



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 01:33 PM JST

PDB ID : 7W4Q / pdb_00007w4q
EMDB ID : EMD-32312
Title : Deactive state CI from Q1-NADH dataset, Subclass 6
Authors : Gu, J.; Yang, M.
Deposited on : 2021-11-28
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

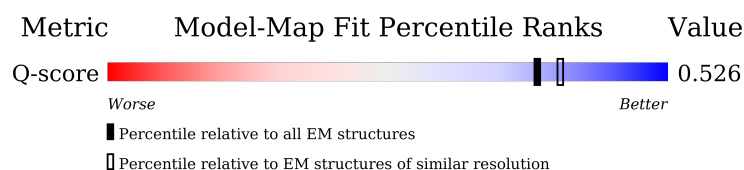
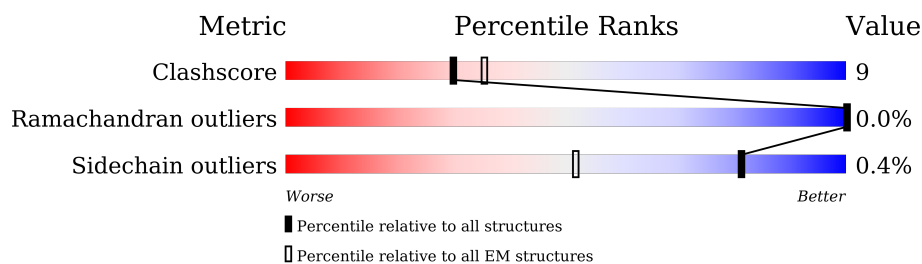
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	A	433	28% 70% 30%
2	B	176	77% 23%
3	C	156	5% 75% 24%
4	E	115	22% 83% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	86	50% 70% 30%
6	G	88	73% 67% 33%
6	X	88	8% 70% 30%
7	H	112	19% 76% 24%
8	I	112	14% 69% 18% 13%
9	J	342	24% 65% 21% 13%
10	K	43	30% 70% 28% .
11	L	125	8% 86% 14%
12	M	690	11% 83% 17%
13	N	144	12% 80% 20%
14	O	217	29% 71% 28% .
15	P	208	. 77% 23%
16	Q	430	. 73% 23% ..
17	S	70	. 87% 13%
18	T	96	12% 83% 17%
19	U	83	10% 93% 7%
20	V	140	37% 81% 19%
21	W	142	9% 77% 23%
22	Y	70	29% 79% 21%
23	Z	84	27% 88% 11% .
24	a	140	. 79% 21%
25	b	126	14% 67% 15% 18%
26	c	156	11% 88% 12%
27	d	175	9% 86% 14%
28	e	107	16% 79% 20% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	f	49	
30	g	122	
31	h	105	
32	i	347	
33	j	115	
34	k	98	
35	l	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
50	CDL	l	701	-	-	X	-

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 66581 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
			1248	794	227	213	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	115	Total	C	N	O	S	0	0
			961	614	176	166	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
			693	447	102	139	5		
6	X	88	Total	C	N	O	S	0	0
			696	449	103	139	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
			2348	1509	420	411	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
			5296	3320	923	1014	39		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	217	Total	C	N	O	S	0	0
			1664	1060	281	313	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1734	1122	298	312	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
			1011	645	171	189	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
			1173	755	203	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
			879	573	158	147	1		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	107	Total	C	N	O	S	0	0
			890	568	145	173	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	42	Total	C	N	O	0	0
			342	225	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
			847	537	160	144	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
			800	545	118	132	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
			4781	3172	740	818	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
			948	636	138	166	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
			1520	974	275	263	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
			3630	2412	572	608	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
			1386	881	250	245	10		

- Molecule 43 is a protein called Complex I-B18.

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.

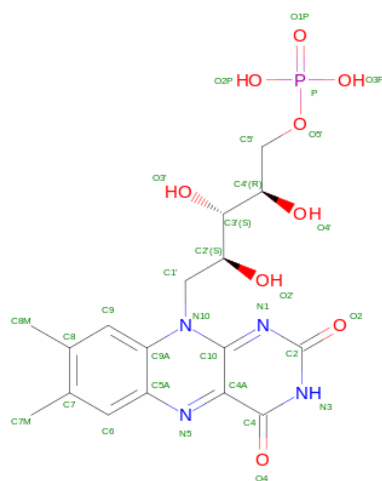
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2582	1643	438	491	10		

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



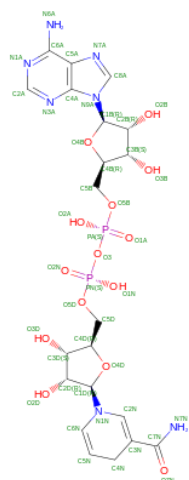
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

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



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

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



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

- Molecule 48 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $\text{C}_{41}\text{H}_{78}\text{NO}_8\text{P}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	Q	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	r	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	s	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



- Molecule 50 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).

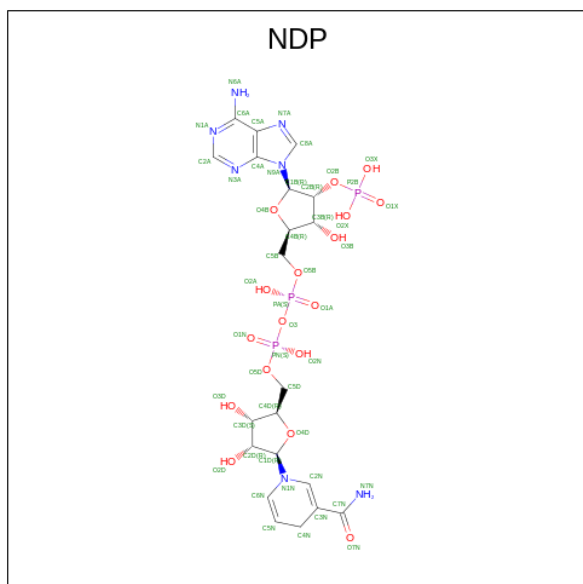


Continued on next page...

Continued from previous page...

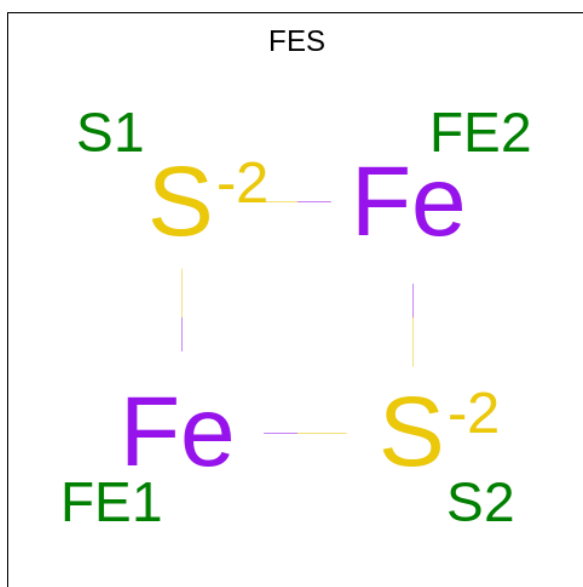
Mol	Chain	Residues	Atoms				AltConf
50	a	1	Total	C	O	P	0
			91	72	17	2	
50	i	1	Total	C	O	P	0
			66	47	17	2	
50	l	1	Total	C	O	P	0
			99	80	17	2	
50	l	1	Total	C	O	P	0
			100	81	17	2	
50	r	1	Total	C	O	P	0
			100	81	17	2	

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



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

- Molecule 52 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

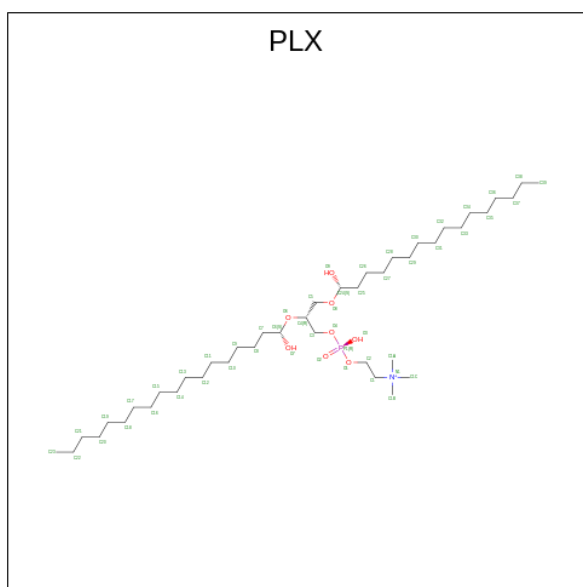


Mol	Chain	Residues	Atoms			AltConf
52	M	1	Total	Fe	S	0
			4	2	2	
52	O	1	Total	Fe	S	0
			4	2	2	

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 54 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).

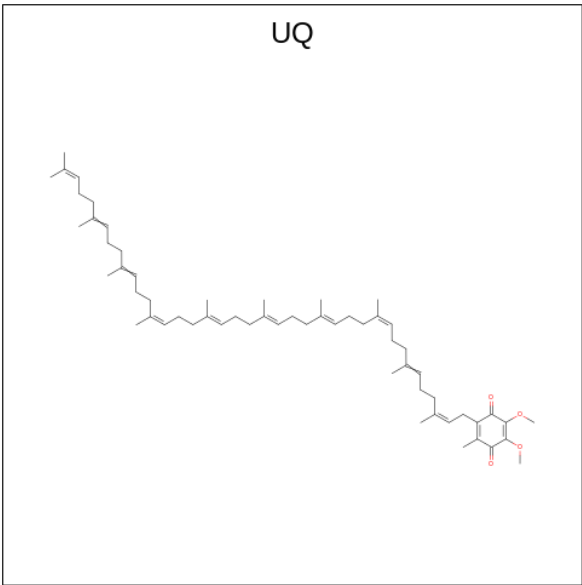


Mol	Chain	Residues	Atoms					AltConf
54	N	1	Total	C	N	O	P	0
			52	42	1	8	1	
54	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
54	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
54	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
54	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
54	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

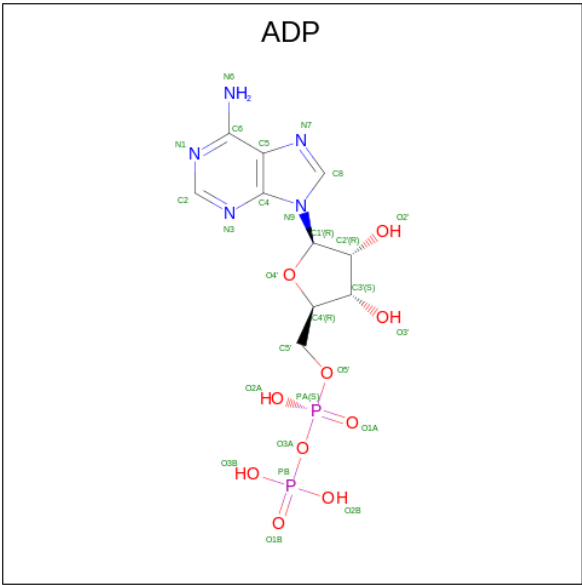
Mol	Chain	Residues	Atoms		AltConf
55	T	1	Total	Zn	0
			1	1	

- Molecule 56 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
56	s	1	Total	C	O	0
			28	24	4	

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

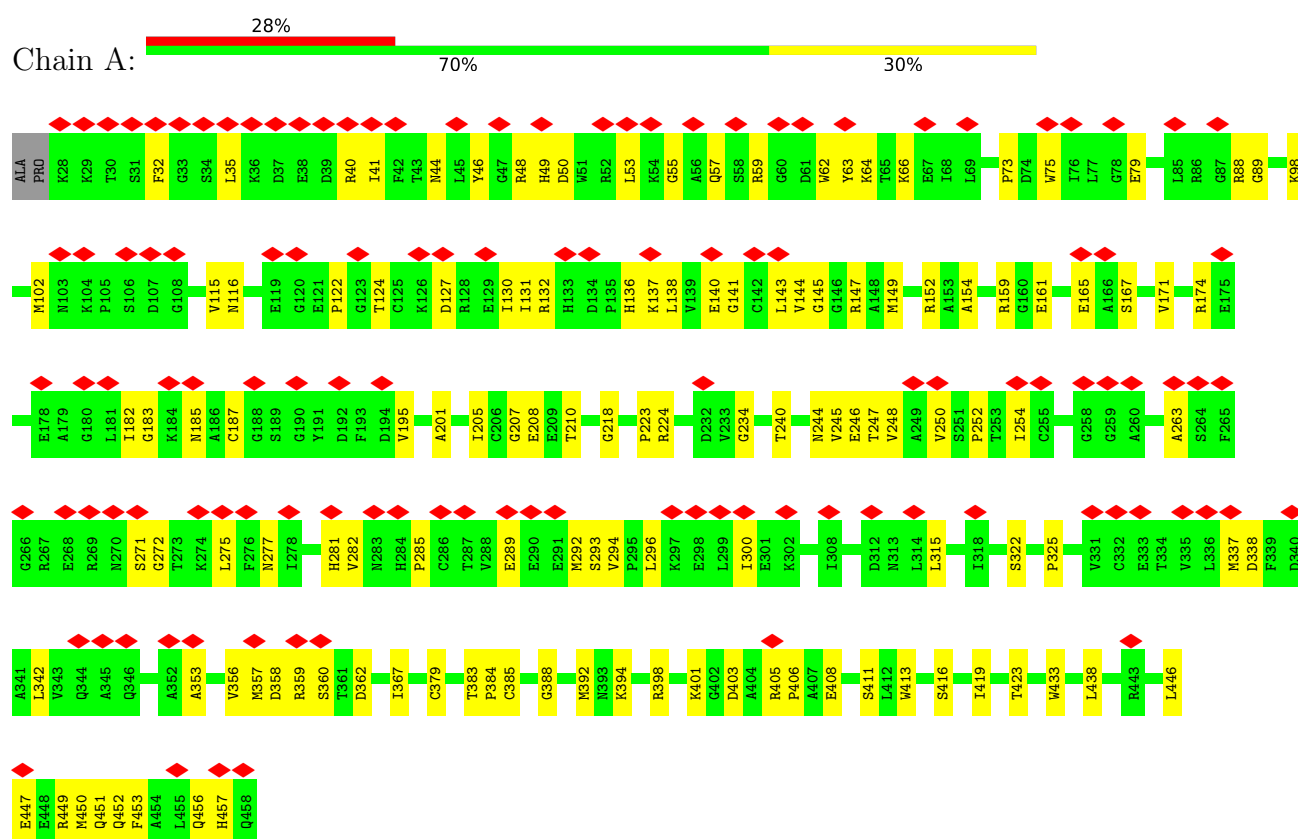


Mol	Chain	Residues	Atoms					AltConf
57	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

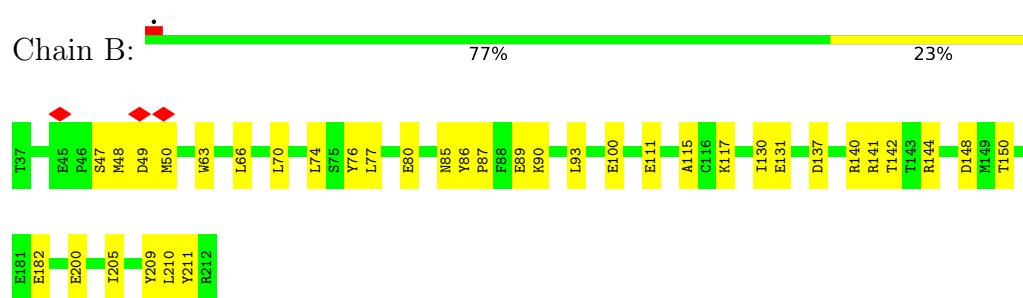
3 Residue-property plots

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

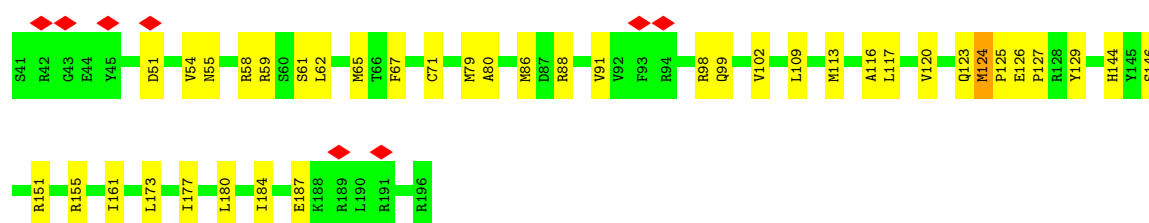
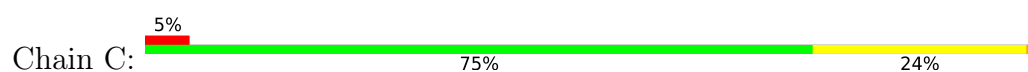
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



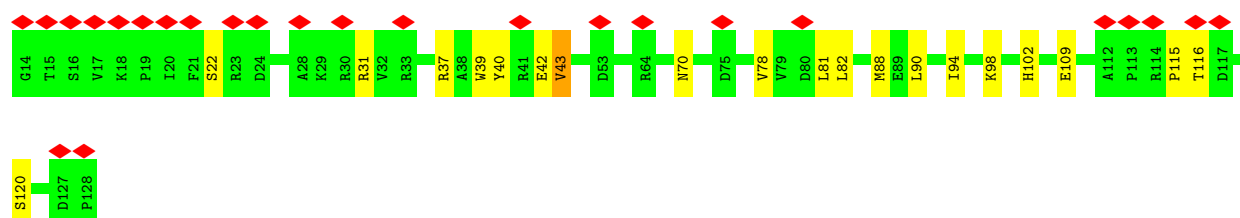
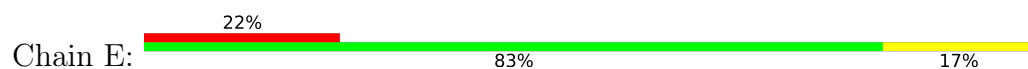
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



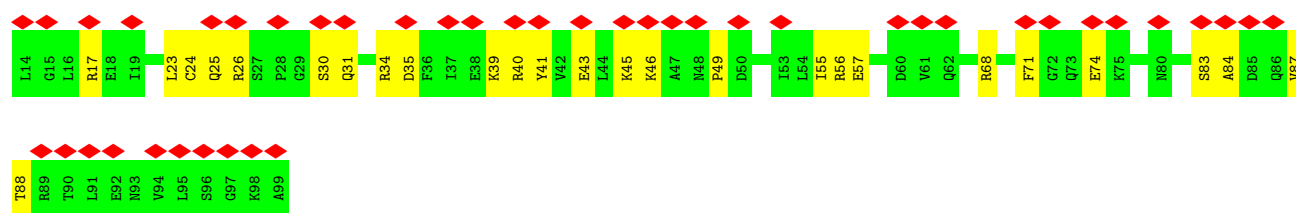
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



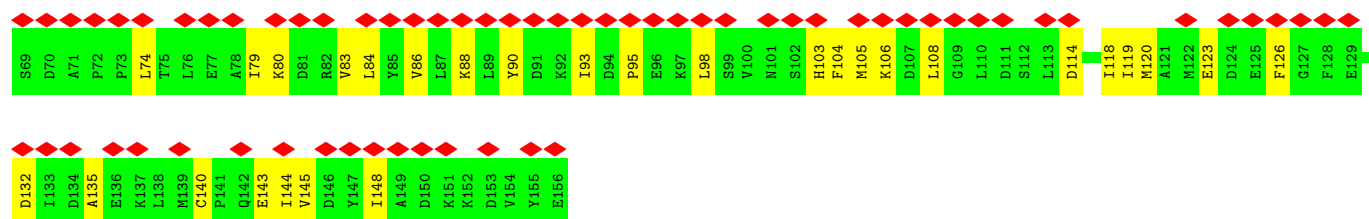
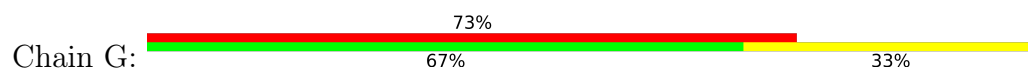
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



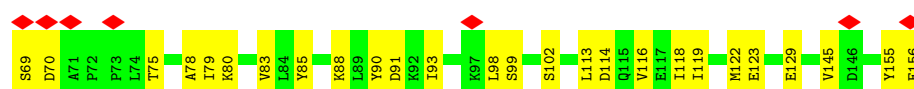
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



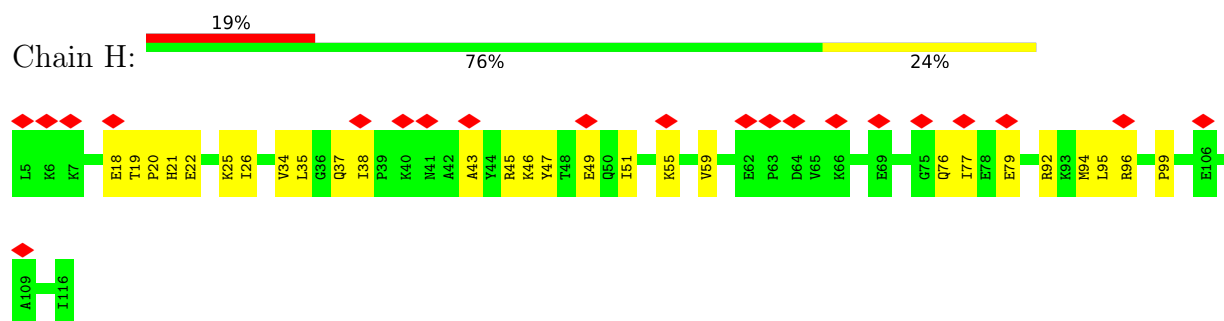
- Molecule 6: Acyl carrier protein



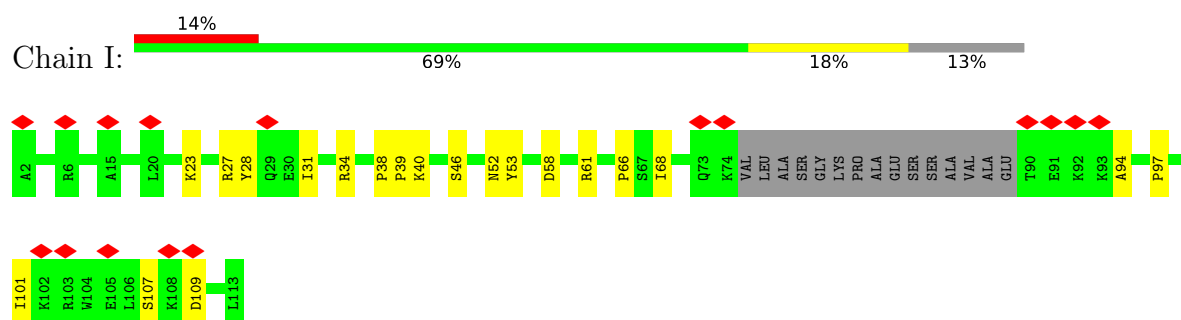
- Molecule 6: Acyl carrier protein



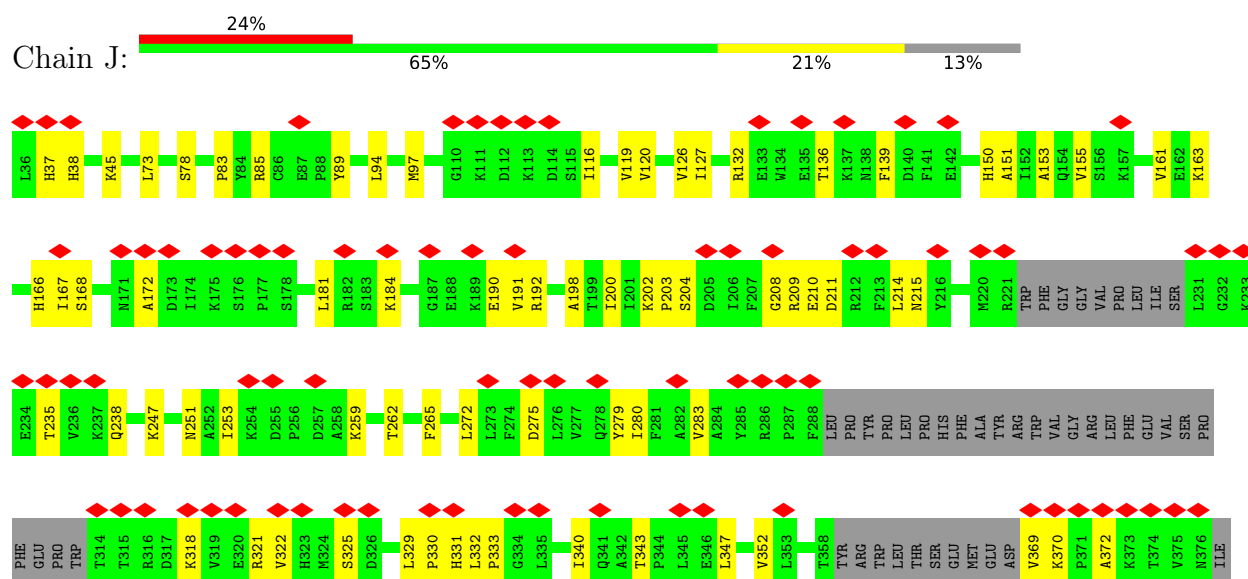
- Molecule 7: Complex I subunit B13



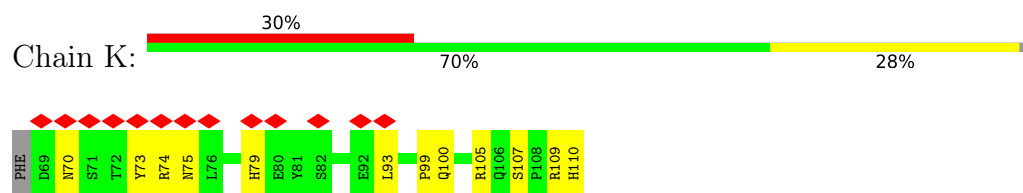
- Molecule 8: Complex I-B14.5a



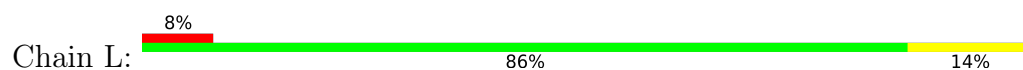
- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial



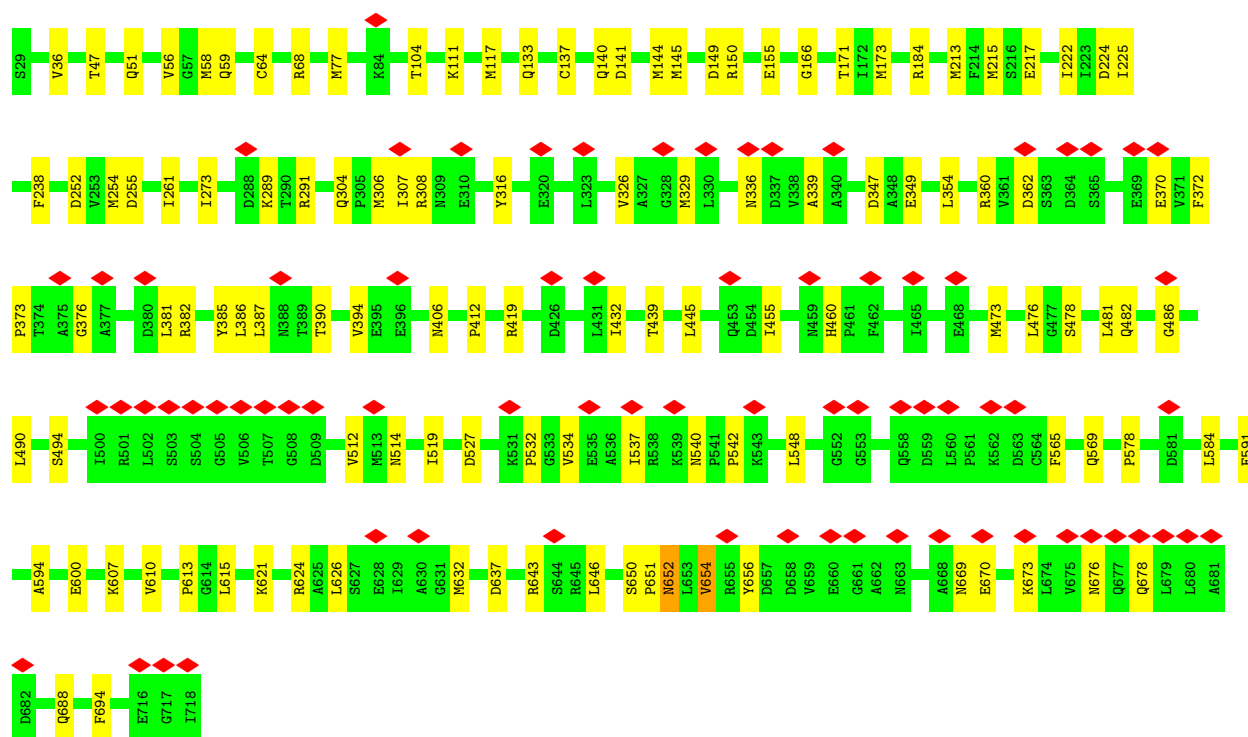
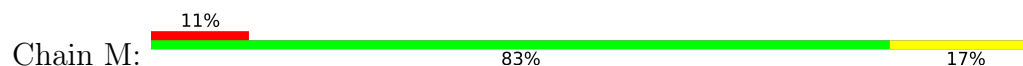
- Molecule 10: Complex I-9kD



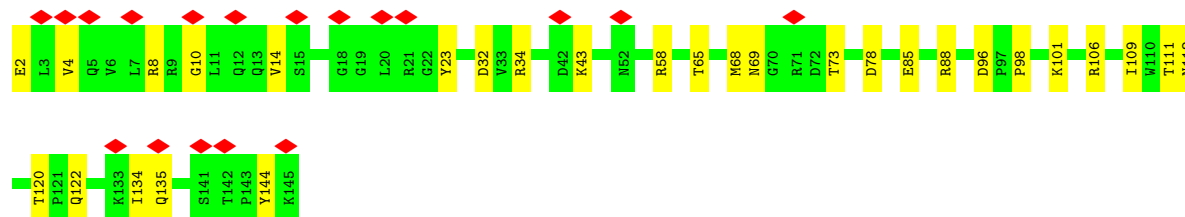
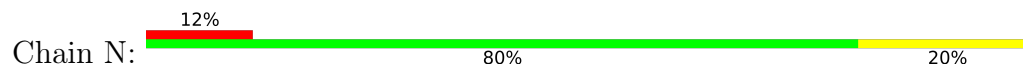
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



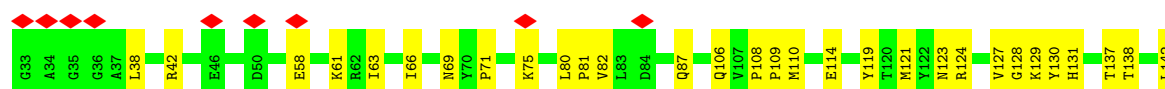
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

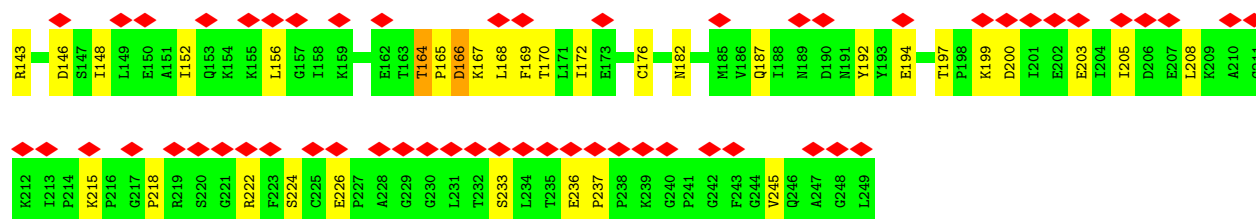


- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

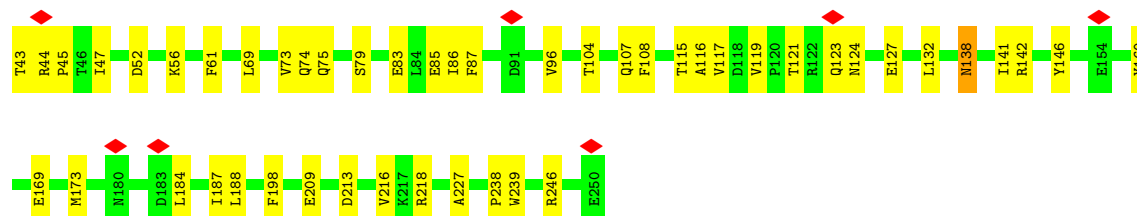
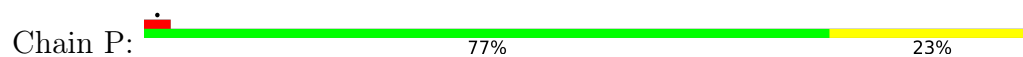


- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

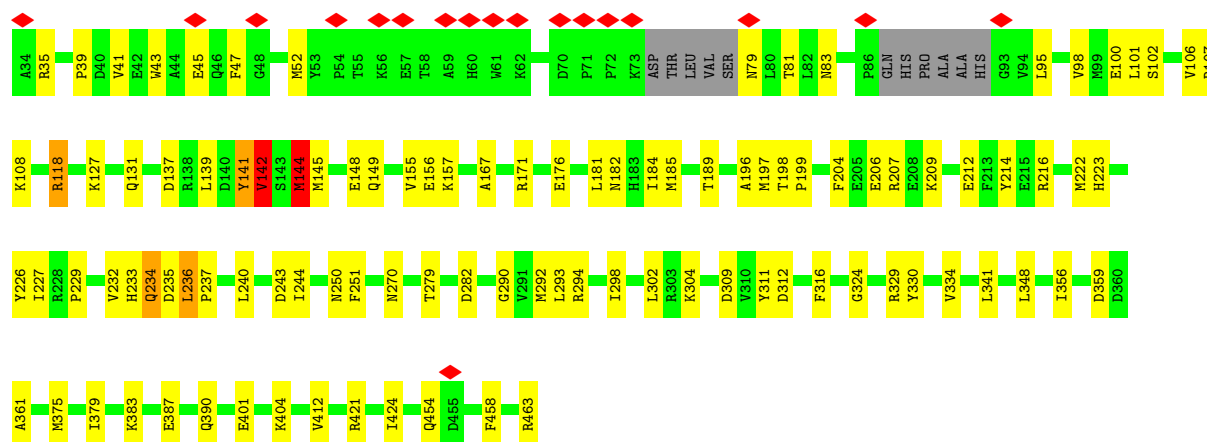




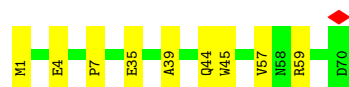
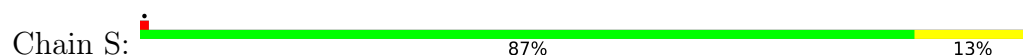
• Molecule 15: Complex I-30kD



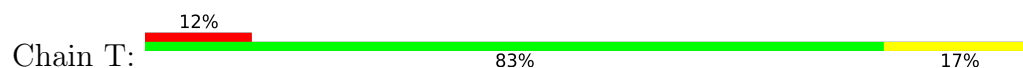
• Molecule 16: Complex I-49kD

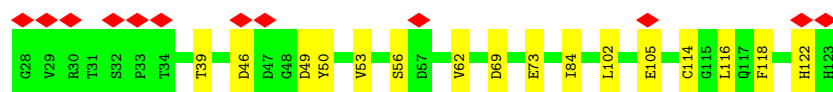


• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

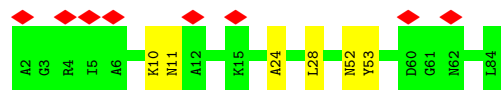


• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

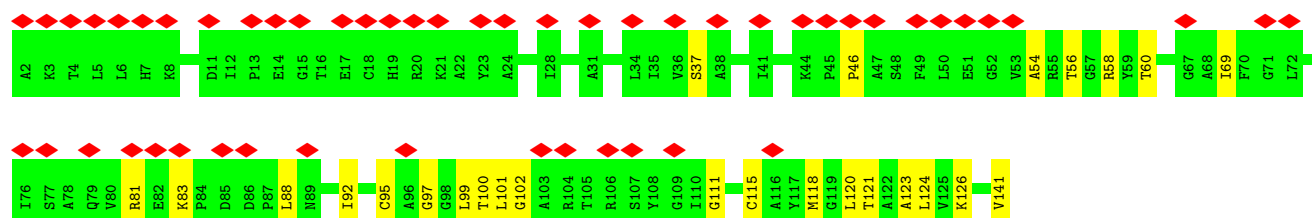
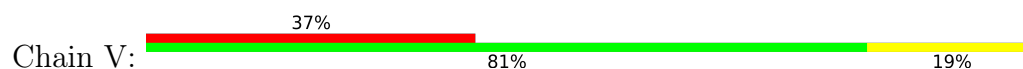




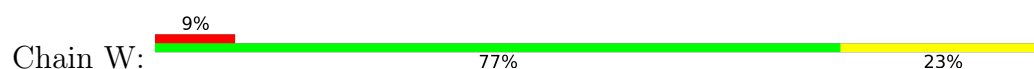
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



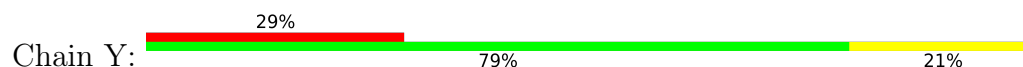
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



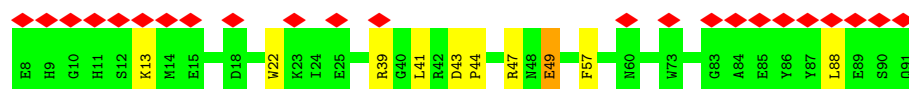
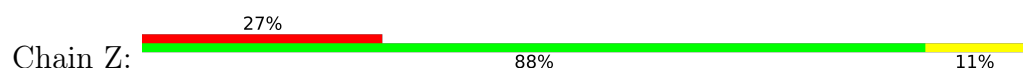
- Molecule 21: Complex I-B16.6



- Molecule 22: Complex I-AGGG

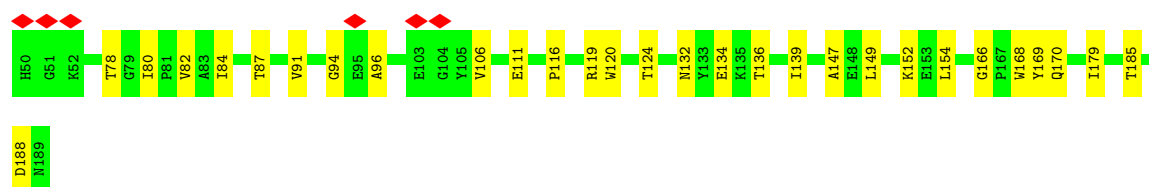


- Molecule 23: Complex I-B12



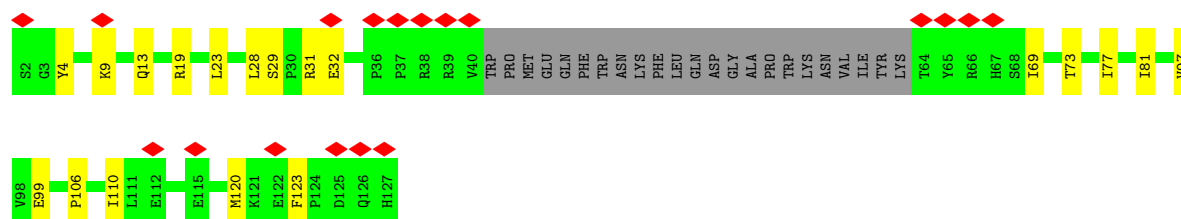
- Molecule 24: Complex I-SGDH

Chain a:  79% 21%



• Molecule 25: Complex I-B17

Chain b:  14% 67% 15% 18%



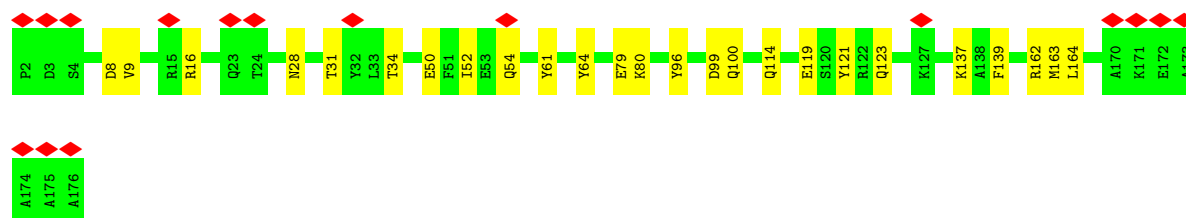
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c:  11% 88% 12%



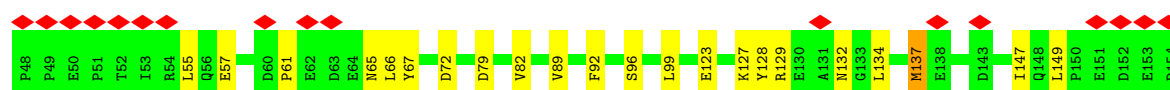
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d:  9% 86% 14%

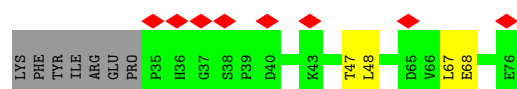
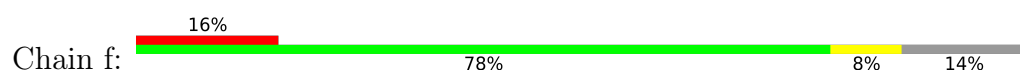


• Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

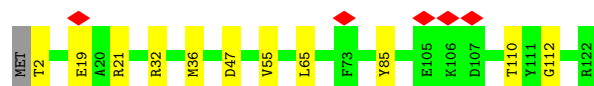
Chain e:  16% 79% 20%



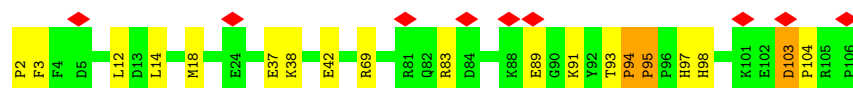
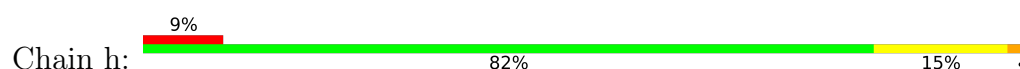
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



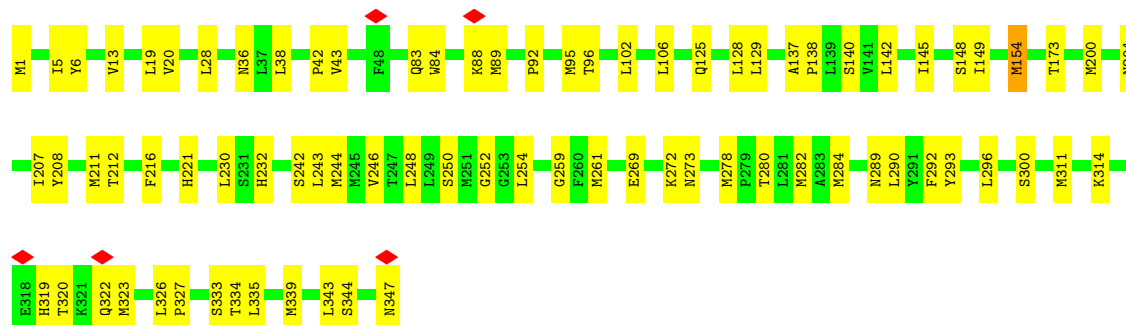
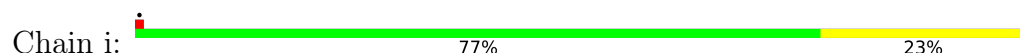
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



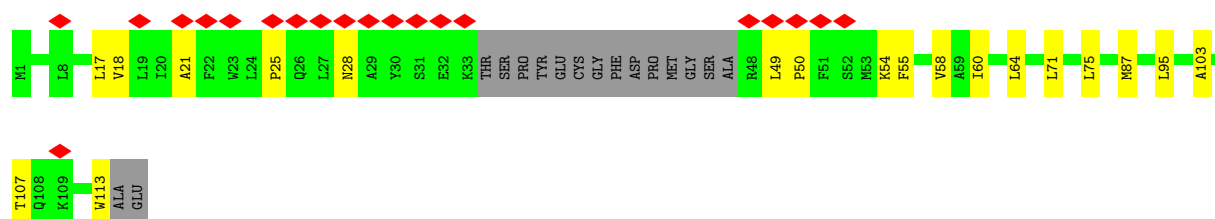
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

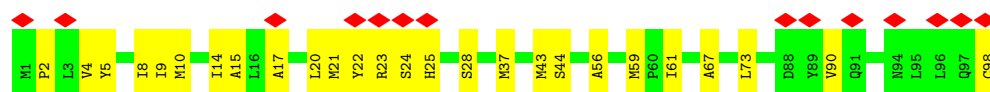


- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

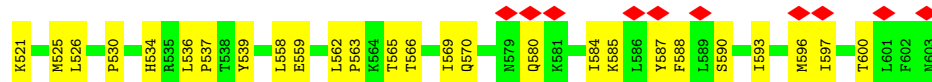
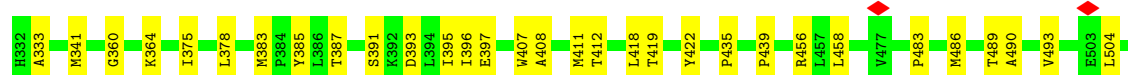
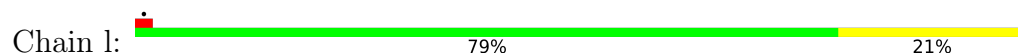


- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

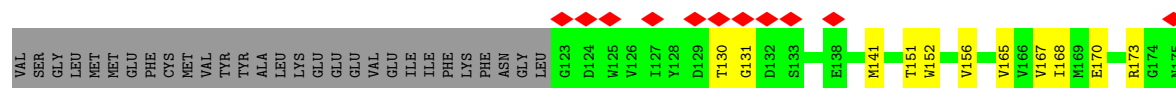
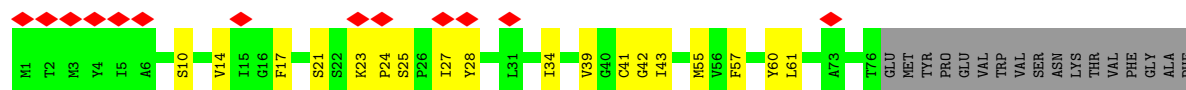




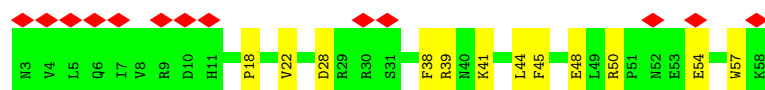
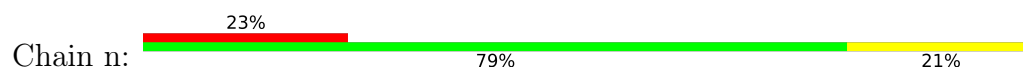
• Molecule 35: NADH-ubiquinone oxidoreductase chain 5



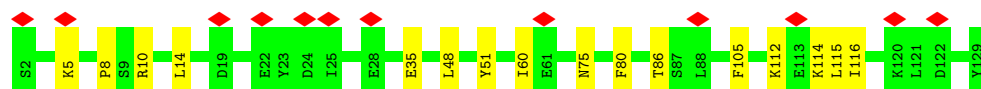
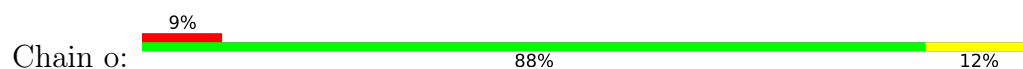
• Molecule 36: NADH-ubiquinone oxidoreductase chain 6



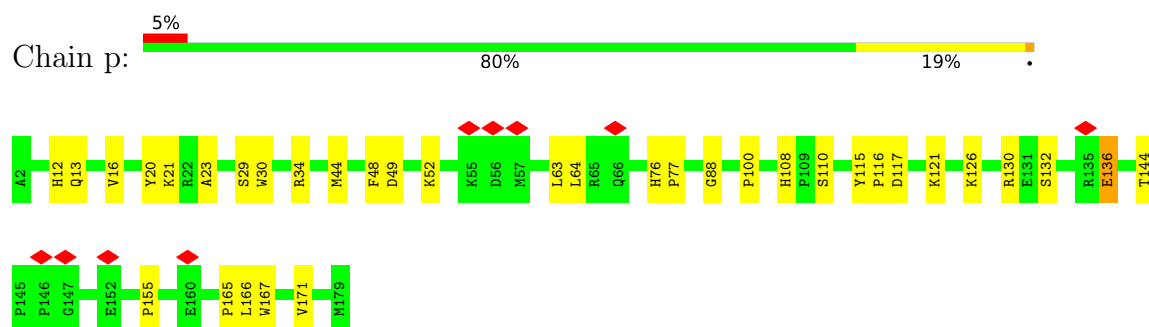
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



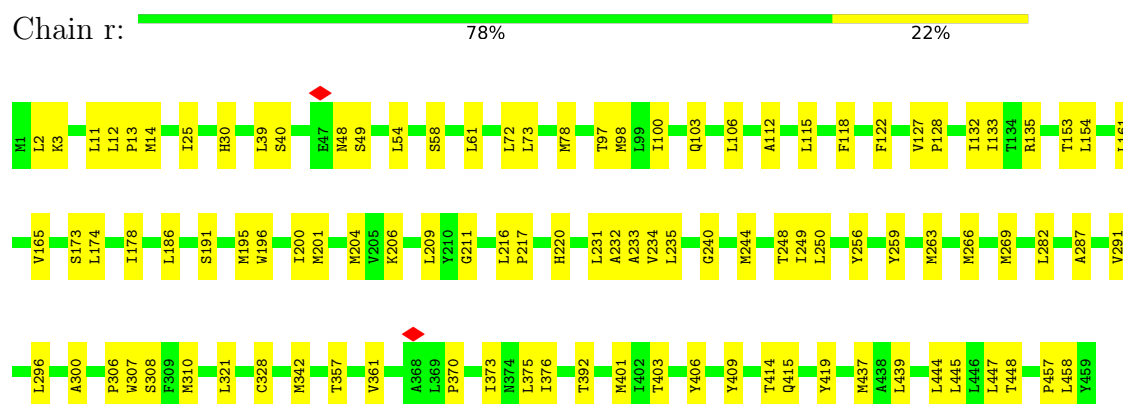
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



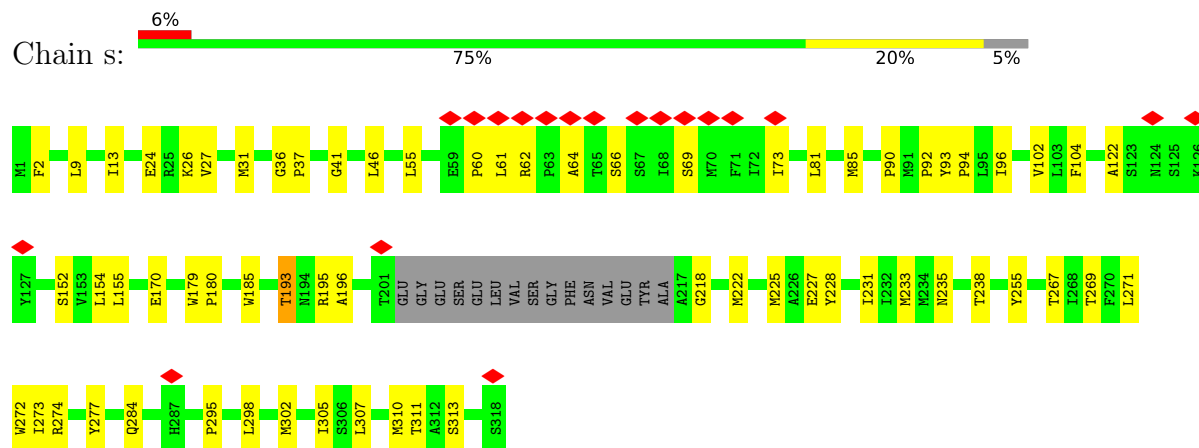
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



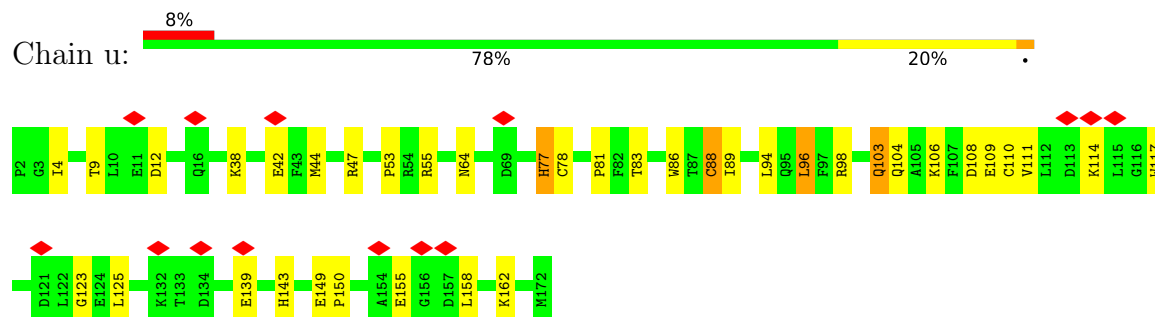
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4



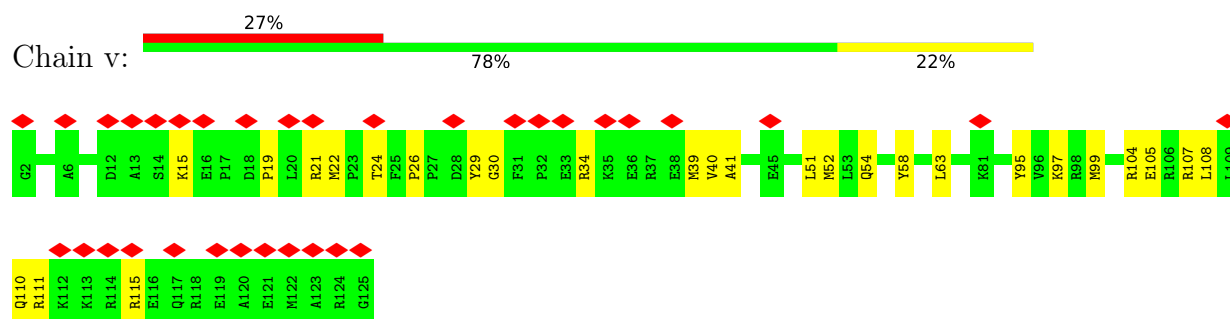
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1



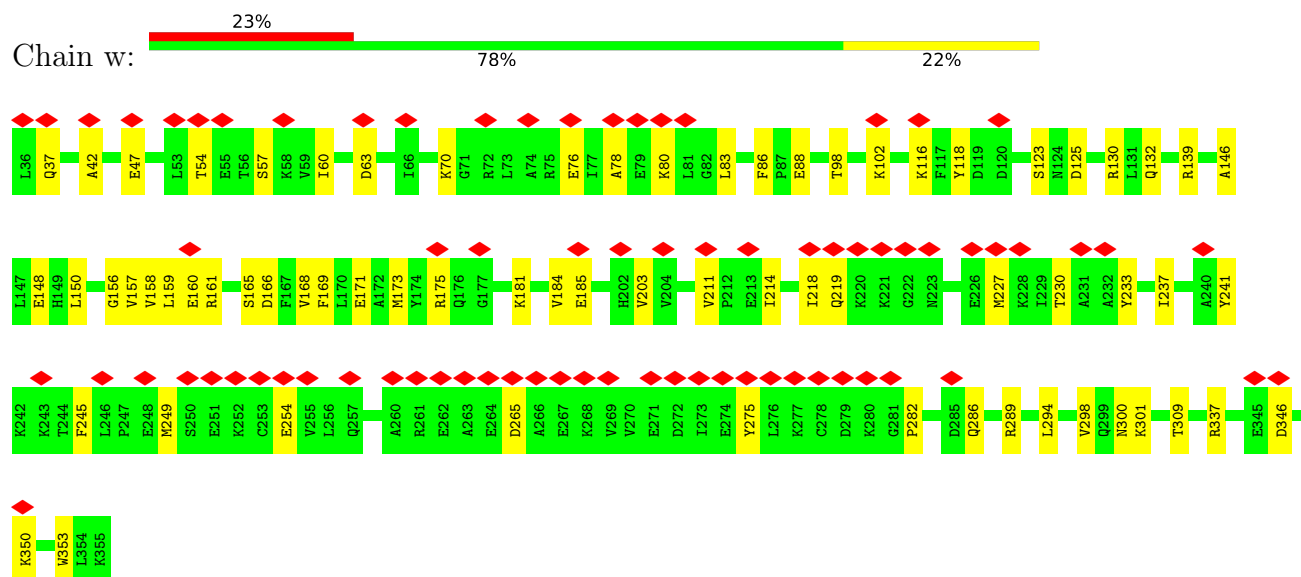
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 43: Complex I-B18



- 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	24259	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	0.226	Depositor
Minimum map value	-0.088	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0282	Depositor
Map size ($\text{\AA}$)	333.7616, 333.7616, 333.7616	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAI, UQ, 8Q1, FES, MG, CDL, FMN, NDP, 2MR, PLX, PEE, ADP, ZN, 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	0.13	0/3393	0.35	0/4584
2	B	0.11	0/1443	0.31	0/1952
3	C	0.15	0/1279	0.43	2/1730 (0.1%)
4	E	0.17	0/985	0.52	2/1328 (0.2%)
5	F	0.16	0/702	0.47	1/945 (0.1%)
6	G	0.13	0/705	0.37	0/956
6	X	0.12	0/708	0.35	0/959
7	H	0.12	0/929	0.34	0/1258
8	I	0.13	0/798	0.36	0/1079
9	J	0.13	0/2400	0.40	1/3240 (0.0%)
10	K	0.12	0/365	0.33	0/493
11	L	0.09	0/1039	0.28	0/1403
12	M	0.12	0/5384	0.34	2/7295 (0.0%)
13	N	0.13	0/1245	0.34	0/1694
14	O	0.15	0/1704	0.43	2/2319 (0.1%)
15	P	0.12	0/1785	0.36	0/2431
16	Q	0.17	0/3451	0.45	6/4672 (0.1%)
17	S	0.13	0/582	0.37	0/783
18	T	0.10	0/755	0.30	0/1018
19	U	0.13	0/664	0.34	0/912
20	V	0.20	0/1032	0.44	0/1399
21	W	0.13	0/1204	0.29	0/1624
22	Y	0.16	0/623	0.38	0/853
23	Z	0.10	0/695	0.29	0/939
24	a	0.12	0/1199	0.34	1/1623 (0.1%)
25	b	0.13	0/906	0.37	0/1232
26	c	0.11	0/1371	0.31	0/1875
27	d	0.12	0/1494	0.30	0/2015
28	e	0.11	0/916	0.35	0/1246
29	f	0.11	0/350	0.23	0/473
30	g	0.11	0/1031	0.27	0/1394
31	h	0.19	0/868	0.68	6/1163 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.13	0/2773	0.33	0/3768
33	j	0.17	0/819	0.37	0/1117
34	k	0.15	0/759	0.35	0/1029
35	l	0.15	0/4910	0.38	2/6678 (0.0%)
36	m	0.14	0/970	0.36	0/1316
37	n	0.12	0/491	0.33	0/663
38	o	0.11	0/1092	0.30	0/1481
39	p	0.17	0/1576	0.46	3/2139 (0.1%)
40	r	0.13	0/3722	0.32	0/5077
41	s	0.15	0/2464	0.35	0/3369
42	u	0.20	0/1424	0.57	1/1923 (0.1%)
43	v	0.15	0/1052	0.42	0/1411
44	w	0.13	0/2642	0.35	0/3580
All	All	0.14	0/66699	0.38	29/90438 (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 (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	u	77	HIS	N-CA-C	10.26	122.22	111.14
16	Q	233	HIS	N-CA-C	10.24	122.44	111.28
31	h	103	ASP	CA-C-N	8.67	128.81	120.31
31	h	103	ASP	C-N-CA	8.67	128.81	120.31
16	Q	234	GLN	N-CA-C	7.46	125.21	114.39
16	Q	144	MET	N-CA-C	7.38	119.32	111.28
35	l	2	ASN	CA-C-N	7.07	127.06	119.28
35	l	2	ASN	C-N-CA	7.07	127.06	119.28
39	p	144	THR	CA-C-N	6.96	127.54	120.38
39	p	144	THR	C-N-CA	6.96	127.54	120.38
4	E	42	GLU	N-CA-C	6.15	117.98	111.28
31	h	94	PRO	CA-C-N	6.12	126.68	120.38
31	h	94	PRO	C-N-CA	6.12	126.68	120.38
12	M	652	ASN	N-CA-C	5.93	118.53	111.71
31	h	95	PRO	CA-C-N	5.88	125.58	119.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	h	95	PRO	C-N-CA	5.88	125.58	119.05
4	E	43	VAL	CB-CA-C	-5.88	108.12	114.35
9	J	331	HIS	N-CA-C	5.84	117.64	111.28
14	O	164	THR	CA-C-N	5.83	125.52	119.05
14	O	164	THR	C-N-CA	5.83	125.52	119.05
16	Q	236	LEU	CA-C-N	5.78	125.75	120.03
16	Q	236	LEU	C-N-CA	5.78	125.75	120.03
12	M	654	VAL	N-CA-C	5.72	116.45	110.62
3	C	124	MET	CA-C-N	5.50	125.41	119.85
3	C	124	MET	C-N-CA	5.50	125.41	119.85
16	Q	142	VAL	N-CA-C	5.49	116.22	110.62
5	F	49	PRO	CA-N-CD	-5.41	104.43	112.00
24	a	94	GLY	N-CA-C	5.29	120.61	111.98
39	p	136	GLU	N-CA-C	5.04	116.77	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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3318	0	3280	96	0
2	B	1412	0	1363	32	0
3	C	1248	0	1254	32	0
4	E	961	0	960	20	0
5	F	691	0	704	28	0
6	G	693	0	671	28	0
6	X	696	0	680	22	0
7	H	910	0	950	17	0
8	I	780	0	808	17	0
9	J	2348	0	2390	46	0
10	K	355	0	329	11	0
11	L	1016	0	1016	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	M	5296	0	5326	94	0
13	N	1204	0	1162	21	0
14	O	1664	0	1660	55	0
15	P	1734	0	1689	37	0
16	Q	3377	0	3320	80	0
17	S	567	0	565	6	0
18	T	741	0	702	11	0
19	U	643	0	642	9	0
20	V	1011	0	1006	21	0
21	W	1173	0	1166	28	0
22	Y	597	0	537	14	0
23	Z	674	0	643	10	0
24	a	1165	0	1174	25	0
25	b	879	0	899	18	0
26	c	1315	0	1208	14	0
27	d	1461	0	1429	21	0
28	e	890	0	837	19	0
29	f	342	0	341	4	0
30	g	1000	0	994	11	0
31	h	847	0	842	15	0
32	i	2710	0	2874	58	0
33	j	800	0	855	16	0
34	k	748	0	799	24	0
35	l	4781	0	4926	93	0
36	m	948	0	960	23	0
37	n	479	0	486	10	0
38	o	1062	0	1072	12	0
39	p	1520	0	1444	29	0
40	r	3630	0	3836	74	0
41	s	2394	0	2508	55	0
42	u	1386	0	1366	30	0
43	v	1028	0	980	23	0
44	w	2582	0	2531	46	0
45	A	8	0	0	1	0
45	B	16	0	0	0	0
45	C	8	0	0	1	0
45	M	16	0	0	0	0
46	A	31	0	19	5	0
47	A	44	0	27	5	0
48	B	51	0	82	0	0
48	C	47	0	71	1	0
48	Q	47	0	71	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	l	92	0	138	4	0
48	m	41	0	59	3	0
48	r	51	0	82	3	0
48	s	51	0	82	2	0
49	G	35	0	0	1	0
49	X	35	0	0	2	0
50	I	51	0	46	0	0
50	a	91	0	132	4	0
50	i	66	0	76	4	0
50	l	199	0	307	32	0
50	r	100	0	156	10	0
51	J	48	0	25	4	0
52	M	4	0	0	0	0
52	O	4	0	0	0	0
53	M	1	0	0	0	0
54	N	52	0	88	2	0
54	a	52	0	88	2	0
54	g	52	0	88	6	0
54	j	52	0	88	3	0
54	r	104	0	176	18	0
55	T	1	0	0	0	0
56	s	28	0	31	2	0
57	w	27	0	11	2	0
All	All	66581	0	67127	1214	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 (1214) 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)
39:p:132:SER:O	39:p:136:GLU:HG3	1.37	1.19
51:J:401:NDP:O4D	51:J:401:NDP:C4D	1.68	1.18
35:l:5:ALA:CB	35:l:61:MET:HE1	1.71	1.18
4:E:40:TYR:CD2	6:G:120:MET:HE1	1.83	1.13
20:V:95:CYS:HB2	20:V:115:CYS:SG	1.89	1.12
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.11
50:l:701:CDL:H312	50:l:701:CDL:H742	1.17	1.11
35:l:5:ALA:HB2	35:l:61:MET:HE1	1.17	1.10
16:Q:235:ASP:HB2	16:Q:356:ILE:HD13	1.35	1.08
50:l:701:CDL:H422	40:r:448:THR:HG21	1.40	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:382:ARG:NH2	12:M:652:ASN:HD22	1.59	1.00
35:l:5:ALA:HB2	35:l:61:MET:CE	1.94	0.97
50:l:701:CDL:H742	50:l:701:CDL:C31	1.96	0.95
16:Q:144:MET:CE	16:Q:214:TYR:CE2	2.51	0.92
12:M:382:ARG:CZ	12:M:652:ASN:HD22	1.82	0.92
45:C:301:SF4:S4	16:Q:223:HIS:CD2	2.63	0.91
4:E:40:TYR:CD2	6:G:120:MET:CE	2.52	0.91
4:E:115:PRO:HB2	4:E:120:SER:OG	1.70	0.90
42:u:96:LEU:HD12	42:u:96:LEU:H	1.33	0.90
5:F:56:ARG:HB3	12:M:651:PRO:CG	2.02	0.89
4:E:40:TYR:HD2	6:G:120:MET:HE1	1.36	0.88
50:l:701:CDL:H812	54:r:503:PLX:H212	1.57	0.85
16:Q:144:MET:HE1	16:Q:214:TYR:CE2	2.12	0.84
5:F:57:GLU:O	12:M:651:PRO:HB2	1.78	0.83
35:l:11:THR:O	35:l:15:LEU:HD23	1.78	0.83
4:E:40:TYR:HD2	6:G:120:MET:CE	1.89	0.82
20:V:81:ARG:NH1	20:V:88:LEU:HD23	1.95	0.82
4:E:115:PRO:HB2	4:E:120:SER:HG	1.45	0.81
14:O:166:ASP:OD1	14:O:166:ASP:N	2.13	0.80
16:Q:144:MET:CE	16:Q:214:TYR:HE2	1.93	0.79
40:r:191:SER:HB3	48:r:501:PEE:H3	1.64	0.79
14:O:128:GLY:H	14:O:170:THR:HG21	1.46	0.79
35:l:5:ALA:HB1	35:l:61:MET:HE1	1.66	0.78
16:Q:81:THR:HG22	16:Q:100:GLU:HG2	1.66	0.78
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.67	0.77
50:l:701:CDL:H541	50:l:701:CDL:HA62	1.66	0.76
5:F:56:ARG:HB3	12:M:651:PRO:CD	2.16	0.75
40:r:328:CYS:HB3	40:r:437:MET:HE1	1.69	0.75
35:l:504:LEU:HD12	50:l:702:CDL:H522	1.69	0.75
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.68	0.74
7:H:18:GLU:HG2	7:H:19:THR:HG23	1.68	0.74
11:L:78:ARG:HE	12:M:607:LYS:HE3	1.52	0.74
16:Q:144:MET:HE3	16:Q:222:MET:O	1.87	0.74
20:V:101:LEU:HD23	20:V:101:LEU:O	1.87	0.74
4:E:39:TRP:O	4:E:43:VAL:HG23	1.87	0.74
4:E:70:ASN:ND2	49:G:201:8Q1:O4	2.20	0.74
43:v:111:ARG:HE	43:v:115:ARG:HH22	1.34	0.73
12:M:382:ARG:NH2	12:M:652:ASN:ND2	2.36	0.73
50:l:701:CDL:HA62	50:l:701:CDL:C54	2.18	0.73
40:r:370:PRO:HB3	40:r:375:LEU:HD22	1.68	0.73
43:v:52:MET:SD	43:v:54:GLN:NE2	2.61	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:96:LEU:HD12	42:u:96:LEU:N	2.03	0.73
36:m:170:GLU:OE1	36:m:173:ARG:NH2	2.21	0.73
1:A:41:ILE:O	1:A:137:LYS:NZ	2.21	0.72
33:j:95:LEU:HD13	41:s:302:MET:HG2	1.72	0.72
12:M:360:ARG:HG2	12:M:632:MET:HG2	1.72	0.71
20:V:99:LEU:C	20:V:99:LEU:HD23	2.15	0.71
34:k:22:TYR:O	35:l:585:LYS:NZ	2.21	0.71
50:l:701:CDL:H792	54:r:503:PLX:H212	1.72	0.70
32:i:1:MET:HA	44:w:289:ARG:HH21	1.56	0.70
35:l:331:MET:HB3	35:l:387:THR:HG22	1.72	0.70
11:L:88:GLN:NE2	12:M:141:ASP:OD2	2.24	0.70
12:M:382:ARG:CZ	12:M:652:ASN:ND2	2.53	0.70
1:A:159:ARG:NH2	14:O:176:CYS:O	2.25	0.70
13:N:69:ASN:OD1	13:N:112:ASN:ND2	2.23	0.70
2:B:131:GLU:HG3	2:B:144:ARG:HD2	1.73	0.69
32:i:232:HIS:HB3	32:i:311:MET:HE1	1.74	0.69
3:C:71:CYS:HB3	16:Q:141:TYR:HB3	1.73	0.69
8:I:68:ILE:HD11	15:P:75:GLN:HE21	1.58	0.69
14:O:218:PRO:HG3	14:O:224:SER:H	1.57	0.69
10:K:107:SER:HG	10:K:110:HIS:HD1	1.35	0.69
24:a:134:GLU:OE1	37:n:57:TRP:NE1	2.25	0.68
1:A:282:VAL:HG13	1:A:356:VAL:HG21	1.75	0.68
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.75	0.68
41:s:24:GLU:HG3	41:s:271:LEU:HD22	1.75	0.68
2:B:111:GLU:O	2:B:141:ARG:NH1	2.27	0.68
12:M:643:ARG:HA	12:M:646:LEU:HD12	1.75	0.68
16:Q:137:ASP:OD1	16:Q:144:MET:HB3	1.94	0.68
40:r:14:MET:SD	40:r:30:HIS:ND1	2.66	0.68
43:v:26:PRO:HG2	43:v:29:TYR:HB2	1.75	0.68
1:A:456:GLN:HE22	1:A:457:HIS:HD2	1.42	0.68
12:M:676:ASN:O	12:M:678:GLN:NE2	2.27	0.68
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.75	0.68
35:l:161:ARG:NH1	35:l:238:GLU:OE1	2.28	0.67
50:l:701:CDL:H812	54:r:503:PLX:C21	2.23	0.67
42:u:94:LEU:HB2	42:u:96:LEU:HD11	1.77	0.67
32:i:89:MET:HG3	32:i:95:MET:HE2	1.76	0.67
40:r:201:MET:HE1	54:r:502:PLX:H191	1.77	0.66
14:O:164:THR:HG23	14:O:167:LYS:H	1.60	0.66
1:A:205:ILE:HD13	1:A:379:CYS:HB3	1.77	0.66
34:k:22:TYR:CE2	35:l:584:ILE:HD12	2.30	0.66
35:l:7:LEU:HD22	35:l:46:LEU:HD11	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:414:THR:OG1	40:r:415:GLN:OE1	2.12	0.66
12:M:373:PRO:HG2	12:M:490:LEU:HD22	1.76	0.66
21:W:93:GLU:HG3	31:h:98:HIS:NE2	2.11	0.66
4:E:22:SER:OG	4:E:31:ARG:NH1	2.26	0.66
50:l:701:CDL:H532	50:l:701:CDL:H791	1.76	0.66
15:P:85:GLU:OE2	15:P:142:ARG:NH1	2.28	0.66
1:A:392:MET:HE2	1:A:419:ILE:HD12	1.78	0.65
11:L:156:LYS:HE2	12:M:68:ARG:HE	1.61	0.65
30:g:110:THR:HG22	30:g:112:GLY:H	1.61	0.65
40:r:282:LEU:HG	40:r:342:MET:HG3	1.77	0.65
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.78	0.65
50:l:701:CDL:H122	50:l:701:CDL:OA9	1.95	0.65
36:m:34:ILE:HD13	36:m:61:LEU:HD22	1.77	0.65
24:a:149:LEU:HD11	42:u:162:LYS:HD3	1.77	0.65
30:g:32:ARG:HB3	32:i:339:MET:HE1	1.79	0.65
41:s:24:GLU:OE2	41:s:274:ARG:NH1	2.29	0.65
12:M:624:ARG:NH2	12:M:637:ASP:OD1	2.30	0.65
3:C:102:VAL:HG23	3:C:129:TYR:O	1.96	0.65
9:J:83:PRO:HG3	9:J:119:VAL:HG11	1.79	0.65
9:J:318:LYS:HD2	9:J:321:ARG:HH12	1.62	0.65
20:V:101:LEU:HD23	20:V:101:LEU:C	2.21	0.65
1:A:127:ASP:HA	1:A:130:ILE:HG12	1.78	0.65
32:i:221:HIS:HB2	32:i:323:MET:HE1	1.79	0.65
15:P:74:GLN:HE22	15:P:146:TYR:HE1	1.44	0.64
35:l:391:SER:O	35:l:395:ILE:HG12	1.97	0.64
12:M:476:LEU:HD21	12:M:481:LEU:HD21	1.78	0.64
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.80	0.64
5:F:24:CYS:O	5:F:34:ARG:NH1	2.31	0.63
22:Y:72:ARG:NH1	22:Y:76:ASP:OD2	2.31	0.63
6:G:126:PHE:HE2	6:G:148:ILE:HG13	1.63	0.63
15:P:44:ARG:HE	15:P:45:PRO:HD3	1.63	0.63
32:i:128:LEU:HD12	32:i:216:PHE:HB3	1.80	0.63
34:k:44:SER:HB2	34:k:59:MET:HE1	1.79	0.63
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.32	0.63
33:j:18:VAL:HG22	41:s:222:MET:HG3	1.80	0.63
50:l:701:CDL:H541	50:l:701:CDL:CA6	2.28	0.63
9:J:211:ASP:O	9:J:215:ASN:ND2	2.32	0.62
35:l:97:THR:O	35:l:101:MET:HG3	1.97	0.62
6:G:120:MET:HA	6:G:123:GLU:HG3	1.80	0.62
35:l:407:TRP:O	35:l:411:MET:HG2	2.00	0.62
22:Y:100:LEU:HB2	43:v:111:ARG:HH22	1.63	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.39	0.62
9:J:192:ARG:NH1	9:J:198:ALA:O	2.33	0.62
12:M:166:GLY:HA2	12:M:213:MET:HE2	1.81	0.62
34:k:10:MET:O	34:k:14:ILE:HG13	1.99	0.62
40:r:306:PRO:HA	40:r:458:LEU:HD23	1.82	0.62
41:s:310:MET:HG3	41:s:311:THR:HG23	1.80	0.62
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.82	0.62
9:J:369:VAL:HG12	9:J:370:LYS:HG2	1.80	0.62
6:X:123:GLU:HG2	6:X:129:GLU:HA	1.82	0.62
1:A:116:ASN:ND2	1:A:207:GLY:O	2.28	0.62
9:J:150:HIS:HB2	9:J:190:GLU:HG2	1.82	0.62
14:O:87:GLN:OE1	14:O:123:ASN:ND2	2.32	0.62
9:J:203:PRO:HA	9:J:265:PHE:HB2	1.82	0.61
44:w:139:ARG:NH1	44:w:166:ASP:OD2	2.33	0.61
43:v:15:LYS:HE2	43:v:110:GLN:HG3	1.82	0.61
10:K:100:GLN:HB3	14:O:71:PRO:HA	1.83	0.61
35:l:161:ARG:NH2	39:p:88:GLY:O	2.34	0.61
35:l:526:LEU:HD12	35:l:530:PRO:HG2	1.82	0.61
5:F:56:ARG:HB3	12:M:651:PRO:HD2	1.81	0.61
13:N:120:THR:HG22	13:N:122:GLN:H	1.64	0.61
16:Q:184:ILE:HD11	16:Q:251:PHE:HZ	1.65	0.61
32:i:149:ILE:HD12	32:i:154:MET:HG3	1.82	0.61
44:w:76:GLU:O	44:w:80:LYS:HG2	2.01	0.61
20:V:97:GLY:O	20:V:100:THR:HG22	2.01	0.61
12:M:336:ASN:HD21	12:M:540:ASN:HB3	1.66	0.61
32:i:125:GLN:HG2	50:i:401:CDL:HA21	1.81	0.61
9:J:168:SER:HA	9:J:184:LYS:HE2	1.83	0.60
1:A:152:ARG:NH2	10:K:99:PRO:O	2.33	0.60
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.34	0.60
4:E:90:LEU:O	4:E:94:ILE:HG13	2.01	0.60
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.27	0.60
35:l:102:GLU:OE1	35:l:456:ARG:NH2	2.33	0.60
35:l:250:SER:HB2	35:l:333:ALA:HA	1.83	0.60
32:i:207:ILE:HG22	32:i:211:MET:HE2	1.84	0.60
35:l:221:ALA:HA	35:l:226:GLN:HG2	1.83	0.60
14:O:38:LEU:HD23	14:O:42:ARG:HH22	1.66	0.60
22:Y:94:ASP:HB3	22:Y:99:ILE:HB	1.82	0.60
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.34	0.60
25:b:77:ILE:O	25:b:81:ILE:HG12	2.02	0.60
50:l:701:CDL:C81	54:r:503:PLX:H212	2.28	0.60
8:I:101:ILE:HD13	15:P:138:ASN:HB2	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:84:ARG:NH1	11:L:88:GLN:O	2.35	0.60
35:l:419:THR:HA	35:l:422:TYR:CE2	2.36	0.60
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.36	0.60
24:a:106:VAL:HG13	37:n:50:ARG:HH21	1.67	0.60
25:b:31:ARG:HH21	39:p:116:PRO:HG2	1.67	0.60
6:X:75:THR:HG23	6:X:78:ALA:H	1.66	0.60
33:j:64:LEU:HD13	36:m:165:VAL:HG22	1.84	0.60
12:M:394:VAL:HG22	12:M:473:MET:HE1	1.84	0.60
16:Q:375:MET:HE3	16:Q:379:ILE:HG13	1.83	0.60
7:H:43:ALA:HA	7:H:46:LYS:HE3	1.84	0.59
39:p:29:SER:HB3	39:p:76:HIS:HD2	1.66	0.59
40:r:220:HIS:HE1	40:r:232:ALA:HB2	1.67	0.59
1:A:453:PHE:HA	1:A:456:GLN:HE21	1.67	0.59
32:i:211:MET:HG2	32:i:333:SER:HB2	1.84	0.59
41:s:273:ILE:HG23	41:s:277:TYR:HD2	1.67	0.59
41:s:295:PRO:HB3	48:s:401:PEE:H26	1.84	0.59
39:p:12:HIS:O	39:p:16:VAL:HG23	2.01	0.59
41:s:62:ARG:HD3	41:s:64:ALA:H	1.68	0.59
7:H:21:HIS:O	7:H:25:LYS:HG3	2.02	0.59
41:s:26:LYS:HG2	41:s:36:GLY:HA3	1.82	0.59
22:Y:65:MET:HE2	35:l:375:ILE:HG12	1.84	0.59
44:w:118:TYR:OH	57:w:401:ADP:O2'	2.20	0.59
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.84	0.59
1:A:447:GLU:O	1:A:451:GLN:HG3	2.02	0.59
22:Y:43:ARG:HG3	22:Y:48:PRO:HA	1.85	0.59
12:M:307:ILE:HG22	12:M:308:ARG:H	1.68	0.59
12:M:382:ARG:HD3	12:M:386:LEU:HD11	1.84	0.59
28:e:72:ASP:OD1	39:p:108:HIS:NE2	2.35	0.59
35:l:534:HIS:CD2	48:l:703:PEE:H13	2.38	0.59
41:s:85:MET:HG3	41:s:233:MET:HE2	1.84	0.59
9:J:127:ILE:HD11	9:J:253:ILE:HD11	1.85	0.59
50:l:701:CDL:H641	54:r:503:PLX:H122	1.85	0.59
2:B:47:SER:OG	2:B:49:ASP:OD1	2.21	0.58
7:H:38:ILE:O	7:H:45:ARG:NH1	2.36	0.58
24:a:87:THR:O	24:a:91:VAL:HG23	2.02	0.58
1:A:138:LEU:HD12	1:A:245:VAL:HG13	1.85	0.58
2:B:89:GLU:OE1	13:N:34:ARG:NH2	2.36	0.58
16:Q:235:ASP:CG	16:Q:356:ILE:HG21	2.27	0.58
16:Q:387:GLU:OE2	16:Q:390:GLN:NE2	2.37	0.58
44:w:203:VAL:HG12	44:w:254:GLU:HB2	1.85	0.58
1:A:159:ARG:NE	1:A:161:GLU:OE1	2.35	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:35:LEU:HD13	7:H:49:GLU:HG3	1.85	0.58
14:O:131:HIS:CD2	14:O:170:THR:OG1	2.55	0.58
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.36	0.58
50:l:701:CDL:H452	40:r:445:LEU:HB3	1.85	0.58
39:p:29:SER:HB3	39:p:76:HIS:CD2	2.39	0.58
40:r:61:LEU:HB2	40:r:457:PRO:HD3	1.85	0.58
3:C:109:LEU:HD13	3:C:117:LEU:HD13	1.85	0.58
3:C:123:GLN:O	41:s:61:LEU:HD11	2.04	0.58
4:E:78:VAL:O	4:E:82:LEU:HG	2.04	0.58
22:Y:51:THR:HG22	22:Y:53:SER:H	1.68	0.58
27:d:96:TYR:O	27:d:100:GLN:HG3	2.03	0.58
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.85	0.58
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.37	0.58
32:i:280:THR:O	32:i:284:MET:HG2	2.03	0.58
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.36	0.58
6:X:114:ASP:O	6:X:118:ILE:HG12	2.04	0.58
19:U:52:ASN:HB3	24:a:185:THR:HG22	1.86	0.58
25:b:69:ILE:O	25:b:73:THR:OG1	2.20	0.58
6:G:126:PHE:CE2	6:G:148:ILE:HG13	2.39	0.58
14:O:146:ASP:OD1	14:O:146:ASP:N	2.37	0.58
6:X:79:ILE:O	6:X:83:VAL:HG23	2.02	0.58
6:G:104:PHE:HA	6:G:108:LEU:HD12	1.85	0.58
15:P:169:GLU:OE2	16:Q:463:ARG:NH2	2.36	0.58
16:Q:235:ASP:CB	16:Q:356:ILE:HG21	2.33	0.58
20:V:123:ALA:O	20:V:126:LYS:N	2.37	0.58
22:Y:76:ASP:O	35:l:385:TYR:OH	2.21	0.58
5:F:25:GLN:OE1	5:F:26:ARG:NH1	2.36	0.57
14:O:148:ILE:O	14:O:152:ILE:HG13	2.04	0.57
16:Q:182:ASN:OD1	16:Q:404:LYS:NZ	2.37	0.57
41:s:273:ILE:HG23	41:s:277:TYR:CD2	2.39	0.57
2:B:177:THR:HG22	2:B:179:THR:H	1.68	0.57
40:r:133:ILE:HD11	40:r:231:LEU:HD11	1.86	0.57
11:L:109:ASN:ND2	11:L:111:LEU:O	2.36	0.57
44:w:294:LEU:O	44:w:298:VAL:HG13	2.04	0.57
20:V:88:LEU:O	20:V:92:ILE:HG13	2.05	0.57
6:X:83:VAL:HG13	6:X:122:MET:HE2	1.84	0.57
36:m:10:SER:O	36:m:14:VAL:HG23	2.03	0.57
44:w:70:LYS:NZ	44:w:88:GLU:OE2	2.37	0.57
16:Q:52:MET:HE2	32:i:173:THR:HG22	1.87	0.57
36:m:25:SER:O	36:m:28:TYR:N	2.37	0.57
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.40	0.57
49:X:201:8Q1:O3	39:p:13:GLN:NE2	2.37	0.57
1:A:137:LYS:HA	1:A:140:GLU:HG2	1.87	0.57
7:H:51:ILE:HD11	8:I:94:ALA:HB3	1.87	0.57
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.87	0.57
12:M:255:ASP:N	12:M:255:ASP:OD1	2.38	0.57
6:X:90:TYR:CE1	23:Z:44:PRO:HB2	2.40	0.57
1:A:102:MET:HG2	1:A:149:MET:HB3	1.87	0.57
13:N:65:THR:O	13:N:73:THR:OG1	2.22	0.57
37:n:39:ARG:O	37:n:41:LYS:NZ	2.35	0.57
21:W:97:ILE:HD13	31:h:83:ARG:HB2	1.86	0.56
2:B:177:THR:HG21	2:B:182:GLU:HB2	1.87	0.56
9:J:85:ARG:HH12	51:J:401:NDP:C6A	2.18	0.56
20:V:54:ALA:O	20:V:58:ARG:HG2	2.04	0.56
42:u:96:LEU:H	42:u:96:LEU:CD1	2.11	0.56
12:M:354:LEU:HD22	12:M:548:LEU:HD22	1.88	0.56
48:Q:501:PEE:H27	35:l:563:PRO:HA	1.87	0.56
24:a:132:ASN:ND2	40:r:49:SER:O	2.38	0.56
24:a:154:LEU:HD21	32:i:272:LYS:HD3	1.88	0.56
29:f:47:THR:HG23	30:g:65:LEU:HD22	1.88	0.56
33:j:60:ILE:HG21	36:m:168:ILE:HG21	1.87	0.56
34:k:5:TYR:O	34:k:9:ILE:HG12	2.05	0.56
6:G:74:LEU:H	6:G:74:LEU:HD23	1.70	0.56
6:X:69:SER:OG	6:X:70:ASP:N	2.39	0.56
24:a:116:PRO:HA	24:a:119:ARG:HG3	1.87	0.56
50:r:504:CDL:H271	50:r:504:CDL:H742	1.87	0.56
48:m:201:PEE:H52	41:s:104:PHE:HE1	1.70	0.56
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.86	0.56
15:P:124:ASN:HD22	15:P:146:TYR:HD2	1.54	0.56
21:W:144:THR:HB	41:s:96:ILE:HG23	1.88	0.56
16:Q:141:TYR:N	16:Q:141:TYR:CD2	2.73	0.56
16:Q:236:LEU:HD22	16:Q:240:LEU:HD23	1.86	0.56
36:m:41:CYS:HG	36:m:57:PHE:HD1	1.51	0.56
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.87	0.56
16:Q:100:GLU:HG3	16:Q:108:LYS:HE2	1.86	0.56
2:B:74:LEU:HB2	41:s:272:TRP:CZ2	2.41	0.56
5:F:56:ARG:CB	12:M:651:PRO:CD	2.83	0.56
16:Q:142:VAL:HG12	16:Q:182:ASN:HA	1.86	0.56
54:a:202:PLX:H102	40:r:40:SER:HB3	1.86	0.56
54:g:201:PLX:H301	32:i:347:ASN:HB3	1.86	0.56
31:h:38:LYS:O	31:h:42:GLU:HG2	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:227:PHE:O	35:l:230:HIS:ND1	2.35	0.56
2:B:87:PRO:O	2:B:90:LYS:NZ	2.39	0.56
36:m:141:MET:HE3	36:m:141:MET:HA	1.87	0.55
44:w:132:GLN:OE1	57:w:401:ADP:N6	2.35	0.55
9:J:204:SER:OG	9:J:238:GLN:O	2.23	0.55
9:J:247:LYS:HB2	9:J:340:ILE:HD13	1.87	0.55
15:P:138:ASN:C	15:P:138:ASN:HD22	2.14	0.55
40:r:373:ILE:HD11	40:r:444:LEU:HD23	1.87	0.55
50:l:701:CDL:OA9	50:l:701:CDL:H331	2.06	0.55
12:M:419:ARG:NH1	12:M:439:THR:O	2.40	0.55
35:l:558:LEU:HD13	40:r:211:GLY:HA2	1.89	0.55
9:J:214:LEU:HD13	9:J:352:VAL:HG11	1.88	0.55
26:c:182:VAL:HG22	43:v:34:ARG:NH2	2.21	0.55
36:m:42:GLY:HA2	48:m:201:PEE:H23	1.89	0.55
50:r:504:CDL:H401	50:r:504:CDL:H211	1.87	0.55
3:C:55:ASN:ND2	3:C:187:GLU:O	2.39	0.55
25:b:31:ARG:NH2	39:p:117:ASP:OD2	2.40	0.55
40:r:403:THR:HA	40:r:406:TYR:CE2	2.41	0.55
42:u:106:LYS:O	42:u:109:GLU:HG3	2.07	0.55
12:M:406:ASN:ND2	12:M:688:GLN:O	2.36	0.55
13:N:85:GLU:HB2	13:N:98:PRO:HB3	1.87	0.55
44:w:42:ALA:HB1	44:w:47:GLU:HG3	1.87	0.55
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.24	0.55
34:k:61:ILE:HG12	36:m:55:MET:HE1	1.88	0.55
35:l:566:THR:O	35:l:570:GLN:HG2	2.06	0.55
1:A:234:GLY:HA3	1:A:240:THR:HG22	1.87	0.54
12:M:58:MET:HE1	12:M:104:THR:HB	1.88	0.54
12:M:370:GLU:HG3	12:M:519:ILE:HD13	1.89	0.54
14:O:164:THR:OG1	14:O:165:PRO:HD2	2.07	0.54
21:W:90:ASN:ND2	21:W:123:GLU:O	2.40	0.54
25:b:123:PHE:HB3	43:v:40:VAL:HG21	1.89	0.54
32:i:246:VAL:HG21	50:r:504:CDL:H362	1.88	0.54
40:r:13:PRO:HB3	50:r:504:CDL:H581	1.89	0.54
40:r:39:LEU:HD11	54:r:503:PLX:H321	1.89	0.54
41:s:69:SER:O	41:s:73:ILE:HG12	2.07	0.54
6:G:114:ASP:O	6:G:118:ILE:HG13	2.07	0.54
44:w:227:MET:SD	44:w:227:MET:N	2.81	0.54
21:W:129:THR:OG1	21:W:131:GLU:OE2	2.25	0.54
2:B:93:LEU:O	8:I:34:ARG:NH2	2.40	0.54
5:F:56:ARG:CB	12:M:651:PRO:CG	2.83	0.54
14:O:129:LYS:HB3	14:O:168:LEU:HD12	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:108:HIS:ND1	39:p:110:SER:OG	2.31	0.54
41:s:170:GLU:OE2	42:u:98:ARG:NH1	2.41	0.54
1:A:127:ASP:O	1:A:131:ILE:HG23	2.07	0.54
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	1.89	0.54
26:c:110:ASP:OD1	26:c:110:ASP:N	2.40	0.54
14:O:63:ILE:HG12	14:O:82:VAL:HG23	1.88	0.54
18:T:53:VAL:O	18:T:56:SER:OG	2.25	0.54
50:l:701:CDL:H792	54:r:503:PLX:H233	1.90	0.54
22:Y:97:LEU:HG	43:v:107:ARG:HH12	1.71	0.54
44:w:214:ILE:O	44:w:218:ILE:HG13	2.08	0.54
3:C:144:HIS:O	3:C:151:ARG:NH1	2.41	0.54
7:H:47:TYR:O	7:H:51:ILE:HG12	2.07	0.54
12:M:224:ASP:OD1	12:M:291:ARG:NH1	2.38	0.54
50:l:701:CDL:H432	50:l:701:CDL:H602	1.90	0.54
49:X:201:8Q1:N36	49:X:201:8Q1:O40	2.41	0.54
35:l:146:GLY:O	35:l:150:MET:HG2	2.08	0.54
39:p:136:GLU:OE1	39:p:165:PRO:HA	2.08	0.54
5:F:45:LYS:NZ	12:M:376:GLY:O	2.40	0.54
14:O:128:GLY:H	14:O:170:THR:CG2	2.18	0.54
32:i:278:MET:O	32:i:282:MET:HG3	2.08	0.54
42:u:77:HIS:ND1	42:u:114:LYS:HG3	2.22	0.54
4:E:109:GLU:CD	4:E:109:GLU:H	2.16	0.53
42:u:155:GLU:N	42:u:155:GLU:OE1	2.40	0.53
1:A:48:ARG:O	10:K:74:ARG:NH1	2.40	0.53
9:J:247:LYS:O	9:J:251:ASN:ND2	2.38	0.53
20:V:99:LEU:HD23	20:V:99:LEU:O	2.06	0.53
40:r:49:SER:OG	40:r:58:SER:O	2.26	0.53
40:r:72:LEU:HD11	40:r:233:ALA:HB3	1.90	0.53
48:r:501:PEE:H26	48:r:501:PEE:H60	1.89	0.53
11:L:80:PHE:HE1	11:L:100:GLU:HG2	1.72	0.53
15:P:69:LEU:HD22	15:P:96:VAL:HG22	1.90	0.53
3:C:116:ALA:O	3:C:120:VAL:HG23	2.09	0.53
5:F:17:ARG:NH2	12:M:362:ASP:OD1	2.42	0.53
6:G:119:ILE:HD13	6:G:135:ALA:HB1	1.90	0.53
12:M:512:VAL:O	12:M:514:ASN:ND2	2.41	0.53
12:M:36:VAL:HB	12:M:56:VAL:HG21	1.91	0.53
1:A:66:LYS:HE2	1:A:187:CYS:HB3	1.90	0.53
6:X:91:ASP:HB3	23:Z:47:ARG:HH12	1.72	0.53
1:A:143:LEU:HD13	1:A:182:ILE:HD13	1.91	0.53
3:C:80:ALA:HA	3:C:86:MET:HG2	1.90	0.53
5:F:84:ALA:O	5:F:88:THR:OG1	2.25	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:114:THR:OG1	42:u:143:HIS:ND1	2.35	0.53
48:m:201:PEE:H56	48:m:201:PEE:H25	1.90	0.53
44:w:346:ASP:OD1	44:w:346:ASP:N	2.41	0.53
44:w:353:TRP:H	44:w:353:TRP:CD1	2.25	0.53
9:J:153:ALA:HB2	9:J:191:VAL:HG23	1.91	0.53
16:Q:41:VAL:O	16:Q:45:GLU:HG2	2.08	0.53
18:T:50:TYR:O	18:T:53:VAL:HG12	2.09	0.53
25:b:29:SER:OG	25:b:32:GLU:OE1	2.23	0.53
35:l:4:PHE:C	35:l:4:PHE:CD2	2.86	0.53
27:d:79:GLU:HG3	27:d:80:LYS:HG2	1.90	0.53
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.89	0.53
1:A:338:ASP:OD1	1:A:338:ASP:N	2.39	0.53
6:G:103:HIS:HE1	6:G:105:MET:HE2	1.73	0.53
19:U:11:ASN:O	19:U:11:ASN:ND2	2.40	0.53
31:h:37:GLU:OE2	32:i:83:GLN:NE2	2.42	0.53
21:W:105:LYS:HZ1	42:u:4:ILE:HB	1.74	0.52
34:k:98:CYS:HB2	35:l:580:GLN:HB2	1.90	0.52
35:l:5:ALA:CB	35:l:61:MET:CE	2.63	0.52
50:l:701:CDL:C34	50:l:701:CDL:H392	2.39	0.52
44:w:70:LYS:NZ	44:w:161:ARG:HH21	2.08	0.52
6:G:140:CYS:SG	6:G:143:GLU:HG3	2.50	0.52
12:M:155:GLU:N	12:M:155:GLU:OE2	2.42	0.52
25:b:97:VAL:HG22	35:l:63:ILE:HG23	1.91	0.52
35:l:298:ILE:O	35:l:302:VAL:HG23	2.10	0.52
42:u:104:GLN:O	42:u:108:ASP:OD1	2.27	0.52
43:v:95:TYR:O	43:v:99:MET:HG3	2.08	0.52
1:A:246:GLU:OE1	1:A:275:LEU:HD23	2.08	0.52
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.90	0.52
20:V:69:ILE:HG22	20:V:97:GLY:HA2	1.91	0.52
35:l:222:GLY:HA2	35:l:229:LEU:HD12	1.91	0.52
2:B:85:ASN:HB2	13:N:58:ARG:HH12	1.75	0.52
3:C:59:ARG:NH1	54:N:201:PLX:O3	2.36	0.52
26:c:58:ARG:NE	38:o:35:GLU:OE2	2.40	0.52
1:A:124:THR:HA	1:A:277:ASN:HD21	1.73	0.52
1:A:250:VAL:O	1:A:254:ILE:HG12	2.10	0.52
12:M:304:GLN:HG2	12:M:615:LEU:HD12	1.91	0.52
35:l:489:THR:O	35:l:493:VAL:HG13	2.09	0.52
1:A:277:ASN:OD1	1:A:277:ASN:N	2.43	0.52
32:i:88:LYS:HD2	32:i:148:SER:OG	2.09	0.52
35:l:559:GLU:O	35:l:563:PRO:HD2	2.10	0.52
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:169:PHE:O	44:w:173:MET:HG3	2.10	0.52
5:F:56:ARG:HB3	12:M:651:PRO:HG3	1.90	0.52
10:K:79:HIS:CE1	14:O:215:LYS:HB3	2.44	0.52
15:P:173:MET:HB3	15:P:198:PHE:HB2	1.91	0.52
21:W:81:ARG:HH22	42:u:64:ASN:ND2	2.07	0.52
28:e:79:ASP:HB3	28:e:82:VAL:HG12	1.91	0.52
41:s:269:THR:O	41:s:273:ILE:HD12	2.09	0.52
3:C:88:ARG:HA	41:s:37:PRO:HA	1.92	0.52
12:M:77:MET:HE1	12:M:117:MET:HG2	1.90	0.52
12:M:213:MET:HG2	12:M:215:MET:HG2	1.90	0.52
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.91	0.52
25:b:4:TYR:HB2	25:b:9:LYS:HG2	1.90	0.52
32:i:84:TRP:HH2	34:k:59:MET:HE2	1.74	0.52
48:C:302:PEE:H1	33:j:28:ASN:HB3	1.91	0.52
9:J:163:LYS:HG2	9:J:259:LYS:HZ3	1.75	0.52
10:K:105:ARG:NH1	11:L:167:ASN:O	2.43	0.52
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.91	0.52
35:l:393:ASP:O	35:l:397:GLU:HG3	2.10	0.52
39:p:49:ASP:HB2	39:p:52:LYS:HE2	1.90	0.52
41:s:81:LEU:O	41:s:85:MET:HG2	2.10	0.52
14:O:127:VAL:HG22	14:O:170:THR:HG21	1.92	0.52
20:V:141:VAL:O	24:a:169:TYR:OH	2.25	0.52
32:i:204:ASN:C	32:i:204:ASN:HD22	2.18	0.52
41:s:307:LEU:HA	41:s:310:MET:HG2	1.92	0.52
12:M:144:MET:HG3	16:Q:383:LYS:HG3	1.91	0.51
27:d:121:TYR:HD2	35:l:203:MET:HE2	1.73	0.51
32:i:243:LEU:HD23	50:r:504:CDL:H361	1.91	0.51
35:l:309:GLN:O	35:l:313:MET:HG3	2.09	0.51
3:C:79:MET:HE3	3:C:86:MET:HE3	1.90	0.51
7:H:19:THR:O	7:H:19:THR:OG1	2.27	0.51
35:l:286:LEU:HD22	35:l:411:MET:SD	2.50	0.51
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.38	0.51
12:M:171:THR:HG23	12:M:173:MET:HE3	1.93	0.51
14:O:131:HIS:HA	14:O:170:THR:OG1	2.10	0.51
34:k:23:ARG:HG2	36:m:23:LYS:HE2	1.91	0.51
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.45	0.51
6:G:88:LYS:HE3	6:G:95:PRO:HB3	1.93	0.51
6:X:123:GLU:OE1	39:p:21:LYS:NZ	2.43	0.51
22:Y:95:GLU:OE2	22:Y:95:GLU:N	2.38	0.51
35:l:99:SER:HB3	35:l:341:MET:HE1	1.92	0.51
39:p:100:PRO:HG3	40:r:419:TYR:CZ	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ALA:HB1	14:O:121:MET:HB2	1.92	0.51
1:A:360:SER:O	1:A:360:SER:OG	2.25	0.51
2:B:137:ASP:OD1	2:B:137:ASP:N	2.35	0.51
4:E:116:THR:HG22	4:E:116:THR:O	2.09	0.51
12:M:478:SER:O	12:M:482:GLN:HG2	2.10	0.51
32:i:334:THR:HG22	32:i:335:LEU:HG	1.92	0.51
50:l:701:CDL:H792	54:r:503:PLX:C21	2.41	0.51
44:w:125:ASP:O	44:w:130:ARG:NH2	2.44	0.51
1:A:44:ASN:HD22	1:A:59:ARG:NH1	2.09	0.51
1:A:98:LYS:NZ	47:A:503:NAI:O3B	2.44	0.51
40:r:112:ALA:HB1	40:r:118:PHE:HB2	1.93	0.51
41:s:2:PHE:HZ	41:s:96:ILE:HD11	1.75	0.51
41:s:185:TRP:NE1	41:s:238:THR:OG1	2.38	0.51
1:A:50:ASP:HB3	1:A:55:GLY:HA3	1.91	0.51
35:l:327:LEU:O	35:l:331:MET:HG2	2.10	0.51
41:s:102:VAL:HG11	41:s:154:LEU:HD11	1.92	0.51
9:J:279:TYR:O	9:J:283:VAL:HG22	2.11	0.51
32:i:20:VAL:HG11	32:i:137:ALA:HB1	1.93	0.51
9:J:275:ASP:OD1	9:J:275:ASP:N	2.41	0.51
32:i:154:MET:HA	32:i:154:MET:HE2	1.93	0.51
35:l:190:LEU:HB2	35:l:196:TRP:NE1	2.26	0.51
40:r:269:MET:HE1	40:r:296:LEU:HD13	1.93	0.51
1:A:63:TYR:HE1	14:O:245:VAL:HG21	1.75	0.50
16:Q:102:SER:OG	16:Q:107:ARG:NH1	2.44	0.50
16:Q:330:TYR:O	16:Q:334:VAL:HG23	2.11	0.50
1:A:89:GLY:O	47:A:503:NAI:H2N	2.11	0.50
7:H:76:GLN:O	7:H:79:GLU:HG2	2.11	0.50
6:G:103:HIS:CE1	6:G:105:MET:HG3	2.47	0.50
12:M:64:CYS:O	12:M:184:ARG:NH2	2.35	0.50
12:M:385:TYR:OH	12:M:527:ASP:OD1	2.26	0.50
25:b:9:LYS:O	25:b:13:GLN:HG2	2.10	0.50
25:b:19:ARG:HA	39:p:171:VAL:HG13	1.93	0.50
34:k:2:PRO:HD2	34:k:5:TYR:CD2	2.47	0.50
1:A:63:TYR:CE1	1:A:64:LYS:HG3	2.47	0.50
1:A:362:ASP:OD1	1:A:449:ARG:NH2	2.38	0.50
1:A:388:GLY:HA3	1:A:419:ILE:HD11	1.93	0.50
6:X:155:TYR:HE1	25:b:23:LEU:HB3	1.76	0.50
35:l:290:LEU:O	35:l:293:ILE:HG22	2.12	0.50
35:l:562:LEU:HB2	35:l:563:PRO:HD3	1.93	0.50
40:r:11:LEU:HB3	40:r:100:ILE:HD13	1.92	0.50
6:G:88:LYS:HD3	6:G:98:LEU:HD21	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:75:GLN:HB3	15:P:87:PHE:HB2	1.94	0.50
50:l:701:CDL:HA62	50:l:701:CDL:H542	1.94	0.50
42:u:103:GLN:N	42:u:103:GLN:OE1	2.45	0.50
8:I:46:SER:O	8:I:52:ASN:ND2	2.43	0.50
9:J:37:HIS:CE1	18:T:49:ASP:HA	2.47	0.50
12:M:360:ARG:HB2	12:M:360:ARG:HH11	1.77	0.50
13:N:78:ASP:OD1	13:N:78:ASP:N	2.43	0.50
15:P:43:THR:HA	15:P:47:ILE:HD12	1.93	0.50
16:Q:156:GLU:OE2	16:Q:171:ARG:NH2	2.41	0.50
24:a:91:VAL:HG13	27:d:52:ILE:HG12	1.92	0.50
12:M:670:GLU:HA	12:M:673:LYS:HD3	1.94	0.50
26:c:143:MET:HE2	26:c:143:MET:HA	1.93	0.50
40:r:231:LEU:HA	40:r:235:LEU:HB2	1.94	0.50
40:r:357:THR:O	40:r:361:VAL:HG23	2.12	0.50
42:u:88:CYS:SG	42:u:89:ILE:N	2.85	0.50
44:w:181:LYS:O	44:w:185:GLU:HG3	2.12	0.50
1:A:46:TYR:CE1	14:O:226:GLU:HB3	2.47	0.50
39:p:20:TYR:HB2	39:p:48:PHE:CZ	2.47	0.50
42:u:149:GLU:HG2	42:u:150:PRO:HD2	1.94	0.50
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.93	0.49
16:Q:244:ILE:HG22	16:Q:348:LEU:HD11	1.93	0.49
1:A:48:ARG:NH2	14:O:226:GLU:OE2	2.45	0.49
16:Q:139:LEU:HD11	16:Q:424:ILE:HD13	1.94	0.49
40:r:220:HIS:CE1	40:r:232:ALA:HB2	2.47	0.49
6:G:144:ILE:O	6:G:148:ILE:HG12	2.13	0.49
9:J:94:LEU:HD23	9:J:97:MET:HE3	1.93	0.49
12:M:390:THR:HA	12:M:600:GLU:HG2	1.93	0.49
15:P:108:PHE:O	15:P:160:TYR:OH	2.25	0.49
37:n:28:ASP:OD2	40:r:3:LYS:NZ	2.31	0.49
6:G:93:ILE:HD11	6:G:108:LEU:HB3	1.93	0.49
13:N:4:VAL:O	13:N:8:ARG:HG2	2.12	0.49
16:Q:176:GLU:OE2	16:Q:311:TYR:OH	2.22	0.49
35:l:66:TRP:HZ3	48:l:704:PEE:H38	1.78	0.49
35:l:539:TYR:OH	38:o:10:ARG:NH1	2.46	0.49
40:r:259:TYR:O	40:r:263:MET:HG2	2.13	0.49
1:A:272:GLY:O	1:A:292:MET:HG3	2.13	0.49
3:C:113:MET:HE3	3:C:116:ALA:HB3	1.94	0.49
11:L:163:ASN:O	11:L:171:ARG:HA	2.13	0.49
12:M:654:VAL:O	12:M:656:TYR:CD2	2.66	0.49
15:P:104:THR:O	15:P:107:GLN:NE2	2.44	0.49
24:a:136:THR:HG21	40:r:48:ASN:HD22	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:o:105:PHE:CD2	40:r:263:MET:HE1	2.48	0.49
41:s:152:SER:HA	41:s:155:LEU:HD12	1.92	0.49
1:A:44:ASN:HD22	1:A:59:ARG:CZ	2.24	0.49
1:A:394:LYS:HB3	12:M:155:GLU:HG2	1.95	0.49
7:H:34:VAL:HG21	7:H:92:ARG:HG2	1.94	0.49
8:I:66:PRO:HB3	15:P:79:SER:HA	1.94	0.49
12:M:347:ASP:OD1	12:M:347:ASP:N	2.35	0.49
17:S:39:ALA:HA	17:S:44:GLN:HG3	1.95	0.49
27:d:119:GLU:HG2	43:v:52:MET:HA	1.94	0.49
1:A:452:GLN:NE2	1:A:452:GLN:O	2.46	0.49
20:V:102:GLY:HA3	20:V:111:GLY:CA	2.43	0.49
40:r:266:MET:HE1	40:r:392:THR:HB	1.94	0.49
1:A:413:TRP:O	1:A:416:SER:OG	2.26	0.49
5:F:56:ARG:HB3	12:M:651:PRO:HG2	1.92	0.49
20:V:101:LEU:C	20:V:101:LEU:CD2	2.86	0.49
21:W:85:GLN:O	21:W:89:GLU:HG3	2.12	0.49
9:J:235:THR:HG23	9:J:325:SER:HA	1.95	0.49
12:M:494:SER:OG	12:M:669:ASN:ND2	2.46	0.49
32:i:320:THR:OG1	44:w:300:ASN:HB2	2.13	0.49
33:j:55:PHE:O	33:j:58:VAL:HG12	2.13	0.49
41:s:24:GLU:OE1	41:s:228:TYR:OH	2.25	0.49
3:C:102:VAL:HA	3:C:129:TYR:O	2.13	0.48
9:J:132:ARG:NH2	51:J:401:NDP:O2X	2.46	0.48
9:J:209:ARG:HB3	9:J:210:GLU:OE1	2.13	0.48
13:N:10:GLY:O	13:N:14:VAL:HG23	2.13	0.48
16:Q:251:PHE:HB3	16:Q:341:LEU:HD11	1.95	0.48
5:F:56:ARG:CB	12:M:651:PRO:HD2	2.44	0.48
12:M:347:ASP:HB3	12:M:594:ALA:HB1	1.96	0.48
14:O:130:TYR:HB2	14:O:169:PHE:HD1	1.78	0.48
25:b:123:PHE:HD2	43:v:40:VAL:HG11	1.78	0.48
50:l:701:CDL:H422	40:r:448:THR:CG2	2.29	0.48
1:A:41:ILE:H	1:A:289:GLU:CD	2.21	0.48
1:A:44:ASN:ND2	1:A:49:HIS:HB2	2.29	0.48
1:A:185:ASN:C	1:A:187:CYS:H	2.21	0.48
3:C:184:ILE:O	3:C:187:GLU:HG2	2.13	0.48
6:G:84:LEU:O	6:G:88:LYS:HG2	2.12	0.48
12:M:261:ILE:HD12	12:M:273:ILE:HD12	1.96	0.48
12:M:360:ARG:HB2	12:M:360:ARG:NH1	2.28	0.48
20:V:102:GLY:HA3	20:V:111:GLY:HA2	1.94	0.48
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.95	0.48
34:k:37:MET:HG3	34:k:67:ALA:CB	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:292:ALA:HB2	35:l:304:PHE:HB3	1.95	0.48
35:l:408:ALA:O	35:l:412:THR:HG23	2.13	0.48
35:l:521:LYS:O	35:l:525:MET:HG2	2.14	0.48
44:w:83:LEU:HD22	44:w:156:GLY:HA3	1.95	0.48
2:B:50:MET:HE2	2:B:50:MET:HA	1.95	0.48
9:J:172:ALA:HA	9:J:181:LEU:HB3	1.96	0.48
25:b:31:ARG:O	25:b:31:ARG:HG2	2.13	0.48
35:l:565:THR:O	35:l:569:ILE:HG13	2.13	0.48
2:B:115:ALA:HB2	2:B:142:THR:HG23	1.95	0.48
12:M:534:VAL:HG22	12:M:537:ILE:HB	1.96	0.48
13:N:96:ASP:OD2	13:N:101:LYS:HD2	2.13	0.48
14:O:131:HIS:HD2	14:O:170:THR:OG1	1.96	0.48
7:H:55:LYS:O	7:H:59:VAL:HG12	2.13	0.48
11:L:90:GLY:HA3	15:P:238:PRO:HB2	1.94	0.48
12:M:47:THR:HG23	12:M:51:GLN:HB2	1.95	0.48
20:V:69:ILE:CG2	20:V:97:GLY:HA2	2.44	0.48
24:a:188:ASP:OD1	24:a:188:ASP:N	2.35	0.48
30:g:32:ARG:O	30:g:36:MET:HG2	2.13	0.48
43:v:21:ARG:HH21	43:v:24:THR:HG21	1.77	0.48
44:w:54:THR:HG22	44:w:54:THR:O	2.12	0.48
1:A:182:ILE:HD12	1:A:183:GLY:H	1.79	0.48
4:E:37:ARG:HH22	6:G:132:ASP:HB2	1.79	0.48
9:J:166:HIS:HB3	9:J:200:ILE:HD13	1.95	0.48
19:U:11:ASN:HD22	19:U:11:ASN:C	2.22	0.48
21:W:36:PHE:O	21:W:40:ILE:HG12	2.13	0.48
40:r:240:GLY:O	40:r:244:MET:HG3	2.13	0.48
56:s:402:UQ:H152	56:s:402:UQ:H101	1.96	0.48
14:O:182:ASN:ND2	14:O:194:GLU:OE2	2.47	0.48
15:P:115:THR:OG1	15:P:116:ALA:N	2.46	0.48
19:U:53:TYR:CZ	42:u:44:MET:HG3	2.49	0.48
32:i:252:GLY:HA3	32:i:290:LEU:HD13	1.96	0.48
41:s:179:TRP:CG	41:s:180:PRO:HD3	2.48	0.48
43:v:51:LEU:HD13	43:v:63:LEU:HD23	1.96	0.48
27:d:114:GLN:HG3	35:l:203:MET:HG2	1.94	0.48
34:k:5:TYR:HA	34:k:43:MET:HE1	1.96	0.48
50:l:701:CDL:H392	50:l:701:CDL:H342	1.95	0.48
38:o:112:LYS:O	38:o:116:ILE:HG13	2.14	0.48
39:p:136:GLU:OE2	39:p:167:TRP:NE1	2.46	0.48
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.95	0.48
16:Q:145:MET:HE2	16:Q:226:TYR:HB3	1.94	0.48
40:r:153:THR:HG23	40:r:206:LYS:HD2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:216:LEU:HD23	40:r:287:ALA:HB1	1.96	0.48
44:w:237:ILE:O	44:w:241:TYR:HB2	2.14	0.48
25:b:99:GLU:OE2	35:l:59:GLN:NE2	2.44	0.47
43:v:22:MET:HG3	43:v:105:GLU:HG2	1.95	0.47
5:F:40:ARG:O	5:F:43:GLU:HG3	2.14	0.47
12:M:308:ARG:NH2	12:M:578:PRO:O	2.47	0.47
16:Q:270:ASN:HB3	41:s:284:GLN:NE2	2.29	0.47
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.49	0.47
3:C:67:PHE:HE2	3:C:113:MET:HE2	1.80	0.47
14:O:131:HIS:NE2	14:O:172:ILE:HG13	2.30	0.47
32:i:1:MET:HE3	32:i:6:TYR:HD1	1.78	0.47
35:l:5:ALA:HB2	35:l:61:MET:SD	2.53	0.47
12:M:569:GLN:HG3	12:M:584:LEU:HB2	1.95	0.47
27:d:50:GLU:O	27:d:54:GLN:HG3	2.15	0.47
34:k:90:VAL:HG11	35:l:585:LYS:HG3	1.96	0.47
36:m:25:SER:O	36:m:27:ILE:N	2.47	0.47
39:p:121:LYS:HD2	39:p:121:LYS:HA	1.61	0.47
41:s:27:VAL:HG13	41:s:31:MET:HE3	1.96	0.47
14:O:182:ASN:HA	14:O:222:ARG:HH21	1.79	0.47
8:I:23:LYS:HD3	16:Q:250:ASN:HA	1.95	0.47
12:M:252:ASP:OD1	12:M:254:MET:HG2	2.14	0.47
54:j:201:PLX:H282	54:j:201:PLX:H312	1.53	0.47
54:j:201:PLX:H381	54:j:201:PLX:H322	1.96	0.47
35:l:364:LYS:HA	35:l:364:LYS:HD3	1.76	0.47
39:p:136:GLU:OE2	39:p:167:TRP:CD1	2.68	0.47
42:u:9:THR:OG1	42:u:12:ASP:OD2	2.27	0.47
44:w:86:PHE:HB2	44:w:159:LEU:HD23	1.96	0.47
3:C:67:PHE:HE1	3:C:120:VAL:HG11	1.79	0.47
9:J:168:SER:O	9:J:202:LYS:HA	2.14	0.47
11:L:89:SER:O	12:M:59:GLN:NE2	2.46	0.47
12:M:613:PRO:HB3	13:N:134:ILE:HD13	1.96	0.47
14:O:137:THR:HG22	14:O:138:THR:H	1.78	0.47
16:Q:236:LEU:HD22	16:Q:240:LEU:CD2	2.45	0.47
26:c:117:VAL:HG21	35:l:539:TYR:HB2	1.96	0.47
30:g:19:GLU:HG2	42:u:158:LEU:HD12	1.97	0.47
31:h:95:PRO:HD2	31:h:98:HIS:HD2	1.80	0.47
35:l:289:ALA:HB1	35:l:418:LEU:HB3	1.96	0.47
41:s:231:ILE:O	41:s:235:ASN:ND2	2.47	0.47
42:u:83:THR:HA	42:u:86:TRP:CD1	2.50	0.47
44:w:78:ALA:HB2	44:w:158:VAL:HG21	1.96	0.47
33:j:49:LEU:N	33:j:50:PRO:HD2	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:17:ALA:O	34:k:21:MET:HG2	2.15	0.47
50:l:701:CDL:H432	50:l:701:CDL:C60	2.45	0.47
46:A:502:FMN:O4'	46:A:502:FMN:O2'	2.32	0.47
2:B:148:ASP:OD1	2:B:150:THR:OG1	2.30	0.47
16:Q:83:ASN:OD1	16:Q:98:VAL:HG22	2.15	0.47
16:Q:235:ASP:HB2	16:Q:356:ILE:HG21	1.96	0.47
22:Y:100:LEU:H	43:v:111:ARG:HH12	1.62	0.47
32:i:254:LEU:HD21	40:r:154:LEU:HD11	1.96	0.47
40:r:73:LEU:HD22	40:r:103:GLN:OE1	2.14	0.47
3:C:58:ARG:NH1	3:C:127:PRO:HG3	2.30	0.47
9:J:214:LEU:HD23	9:J:280:ILE:HG12	1.97	0.47
16:Q:101:LEU:HD22	16:Q:106:VAL:HA	1.97	0.47
6:X:118:ILE:O	6:X:122:MET:HG2	2.15	0.47
33:j:54:LYS:HD3	33:j:113:TRP:HA	1.97	0.47
35:l:233:LEU:HB3	35:l:234:PRO:HD3	1.96	0.47
5:F:43:GLU:HA	5:F:46:LYS:HG3	1.97	0.46
12:M:432:ILE:HD11	12:M:445:LEU:HD12	1.97	0.46
16:Q:236:LEU:HA	16:Q:237:PRO:HD3	1.79	0.46
20:V:99:LEU:C	20:V:99:LEU:CD2	2.86	0.46
24:a:111:GLU:HG2	27:d:64:TYR:HE1	1.80	0.46
39:p:16:VAL:HG12	39:p:48:PHE:CZ	2.51	0.46
24:a:96:ALA:HB2	27:d:61:TYR:CE2	2.50	0.46
26:c:84:GLN:O	26:c:98:ARG:NH1	2.48	0.46
26:c:176:LYS:HD2	26:c:176:LYS:HA	1.72	0.46
32:i:102:LEU:HD13	32:i:142:LEU:HG	1.97	0.46
41:s:227:GLU:O	41:s:231:ILE:HG13	2.16	0.46
42:u:139:GLU:N	42:u:139:GLU:OE2	2.47	0.46
44:w:57:SER:HB3	44:w:150:LEU:HD21	1.98	0.46
9:J:272:LEU:HB2	9:J:275:ASP:OD1	2.15	0.46
25:b:106:PRO:HG2	25:b:120:MET:SD	2.56	0.46
54:g:201:PLX:H312	54:g:201:PLX:H211	1.95	0.46
34:k:22:TYR:HB3	35:l:585:LYS:HG2	1.98	0.46
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.95	0.46
37:n:28:ASP:OD1	40:r:2:LEU:HB2	2.16	0.46
40:r:106:LEU:HD13	40:r:234:VAL:HG11	1.97	0.46
42:u:55:ARG:HG3	42:u:55:ARG:HH11	1.79	0.46
44:w:265:ASP:OD1	44:w:265:ASP:N	2.41	0.46
4:E:88:MET:HE2	15:P:184:LEU:O	2.15	0.46
9:J:262:THR:O	9:J:333:PRO:HD2	2.15	0.46
12:M:213:MET:SD	12:M:215:MET:HE2	2.56	0.46
14:O:130:TYR:CE2	14:O:208:LEU:HD22	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:69:ASP:O	18:T:73:GLU:HG3	2.15	0.46
50:l:701:CDL:H312	50:l:701:CDL:C74	2.12	0.46
38:o:105:PHE:HD2	40:r:263:MET:HE1	1.80	0.46
7:H:20:PRO:HB2	7:H:77:ILE:HG21	1.98	0.46
48:r:501:PEE:H81	54:r:502:PLX:H393	1.97	0.46
43:v:19:PRO:HA	43:v:22:MET:HE3	1.97	0.46
1:A:145:GLY:O	1:A:149:MET:HG3	2.16	0.46
5:F:31:GLN:O	5:F:34:ARG:HB2	2.16	0.46
14:O:110:MET:O	14:O:114:GLU:HG3	2.15	0.46
14:O:199:LYS:NZ	14:O:203:GLU:OE2	2.47	0.46
23:Z:39:ARG:HG3	23:Z:41:LEU:HD12	1.96	0.46
32:i:230:LEU:HD11	32:i:244:MET:HE1	1.98	0.46
40:r:373:ILE:HA	40:r:376:ILE:HD12	1.97	0.46
2:B:74:LEU:HD12	2:B:77:LEU:HD23	1.98	0.46
2:B:80:GLU:HG3	17:S:1:MET:HG2	1.98	0.46
16:Q:144:MET:HE2	16:Q:144:MET:HB2	1.78	0.46
6:X:90:TYR:HE1	23:Z:44:PRO:HB2	1.78	0.46
28:e:128:TYR:HE1	28:e:132:ASN:HD22	1.64	0.46
50:l:701:CDL:H451	50:l:701:CDL:H612	1.97	0.46
42:u:38:LYS:O	42:u:42:GLU:HG2	2.16	0.46
5:F:55:ILE:HD13	12:M:381:LEU:HD23	1.98	0.46
8:I:58:ASP:OD2	8:I:61:ARG:HB2	2.16	0.46
9:J:116:ILE:O	9:J:120:VAL:HG22	2.16	0.46
12:M:382:ARG:HA	12:M:385:TYR:CE1	2.51	0.46
14:O:66:ILE:HD13	14:O:81:PRO:HB2	1.98	0.46
15:P:119:VAL:HG12	15:P:121:THR:HG22	1.97	0.46
24:a:168:TRP:HB3	30:g:2:THR:O	2.16	0.46
50:a:201:CDL:H531	48:l:704:PEE:H56	1.98	0.46
35:l:596:MET:O	35:l:600:THR:HG23	2.16	0.46
41:s:55:LEU:HD12	56:s:402:UQ:H112	1.98	0.46
1:A:130:ILE:HD11	1:A:245:VAL:HG12	1.97	0.46
9:J:329:LEU:HD12	9:J:329:LEU:N	2.31	0.46
15:P:173:MET:HE3	15:P:188:LEU:HD12	1.96	0.46
24:a:78:THR:HG21	28:e:96:SER:O	2.16	0.46
54:g:201:PLX:H101	54:g:201:PLX:H72	1.64	0.46
31:h:2:PRO:HB2	31:h:3:PHE:H	1.54	0.46
32:i:242:SER:O	32:i:246:VAL:HG23	2.15	0.46
35:l:173:LEU:HG	40:r:401:MET:HE3	1.98	0.46
42:u:111:VAL:CG1	42:u:117:TRP:HB2	2.46	0.46
44:w:63:ASP:HB3	44:w:241:TYR:OH	2.16	0.46
1:A:210:THR:HB	1:A:224:ARG:H	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.51	0.45
9:J:136:THR:OG1	9:J:139:PHE:O	2.33	0.45
12:M:326:VAL:HG23	12:M:626:LEU:HD13	1.97	0.45
14:O:156:LEU:HD11	14:O:169:PHE:HD2	1.81	0.45
21:W:74:LEU:O	21:W:78:GLU:HG3	2.16	0.45
44:w:60:ILE:HG23	44:w:203:VAL:HG23	1.98	0.45
1:A:405:ARG:HD3	1:A:406:PRO:HD2	1.98	0.45
2:B:179:THR:OG1	2:B:182:GLU:OE2	2.27	0.45
6:G:90:TYR:OH	6:G:114:ASP:OD1	2.29	0.45
9:J:126:VAL:HG23	9:J:161:VAL:HG11	1.98	0.45
14:O:128:GLY:CA	14:O:167:LYS:O	2.65	0.45
35:l:151:SER:OG	35:l:248:HIS:NE2	2.45	0.45
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.98	0.45
40:r:287:ALA:O	40:r:291:VAL:HG23	2.17	0.45
54:r:502:PLX:H301	54:r:502:PLX:H331	1.79	0.45
41:s:195:ARG:HD3	41:s:231:ILE:HD11	1.98	0.45
1:A:40:ARG:NE	14:O:233:SER:OG	2.50	0.45
1:A:244:ASN:N	46:A:502:FMN:O1P	2.42	0.45
3:C:127:PRO:HA	9:J:89:TYR:OH	2.17	0.45
16:Q:47:PHE:HD2	16:Q:52:MET:HE1	1.80	0.45
16:Q:142:VAL:CG1	16:Q:182:ASN:HA	2.47	0.45
28:e:65:ASN:OD1	28:e:67:TYR:N	2.43	0.45
35:l:293:ILE:HG23	35:l:294:THR:HG23	1.97	0.45
44:w:98:THR:OG1	44:w:337:ARG:NH2	2.44	0.45
44:w:181:LYS:O	44:w:184:VAL:HG22	2.16	0.45
1:A:294:VAL:O	1:A:337:MET:HG2	2.17	0.45
3:C:124:MET:HA	3:C:125:PRO:HD3	1.77	0.45
8:I:68:ILE:HD11	15:P:75:GLN:NE2	2.29	0.45
9:J:45:LYS:HE3	9:J:45:LYS:HB2	1.77	0.45
12:M:306:MET:HE3	12:M:316:TYR:CE1	2.52	0.45
21:W:119:PRO:O	36:m:130:THR:OG1	2.26	0.45
28:e:55:LEU:HD11	28:e:57:GLU:HB2	1.99	0.45
32:i:92:PRO:O	32:i:96:THR:HG22	2.16	0.45
32:i:200:MET:HE1	32:i:343:LEU:HD13	1.98	0.45
36:m:23:LYS:N	36:m:24:PRO:HD3	2.32	0.45
36:m:39:VAL:O	36:m:43:ILE:HG13	2.17	0.45
40:r:12:LEU:HB2	40:r:13:PRO:HD3	1.99	0.45
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.98	0.45
16:Q:237:PRO:O	21:W:9:ASP:OD2	2.34	0.45
16:Q:293:LEU:HD22	16:Q:298:ILE:HD12	1.98	0.45
20:V:123:ALA:O	20:V:124:LEU:C	2.57	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:169:GLU:HA	27:d:123:GLN:HB2	1.98	0.45
32:i:250:SER:O	32:i:259:GLY:HA3	2.17	0.45
38:o:48:LEU:HB3	39:p:166:LEU:HD13	1.97	0.45
2:B:100:GLU:O	2:B:170:GLY:N	2.47	0.45
13:N:144:TYR:H	13:N:144:TYR:HD1	1.65	0.45
16:Q:232:VAL:CG2	16:Q:356:ILE:HB	2.47	0.45
21:W:82:ARG:O	21:W:86:MET:HG3	2.17	0.45
54:g:201:PLX:H361	54:g:201:PLX:H311	1.99	0.45
33:j:75:LEU:HD13	41:s:305:ILE:HD11	1.99	0.45
41:s:9:LEU:O	41:s:13:ILE:HG12	2.16	0.45
9:J:329:LEU:HD22	9:J:332:LEU:HD12	1.98	0.45
15:P:213:ASP:HB3	15:P:216:VAL:HG22	1.98	0.45
32:i:296:LEU:O	32:i:300:SER:HB3	2.17	0.45
50:l:701:CDL:H271	50:l:701:CDL:H232	1.99	0.45
42:u:77:HIS:ND1	42:u:114:LYS:CG	2.79	0.45
5:F:35:ASP:O	5:F:39:LYS:HG2	2.17	0.45
16:Q:148:GLU:HB3	16:Q:227:ILE:HB	1.99	0.45
6:X:83:VAL:HA	6:X:122:MET:HE1	1.99	0.45
27:d:99:ASP:HB3	28:e:137:MET:SD	2.57	0.45
5:F:56:ARG:CB	12:M:651:PRO:HG3	2.46	0.45
6:G:74:LEU:HD12	6:G:79:ILE:HD11	1.98	0.45
40:r:115:LEU:HD12	40:r:174:LEU:HD22	1.99	0.45
41:s:179:TRP:CD2	41:s:180:PRO:HD3	2.51	0.45
1:A:218:GLY:HA2	14:O:80:LEU:HD23	1.99	0.45
1:A:325:PRO:HG3	1:A:433:TRP:HB3	1.98	0.45
8:I:27:ARG:NH1	16:Q:212:GLU:OE2	2.48	0.45
11:L:92:ASN:HB3	15:P:238:PRO:HA	1.98	0.45
16:Q:35:ARG:HD3	28:e:61:PRO:HD2	1.99	0.45
19:U:24:ALA:O	19:U:28:LEU:HD23	2.18	0.45
24:a:152:LYS:HB2	24:a:152:LYS:HE3	1.72	0.45
26:c:96:ASP:OD1	26:c:97:LEU:N	2.49	0.45
27:d:137:LYS:HD2	27:d:137:LYS:HA	1.78	0.45
36:m:21:SER:O	36:m:23:LYS:NZ	2.49	0.45
38:o:8:PRO:HG3	38:o:14:LEU:HD13	1.99	0.45
44:w:350:LYS:HA	44:w:350:LYS:HD3	1.79	0.45
17:S:35:GLU:OE1	41:s:93:TYR:OH	2.20	0.44
17:S:45:TRP:CD1	21:W:140:PHE:HB2	2.52	0.44
18:T:114:CYS:SG	18:T:116:LEU:HG	2.57	0.44
26:c:167:TYR:CD2	26:c:178:PRO:HG3	2.53	0.44
27:d:164:LEU:HD21	28:e:149:LEU:HD22	1.99	0.44
32:i:269:GLU:O	32:i:273:ASN:ND2	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:263:MET:HA	40:r:263:MET:HE3	1.97	0.44
3:C:67:PHE:CZ	3:C:120:VAL:HG21	2.52	0.44
10:K:73:TYR:CZ	10:K:75:ASN:HB3	2.52	0.44
16:Q:234:GLN:O	16:Q:234:GLN:HG2	2.17	0.44
31:h:2:PRO:HA	32:i:140:SER:HB2	2.00	0.44
40:r:186:LEU:HD21	40:r:195:MET:HE2	1.99	0.44
1:A:40:ARG:NH1	1:A:289:GLU:O	2.50	0.44
1:A:357:MET:HG2	14:O:142:LEU:HD11	1.99	0.44
14:O:197:THR:H	14:O:200:ASP:HB2	1.82	0.44
19:U:53:TYR:HB2	21:W:72:MET:HE1	1.99	0.44
32:i:319:HIS:HB2	32:i:322:GLN:NE2	2.31	0.44
35:l:593:ILE:O	35:l:597:ILE:HG13	2.18	0.44
37:n:18:PRO:O	37:n:22:VAL:HG23	2.17	0.44
41:s:92:PRO:HB3	41:s:255:TYR:CD1	2.52	0.44
1:A:35:LEU:HD23	1:A:40:ARG:HH11	1.81	0.44
10:K:109:ARG:NH2	14:O:106:GLN:O	2.50	0.44
16:Q:185:MET:O	16:Q:189:THR:OG1	2.25	0.44
16:Q:198:THR:HB	16:Q:199:PRO:HD3	1.99	0.44
27:d:31:THR:O	27:d:34:THR:HG22	2.16	0.44
50:i:401:CDL:H142	50:i:401:CDL:H171	1.78	0.44
1:A:296:LEU:O	1:A:300:ILE:HG23	2.17	0.44
15:P:117:VAL:HB	15:P:127:GLU:HG2	1.98	0.44
25:b:28:LEU:HG	25:b:32:GLU:HG2	2.00	0.44
42:u:81:PRO:HG2	42:u:110:CYS:SG	2.58	0.44
43:v:39:MET:HE3	43:v:41:ALA:H	1.82	0.44
44:w:211:VAL:O	44:w:214:ILE:HG22	2.17	0.44
3:C:67:PHE:HZ	3:C:120:VAL:HG21	1.83	0.44
5:F:57:GLU:O	12:M:651:PRO:CB	2.57	0.44
9:J:167:ILE:HG21	51:J:401:NDP:H4D	2.00	0.44
12:M:591:GLU:HG2	12:M:610:VAL:HG23	1.99	0.44
16:Q:324:GLY:O	16:Q:329:ARG:NH2	2.50	0.44
18:T:122:HIS:O	18:T:122:HIS:ND1	2.50	0.44
23:Z:49:GLU:OE2	39:p:34:ARG:NE	2.44	0.44
36:m:60:TYR:HD2	36:m:61:LEU:HD23	1.83	0.44
39:p:126:LYS:O	39:p:130:ARG:HG3	2.17	0.44
40:r:204:MET:HE3	40:r:209:LEU:HB2	1.99	0.44
41:s:90:PRO:HB3	41:s:94:PRO:HD3	2.00	0.44
1:A:205:ILE:HD11	1:A:223:PRO:HD3	1.99	0.44
2:B:117:LYS:HE3	2:B:130:ILE:HG22	1.99	0.44
3:C:98:ARG:HG3	3:C:99:GLN:OE1	2.17	0.44
8:I:97:PRO:HD3	15:P:61:PHE:CE1	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:129:LYS:HD3	14:O:168:LEU:CD1	2.47	0.44
31:h:18:MET:HE3	34:k:56:ALA:HA	2.00	0.44
40:r:127:VAL:HB	40:r:128:PRO:HD3	1.99	0.44
5:F:23:LEU:O	5:F:57:GLU:HA	2.18	0.44
7:H:37:GLN:HB2	7:H:95:LEU:HD11	1.99	0.44
14:O:58:GLU:HA	14:O:61:LYS:HG3	2.00	0.44
16:Q:102:SER:OG	16:Q:102:SER:O	2.33	0.44
20:V:81:ARG:O	20:V:83:LYS:HG3	2.18	0.44
24:a:139:ILE:HG23	40:r:54:LEU:HD23	1.99	0.44
28:e:134:LEU:HD12	28:e:134:LEU:H	1.83	0.44
32:i:326:LEU:HB3	32:i:327:PRO:HD3	1.99	0.44
38:o:5:LYS:HA	38:o:5:LYS:HD2	1.87	0.44
1:A:73:PRO:HD3	1:A:147:ARG:NH2	2.33	0.44
1:A:446:LEU:O	1:A:450:MET:HG3	2.18	0.44
3:C:58:ARG:HD3	3:C:127:PRO:HG2	1.98	0.44
8:I:28:TYR:O	8:I:31:ILE:HG12	2.18	0.44
14:O:187:GLN:HG3	14:O:192:TYR:CE1	2.53	0.44
15:P:52:ASP:O	15:P:56:LYS:HG3	2.18	0.44
31:h:89:GLU:OE2	31:h:91:LYS:HB3	2.18	0.44
50:l:701:CDL:C79	54:r:503:PLX:H212	2.46	0.44
1:A:315:LEU:HB2	1:A:359:ARG:HG2	1.99	0.43
15:P:123:GLN:NE2	15:P:124:ASN:OD1	2.51	0.43
24:a:179:ILE:HG21	31:h:38:LYS:HG3	2.00	0.43
26:c:63:GLU:HG3	26:c:77:LYS:HB3	2.00	0.43
31:h:12:LEU:HD13	31:h:14:LEU:HD21	2.00	0.43
35:l:65:ASN:OD1	35:l:66:TRP:N	2.51	0.43
41:s:66:SER:HB2	41:s:122:ALA:O	2.18	0.43
42:u:47:ARG:NH2	42:u:53:PRO:HG3	2.33	0.43
1:A:263:ALA:HA	1:A:271:SER:HB3	1.98	0.43
1:A:401:LYS:HE2	1:A:401:LYS:HB3	1.73	0.43
9:J:318:LYS:O	9:J:322:VAL:HG13	2.18	0.43
14:O:80:LEU:HD11	14:O:119:TYR:CE2	2.53	0.43
21:W:51:MET:HA	41:s:313:SER:HB2	2.00	0.43
39:p:23:ALA:HB1	39:p:44:MET:HE2	2.00	0.43
40:r:307:TRP:HA	40:r:310:MET:HE2	2.00	0.43
41:s:273:ILE:HD12	41:s:273:ILE:H	1.83	0.43
1:A:281:HIS:ND1	1:A:358:ASP:OD2	2.51	0.43
6:G:80:LYS:HB3	6:G:80:LYS:HE3	1.71	0.43
16:Q:196:ALA:O	16:Q:197:MET:HG2	2.18	0.43
18:T:102:LEU:HD21	18:T:118:PHE:HB2	1.99	0.43
32:i:106:LEU:HG	32:i:138:PRO:HB2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:63:LEU:O	39:p:64:LEU:HB3	2.17	0.43
44:w:116:LYS:NZ	44:w:123:SER:OG	2.51	0.43
1:A:408:GLU:O	1:A:411:SER:HB3	2.18	0.43
7:H:96:ARG:O	7:H:96:ARG:NH1	2.51	0.43
21:W:120:MET:SD	31:h:69:ARG:NE	2.82	0.43
32:i:38:LEU:HD12	34:k:73:LEU:HD22	1.99	0.43
54:j:201:PLX:H251	36:m:151:THR:HG21	1.99	0.43
54:r:503:PLX:H121	54:r:503:PLX:H152	1.54	0.43
41:s:298:LEU:O	41:s:302:MET:HG3	2.18	0.43
1:A:154:ALA:HB3	1:A:195:VAL:HG22	1.99	0.43
3:C:146:SER:OG	16:Q:118:2MR:O	2.27	0.43
4:E:109:GLU:OE1	15:P:218:ARG:NH2	2.52	0.43
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	1.99	0.43
18:T:84:ILE:HD12	18:T:84:ILE:HA	1.90	0.43
6:X:83:VAL:HG21	6:X:145:VAL:HG22	2.00	0.43
30:g:55:VAL:HG11	50:r:504:CDL:H711	2.01	0.43
34:k:15:ALA:HB2	36:m:17:PHE:HE2	1.82	0.43
34:k:23:ARG:HD3	36:m:23:LYS:HB2	2.01	0.43
38:o:80:PHE:HE1	38:o:86:THR:HG21	1.84	0.43
44:w:70:LYS:HZ1	44:w:161:ARG:HH21	1.66	0.43
44:w:230:THR:HG23	44:w:233:TYR:H	1.82	0.43
3:C:155:ARG:NH1	15:P:209:GLU:OE2	2.44	0.43
24:a:80:ILE:O	24:a:84:ILE:HG12	2.18	0.43
29:f:68:GLU:HG3	30:g:21:ARG:NH2	2.33	0.43
33:j:25:PRO:HB2	41:s:60:PRO:HD3	2.00	0.43
35:l:270:ASN:O	35:l:274:GLN:HG3	2.19	0.43
50:l:701:CDL:H401	40:r:445:LEU:HD22	2.01	0.43
37:n:54:GLU:N	37:n:54:GLU:OE1	2.51	0.43
40:r:98:MET:HB3	40:r:132:ILE:HD11	2.01	0.43
43:v:29:TYR:HE2	43:v:108:LEU:HD22	1.82	0.43
9:J:151:ALA:O	9:J:155:VAL:HG23	2.17	0.43
16:Q:95:LEU:HD22	16:Q:458:PHE:HZ	1.84	0.43
21:W:77:ALA:O	21:W:81:ARG:HG3	2.18	0.43
50:a:201:CDL:HB61	54:r:503:PLX:H72	2.00	0.43
32:i:208:TYR:O	32:i:212:THR:HG22	2.19	0.43
3:C:173:LEU:O	3:C:177:ILE:HG12	2.19	0.43
9:J:208:GLY:H	9:J:211:ASP:CG	2.26	0.43
11:L:99:MET:HE3	11:L:128:PHE:CE2	2.54	0.43
33:j:75:LEU:HB3	41:s:155:LEU:HD21	2.01	0.43
33:j:103:ALA:O	33:j:107:THR:HG23	2.18	0.43
35:l:37:LYS:HD3	35:l:98:TRP:HE1	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ARG:HA	1:A:147:ARG:HD2	1.85	0.43
1:A:292:MET:HE2	1:A:292:MET:HB3	1.82	0.43
5:F:30:SER:HB2	5:F:34:ARG:NH1	2.33	0.43
6:G:79:ILE:HG22	6:G:145:VAL:HG22	2.01	0.43
54:N:201:PLX:H1C3	54:N:201:PLX:H21	1.68	0.43
16:Q:79:ASN:HA	16:Q:101:LEU:O	2.19	0.43
30:g:36:MET:SD	32:i:339:MET:HE2	2.59	0.43
35:l:483:PRO:HD2	35:l:486:MET:HE2	2.01	0.43
40:r:135:ARG:HD3	50:r:504:CDL:H141	2.00	0.43
40:r:200:ILE:O	40:r:204:MET:HG2	2.19	0.43
41:s:193:THR:HG21	41:s:231:ILE:HG12	2.01	0.43
48:s:401:PEE:H35	48:s:401:PEE:H30	1.81	0.43
13:N:2:GLU:HG3	13:N:4:VAL:HG22	2.01	0.43
15:P:73:VAL:HG13	15:P:86:ILE:HG23	2.00	0.43
33:j:71:LEU:HD23	33:j:71:LEU:HA	1.91	0.43
50:l:701:CDL:C64	54:r:503:PLX:H122	2.48	0.43
40:r:342:MET:HE1	40:r:409:TYR:CE2	2.54	0.43
44:w:165:SER:HB3	44:w:245:PHE:CZ	2.54	0.43
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.54	0.42
3:C:65:MET:HE3	3:C:65:MET:HB3	1.87	0.42
7:H:35:LEU:HA	7:H:38:ILE:HD13	2.01	0.42
12:M:349:GLU:HG3	12:M:646:LEU:HD11	2.01	0.42
14:O:236:GLU:HG2	14:O:237:PRO:HD2	2.01	0.42
17:S:57:VAL:HG23	17:S:59:ARG:HG3	1.99	0.42
18:T:46:ASP:OD1	18:T:49:ASP:HB2	2.19	0.42
18:T:105:GLU:H	18:T:105:GLU:HG2	1.69	0.42
50:a:201:CDL:H762	50:a:201:CDL:H792	1.63	0.42
40:r:161:LEU:O	40:r:165:VAL:HG13	2.18	0.42
44:w:37:GLN:OE1	44:w:37:GLN:N	2.35	0.42
44:w:171:GLU:O	44:w:175:ARG:HG2	2.19	0.42
1:A:338:ASP:O	1:A:342:LEU:HB2	2.19	0.42
1:A:383:THR:HG23	1:A:384:PRO:HD3	2.01	0.42
2:B:50:MET:HG3	21:W:33:TYR:OH	2.19	0.42
12:M:486:GLY:O	12:M:490:LEU:HB2	2.19	0.42
15:P:44:ARG:HB3	15:P:45:PRO:CD	2.49	0.42
23:Z:57:PHE:CG	35:l:435:PRO:HG3	2.54	0.42
24:a:120:TRP:O	24:a:124:THR:HG22	2.18	0.42
32:i:95:MET:HE1	32:i:145:ILE:HD12	2.01	0.42
35:l:169:LEU:HD12	35:l:169:LEU:HA	1.88	0.42
39:p:30:TRP:NE1	39:p:76:HIS:HB2	2.34	0.42
40:r:447:LEU:HD11	54:r:503:PLX:H371	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:PHE:HB2	1:A:293:SER:O	2.20	0.42
1:A:141:GLY:HA2	1:A:144:VAL:HG22	2.00	0.42
47:A:503:NAI:H6N	47:A:503:NAI:H2D	1.80	0.42
2:B:48:MET:HE3	2:B:48:MET:HB3	1.88	0.42
5:F:30:SER:HB2	5:F:34:ARG:HH12	1.85	0.42
16:Q:127:LYS:HB3	16:Q:131:GLN:HB3	2.01	0.42
40:r:300:ALA:O	40:r:308:SER:HB3	2.19	0.42
41:s:196:ALA:HB3	41:s:274:ARG:HA	2.01	0.42
44:w:165:SER:O	44:w:168:VAL:HG22	2.19	0.42
1:A:367:ILE:HG13	1:A:438:LEU:HD13	2.02	0.42
5:F:71:PHE:N	12:M:362:ASP:OD2	2.47	0.42
26:c:185:GLU:OE1	43:v:97:LYS:NZ	2.50	0.42
54:g:201:PLX:H342	32:i:261:MET:HE1	2.01	0.42
34:k:20:LEU:HD22	35:l:588:PHE:HB3	2.02	0.42
38:o:114:LYS:HB3	38:o:114:LYS:HE3	1.57	0.42
43:v:30:GLY:HA3	43:v:104:ARG:HH12	1.84	0.42
13:N:68:MET:HE2	13:N:69:ASN:ND2	2.34	0.42
16:Q:290:GLY:HA2	16:Q:294:ARG:HH21	1.84	0.42
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.84	0.42
6:X:99:SER:O	6:X:102:SER:OG	2.32	0.42
24:a:82:VAL:HG23	54:a:202:PLX:H232	2.01	0.42
31:h:103:ASP:HA	31:h:104:PRO:HD3	1.62	0.42
33:j:21:ALA:HB1	41:s:218:GLY:HA3	2.01	0.42
34:k:4:VAL:O	34:k:8:ILE:HG12	2.19	0.42
2:B:210:LEU:HD12	8:I:38:PRO:HB3	2.01	0.42
5:F:68:ARG:HG3	5:F:74:GLU:HG2	2.02	0.42
8:I:40:LYS:HB2	21:W:7:LYS:H	1.83	0.42
11:L:116:SER:OG	15:P:227:ALA:O	2.26	0.42
16:Q:292:MET:HE2	16:Q:454:GLN:HG2	2.01	0.42
6:X:116:VAL:HA	6:X:119:ILE:HG22	2.01	0.42
32:i:43:VAL:HG11	32:i:129:LEU:HD23	2.02	0.42
35:l:396:ILE:HG21	35:l:490:ALA:HB2	2.00	0.42
39:p:155:PRO:O	39:p:165:PRO:HD2	2.19	0.42
6:G:93:ILE:HD11	6:G:108:LEU:HD22	2.01	0.42
6:G:106:LYS:HE2	6:G:106:LYS:HB3	1.90	0.42
9:J:73:LEU:O	9:J:78:SER:OG	2.28	0.42
9:J:168:SER:O	9:J:203:PRO:HD2	2.20	0.42
14:O:75:LYS:HE2	14:O:75:LYS:HB3	1.69	0.42
14:O:130:TYR:N	14:O:168:LEU:O	2.44	0.42
20:V:56:THR:O	20:V:60:THR:OG1	2.31	0.42
6:X:93:ILE:HD11	6:X:98:LEU:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:162:PRO:HB3	43:v:58:TYR:CE1	2.55	0.42
32:i:5:ILE:HD13	32:i:5:ILE:HA	1.90	0.42
44:w:146:ALA:HB1	44:w:157:VAL:HG21	2.01	0.42
1:A:122:PRO:HD2	1:A:322:SER:OG	2.20	0.42
5:F:83:SER:O	5:F:87:VAL:HG13	2.20	0.42
7:H:94:MET:SD	7:H:99:PRO:HG3	2.60	0.42
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.54	0.42
16:Q:235:ASP:CG	16:Q:356:ILE:CG2	2.92	0.42
21:W:79:LYS:NZ	36:m:131:GLY:HA2	2.35	0.42
24:a:166:GLY:O	24:a:170:GLN:NE2	2.53	0.42
25:b:32:GLU:HG3	39:p:115:TYR:HA	2.01	0.42
35:l:2:ASN:ND2	35:l:61:MET:SD	2.93	0.42
41:s:222:MET:HA	41:s:225:MET:HG3	2.02	0.42
44:w:102:LYS:HB2	44:w:102:LYS:HE3	1.87	0.42
1:A:453:PHE:CA	1:A:456:GLN:HE21	2.32	0.42
10:K:100:GLN:NE2	14:O:69:ASN:O	2.53	0.42
16:Q:312:ASP:OD1	16:Q:312:ASP:N	2.53	0.42
21:W:120:MET:HE2	21:W:120:MET:HB2	1.89	0.42
23:Z:13:LYS:HD2	23:Z:13:LYS:HA	1.85	0.42
32:i:246:VAL:HG11	50:r:504:CDL:H392	2.01	0.42
50:i:401:CDL:H342	50:i:401:CDL:HA62	2.02	0.42
40:r:321:LEU:HD13	40:r:444:LEU:HG	2.01	0.42
44:w:148:GLU:OE1	44:w:301:LYS:NZ	2.37	0.42
1:A:115:VAL:HG22	1:A:248:VAL:HG21	2.02	0.42
2:B:200:GLU:HG3	13:N:88:ARG:HD3	2.02	0.42
12:M:145:MET:HG3	15:P:239:TRP:O	2.20	0.42
20:V:81:ARG:HH12	20:V:88:LEU:HD23	1.82	0.42
22:Y:60:PHE:CD1	22:Y:60:PHE:C	2.98	0.42
36:m:152:TRP:O	36:m:156:VAL:HG22	2.20	0.42
40:r:97:THR:HG21	50:r:504:CDL:H242	2.02	0.42
40:r:118:PHE:O	40:r:122:PHE:HB3	2.19	0.42
44:w:245:PHE:CE1	44:w:249:MET:HG3	2.55	0.42
3:C:58:ARG:HD3	3:C:127:PRO:CG	2.50	0.41
8:I:53:TYR:CD2	12:M:111:LYS:HG2	2.55	0.41
13:N:135:GLN:OE1	13:N:135:GLN:HA	2.20	0.41
16:Q:157:LYS:HE3	16:Q:157:LYS:HB2	1.88	0.41
24:a:134:GLU:HG2	37:n:38:PHE:O	2.19	0.41
32:i:347:ASN:OD1	32:i:347:ASN:N	2.53	0.41
35:l:378:LEU:HD22	35:l:383:MET:HE2	2.02	0.41
48:l:704:PEE:H55	48:l:704:PEE:H60	1.86	0.41
38:o:115:LEU:HD23	38:o:115:LEU:HA	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:115:LEU:HB2	40:r:174:LEU:HB3	2.01	0.41
41:s:267:THR:O	41:s:271:LEU:HG	2.19	0.41
1:A:48:ARG:NH1	10:K:70:ASN:O	2.40	0.41
1:A:140:GLU:HG3	1:A:252:PRO:HG3	2.02	0.41
1:A:285:PRO:HG3	14:O:143:ARG:NH1	2.35	0.41
6:G:83:VAL:O	6:G:86:VAL:HG22	2.19	0.41
12:M:329:MET:HG3	12:M:565:PHE:CE2	2.55	0.41
13:N:14:VAL:HA	13:N:23:TYR:CD2	2.55	0.41
14:O:148:ILE:H	14:O:148:ILE:HG13	1.71	0.41
16:Q:304:LYS:NZ	16:Q:316:PHE:O	2.48	0.41
19:U:11:ASN:ND2	19:U:11:ASN:C	2.77	0.41
35:l:272:LEU:O	35:l:276:MET:HG3	2.20	0.41
35:l:525:MET:SD	39:p:77:PRO:HB2	2.60	0.41
16:Q:167:ALA:HB2	16:Q:356:ILE:O	2.21	0.41
17:S:4:GLU:O	17:S:7:PRO:HD2	2.20	0.41
34:k:23:ARG:HG3	34:k:24:SER:H	1.84	0.41
50:r:504:CDL:H772	50:r:504:CDL:H741	1.72	0.41
2:B:70:LEU:HG	41:s:277:TYR:OH	2.19	0.41
4:E:40:TYR:CG	6:G:120:MET:HE1	2.47	0.41
7:H:22:GLU:O	7:H:26:ILE:HG12	2.21	0.41
9:J:163:LYS:NZ	9:J:253:ILE:O	2.44	0.41
12:M:455:ILE:HD13	12:M:460:HIS:HB3	2.03	0.41
12:M:621:LYS:HB3	12:M:621:LYS:HE3	1.85	0.41
16:Q:144:MET:HE3	16:Q:214:TYR:HE2	1.80	0.41
22:Y:100:LEU:H	43:v:111:ARG:NH1	2.18	0.41
28:e:99:LEU:HD12	28:e:99:LEU:HA	1.87	0.41
35:l:292:ALA:HB2	35:l:304:PHE:CB	2.50	0.41
44:w:219:GLN:HA	44:w:227:MET:HE1	2.02	0.41
1:A:277:ASN:OD1	1:A:353:ALA:HA	2.21	0.41
3:C:51:ASP:HA	3:C:54:VAL:HG12	2.01	0.41
4:E:81:LEU:HD12	4:E:81:LEU:HA	1.91	0.41
13:N:32:ASP:OD2	13:N:34:ARG:NE	2.37	0.41
27:d:163:MET:HE1	28:e:147:ILE:HG21	2.02	0.41
28:e:66:LEU:HD23	28:e:66:LEU:HA	1.94	0.41
29:f:48:LEU:HD23	29:f:48:LEU:HA	1.87	0.41
35:l:174:TYR:HD1	35:l:229:LEU:HB3	1.85	0.41
40:r:216:LEU:HB3	40:r:217:PRO:HD3	2.03	0.41
9:J:343:THR:HG23	9:J:347:LEU:HD12	2.01	0.41
14:O:152:ILE:HG23	14:O:205:ILE:HD11	2.03	0.41
16:Q:206:GLU:OE2	16:Q:209:LYS:NZ	2.53	0.41
21:W:70:ALA:HB2	42:u:125:LEU:HD13	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:80:LYS:HE3	6:X:80:LYS:HB3	1.79	0.41
34:k:25:HIS:O	34:k:28:SER:N	2.44	0.41
37:n:48:GLU:H	37:n:48:GLU:CD	2.28	0.41
43:v:30:GLY:H	43:v:104:ARG:HH22	1.69	0.41
1:A:367:ILE:HG21	1:A:438:LEU:HD22	2.03	0.41
46:A:502:FMN:N5	47:A:503:NAI:H4N	2.35	0.41
2:B:86:TYR:CG	2:B:87:PRO:HA	2.55	0.41
16:Q:155:VAL:HB	16:Q:229:PRO:HB3	2.03	0.41
19:U:10:LYS:O	19:U:10:LYS:HD3	2.20	0.41
21:W:81:ARG:HH22	42:u:64:ASN:HD21	1.69	0.41
25:b:110:ILE:HG12	27:d:16:ARG:HB2	2.01	0.41
26:c:127:ASN:O	26:c:131:LYS:HG3	2.20	0.41
27:d:28:ASN:OD1	27:d:28:ASN:C	2.64	0.41
30:g:47:ASP:HB2	32:i:327:PRO:HG2	2.03	0.41
31:h:93:THR:HA	31:h:94:PRO:HD3	1.93	0.41
50:l:701:CDL:H322	50:l:701:CDL:H351	1.87	0.41
44:w:282:PRO:O	44:w:286:GLN:HG2	2.21	0.41
4:E:98:LYS:HB3	4:E:102:HIS:HB2	2.03	0.41
4:E:98:LYS:HD3	4:E:102:HIS:HB3	2.02	0.41
16:Q:279:THR:HG1	16:Q:282:ASP:HB2	1.86	0.41
21:W:66:GLU:OE2	42:u:123:GLY:N	2.39	0.41
24:a:147:ALA:HB2	40:r:173:SER:HB2	2.02	0.41
30:g:85:TYR:CZ	32:i:344:SER:HB3	2.56	0.41
31:h:95:PRO:HD2	31:h:98:HIS:CD2	2.56	0.41
41:s:92:PRO:HG2	41:s:93:TYR:CE2	2.55	0.41
1:A:53:LEU:O	1:A:57:GLN:HG3	2.21	0.41
1:A:75:TRP:CH2	1:A:79:GLU:HG3	2.56	0.41
1:A:88:ARG:HB2	1:A:247:THR:OG1	2.21	0.41
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.78	0.41
2:B:205:ILE:O	2:B:209:TYR:HB3	2.21	0.41
12:M:372:PHE:H	12:M:532:PRO:HB2	1.85	0.41
14:O:130:TYR:HB2	14:O:169:PHE:CD1	2.55	0.41
19:U:10:LYS:HD3	19:U:10:LYS:C	2.46	0.41
23:Z:43:ASP:HA	23:Z:44:PRO:HD3	1.93	0.41
23:Z:88:LEU:HD23	23:Z:88:LEU:HA	1.94	0.41
27:d:9:VAL:HG11	28:e:123:GLU:HG2	2.03	0.41
27:d:139:PHE:HB2	28:e:137:MET:HE1	2.02	0.41
27:d:162:ARG:NH1	27:d:162:ARG:HB3	2.35	0.41
28:e:92:PHE:O	28:e:96:SER:HB2	2.20	0.41
29:f:67:LEU:HD23	29:f:67:LEU:HA	1.84	0.41
35:l:27:TYR:O	35:l:115:ASN:ND2	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:l:701:CDL:C63	54:r:503:PLX:H122	2.50	0.41
40:r:78:MET:HE1	40:r:439:LEU:HD12	2.03	0.41
40:r:248:THR:HG23	40:r:249:ILE:HG23	2.03	0.41
40:r:445:LEU:O	40:r:448:THR:HG22	2.21	0.41
54:r:502:PLX:H22	54:r:502:PLX:H1C3	1.91	0.41
41:s:41:GLY:HA2	41:s:46:LEU:HD12	2.03	0.41
44:w:160:GLU:N	44:w:160:GLU:OE2	2.53	0.41
2:B:200:GLU:HG3	13:N:88:ARG:HB2	2.02	0.41
5:F:41:TYR:CZ	5:F:55:ILE:HD11	2.56	0.41
9:J:329:LEU:HA	9:J:330:PRO:HD3	1.93	0.41
12:M:339:ALA:HB3	12:M:542:PRO:HG3	2.02	0.41
14:O:164:THR:HA	14:O:165:PRO:HD3	1.90	0.41
22:Y:45:ARG:HG2	35:l:439:PRO:HB3	2.03	0.41
54:g:201:PLX:H322	32:i:347:ASN:HD22	1.85	0.41
32:i:19:LEU:HD11	32:i:28:LEU:HD12	2.02	0.41
32:i:314:LYS:NZ	44:w:309:THR:OG1	2.54	0.41
35:l:587:TYR:O	35:l:590:SER:OG	2.39	0.41
3:C:161:ILE:HG13	3:C:180:LEU:HB2	2.03	0.40
12:M:289:LYS:NZ	12:M:694:PHE:O	2.54	0.40
18:T:39:THR:HG22	18:T:62:VAL:HG23	2.03	0.40
6:X:88:LYS:HG2	6:X:98:LEU:HD21	2.03	0.40
33:j:87:MET:HE3	33:j:87:MET:HB3	1.89	0.40
34:k:43:MET:HE2	34:k:43:MET:HB2	1.89	0.40
38:o:51:TYR:HA	38:o:60:ILE:HD11	2.02	0.40
6:X:113:LEU:O	6:X:116:VAL:HG12	2.21	0.40
22:Y:61:PHE:CD1	35:l:458:LEU:HD23	2.56	0.40
50:i:401:CDL:H342	50:i:401:CDL:H312	1.78	0.40
35:l:44:PHE:HB2	35:l:94:LEU:HB3	2.03	0.40
1:A:167:SER:O	1:A:171:VAL:HG13	2.22	0.40
1:A:398:ARG:HG2	1:A:403:ASP:HB2	2.03	0.40
2:B:150:THR:HG21	2:B:180:HIS:CD2	2.57	0.40
3:C:61:SER:O	3:C:61:SER:OG	2.37	0.40
8:I:107:SER:C	8:I:109:ASP:H	2.29	0.40
12:M:213:MET:HE3	12:M:213:MET:HB2	1.83	0.40
13:N:43:LYS:NZ	13:N:111:THR:O	2.52	0.40
14:O:108:PRO:HA	14:O:109:PRO:HD3	2.00	0.40
21:W:58:ARG:HA	21:W:58:ARG:HD2	1.80	0.40
6:X:75:THR:OG1	6:X:156:GLU:O	2.31	0.40
27:d:8:ASP:HB2	28:e:127:LYS:HD3	2.03	0.40
35:l:76:LEU:HD23	35:l:76:LEU:HA	1.92	0.40
35:l:90:ILE:HG12	35:l:129:MET:SD	2.61	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:58:MET:HB2	15:P:246:ARG:CZ	2.51	0.40
12:M:133:GLN:O	12:M:137:CYS:HB2	2.21	0.40
14:O:38:LEU:O	14:O:124:ARG:NH2	2.53	0.40
28:e:129:ARG:HA	28:e:134:LEU:HD13	2.02	0.40
32:i:13:VAL:O	32:i:36:ASN:ND2	2.53	0.40
35:l:49:VAL:HB	35:l:50:PRO:HD3	2.03	0.40
35:l:174:TYR:CD1	35:l:229:LEU:HB3	2.57	0.40
37:n:44:LEU:HD23	37:n:45:PHE:CE2	2.55	0.40
40:r:178:ILE:HD13	40:r:178:ILE:HA	1.96	0.40
1:A:62:TRP:HE1	1:A:136:HIS:HB3	1.87	0.40
3:C:62:LEU:O	3:C:91:VAL:HA	2.21	0.40
50:a:201:CDL:H311	50:a:201:CDL:H342	1.76	0.40
32:i:248:LEU:HD22	32:i:293:TYR:HD1	1.86	0.40
33:j:17:LEU:HA	33:j:17:LEU:HD23	1.88	0.40
35:l:271:LYS:HB3	35:l:271:LYS:HE3	1.87	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	429/433 (99%)	413 (96%)	16 (4%)	0	100	100
2	B	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
3	C	154/156 (99%)	147 (96%)	7 (4%)	0	100	100
4	E	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
5	F	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
6	G	86/88 (98%)	86 (100%)	0	0	100	100
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	101 (92%)	9 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	I	93/112 (83%)	84 (90%)	9 (10%)	0	100	100
9	J	289/342 (84%)	275 (95%)	13 (4%)	1 (0%)	36	65
10	K	40/43 (93%)	39 (98%)	1 (2%)	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	663 (96%)	25 (4%)	0	100	100
13	N	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
14	O	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
15	P	206/208 (99%)	194 (94%)	12 (6%)	0	100	100
16	Q	412/430 (96%)	398 (97%)	14 (3%)	0	100	100
17	S	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
18	T	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
19	U	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
20	V	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	18	49
21	W	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
22	Y	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
23	Z	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
24	a	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
25	b	99/126 (79%)	92 (93%)	7 (7%)	0	100	100
26	c	154/156 (99%)	146 (95%)	8 (5%)	0	100	100
27	d	173/175 (99%)	171 (99%)	2 (1%)	0	100	100
28	e	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
29	f	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
30	g	119/122 (98%)	115 (97%)	4 (3%)	0	100	100
31	h	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
32	i	345/347 (99%)	332 (96%)	13 (4%)	0	100	100
33	j	95/115 (83%)	90 (95%)	5 (5%)	0	100	100
34	k	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
35	l	601/603 (100%)	574 (96%)	27 (4%)	0	100	100
36	m	125/175 (71%)	114 (91%)	11 (9%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	119 (94%)	7 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	p	176/178 (99%)	170 (97%)	6 (3%)	0	100	100
40	r	457/459 (100%)	447 (98%)	10 (2%)	0	100	100
41	s	299/318 (94%)	285 (95%)	14 (5%)	0	100	100
42	u	169/171 (99%)	164 (97%)	5 (3%)	0	100	100
43	v	122/124 (98%)	114 (93%)	8 (7%)	0	100	100
44	w	318/320 (99%)	303 (95%)	15 (5%)	0	100	100
All	All	8029/8322 (96%)	7709 (96%)	318 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	38	HIS
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	345/346 (100%)	345 (100%)	0	100	100
2	B	151/151 (100%)	150 (99%)	1 (1%)	76	80
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	105/107 (98%)	105 (100%)	0	100	100
5	F	76/76 (100%)	76 (100%)	0	100	100
6	G	76/81 (94%)	76 (100%)	0	100	100
6	X	77/81 (95%)	77 (100%)	0	100	100
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	87 (100%)	0	100	100
9	J	252/296 (85%)	252 (100%)	0	100	100
10	K	41/42 (98%)	41 (100%)	0	100	100
11	L	113/113 (100%)	112 (99%)	1 (1%)	70	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	M	580/580 (100%)	579 (100%)	1 (0%)	87	88
13	N	130/130 (100%)	130 (100%)	0	100	100
14	O	181/183 (99%)	180 (99%)	1 (1%)	78	81
15	P	189/190 (100%)	188 (100%)	1 (0%)	81	83
16	Q	361/370 (98%)	358 (99%)	3 (1%)	73	79
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	98/101 (97%)	94 (96%)	4 (4%)	27	55
21	W	123/123 (100%)	123 (100%)	0	100	100
22	Y	62/63 (98%)	62 (100%)	0	100	100
23	Z	65/65 (100%)	64 (98%)	1 (2%)	57	72
24	a	122/122 (100%)	122 (100%)	0	100	100
25	b	98/119 (82%)	98 (100%)	0	100	100
26	c	141/141 (100%)	141 (100%)	0	100	100
27	d	155/155 (100%)	155 (100%)	0	100	100
28	e	99/99 (100%)	98 (99%)	1 (1%)	68	76
29	f	35/45 (78%)	35 (100%)	0	100	100
30	g	108/109 (99%)	108 (100%)	0	100	100
31	h	88/93 (95%)	87 (99%)	1 (1%)	65	76
32	i	311/311 (100%)	310 (100%)	1 (0%)	86	86
33	j	88/100 (88%)	88 (100%)	0	100	100
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	535/537 (100%)	534 (100%)	1 (0%)	87	88
36	m	98/141 (70%)	98 (100%)	0	100	100
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	113/113 (100%)	112 (99%)	1 (1%)	70	78
39	p	156/159 (98%)	156 (100%)	0	100	100
40	r	409/410 (100%)	408 (100%)	1 (0%)	87	88
41	s	263/275 (96%)	262 (100%)	1 (0%)	84	84
42	u	150/153 (98%)	146 (97%)	4 (3%)	39	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	v	104/111 (94%)	104 (100%)	0	100	100
44	w	281/283 (99%)	280 (100%)	1 (0%)	84	84
All	All	7041/7246 (97%)	7016 (100%)	25 (0%)	81	84

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	76	TYR
11	L	149	GLU
12	M	650	SER
14	O	166	ASP
15	P	138	ASN
16	Q	141	TYR
16	Q	142	VAL
16	Q	144	MET
20	V	37	SER
20	V	118	MET
20	V	120	LEU
20	V	121	THR
23	Z	49	GLU
28	e	137	MET
31	h	97	HIS
32	i	154	MET
35	l	190	LEU
38	o	75	ASN
40	r	256	TYR
41	s	193	THR
42	u	78	CYS
42	u	88	CYS
42	u	96	LEU
42	u	103	GLN
44	w	275	TYR

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	44	ASN
1	A	270	ASN
1	A	393	ASN
1	A	456	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	457	HIS
3	C	123	GLN
4	E	108	HIS
5	F	93	ASN
6	G	103	HIS
6	G	142	GLN
7	H	73	GLN
7	H	110	ASN
9	J	128	ASN
9	J	376	ASN
10	K	79	HIS
10	K	90	ASN
12	M	123	ASN
12	M	334	GLN
14	O	41	HIS
14	O	69	ASN
14	O	131	HIS
14	O	133	GLN
14	O	189	ASN
15	P	55	HIS
15	P	74	GLN
15	P	75	GLN
15	P	77	GLN
15	P	123	GLN
15	P	181	HIS
15	P	196	HIS
15	P	236	ASN
16	Q	160	ASN
16	Q	250	ASN
17	S	61	HIS
18	T	123	HIS
19	U	52	ASN
19	U	83	ASN
20	V	7	HIS
20	V	89	ASN
21	W	76	GLN
24	a	132	ASN
24	a	170	GLN
26	c	154	GLN
28	e	132	ASN
32	i	134	GLN
32	i	322	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	k	25	HIS
34	k	57	ASN
35	l	34	ASN
35	l	67	HIS
35	l	165	ASN
35	l	295	GLN
35	l	348	HIS
35	l	354	GLN
35	l	447	ASN
35	l	580	GLN
37	n	3	ASN
38	o	75	ASN
38	o	123	GLN
39	p	75	GLN
40	r	144	ASN
40	r	168	GLN
40	r	175	ASN
40	r	251	ASN
40	r	304	GLN
40	r	366	ASN
41	s	317	GLN
42	u	30	HIS
42	u	151	ASN
43	v	84	GLN
43	v	85	HIS
44	w	65	ASN
44	w	127	ASN
44	w	149	HIS
44	w	176	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	1.97	1 (10%)	5,13,15	5.96	3 (60%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.70	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	12.16	130.63	119.48
16	Q	118	2MR	CD-NE-CZ	4.34	131.53	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.10	130.71	123.86

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Q	118	2MR	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 37 ligands modelled in this entry, 2 are monoatomic - leaving 35 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$
54	PLX	g	201	-	51,51,51	1.15	3 (5%)	55,59,59	0.58	1 (1%)
54	PLX	a	202	-	51,51,51	1.14	4 (7%)	55,59,59	0.60	1 (1%)
48	PEE	s	401	-	50,50,50	1.16	6 (12%)	53,55,55	0.94	2 (3%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
51	NDP	J	401	-	49,52,52	4.40	23 (46%)	66,80,80	2.16	14 (21%)
48	PEE	B	303	-	50,50,50	1.16	6 (12%)	53,55,55	0.96	2 (3%)
48	PEE	l	704	-	45,45,50	1.22	6 (13%)	48,50,55	0.98	2 (4%)
50	CDL	l	702	-	99,99,99	1.09	8 (8%)	105,111,111	0.84	4 (3%)
54	PLX	r	503	-	51,51,51	1.14	4 (7%)	55,59,59	0.59	1 (1%)
52	FES	O	301	14	0,4,4	-	-	-	-	-
54	PLX	N	201	-	51,51,51	1.15	4 (7%)	55,59,59	0.60	1 (1%)
46	FMN	A	502	-	33,33,33	1.07	2 (6%)	48,50,50	1.21	7 (14%)
50	CDL	i	401	-	65,65,99	1.28	8 (12%)	71,77,111	1.01	4 (5%)
50	CDL	l	701	-	98,98,99	0.92	4 (4%)	104,110,111	1.15	7 (6%)
56	UQ	s	402	-	28,28,63	3.30	6 (21%)	34,37,79	2.72	9 (26%)
45	SF4	A	501	1	0,12,12	-	-	-	-	-
48	PEE	m	201	-	40,40,50	1.15	5 (12%)	43,45,55	0.99	2 (4%)
57	ADP	w	401	-	27,29,29	2.96	8 (29%)	42,45,45	2.01	9 (21%)
49	8Q1	X	201	-	31,34,34	1.70	6 (19%)	40,43,43	1.53	6 (15%)
47	NAI	A	503	-	45,48,48	3.90	20 (44%)	60,73,73	1.78	12 (20%)
50	CDL	r	504	-	99,99,99	1.09	8 (8%)	105,111,111	0.86	4 (3%)
50	CDL	I	201	-	50,50,99	1.41	8 (16%)	56,62,111	1.13	4 (7%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PEE	Q	501	-	46,46,50	1.21	6 (13%)	49,51,55	0.99	2 (4%)
45	SF4	M	801	12	0,12,12	-	-	-		
50	CDL	a	201	-	90,90,99	1.14	9 (10%)	96,102,111	0.92	4 (4%)
52	FES	M	803	12	0,4,4	-	-	-		
54	PLX	j	201	-	51,51,51	1.15	4 (7%)	55,59,59	0.58	1 (1%)
49	8Q1	G	201	-	31,34,34	1.70	6 (19%)	40,43,43	1.55	6 (15%)
45	SF4	C	301	16,3	0,12,12	-	-	-		
48	PEE	l	703	-	45,45,50	1.22	6 (13%)	48,50,55	0.97	2 (4%)
48	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	0.94	2 (3%)
48	PEE	C	302	-	46,46,50	1.21	6 (13%)	49,51,55	0.99	2 (4%)
54	PLX	r	502	-	51,51,51	1.15	5 (9%)	55,59,59	0.62	1 (1%)
45	SF4	B	302	2	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PLX	g	201	-	-	21/55/55/55	-
54	PLX	a	202	-	-	22/55/55/55	-
48	PEE	s	401	-	-	25/54/54/54	-
45	SF4	M	802	12	-	-	0/6/5/5
51	NDP	J	401	-	-	6/34/77/77	0/4/5/5
48	PEE	B	303	-	-	24/54/54/54	-
48	PEE	l	704	-	-	22/49/49/54	-
50	CDL	l	702	-	-	51/110/110/110	-
54	PLX	r	503	-	-	34/55/55/55	-
52	FES	O	301	14	-	-	0/1/1/1
54	PLX	N	201	-	-	26/55/55/55	-
46	FMN	A	502	-	-	6/18/18/18	0/3/3/3
50	CDL	i	401	-	-	35/76/76/110	-
50	CDL	l	701	-	-	33/109/109/110	-
56	UQ	s	402	-	-	9/21/45/87	0/1/1/1
45	SF4	A	501	1	-	-	0/6/5/5
48	PEE	m	201	-	-	21/44/44/54	-
57	ADP	w	401	-	-	3/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	8Q1	X	201	-	-	22/41/41/41	-
47	NAI	A	503	-	-	7/29/72/72	0/5/5/5
50	CDL	r	504	-	-	64/110/110/110	-
50	CDL	I	201	-	-	39/61/61/110	-
45	SF4	B	301	2	-	-	0/6/5/5
48	PEE	Q	501	-	-	19/50/50/54	-
45	SF4	M	801	12	-	-	0/6/5/5
50	CDL	a	201	-	-	53/101/101/110	-
52	FES	M	803	12	-	-	0/1/1/1
54	PLX	j	201	-	-	28/55/55/55	-
49	8Q1	G	201	-	-	19/41/41/41	-
48	PEE	l	703	-	-	27/49/49/54	-
48	PEE	r	501	-	-	20/54/54/54	-
45	SF4	C	301	16,3	-	-	0/6/5/5
48	PEE	C	302	-	-	28/50/50/54	-
54	PLX	r	502	-	-	28/55/55/55	-
45	SF4	B	302	2	-	-	0/6/5/5

All (187) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	J	401	NDP	C3B-C2B	-12.87	1.24	1.52
51	J	401	NDP	C6N-C5N	12.49	1.55	1.33
51	J	401	NDP	O4D-C4D	10.71	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.26	1.26	1.53
51	J	401	NDP	C3D-C4D	-9.82	1.27	1.53
56	s	402	UQ	C13-C14	9.37	1.55	1.33
47	A	503	NAI	O4B-C1B	9.15	1.63	1.42
56	s	402	UQ	C8-C9	9.02	1.54	1.33
57	w	401	ADP	C3'-C4'	-8.84	1.30	1.53
47	A	503	NAI	O4B-C4B	-8.21	1.26	1.45
56	s	402	UQ	C18-C19	8.20	1.55	1.32
51	J	401	NDP	O4B-C4B	-7.83	1.27	1.45
57	w	401	ADP	O4'-C4'	7.77	1.62	1.45
47	A	503	NAI	C2D-C1D	-7.45	1.29	1.53
51	J	401	NDP	C2N-C3N	7.44	1.55	1.34
47	A	503	NAI	C2B-C1B	-7.21	1.30	1.53
47	A	503	NAI	O4D-C4D	6.94	1.60	1.45
47	A	503	NAI	C2D-C3D	5.99	1.69	1.53
51	J	401	NDP	C6A-N6A	5.96	1.49	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	J	401	NDP	P2B-O2B	5.80	1.70	1.59
47	A	503	NAI	C7N-N7N	5.78	1.48	1.33
57	w	401	ADP	C6-N6	5.56	1.48	1.34
49	X	201	8Q1	C34-N36	5.50	1.45	1.33
47	A	503	NAI	O4D-C1D	5.49	1.55	1.42
49	G	201	8Q1	C34-N36	5.46	1.45	1.33
51	J	401	NDP	C3B-C4B	5.45	1.66	1.53
49	X	201	8Q1	C39-N41	5.39	1.45	1.33
49	G	201	8Q1	C39-N41	5.35	1.45	1.33
47	A	503	NAI	C6A-N6A	5.18	1.47	1.34
47	A	503	NAI	C4N-C3N	-4.95	1.40	1.49
51	J	401	NDP	C6N-N1N	4.92	1.49	1.37
51	J	401	NDP	O4D-C1D	-4.90	1.30	1.42
51	J	401	NDP	O4B-C1B	4.66	1.53	1.42
47	A	503	NAI	O2B-C2B	4.51	1.53	1.43
57	w	401	ADP	O4'-C1'	-4.42	1.31	1.42
51	J	401	NDP	C1B-N9A	-4.41	1.33	1.46
50	l	701	CDL	OA8-CA7	4.37	1.46	1.33
50	l	701	CDL	OB8-CB7	4.23	1.45	1.33
51	J	401	NDP	C7N-N7N	4.22	1.44	1.33
51	J	401	NDP	O2D-C2D	-4.12	1.33	1.43
47	A	503	NAI	C6N-C5N	4.12	1.40	1.33
50	l	701	CDL	OB6-CB5	4.06	1.45	1.34
50	l	701	CDL	OA6-CA5	3.96	1.45	1.34
46	A	502	FMN	C4A-N5	3.85	1.38	1.30
48	C	302	PEE	C18-C19	3.75	1.53	1.31
48	B	303	PEE	C18-C19	3.74	1.53	1.31
48	l	703	PEE	C18-C19	3.73	1.53	1.31
48	s	401	PEE	C18-C19	3.73	1.53	1.31
48	r	501	PEE	C18-C19	3.73	1.53	1.31
48	l	704	PEE	C18-C19	3.72	1.53	1.31
48	m	201	PEE	C18-C19	3.72	1.53	1.31
48	Q	501	PEE	C18-C19	3.72	1.53	1.31
48	l	704	PEE	C39-C38	3.67	1.53	1.31
48	C	302	PEE	C39-C38	3.67	1.53	1.31
48	Q	501	PEE	C39-C38	3.66	1.53	1.31
48	s	401	PEE	C39-C38	3.66	1.53	1.31
48	r	501	PEE	C39-C38	3.66	1.53	1.31
48	l	703	PEE	C39-C38	3.65	1.52	1.31
48	B	303	PEE	C39-C38	3.64	1.52	1.31
47	A	503	NAI	C7N-C3N	3.60	1.56	1.48
50	I	201	CDL	OA8-CA7	3.46	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	r	504	CDL	OA8-CA7	3.46	1.43	1.33
50	a	201	CDL	OA8-CA7	3.45	1.43	1.33
50	l	702	CDL	OA8-CA7	3.44	1.43	1.33
50	i	401	CDL	OA8-CA7	3.44	1.43	1.33
57	w	401	ADP	O2'-C2'	-3.35	1.35	1.43
47	A	503	NAI	C4N-C5N	-3.24	1.40	1.48
57	w	401	ADP	O3'-C3'	3.11	1.50	1.43
51	J	401	NDP	O3D-C3D	3.10	1.50	1.43
57	w	401	ADP	C8-N9	-3.08	1.32	1.37
50	I	201	CDL	OB6-CB5	3.05	1.42	1.34
51	J	401	NDP	C7N-C3N	3.05	1.55	1.48
50	a	201	CDL	OB6-CB5	3.05	1.42	1.34
50	r	504	CDL	OB8-CB7	3.04	1.42	1.33
50	l	702	CDL	OB8-CB7	3.04	1.42	1.33
50	a	201	CDL	OA6-CA5	3.04	1.42	1.34
50	I	201	CDL	OB8-CB7	3.03	1.42	1.33
50	i	401	CDL	OB6-CB5	3.03	1.42	1.34
50	l	702	CDL	OB6-CB5	3.02	1.42	1.34
50	l	702	CDL	OA6-CA5	3.02	1.42	1.34
50	r	504	CDL	OB6-CB5	3.01	1.42	1.34
50	i	401	CDL	OB8-CB7	3.00	1.42	1.33
50	a	201	CDL	OB8-CB7	2.99	1.42	1.33
50	i	401	CDL	OA6-CA5	2.95	1.42	1.34
50	r	504	CDL	OA6-CA5	2.94	1.42	1.34
50	I	201	CDL	OA6-CA5	2.93	1.42	1.34
51	J	401	NDP	C8A-N9A	-2.93	1.32	1.37
51	J	401	NDP	C5A-N7A	-2.81	1.33	1.39
54	N	201	PLX	O6-C4	-2.76	1.40	1.44
54	g	201	PLX	O6-C4	-2.76	1.40	1.44
56	s	402	UQ	C6-C1	2.74	1.54	1.46
54	r	503	PLX	O6-C4	-2.67	1.41	1.44
54	a	202	PLX	O6-C4	-2.61	1.41	1.44
54	j	201	PLX	O6-C4	-2.55	1.41	1.44
46	A	502	FMN	C10-N1	2.51	1.38	1.33
51	J	401	NDP	O2B-C2B	2.50	1.53	1.44
48	l	704	PEE	O3-C30	2.49	1.40	1.33
48	Q	501	PEE	O3-C30	2.49	1.40	1.33
47	A	503	NAI	PN-O5D	2.49	1.69	1.59
48	s	401	PEE	O3-C30	2.46	1.40	1.33
47	A	503	NAI	O3B-C3B	-2.46	1.37	1.43
48	m	201	PEE	O3-C30	2.46	1.40	1.33
48	C	302	PEE	O3-C30	2.46	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	C8A-N9A	-2.45	1.33	1.37
49	G	201	8Q1	C1-S44	2.44	1.82	1.76
48	r	501	PEE	O3-C30	2.44	1.40	1.33
48	B	303	PEE	O3-C30	2.44	1.40	1.33
50	I	201	CDL	OA6-CA4	-2.43	1.40	1.46
48	l	703	PEE	O3-C30	2.43	1.40	1.33
49	X	201	8Q1	C1-S44	2.42	1.82	1.76
48	r	501	PEE	O2-C2	-2.42	1.40	1.46
51	J	401	NDP	C2D-C3D	2.42	1.60	1.53
48	l	704	PEE	O2-C2	-2.39	1.40	1.46
54	r	502	PLX	C7-C6	2.39	1.55	1.50
50	r	504	CDL	OA6-CA4	-2.39	1.40	1.46
48	C	302	PEE	O2-C2	-2.39	1.40	1.46
48	s	401	PEE	O2-C2	-2.39	1.40	1.46
48	Q	501	PEE	O2-C2	-2.38	1.40	1.46
56	s	402	UQ	C7-C8	2.38	1.54	1.50
54	j	201	PLX	C7-C6	2.38	1.55	1.50
48	B	303	PEE	O2-C2	-2.37	1.40	1.46
48	l	703	PEE	O2-C2	-2.35	1.40	1.46
48	m	201	PEE	O2-C10	2.35	1.40	1.34
50	i	401	CDL	OA6-CA4	-2.35	1.40	1.46
50	a	201	CDL	OA6-CA4	-2.34	1.40	1.46
48	l	703	PEE	O2-C10	2.33	1.40	1.34
54	r	503	PLX	C7-C6	2.33	1.55	1.50
48	C	302	PEE	O2-C10	2.32	1.40	1.34
47	A	503	NAI	C5B-C4B	2.31	1.58	1.51
48	s	401	PEE	O2-C10	2.30	1.40	1.34
50	l	702	CDL	OA6-CA4	-2.30	1.40	1.46
54	N	201	PLX	C7-C6	2.29	1.55	1.50
48	Q	501	PEE	O2-C10	2.29	1.40	1.34
48	l	704	PEE	O2-C10	2.28	1.40	1.34
54	a	202	PLX	C7-C6	2.28	1.55	1.50
48	B	303	PEE	O2-C10	2.27	1.40	1.34
54	g	201	PLX	C7-C6	2.27	1.55	1.50
48	m	201	PEE	O2-C2	-2.26	1.41	1.46
56	s	402	UQ	O4-C4	-2.25	1.18	1.23
49	G	201	8Q1	C6-C1	2.25	1.53	1.50
50	i	401	CDL	PB2-OB2	2.25	1.68	1.59
49	X	201	8Q1	C6-C1	2.24	1.53	1.50
49	G	201	8Q1	O35-C34	-2.24	1.18	1.23
54	r	502	PLX	O6-C4	-2.24	1.41	1.44
57	w	401	ADP	C5-N7	-2.24	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	X	201	8Q1	O35-C34	-2.22	1.19	1.23
50	l	702	CDL	PB2-OB2	2.21	1.68	1.59
48	r	501	PEE	O2-C10	2.21	1.40	1.34
50	i	401	CDL	PB2-OB5	2.21	1.68	1.59
50	r	504	CDL	PB2-OB2	2.20	1.68	1.59
50	r	504	CDL	PB2-OB5	2.20	1.68	1.59
50	I	201	CDL	PB2-OB2	2.20	1.68	1.59
50	a	201	CDL	PB2-OB2	2.19	1.68	1.59
49	G	201	8Q1	O40-C39	-2.19	1.18	1.23
50	a	201	CDL	PB2-OB5	2.18	1.68	1.59
50	I	201	CDL	PB2-OB5	2.18	1.68	1.59
49	X	201	8Q1	O40-C39	-2.18	1.18	1.23
54	N	201	PLX	P1-O4	2.17	1.68	1.59
54	j	201	PLX	P1-O4	2.17	1.68	1.59
50	l	702	CDL	PB2-OB5	2.16	1.68	1.59
51	J	401	NDP	PA-O5B	2.16	1.68	1.59
54	r	502	PLX	P1-O4	2.15	1.68	1.59
50	i	401	CDL	OB6-CB4	-2.14	1.41	1.46
50	l	702	CDL	OB6-CB4	-2.14	1.41	1.46
54	a	202	PLX	P1-O4	2.14	1.68	1.59
50	I	201	CDL	OB6-CB4	-2.13	1.41	1.46
50	r	504	CDL	OB6-CB4	-2.13	1.41	1.46
50	a	201	CDL	OB6-CB4	-2.13	1.41	1.46
51	J	401	NDP	O7N-C7N	-2.12	1.19	1.24
54	r	503	PLX	P1-O4	2.10	1.67	1.59
48	B	303	PEE	O3-C3	-2.10	1.40	1.45
48	s	401	PEE	O3-C3	-2.09	1.40	1.45
48	l	703	PEE	O3-C3	-2.08	1.40	1.45
54	g	201	PLX	P1-O4	2.08	1.67	1.59
48	m	201	PEE	O3-C3	-2.07	1.40	1.45
54	r	502	PLX	P1-O1	2.07	1.67	1.59
54	j	201	PLX	P1-O1	2.06	1.67	1.59
48	Q	501	PEE	O3-C3	-2.05	1.40	1.45
54	r	503	PLX	P1-O1	2.04	1.67	1.59
48	r	501	PEE	O3-C3	-2.04	1.40	1.45
54	N	201	PLX	P1-O1	2.04	1.67	1.59
47	A	503	NAI	C2N-C3N	2.03	1.40	1.34
54	a	202	PLX	P1-O1	2.03	1.67	1.59
48	l	704	PEE	O3-C3	-2.02	1.40	1.45
54	r	502	PLX	C25-C24	2.01	1.55	1.50
50	a	201	CDL	C11-CA5	2.01	1.56	1.50
48	C	302	PEE	O3-C3	-2.01	1.40	1.45

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	s	402	UQ	C7-C8-C9	-9.16	111.53	126.79
51	J	401	NDP	C3N-C2N-N1N	-7.52	112.37	123.10
51	J	401	NDP	C1D-N1N-C2N	-7.28	109.00	121.11
56	s	402	UQ	C12-C13-C14	-6.17	112.81	127.66
49	X	201	8Q1	C6-C1-S44	5.98	120.42	113.46
51	J	401	NDP	C5A-C4A-N3A	-5.87	119.10	126.75
49	G	201	8Q1	C6-C1-S44	5.82	120.23	113.46
47	A	503	NAI	C5A-C4A-N3A	-5.79	119.20	126.75
57	w	401	ADP	C5-C4-N3	-5.78	119.22	126.75
51	J	401	NDP	C1D-N1N-C6N	-5.12	109.79	120.83
50	l	701	CDL	OA6-CA5-C11	4.66	121.54	111.50
56	s	402	UQ	C10-C9-C8	-4.57	111.96	123.68
57	w	401	ADP	N3-C4-N9	4.50	134.50	127.08
56	s	402	UQ	C11-C9-C8	-4.47	112.06	121.12
57	w	401	ADP	N3-C2-N1	-4.46	121.63	128.60
50	l	701	CDL	OB6-CB5-C51	4.30	120.77	111.50
47	A	503	NAI	N3A-C2A-N1A	-4.27	121.93	128.60
50	a	201	CDL	OA6-CA5-C11	4.24	120.64	111.50
56	s	402	UQ	C15-C14-C13	-4.19	112.94	123.68
48	B	303	PEE	O2-C10-C11	4.10	120.34	111.50
50	l	702	CDL	OA6-CA5-C11	4.10	120.34	111.50
56	s	402	UQ	C17-C18-C19	-4.07	113.83	127.75
51	J	401	NDP	N3A-C4A-N9A	4.07	133.79	127.08
50	I	201	CDL	OB6-CB5-C51	4.05	120.23	111.50
50	i	401	CDL	OA6-CA5-C11	4.04	120.21	111.50
51	J	401	NDP	N3A-C2A-N1A	-4.03	122.29	128.60
50	a	201	CDL	OB6-CB5-C51	4.03	120.19	111.50
48	m	201	PEE	O2-C10-C11	4.02	120.16	111.50
50	r	504	CDL	OA6-CA5-C11	3.98	120.08	111.50
47	A	503	NAI	N3A-C4A-N9A	3.97	133.63	127.08
48	Q	501	PEE	O2-C10-C11	3.97	120.06	111.50
48	C	302	PEE	O2-C10-C11	3.93	119.97	111.50
50	r	504	CDL	OB6-CB5-C51	3.92	119.94	111.50
50	I	201	CDL	OA6-CA5-C11	3.91	119.94	111.50
48	s	401	PEE	O2-C10-C11	3.88	119.86	111.50
50	i	401	CDL	OB6-CB5-C51	3.86	119.81	111.50
48	l	704	PEE	O2-C10-C11	3.85	119.80	111.50
47	A	503	NAI	C2A-N3A-C4A	3.84	120.83	111.75
48	r	501	PEE	O2-C10-C11	3.84	119.78	111.50
48	l	703	PEE	O2-C10-C11	3.78	119.64	111.50
51	J	401	NDP	C2A-N3A-C4A	3.74	120.59	111.75
47	A	503	NAI	C5A-N7A-C8A	3.73	108.81	103.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	w	401	ADP	C2-N3-C4	3.72	120.53	111.75
56	s	402	UQ	C16-C14-C13	-3.71	113.61	121.12
56	s	402	UQ	C21-C19-C18	-3.71	111.93	122.65
57	w	401	ADP	N9-C8-N7	-3.67	108.90	113.91
50	l	702	CDL	OB6-CB5-C51	3.63	119.33	111.50
57	w	401	ADP	C5-N7-C8	3.49	108.46	103.51
49	X	201	8Q1	O4-C1-C6	-3.48	119.88	123.99
49	G	201	8Q1	O4-C1-C6	-3.43	119.94	123.99
47	A	503	NAI	N9A-C8A-N7A	-3.39	109.27	113.91
51	J	401	NDP	C5A-N7A-C8A	3.32	108.22	103.51
47	A	503	NAI	C4A-C5A-N7A	-3.31	106.59	110.62
47	A	503	NAI	C3D-C2D-C1D	3.17	107.45	101.43
50	l	701	CDL	CA4-OA6-CA5	-3.16	110.02	117.79
51	J	401	NDP	N9A-C8A-N7A	-3.13	109.63	113.91
47	A	503	NAI	C4D-O4D-C1D	-3.13	102.57	109.47
57	w	401	ADP	C4-N9-C8	3.12	109.11	105.73
46	A	502	FMN	C4-N3-C2	-3.11	119.90	125.64
51	J	401	NDP	C4A-C5A-N7A	-3.09	106.86	110.62
56	s	402	UQ	C20-C19-C18	-3.05	113.83	122.65
49	G	201	8Q1	C37-C38-C39	3.04	117.42	112.36
50	l	701	CDL	OA8-CA7-C31	2.94	121.14	111.91
50	l	701	CDL	OB8-CB7-C71	2.91	121.03	111.91
57	w	401	ADP	C4-C5-N7	-2.77	107.24	110.62
50	l	701	CDL	CB4-OB6-CB5	-2.74	111.05	117.79
48	l	704	PEE	O3-C30-C31	2.68	120.31	111.91
46	A	502	FMN	C4A-C4-N3	2.67	119.97	113.19
51	J	401	NDP	PN-O3-PA	-2.67	123.67	132.83
50	i	401	CDL	OB8-CB7-C71	2.65	120.24	111.91
48	r	501	PEE	O3-C30-C31	2.65	120.23	111.91
50	a	201	CDL	OB8-CB7-C71	2.65	120.23	111.91
50	i	401	CDL	OA8-CA7-C31	2.64	120.21	111.91
48	l	703	PEE	O3-C30-C31	2.63	120.17	111.91
50	I	201	CDL	OA8-CA7-C31	2.61	120.11	111.91
48	C	302	PEE	O3-C30-C31	2.61	120.08	111.91
48	s	401	PEE	O3-C30-C31	2.59	120.05	111.91
50	r	504	CDL	OB8-CB7-C71	2.59	120.02	111.91
48	B	303	PEE	O3-C30-C31	2.57	119.97	111.91
48	Q	501	PEE	O3-C30-C31	2.56	119.95	111.91
50	l	702	CDL	OB8-CB7-C71	2.56	119.94	111.91
47	A	503	NAI	PN-O3-PA	-2.55	124.07	132.83
50	r	504	CDL	OA8-CA7-C31	2.54	119.89	111.91
50	I	201	CDL	OB8-CB7-C71	2.54	119.88	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	a	201	CDL	OA8-CA7-C31	2.54	119.86	111.91
50	l	702	CDL	OA8-CA7-C31	2.52	119.81	111.91
48	m	201	PEE	O3-C30-C31	2.51	119.79	111.91
49	X	201	8Q1	C37-C38-C39	2.51	116.54	112.36
46	A	502	FMN	O4-C4-C4A	-2.49	120.00	126.60
49	G	201	8Q1	C38-C39-N41	2.48	120.59	116.42
54	r	503	PLX	C1A-N1-C1	2.44	119.89	109.92
54	a	202	PLX	C1A-N1-C1	2.43	119.86	109.92
57	w	401	ADP	PA-O3A-PB	-2.43	124.50	132.83
54	r	502	PLX	C1A-N1-C1	2.43	119.84	109.92
54	g	201	PLX	C1A-N1-C1	2.37	119.62	109.92
49	G	201	8Q1	C43-S44-C1	2.37	109.24	101.87
51	J	401	NDP	C2B-C3B-C4B	2.36	107.12	101.99
46	A	502	FMN	C4A-C10-N10	2.34	119.91	116.48
54	j	201	PLX	C1A-N1-C1	2.32	119.42	109.92
47	A	503	NAI	C2D-C3D-C4D	2.31	107.12	102.64
54	N	201	PLX	C1A-N1-C1	2.29	119.30	109.92
49	X	201	8Q1	C38-C39-N41	2.27	120.25	116.42
46	A	502	FMN	C9A-C5A-N5	-2.27	119.97	122.43
50	l	701	CDL	OA6-CA5-OA7	-2.26	118.25	123.70
51	J	401	NDP	C4A-N9A-C8A	2.26	108.17	105.73
46	A	502	FMN	C4A-C10-N1	-2.25	119.51	124.73
49	X	201	8Q1	O4-C1-S44	-2.25	119.69	122.61
49	X	201	8Q1	C43-S44-C1	2.24	108.84	101.87
47	A	503	NAI	C4A-N9A-C8A	2.24	108.15	105.73
46	A	502	FMN	C10-C4A-N5	-2.22	120.14	124.86
49	G	201	8Q1	O4-C1-S44	-2.14	119.83	122.61
51	J	401	NDP	C2D-C3D-C4D	2.09	106.69	102.64

There are no chirality outliers.

All (692) 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'
47	A	503	NAI	C5B-O5B-PA-O1A
47	A	503	NAI	C5B-O5B-PA-O3
48	B	303	PEE	C1-O3P-P-O1P
48	C	302	PEE	C11-C10-O2-C2
48	C	302	PEE	C1-O3P-P-O1P
48	C	302	PEE	C4-O4P-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	Q	501	PEE	C11-C10-O2-C2
48	l	704	PEE	C1-O3P-P-O1P
48	m	201	PEE	C11-C10-O2-C2
48	m	201	PEE	O4P-C4-C5-N
48	s	401	PEE	C1-O3P-P-O2P
48	s	401	PEE	C1-O3P-P-O1P
49	G	201	8Q1	C1-C6-C7-C8
49	G	201	8Q1	O4-C1-S44-C43
49	G	201	8Q1	C6-C1-S44-C43
49	G	201	8Q1	C28-C29-C32-C34
49	G	201	8Q1	C28-C29-C32-O33
49	G	201	8Q1	C31-C29-C32-O33
49	G	201	8Q1	N36-C37-C38-C39
49	G	201	8Q1	N41-C42-C43-S44
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	C6-C1-S44-C43
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	C29-C32-C34-O35
49	X	201	8Q1	N36-C37-C38-C39
49	X	201	8Q1	C42-C43-S44-C1
49	X	201	8Q1	C28-O27-P24-O2
49	X	201	8Q1	C28-O27-P24-O1
50	I	201	CDL	O1-C1-CA2-OA2
50	I	201	CDL	CB2-C1-CA2-OA2
50	I	201	CDL	OA5-CA3-CA4-OA6
50	I	201	CDL	CB2-OB2-PB2-OB3
50	I	201	CDL	CB3-OB5-PB2-OB3
50	a	201	CDL	CA2-OA2-PA1-OA3
50	a	201	CDL	CA2-OA2-PA1-OA4
50	a	201	CDL	OA5-CA3-CA4-OA6
50	a	201	CDL	CB2-OB2-PB2-OB3
50	i	401	CDL	CA2-OA2-PA1-OA5
50	i	401	CDL	CA3-OA5-PA1-OA2
50	i	401	CDL	CA3-OA5-PA1-OA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
50	i	401	CDL	CA3-OA5-PA1-OA4
50	i	401	CDL	CB2-OB2-PB2-OB3
50	i	401	CDL	CB2-OB2-PB2-OB4
50	l	701	CDL	O1-C1-CB2-OB2
50	l	701	CDL	CA3-OA5-PA1-OA3
50	l	701	CDL	CB2-OB2-PB2-OB3
50	l	701	CDL	CB2-OB2-PB2-OB4
50	l	702	CDL	O1-C1-CA2-OA2
50	l	702	CDL	CA3-OA5-PA1-OA4
50	l	702	CDL	OA6-CA4-CA6-OA8
50	l	702	CDL	CB2-OB2-PB2-OB3
50	l	702	CDL	CB2-OB2-PB2-OB4
50	l	702	CDL	CB2-OB2-PB2-OB5
50	l	702	CDL	CB3-OB5-PB2-OB3
50	r	504	CDL	CA2-OA2-PA1-OA3
50	r	504	CDL	CA2-OA2-PA1-OA4
50	r	504	CDL	CA3-OA5-PA1-OA3
50	r	504	CDL	CA3-OA5-PA1-OA4
50	r	504	CDL	OA6-CA4-CA6-OA8
50	r	504	CDL	CB2-OB2-PB2-OB3
50	r	504	CDL	CB3-OB5-PB2-OB3
50	r	504	CDL	C51-CB5-OB6-CB4
51	J	401	NDP	C2B-O2B-P2B-O1X
54	N	201	PLX	O7-C6-C7-C8
54	N	201	PLX	O4-C3-C4-O6
54	N	201	PLX	C3-O4-P1-O1
54	N	201	PLX	C3-O4-P1-O2
54	N	201	PLX	C3-O4-P1-O3
54	N	201	PLX	N1-C1-C2-O1
54	g	201	PLX	O7-C6-O6-C4
54	g	201	PLX	O9-C24-O8-C5
54	j	201	PLX	O7-C6-C7-C8
54	j	201	PLX	O9-C24-O8-C5
54	j	201	PLX	C25-C24-O8-C5
54	r	502	PLX	O7-C6-O6-C4
54	r	502	PLX	C5-C4-O6-C6
54	r	502	PLX	C3-O4-P1-O2
54	r	502	PLX	C2-O1-P1-O2
54	r	502	PLX	O9-C24-O8-C5
54	r	502	PLX	O9-C24-C25-C26
54	r	503	PLX	C5-C4-O6-C6
54	r	503	PLX	C2-O1-P1-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	r	503	PLX	C2-O1-P1-O2
54	r	503	PLX	C2-O1-P1-O3
54	r	503	PLX	O9-C24-O8-C5
56	s	402	UQ	C7-C8-C9-C11
56	s	402	UQ	C12-C11-C9-C8
56	s	402	UQ	C12-C11-C9-C10
56	s	402	UQ	C12-C13-C14-C16
56	s	402	UQ	C14-C16-C17-C18
56	s	402	UQ	C17-C18-C19-C21
57	w	401	ADP	C5'-O5'-PA-O2A
57	w	401	ADP	C5'-O5'-PA-O3A
50	i	401	CDL	OA9-CA7-OA8-CA6
48	C	302	PEE	O4-C10-O2-C2
48	Q	501	PEE	O4-C10-O2-C2
48	l	703	PEE	O4-C10-O2-C2
48	m	201	PEE	O4-C10-O2-C2
50	i	401	CDL	C31-CA7-OA8-CA6
48	l	703	PEE	C11-C10-O2-C2
48	l	703	PEE	C31-C30-O3-C3
48	l	704	PEE	C31-C30-O3-C3
48	B	303	PEE	C37-C38-C39-C40
48	Q	501	PEE	C37-C38-C39-C40
48	l	704	PEE	C37-C38-C39-C40
48	r	501	PEE	C17-C18-C19-C20
48	s	401	PEE	C17-C18-C19-C20
56	s	402	UQ	C7-C8-C9-C10
50	r	504	CDL	OB7-CB5-OB6-CB4
48	l	703	PEE	O5-C30-O3-C3
48	l	704	PEE	O5-C30-O3-C3
50	a	201	CDL	O1-C1-CB2-OB2
48	m	201	PEE	C31-C30-O3-C3
50	l	702	CDL	C59-C60-C61-C62
54	N	201	PLX	C28-C29-C30-C31
54	r	502	PLX	C9-C10-C11-C12
54	r	503	PLX	C12-C13-C14-C15
54	a	202	PLX	C33-C34-C35-C36
56	s	402	UQ	C13-C14-C16-C17
48	m	201	PEE	O5-C30-O3-C3
54	g	201	PLX	C7-C8-C9-C10
54	j	201	PLX	C28-C29-C30-C31
50	a	201	CDL	CA2-C1-CB2-OB2
50	l	701	CDL	CA2-C1-CB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
50	r	504	CDL	CB2-C1-CA2-OA2
54	r	502	PLX	C30-C31-C32-C33
50	a	201	CDL	C71-CB7-OB8-CB6
50	l	701	CDL	C31-CA7-OA8-CA6
50	l	702	CDL	C71-CB7-OB8-CB6
50	r	504	CDL	C71-CB7-OB8-CB6
48	Q	501	PEE	C10-C11-C12-C13
50	a	201	CDL	CA7-C31-C32-C33
50	r	504	CDL	C74-C75-C76-C77
50	l	702	CDL	C35-C36-C37-C38
48	m	201	PEE	C33-C34-C35-C36
50	I	201	CDL	O1-C1-CB2-OB2
50	i	401	CDL	O1-C1-CA2-OA2
50	l	702	CDL	O1-C1-CB2-OB2
50	i	401	CDL	OB6-CB4-CB6-OB8
48	s	401	PEE	C31-C30-O3-C3
50	r	504	CDL	OB9-CB7-OB8-CB6
50	i	401	CDL	C31-C32-C33-C34
50	l	701	CDL	CB5-C51-C52-C53
51	J	401	NDP	C2D-C1D-N1N-C6N
50	l	701	CDL	OA9-CA7-OA8-CA6
50	l	702	CDL	OB9-CB7-OB8-CB6
48	B	303	PEE	C31-C30-O3-C3
50	I	201	CDL	CB5-C51-C52-C53
50	r	504	CDL	CB5-C51-C52-C53
48	B	303	PEE	C17-C18-C19-C20
54	r	502	PLX	C11-C12-C13-C14
50	i	401	CDL	CA7-C31-C32-C33
50	i	401	CDL	CB7-C71-C72-C73
50	l	702	CDL	CB5-C51-C52-C53
50	r	504	CDL	CB7-C71-C72-C73
50	l	702	CDL	C11-C12-C13-C14
54	r	503	PLX	C2-C1-N1-C1A
48	B	303	PEE	C10-C11-C12-C13
48	l	703	PEE	C30-C31-C32-C33
48	r	501	PEE	C10-C11-C12-C13
50	a	201	CDL	C76-C77-C78-C79
50	a	201	CDL	C31-C32-C33-C34
54	a	202	PLX	C29-C30-C31-C32
50	a	201	CDL	OB9-CB7-OB8-CB6
50	r	504	CDL	C78-C79-C80-C81
50	a	201	CDL	O1-C1-CA2-OA2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
50	r	504	CDL	O1-C1-CA2-OA2
48	B	303	PEE	O5-C30-O3-C3
48	s	401	PEE	O5-C30-O3-C3
48	s	401	PEE	C11-C10-O2-C2
48	C	302	PEE	C4-O4P-P-O3P
48	l	703	PEE	C4-O4P-P-O3P
48	m	201	PEE	C4-O4P-P-O3P
48	s	401	PEE	C1-O3P-P-O4P
50	I	201	CDL	CA2-OA2-PA1-OA5
50	I	201	CDL	CB2-OB2-PB2-OB5
50	a	201	CDL	CA2-OA2-PA1-OA5
50	a	201	CDL	CA3-OA5-PA1-OA2
50	a	201	CDL	CB3-OB5-PB2-OB2
50	i	401	CDL	CB2-OB2-PB2-OB5
50	l	701	CDL	CA2-OA2-PA1-OA5
50	l	701	CDL	CA3-OA5-PA1-OA2
50	l	701	CDL	CB2-OB2-PB2-OB5
50	l	702	CDL	CA2-OA2-PA1-OA5
50	l	702	CDL	CA3-OA5-PA1-OA2
50	l	702	CDL	CB3-OB5-PB2-OB2
50	r	504	CDL	CA2-OA2-PA1-OA5
50	r	504	CDL	CA3-OA5-PA1-OA2
50	r	504	CDL	CB2-OB2-PB2-OB5
54	r	502	PLX	C3-O4-P1-O1
48	m	201	PEE	C12-C13-C14-C15
50	a	201	CDL	CB2-C1-CA2-OA2
50	i	401	CDL	CB2-C1-CA2-OA2
50	l	702	CDL	CB2-C1-CA2-OA2
48	s	401	PEE	O4-C10-O2-C2
54	j	201	PLX	C15-C16-C17-C18
48	Q	501	PEE	C19-C20-C21-C22
50	r	504	CDL	CA7-C31-C32-C33
54	g	201	PLX	C33-C34-C35-C36
48	r	501	PEE	C31-C32-C33-C34
50	r	504	CDL	C71-C72-C73-C74
54	a	202	PLX	C28-C29-C30-C31
54	j	201	PLX	C27-C28-C29-C30
50	a	201	CDL	C32-C33-C34-C35
50	a	201	CDL	C52-C53-C54-C55
50	l	702	CDL	C55-C56-C57-C58
54	N	201	PLX	C11-C12-C13-C14
54	N	201	PLX	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	g	201	PLX	C11-C10-C9-C8
54	r	502	PLX	C27-C28-C29-C30
54	r	503	PLX	C13-C14-C15-C16
50	l	701	CDL	C35-C36-C37-C38
50	r	504	CDL	C55-C56-C57-C58
54	a	202	PLX	C26-C27-C28-C29
50	a	201	CDL	C37-C38-C39-C40
50	l	702	CDL	C75-C76-C77-C78
50	r	504	CDL	C73-C74-C75-C76
54	N	201	PLX	C16-C17-C18-C19
54	g	201	PLX	C14-C15-C16-C17
54	j	201	PLX	C7-C8-C9-C10
54	j	201	PLX	C25-C26-C27-C28
54	r	503	PLX	C27-C28-C29-C30
54	g	201	PLX	C27-C28-C29-C30
48	Q	501	PEE	C23-C24-C25-C26
48	l	704	PEE	C31-C32-C33-C34
50	a	201	CDL	C11-C12-C13-C14
50	a	201	CDL	C73-C74-C75-C76
50	a	201	CDL	C75-C76-C77-C78
54	g	201	PLX	C28-C29-C30-C31
54	g	201	PLX	C32-C33-C34-C35
48	r	501	PEE	C12-C13-C14-C15
54	N	201	PLX	C17-C18-C19-C20
54	g	201	PLX	C9-C10-C11-C12
49	G	201	8Q1	C11-C12-C13-C14
50	i	401	CDL	C32-C33-C34-C35
50	r	504	CDL	C52-C53-C54-C55
50	r	504	CDL	C56-C57-C58-C59
54	a	202	PLX	C16-C17-C18-C19
54	j	201	PLX	C10-C11-C12-C13
48	Q	501	PEE	C12-C13-C14-C15
50	i	401	CDL	C73-C74-C75-C76
54	r	503	PLX	C26-C27-C28-C29
50	I	201	CDL	C51-CB5-OB6-CB4
50	r	504	CDL	C75-C76-C77-C78
50	I	201	CDL	CA7-C31-C32-C33
56	s	402	UQ	C17-C18-C19-C20
48	l	704	PEE	C22-C23-C24-C25
48	s	401	PEE	C21-C22-C23-C24
50	I	201	CDL	C11-C12-C13-C14
50	a	201	CDL	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
50	i	401	CDL	C71-C72-C73-C74
54	a	202	PLX	C18-C19-C20-C21
54	a	202	PLX	C11-C10-C9-C8
54	r	503	PLX	C14-C15-C16-C17
54	r	503	PLX	C2-C1-N1-C1C
48	r	501	PEE	C41-C42-C43-C44
50	i	401	CDL	C37-C38-C39-C40
50	l	702	CDL	C60-C61-C62-C63
48	l	704	PEE	O4P-C4-C5-N
49	G	201	8Q1	C7-C8-C9-C10
50	l	702	CDL	C73-C74-C75-C76
54	r	502	PLX	C33-C34-C35-C36
48	B	303	PEE	C33-C34-C35-C36
50	i	401	CDL	C52-C53-C54-C55
50	r	504	CDL	C15-C16-C17-C18
54	N	201	PLX	C9-C10-C11-C12
54	a	202	PLX	C25-C26-C27-C28
54	g	201	PLX	C10-C11-C12-C13
54	r	502	PLX	C31-C32-C33-C34
48	l	704	PEE	C33-C34-C35-C36
50	a	201	CDL	C71-C72-C73-C74
50	l	702	CDL	C58-C59-C60-C61
54	N	201	PLX	C14-C15-C16-C17
49	X	201	8Q1	C9-C10-C11-C12
54	r	503	PLX	C10-C11-C12-C13
48	s	401	PEE	C43-C44-C45-C46
54	N	201	PLX	C25-C26-C27-C28
54	a	202	PLX	C10-C11-C12-C13
54	r	502	PLX	C16-C17-C18-C19
48	l	704	PEE	C17-C18-C19-C20
50	l	702	CDL	C52-C53-C54-C55
50	r	504	CDL	C59-C60-C61-C62
54	a	202	PLX	O7-C6-C7-C8
54	j	201	PLX	O9-C24-C25-C26
50	r	504	CDL	C43-C44-C45-C46
54	r	502	PLX	C7-C8-C9-C10
50	I	201	CDL	CB7-C71-C72-C73
50	I	201	CDL	C71-C72-C73-C74
50	r	504	CDL	C82-C83-C84-C85
54	r	503	PLX	C25-C26-C27-C28
50	I	201	CDL	OB7-CB5-OB6-CB4
54	r	502	PLX	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	l	703	PEE	C11-C12-C13-C14
54	N	201	PLX	C35-C36-C37-C38
48	r	501	PEE	C11-C10-O2-C2
48	l	703	PEE	C31-C32-C33-C34
49	X	201	8Q1	C7-C8-C9-C10
50	l	702	CDL	C18-C19-C20-C21
50	r	504	CDL	C41-C42-C43-C44
54	j	201	PLX	C12-C13-C14-C15
48	l	704	PEE	C32-C33-C34-C35
54	r	502	PLX	C14-C15-C16-C17
48	C	302	PEE	C37-C38-C39-C40
48	Q	501	PEE	C17-C18-C19-C20
50	r	504	CDL	C13-C14-C15-C16
48	C	302	PEE	C15-C16-C17-C18
48	s	401	PEE	C19-C20-C21-C22
50	I	201	CDL	OA7-CA5-OA6-CA4
50	i	401	CDL	C71-CB7-OB8-CB6
54	N	201	PLX	C26-C27-C28-C29
54	r	502	PLX	C28-C29-C30-C31
50	i	401	CDL	C36-C37-C38-C39
54	r	503	PLX	C28-C29-C30-C31
50	r	504	CDL	C51-C52-C53-C54
50	l	702	CDL	C37-C38-C39-C40
54	r	503	PLX	C15-C16-C17-C18
48	l	704	PEE	C10-C11-C12-C13
48	l	704	PEE	C11-C10-O2-C2
50	I	201	CDL	C11-CA5-OA6-CA4
50	l	701	CDL	C11-CA5-OA6-CA4
48	B	303	PEE	C21-C22-C23-C24
54	j	201	PLX	C13-C14-C15-C16
54	a	202	PLX	C12-C13-C14-C15
48	l	704	PEE	O4-C10-O2-C2
48	r	501	PEE	O4-C10-O2-C2
50	l	701	CDL	OA7-CA5-OA6-CA4
50	i	401	CDL	C14-C15-C16-C17
50	l	702	CDL	C32-C33-C34-C35
54	N	201	PLX	C30-C31-C32-C33
54	r	503	PLX	C2-C1-N1-C1B
48	s	401	PEE	C22-C23-C24-C25
54	j	201	PLX	C31-C32-C33-C34
48	B	303	PEE	C22-C23-C24-C25
54	j	201	PLX	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
50	i	401	CDL	OB9-CB7-OB8-CB6
50	a	201	CDL	C16-C17-C18-C19
48	s	401	PEE	C36-C37-C38-C39
46	A	502	FMN	O2'-C2'-C3'-C4'
48	C	302	PEE	C1-O3P-P-O4P
54	r	502	PLX	C2-O1-P1-O4
50	I	201	CDL	OA5-CA3-CA4-CA6
50	I	201	CDL	OB5-CB3-CB4-CB6
54	N	201	PLX	O4-C3-C4-C5
54	r	503	PLX	C16-C17-C18-C19
50	l	701	CDL	C20-C21-C22-C23
54	N	201	PLX	C27-C28-C29-C30
54	g	201	PLX	C25-C26-C27-C28
50	a	201	CDL	C21-C22-C23-C24
50	l	702	CDL	C56-C57-C58-C59
54	r	503	PLX	C7-C8-C9-C10
50	i	401	CDL	CB3-CB4-CB6-OB8
54	j	201	PLX	C3-C4-C5-O8
54	r	502	PLX	C3-C4-C5-O8
54	r	503	PLX	C3-C4-C5-O8
54	r	502	PLX	C12-C13-C14-C15
50	I	201	CDL	C72-C73-C74-C75
48	m	201	PEE	C11-C12-C13-C14
50	i	401	CDL	CB5-C51-C52-C53
50	I	201	CDL	C52-C53-C54-C55
50	r	504	CDL	C81-C82-C83-C84
48	Q	501	PEE	C24-C25-C26-C27
48	l	703	PEE	C32-C33-C34-C35
50	r	504	CDL	C60-C61-C62-C63
50	r	504	CDL	C62-C63-C64-C65
48	B	303	PEE	C39-C40-C41-C42
48	C	302	PEE	C35-C36-C37-C38
50	l	702	CDL	C64-C65-C66-C67
54	g	201	PLX	C30-C31-C32-C33
50	r	504	CDL	C84-C85-C86-C87
49	X	201	8Q1	C13-C14-C15-C16
54	j	201	PLX	C30-C31-C32-C33
48	r	501	PEE	C44-C45-C46-C47
54	g	201	PLX	C13-C14-C15-C16
49	X	201	8Q1	C28-O27-P24-O3
54	N	201	PLX	C33-C34-C35-C36
54	a	202	PLX	C30-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	l	703	PEE	O3P-C1-C2-O2
54	j	201	PLX	C26-C27-C28-C29
54	r	503	PLX	C31-C32-C33-C34
48	l	703	PEE	C15-C16-C17-C18
48	r	501	PEE	C36-C37-C38-C39
50	a	201	CDL	C35-C36-C37-C38
54	r	503	PLX	C33-C34-C35-C36
48	C	302	PEE	C11-C12-C13-C14
54	j	201	PLX	C14-C15-C16-C17
50	I	201	CDL	C31-C32-C33-C34
48	C	302	PEE	C31-C30-O3-C3
48	m	201	PEE	C13-C14-C15-C16
48	l	703	PEE	C19-C20-C21-C22
50	i	401	CDL	C75-C76-C77-C78
50	a	201	CDL	OA5-CA3-CA4-CA6
50	a	201	CDL	CB5-C51-C52-C53
48	B	303	PEE	O4P-C4-C5-N
50	a	201	CDL	C60-C61-C62-C63
54	g	201	PLX	C12-C13-C14-C15
50	r	504	CDL	C11-CA5-OA6-CA4
50	r	504	CDL	C42-C43-C44-C45
48	r	501	PEE	C13-C14-C15-C16
48	l	704	PEE	C1-C2-C3-O3
50	I	201	CDL	CA3-CA4-CA6-OA8
50	l	702	CDL	CA3-CA4-CA6-OA8
50	l	702	CDL	CB3-CB4-CB6-OB8
54	g	201	PLX	C3-C4-C5-O8
48	m	201	PEE	C24-C25-C26-C27
49	X	201	8Q1	C29-C32-C34-N36
50	I	201	CDL	CB3-OB5-PB2-OB2
50	a	201	CDL	CB2-OB2-PB2-OB5
50	l	702	CDL	C39-C40-C41-C42
50	l	702	CDL	OA5-CA3-CA4-OA6
54	j	201	PLX	O4-C3-C4-O6
50	r	504	CDL	C54-C55-C56-C57
50	l	702	CDL	OB6-CB4-CB6-OB8
54	r	502	PLX	O6-C4-C5-O8
54	r	503	PLX	O6-C4-C5-O8
50	l	701	CDL	C51-CB5-OB6-CB4
50	l	701	CDL	CB7-C71-C72-C73
48	s	401	PEE	C34-C35-C36-C37
54	a	202	PLX	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
50	l	701	CDL	CA4-CA3-OA5-PA1
54	a	202	PLX	C13-C14-C15-C16
48	Q	501	PEE	C18-C19-C20-C21
49	X	201	8Q1	O4-C1-S44-C43
54	a	202	PLX	C7-C8-C9-C10
50	l	702	CDL	C71-C72-C73-C74
48	C	302	PEE	C10-C11-C12-C13
54	N	201	PLX	O6-C6-C7-C8
54	a	202	PLX	O6-C6-C7-C8
48	r	501	PEE	O3P-C1-C2-C3
50	a	201	CDL	OB5-CB3-CB4-CB6
50	l	702	CDL	OA5-CA3-CA4-CA6
54	g	201	PLX	O4-C3-C4-C5
48	l	703	PEE	C37-C38-C39-C40
48	s	401	PEE	C38-C39-C40-C41
50	l	702	CDL	C74-C75-C76-C77
54	r	503	PLX	C11-C12-C13-C14
48	C	302	PEE	C33-C34-C35-C36
49	X	201	8Q1	O33-C32-C34-N36
50	a	201	CDL	C58-C59-C60-C61
49	X	201	8Q1	O27-C28-C29-C30
49	X	201	8Q1	O27-C28-C29-C31
50	a	201	CDL	C59-C60-C61-C62
54	a	202	PLX	C9-C10-C11-C12
50	a	201	CDL	C55-C56-C57-C58
50	r	504	CDL	C72-C73-C74-C75
48	l	703	PEE	C20-C21-C22-C23
50	l	701	CDL	C24-C25-C26-C27
48	m	201	PEE	C3-C2-O2-C10
50	r	504	CDL	OA7-CA5-OA6-CA4
54	N	201	PLX	C13-C14-C15-C16
48	r	501	PEE	C1-C2-C3-O3
50	r	504	CDL	CA3-CA4-CA6-OA8
48	C	302	PEE	O5-C30-O3-C3
48	l	704	PEE	C12-C13-C14-C15
48	B	303	PEE	O3P-C1-C2-O2
48	r	501	PEE	O3P-C1-C2-O2
50	a	201	CDL	OB5-CB3-CB4-OB6
50	I	201	CDL	C31-CA7-OA8-CA6
48	Q	501	PEE	C16-C17-C18-C19
48	Q	501	PEE	C32-C33-C34-C35
50	l	701	CDL	O1-C1-CA2-OA2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
50	l	701	CDL	OB7-CB5-OB6-CB4
49	G	201	8Q1	C31-C29-C32-C34
50	l	701	CDL	C36-C37-C38-C39
48	l	704	PEE	O2-C2-C3-O3
48	r	501	PEE	O2-C2-C3-O3
50	I	201	CDL	OA6-CA4-CA6-OA8
50	i	401	CDL	C33-C34-C35-C36
50	i	401	CDL	C15-C16-C17-C18
48	B	303	PEE	C15-C16-C17-C18
48	l	703	PEE	C22-C23-C24-C25
48	l	704	PEE	C23-C24-C25-C26
48	r	501	PEE	C24-C25-C26-C27
50	r	504	CDL	C39-C40-C41-C42
48	l	703	PEE	C23-C24-C25-C26
50	l	701	CDL	C75-C76-C77-C78
50	a	201	CDL	C15-C16-C17-C18
54	j	201	PLX	C11-C12-C13-C14
54	j	201	PLX	C33-C34-C35-C36
50	r	504	CDL	CB3-OB5-PB2-OB2
47	A	503	NAI	C2D-C1D-N1N-C2N
48	C	302	PEE	C42-C43-C44-C45
48	C	302	PEE	C1-O3P-P-O2P
48	C	302	PEE	C4-O4P-P-O2P
48	l	703	PEE	C4-O4P-P-O2P
48	m	201	PEE	C4-O4P-P-O2P
48	m	201	PEE	C4-O4P-P-O1P
50	I	201	CDL	CA2-OA2-PA1-OA4
50	I	201	CDL	CB2-OB2-PB2-OB4
50	I	201	CDL	CB3-OB5-PB2-OB4
50	a	201	CDL	CA3-OA5-PA1-OA4
50	a	201	CDL	CB2-OB2-PB2-OB4
50	a	201	CDL	CB3-OB5-PB2-OB3
50	l	701	CDL	CA2-OA2-PA1-OA3
50	l	701	CDL	CA3-OA5-PA1-OA4
50	l	702	CDL	CA2-OA2-PA1-OA3
50	l	702	CDL	CA2-OA2-PA1-OA4
50	r	504	CDL	CB2-OB2-PB2-OB4
54	N	201	PLX	C2-O1-P1-O3
54	r	502	PLX	C2-O1-P1-O3
57	w	401	ADP	C5'-O5'-PA-O1A
48	s	401	PEE	C30-C31-C32-C33
48	B	303	PEE	O3P-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	l	703	PEE	O3P-C1-C2-C3
54	j	201	PLX	O4-C3-C4-C5
50	r	504	CDL	C64-C65-C66-C67
48	C	302	PEE	C13-C14-C15-C16
48	B	303	PEE	C19-C20-C21-C22
48	m	201	PEE	C15-C16-C17-C18
50	r	504	CDL	C44-C45-C46-C47
50	I	201	CDL	CA2-C1-CB2-OB2
50	l	702	CDL	CA2-C1-CB2-OB2
50	l	702	CDL	C40-C41-C42-C43
50	r	504	CDL	OB5-CB3-CB4-OB6
54	g	201	PLX	O4-C3-C4-O6
50	a	201	CDL	C22-C23-C24-C25
50	i	401	CDL	C35-C36-C37-C38
50	r	504	CDL	C14-C15-C16-C17
50	I	201	CDL	OA9-CA7-OA8-CA6
46	A	502	FMN	C1'-C2'-C3'-C4'
48	Q	501	PEE	O2-C2-C3-O3
54	g	201	PLX	O6-C4-C5-O8
54	j	201	PLX	O6-C4-C5-O8
54	a	202	PLX	C19-C20-C21-C22
54	a	202	PLX	C27-C28-C29-C30
54	r	503	PLX	O9-C24-C25-C26
50	l	702	CDL	C33-C34-C35-C36
47	A	503	NAI	O4D-C1D-N1N-C2N
48	B	303	PEE	C32-C33-C34-C35
48	r	501	PEE	C33-C34-C35-C36
50	r	504	CDL	C80-C81-C82-C83
54	r	503	PLX	C20-C21-C22-C23
50	r	504	CDL	CB4-CB3-OB5-PB2
50	r	504	CDL	C11-C12-C13-C14
50	I	201	CDL	OB5-CB3-CB4-OB6
50	l	701	CDL	OA5-CA3-CA4-OA6
50	l	702	CDL	C20-C21-C22-C23
50	a	201	CDL	C36-C37-C38-C39
48	m	201	PEE	O3-C30-C31-C32
50	a	201	CDL	C44-C45-C46-C47
46	A	502	FMN	O2'-C2'-C3'-O3'
48	l	703	PEE	C13-C14-C15-C16
48	B	303	PEE	C1-O3P-P-O4P
50	i	401	CDL	CB3-OB5-PB2-OB2
50	l	701	CDL	CB3-OB5-PB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	a	202	PLX	C2-O1-P1-O4
54	g	201	PLX	C3-O4-P1-O1
54	r	503	PLX	C3-O4-P1-O1
54	r	502	PLX	C15-C16-C17-C18
49	G	201	8Q1	C6-C7-C8-C9
49	G	201	8Q1	C30-C29-C32-O33
50	l	702	CDL	C12-C13-C14-C15
48	C	302	PEE	C38-C39-C40-C41
48	l	704	PEE	C18-C19-C20-C21
54	N	201	PLX	C11-C10-C9-C8
54	r	503	PLX	C9-C10-C11-C12
54	r	503	PLX	C29-C30-C31-C32
50	r	504	CDL	C31-C32-C33-C34
48	s	401	PEE	C12-C13-C14-C15
48	l	703	PEE	C33-C34-C35-C36
48	r	501	PEE	C31-C30-O3-C3
50	r	504	CDL	C20-C21-C22-C23
48	r	501	PEE	C38-C39-C40-C41
54	j	201	PLX	C34-C35-C36-C37
48	r	501	PEE	O5-C30-O3-C3
48	C	302	PEE	C39-C40-C41-C42
48	m	201	PEE	C14-C15-C16-C17
48	l	703	PEE	C39-C40-C41-C42
54	r	503	PLX	C24-C25-C26-C27
50	a	201	CDL	C43-C44-C45-C46
54	j	201	PLX	O6-C6-C7-C8
54	r	502	PLX	O8-C24-C25-C26
50	r	504	CDL	C37-C38-C39-C40
50	i	401	CDL	CA4-CA3-OA5-PA1
51	J	401	NDP	O4D-C1D-N1N-C6N
48	B	303	PEE	C30-C31-C32-C33
50	a	201	CDL	C34-C35-C36-C37
48	C	302	PEE	C1-C2-C3-O3
50	a	201	CDL	C53-C54-C55-C56
54	a	202	PLX	C14-C15-C16-C17
54	r	503	PLX	C30-C31-C32-C33
48	l	703	PEE	C3-C2-O2-C10
54	r	503	PLX	C19-C20-C21-C22
50	a	201	CDL	C32-C31-CA7-OA8
47	A	503	NAI	C2D-C1D-N1N-C6N
50	r	504	CDL	C1-CB2-OB2-PB2
50	a	201	CDL	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
50	l	701	CDL	OA5-CA3-CA4-CA6
50	r	504	CDL	OB5-CB3-CB4-CB6
48	B	303	PEE	C16-C17-C18-C19
48	m	201	PEE	C18-C19-C20-C21
54	N	201	PLX	C31-C32-C33-C34
48	B	303	PEE	C13-C14-C15-C16
49	G	201	8Q1	C42-C43-S44-C1
50	I	201	CDL	OB6-CB4-CB6-OB8
50	l	702	CDL	C43-C44-C45-C46
50	a	201	CDL	C18-C19-C20-C21
50	a	201	CDL	C23-C24-C25-C26
50	i	401	CDL	C12-C13-C14-C15
48	m	201	PEE	C16-C17-C18-C19
49	G	201	8Q1	C10-C11-C12-C13
54	j	201	PLX	C18-C19-C20-C21
48	C	302	PEE	C20-C21-C22-C23
54	r	502	PLX	C26-C27-C28-C29
48	s	401	PEE	C15-C16-C17-C18
48	l	703	PEE	C36-C37-C38-C39
54	a	202	PLX	O8-C24-C25-C26
54	r	503	PLX	O8-C24-C25-C26
48	s	401	PEE	O4P-C4-C5-N
48	Q	501	PEE	C2-C1-O3P-P
50	l	702	CDL	C76-C77-C78-C79
48	l	704	PEE	C34-C35-C36-C37
48	C	302	PEE	C14-C15-C16-C17
48	C	302	PEE	C17-C18-C19-C20
48	r	501	PEE	C39-C40-C41-C42
48	s	401	PEE	C44-C45-C46-C47
48	Q	501	PEE	C36-C37-C38-C39
48	Q	501	PEE	C38-C39-C40-C41
48	l	703	PEE	C1-C2-O2-C10
47	A	503	NAI	O4D-C1D-N1N-C6N
48	l	703	PEE	C10-C11-C12-C13
54	N	201	PLX	C18-C19-C20-C21
50	a	201	CDL	C74-C75-C76-C77
48	B	303	PEE	C18-C19-C20-C21
48	s	401	PEE	C16-C17-C18-C19
48	C	302	PEE	C19-C20-C21-C22
48	Q	501	PEE	C1-C2-C3-O3
54	g	201	PLX	C7-C6-O6-C4
54	j	201	PLX	C7-C6-O6-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
50	r	504	CDL	OA9-CA7-OA8-CA6
54	r	502	PLX	C10-C11-C12-C13
48	s	401	PEE	O2-C10-C11-C12
48	s	401	PEE	C31-C32-C33-C34
50	r	504	CDL	C31-CA7-OA8-CA6
48	B	303	PEE	C12-C13-C14-C15
54	r	503	PLX	C35-C36-C37-C38
48	C	302	PEE	O3-C30-C31-C32
48	C	302	PEE	C36-C37-C38-C39
50	I	201	CDL	C12-C11-CA5-OA6
50	r	504	CDL	C52-C51-CB5-OB6
51	J	401	NDP	C2B-O2B-P2B-O2X
50	I	201	CDL	C12-C13-C14-C15
49	G	201	8Q1	C9-C10-C11-C12
50	l	701	CDL	C51-C52-C53-C54
48	B	303	PEE	C36-C37-C38-C39
48	s	401	PEE	O4-C10-C11-C12
50	l	702	CDL	C38-C39-C40-C41
48	l	703	PEE	C18-C19-C20-C21
48	l	704	PEE	C16-C17-C18-C19
50	i	401	CDL	CA3-CA4-CA6-OA8
50	a	201	CDL	C13-C14-C15-C16
50	l	701	CDL	C23-C24-C25-C26
48	m	201	PEE	C23-C24-C25-C26
47	A	503	NAI	C2N-C3N-C7N-N7N
48	Q	501	PEE	C1-O3P-P-O1P
48	m	201	PEE	C1-O3P-P-O1P
50	I	201	CDL	CA3-OA5-PA1-OA3
50	i	401	CDL	CB3-OB5-PB2-OB3
50	l	701	CDL	CB3-OB5-PB2-OB3
51	J	401	NDP	C5B-O5B-PA-O1A
51	J	401	NDP	O4B-C4B-C5B-O5B
50	I	201	CDL	C12-C11-CA5-OA7
50	I	201	CDL	C72-C71-CB7-OB8
54	r	502	PLX	C25-C24-O8-C5
48	l	704	PEE	O3-C30-C31-C32
50	I	201	CDL	C52-C51-CB5-OB6
50	l	701	CDL	C12-C11-CA5-OA6
48	s	401	PEE	C23-C24-C25-C26
54	j	201	PLX	C24-C25-C26-C27
48	Q	501	PEE	C30-C31-C32-C33
48	C	302	PEE	O5-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
50	l	701	CDL	C12-C11-CA5-OA7
50	l	702	CDL	C72-C71-CB7-OB8
48	B	303	PEE	C43-C44-C45-C46
50	l	702	CDL	C32-C31-CA7-OA8
48	l	704	PEE	O5-C30-C31-C32
50	l	702	CDL	C72-C71-CB7-OB9
50	r	504	CDL	C52-C51-CB5-OB7
50	l	702	CDL	C44-C45-C46-C47
50	r	504	CDL	C72-C71-CB7-OB8
48	l	703	PEE	C16-C17-C18-C19
50	a	201	CDL	C72-C71-CB7-OB8

There are no ring outliers.

27 monomers are involved in 104 short contacts:

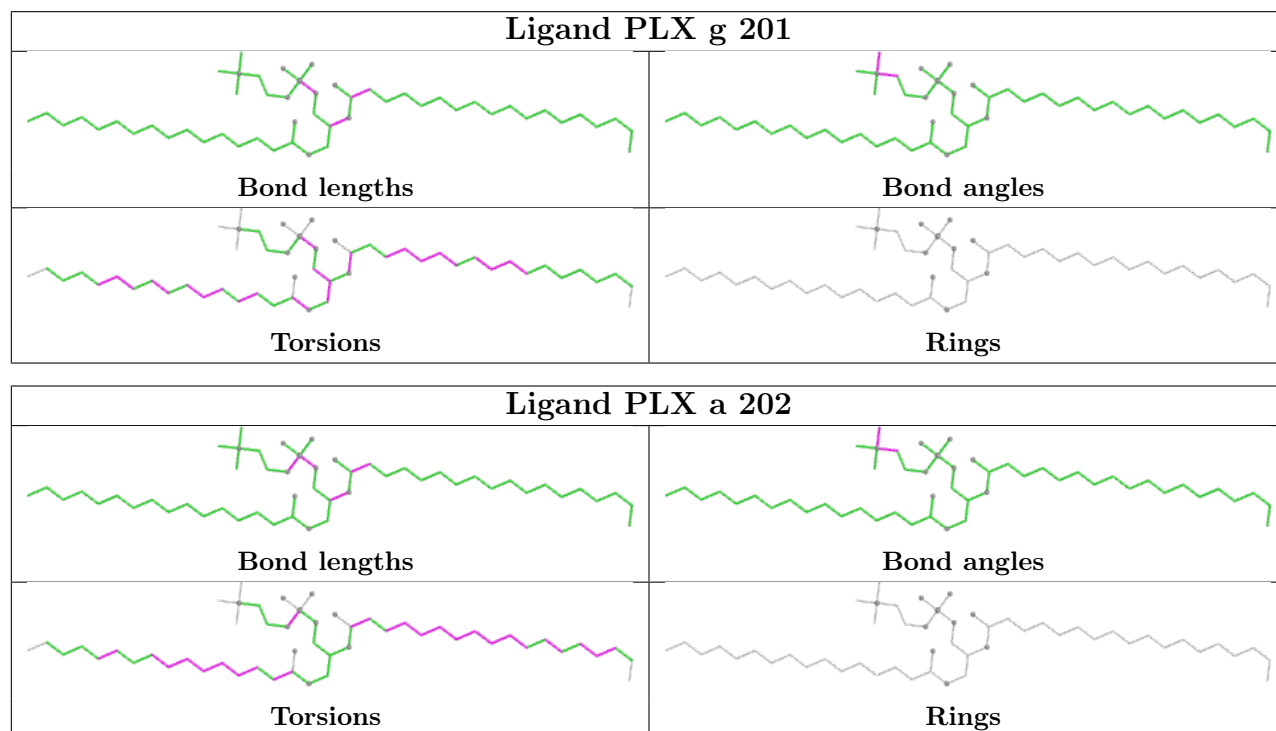
Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	g	201	PLX	6	0
54	a	202	PLX	2	0
48	s	401	PEE	2	0
51	J	401	NDP	4	0
48	l	704	PEE	3	0
50	l	702	CDL	1	0
54	r	503	PLX	14	0
54	N	201	PLX	2	0
46	A	502	FMN	5	0
50	i	401	CDL	4	0
50	l	701	CDL	31	0
56	s	402	UQ	2	0
45	A	501	SF4	1	0
48	m	201	PEE	3	0
57	w	401	ADP	2	0
49	X	201	8Q1	2	0
47	A	503	NAI	5	0
50	r	504	CDL	10	0
48	Q	501	PEE	1	0
50	a	201	CDL	4	0
54	j	201	PLX	3	0
49	G	201	8Q1	1	0
45	C	301	SF4	1	0
48	l	703	PEE	1	0
48	r	501	PEE	3	0
48	C	302	PEE	1	0

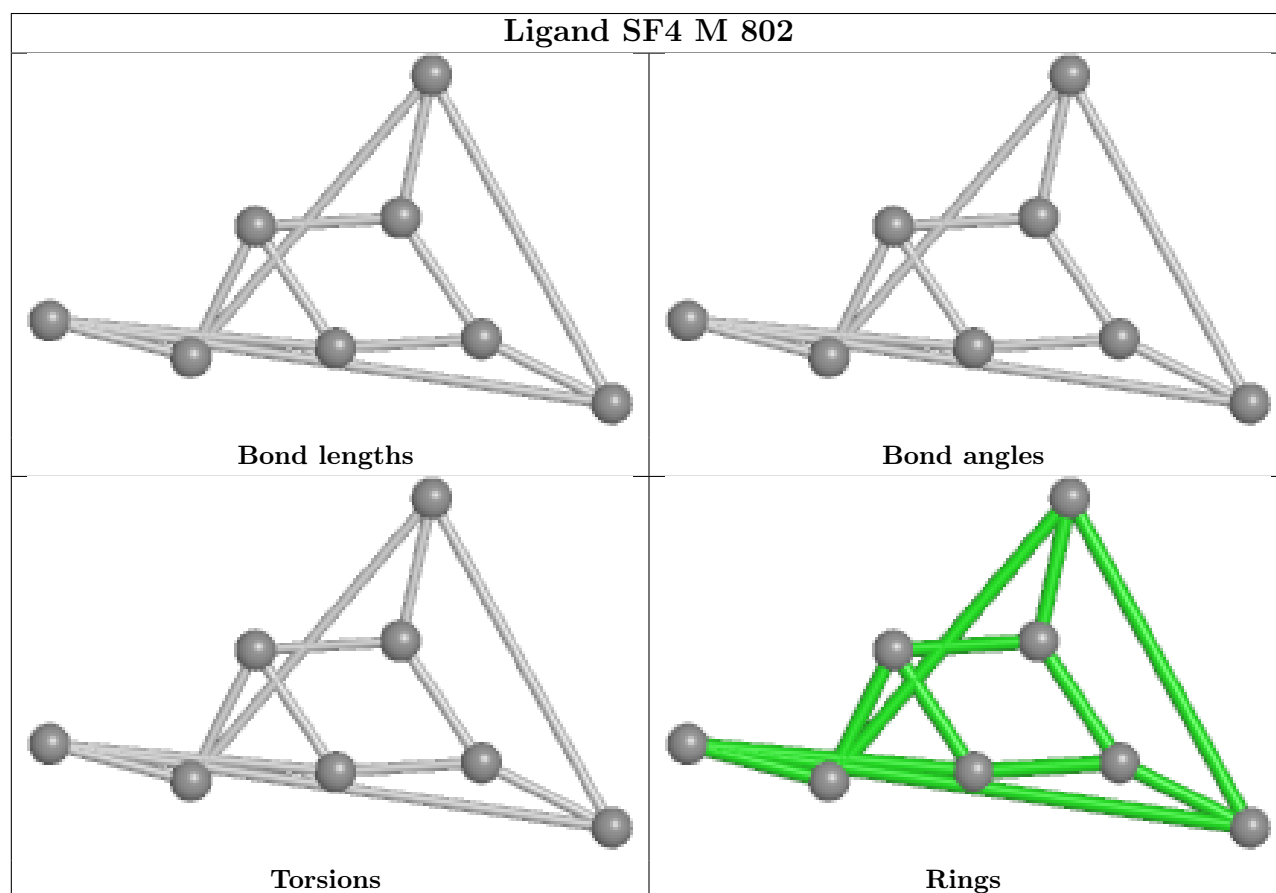
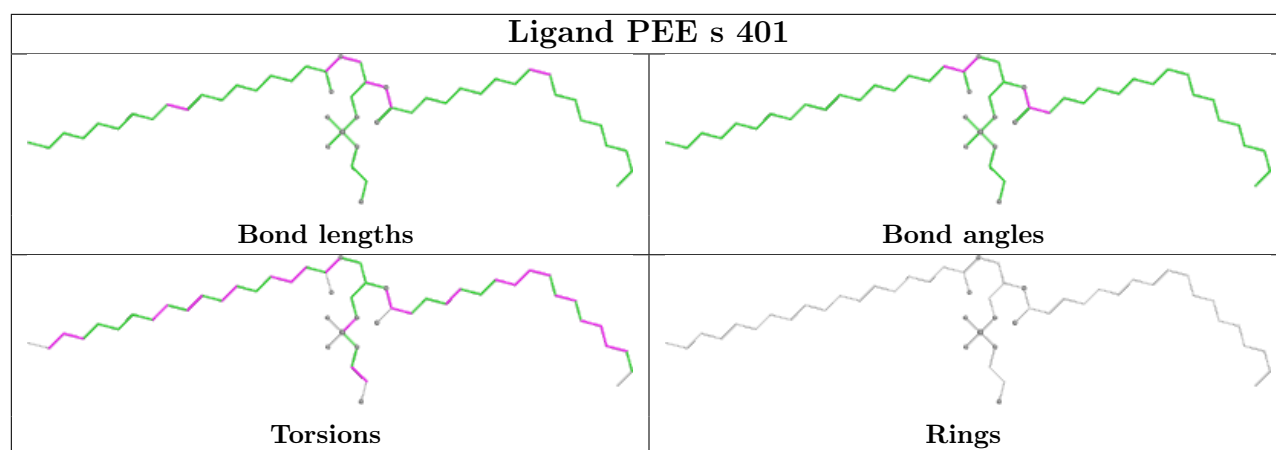
Continued on next page...

Continued from previous page...

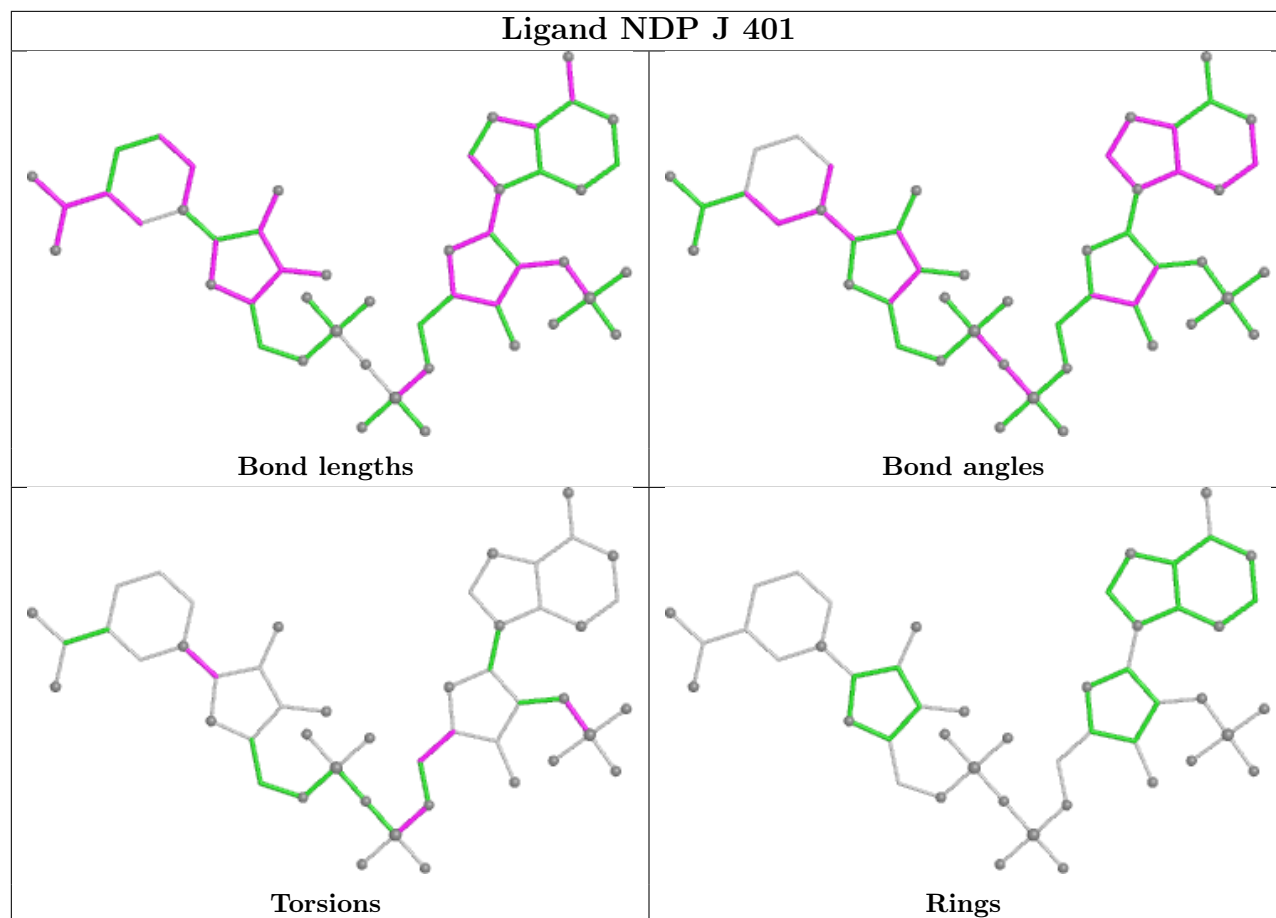
Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	r	502	PLX	4	0

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

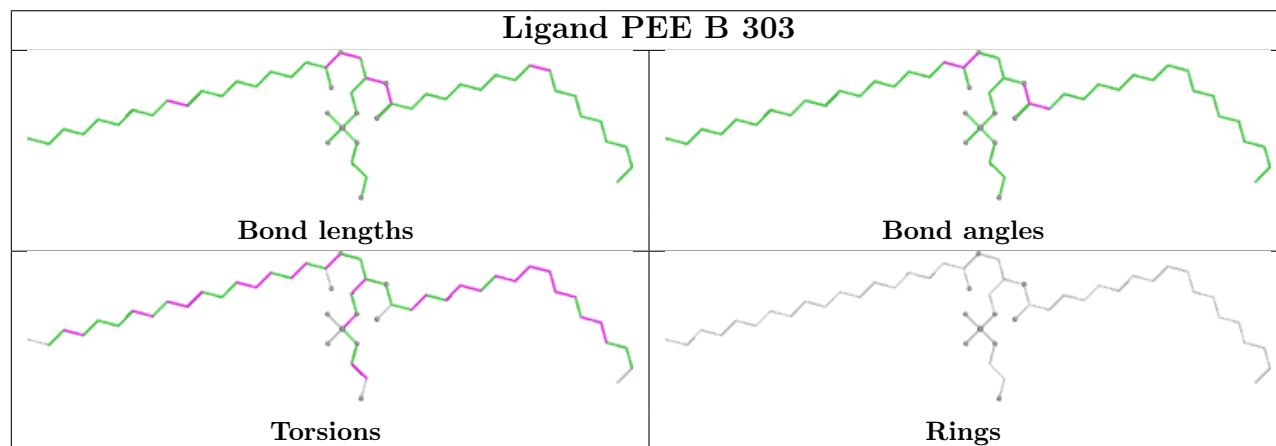


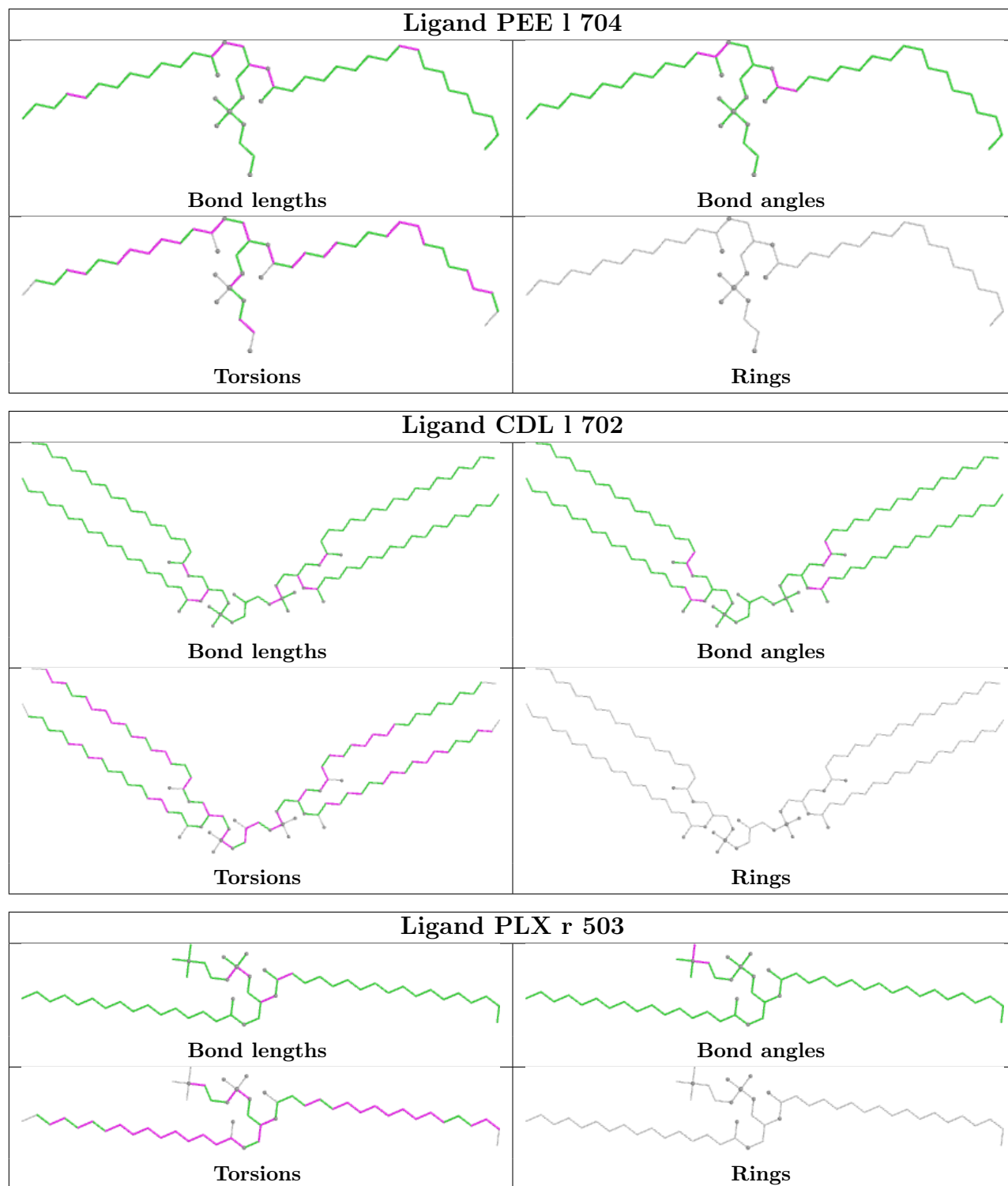


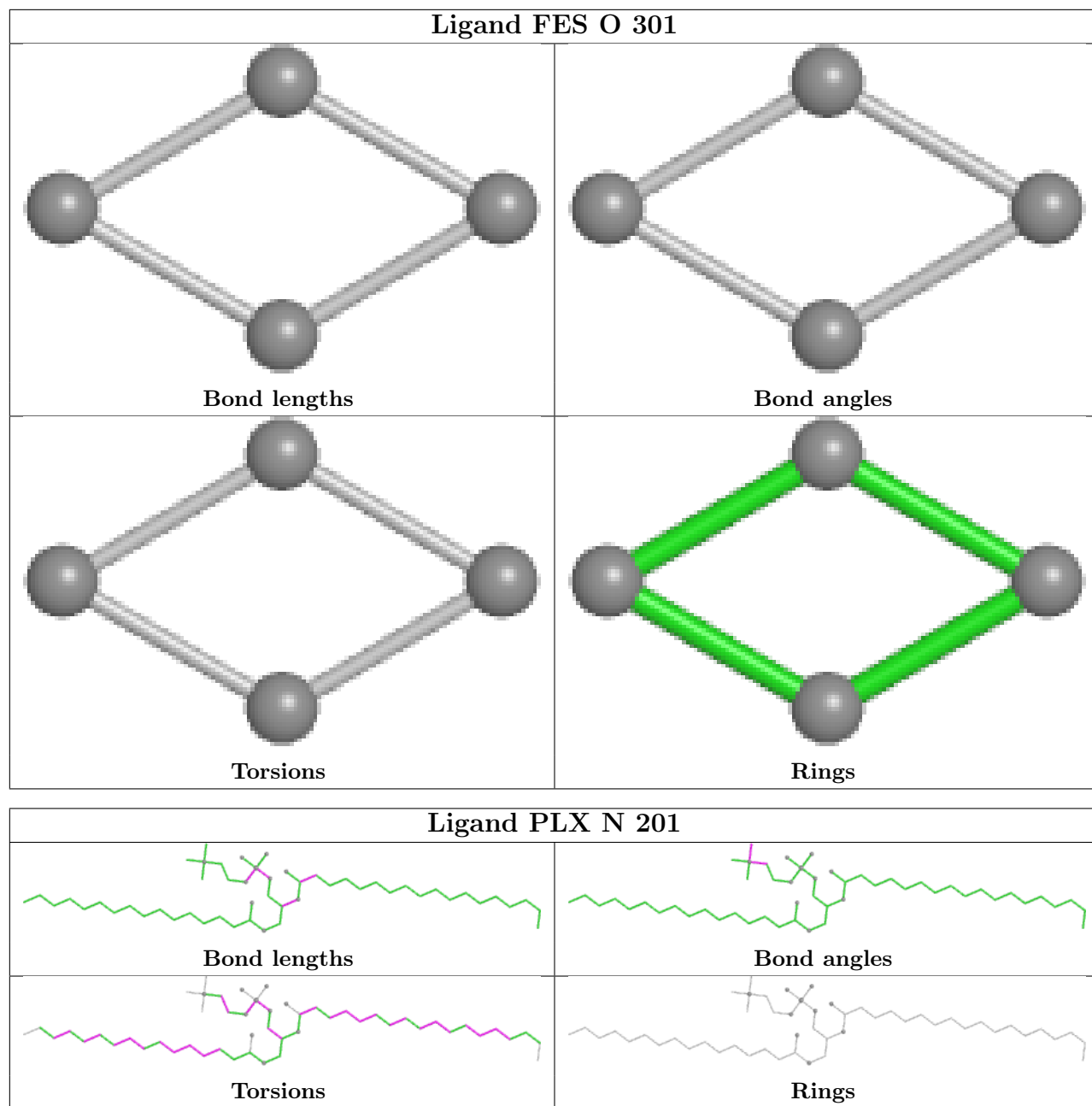
Ligand NDP J 401

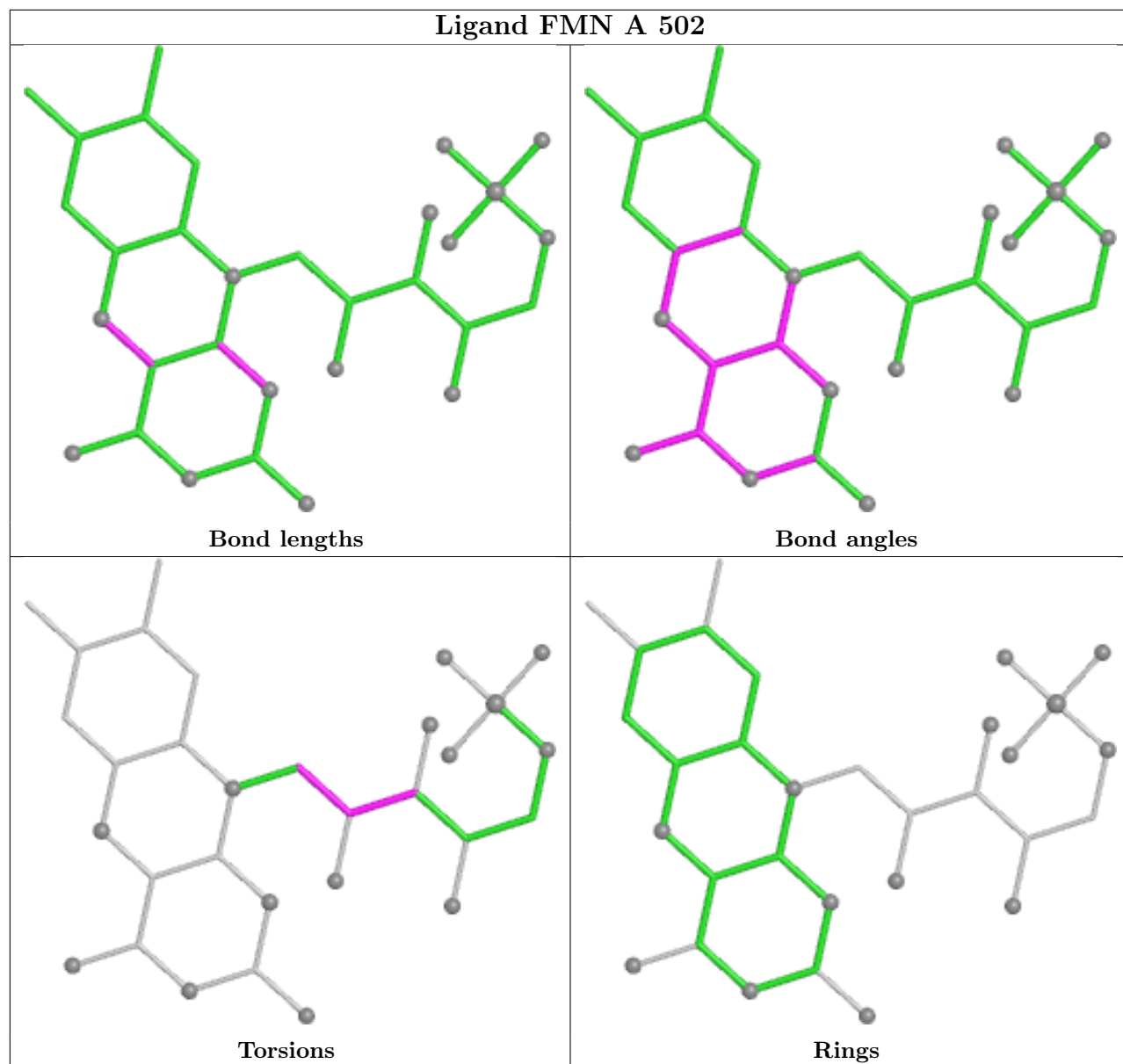


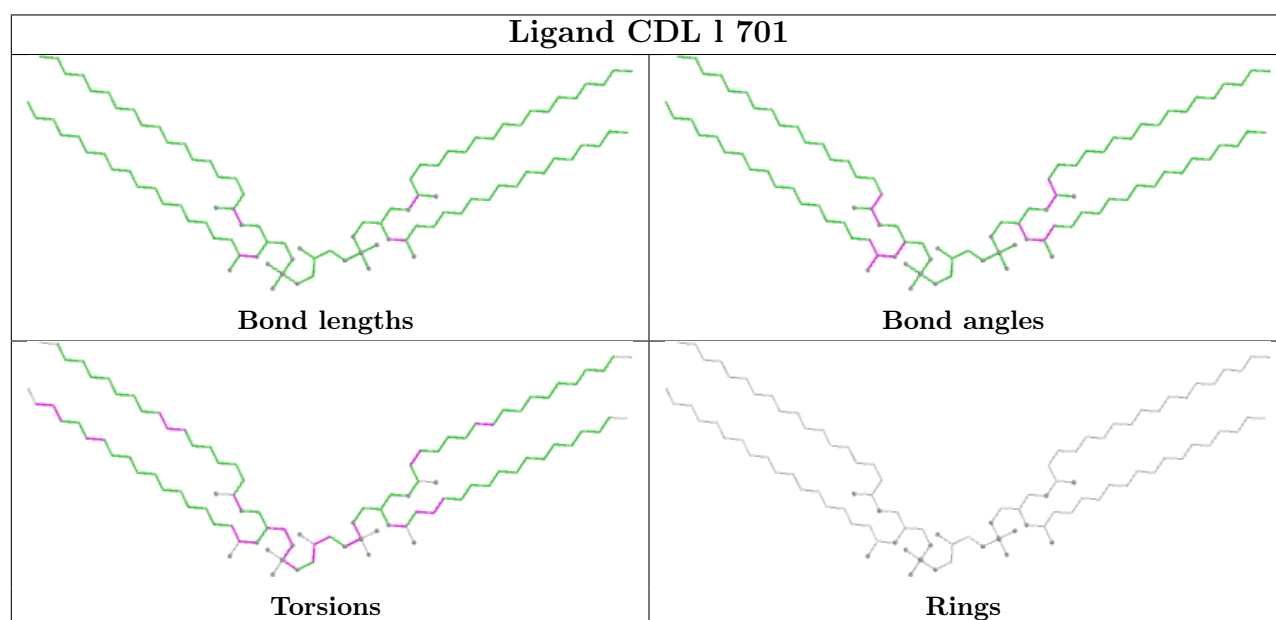
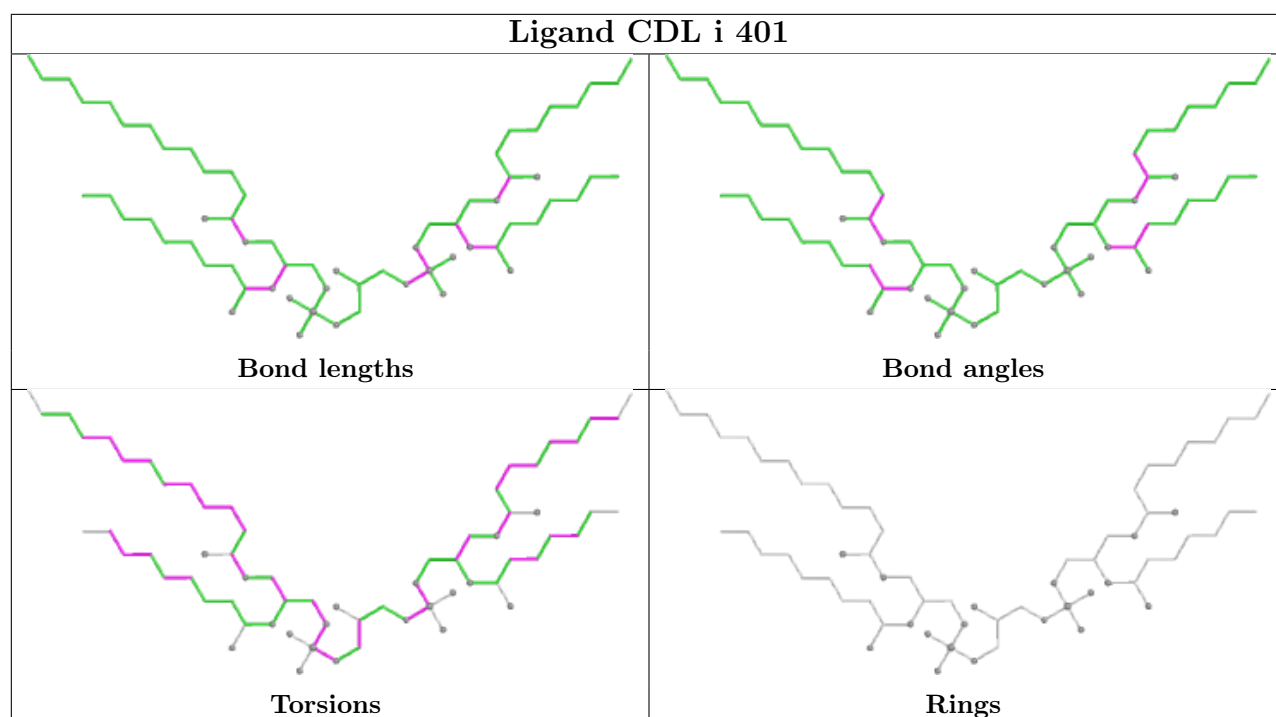
Ligand PEE B 303

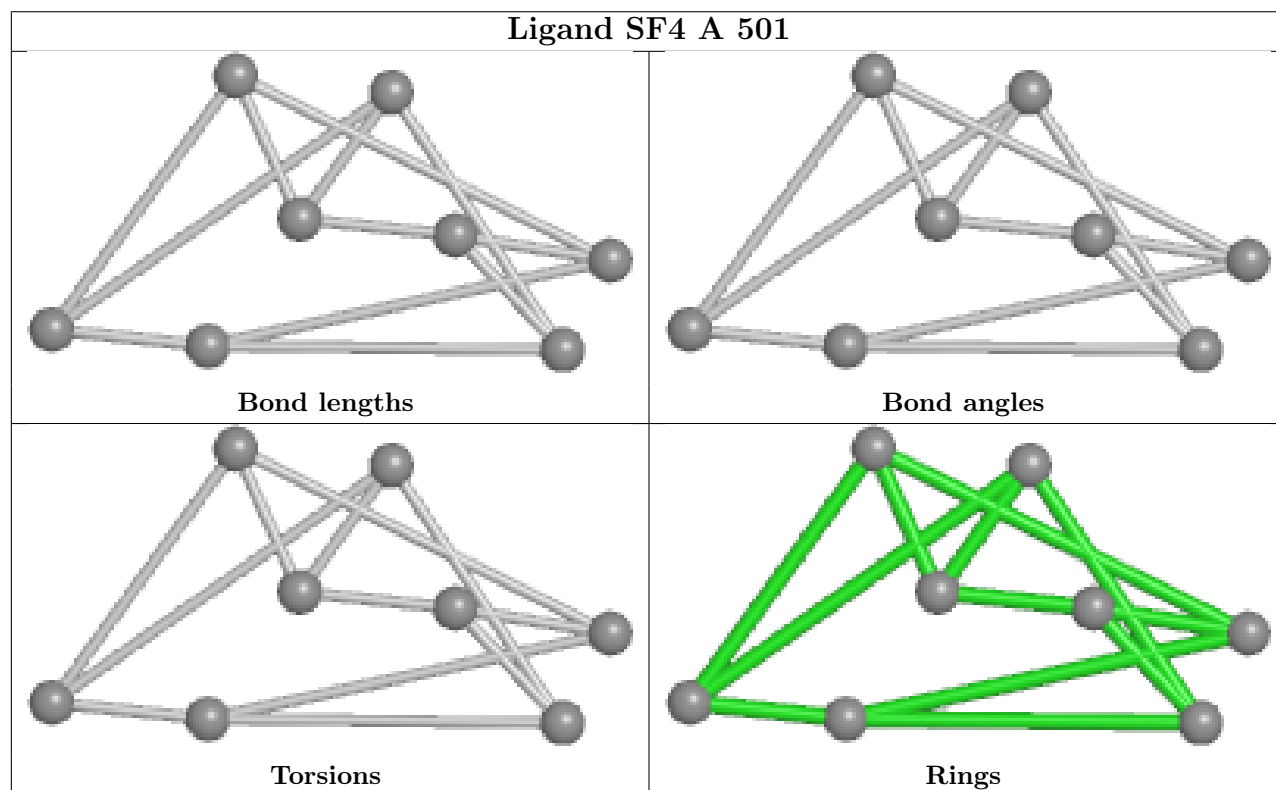
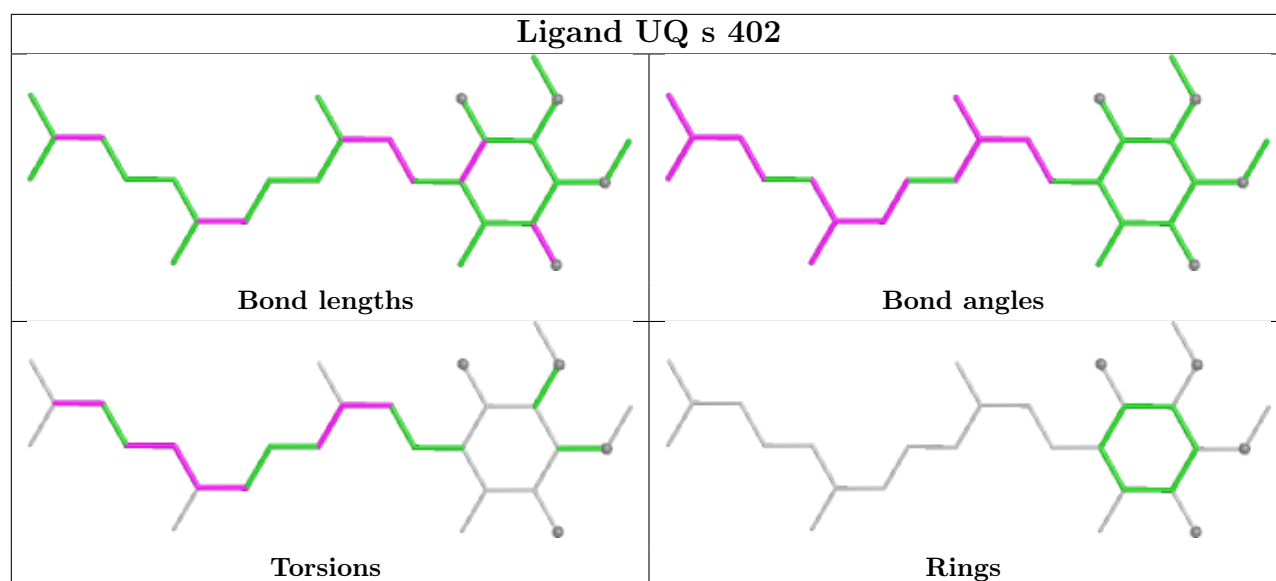


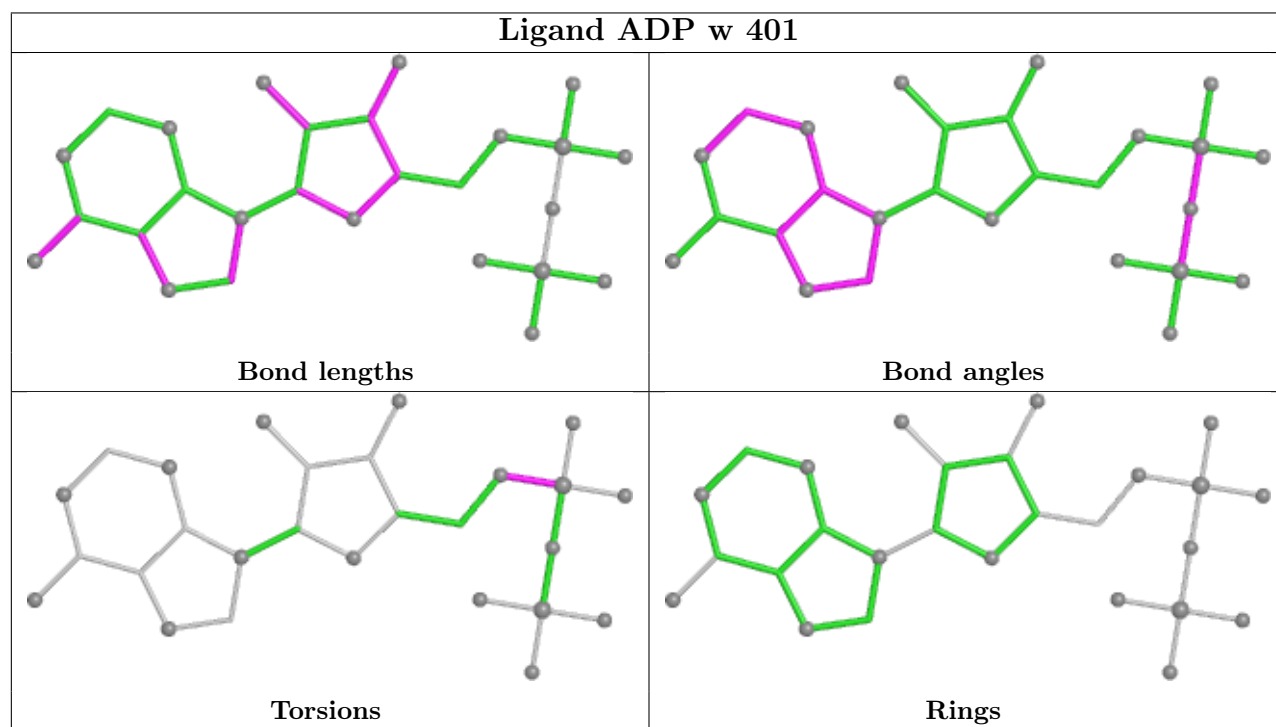
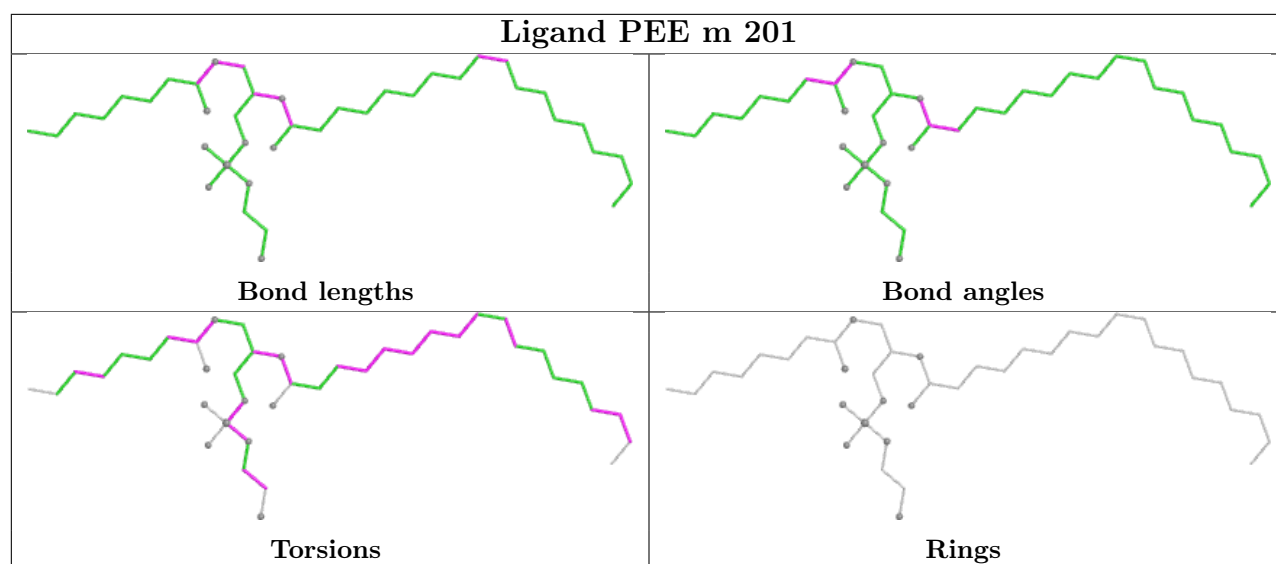


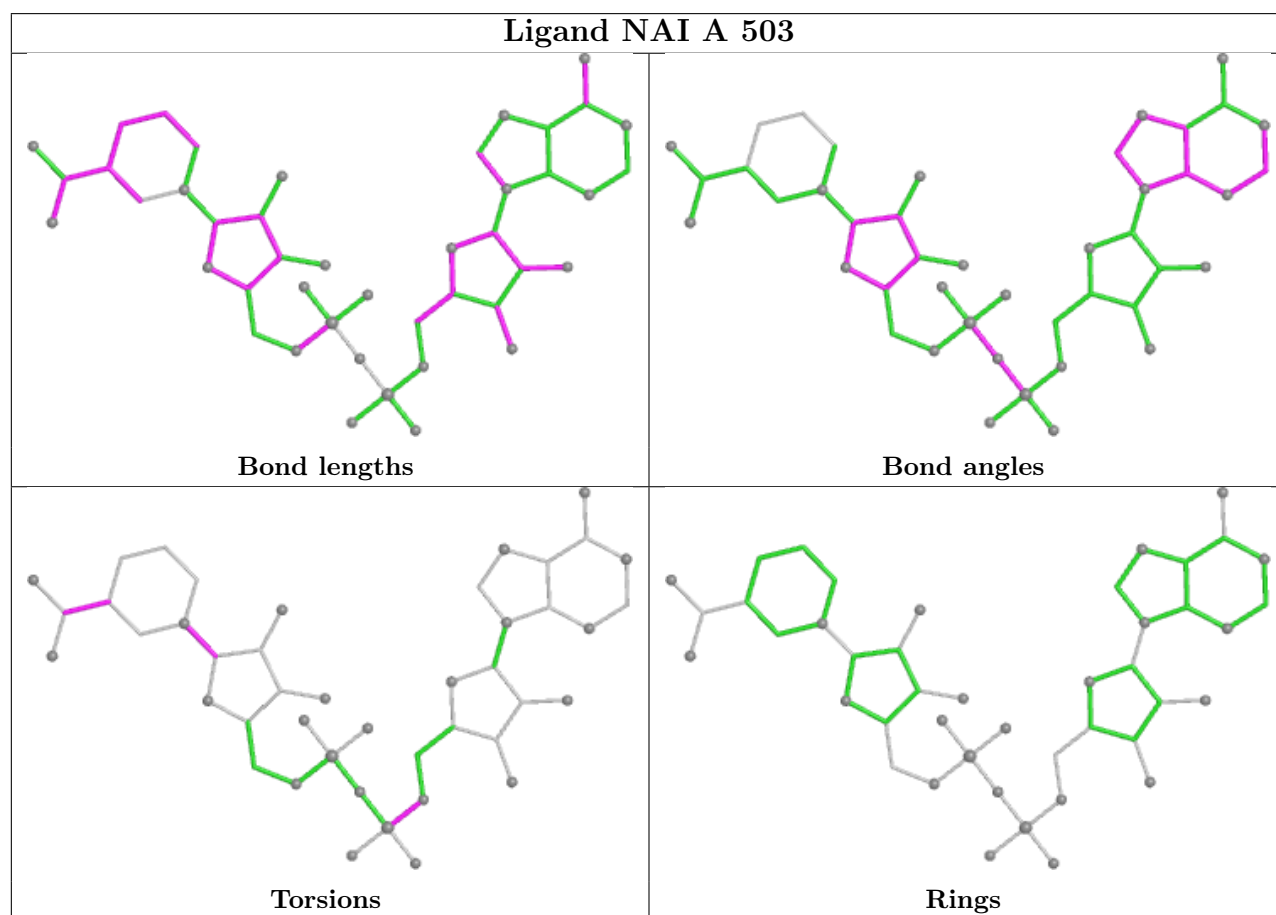
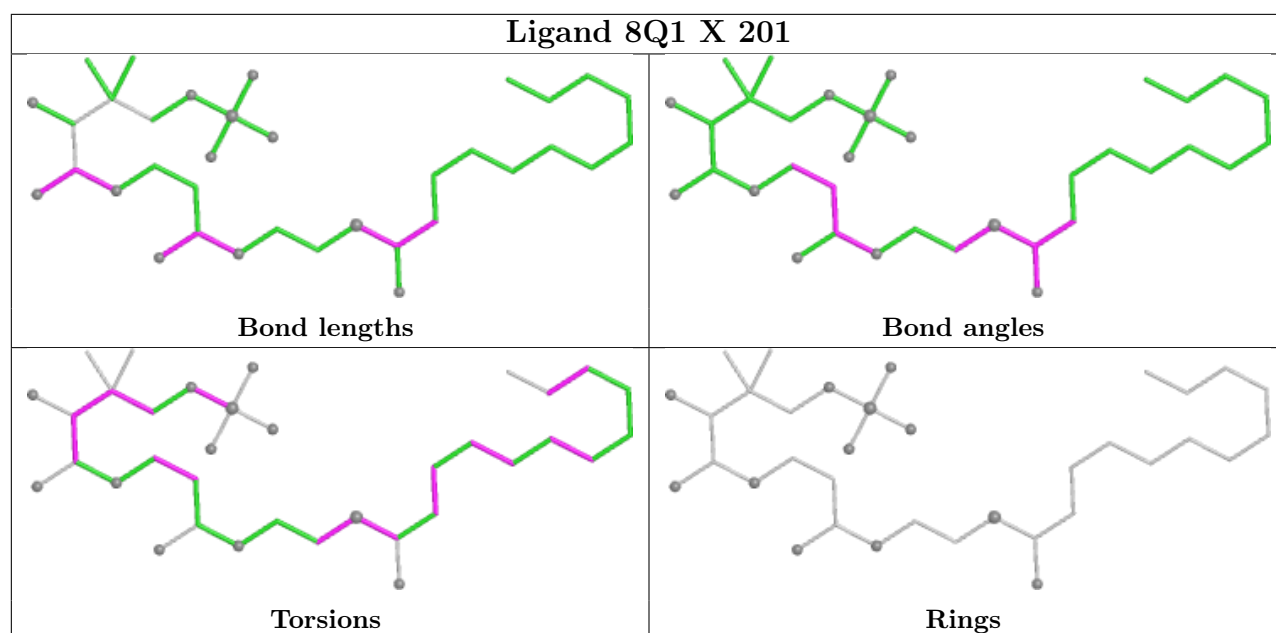


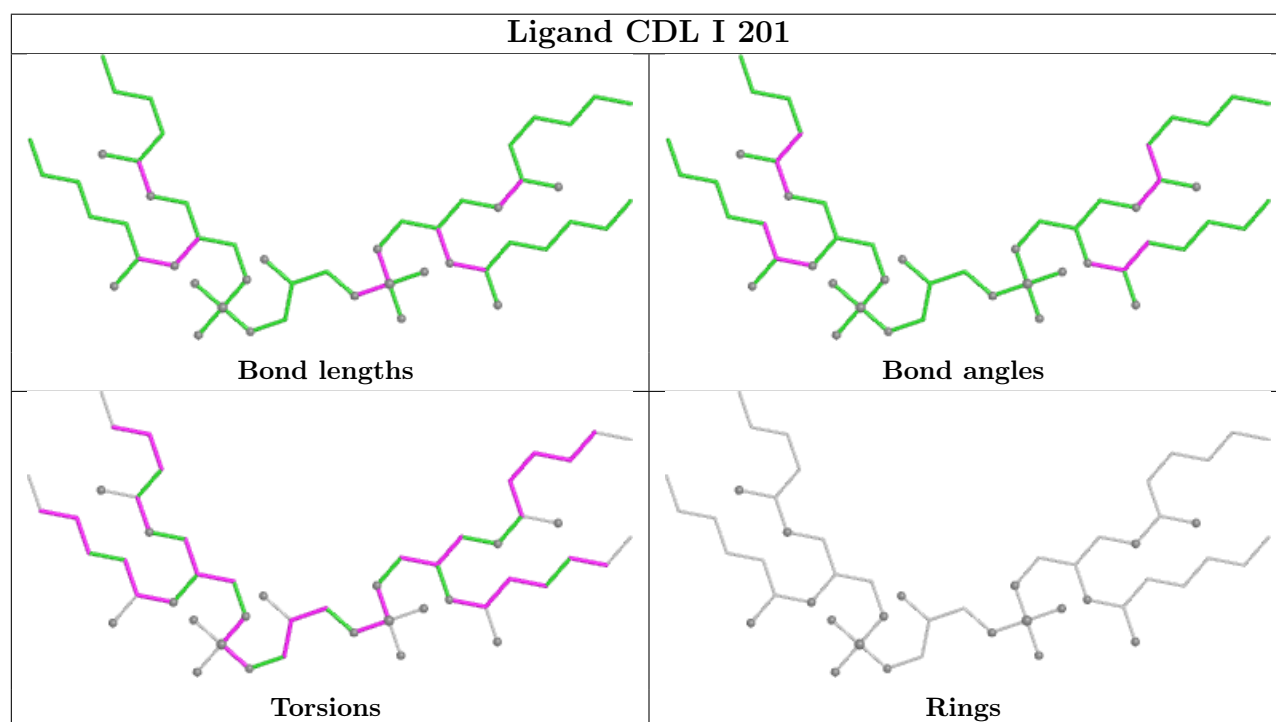
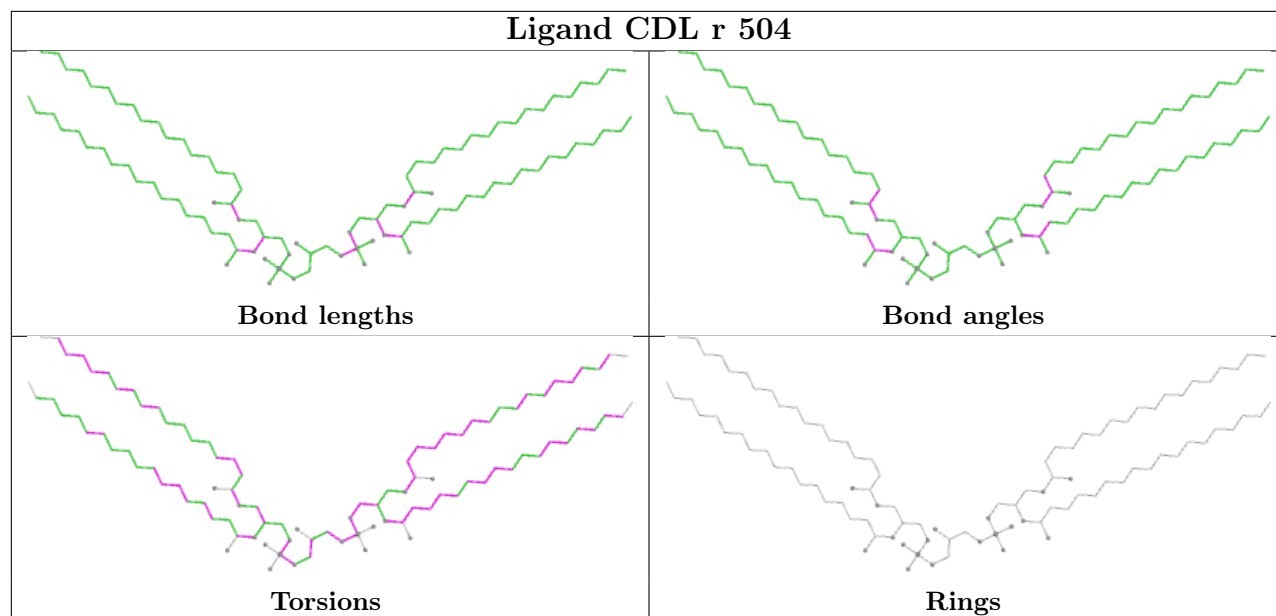


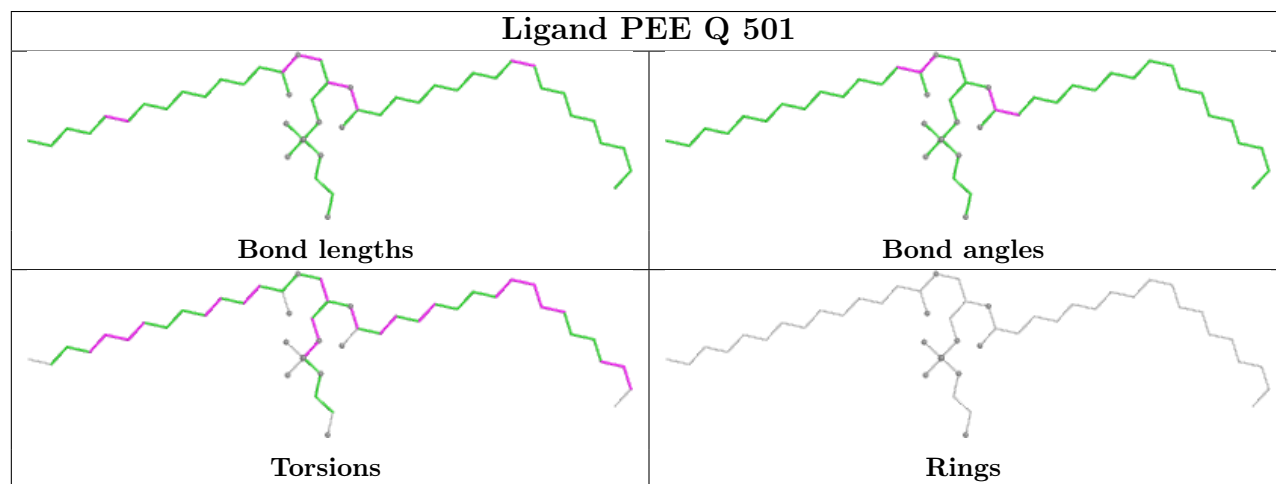
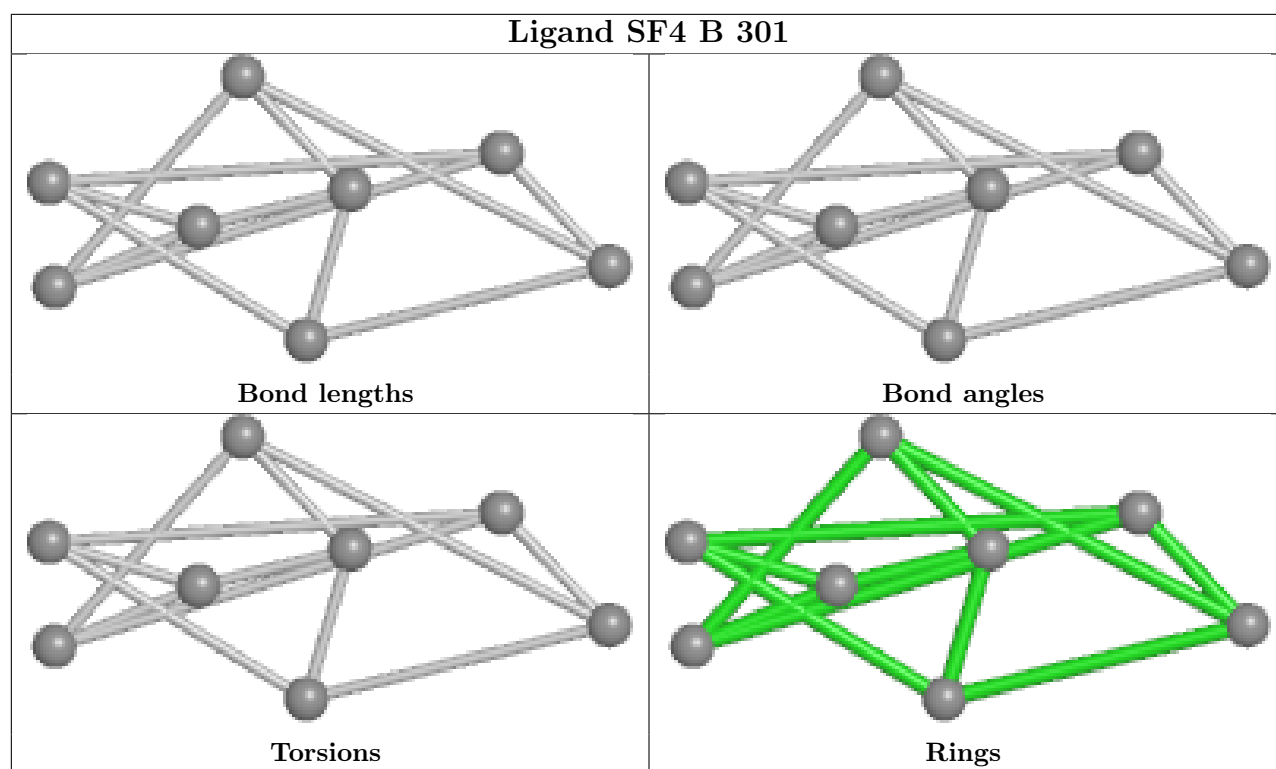


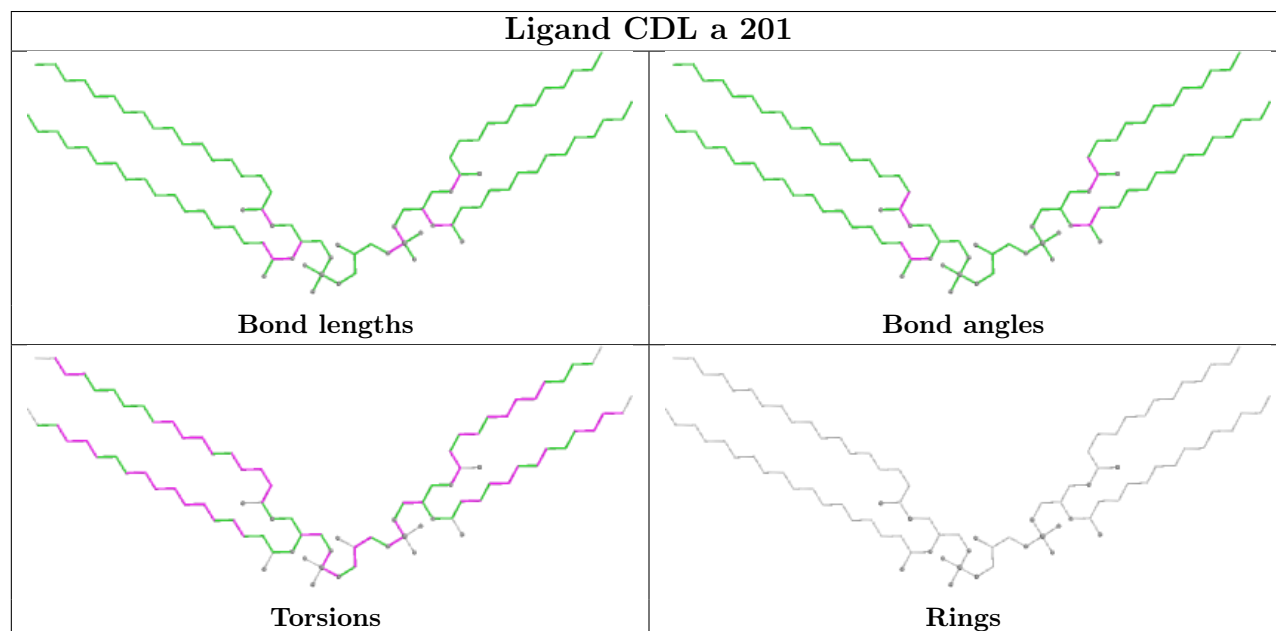
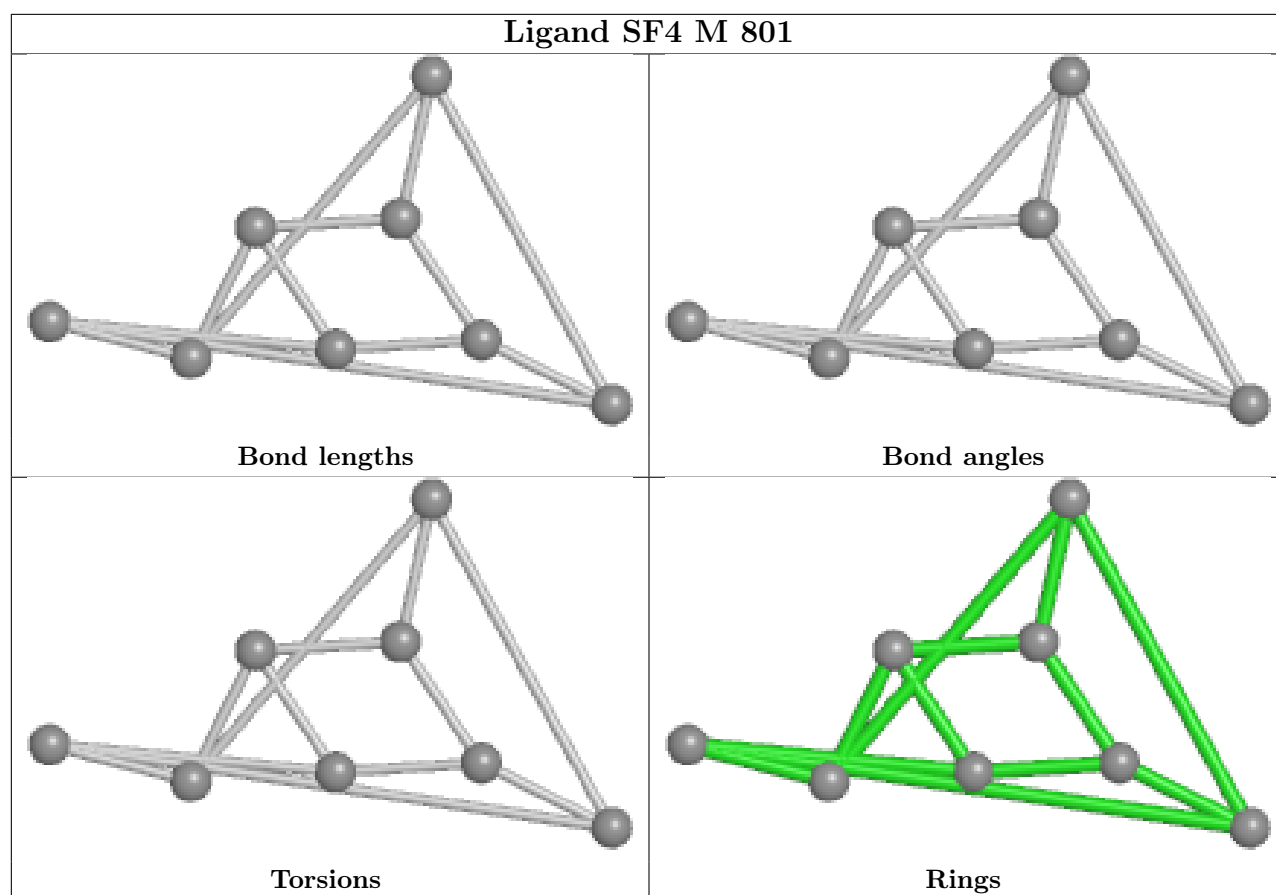


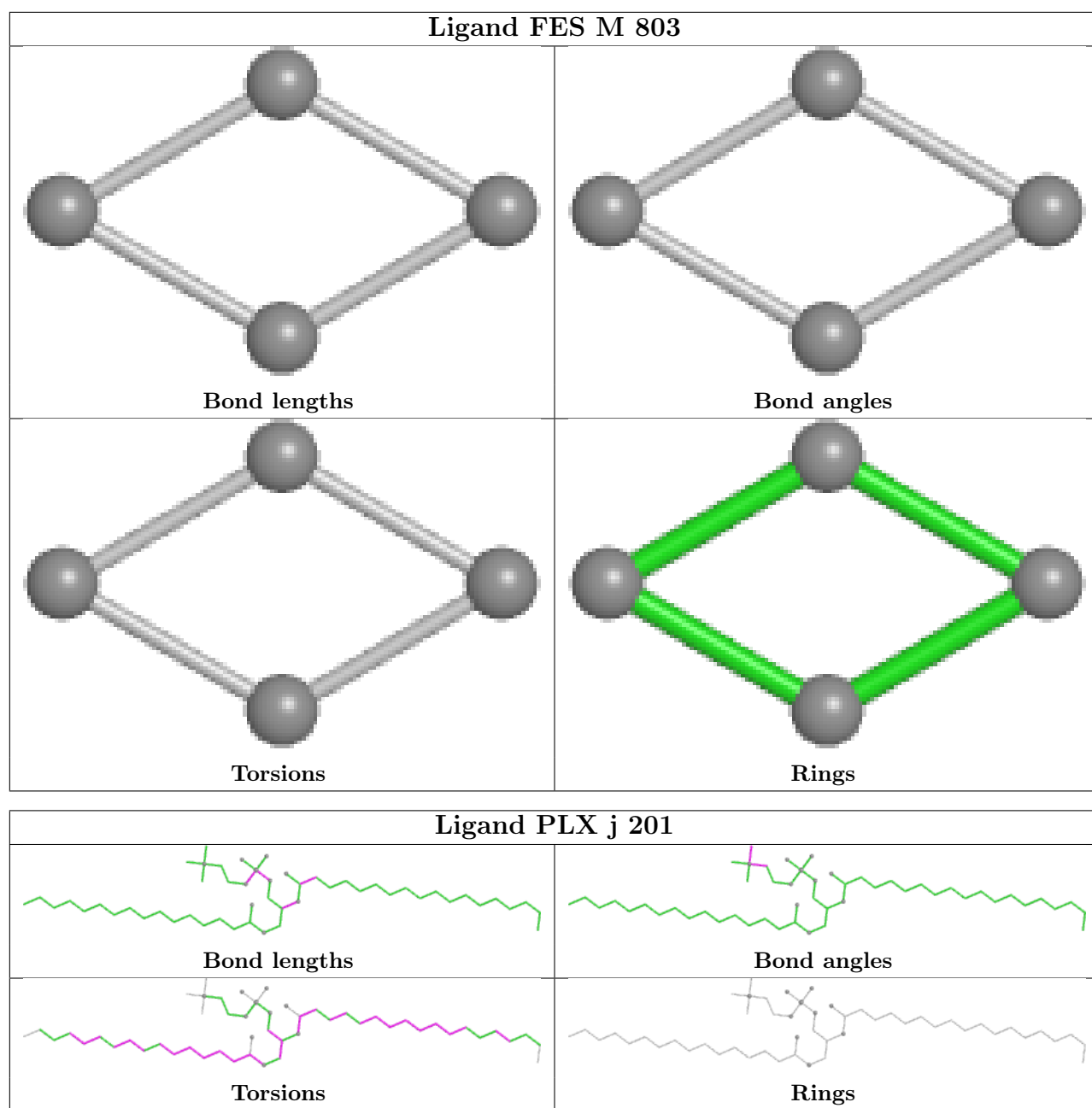




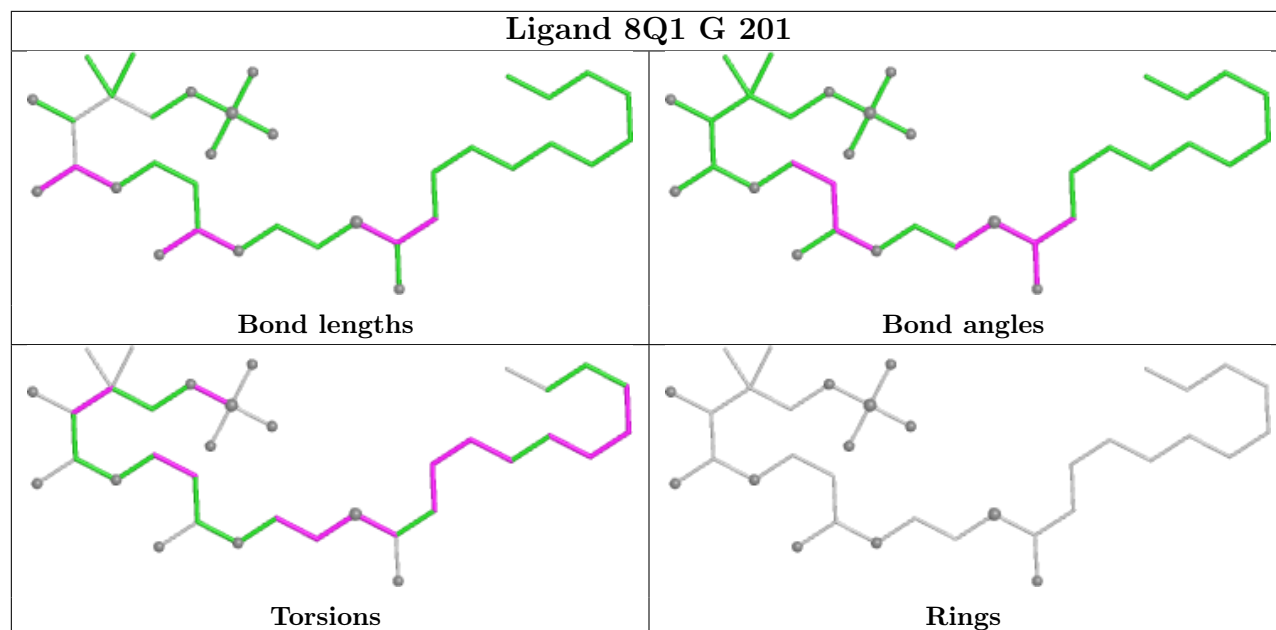




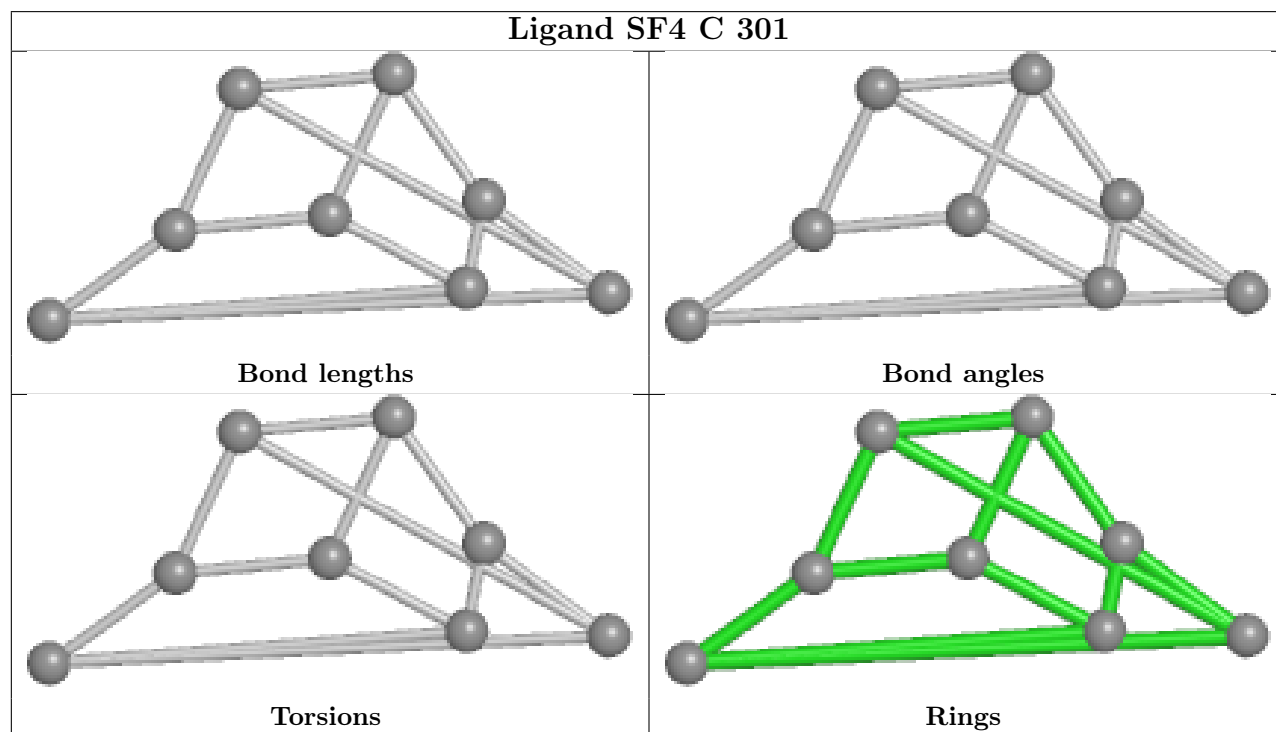


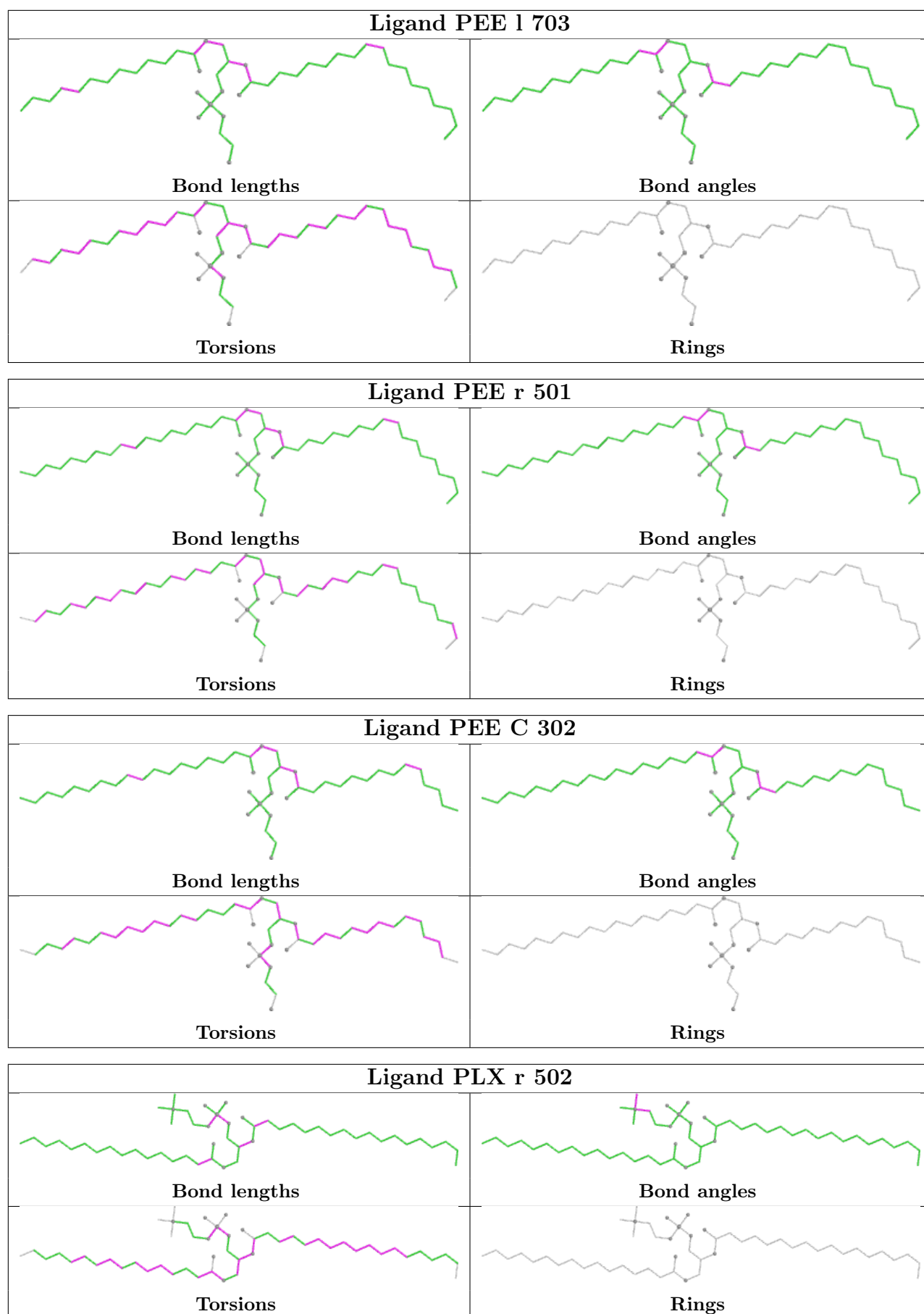


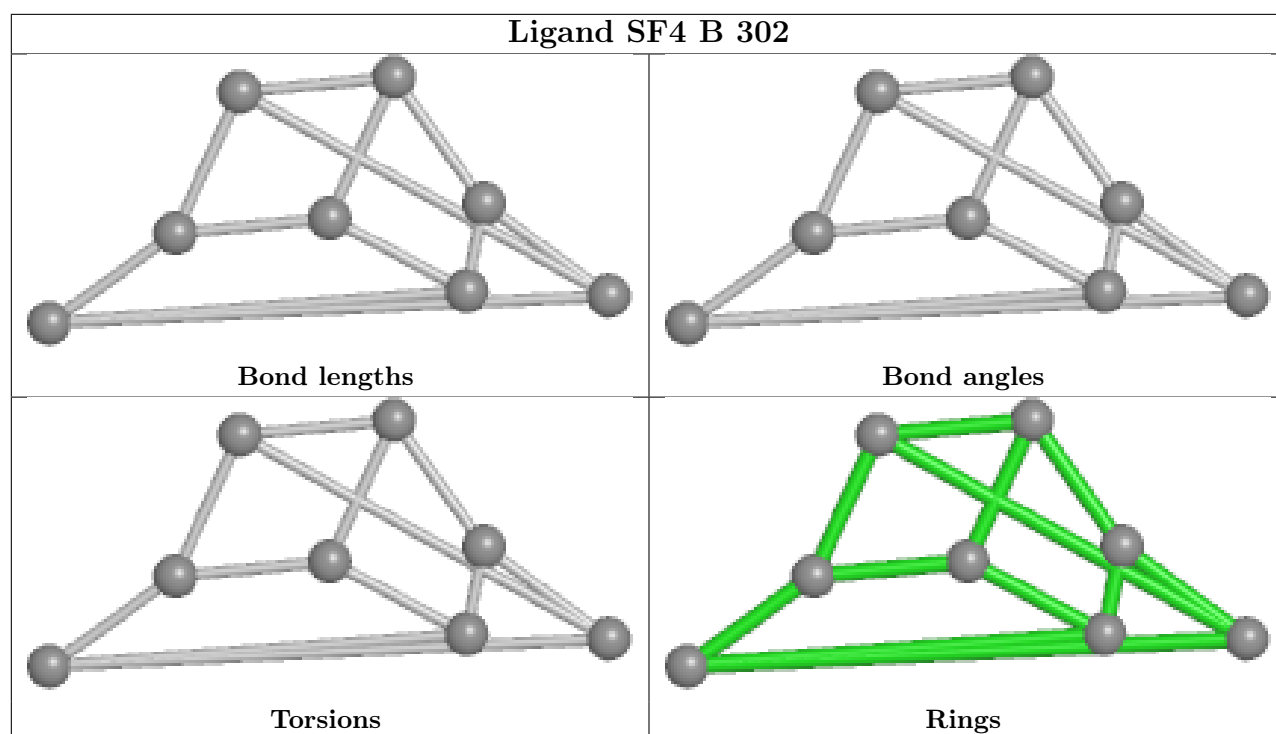
Ligand 8Q1 G 201



Ligand SF4 C 301







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

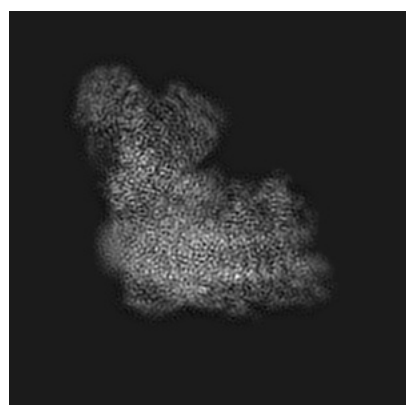
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32312. These allow visual inspection of the internal detail of the map and identification of artifacts.

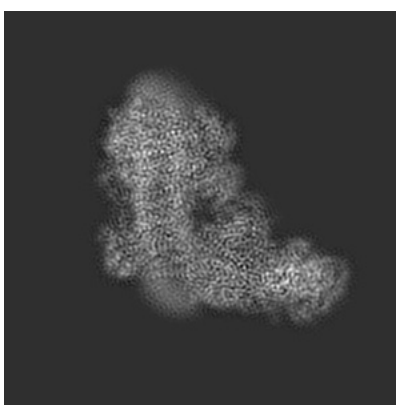
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

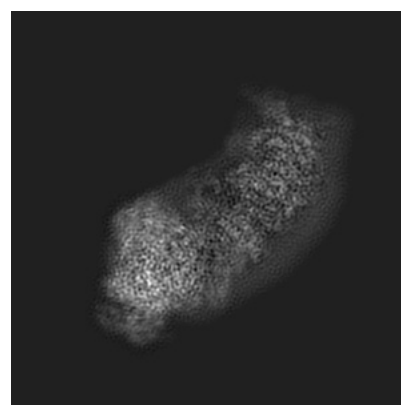
6.1.1 Primary map



X



Y

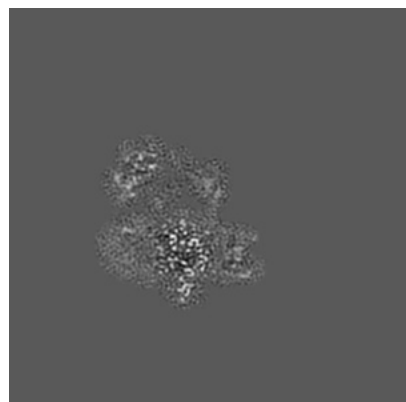


Z

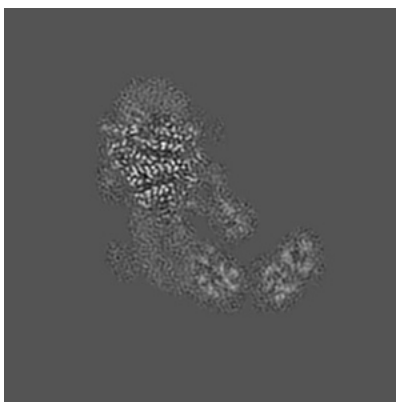
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

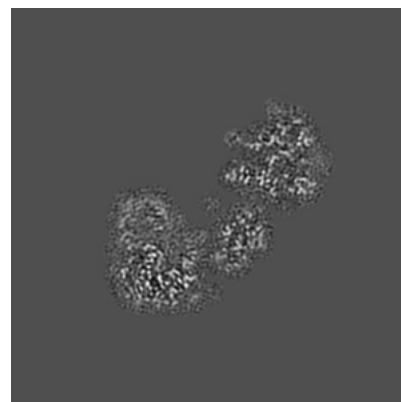
6.2.1 Primary map



X Index: 152



Y Index: 152

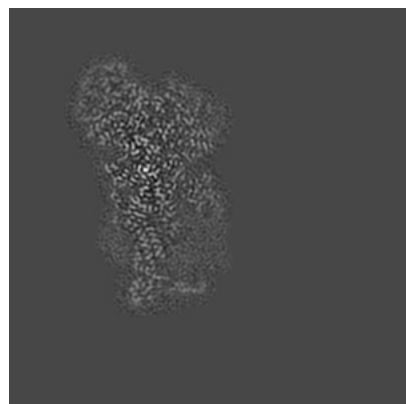


Z Index: 152

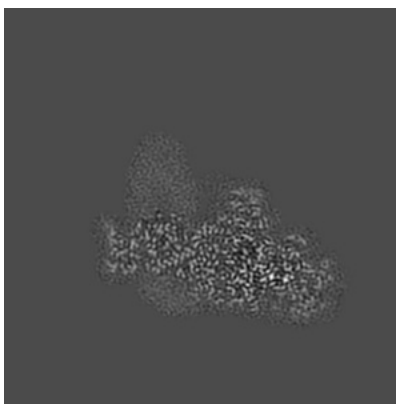
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

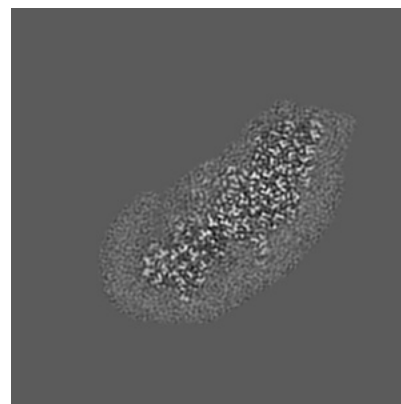
6.3.1 Primary map



X Index: 104



Y Index: 98

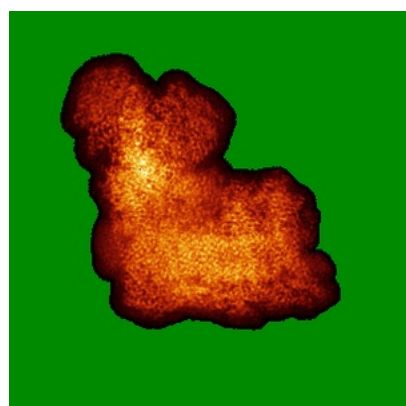


Z Index: 127

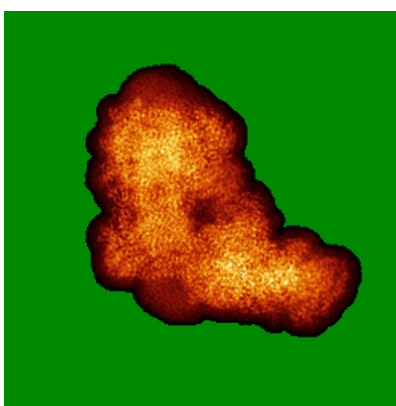
The images above show the largest variance slices of the map in three orthogonal directions.

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

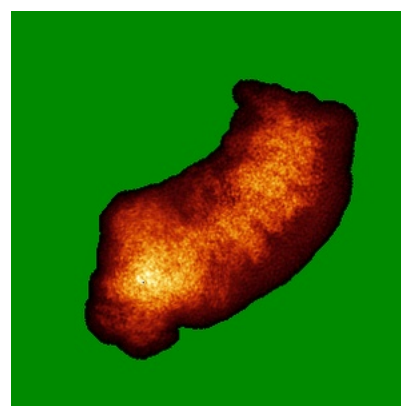
6.4.1 Primary map



X



Y

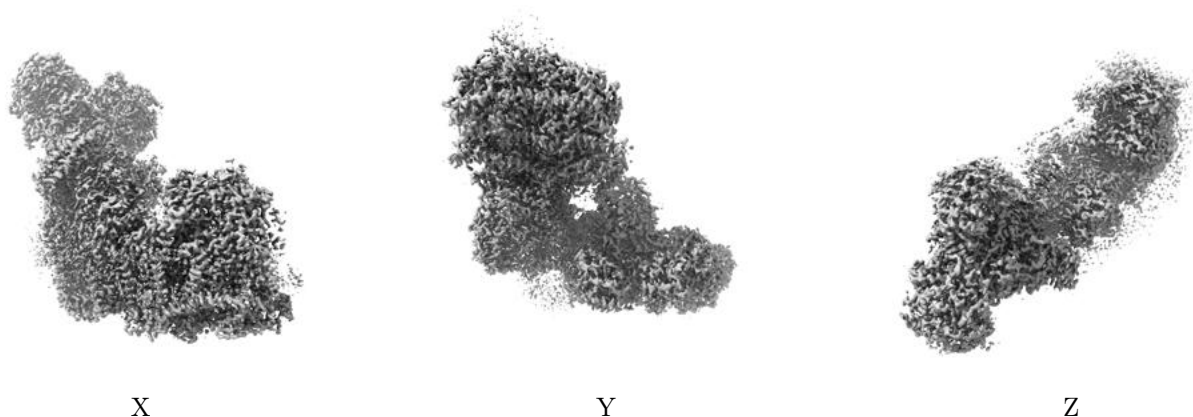


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0282. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

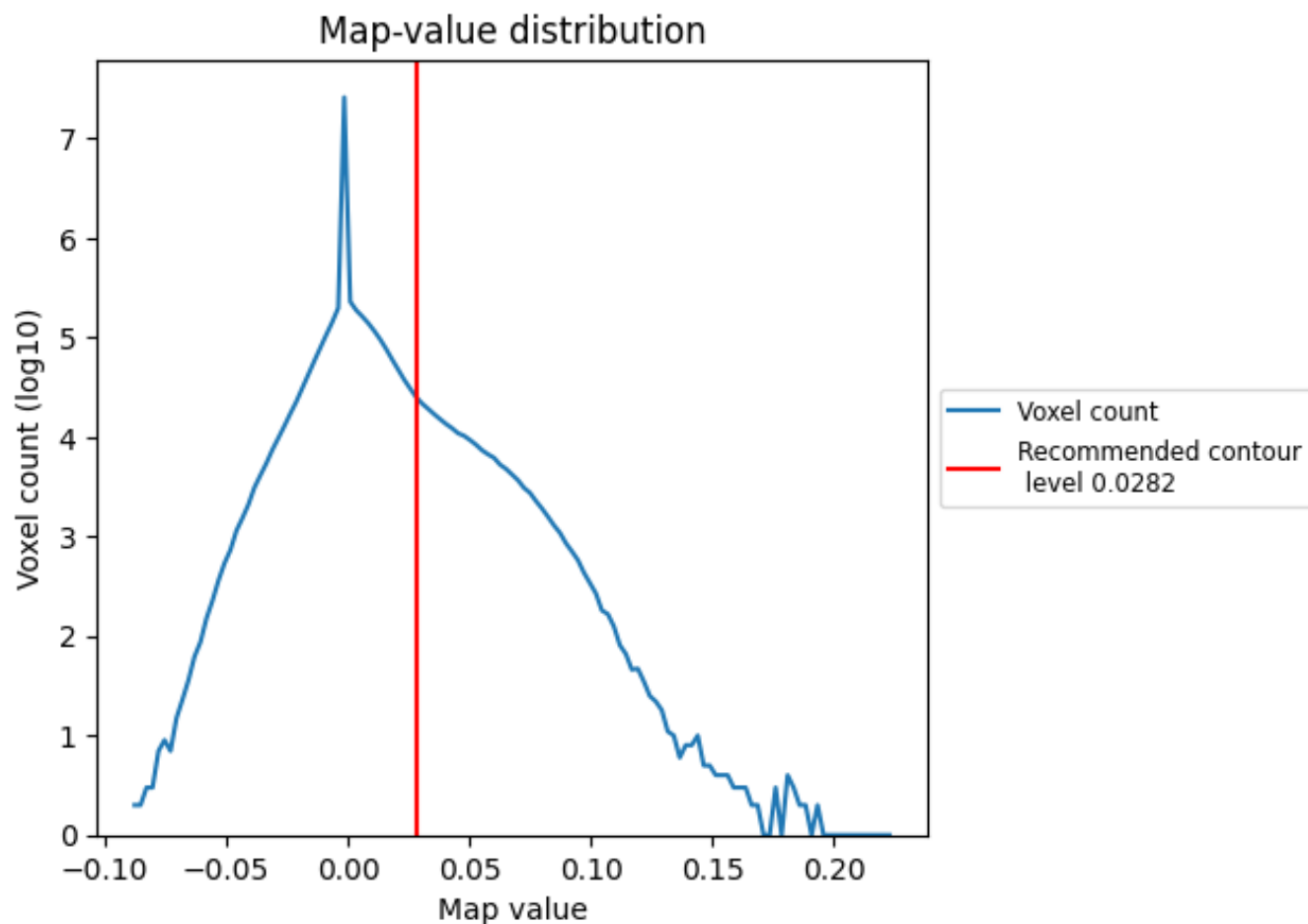
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

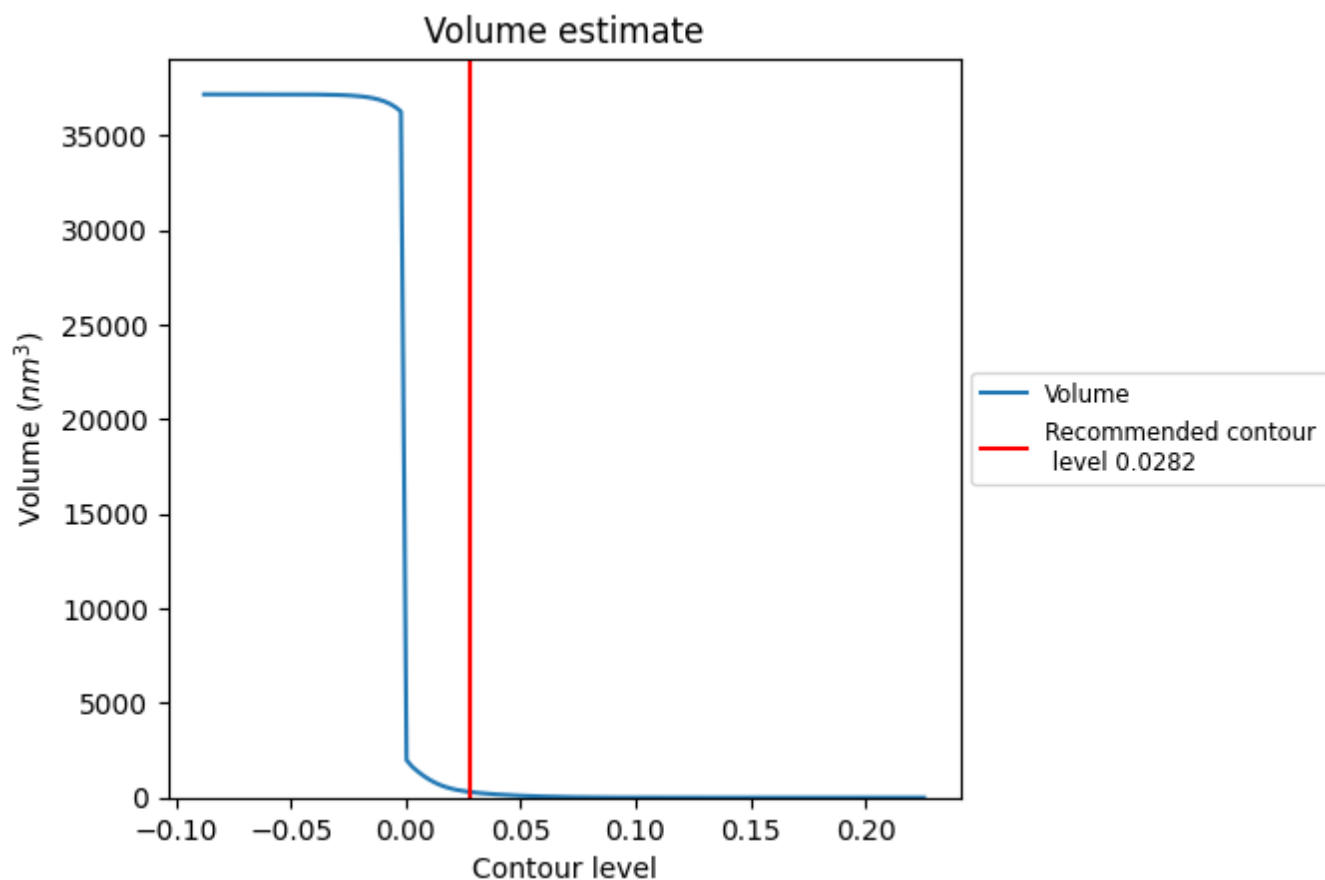
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

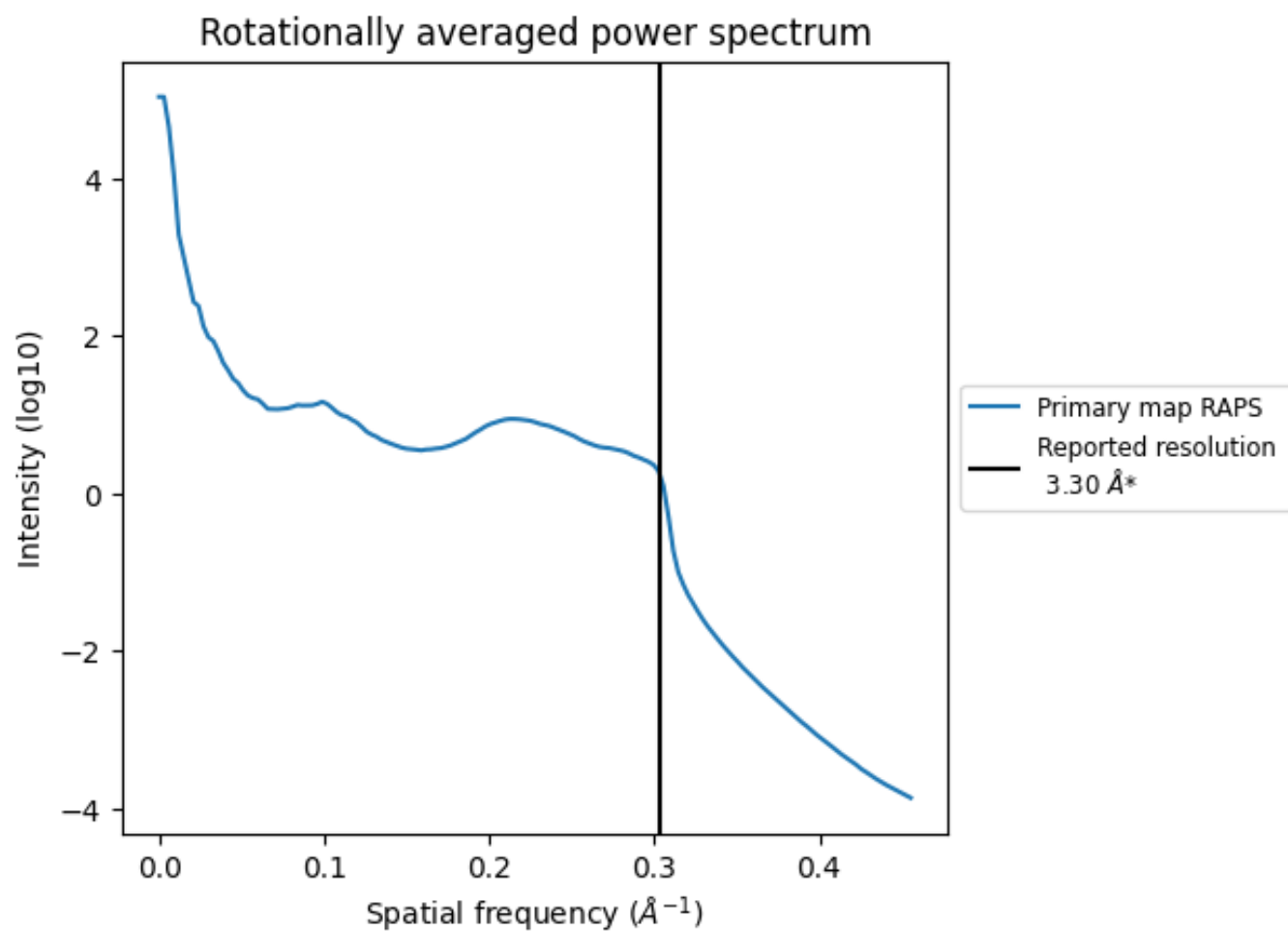
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 291 nm³; this corresponds to an approximate mass of 263 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 0.303 Å⁻¹

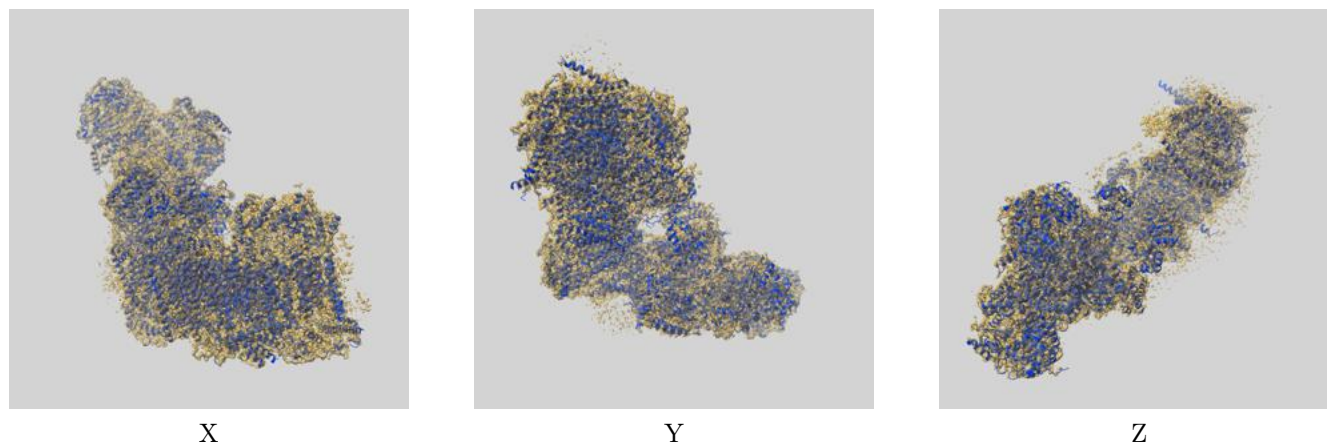
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

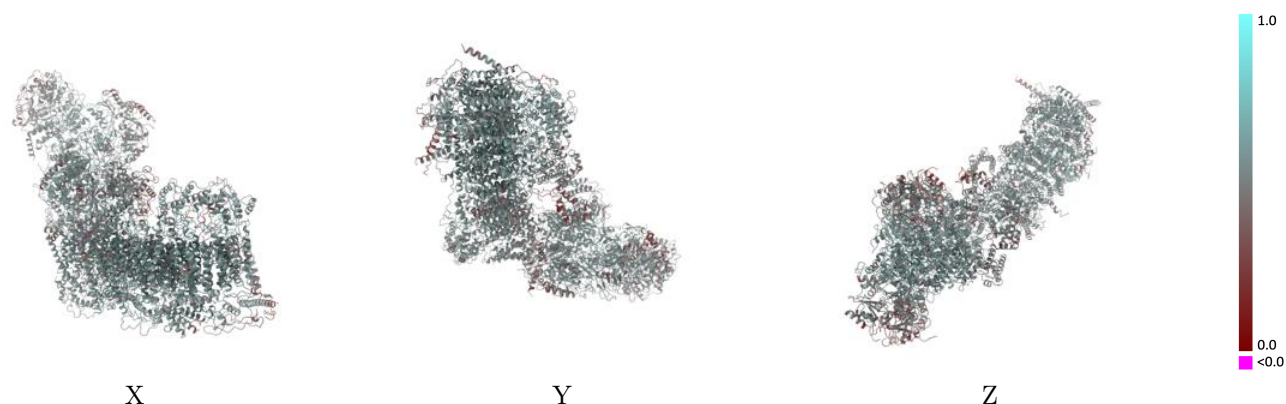
This section contains information regarding the fit between EMDB map EMD-32312 and PDB model 7W4Q. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



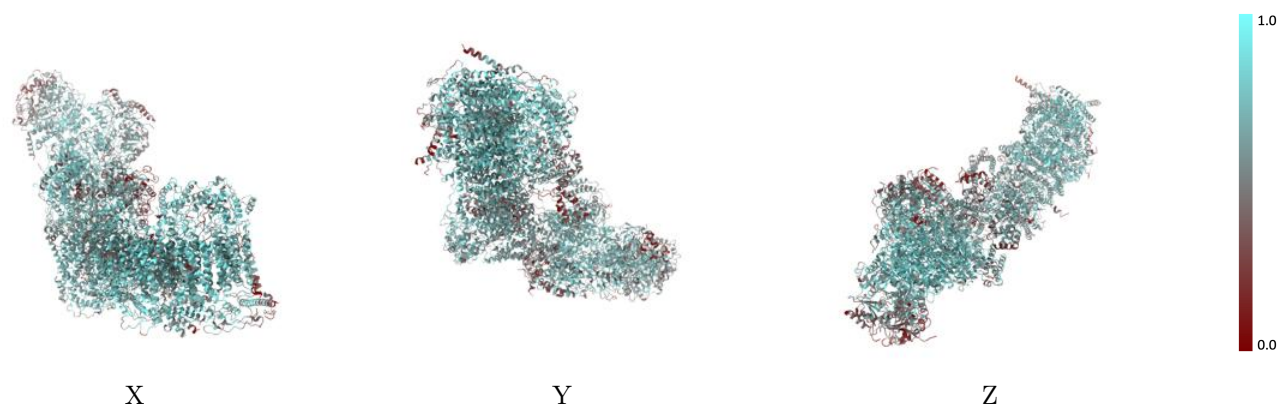
The images above show the 3D surface view of the map at the recommended contour level 0.0282 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



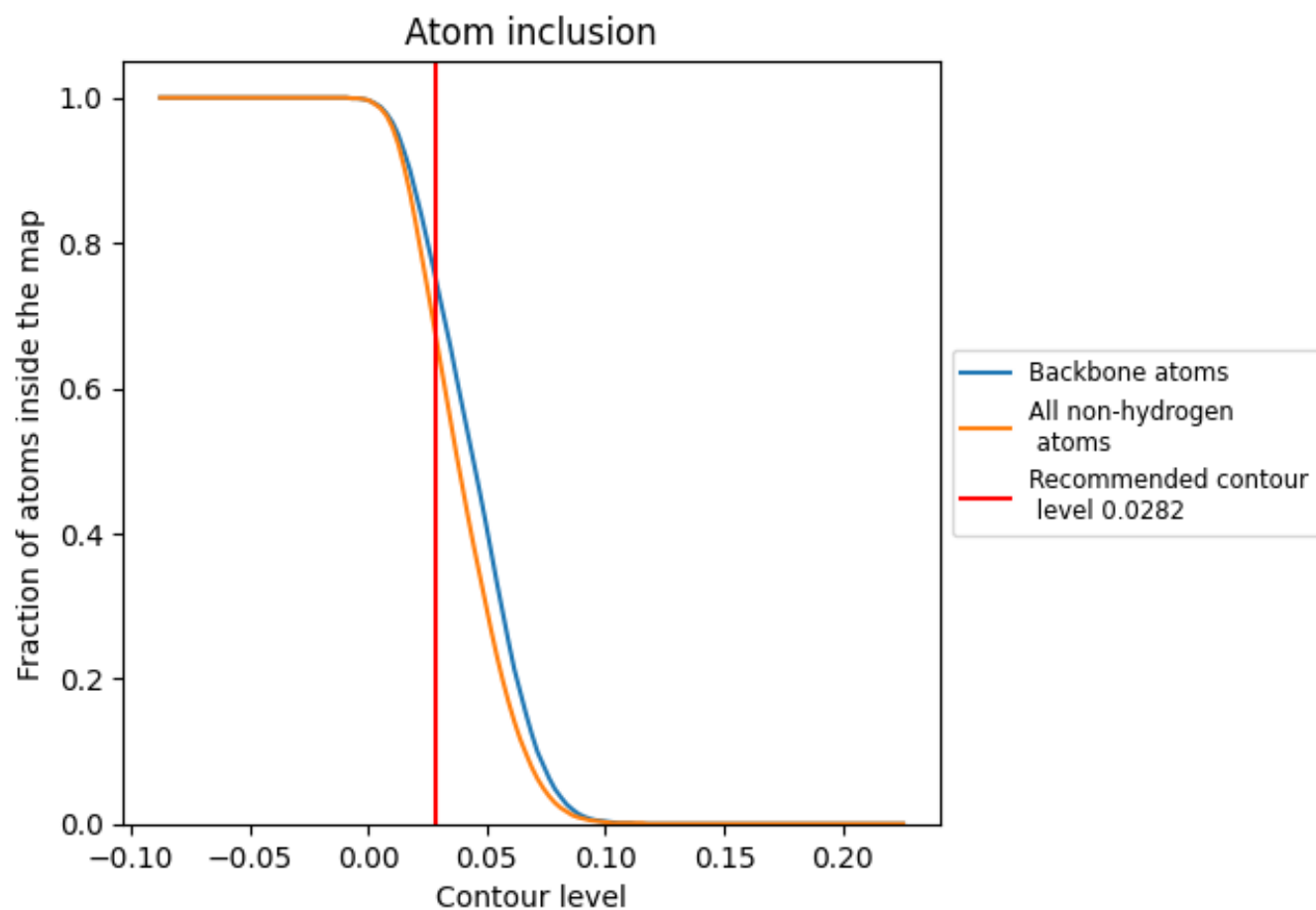
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0282).

9.4 Atom inclusion ⓘ



At the recommended contour level, 75% of all backbone atoms, 68% 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 (0.0282) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6760	 0.5260
A	 0.5470	 0.4760
B	 0.8180	 0.5740
C	 0.7590	 0.5560
E	 0.6140	 0.5170
F	 0.4110	 0.4050
G	 0.3060	 0.3630
H	 0.5890	 0.4780
I	 0.6570	 0.5270
J	 0.5560	 0.4770
K	 0.4830	 0.4680
L	 0.7210	 0.5510
M	 0.6840	 0.5280
N	 0.6940	 0.5380
O	 0.5420	 0.4750
P	 0.7820	 0.5640
Q	 0.7820	 0.5660
S	 0.7560	 0.5440
T	 0.6730	 0.5330
U	 0.6710	 0.5210
V	 0.4990	 0.4730
W	 0.7060	 0.5330
X	 0.6630	 0.5100
Y	 0.6080	 0.4940
Z	 0.5550	 0.4620
a	 0.7200	 0.5510
b	 0.6200	 0.4970
c	 0.7150	 0.5420
d	 0.6870	 0.5230
e	 0.6370	 0.5200
f	 0.5780	 0.4850
g	 0.7470	 0.5560
h	 0.6980	 0.5320
i	 0.7790	 0.5690
j	 0.5840	 0.4970



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	 0.6510	 0.5230
l	 0.7370	 0.5570
m	 0.6250	 0.5170
n	 0.6230	 0.5090
o	 0.7020	 0.5330
p	 0.7320	 0.5410
r	 0.7840	 0.5680
s	 0.7210	 0.5370
u	 0.6960	 0.5300
v	 0.5850	 0.4860
w	 0.5840	 0.4930