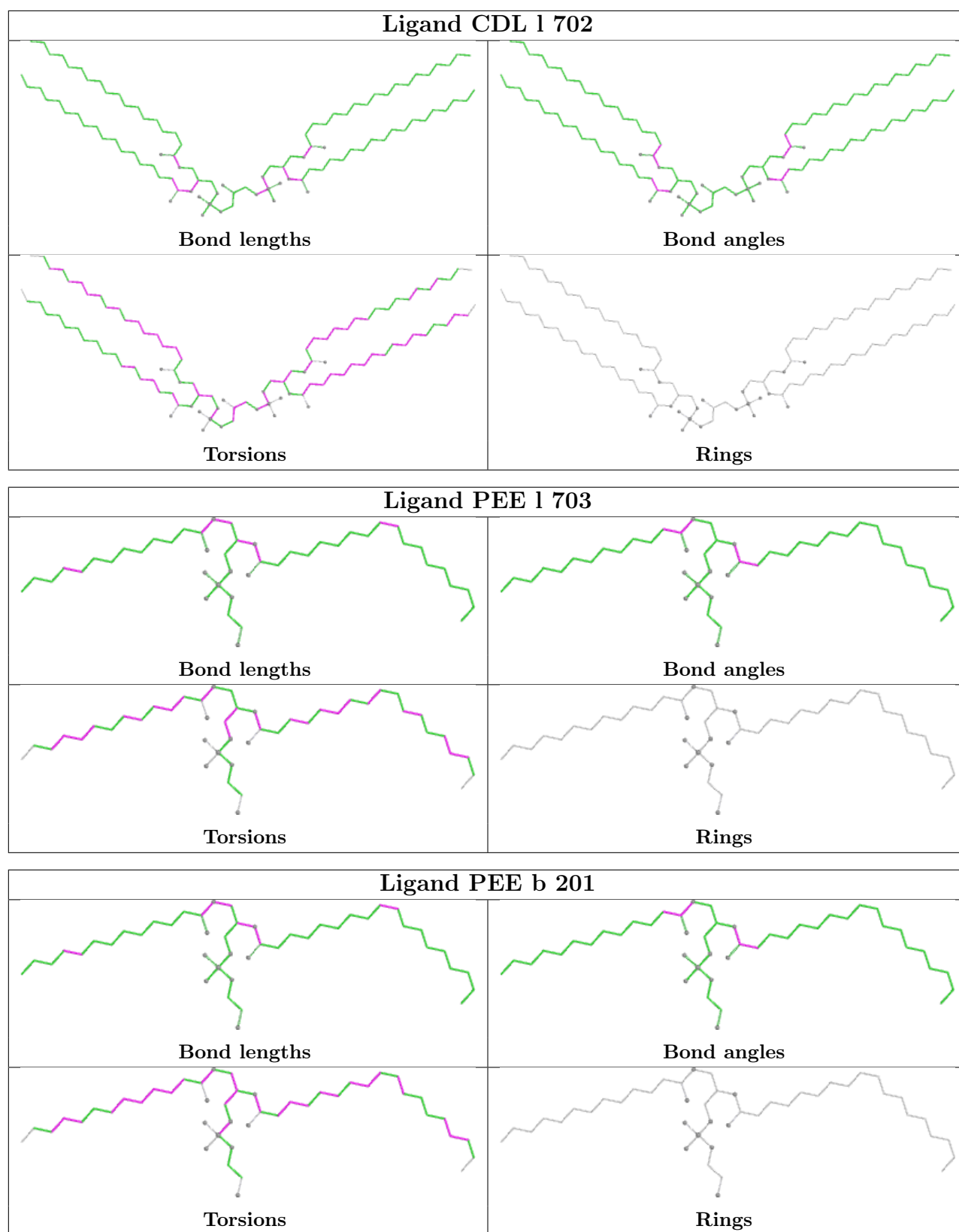












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

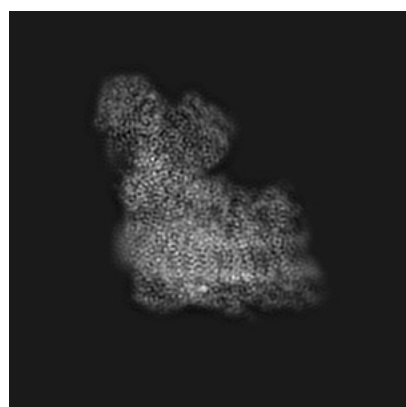
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32242. These allow visual inspection of the internal detail of the map and identification of artifacts.

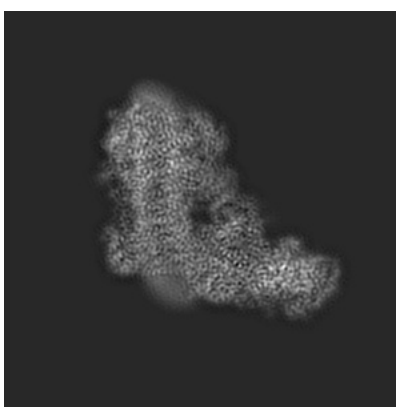
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

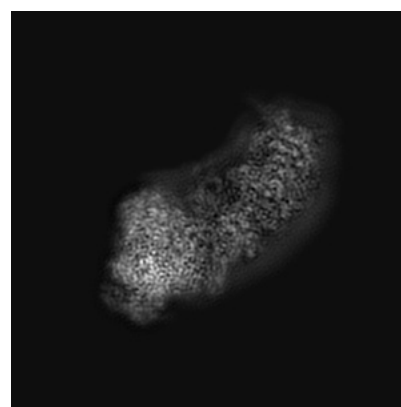
6.1.1 Primary map



X



Y

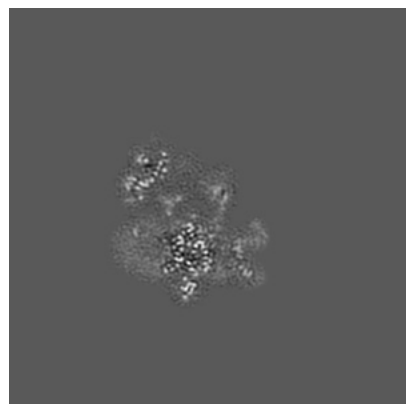


Z

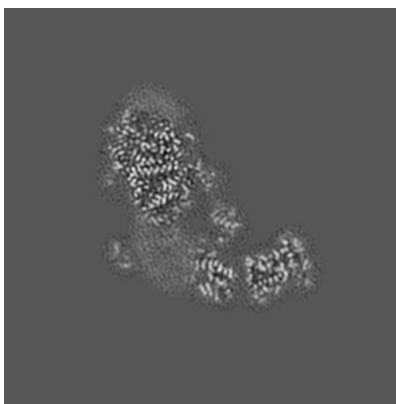
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

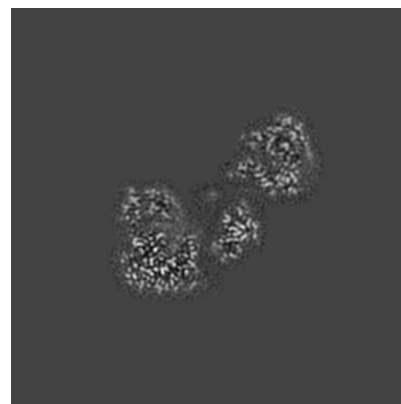
6.2.1 Primary map



X Index: 165



Y Index: 165



Z Index: 165

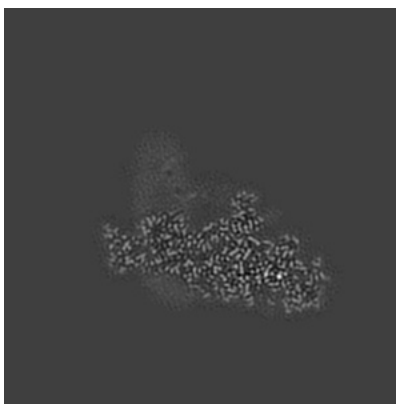
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

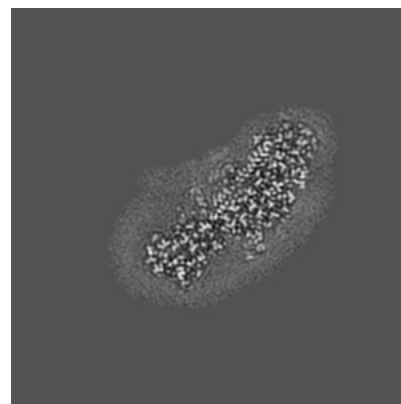
6.3.1 Primary map



X Index: 115



Y Index: 120

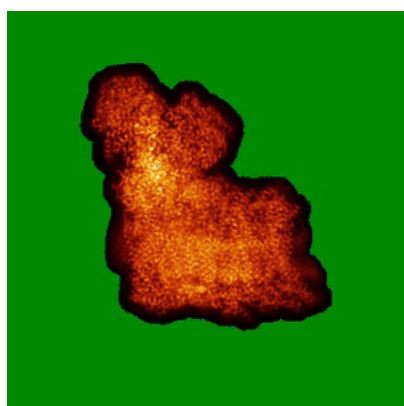


Z Index: 137

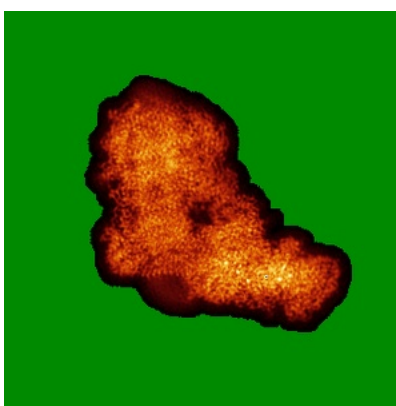
The images above show the largest variance slices of the map in three orthogonal directions.

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

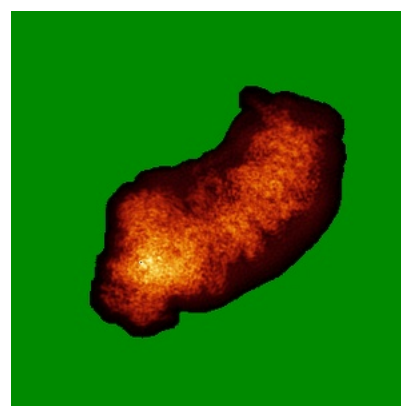
6.4.1 Primary map



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

This section was not generated.

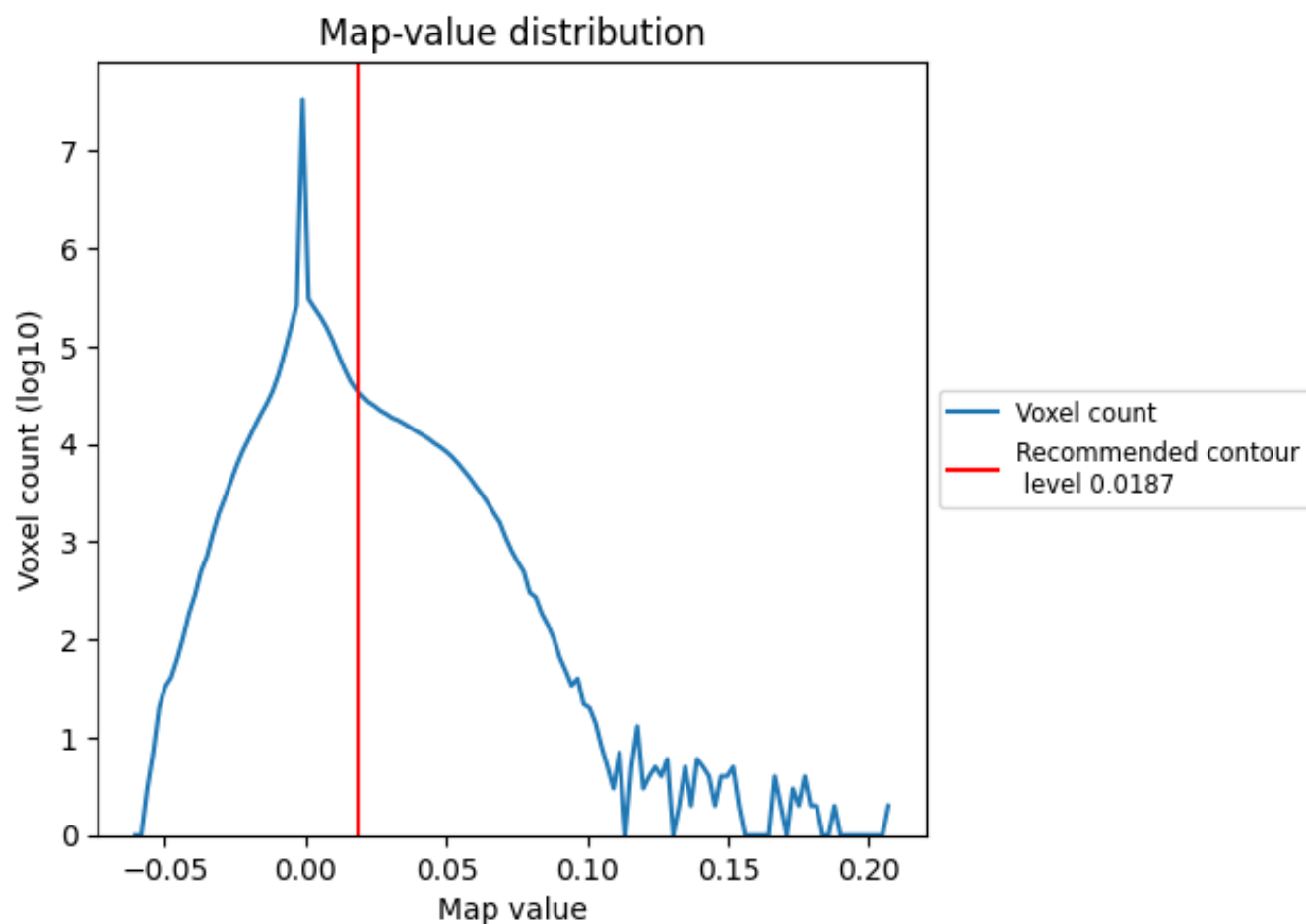
6.6 Mask visualisation

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

7 Map analysis [i](#)

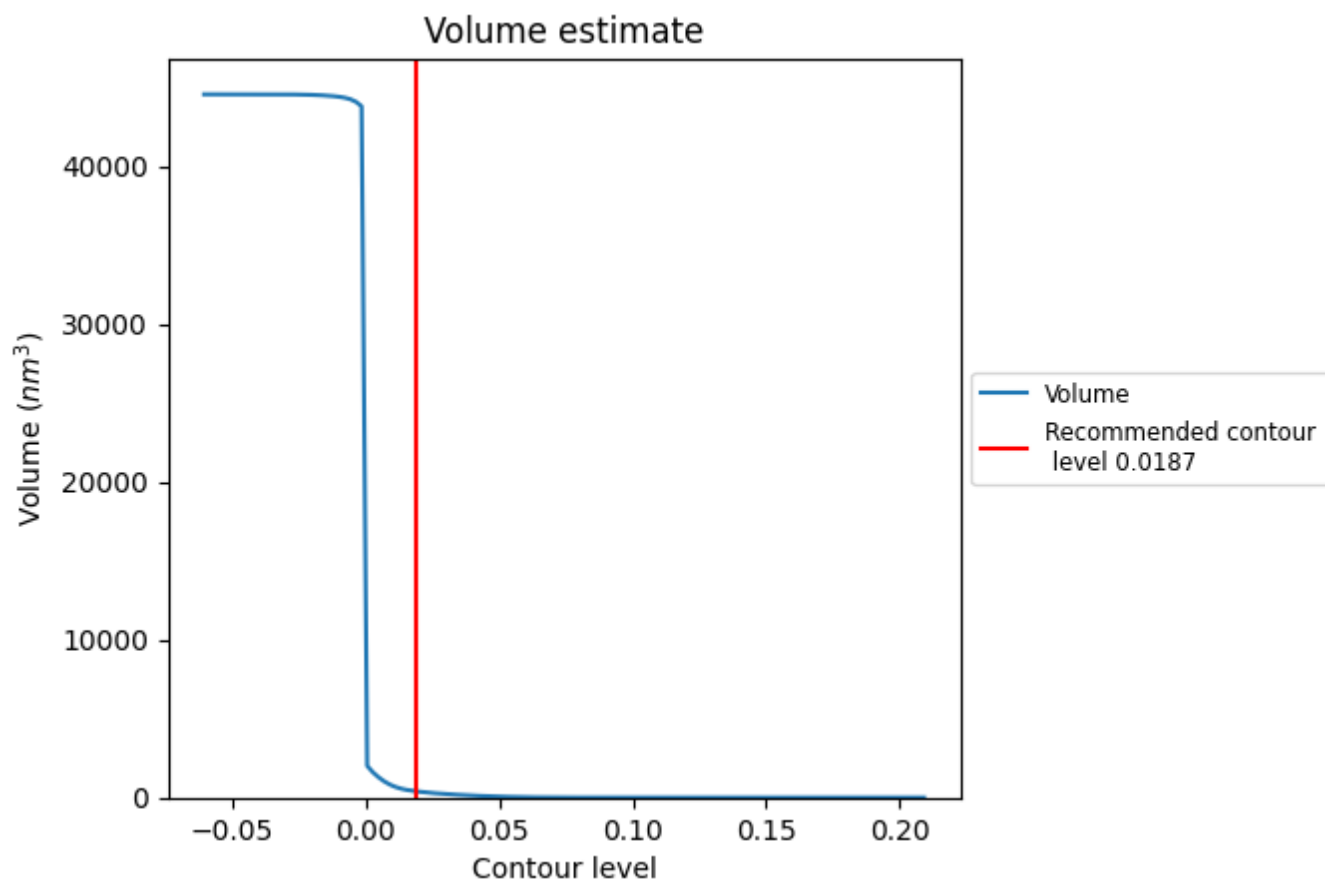
This section contains the results of statistical analysis of the map.

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.

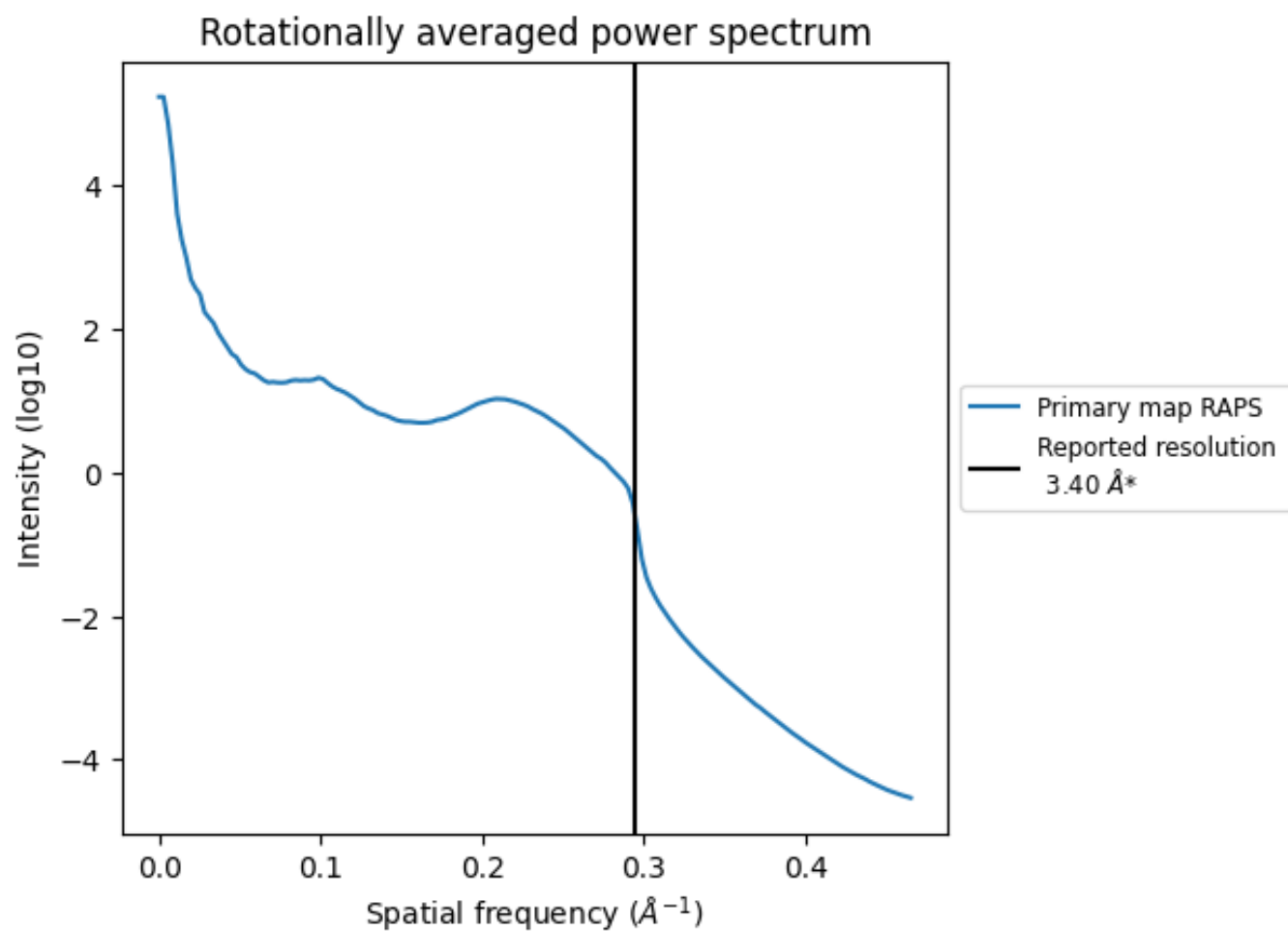
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 399 nm^3 ; this corresponds to an approximate mass of 360 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 0.294 Å⁻¹

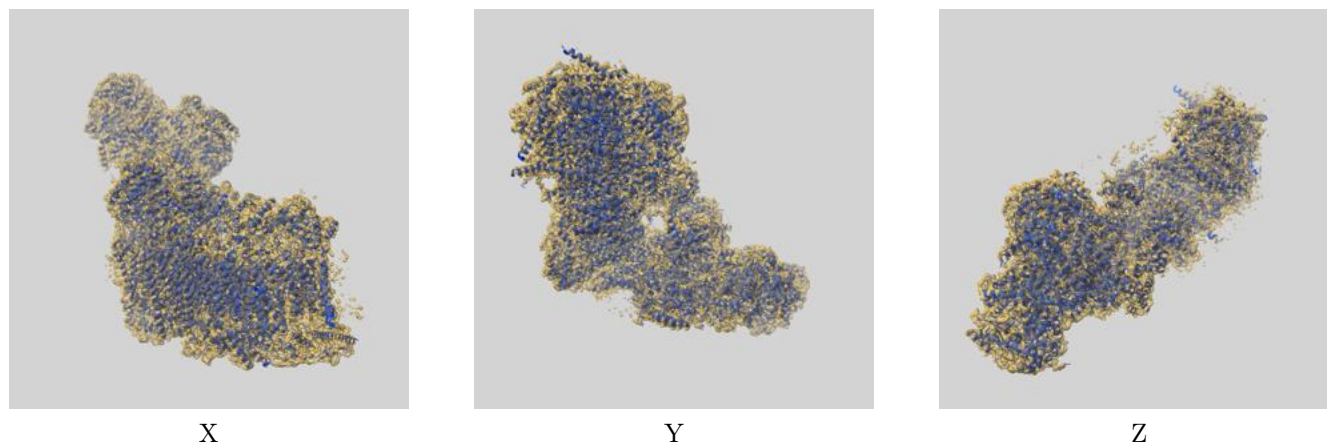
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

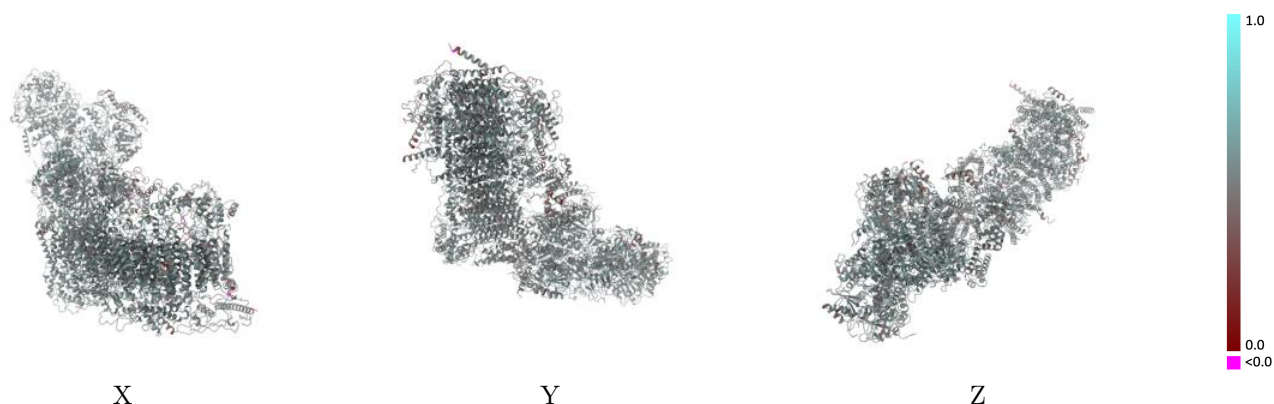
This section contains information regarding the fit between EMDB map EMD-32242 and PDB model 7W0H. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0187 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

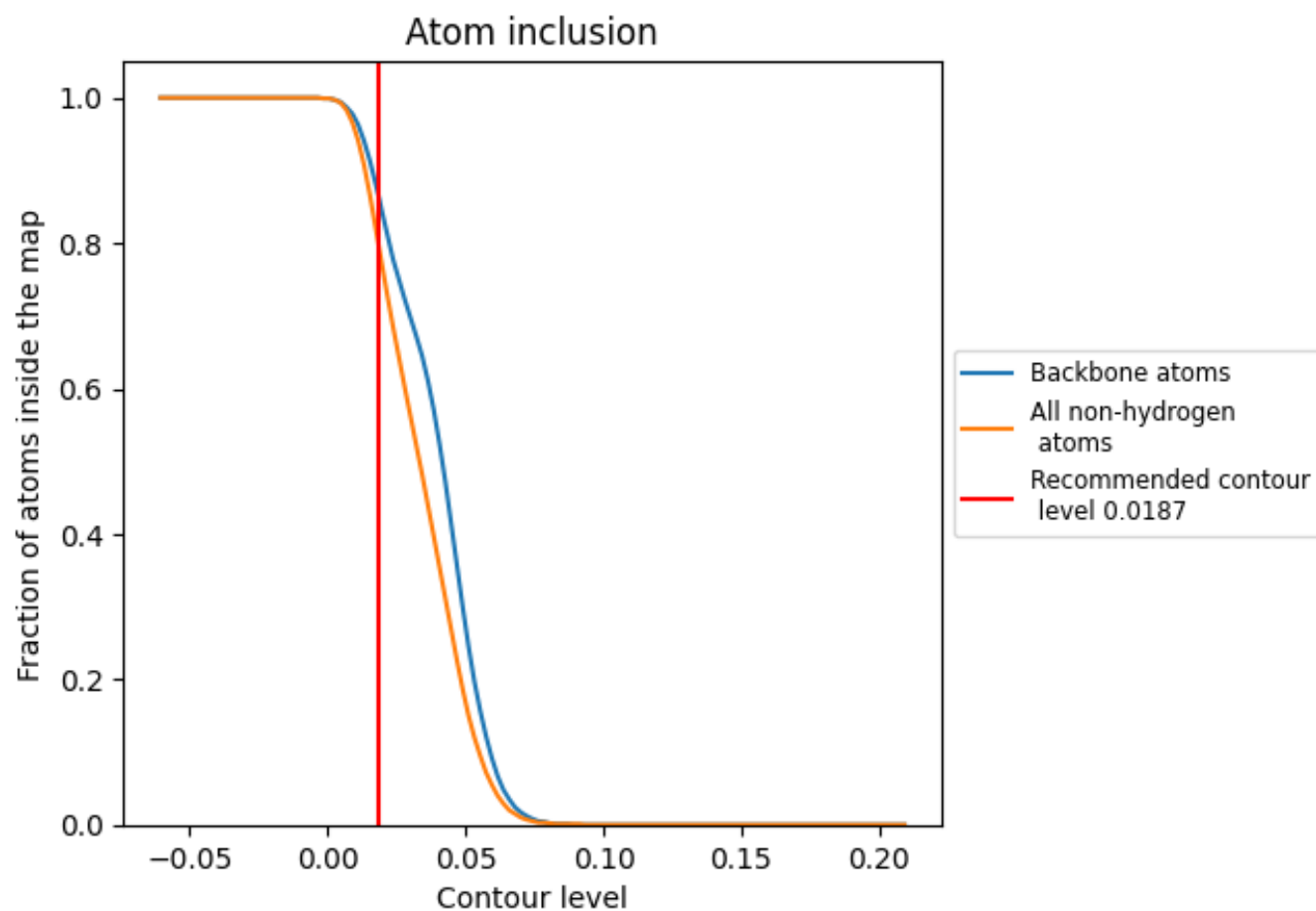


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0187) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7930	 0.5260
A	 0.8190	 0.5230
B	 0.8870	 0.5560
C	 0.8230	 0.5470
E	 0.7780	 0.5220
F	 0.7600	 0.4780
G	 0.6280	 0.4370
H	 0.8040	 0.5120
I	 0.7780	 0.5360
J	 0.7860	 0.5190
K	 0.8110	 0.5260
L	 0.8080	 0.5490
M	 0.8300	 0.5370
N	 0.7480	 0.5310
O	 0.8010	 0.5130
P	 0.8530	 0.5550
Q	 0.8410	 0.5510
S	 0.8410	 0.5430
T	 0.8060	 0.5470
U	 0.8060	 0.5260
V	 0.6060	 0.4940
W	 0.8270	 0.5330
X	 0.7530	 0.5000
Y	 0.7390	 0.4830
Z	 0.6530	 0.4570
a	 0.7940	 0.5360
b	 0.7080	 0.4950
c	 0.8080	 0.5210
d	 0.7840	 0.5120
e	 0.7250	 0.5070
f	 0.7320	 0.4990
g	 0.8270	 0.5450
h	 0.8170	 0.5330
i	 0.8150	 0.5430
j	 0.7050	 0.5030



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	 0.7430	 0.5220
l	 0.7860	 0.5300
m	 0.7520	 0.5040
n	 0.7130	 0.5080
o	 0.7430	 0.5210
p	 0.8040	 0.5180
r	 0.7930	 0.5440
s	 0.8090	 0.5320
u	 0.8170	 0.5330
v	 0.7650	 0.4890
w	 0.7810	 0.5120