



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:48 PM UTC

PDB ID : 7W2U / pdb_00007w2u
EMDB ID : EMD-32266
Title : Active state CI from DQ-NADH dataset, Subclass 2
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-24
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

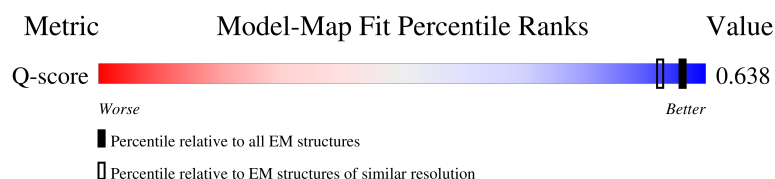
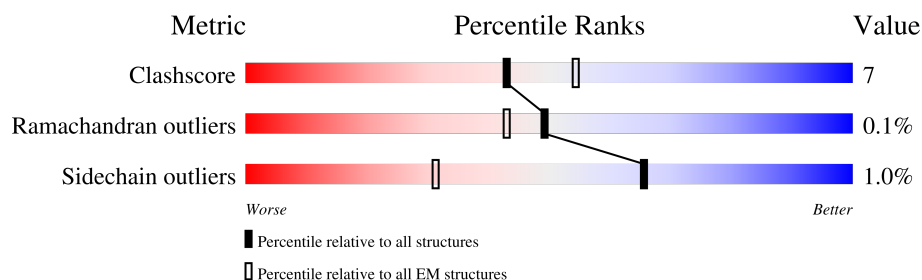
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 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	8728 (2.10 - 3.10)

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

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

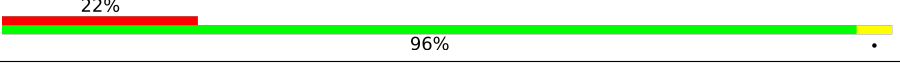
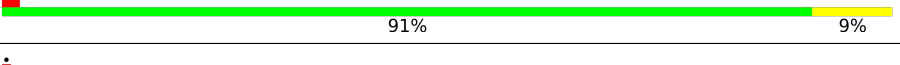
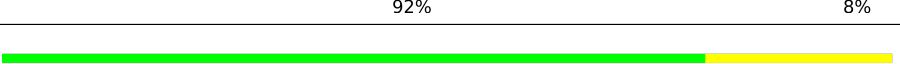
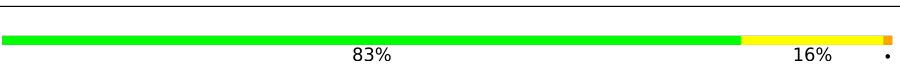
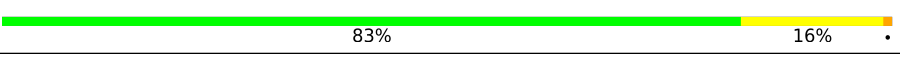
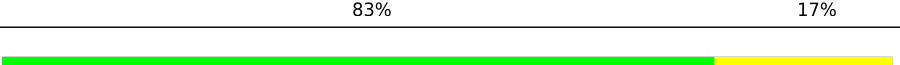
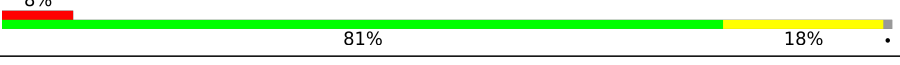
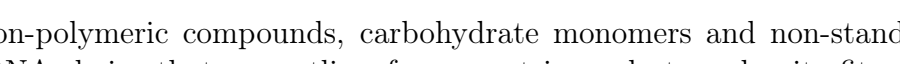
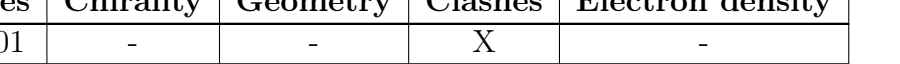
Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	A	501	-	-	X	-

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 68170 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	86	Total	C	N	O	S	0	0
			681	429	126	124	2		

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			693	447	102	139	5		
6	X	88	Total	C	N	O	S	0	0
			693	447	103	138	5		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	690	Total	C	N	O	S	0	0
			5296	3320	923	1014	39		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1732	1121	295	314	2		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	98	Total	C	N	O	S	0	0
			815	535	144	135	1		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	49	Total	C	N	O	0	0
			378	246	65	67		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	606	Total	C	N	O	S	0	0
			4800	3182	744	823	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	175	Total	C	N	O	S	0	0
			1277	852	187	225	13		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	o	128	Total	C	N	O	0	0
			1062	691	182	189		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	318	Total	C	N	O	S	0	0
			2508	1678	385	424	21		

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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



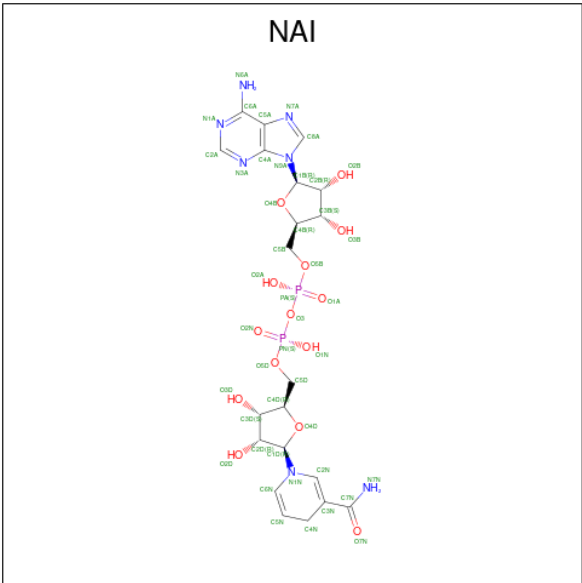
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

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



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

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



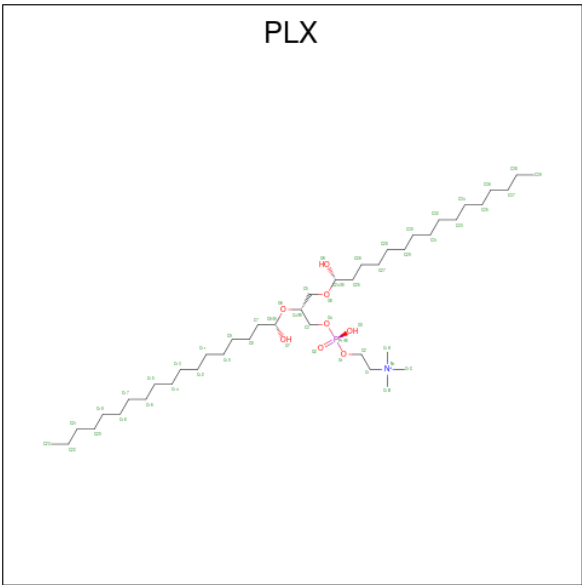
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

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



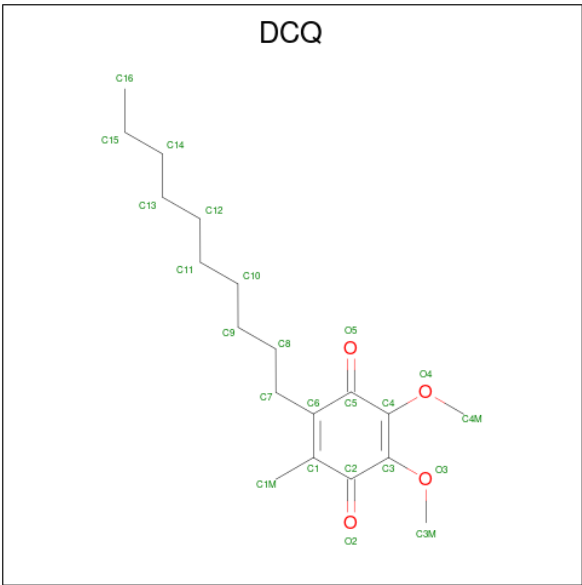
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	V	1	Total	C	N	O	P	0
			40	30	1	8	1	
48	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	j	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	l	1	Total	C	N	O	P	0
			51	41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

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



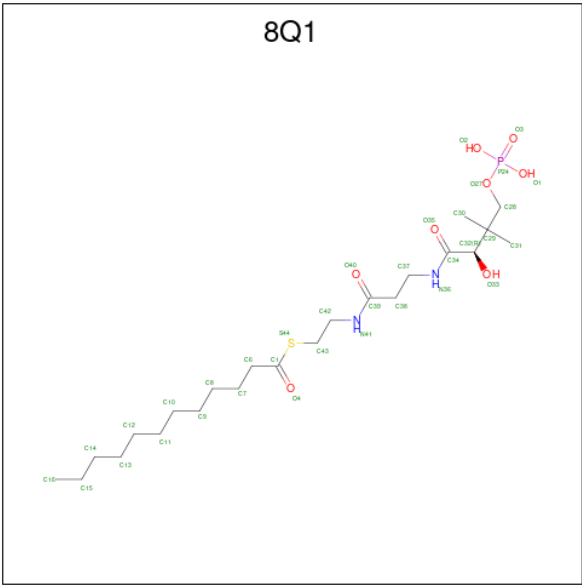
Mol	Chain	Residues	Atoms					AltConf
49	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	J	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	e	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	j	1	Total	C	N	O	P	0
			52	42	1	8	1	

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



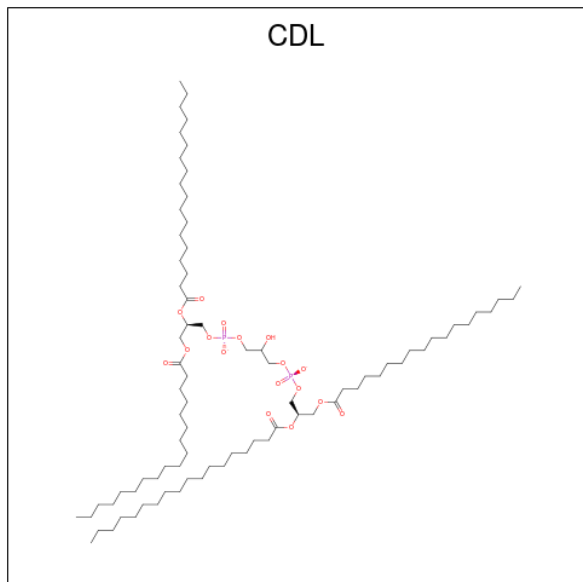
Mol	Chain	Residues	Atoms			AltConf
50	C	1	Total	C	O	0
			23	19	4	

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



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

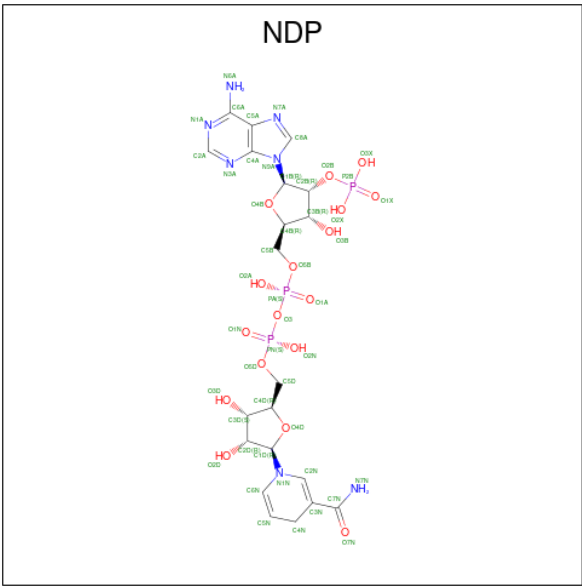
- Molecule 52 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
52	I	1	Total	C	O	P	0
			51	32	17	2	
52	V	1	Total	C	O	P	0
			94	75	17	2	
52	a	1	Total	C	O	P	0
			100	81	17	2	
52	g	1	Total	C	O	P	0
			100	81	17	2	
52	i	1	Total	C	O	P	0
			87	68	17	2	
52	k	1	Total	C	O	P	0
			100	81	17	2	
52	l	1	Total	C	O	P	0
			92	73	17	2	
52	o	1	Total	C	O	P	0
			100	81	17	2	
52	r	1	Total	C	O	P	0
			99	80	17	2	
52	s	1	Total	C	O	P	0
			89	70	17	2	
52	u	1	Total	C	O	P	0
			55	36	17	2	

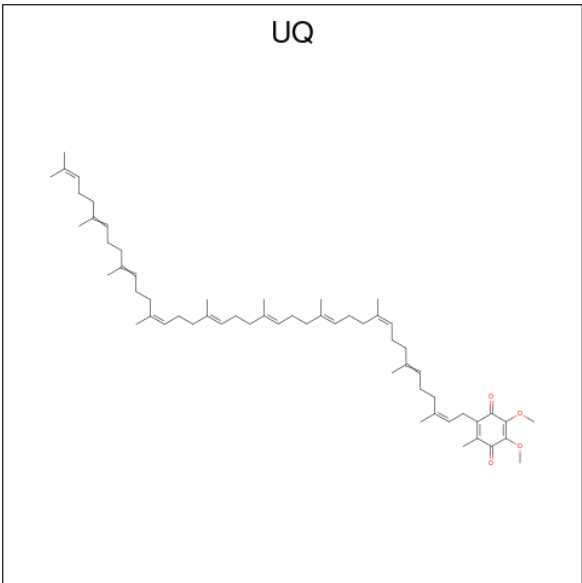
- Molecule 53 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest"

by depositor).



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

- Molecule 54 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



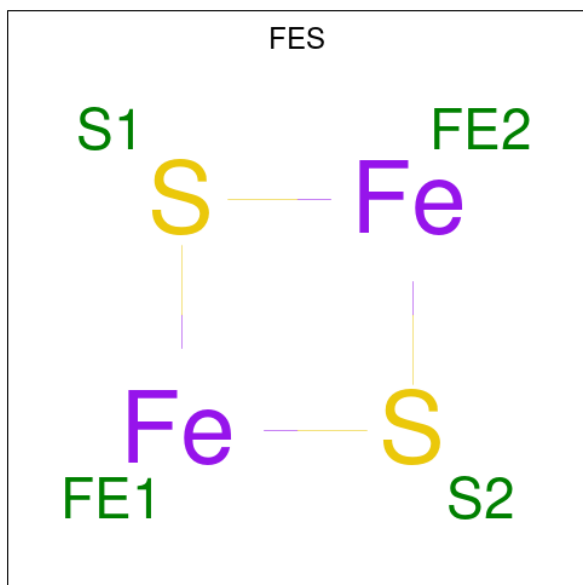
Mol	Chain	Residues	Atoms			AltConf
54	J	1	Total	C	O	0
			33	29	4	

Continued on next page...

Continued from previous page...

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

- Molecule 55 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



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

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

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

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

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

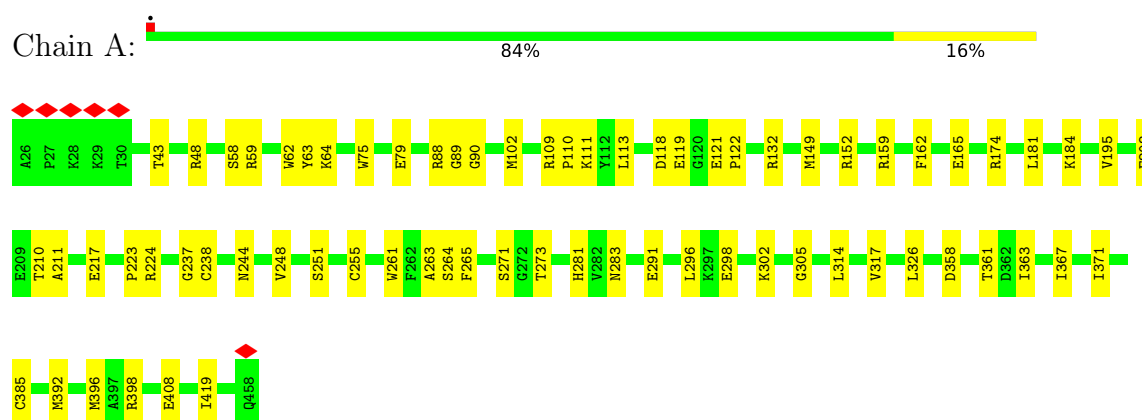
- # ADP



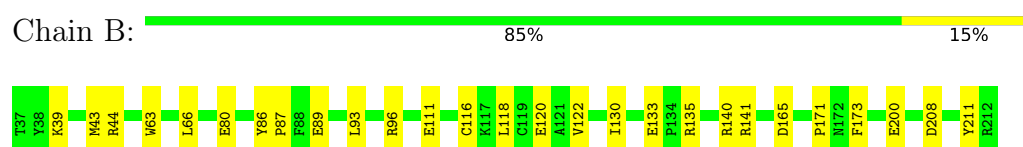
3 Residue-property plots

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

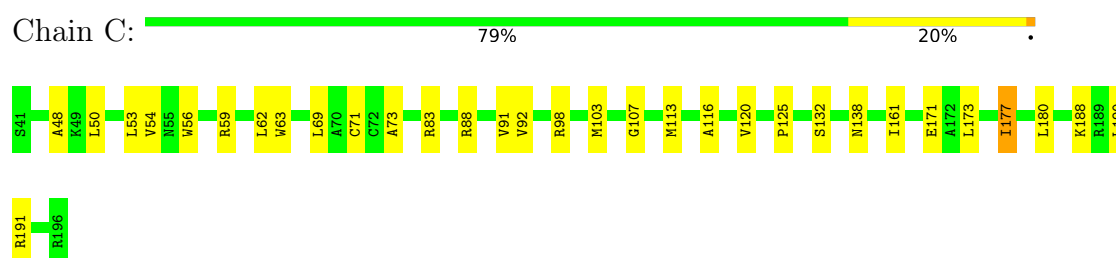
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



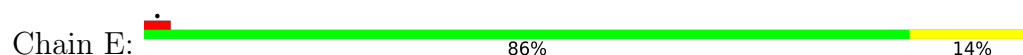
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



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

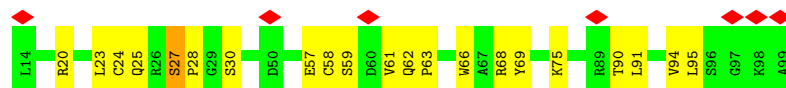
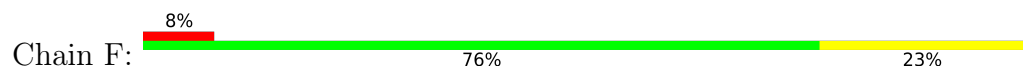


- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

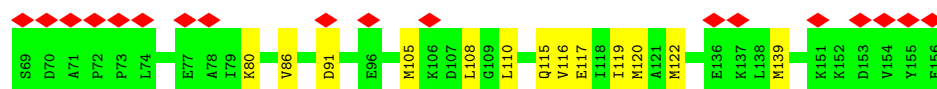
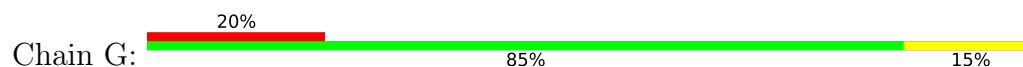




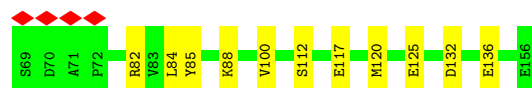
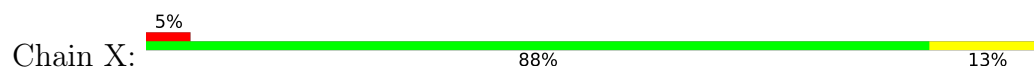
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



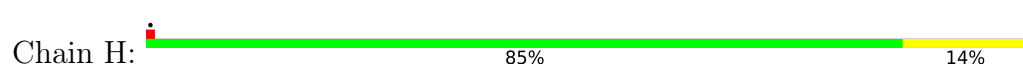
- Molecule 6: Acyl carrier protein



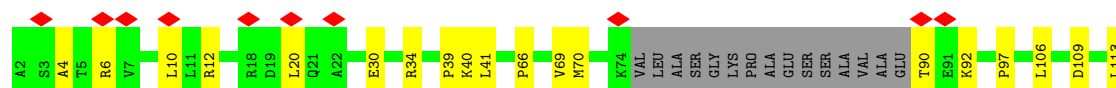
- Molecule 6: Acyl carrier protein



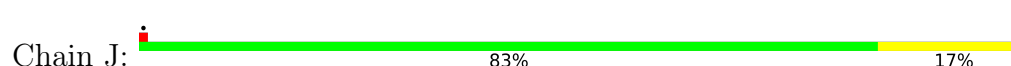
- Molecule 7: Complex I subunit B13



- Molecule 8: Complex I-B14.5a



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

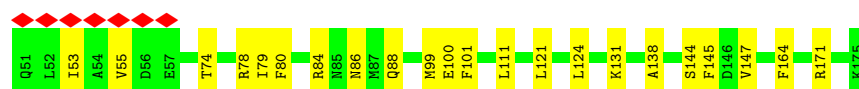
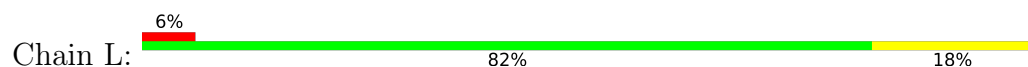




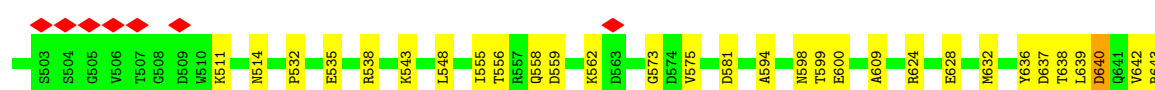
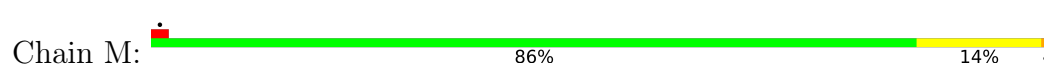
• Molecule 10: Complex I-9kD



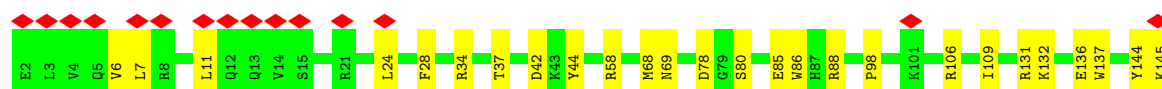
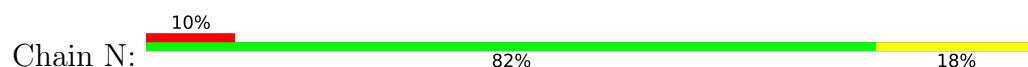
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



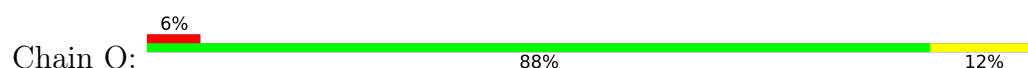
• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

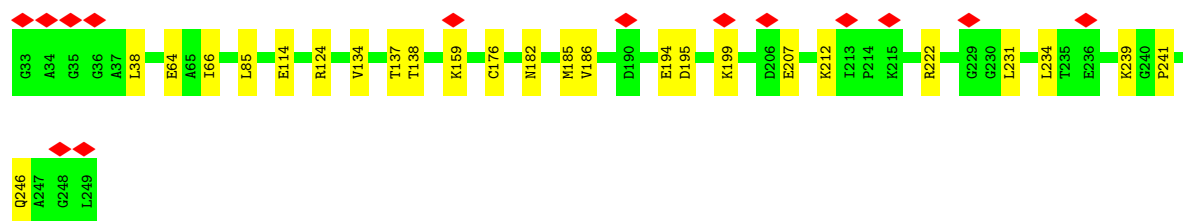


• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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





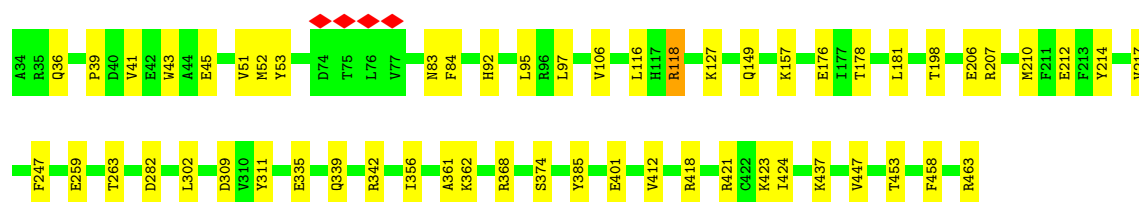
- Molecule 15: Complex I-30kD

Chain P: 85% 13%



- Molecule 16: Complex I-49kD

Chain Q: 87% 13%



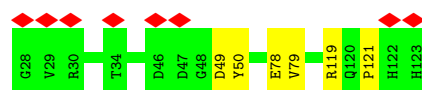
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S: 89% 10%



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

Chain T: 8% 94% 6%

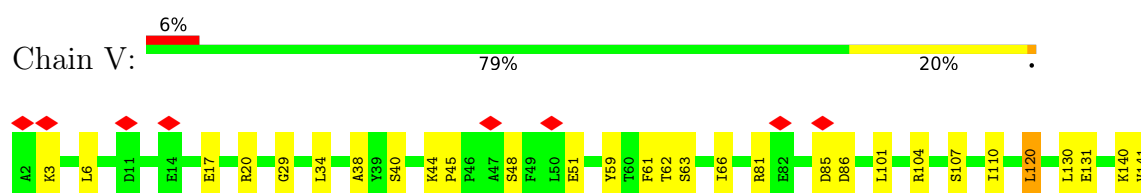


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

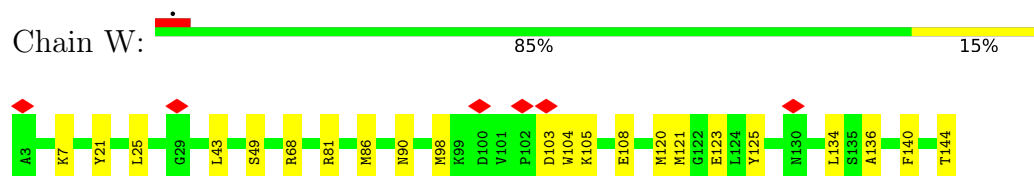
Chain U: 5% 93% 7%



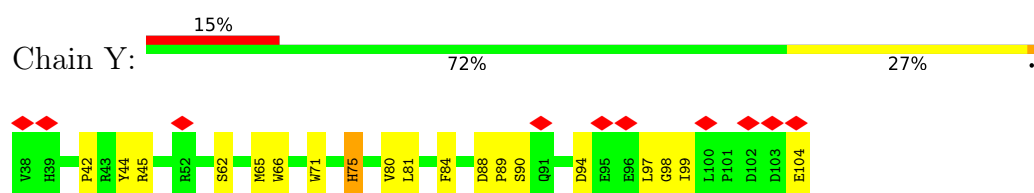
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



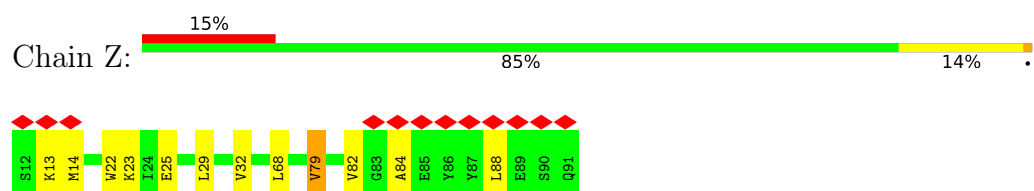
- Molecule 21: Complex I-B16.6



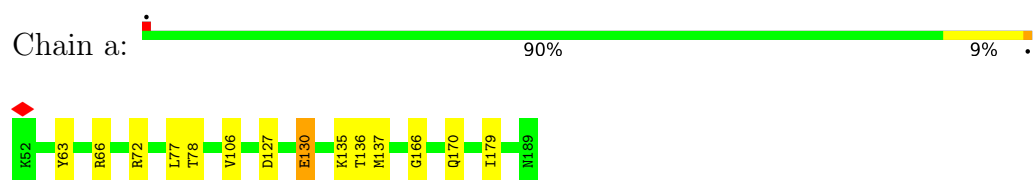
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



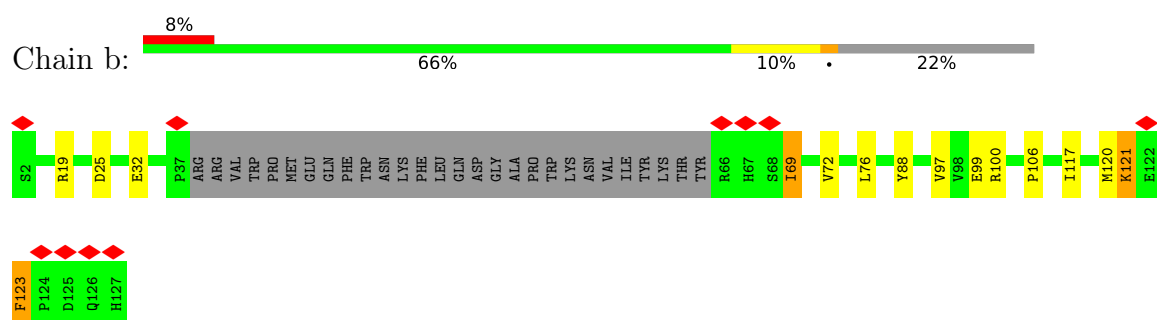
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



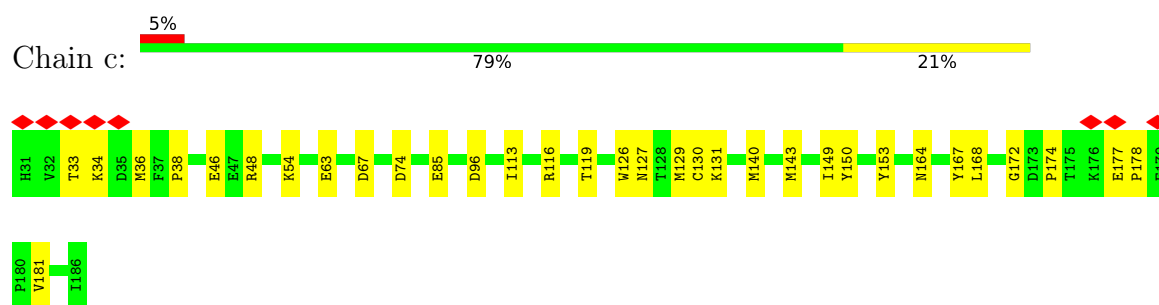
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



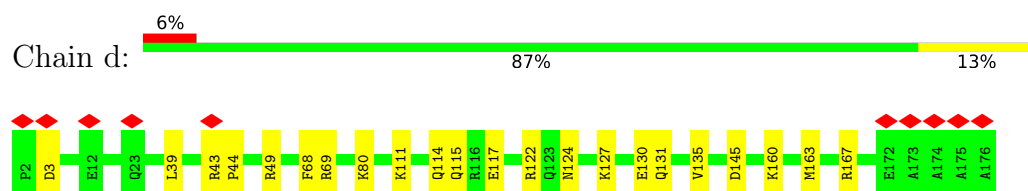
- Molecule 25: Complex I-B17



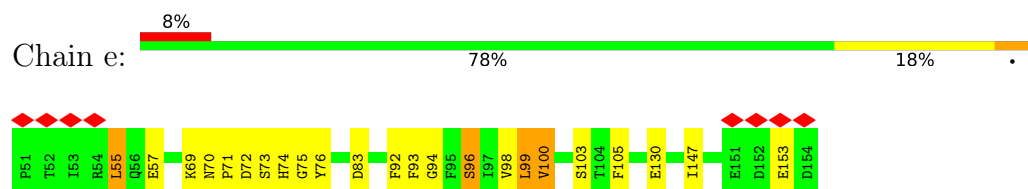
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



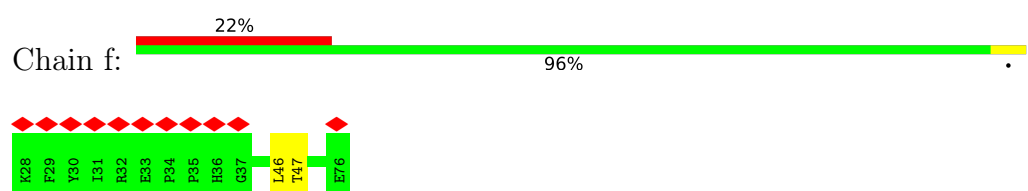
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



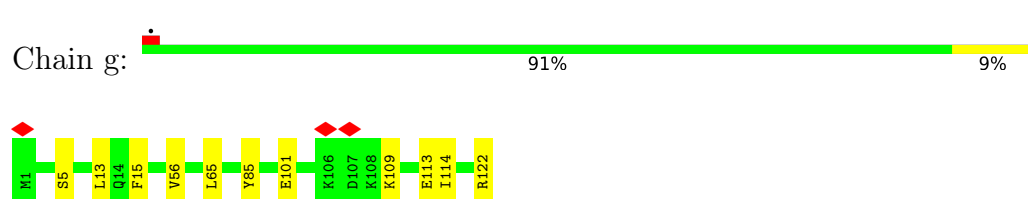
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



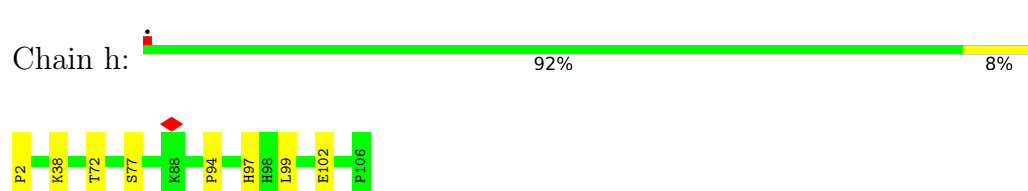
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



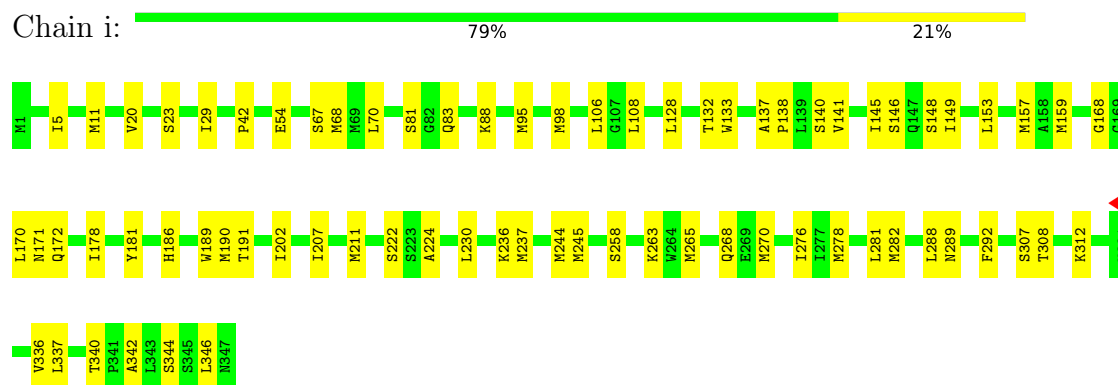
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



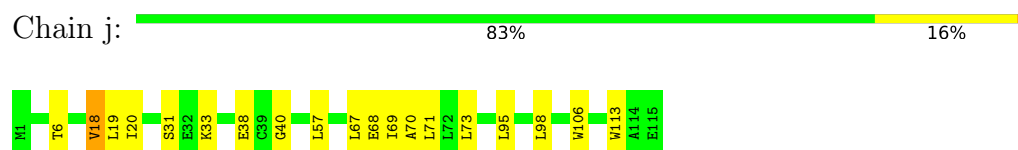
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



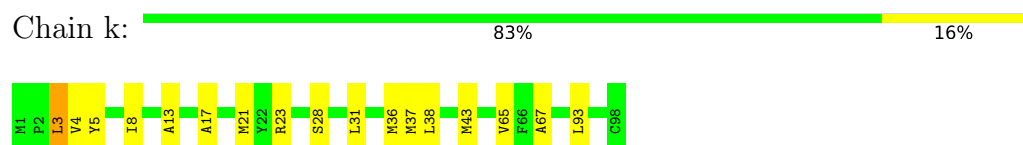
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



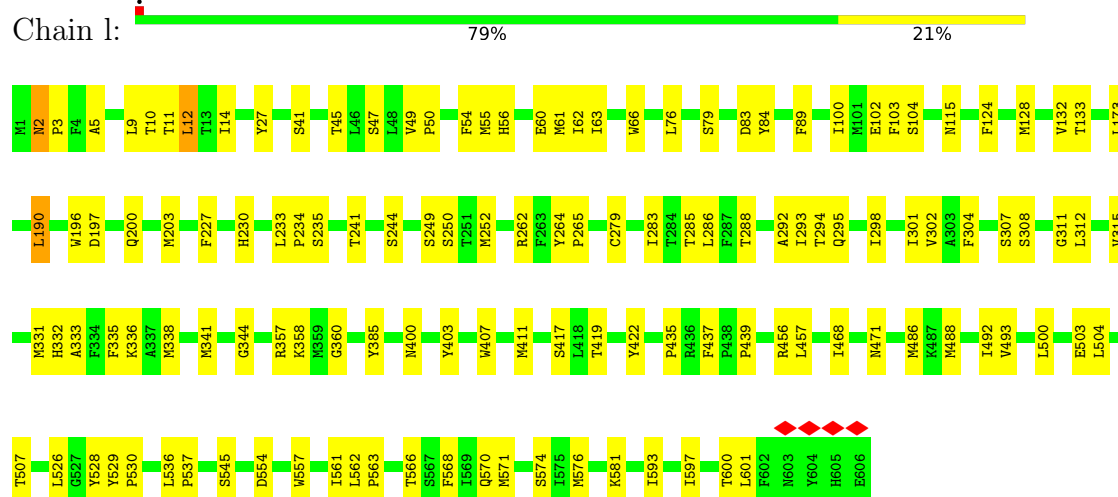
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3



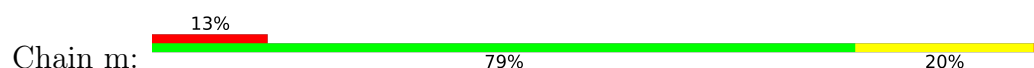
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

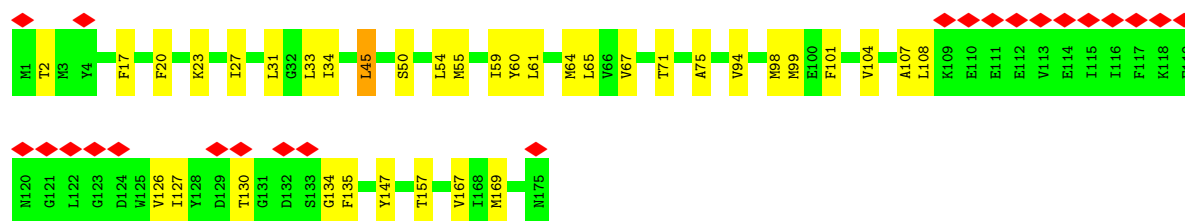


- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

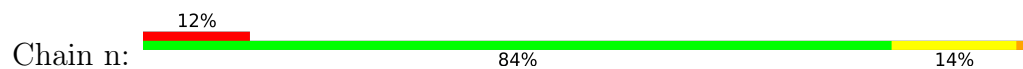


- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

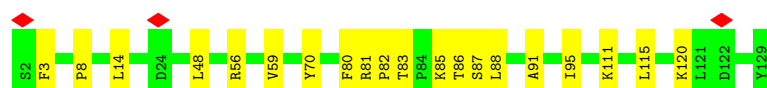
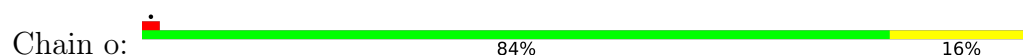




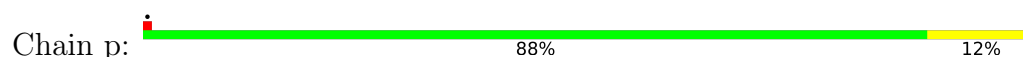
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



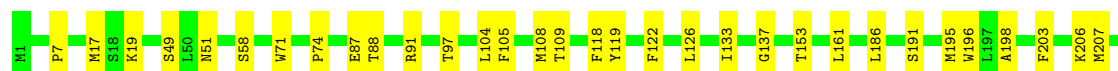
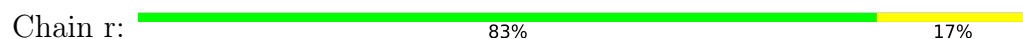
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



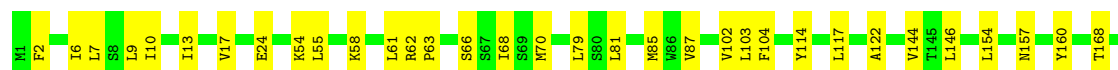
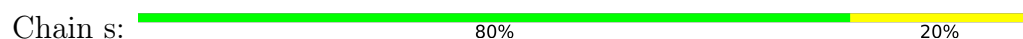
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

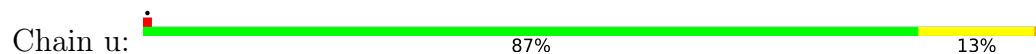


- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

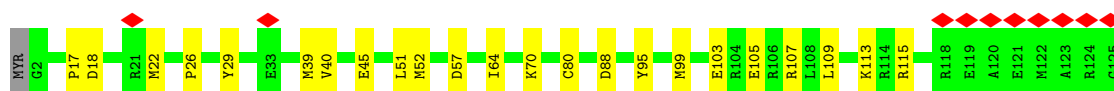
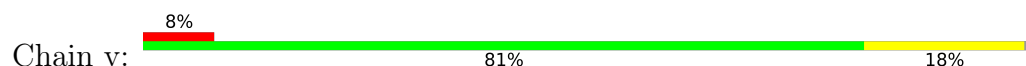




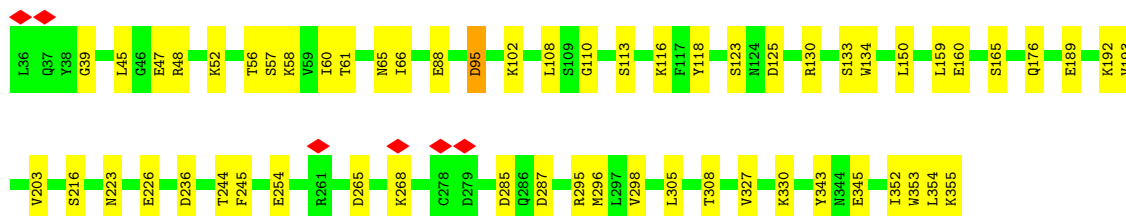
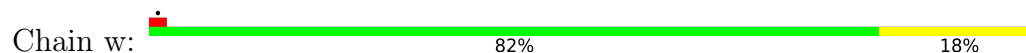
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	187567	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	0.202	Depositor
Minimum map value	-0.109	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0265	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.13	0/3406	0.32	0/4603
2	B	0.14	0/1443	0.32	0/1952
3	C	0.14	0/1279	0.32	0/1730
4	E	0.13	0/995	0.30	0/1340
5	F	0.19	0/692	0.65	3/933 (0.3%)
6	G	0.12	0/705	0.34	0/956
6	X	0.11	0/704	0.28	0/953
7	H	0.14	0/929	0.34	0/1258
8	I	0.14	0/798	0.35	0/1079
9	J	0.13	0/2828	0.33	0/3834
10	K	0.12	0/377	0.29	0/509
11	L	0.17	0/1039	0.39	1/1403 (0.1%)
12	M	0.13	0/5384	0.35	2/7295 (0.0%)
13	N	0.12	0/1245	0.30	0/1694
14	O	0.13	0/1711	0.31	0/2328
15	P	0.16	0/1783	0.44	3/2429 (0.1%)
16	Q	0.15	0/3538	0.32	0/4796
17	S	0.16	0/581	0.39	0/781
18	T	0.11	0/755	0.30	0/1018
19	U	0.12	0/664	0.29	0/912
20	V	0.12	0/1042	0.24	0/1411
21	W	0.15	0/1192	0.32	0/1610
22	Y	0.22	0/610	0.55	1/836 (0.1%)
23	Z	0.11	0/660	0.26	0/892
24	a	0.14	0/1184	0.31	0/1603
25	b	0.17	0/840	0.72	3/1144 (0.3%)
26	c	0.14	0/1371	0.39	2/1875 (0.1%)
27	d	0.13	0/1494	0.28	0/2015
28	e	0.18	0/891	0.51	3/1210 (0.2%)
29	f	0.11	0/386	0.24	0/523
30	g	0.13	0/1036	0.30	0/1401
31	h	0.12	0/889	0.30	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.16	0/2773	0.34	0/3768
33	j	0.16	0/938	0.36	0/1281
34	k	0.16	0/759	0.31	0/1029
35	l	0.15	0/4929	0.38	3/6704 (0.0%)
36	m	0.16	0/1309	0.37	0/1780
37	n	0.12	0/491	0.28	0/663
38	o	0.14	0/1092	0.30	0/1481
39	p	0.12	0/1590	0.28	0/2155
40	r	0.16	0/3723	0.36	0/5078
41	s	0.18	0/2581	0.39	0/3529
42	u	0.13	0/1436	0.35	0/1938
43	v	0.13	0/1052	0.40	0/1411
44	w	0.12	0/2642	0.32	0/3580
All	All	0.14	0/67766	0.36	21/91910 (0.0%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	123	PHE	CA-C-N	13.44	133.84	119.87
25	b	123	PHE	C-N-CA	13.44	133.84	119.87
5	F	27	SER	CA-C-N	7.90	127.82	119.05
5	F	27	SER	C-N-CA	7.90	127.82	119.05
5	F	25	GLN	N-CA-C	7.77	119.75	111.28
15	P	44	ARG	CA-C-N	7.64	127.54	119.05
15	P	44	ARG	C-N-CA	7.64	127.54	119.05
12	M	460	HIS	CA-C-N	6.79	126.58	119.05
12	M	460	HIS	C-N-CA	6.79	126.58	119.05
35	l	2	ASN	CA-C-N	6.52	126.45	119.28
35	l	2	ASN	C-N-CA	6.52	126.45	119.28
28	e	100	VAL	N-CA-C	6.14	116.30	110.53
11	L	111	LEU	N-CA-C	6.07	117.70	111.14
28	e	96	SER	N-CA-C	5.98	117.88	111.36
28	e	99	LEU	N-CA-C	5.67	117.27	111.14
35	l	56	HIS	N-CA-C	5.60	117.19	111.14
22	Y	75	HIS	N-CA-C	5.56	117.42	111.36
15	P	45	PRO	N-CA-C	5.39	121.03	113.53
25	b	121	LYS	N-CA-C	5.31	120.95	113.56
26	c	126	TRP	CA-C-N	5.16	131.39	121.54
26	c	126	TRP	C-N-CA	5.16	131.39	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3330	0	3292	54	0
2	B	1412	0	1363	24	0
3	C	1248	0	1254	27	0
4	E	971	0	975	19	0
5	F	681	0	689	11	0
6	G	693	0	671	9	0
6	X	693	0	671	11	0
7	H	910	0	950	11	0
8	I	780	0	808	16	0
9	J	2751	0	2773	33	0
10	K	366	0	338	14	0
11	L	1016	0	1016	20	0
12	M	5296	0	5326	68	0
13	N	1204	0	1162	17	0
14	O	1671	0	1673	18	0
15	P	1732	0	1682	20	0
16	Q	3459	0	3396	36	0
17	S	566	0	561	7	0
18	T	741	0	701	4	0
19	U	643	0	642	5	0
20	V	1021	0	1025	20	0
21	W	1161	0	1144	19	0
22	Y	584	0	529	25	0
23	Z	641	0	620	9	0
24	a	1151	0	1164	16	0
25	b	815	0	831	20	0
26	c	1315	0	1208	24	0
27	d	1461	0	1429	19	0
28	e	867	0	817	22	0
29	f	378	0	356	2	0
30	g	1005	0	999	10	0
31	h	867	0	871	5	0
32	i	2710	0	2874	46	0
33	j	914	0	951	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	k	748	0	799	15	0
35	l	4800	0	4939	92	0
36	m	1277	0	1239	32	0
37	n	479	0	486	11	0
38	o	1062	0	1072	16	0
39	p	1534	0	1470	18	0
40	r	3631	0	3839	53	0
41	s	2508	0	2607	50	0
42	u	1398	0	1374	16	0
43	v	1028	0	982	18	0
44	w	2582	0	2531	34	0
45	A	8	0	0	2	0
45	B	16	0	0	0	0
45	C	8	0	0	1	0
45	M	16	0	0	0	0
46	A	31	0	19	5	0
47	A	44	0	27	6	0
48	B	51	0	82	4	0
48	C	47	0	71	1	0
48	V	40	0	54	2	0
48	W	41	0	59	1	0
48	j	92	0	141	9	0
48	l	97	0	151	3	0
48	r	51	0	82	3	0
49	C	52	0	88	4	0
49	J	52	0	88	5	0
49	a	52	0	88	1	0
49	e	52	0	88	2	0
49	g	52	0	88	6	0
49	j	52	0	88	3	0
50	C	23	0	30	4	0
51	G	35	0	0	0	0
51	X	35	0	0	3	0
52	I	51	0	46	1	0
52	V	94	0	138	7	0
52	a	100	0	156	5	0
52	g	100	0	156	7	0
52	i	87	0	124	2	0
52	k	100	0	156	7	0
52	l	92	0	137	6	0
52	o	100	0	156	10	0
52	r	99	0	151	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	s	89	0	125	7	0
52	u	55	0	54	4	0
53	J	48	0	25	2	0
54	J	33	0	39	2	0
54	s	38	0	47	5	0
55	M	4	0	0	0	0
55	O	4	0	0	0	0
56	M	1	0	0	0	0
57	T	1	0	0	0	0
58	w	27	0	11	1	0
All	All	68170	0	68864	901	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (901) 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)
6:X:112:SER:CB	51:X:201:8Q1:O1	1.68	1.42
15:P:44:ARG:CB	15:P:45:PRO:HD3	1.42	1.37
15:P:44:ARG:CB	15:P:45:PRO:CD	2.16	1.23
22:Y:71:TRP:CZ2	22:Y:75:HIS:CE1	2.26	1.23
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.18
53:J:401:NDP:O4D	53:J:401:NDP:C4D	1.68	1.16
22:Y:71:TRP:CZ2	22:Y:75:HIS:HE1	1.63	1.15
4:E:128:PRO:HG2	11:L:74:THR:CG2	1.77	1.14
22:Y:71:TRP:CH2	22:Y:75:HIS:HE1	1.66	1.11
22:Y:71:TRP:CE2	22:Y:75:HIS:CE1	2.51	0.98
35:l:2:ASN:OD1	35:l:3:PRO:HD2	1.69	0.93
4:E:128:PRO:HG2	11:L:74:THR:HG21	1.55	0.89
4:E:128:PRO:HG2	11:L:74:THR:HG23	1.55	0.87
41:s:24:GLU:OE2	41:s:271:LEU:HD22	1.74	0.87
44:w:223:ASN:HD22	44:w:226:GLU:HG3	1.41	0.84
15:P:43:THR:HA	15:P:47:ILE:HD12	1.60	0.83
22:Y:71:TRP:CH2	22:Y:75:HIS:CE1	2.58	0.82
1:A:121:GLU:HG2	47:A:503:NAI:H42N	1.60	0.82
12:M:213:MET:HE1	12:M:713:ALA:HB1	1.63	0.80
28:e:93:PHE:O	28:e:98:VAL:HG23	1.81	0.80
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.64	0.79
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.65	0.77
9:J:308:SER:HB2	49:J:403:PLX:H252	1.65	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:40:LYS:HB3	21:W:7:LYS:H	1.50	0.74
44:w:47:GLU:OE2	44:w:52:LYS:NZ	2.21	0.73
12:M:456:ALA:O	12:M:499:ASN:ND2	2.21	0.73
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.21	0.73
24:a:78:THR:CG2	28:e:100:VAL:HG21	2.19	0.72
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.72	0.72
20:V:140:LYS:HG3	20:V:141:VAL:HG13	1.71	0.72
22:Y:71:TRP:CE2	22:Y:75:HIS:ND1	2.57	0.72
41:s:85:MET:HE3	41:s:233:MET:HE2	1.72	0.72
1:A:184:LYS:HB2	10:K:98:MET:HE1	1.71	0.72
25:b:123:PHE:HB3	43:v:40:VAL:HG11	1.73	0.71
21:W:121:MET:HE2	21:W:136:ALA:HB1	1.72	0.71
52:r:502:CDL:H591	52:r:502:CDL:H332	1.73	0.70
44:w:125:ASP:O	44:w:130:ARG:NH2	2.25	0.70
36:m:45:LEU:HD22	36:m:50:SER:HA	1.72	0.70
32:i:236:LYS:HG3	32:i:237:MET:HG3	1.74	0.70
1:A:58:SER:O	14:O:241:PRO:HD3	1.92	0.69
4:E:128:PRO:CG	11:L:74:THR:CG2	2.63	0.69
44:w:113:SER:HB3	44:w:116:LYS:HG2	1.73	0.69
30:g:15:PHE:HB2	49:g:201:PLX:H6	1.74	0.69
20:V:48:SER:HB3	20:V:51:GLU:HG3	1.74	0.69
25:b:121:LYS:O	25:b:121:LYS:HG2	1.92	0.69
20:V:61:PHE:HD2	20:V:104:ARG:HH21	1.39	0.69
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.75	0.69
41:s:307:LEU:HA	41:s:310:MET:HE2	1.74	0.68
27:d:111:LYS:NZ	35:l:200:GLN:OE1	2.27	0.68
36:m:54:LEU:HB3	41:s:103:LEU:HD22	1.75	0.68
10:K:77:GLN:OE1	10:K:77:GLN:N	2.21	0.67
43:v:26:PRO:HG2	43:v:29:TYR:HB2	1.75	0.67
9:J:299:ARG:NH1	9:J:320:GLU:OE2	2.27	0.67
14:O:38:LEU:O	14:O:124:ARG:NH2	2.28	0.67
7:H:38:ILE:O	7:H:45:ARG:NH1	2.25	0.67
20:V:3:LYS:HA	20:V:6:LEU:HD12	1.75	0.67
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.76	0.66
12:M:460:HIS:CG	12:M:461:PRO:HD2	2.31	0.66
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.27	0.66
21:W:81:ARG:NH2	42:u:64:ASN:OD1	2.28	0.66
10:K:106:GLN:OE1	10:K:106:GLN:N	2.29	0.65
34:k:65:VAL:HG11	36:m:157:THR:HG23	1.78	0.65
52:s:401:CDL:H552	52:s:401:CDL:H202	1.77	0.65
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.78	0.64
1:A:102:MET:O	1:A:111:LYS:NZ	2.29	0.64
14:O:182:ASN:HB3	14:O:194:GLU:HB2	1.78	0.64
26:c:164:ASN:HA	26:c:181:VAL:HB	1.78	0.64
24:a:135:LYS:NZ	37:n:32:ASP:OD1	2.27	0.64
12:M:624:ARG:NH2	12:M:637:ASP:OD1	2.29	0.64
5:F:68:ARG:NH2	12:M:364:ASP:OD1	2.31	0.63
52:a:201:CDL:H171	52:a:201:CDL:H712	1.79	0.63
26:c:36:MET:HA	26:c:36:MET:HE2	1.81	0.63
20:V:107:SER:HB2	20:V:110:ILE:HB	1.80	0.63
35:l:173:LEU:HD12	40:r:405:LEU:HD21	1.81	0.63
9:J:192:ARG:NH1	9:J:198:ALA:O	2.31	0.63
1:A:263:ALA:HA	1:A:271:SER:HB3	1.81	0.63
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.32	0.63
1:A:255:CYS:O	14:O:246:GLN:NE2	2.32	0.62
27:d:163:MET:HE1	28:e:147:ILE:HG21	1.81	0.62
49:g:201:PLX:H332	32:i:342:ALA:HB3	1.81	0.62
52:g:202:CDL:H232	52:g:202:CDL:H782	1.79	0.62
40:r:231:LEU:HD23	40:r:235:LEU:HD12	1.80	0.62
10:K:110:HIS:HA	12:M:441:ARG:HD2	1.82	0.62
39:p:95:GLU:HA	39:p:98:LYS:HD2	1.82	0.62
16:Q:259:GLU:HG2	21:W:25:LEU:HD11	1.82	0.62
3:C:125:PRO:HG2	41:s:58:LYS:HE3	1.81	0.62
34:k:17:ALA:HB2	52:k:101:CDL:H812	1.81	0.62
3:C:98:ARG:HD2	41:s:61:LEU:HD21	1.80	0.62
11:L:84:ARG:NH1	11:L:88:GLN:O	2.33	0.61
1:A:152:ARG:NH2	10:K:99:PRO:O	2.33	0.61
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.81	0.61
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.83	0.61
35:l:227:PHE:O	35:l:230:HIS:ND1	2.32	0.61
36:m:94:VAL:HG13	36:m:98:MET:HE3	1.81	0.61
22:Y:89:PRO:HB3	43:v:103:GLU:HG3	1.83	0.61
40:r:306:PRO:HB3	40:r:458:LEU:HD12	1.81	0.61
15:P:122:ARG:NH1	15:P:127:GLU:OE1	2.33	0.61
34:k:23:ARG:HG3	36:m:23:LYS:HE2	1.82	0.61
32:i:265:MET:O	32:i:268:GLN:HG3	2.00	0.60
1:A:48:ARG:NH1	10:K:70:ASN:O	2.33	0.60
9:J:174:ILE:HG23	9:J:175:LYS:HD3	1.82	0.60
22:Y:81:LEU:HD23	35:l:488:MET:HE1	1.82	0.60
27:d:167:ARG:HH21	28:e:153:GLU:HG3	1.66	0.60
20:V:40:SER:HA	52:V:201:CDL:HB62	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:331:MET:HE1	35:l:468:ILE:HD12	1.83	0.60
10:K:76:LEU:HD13	10:K:79:HIS:HD2	1.66	0.60
20:V:85:ASP:HB3	20:V:130:LEU:HD21	1.82	0.60
36:m:61:LEU:O	41:s:114:TYR:OH	2.20	0.60
34:k:31:LEU:HD21	36:m:67:VAL:HG11	1.83	0.60
36:m:126:VAL:HG23	36:m:127:ILE:HG23	1.84	0.60
11:L:78:ARG:HH22	12:M:249:GLU:HG3	1.65	0.60
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.28	0.59
39:p:117:ASP:O	39:p:121:LYS:HG3	2.02	0.59
15:P:113:ASP:OD1	16:Q:423:LYS:NZ	2.35	0.59
34:k:3:LEU:HD11	36:m:107:ALA:HB1	1.83	0.59
40:r:191:SER:HB3	48:r:501:PEE:H2	1.84	0.59
1:A:43:THR:OG1	1:A:59:ARG:HD3	2.02	0.59
1:A:210:THR:HB	1:A:224:ARG:HG3	1.84	0.59
35:l:562:LEU:HB3	35:l:563:PRO:HD3	1.84	0.59
41:s:146:LEU:HD12	41:s:188:SER:HB3	1.83	0.59
9:J:173:ASP:HB3	9:J:176:SER:HB2	1.83	0.59
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.21	0.59
3:C:73:ALA:HB3	50:C:304:DCQ:H4MB	1.83	0.59
26:c:54:LYS:NZ	26:c:74:ASP:OD2	2.35	0.59
52:r:502:CDL:H621	52:r:502:CDL:H432	1.84	0.59
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.83	0.59
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	1.83	0.59
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.21	0.59
36:m:94:VAL:O	36:m:98:MET:HG2	2.03	0.59
52:o:201:CDL:H601	52:o:201:CDL:H742	1.83	0.59
2:B:173:PHE:HE2	3:C:171:GLU:HG2	1.67	0.59
12:M:535:GLU:OE1	12:M:538:ARG:NH1	2.35	0.58
41:s:228:TYR:HA	41:s:231:ILE:HD12	1.85	0.58
16:Q:83:ASN:HB2	33:j:38:GLU:HG2	1.85	0.58
24:a:136:THR:OG1	40:r:51:ASN:ND2	2.34	0.58
3:C:63:TRP:HH2	54:s:402:UQ:H153	1.67	0.58
23:Z:23:LYS:HB3	23:Z:25:GLU:HG2	1.84	0.58
26:c:149:ILE:HG22	26:c:150:TYR:CD1	2.39	0.58
36:m:33:LEU:HD23	36:m:64:MET:HE3	1.86	0.58
2:B:43:MET:HA	2:B:43:MET:HE2	1.85	0.58
21:W:105:LYS:HE3	42:u:4:ILE:HD11	1.86	0.58
25:b:69:ILE:HD12	25:b:69:ILE:H	1.68	0.58
28:e:92:PHE:O	28:e:96:SER:HB2	2.04	0.58
32:i:95:MET:HE1	32:i:145:ILE:HD12	1.84	0.57
43:v:51:LEU:O	43:v:52:MET:HG2	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:GLU:O	1:A:302:LYS:HB2	2.05	0.57
3:C:48:ALA:HA	3:C:191:ARG:HE	1.69	0.57
11:L:74:THR:O	11:L:74:THR:HG22	2.04	0.57
48:j:202:PEE:H7	52:s:401:CDL:H112	1.85	0.57
35:l:294:THR:HG22	52:l:701:CDL:HB61	1.85	0.57
35:l:503:GLU:O	35:l:507:THR:HG23	2.04	0.57
24:a:66:ARG:HH12	28:e:72:ASP:HB2	1.69	0.57
7:H:76:GLN:O	7:H:78:GLU:N	2.38	0.57
36:m:31:LEU:HD21	52:s:401:CDL:H542	1.87	0.57
44:w:118:TYR:OH	58:w:401:ADP:O2'	2.23	0.57
27:d:115:GLN:HG2	35:l:62:ILE:HG12	1.87	0.57
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.87	0.57
44:w:176:GLN:NE2	44:w:236:ASP:OD2	2.35	0.57
4:E:64:ARG:NH2	6:G:117:GLU:OE2	2.34	0.57
20:V:17:GLU:OE1	20:V:20:ARG:NH1	2.37	0.57
9:J:306:GLU:HG2	9:J:315:THR:HG22	1.87	0.56
40:r:133:ILE:HD11	40:r:231:LEU:HD11	1.87	0.56
26:c:129:MET:HB3	35:l:528:TYR:CG	2.40	0.56
35:l:400:ASN:HB3	35:l:486:MET:HE3	1.86	0.56
35:l:417:SER:OG	35:l:493:VAL:HG13	2.05	0.56
40:r:371:PRO:HD2	52:r:502:CDL:H391	1.86	0.56
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.88	0.56
9:J:157:LYS:NZ	9:J:197:GLU:OE1	2.33	0.56
12:M:598:ASN:HD22	12:M:599:THR:H	1.52	0.56
24:a:166:GLY:O	24:a:170:GLN:NE2	2.37	0.56
41:s:79:LEU:HD22	41:s:222:MET:HG2	1.87	0.56
44:w:95:ASP:OD1	44:w:95:ASP:N	2.37	0.56
9:J:117:ARG:O	9:J:121:GLU:HG3	2.05	0.56
6:X:117:GLU:OE2	39:p:45:ARG:NH1	2.38	0.56
6:X:132:ASP:O	6:X:136:GLU:HG3	2.05	0.56
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.87	0.56
6:X:112:SER:CA	51:X:201:8Q1:O1	2.49	0.56
40:r:403:THR:HA	40:r:406:TYR:CE2	2.40	0.56
32:i:54:GLU:HG3	34:k:93:LEU:HB3	1.88	0.56
26:c:38:PRO:HG2	38:o:70:TYR:HD2	1.71	0.56
3:C:83:ARG:NH1	16:Q:212:GLU:OE1	2.33	0.56
24:a:78:THR:HG23	28:e:100:VAL:HG11	1.88	0.56
3:C:59:ARG:NH1	49:C:303:PLX:O3	2.25	0.55
16:Q:282:ASP:OD2	16:Q:437:LYS:NZ	2.39	0.55
37:n:10:ASP:HB2	40:r:19:LYS:NZ	2.21	0.55
5:F:24:CYS:N	5:F:58:CYS:SG	2.79	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:g:202:CDL:H201	52:g:202:CDL:H332	1.89	0.55
34:k:21:MET:HE3	52:k:101:CDL:H731	1.88	0.55
9:J:171:ASN:HA	9:J:327:MET:HE3	1.88	0.55
18:T:78:GLU:OE2	18:T:119:ARG:NH1	2.33	0.55
20:V:66:ILE:HD11	20:V:101:LEU:HB2	1.86	0.55
35:l:55:MET:HG2	35:l:471:ASN:O	2.06	0.55
44:w:58:LYS:O	44:w:60:ILE:HG13	2.07	0.55
3:C:98:ARG:NH1	33:j:33:LYS:O	2.35	0.55
35:l:233:LEU:HB3	35:l:234:PRO:HD3	1.89	0.55
35:l:419:THR:HA	35:l:422:TYR:CE2	2.42	0.55
9:J:75:ARG:NH2	15:P:215:GLU:OE1	2.40	0.55
12:M:275:PRO:HG3	12:M:286:ILE:HG12	1.87	0.55
4:E:128:PRO:CG	11:L:74:THR:HG23	2.33	0.55
12:M:372:PHE:H	12:M:532:PRO:HB2	1.71	0.55
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.46	0.55
14:O:195:ASP:OD2	14:O:222:ARG:NH1	2.40	0.55
24:a:179:ILE:HG21	31:h:38:LYS:HG3	1.89	0.55
33:j:113:TRP:HZ2	41:s:286:MET:HE3	1.72	0.55
35:l:597:ILE:HG23	35:l:601:LEU:HD22	1.89	0.55
35:l:11:THR:HG21	35:l:47:SER:HB3	1.89	0.54
12:M:340:ALA:HB3	12:M:366:LEU:HD13	1.90	0.54
5:F:30:SER:OG	5:F:63:PRO:HG3	2.07	0.54
9:J:174:ILE:HG23	9:J:175:LYS:CD	2.37	0.54
40:r:122:PHE:CE2	40:r:206:LYS:HD2	2.41	0.54
44:w:295:ARG:HA	44:w:298:VAL:HG22	1.90	0.54
3:C:132:SER:OG	3:C:138:ASN:OD1	2.23	0.54
22:Y:88:ASP:OD2	22:Y:90:SER:OG	2.23	0.54
40:r:105:PHE:O	40:r:109:THR:OG1	2.25	0.54
1:A:89:GLY:O	47:A:503:NAI:H2N	2.07	0.54
8:I:6:ARG:HH21	8:I:10:LEU:HD11	1.73	0.54
41:s:63:PRO:HB2	41:s:66:SER:HB3	1.89	0.54
1:A:283:ASN:ND2	1:A:305:GLY:O	2.38	0.54
44:w:61:THR:HG22	44:w:159:LEU:HB2	1.90	0.54
21:W:134:LEU:HD21	36:m:2:THR:HB	1.90	0.54
9:J:135:GLU:HG2	9:J:140:ASP:HA	1.90	0.54
14:O:207:GLU:HG2	14:O:212:LYS:HB2	1.88	0.54
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.43	0.54
42:u:77:HIS:CE1	42:u:115:LEU:HD21	2.43	0.54
4:E:87:LYS:HE3	4:E:90:LEU:HD23	1.89	0.53
1:A:90:GLY:HA3	47:A:503:NAI:H1D	1.90	0.53
1:A:121:GLU:HG2	47:A:503:NAI:C4N	2.34	0.53

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	2.42	0.53
35:l:488:MET:O	35:l:492:ILE:HG13	2.08	0.53
39:p:123:GLU:OE2	39:p:126:LYS:NZ	2.35	0.53
10:K:87:LEU:HD13	14:O:85:LEU:HD13	1.90	0.53
16:Q:36:GLN:NE2	40:r:137:GLY:O	2.41	0.53
1:A:122:PRO:HA	14:O:176:CYS:SG	2.49	0.53
30:g:101:GLU:OE1	30:g:101:GLU:N	2.25	0.53
25:b:106:PRO:HG2	25:b:120:MET:HE2	1.89	0.53
12:M:647:GLU:HB2	12:M:654:VAL:HG11	1.91	0.53
52:g:202:CDL:H221	52:g:202:CDL:H401	1.90	0.53
10:K:105:ARG:NH2	12:M:426:ASP:OD2	2.34	0.53
13:N:68:MET:HG3	13:N:69:ASN:H	1.73	0.53
40:r:203:PHE:O	40:r:207:MET:HG2	2.09	0.53
22:Y:44:TYR:HB2	23:Z:14:MET:HE1	1.90	0.52
32:i:276:ILE:HG21	48:r:501:PEE:H7	1.90	0.52
3:C:92:VAL:HG11	54:s:402:UQ:H103	1.90	0.52
9:J:369:VAL:HG12	9:J:369:VAL:O	2.09	0.52
12:M:466:LEU:HD13	12:M:500:ILE:HD11	1.92	0.52
21:W:120:MET:HB3	21:W:123:GLU:OE1	2.09	0.52
35:l:293:ILE:HG13	35:l:294:THR:HG23	1.91	0.52
37:n:26:TYR:OH	37:n:30:ARG:NH1	2.41	0.52
44:w:60:ILE:HG12	44:w:203:VAL:HB	1.89	0.52
1:A:385:CYS:HB3	45:A:501:SF4:S2	2.48	0.52
22:Y:71:TRP:CZ3	22:Y:75:HIS:HE1	2.23	0.52
26:c:96:ASP:N	26:c:96:ASP:OD1	2.43	0.52
37:n:17:VAL:HG13	40:r:7:PRO:HB3	1.90	0.52
38:o:59:VAL:HG22	40:r:423:ILE:HG12	1.91	0.52
11:L:78:ARG:NH2	12:M:249:GLU:HG3	2.24	0.52
52:a:201:CDL:H751	28:e:103:SER:HB2	1.92	0.52
26:c:85:GLU:OE1	26:c:119:THR:OG1	2.20	0.52
2:B:133:GLU:OE2	13:N:131:ARG:NH2	2.41	0.52
8:I:109:ASP:OD2	21:W:21:TYR:OH	2.23	0.52
26:c:46:GLU:CD	26:c:46:GLU:H	2.17	0.52
36:m:71:THR:HA	36:m:75:ALA:HB3	1.92	0.52
46:A:502:FMN:N5	47:A:503:NAI:H4N	2.25	0.52
32:i:278:MET:O	32:i:282:MET:HG3	2.10	0.52
39:p:98:LYS:HG3	39:p:178:PRO:HG3	1.91	0.52
40:r:257:MET:O	40:r:260:PRO:HD2	2.10	0.52
3:C:188:LYS:HB3	3:C:191:ARG:HH11	1.74	0.52
6:X:82:ARG:HD3	22:Y:44:TYR:CE1	2.45	0.52
3:C:188:LYS:HB3	3:C:191:ARG:NH1	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:68:MET:HE2	32:i:68:MET:HA	1.91	0.51
36:m:27:ILE:HG22	41:s:70:MET:HE1	1.91	0.51
26:c:168:LEU:HA	26:c:172:GLY:HA2	1.92	0.51
32:i:95:MET:HE2	32:i:149:ILE:HD13	1.92	0.51
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.45	0.51
6:X:120:MET:HE1	39:p:24:LEU:HB3	1.93	0.51
26:c:140:MET:HE2	35:l:283:ILE:HD13	1.93	0.51
32:i:202:ILE:HG22	32:i:346:LEU:HD13	1.92	0.51
1:A:88:ARG:NH2	1:A:273:THR:O	2.40	0.51
5:F:91:LEU:O	5:F:95:LEU:HD12	2.11	0.51
12:M:390:THR:HA	12:M:600:GLU:HG2	1.93	0.51
23:Z:29:LEU:HA	23:Z:32:VAL:HG12	1.93	0.51
25:b:25:ASP:OD2	39:p:125:TRP:NE1	2.36	0.51
7:H:77:ILE:HD12	7:H:78:GLU:N	2.26	0.51
9:J:87:GLU:HG3	9:J:89:TYR:H	1.76	0.51
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.92	0.51
33:j:71:LEU:O	36:m:147:TYR:OH	2.24	0.51
44:w:165:SER:HB3	44:w:245:PHE:CE1	2.46	0.51
48:V:202:PEE:H7	35:l:568:PHE:HE2	1.75	0.51
35:l:249:SER:OG	35:l:336:LYS:HG3	2.12	0.51
35:l:545:SER:OG	40:r:274:SER:O	2.25	0.51
1:A:43:THR:HA	14:O:234:LEU:HD21	1.93	0.50
15:P:147:THR:HB	15:P:153:ILE:HD11	1.94	0.50
52:k:101:CDL:H192	35:l:593:ILE:HD11	1.94	0.50
12:M:224:ASP:OD2	12:M:291:ARG:NH2	2.37	0.50
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.93	0.50
32:i:258:SER:OG	32:i:336:VAL:HG22	2.11	0.50
33:j:18:VAL:HG23	41:s:222:MET:HE1	1.94	0.50
35:l:103:PHE:HB2	35:l:341:MET:HE3	1.93	0.50
52:s:401:CDL:H182	52:s:401:CDL:H362	1.93	0.50
35:l:298:ILE:O	35:l:302:VAL:HG23	2.11	0.50
27:d:117:GLU:HG3	27:d:124:ASN:HB2	1.94	0.50
42:u:83:THR:HA	42:u:86:TRP:CD1	2.46	0.50
27:d:127:LYS:O	27:d:130:GLU:HG3	2.11	0.50
31:h:2:PRO:HA	32:i:140:SER:HB2	1.94	0.50
23:Z:84:ALA:O	23:Z:88:LEU:HB2	2.12	0.50
32:i:11:MET:HE1	52:i:401:CDL:H771	1.94	0.50
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.47	0.49
25:b:99:GLU:HG2	35:l:61:MET:HG3	1.94	0.49
32:i:337:LEU:O	32:i:340:THR:OG1	2.26	0.49
37:n:30:ARG:NH2	52:u:201:CDL:OA4	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:v:95:TYR:O	43:v:99:MET:HG3	2.12	0.49
1:A:281:HIS:HD2	1:A:358:ASP:H	1.60	0.49
3:C:53:LEU:HD11	49:C:303:PLX:H151	1.94	0.49
5:F:69:TYR:HE2	5:F:75:LYS:HG3	1.77	0.49
21:W:90:ASN:ND2	21:W:123:GLU:O	2.45	0.49
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.95	0.49
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.47	0.49
8:I:30:GLU:OE2	8:I:30:GLU:N	2.23	0.49
12:M:265:THR:HG21	12:M:609:ALA:HB1	1.93	0.49
27:d:114:GLN:HG3	35:l:203:MET:HG2	1.93	0.49
35:l:312:LEU:O	35:l:315:VAL:HG22	2.13	0.49
4:E:64:ARG:O	4:E:68:MET:HG2	2.12	0.49
8:I:30:GLU:H	8:I:30:GLU:CD	2.17	0.49
12:M:171:THR:HG23	12:M:173:MET:HE3	1.94	0.49
12:M:257:VAL:O	12:M:598:ASN:ND2	2.45	0.49
13:N:42:ASP:HB3	13:N:44:TYR:H	1.75	0.49
17:S:69:ILE:HD11	42:u:75:LYS:HD2	1.95	0.49
20:V:131:GLU:OE2	40:r:191:SER:OG	2.27	0.49
6:X:112:SER:N	51:X:201:8Q1:O1	2.45	0.49
26:c:127:ASN:HA	26:c:130:CYS:HB2	1.95	0.49
41:s:179:TRP:O	41:s:183:MET:HG3	2.12	0.49
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.94	0.49
27:d:68:PHE:HD1	37:n:44:LEU:HD11	1.78	0.49
12:M:638:THR:O	12:M:642:VAL:HG23	2.13	0.49
48:j:202:PEE:H31	52:s:401:CDL:H222	1.95	0.49
46:A:502:FMN:N1	46:A:502:FMN:O3'	2.31	0.48
2:B:93:LEU:O	8:I:34:ARG:NH2	2.45	0.48
9:J:168:SER:O	9:J:203:PRO:HD2	2.12	0.48
35:l:311:GLY:O	35:l:315:VAL:HG13	2.13	0.48
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.47	0.48
20:V:29:GLY:O	20:V:63:SER:HB3	2.13	0.48
32:i:159:MET:SD	32:i:281:LEU:HD23	2.52	0.48
52:r:502:CDL:H311	52:r:502:CDL:H561	1.95	0.48
6:G:116:VAL:HG12	6:G:120:MET:HE2	1.94	0.48
10:K:76:LEU:HD13	10:K:79:HIS:CD2	2.46	0.48
24:a:137:MET:HE2	37:n:42:SER:HB3	1.95	0.48
27:d:69:ARG:NH2	37:n:46:LYS:O	2.37	0.48
52:o:201:CDL:H561	52:o:201:CDL:H731	1.95	0.48
41:s:102:VAL:HG21	41:s:154:LEU:HD11	1.95	0.48
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.46	0.48
3:C:50:LEU:O	3:C:54:VAL:HG23	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:476:LEU:HD21	12:M:481:LEU:HD21	1.94	0.48
16:Q:210:MET:HE2	16:Q:247:PHE:HZ	1.78	0.48
52:r:502:CDL:H342	52:r:502:CDL:H372	1.59	0.48
4:E:87:LYS:HD2	4:E:87:LYS:HA	1.64	0.48
7:H:55:LYS:HE3	15:P:104:THR:HG21	1.95	0.48
41:s:7:LEU:HD23	41:s:10:ILE:HD11	1.96	0.48
2:B:116:CYS:SG	2:B:118:LEU:HG	2.53	0.48
3:C:69:LEU:HB2	3:C:107:GLY:HA3	1.96	0.48
33:j:19:LEU:HD11	48:j:202:PEE:H52	1.94	0.48
35:l:244:SER:O	35:l:249:SER:HB2	2.14	0.48
37:n:42:SER:O	37:n:46:LYS:HB2	2.13	0.48
40:r:198:ALA:HB2	48:r:501:PEE:H22	1.96	0.48
1:A:248:VAL:O	1:A:251:SER:OG	2.32	0.48
1:A:63:TYR:CD2	1:A:64:LYS:HG2	2.49	0.48
1:A:118:ASP:O	1:A:159:ARG:HD2	2.14	0.48
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.49	0.48
25:b:106:PRO:HA	25:b:117:ILE:HG22	1.96	0.48
27:d:111:LYS:HE3	35:l:197:ASP:OD2	2.13	0.48
35:l:12:LEU:HD21	35:l:133:THR:HG21	1.94	0.48
40:r:269:MET:HE1	40:r:396:MET:SD	2.53	0.48
1:A:261:TRP:O	1:A:264:SER:OG	2.29	0.48
3:C:190:LEU:HD22	48:C:302:PEE:H14	1.95	0.48
4:E:30:ARG:O	4:E:34:GLU:HG3	2.13	0.48
32:i:20:VAL:HG11	32:i:137:ALA:HB1	1.95	0.48
52:o:201:CDL:H331	52:o:201:CDL:H361	1.64	0.48
12:M:151:SER:HB3	16:Q:374:SER:HB3	1.95	0.47
13:N:85:GLU:HG2	13:N:86:TRP:N	2.29	0.47
13:N:132:LYS:NZ	13:N:136:GLU:OE2	2.45	0.47
1:A:62:TRP:CD2	1:A:181:LEU:HD13	2.49	0.47
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.95	0.47
3:C:103:MET:HE1	3:C:120:VAL:HG23	1.95	0.47
12:M:197:THR:O	14:O:114:GLU:HG2	2.14	0.47
29:f:47:THR:HG23	30:g:65:LEU:HD22	1.96	0.47
33:j:57:LEU:HD21	36:m:169:MET:HE3	1.95	0.47
35:l:292:ALA:HB2	35:l:304:PHE:HB3	1.96	0.47
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.96	0.47
18:T:79:VAL:O	18:T:121:PRO:HD3	2.14	0.47
19:U:26:GLY:HA3	48:j:201:PEE:H37	1.95	0.47
33:j:73:LEU:HD12	36:m:55:MET:SD	2.54	0.47
40:r:104:LEU:HG	40:r:108:MET:HE2	1.95	0.47
12:M:419:ARG:NH1	12:M:439:THR:O	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:TYR:O	3:C:88:ARG:NH2	2.47	0.47
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.95	0.47
38:o:56:ARG:NH1	40:r:422:HIS:O	2.37	0.47
12:M:217:GLU:HG2	12:M:218:LEU:HG	1.96	0.47
12:M:250:SER:OG	12:M:251:ILE:N	2.47	0.47
22:Y:104:GLU:O	43:v:115:ARG:NH2	2.48	0.47
35:l:358:LYS:HG3	39:p:80:TYR:CE1	2.49	0.47
40:r:122:PHE:HE2	40:r:206:LYS:HD2	1.78	0.47
41:s:195:ARG:HD3	41:s:231:ILE:HD11	1.97	0.47
3:C:173:LEU:O	3:C:177:ILE:HD12	2.15	0.47
9:J:37:HIS:CE1	18:T:49:ASP:HA	2.50	0.47
9:J:179:ARG:HB2	9:J:179:ARG:CZ	2.44	0.47
9:J:313:TRP:CE2	54:J:402:UQ:H72	2.49	0.47
14:O:185:MET:HE2	14:O:185:MET:HB2	1.77	0.47
16:Q:127:LYS:O	16:Q:418:ARG:HG2	2.13	0.47
19:U:24:ALA:HB2	48:j:201:PEE:H72	1.96	0.47
49:g:201:PLX:H102	49:g:201:PLX:H71	1.59	0.47
40:r:313:THR:HA	40:r:316:MET:HE3	1.97	0.47
41:s:55:LEU:HD13	41:s:221:ALA:HB2	1.97	0.47
9:J:365:GLU:HG2	9:J:368:ASP:HB2	1.96	0.47
42:u:83:THR:HA	42:u:86:TRP:NE1	2.30	0.47
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.95	0.47
1:A:296:LEU:HD21	1:A:317:VAL:HG11	1.96	0.47
8:I:70:MET:HG3	15:P:66:ALA:HB1	1.95	0.47
1:A:211:ALA:HB2	1:A:223:PRO:HG3	1.96	0.47
11:L:131:LYS:HD2	11:L:147:VAL:HG11	1.97	0.47
44:w:39:GLY:HA2	44:w:296:MET:HE1	1.97	0.47
1:A:110:PRO:O	1:A:238:CYS:HB3	2.15	0.46
23:Z:79:VAL:HA	23:Z:82:VAL:HG22	1.97	0.46
25:b:72:VAL:HG23	25:b:76:LEU:HD23	1.97	0.46
30:g:56:VAL:HG21	40:r:17:MET:HE1	1.97	0.46
52:l:701:CDL:H341	52:l:701:CDL:H311	1.65	0.46
38:o:115:LEU:HG	38:o:120:LYS:O	2.15	0.46
52:r:502:CDL:H312	52:r:502:CDL:H742	1.97	0.46
52:s:401:CDL:H141	52:s:401:CDL:H171	1.72	0.46
12:M:460:HIS:ND1	12:M:461:PRO:HD2	2.30	0.46
27:d:131:GLN:NE2	28:e:130:GLU:OE2	2.47	0.46
35:l:83:ASP:CG	35:l:262:ARG:HH12	2.23	0.46
52:l:701:CDL:H711	52:l:701:CDL:H742	1.60	0.46
16:Q:41:VAL:O	16:Q:45:GLU:HG2	2.14	0.46
44:w:343:TYR:OH	44:w:355:LYS:O	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:ARG:HG2	2:B:208:ASP:OD2	2.15	0.46
13:N:85:GLU:HB2	13:N:98:PRO:HB3	1.97	0.46
15:P:209:GLU:HB3	15:P:224:VAL:HG12	1.98	0.46
32:i:207:ILE:O	32:i:211:MET:HG3	2.15	0.46
48:j:201:PEE:H26	41:s:295:PRO:HB3	1.97	0.46
35:l:63:ILE:O	35:l:79:SER:HA	2.15	0.46
11:L:80:PHE:HE1	11:L:100:GLU:HG2	1.80	0.46
34:k:28:SER:HB3	36:m:23:LYS:HG2	1.96	0.46
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.51	0.46
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.51	0.46
38:o:80:PHE:HE1	38:o:86:THR:HG21	1.81	0.46
52:o:201:CDL:H451	52:o:201:CDL:H242	1.97	0.46
11:L:99:MET:HE2	11:L:138:ALA:HB2	1.98	0.46
12:M:389:THR:HB	12:M:473:MET:HE3	1.98	0.46
41:s:13:ILE:O	41:s:17:VAL:HG23	2.16	0.46
1:A:119:GLU:O	1:A:159:ARG:NH1	2.48	0.46
15:P:69:LEU:HD13	15:P:96:VAL:HG22	1.98	0.46
32:i:168:GLY:HA3	32:i:181:TYR:CE1	2.51	0.46
32:i:222:SER:O	32:i:224:ALA:N	2.49	0.46
33:j:18:VAL:HG12	48:j:202:PEE:H16	1.97	0.46
35:l:332:HIS:HA	35:l:335:PHE:CZ	2.50	0.46
8:I:12:ARG:HB3	8:I:20:LEU:HD12	1.97	0.46
9:J:40:LEU:HD21	9:J:55:VAL:HG23	1.98	0.46
13:N:7:LEU:O	13:N:11:LEU:HG	2.16	0.46
14:O:134:VAL:HG22	14:O:186:VAL:HG22	1.97	0.46
20:V:44:LYS:NZ	35:l:581:LYS:HE3	2.31	0.46
21:W:68:ARG:NH2	36:m:134:GLY:H	2.14	0.46
32:i:133:TRP:HE3	52:i:401:CDL:H371	1.81	0.46
49:C:303:PLX:H272	49:C:303:PLX:H102	1.97	0.45
8:I:106:LEU:HD23	8:I:106:LEU:HA	1.81	0.45
12:M:421:SER:OG	12:M:427:LEU:HD22	2.17	0.45
35:l:66:TRP:HZ3	48:l:703:PEE:H38	1.81	0.45
35:l:279:CYS:O	35:l:283:ILE:HG22	2.17	0.45
40:r:306:PRO:O	40:r:310:MET:HG3	2.16	0.45
43:v:17:PRO:HB3	43:v:105:GLU:HG2	1.98	0.45
44:w:189:GLU:O	44:w:193:VAL:HG22	2.16	0.45
50:C:304:DCQ:H3MB	16:Q:92:HIS:ND1	2.31	0.45
6:G:139:MET:HA	6:G:139:MET:HE3	1.99	0.45
52:V:201:CDL:H531	52:V:201:CDL:H562	1.65	0.45
48:V:202:PEE:H7	35:l:568:PHE:CE2	2.51	0.45
6:X:84:LEU:O	6:X:88:LYS:HG3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:g:109:LYS:HB3	30:g:113:GLU:HG3	1.97	0.45
33:j:73:LEU:O	41:s:160:TYR:OH	2.33	0.45
48:j:201:PEE:H35	48:j:201:PEE:H30	1.73	0.45
42:u:169:PHE:CE1	52:u:201:CDL:H542	2.51	0.45
12:M:632:MET:H	12:M:632:MET:HG2	1.60	0.45
22:Y:94:ASP:OD1	43:v:107:ARG:NH1	2.45	0.45
24:a:66:ARG:NH1	28:e:72:ASP:HB2	2.31	0.45
48:B:303:PEE:H59	41:s:277:TYR:CE2	2.51	0.45
50:C:304:DCQ:H1M	50:C:304:DCQ:H7	1.79	0.45
12:M:394:VAL:HG22	12:M:473:MET:HE1	1.99	0.45
28:e:76:TYR:HB2	28:e:83:ASP:OD1	2.16	0.45
33:j:95:LEU:HD13	41:s:302:MET:HG3	1.98	0.45
34:k:4:VAL:O	34:k:8:ILE:HG12	2.16	0.45
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.51	0.45
6:G:80:LYS:HE3	6:G:80:LYS:HB3	1.61	0.45
9:J:317:ASP:OD2	9:J:321:ARG:NH1	2.46	0.45
27:d:145:ASP:OD2	30:g:122:ARG:HD3	2.16	0.45
40:r:357:THR:O	40:r:361:VAL:HG23	2.16	0.45
44:w:223:ASN:ND2	44:w:226:GLU:HG3	2.22	0.45
24:a:78:THR:HG21	28:e:96:SER:O	2.16	0.45
52:a:201:CDL:H772	52:a:201:CDL:H212	1.98	0.45
33:j:69:ILE:HD11	41:s:144:VAL:HG22	1.99	0.45
40:r:126:LEU:HD21	40:r:153:THR:HG21	1.98	0.45
48:B:303:PEE:H55	48:B:303:PEE:H61	1.71	0.45
6:G:115:GLN:O	6:G:119:ILE:HG12	2.17	0.45
8:I:4:ALA:HA	52:I:201:CDL:HA22	1.97	0.45
8:I:69:VAL:O	15:P:76:VAL:HB	2.17	0.45
9:J:178:SER:HB2	9:J:317:ASP:OD1	2.17	0.45
16:Q:116:LEU:O	16:Q:118:2MR:HD3	2.17	0.45
24:a:63:TYR:OH	28:e:71:PRO:O	2.34	0.45
49:g:201:PLX:H122	49:g:201:PLX:H91	1.62	0.45
32:i:245:MET:HE3	32:i:245:MET:HB3	1.78	0.45
10:K:87:LEU:HD22	14:O:66:ILE:HD11	1.99	0.45
13:N:144:TYR:CZ	13:N:145:LYS:HD2	2.52	0.45
20:V:62:THR:O	20:V:66:ILE:HG13	2.17	0.45
31:h:97:HIS:HA	31:h:102:GLU:HB3	1.98	0.45
32:i:81:SER:O	32:i:83:GLN:N	2.47	0.45
34:k:37:MET:HE3	34:k:67:ALA:HB2	1.98	0.45
52:o:201:CDL:H841	52:o:201:CDL:H872	1.79	0.45
42:u:80:GLU:HB2	42:u:81:PRO:HD3	1.99	0.45
12:M:460:HIS:CG	12:M:461:PRO:CD	2.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:460:HIS:HA	12:M:461:PRO:HD3	1.81	0.45
24:a:78:THR:CG2	28:e:100:VAL:CG2	2.92	0.45
30:g:5:SER:HB2	49:g:201:PLX:H1A1	1.98	0.45
35:l:5:ALA:HB2	35:l:61:MET:SD	2.57	0.45
36:m:101:PHE:C	36:m:101:PHE:CD1	2.95	0.45
44:w:65:ASN:OD1	44:w:66:ILE:N	2.37	0.45
7:H:35:LEU:HD23	7:H:38:ILE:HD12	1.99	0.45
16:Q:51:VAL:HG13	16:Q:52:MET:O	2.17	0.45
20:V:59:TYR:CD1	52:V:201:CDL:H112	2.52	0.45
35:l:566:THR:O	35:l:570:GLN:HG2	2.17	0.45
2:B:39:LYS:HD2	16:Q:335:GLU:HG2	1.99	0.44
3:C:107:GLY:HA2	45:C:301:SF4:S1	2.56	0.44
12:M:335:GLY:HA2	12:M:362:ASP:O	2.17	0.44
12:M:573:GLY:HA3	13:N:137:TRP:CD1	2.52	0.44
20:V:104:ARG:HG3	20:V:104:ARG:HH11	1.82	0.44
24:a:106:VAL:HG23	37:n:50:ARG:HH21	1.82	0.44
34:k:13:ALA:HB1	52:k:101:CDL:H821	2.00	0.44
52:o:201:CDL:H812	52:o:201:CDL:H781	1.89	0.44
12:M:559:ASP:N	12:M:559:ASP:OD1	2.50	0.44
14:O:159:LYS:HD2	14:O:159:LYS:HA	1.72	0.44
16:Q:53:TYR:CD2	35:l:571:MET:HG3	2.52	0.44
22:Y:66:TRP:CZ2	23:Z:68:LEU:HD23	2.52	0.44
40:r:233:ALA:HA	40:r:320:GLY:HA2	1.99	0.44
12:M:144:MET:O	16:Q:362:LYS:HE3	2.17	0.44
52:V:201:CDL:H322	52:V:201:CDL:H352	1.40	0.44
28:e:94:GLY:O	28:e:99:LEU:HD13	2.16	0.44
38:o:82:PRO:HB2	52:o:201:CDL:HB4	1.99	0.44
40:r:369:LEU:HD23	52:r:502:CDL:H371	1.99	0.44
52:s:401:CDL:H362	52:s:401:CDL:H201	1.98	0.44
1:A:195:VAL:O	10:K:97:ARG:NH1	2.48	0.44
2:B:89:GLU:OE1	13:N:58:ARG:HD2	2.18	0.44
12:M:562:LYS:HE2	12:M:562:LYS:HB3	1.75	0.44
26:c:168:LEU:HD21	26:c:174:PRO:HB3	1.99	0.44
39:p:27:LEU:HD21	39:p:40:PHE:HB3	1.99	0.44
39:p:138:LYS:HB3	39:p:138:LYS:HE3	1.76	0.44
41:s:2:PHE:CE2	41:s:6:ILE:HD11	2.51	0.44
41:s:62:ARG:NE	41:s:68:ILE:HD13	2.32	0.44
44:w:123:SER:OG	44:w:125:ASP:OD1	2.32	0.44
2:B:171:PRO:HG3	2:B:200:GLU:HG2	2.00	0.44
9:J:179:ARG:NH1	9:J:179:ARG:CB	2.80	0.44
25:b:120:MET:O	25:b:120:MET:HG2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:49:VAL:HB	35:l:50:PRO:HD3	1.99	0.44
35:l:190:LEU:HD22	40:r:383:THR:HG21	1.98	0.44
38:o:8:PRO:HG3	38:o:14:LEU:HB2	1.99	0.44
1:A:224:ARG:HD2	11:L:164:PHE:CZ	2.53	0.44
25:b:123:PHE:HB3	43:v:40:VAL:CG1	2.46	0.44
30:g:13:LEU:HA	49:g:201:PLX:H32	2.00	0.44
42:u:139:GLU:OE2	42:u:139:GLU:N	2.47	0.44
44:w:110:GLY:HA2	44:w:134:TRP:CE2	2.52	0.44
44:w:285:ASP:OD1	44:w:285:ASP:N	2.49	0.44
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.69	0.44
52:V:201:CDL:H542	52:V:201:CDL:H512	1.62	0.44
41:s:186:PHE:O	41:s:189:THR:OG1	2.28	0.44
48:B:303:PEE:H59	41:s:277:TYR:HE2	1.83	0.44
12:M:208:THR:OG1	12:M:210:ILE:O	2.30	0.44
12:M:484:SER:OG	12:M:680:LEU:HD11	2.18	0.44
25:b:32:GLU:HB3	39:p:115:TYR:HD1	1.83	0.44
33:j:67:LEU:HD22	36:m:59:ILE:HD12	2.00	0.44
41:s:70:MET:HB3	41:s:122:ALA:HB2	2.00	0.44
43:v:113:LYS:HE3	43:v:113:LYS:HB3	1.89	0.44
44:w:296:MET:HE2	44:w:296:MET:HA	1.99	0.44
1:A:281:HIS:NE2	1:A:361:THR:OG1	2.50	0.44
1:A:326:LEU:HD23	1:A:367:ILE:HD11	2.00	0.44
50:C:304:DCQ:H16A	50:C:304:DCQ:H13A	1.82	0.44
53:J:401:NDP:H2D	53:J:401:NDP:H2N	1.70	0.44
32:i:146:SER:HA	32:i:149:ILE:HG12	1.99	0.44
1:A:281:HIS:CD2	1:A:358:ASP:H	2.36	0.43
1:A:392:MET:HE2	1:A:419:ILE:HD12	2.00	0.43
12:M:354:LEU:HD22	12:M:548:LEU:HD22	1.98	0.43
12:M:555:ILE:O	12:M:555:ILE:HG13	2.17	0.43
27:d:3:ASP:OD1	27:d:3:ASP:N	2.45	0.43
28:e:73:SER:O	28:e:75:GLY:N	2.51	0.43
31:h:94:PRO:HG2	31:h:99:LEU:HD11	2.00	0.43
35:l:27:TYR:O	35:l:115:ASN:ND2	2.50	0.43
36:m:34:ILE:HG13	36:m:64:MET:HG3	2.00	0.43
40:r:361:VAL:HG13	52:r:502:CDL:H352	2.00	0.43
7:H:37:GLN:HB2	7:H:95:LEU:HD11	2.00	0.43
9:J:129:LEU:HD23	9:J:167:ILE:HG13	1.99	0.43
49:J:403:PLX:H111	49:J:403:PLX:H82	1.47	0.43
11:L:101:PHE:CE2	11:L:121:LEU:HD13	2.53	0.43
26:c:48:ARG:HH22	26:c:63:GLU:CD	2.26	0.43
32:i:307:SER:OG	32:i:308:THR:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:o:201:CDL:H761	52:o:201:CDL:H792	1.54	0.43
41:s:192:GLU:OE2	41:s:234:MET:HE2	2.17	0.43
52:u:201:CDL:H552	52:u:201:CDL:H581	1.62	0.43
44:w:56:THR:O	44:w:56:THR:HG22	2.18	0.43
1:A:59:ARG:O	14:O:239:LYS:O	2.37	0.43
7:H:50:GLN:O	7:H:54:GLU:HG3	2.17	0.43
22:Y:42:PRO:HB2	23:Z:14:MET:HE3	1.99	0.43
25:b:120:MET:HE2	43:v:64:ILE:HG21	1.99	0.43
49:j:203:PLX:H311	49:j:203:PLX:H282	1.42	0.43
38:o:83:THR:HG22	38:o:85:LYS:H	1.82	0.43
40:r:406:TYR:O	40:r:409:TYR:HB3	2.18	0.43
54:s:402:UQ:H202	54:s:402:UQ:H172	1.83	0.43
49:J:403:PLX:H201	33:j:20:ILE:HD11	2.00	0.43
12:M:487:THR:HB	12:M:677:GLN:NE2	2.33	0.43
20:V:45:PRO:HD2	35:l:581:LYS:NZ	2.32	0.43
22:Y:80:VAL:HG23	35:l:385:TYR:OH	2.18	0.43
41:s:85:MET:HE3	41:s:233:MET:CE	2.44	0.43
6:G:105:MET:HG3	6:G:110:LEU:O	2.18	0.43
25:b:32:GLU:OE2	39:p:117:ASP:HB2	2.18	0.43
49:j:203:PLX:H152	49:j:203:PLX:H341	2.01	0.43
43:v:18:ASP:O	43:v:22:MET:HB2	2.19	0.43
44:w:305:LEU:O	44:w:308:THR:OG1	2.34	0.43
2:B:135:ARG:HD3	2:B:141:ARG:HG3	2.01	0.43
48:B:303:PEE:H69	48:B:303:PEE:H62	1.67	0.43
5:F:23:LEU:O	5:F:57:GLU:HA	2.19	0.43
21:W:98:MET:HE2	21:W:104:TRP:CD2	2.53	0.43
27:d:43:ARG:HB3	27:d:44:PRO:HD3	1.99	0.43
32:i:42:PRO:HG3	36:m:167:VAL:HG13	2.00	0.43
32:i:270:MET:HE1	32:i:278:MET:HG2	2.00	0.43
34:k:5:TYR:CD1	34:k:43:MET:HE1	2.53	0.43
35:l:241:THR:HG21	35:l:344:GLY:HA3	1.99	0.43
41:s:179:TRP:CG	41:s:180:PRO:HD3	2.54	0.43
14:O:199:LYS:HE2	14:O:199:LYS:HB2	1.76	0.43
16:Q:206:GLU:O	16:Q:210:MET:HG3	2.18	0.43
21:W:103:ASP:OD1	21:W:103:ASP:N	2.52	0.43
33:j:68:GLU:HG3	33:j:98:LEU:HD13	2.00	0.43
52:k:101:CDL:H671	52:k:101:CDL:H641	1.86	0.43
35:l:557:TRP:O	35:l:561:ILE:HG12	2.18	0.43
40:r:71:TRP:O	40:r:74:PRO:HD2	2.18	0.43
40:r:290:SER:HA	40:r:319:HIS:HE2	1.84	0.43
44:w:354:LEU:HD12	44:w:354:LEU:HA	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:66:PRO:HB3	15:P:79:SER:HA	2.01	0.43
32:i:23:SER:HB2	32:i:29:ILE:HG13	2.01	0.43
52:k:101:CDL:H781	36:m:99:MET:SD	2.59	0.43
35:l:10:THR:O	35:l:14:ILE:HG23	2.18	0.43
35:l:529:TYR:HB3	35:l:530:PRO:HD3	2.00	0.43
4:E:119:LEU:HD22	12:M:628:GLU:HG2	2.00	0.43
7:H:77:ILE:HA	7:H:80:VAL:HB	2.00	0.43
9:J:204:SER:OG	9:J:238:GLN:O	2.37	0.43
24:a:130:GLU:H	24:a:130:GLU:CD	2.27	0.43
32:i:128:LEU:O	32:i:132:THR:OG1	2.26	0.43
40:r:218:LYS:O	40:r:222:GLU:HG2	2.19	0.43
41:s:233:MET:SD	41:s:233:MET:C	3.02	0.43
41:s:267:THR:O	41:s:271:LEU:HG	2.19	0.43
2:B:120:GLU:HB2	2:B:130:ILE:HD12	2.00	0.43
4:E:101:THR:OG1	15:P:219:VAL:O	2.26	0.43
12:M:262:VAL:HG23	12:M:276:ARG:HB2	2.01	0.43
22:Y:44:TYR:O	22:Y:45:ARG:HB2	2.19	0.43
22:Y:99:ILE:O	22:Y:99:ILE:HG13	2.19	0.43
28:e:72:ASP:OD1	28:e:72:ASP:N	2.52	0.43
52:g:202:CDL:H242	40:r:97:THR:HG21	2.01	0.43
32:i:186:HIS:O	32:i:190:MET:HE3	2.19	0.43
35:l:435:PRO:HB3	35:l:437:PHE:CZ	2.54	0.43
39:p:50:GLU:OE2	39:p:51:HIS:NE2	2.52	0.43
42:u:47:ARG:HD2	42:u:47:ARG:HA	1.76	0.43
12:M:137:CYS:HB3	12:M:140:GLN:HB2	2.00	0.42
14:O:137:THR:HG22	14:O:138:THR:H	1.84	0.42
26:c:67:ASP:O	38:o:81:ARG:NH2	2.52	0.42
35:l:503:GLU:OE2	35:l:503:GLU:HA	2.19	0.42
40:r:87:GLU:OE1	40:r:91:ARG:HD2	2.19	0.42
40:r:325:MET:HE2	40:r:362:ALA:HB2	2.01	0.42
40:r:328:CYS:HB3	40:r:437:MET:HE1	2.00	0.42
3:C:56:TRP:CE2	49:C:303:PLX:H91	2.54	0.42
3:C:113:MET:O	3:C:113:MET:HG3	2.18	0.42
54:J:402:UQ:H202	54:J:402:UQ:H221	1.93	0.42
12:M:266:ARG:HG2	12:M:267:THR:HG23	2.00	0.42
22:Y:80:VAL:HG23	35:l:385:TYR:CZ	2.53	0.42
32:i:68:MET:HB3	34:k:36:MET:HE2	2.01	0.42
37:n:46:LYS:HB2	37:n:46:LYS:HE2	1.76	0.42
41:s:307:LEU:HB3	41:s:308:PRO:HD3	2.01	0.42
54:s:402:UQ:H152	54:s:402:UQ:H121	1.80	0.42
44:w:353:TRP:H	44:w:353:TRP:CD1	2.36	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:17:VAL:HG21	11:L:55:VAL:HG22	2.01	0.42
16:Q:157:LYS:HE3	16:Q:157:LYS:HB2	1.83	0.42
25:b:88:TYR:CE1	27:d:49:ARG:HG2	2.54	0.42
38:o:88:LEU:HD21	52:o:201:CDL:H362	2.00	0.42
41:s:24:GLU:OE1	41:s:274:ARG:NH1	2.52	0.42
41:s:209:SER:HB3	41:s:213:VAL:HA	2.00	0.42
43:v:39:MET:HE1	43:v:57:ASP:O	2.19	0.42
44:w:88:GLU:N	44:w:160:GLU:HG3	2.34	0.42
44:w:345:GLU:HB3	44:w:352:ILE:HD12	2.01	0.42
1:A:396:MET:HE3	1:A:396:MET:HB3	1.92	0.42
8:I:113:LEU:HD12	8:I:113:LEU:HA	1.84	0.42
9:J:324:MET:HE3	9:J:324:MET:HB2	1.73	0.42
12:M:241:ARG:O	12:M:244:GLU:HG2	2.18	0.42
32:i:189:TRP:CE2	32:i:263:LYS:HE3	2.55	0.42
35:l:102:GLU:OE1	35:l:456:ARG:NH2	2.46	0.42
35:l:124:PHE:HE1	35:l:252:MET:HB2	1.85	0.42
42:u:38:LYS:HB3	42:u:39:PRO:HD3	2.00	0.42
6:G:86:VAL:HG23	6:G:122:MET:HE1	2.01	0.42
7:H:54:GLU:O	7:H:58:MET:HG3	2.20	0.42
9:J:279:TYR:HB2	9:J:372:ALA:HB2	2.01	0.42
17:S:45:TRP:CD1	21:W:140:PHE:HB2	2.55	0.42
32:i:172:GLN:HB2	32:i:178:ILE:HG13	2.01	0.42
35:l:41:SER:O	35:l:45:THR:HG22	2.19	0.42
36:m:65:LEU:HD12	41:s:117:LEU:HD11	2.00	0.42
38:o:3:PHE:CE2	39:p:70:GLU:HG3	2.54	0.42
38:o:3:PHE:CZ	39:p:70:GLU:HG3	2.54	0.42
40:r:118:PHE:O	40:r:122:PHE:HB3	2.19	0.42
40:r:373:ILE:HD11	40:r:444:LEU:HD12	2.02	0.42
41:s:54:LYS:HE3	41:s:54:LYS:HB3	1.88	0.42
1:A:314:LEU:HD11	1:A:317:VAL:HG23	2.01	0.42
4:E:37:ARG:HA	6:G:120:MET:HE1	2.02	0.42
12:M:389:THR:O	12:M:390:THR:OG1	2.30	0.42
22:Y:94:ASP:O	22:Y:98:GLY:N	2.52	0.42
9:J:229:ILE:HG13	9:J:298:TYR:HD2	1.84	0.42
20:V:38:ALA:HB2	52:k:101:CDL:H251	2.02	0.42
27:d:122:ARG:HA	27:d:122:ARG:HD3	1.85	0.42
28:e:55:LEU:CD2	28:e:57:GLU:HB2	2.49	0.42
32:i:230:LEU:HD11	32:i:244:MET:HE1	2.02	0.42
40:r:329:LEU:O	40:r:332:THR:OG1	2.37	0.42
44:w:57:SER:HB3	44:w:150:LEU:HD11	2.01	0.42
1:A:265:PHE:HB3	1:A:291:GLU:HG3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:161:ILE:HG13	3:C:180:LEU:HB2	2.00	0.42
4:E:21:PHE:HE2	4:E:84:ILE:HD11	1.85	0.42
5:F:90:THR:O	5:F:94:VAL:HG23	2.20	0.42
32:i:170:LEU:HD11	32:i:288:LEU:HD22	2.01	0.42
2:B:44:ARG:HH11	2:B:44:ARG:HG2	1.83	0.42
3:C:116:ALA:O	3:C:120:VAL:HG22	2.19	0.42
4:E:27:GLU:H	4:E:27:GLU:HG3	1.64	0.42
5:F:20:ARG:HB2	5:F:66:TRP:HB2	2.02	0.42
11:L:145:PHE:HD2	11:L:147:VAL:HG23	1.85	0.42
13:N:24:LEU:O	13:N:28:PHE:HD1	2.03	0.42
16:Q:178:THR:OG1	16:Q:214:TYR:OH	2.37	0.42
20:V:120:LEU:HD13	20:V:120:LEU:HA	1.94	0.42
52:a:201:CDL:H182	52:a:201:CDL:H211	1.95	0.42
33:j:70:ALA:HB2	36:m:55:MET:HE2	2.01	0.42
35:l:286:LEU:HD22	35:l:411:MET:SD	2.60	0.42
35:l:500:LEU:HB2	52:l:701:CDL:H551	2.02	0.42
35:l:526:LEU:HD12	35:l:530:PRO:HG2	2.01	0.42
2:B:111:GLU:O	2:B:141:ARG:NH1	2.53	0.42
49:J:403:PLX:H162	49:J:403:PLX:H131	1.90	0.42
17:S:19:PRO:HB3	41:s:9:LEU:HD12	2.01	0.42
32:i:171:ASN:HB2	35:l:574:SER:OG	2.20	0.42
34:k:3:LEU:HD12	34:k:3:LEU:HA	1.85	0.42
35:l:76:LEU:HD21	35:l:196:TRP:HE3	1.84	0.42
41:s:225:MET:HE3	54:s:402:UQ:H221	2.01	0.42
2:B:173:PHE:CE2	3:C:171:GLU:HG2	2.51	0.41
2:B:200:GLU:HG3	13:N:88:ARG:HD3	2.01	0.41
3:C:62:LEU:O	3:C:91:VAL:HA	2.20	0.41
4:E:119:LEU:HA	4:E:119:LEU:HD12	1.83	0.41
12:M:598:ASN:ND2	12:M:599:THR:H	2.17	0.41
49:e:201:PLX:H341	40:r:71:TRP:CG	2.55	0.41
32:i:141:VAL:O	32:i:145:ILE:HG12	2.21	0.41
35:l:457:LEU:HD23	35:l:457:LEU:HA	1.87	0.41
44:w:102:LYS:HB3	44:w:102:LYS:HE3	1.82	0.41
5:F:27:SER:HA	5:F:28:PRO:HD3	1.73	0.41
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.49	0.41
12:M:400:ILE:HD12	12:M:473:MET:SD	2.60	0.41
19:U:38:TYR:HB2	41:s:310:MET:O	2.20	0.41
20:V:81:ARG:NH2	20:V:86:ASP:OD2	2.53	0.41
6:X:125:GLU:OE2	35:l:439:PRO:HG3	2.20	0.41
24:a:78:THR:HG22	28:e:100:VAL:HG21	2.01	0.41
26:c:33:THR:OG1	26:c:34:LYS:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:190:LEU:HB2	35:l:196:TRP:NE1	2.34	0.41
35:l:600:THR:HG22	35:l:601:LEU:HD12	2.02	0.41
52:l:701:CDL:H861	52:l:701:CDL:H201	2.02	0.41
38:o:111:LYS:HB2	38:o:111:LYS:HE3	1.66	0.41
40:r:119:TYR:CZ	40:r:161:LEU:HB2	2.55	0.41
44:w:48:ARG:HD3	44:w:48:ARG:HA	1.75	0.41
9:J:49:SER:HB2	15:P:225:GLU:HB3	2.01	0.41
6:X:82:ARG:HD3	22:Y:44:TYR:HE1	1.85	0.41
52:a:201:CDL:H1	48:l:703:PEE:H48	2.02	0.41
26:c:143:MET:HB3	35:l:407:TRP:CD2	2.55	0.41
52:g:202:CDL:H741	52:g:202:CDL:H772	1.62	0.41
52:l:701:CDL:H371	52:l:701:CDL:H601	2.02	0.41
38:o:48:LEU:HB3	39:p:166:LEU:HD13	2.01	0.41
40:r:186:LEU:HD23	40:r:186:LEU:HA	1.85	0.41
52:r:502:CDL:H812	52:r:502:CDL:H841	1.79	0.41
52:u:201:CDL:H741	52:u:201:CDL:H711	1.75	0.41
1:A:398:ARG:HH22	1:A:408:GLU:CD	2.28	0.41
52:g:202:CDL:H761	52:g:202:CDL:H791	1.52	0.41
35:l:285:THR:HA	35:l:308:SER:HA	2.02	0.41
35:l:295:GLN:HB2	35:l:301:ILE:HG12	2.02	0.41
40:r:346:ARG:O	40:r:419:TYR:HA	2.21	0.41
9:J:122:HIS:HB3	18:T:50:TYR:HA	2.01	0.41
12:M:171:THR:HG23	12:M:173:MET:HG2	2.01	0.41
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.84	0.41
21:W:123:GLU:OE1	31:h:72:THR:HG21	2.20	0.41
23:Z:13:LYS:HD2	23:Z:13:LYS:HA	1.87	0.41
26:c:113:ILE:HD11	26:c:116:ARG:HD2	2.03	0.41
28:e:70:ASN:O	28:e:73:SER:HB3	2.21	0.41
1:A:75:TRP:O	1:A:79:GLU:HG2	2.21	0.41
46:A:502:FMN:HM81	46:A:502:FMN:HM73	1.85	0.41
11:L:145:PHE:CD2	11:L:147:VAL:HG23	2.56	0.41
12:M:639:LEU:O	12:M:643:ARG:HG3	2.21	0.41
12:M:640:ASP:OD1	12:M:640:ASP:N	2.52	0.41
15:P:190:ASP:OD1	15:P:191:TYR:N	2.53	0.41
16:Q:176:GLU:OE2	16:Q:311:TYR:OH	2.24	0.41
16:Q:198:THR:OG1	41:s:275:ALA:O	2.31	0.41
30:g:85:TYR:CZ	32:i:344:SER:HB3	2.56	0.41
32:i:88:LYS:HG2	32:i:148:SER:HB2	2.01	0.41
32:i:312:LYS:HE3	44:w:327:VAL:HG11	2.03	0.41
35:l:128:MET:SD	35:l:252:MET:HA	2.61	0.41
40:r:237:LYS:HD2	40:r:316:MET:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:47:TYR:O	7:H:51:ILE:HG23	2.21	0.41
52:V:201:CDL:H511	35:l:576:MET:O	2.21	0.41
52:V:201:CDL:H641	35:l:597:ILE:HG21	2.03	0.41
22:Y:71:TRP:CD2	22:Y:75:HIS:CE1	3.05	0.41
35:l:9:LEU:HD23	35:l:9:LEU:HA	1.87	0.41
35:l:83:ASP:OD2	35:l:262:ARG:NH1	2.52	0.41
35:l:288:THR:HG21	35:l:307:SER:HB3	2.01	0.41
41:s:207:LEU:O	41:s:209:SER:N	2.53	0.41
43:v:70:LYS:HD3	43:v:80:CYS:SG	2.61	0.41
1:A:109:ARG:NH1	1:A:237:GLY:O	2.49	0.41
5:F:59:SER:O	5:F:61:VAL:N	2.53	0.41
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.56	0.41
19:U:43:ILE:O	19:U:47:ARG:HG3	2.21	0.41
22:Y:84:PHE:HE2	43:v:88:ASP:HB3	1.85	0.41
25:b:106:PRO:HG3	43:v:45:GLU:OE2	2.20	0.41
25:b:120:MET:HE1	43:v:64:ILE:CG2	2.51	0.41
26:c:153:TYR:HB3	35:l:403:TYR:HD2	1.85	0.41
27:d:160:LYS:NZ	30:g:114:ILE:O	2.53	0.41
29:f:46:LEU:HD23	29:f:46:LEU:HA	1.94	0.41
33:j:106:TRP:CE3	48:j:201:PEE:H20	2.56	0.41
35:l:54:PHE:CZ	35:l:84:TYR:HB2	2.56	0.41
40:r:87:GLU:HG3	40:r:88:THR:N	2.35	0.41
40:r:196:TRP:HB2	40:r:253:LEU:HD23	2.02	0.41
41:s:157:ASN:OD1	41:s:168:THR:OG1	2.27	0.41
1:A:326:LEU:HD22	1:A:363:ILE:HD11	2.02	0.41
2:B:80:GLU:HG3	17:S:1:MET:SD	2.61	0.41
4:E:19:PRO:HB3	11:L:53:ILE:HG21	2.02	0.41
5:F:61:VAL:HG23	5:F:62:GLN:H	1.85	0.41
8:I:97:PRO:HD3	15:P:61:PHE:CE1	2.55	0.41
9:J:328:THR:HG22	9:J:330:PRO:HD3	2.02	0.41
49:J:403:PLX:H321	49:J:403:PLX:H291	1.61	0.41
12:M:543:LYS:HB3	12:M:543:LYS:HE2	1.85	0.41
12:M:556:THR:OG1	12:M:558:GLN:HG2	2.21	0.41
17:S:66:LEU:HD13	42:u:75:LYS:HB2	2.03	0.41
21:W:121:MET:SD	36:m:130:THR:HB	2.60	0.41
24:a:72:ARG:HE	24:a:72:ARG:HB3	1.74	0.41
49:a:202:PLX:H141	28:e:105:PHE:HB2	2.02	0.41
25:b:97:VAL:HG22	35:l:63:ILE:HG23	2.02	0.41
26:c:140:MET:HE1	35:l:411:MET:SD	2.61	0.41
26:c:167:TYR:CD2	26:c:178:PRO:HG3	2.55	0.41
27:d:80:LYS:HD3	27:d:80:LYS:HA	1.90	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:e:74:HIS:HB2	28:e:83:ASP:OD2	2.21	0.41
35:l:341:MET:SD	35:l:457:LEU:HD12	2.61	0.41
48:l:703:PEE:H55	48:l:703:PEE:H60	1.86	0.41
40:r:49:SER:HB2	40:r:58:SER:O	2.21	0.41
1:A:367:ILE:O	1:A:371:ILE:HG12	2.21	0.41
12:M:51:GLN:O	12:M:54:GLU:HG2	2.21	0.41
12:M:256:ALA:O	12:M:598:ASN:ND2	2.54	0.41
12:M:581:ASP:OD1	13:N:144:TYR:OH	2.25	0.41
14:O:231:LEU:HD12	14:O:231:LEU:HA	1.91	0.41
15:P:75:GLN:HB3	15:P:87:PHE:CD1	2.56	0.41
52:g:202:CDL:H801	52:g:202:CDL:H241	2.03	0.41
1:A:43:THR:OG1	1:A:59:ARG:CD	2.67	0.40
9:J:64:PHE:HZ	9:J:208:GLY:HA3	1.86	0.40
11:L:79:ILE:HB	11:L:147:VAL:HG22	2.03	0.40
21:W:105:LYS:HB2	21:W:108:GLU:HB2	2.01	0.40
25:b:100:ARG:CD	35:l:60:GLU:HB2	2.50	0.40
44:w:265:ASP:OD1	44:w:268:LYS:HG3	2.20	0.40
44:w:287:ASP:OD1	44:w:287:ASP:N	2.50	0.40
1:A:217:GLU:CD	11:L:171:ARG:HH22	2.28	0.40
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.85	0.40
6:G:91:ASP:OD1	6:G:91:ASP:N	2.53	0.40
20:V:34:LEU:HD23	20:V:34:LEU:HA	1.93	0.40
35:l:250:SER:HB2	35:l:333:ALA:HA	2.02	0.40
35:l:357:ARG:HG2	39:p:32:VAL:HG22	2.03	0.40
1:A:113:LEU:HD13	1:A:149:MET:HE1	2.03	0.40
10:K:88:ASP:OD1	10:K:88:ASP:N	2.52	0.40
13:N:85:GLU:HG2	13:N:86:TRP:H	1.85	0.40
17:S:63:THR:HG23	42:u:21:SER:HB2	2.03	0.40
19:U:66:VAL:O	42:u:130:LYS:HE3	2.21	0.40
21:W:86:MET:HE1	21:W:125:TYR:CZ	2.57	0.40
22:Y:65:MET:HE2	22:Y:65:MET:HB3	1.85	0.40
27:d:124:ASN:OD1	27:d:124:ASN:N	2.55	0.40
32:i:106:LEU:HG	32:i:138:PRO:HB2	2.03	0.40
38:o:91:ALA:O	38:o:95:ILE:HG12	2.21	0.40
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.47	0.40
44:w:108:LEU:HD21	44:w:330:LYS:HB3	2.04	0.40
8:I:90:THR:HG23	8:I:92:LYS:HB2	2.03	0.40
13:N:78:ASP:OD2	13:N:80:SER:OG	2.26	0.40
16:Q:356:ILE:H	16:Q:356:ILE:HG13	1.80	0.40
17:S:12:MET:HG2	41:s:264:LEU:HD21	2.03	0.40
25:b:19:ARG:HA	39:p:171:VAL:HG13	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:e:201:PLX:H341	40:r:71:TRP:CD2	2.55	0.40
32:i:5:ILE:HD13	32:i:5:ILE:HA	1.93	0.40
32:i:153:LEU:O	32:i:157:MET:HG3	2.21	0.40
35:l:89:PHE:CD2	35:l:132:VAL:HG21	2.56	0.40
36:m:104:VAL:O	36:m:108:LEU:HG	2.20	0.40
12:M:388:ASN:HB3	12:M:511:LYS:CD	2.52	0.40
16:Q:335:GLU:O	16:Q:339:GLN:HG2	2.21	0.40
16:Q:342:ARG:HD2	21:W:21:TYR:CZ	2.57	0.40
48:W:201:PEE:H51	41:s:104:PHE:CD1	2.56	0.40
25:b:120:MET:HE1	43:v:64:ILE:HB	2.03	0.40
26:c:127:ASN:O	26:c:131:LYS:HE2	2.21	0.40
26:c:153:TYR:HB3	35:l:403:TYR:CD2	2.57	0.40
26:c:177:GLU:OE2	26:c:177:GLU:HA	2.21	0.40
32:i:70:LEU:HD22	32:i:98:MET:SD	2.62	0.40
49:j:203:PLX:H22	49:j:203:PLX:H1C3	1.83	0.40
34:k:38:LEU:HB2	36:m:60:TYR:CZ	2.57	0.40
38:o:87:SER:HB3	52:o:201:CDL:H732	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/433 (100%)	421 (98%)	10 (2%)	0	100	100
2	B	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
3	C	154/156 (99%)	150 (97%)	4 (3%)	0	100	100
4	E	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
5	F	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
6	G	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
6	X	86/88 (98%)	85 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	110/112 (98%)	106 (96%)	3 (3%)	1 (1%)	14	30
8	I	93/112 (83%)	85 (91%)	8 (9%)	0	100	100
9	J	340/342 (99%)	329 (97%)	10 (3%)	1 (0%)	36	58
10	K	41/43 (95%)	41 (100%)	0	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	676 (98%)	12 (2%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	201 (94%)	14 (6%)	0	100	100
15	P	206/208 (99%)	200 (97%)	5 (2%)	1 (0%)	24	46
16	Q	427/430 (99%)	416 (97%)	11 (3%)	0	100	100
17	S	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
18	T	94/96 (98%)	94 (100%)	0	0	100	100
19	U	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
20	V	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
21	W	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
22	Y	65/67 (97%)	58 (89%)	7 (11%)	0	100	100
23	Z	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
24	a	136/138 (99%)	132 (97%)	4 (3%)	0	100	100
25	b	94/126 (75%)	89 (95%)	5 (5%)	0	100	100
26	c	154/156 (99%)	145 (94%)	9 (6%)	0	100	100
27	d	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
28	e	102/104 (98%)	97 (95%)	5 (5%)	0	100	100
29	f	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
30	g	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
31	h	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
32	i	345/347 (99%)	335 (97%)	10 (3%)	0	100	100
33	j	113/115 (98%)	109 (96%)	3 (3%)	1 (1%)	14	30
34	k	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
35	l	604/606 (100%)	586 (97%)	18 (3%)	0	100	100
36	m	173/175 (99%)	161 (93%)	12 (7%)	0	100	100
37	n	54/56 (96%)	53 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	o	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
39	p	176/178 (99%)	169 (96%)	6 (3%)	1 (1%)	21	42
40	r	457/459 (100%)	449 (98%)	8 (2%)	0	100	100
41	s	316/318 (99%)	305 (96%)	10 (3%)	1 (0%)	36	58
42	u	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	21	42
43	v	122/125 (98%)	118 (97%)	4 (3%)	0	100	100
44	w	318/320 (99%)	305 (96%)	13 (4%)	0	100	100
All	All	8175/8314 (98%)	7917 (97%)	251 (3%)	7 (0%)	49	70

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	P	44	ARG
7	H	77	ILE
9	J	38	HIS
33	j	40	GLY
39	p	174	PRO
41	s	208	VAL
42	u	152	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/346 (100%)	346 (100%)	0	100	100
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	130 (98%)	2 (2%)	57	80
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	74/76 (97%)	74 (100%)	0	100	100
6	G	76/81 (94%)	75 (99%)	1 (1%)	61	82
6	X	75/81 (93%)	74 (99%)	1 (1%)	61	82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	86 (99%)	1 (1%)	65	84
9	J	296/296 (100%)	292 (99%)	4 (1%)	59	81
10	K	42/42 (100%)	41 (98%)	1 (2%)	43	70
11	L	113/113 (100%)	110 (97%)	3 (3%)	39	67
12	M	580/580 (100%)	575 (99%)	5 (1%)	70	87
13	N	130/130 (100%)	128 (98%)	2 (2%)	57	80
14	O	183/183 (100%)	182 (100%)	1 (0%)	81	92
15	P	189/190 (100%)	186 (98%)	3 (2%)	55	79
16	Q	370/370 (100%)	367 (99%)	3 (1%)	73	88
17	S	57/58 (98%)	55 (96%)	2 (4%)	32	59
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	100 (99%)	1 (1%)	68	86
21	W	121/123 (98%)	119 (98%)	2 (2%)	53	78
22	Y	62/62 (100%)	60 (97%)	2 (3%)	34	62
23	Z	62/62 (100%)	61 (98%)	1 (2%)	55	79
24	a	121/121 (100%)	118 (98%)	3 (2%)	42	69
25	b	89/119 (75%)	88 (99%)	1 (1%)	65	84
26	c	141/141 (100%)	141 (100%)	0	100	100
27	d	155/155 (100%)	153 (99%)	2 (1%)	61	82
28	e	96/96 (100%)	94 (98%)	2 (2%)	47	73
29	f	36/45 (80%)	36 (100%)	0	100	100
30	g	108/109 (99%)	108 (100%)	0	100	100
31	h	93/93 (100%)	92 (99%)	1 (1%)	65	84
32	i	311/311 (100%)	310 (100%)	1 (0%)	86	94
33	j	100/100 (100%)	98 (98%)	2 (2%)	48	74
34	k	85/85 (100%)	84 (99%)	1 (1%)	63	83
35	l	537/540 (99%)	529 (98%)	8 (2%)	57	80
36	m	126/141 (89%)	124 (98%)	2 (2%)	55	79
37	n	53/53 (100%)	52 (98%)	1 (2%)	50	75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	o	113/113 (100%)	113 (100%)	0	100	100
39	p	159/159 (100%)	159 (100%)	0	100	100
40	r	410/410 (100%)	407 (99%)	3 (1%)	76	89
41	s	275/275 (100%)	274 (100%)	1 (0%)	84	93
42	u	153/153 (100%)	150 (98%)	3 (2%)	48	74
43	v	104/111 (94%)	103 (99%)	1 (1%)	68	86
44	w	281/283 (99%)	274 (98%)	7 (2%)	42	69
All	All	7147/7241 (99%)	7073 (99%)	74 (1%)	65	86

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	71	CYS
3	C	177	ILE
6	G	108	LEU
8	I	41	LEU
9	J	257	ASP
9	J	304	LEU
9	J	307	VAL
9	J	351	GLU
10	K	76	LEU
11	L	86	ASN
11	L	124	LEU
11	L	144	SER
12	M	171	THR
12	M	400	ILE
12	M	575	VAL
12	M	636	TYR
12	M	640	ASP
13	N	6	VAL
13	N	37	THR
14	O	64	GLU
15	P	75	GLN
15	P	156	SER
15	P	173	MET
16	Q	217	VAL
16	Q	263	THR
16	Q	453	THR
17	S	66	LEU
17	S	68	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	V	120	LEU
21	W	49	SER
21	W	144	THR
6	X	100	VAL
22	Y	62	SER
22	Y	97	LEU
23	Z	79	VAL
24	a	77	LEU
24	a	127	ASP
24	a	130	GLU
25	b	69	ILE
27	d	39	LEU
27	d	135	VAL
28	e	55	LEU
28	e	69	LYS
31	h	77	SER
32	i	67	SER
33	j	18	VAL
33	j	31	SER
34	k	3	LEU
35	l	12	LEU
35	l	100	ILE
35	l	104	SER
35	l	190	LEU
35	l	235	SER
35	l	338	MET
35	l	504	LEU
35	l	554	ASP
36	m	45	LEU
36	m	135	PHE
37	n	46	LYS
40	r	195	MET
40	r	256	TYR
40	r	304	GLN
41	s	81	LEU
42	u	9	THR
42	u	23	SER
42	u	64	ASN
43	v	109	LEU
44	w	45	LEU
44	w	95	ASP
44	w	133	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	w	192	LYS
44	w	216	SER
44	w	244	THR
44	w	254	GLU

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

Mol	Chain	Res	Type
1	A	284	HIS
1	A	393	ASN
1	A	457	HIS
3	C	111	ASN
4	E	70	ASN
4	E	126	HIS
5	F	73	GLN
5	F	86	GLN
8	I	21	GLN
9	J	122	HIS
9	J	295	HIS
12	M	598	ASN
12	M	669	ASN
12	M	677	GLN
13	N	12	GLN
13	N	31	ASN
13	N	112	ASN
14	O	41	HIS
14	O	90	ASN
14	O	131	HIS
14	O	182	ASN
14	O	246	GLN
15	P	51	ASN
15	P	55	HIS
15	P	82	ASN
15	P	131	ASN
15	P	196	HIS
15	P	228	GLN
16	Q	79	ASN
16	Q	190	HIS
16	Q	233	HIS
16	Q	265	ASN
17	S	61	HIS
21	W	24	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	Y	75	HIS
23	Z	21	GLN
25	b	83	HIS
27	d	131	GLN
28	e	86	ASN
29	f	61	GLN
30	g	18	ASN
30	g	90	HIS
32	i	150	ASN
32	i	197	ASN
32	i	204	ASN
32	i	232	HIS
34	k	57	ASN
35	l	135	ASN
35	l	139	GLN
35	l	199	GLN
35	l	296	ASN
35	l	348	HIS
35	l	446	ASN
35	l	470	ASN
39	p	12	HIS
40	r	43	ASN
40	r	51	ASN
40	r	138	ASN
40	r	139	GLN
40	r	175	ASN
40	r	366	ASN
40	r	415	GLN
41	s	47	GLN
41	s	194	ASN
41	s	287	HIS
42	u	151	ASN
43	v	110	GLN
44	w	223	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
16	2MR	Q	118	16	10,12,13	2.00	1 (10%)	5,13,15	5.93	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	5.68	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	12.04	130.52	119.48
16	Q	118	2MR	CD-NE-CZ	3.92	130.74	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.57	131.32	123.65

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 2 are monoatomic - leaving 43 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
46	FMN	A	502	-	33,33,33	1.07	2 (6%)	48,50,50	1.26	8 (16%)
49	PLX	C	303	-	51,51,51	1.20	4 (7%)	53,59,59	0.62	1 (1%)
49	PLX	j	203	-	51,51,51	1.21	4 (7%)	53,59,59	0.62	1 (1%)
51	8Q1	G	201	-	32,34,34	1.63	6 (18%)	39,43,43	1.70	5 (12%)
54	UQ	s	402	-	38,38,63	3.61	9 (23%)	48,49,79	2.80	17 (35%)
52	CDL	I	201	-	50,50,99	1.43	8 (16%)	56,62,111	1.14	4 (7%)
53	NDP	J	401	-	51,52,52	4.27	25 (49%)	71,80,80	2.22	13 (18%)
48	PEE	l	703	-	45,45,50	1.25	6 (13%)	48,50,55	1.03	2 (4%)
49	PLX	e	201	-	51,51,51	1.21	4 (7%)	53,59,59	0.56	1 (1%)
52	CDL	o	201	-	99,99,99	1.11	8 (8%)	105,111,111	0.90	4 (3%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
55	FES	O	301	14	0,4,4	-	-	-	-	-
52	CDL	k	101	-	99,99,99	1.12	8 (8%)	105,111,111	0.85	4 (3%)
52	CDL	a	201	-	99,99,99	1.11	8 (8%)	105,111,111	0.87	4 (3%)
48	PEE	j	201	-	50,50,50	1.17	6 (12%)	53,55,55	0.97	2 (3%)
48	PEE	W	201	-	40,40,50	1.17	5 (12%)	43,45,55	1.01	2 (4%)
49	PLX	g	201	-	51,51,51	1.21	4 (7%)	53,59,59	0.61	1 (1%)
52	CDL	g	202	-	99,99,99	1.11	8 (8%)	105,111,111	0.89	4 (3%)
52	CDL	s	401	-	88,88,99	1.16	8 (9%)	94,100,111	0.93	5 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	CDL	l	701	-	91,91,99	1.14	8 (8%)	97,103,111	0.90	4 (4%)
47	NAI	A	503	-	47,48,48	4.01	22 (46%)	64,73,73	1.70	12 (18%)
58	ADP	w	401	-	28,29,29	3.17	9 (32%)	43,45,45	1.93	9 (20%)
48	PEE	l	702	-	50,50,50	1.18	6 (12%)	53,55,55	0.97	2 (3%)
54	UQ	J	402	-	33,33,63	3.51	9 (27%)	42,43,79	2.74	14 (33%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
45	SF4	M	801	12	0,12,12	-	-	-	-	-
48	PEE	B	303	-	50,50,50	1.19	6 (12%)	53,55,55	1.01	2 (3%)
52	CDL	i	401	-	86,86,99	1.17	8 (9%)	92,98,111	0.90	4 (4%)
52	CDL	V	201	-	93,93,99	1.14	9 (9%)	99,105,111	0.89	4 (4%)
45	SF4	A	501	1	0,12,12	-	-	-	-	-
55	FES	M	803	12	0,4,4	-	-	-	-	-
48	PEE	V	202	-	39,39,50	1.33	6 (15%)	42,44,55	1.11	3 (7%)
48	PEE	j	202	-	40,40,50	1.17	5 (12%)	43,45,55	1.03	2 (4%)
52	CDL	r	502	-	98,98,99	1.11	8 (8%)	104,110,111	0.92	5 (4%)
52	CDL	u	201	-	54,54,99	1.38	8 (14%)	60,66,111	1.11	4 (6%)
49	PLX	a	202	-	51,51,51	1.21	4 (7%)	53,59,59	0.63	1 (1%)
50	DCQ	C	304	-	23,23,23	1.34	3 (13%)	27,29,29	0.99	1 (3%)
48	PEE	C	302	-	46,46,50	1.23	6 (13%)	49,51,55	1.00	2 (4%)
48	PEE	r	501	-	50,50,50	1.18	6 (12%)	53,55,55	0.99	2 (3%)
51	8Q1	X	201	-	32,34,34	1.61	6 (18%)	39,43,43	1.63	8 (20%)
49	PLX	J	403	-	51,51,51	1.21	4 (7%)	53,59,59	0.60	1 (1%)
45	SF4	C	301	3	0,12,12	-	-	-	-	-
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
46	FMN	A	502	-	-	9/18/18/18	0/3/3/3
49	PLX	C	303	-	-	30/55/55/55	-
49	PLX	j	203	-	-	32/55/55/55	-
51	8Q1	G	201	-	-	14/41/41/41	-
54	UQ	s	402	-	-	10/33/57/87	0/1/1/1
52	CDL	I	201	-	-	32/61/61/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	NDP	J	401	-	-	5/34/77/77	0/5/5/5
48	PEE	l	703	-	-	22/49/49/54	-
49	PLX	e	201	-	-	38/55/55/55	-
52	CDL	o	201	-	-	54/110/110/110	-
45	SF4	B	301	2	-	-	0/6/5/5
55	FES	O	301	14	-	-	0/1/1/1
52	CDL	k	101	-	-	61/110/110/110	-
52	CDL	a	201	-	-	52/110/110/110	-
48	PEE	j	201	-	-	25/54/54/54	-
48	PEE	W	201	-	-	14/44/44/54	-
49	PLX	g	201	-	-	32/55/55/55	-
52	CDL	g	202	-	-	59/110/110/110	-
52	CDL	s	401	-	-	60/99/99/110	-
52	CDL	l	701	-	-	53/102/102/110	-
47	NAI	A	503	-	-	7/29/72/72	0/5/5/5
58	ADP	w	401	-	-	2/16/32/32	0/3/3/3
48	PEE	l	702	-	-	29/54/54/54	-
54	UQ	J	402	-	-	14/27/51/87	0/1/1/1
45	SF4	M	802	12	-	-	0/6/5/5
45	SF4	M	801	12	-	-	0/6/5/5
48	PEE	B	303	-	-	24/54/54/54	-
52	CDL	i	401	-	-	53/97/97/110	-
52	CDL	V	201	-	-	61/104/104/110	-
45	SF4	A	501	1	-	-	0/6/5/5
55	FES	M	803	12	-	-	0/1/1/1
48	PEE	V	202	-	-	24/43/43/54	-
48	PEE	j	202	-	-	26/44/44/54	-
52	CDL	r	502	-	-	62/109/109/110	-
52	CDL	u	201	-	-	30/65/65/110	-
49	PLX	a	202	-	-	29/55/55/55	-
50	DCQ	C	304	-	-	4/14/38/38	0/1/1/1
48	PEE	C	302	-	-	23/50/50/54	-
48	PEE	r	501	-	-	24/54/54/54	-
51	8Q1	X	201	-	-	4/41/41/41	-
49	PLX	J	403	-	-	38/55/55/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	C	301	3	-	-	0/6/5/5
45	SF4	B	302	2	-	-	0/6/5/5

All (256) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	J	401	NDP	C3B-C2B	-13.19	1.24	1.53
53	J	401	NDP	O4D-C4D	10.68	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.33	1.26	1.53
54	J	402	UQ	C18-C19	10.00	1.56	1.33
53	J	401	NDP	C3D-C4D	-9.96	1.27	1.53
54	s	402	UQ	C18-C19	9.89	1.55	1.33
54	J	402	UQ	C13-C14	9.57	1.55	1.33
54	s	402	UQ	C13-C14	9.57	1.55	1.33
54	s	402	UQ	C23-C24	9.41	1.54	1.33
47	A	503	NAI	O4B-C1B	9.38	1.63	1.42
54	s	402	UQ	C8-C9	9.22	1.54	1.33
54	J	402	UQ	C8-C9	9.20	1.54	1.33
58	w	401	ADP	C3'-C4'	-8.91	1.30	1.53
47	A	503	NAI	O4B-C4B	-8.35	1.26	1.45
53	J	401	NDP	O4B-C4B	-7.85	1.27	1.45
58	w	401	ADP	O4'-C4'	7.74	1.62	1.45
47	A	503	NAI	C2D-C1D	-7.68	1.29	1.53
54	J	402	UQ	C23-C24	7.53	1.54	1.32
47	A	503	NAI	C2B-C1B	-7.38	1.30	1.53
53	J	401	NDP	C2N-C3N	7.36	1.55	1.35
53	J	401	NDP	C6N-C5N	7.35	1.55	1.33
54	s	402	UQ	C28-C29	7.34	1.54	1.32
47	A	503	NAI	O4D-C4D	6.97	1.60	1.45
53	J	401	NDP	PN-O3	6.53	1.66	1.59
58	w	401	ADP	PA-O3A	6.51	1.66	1.59
47	A	503	NAI	PA-O3	6.18	1.66	1.59
47	A	503	NAI	C2D-C3D	5.98	1.69	1.53
53	J	401	NDP	C6A-N6A	5.78	1.49	1.34
53	J	401	NDP	P2B-O2B	5.73	1.69	1.59
53	J	401	NDP	PA-O3	5.71	1.65	1.59
47	A	503	NAI	O4D-C1D	5.65	1.55	1.42
47	A	503	NAI	PN-O3	5.50	1.65	1.59
58	w	401	ADP	C6-N6	5.40	1.48	1.34
53	J	401	NDP	C3B-C4B	5.38	1.66	1.53
47	A	503	NAI	C7N-N7N	5.29	1.48	1.33
47	A	503	NAI	C4N-C3N	-5.28	1.40	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	G	201	8Q1	C39-N41	5.24	1.45	1.33
51	X	201	8Q1	C34-N36	5.08	1.45	1.33
47	A	503	NAI	C6A-N6A	5.07	1.47	1.34
53	J	401	NDP	C6N-N1N	5.06	1.49	1.37
51	X	201	8Q1	C39-N41	5.03	1.45	1.33
51	G	201	8Q1	C34-N36	5.02	1.45	1.33
53	J	401	NDP	O4D-C1D	-4.95	1.30	1.42
53	J	401	NDP	O4B-C1B	4.71	1.52	1.42
58	w	401	ADP	O4'-C1'	-4.62	1.31	1.42
53	J	401	NDP	C1B-N9A	-4.56	1.33	1.46
47	A	503	NAI	O2B-C2B	4.33	1.53	1.43
53	J	401	NDP	O2D-C2D	-3.96	1.33	1.43
48	V	202	PEE	C18-C19	3.84	1.53	1.31
48	l	702	PEE	C18-C19	3.83	1.53	1.31
48	B	303	PEE	C18-C19	3.83	1.53	1.31
48	r	501	PEE	C18-C19	3.83	1.53	1.31
48	j	202	PEE	C18-C19	3.82	1.53	1.31
53	J	401	NDP	C7N-N7N	3.82	1.44	1.33
48	C	302	PEE	C18-C19	3.81	1.53	1.31
48	l	703	PEE	C18-C19	3.81	1.53	1.31
48	W	201	PEE	C18-C19	3.80	1.53	1.31
48	j	201	PEE	C18-C19	3.79	1.53	1.31
48	C	302	PEE	C39-C38	3.75	1.53	1.31
48	l	703	PEE	C39-C38	3.75	1.53	1.31
48	B	303	PEE	C39-C38	3.74	1.53	1.31
48	r	501	PEE	C39-C38	3.74	1.52	1.31
48	j	201	PEE	C39-C38	3.72	1.52	1.31
48	l	702	PEE	C39-C38	3.72	1.52	1.31
48	V	202	PEE	C39-C38	3.70	1.52	1.31
47	A	503	NAI	C7N-C3N	3.61	1.56	1.48
52	u	201	CDL	OA8-CA7	3.53	1.43	1.33
52	i	401	CDL	OA8-CA7	3.51	1.43	1.33
52	l	701	CDL	OA8-CA7	3.46	1.43	1.33
52	s	401	CDL	OA8-CA7	3.46	1.43	1.33
58	w	401	ADP	C8-N9	-3.46	1.31	1.37
52	k	101	CDL	OA8-CA7	3.45	1.43	1.33
52	r	502	CDL	OA8-CA7	3.44	1.43	1.33
52	V	201	CDL	OA8-CA7	3.44	1.43	1.33
52	I	201	CDL	OA8-CA7	3.43	1.43	1.33
52	a	201	CDL	OA8-CA7	3.43	1.43	1.33
52	g	202	CDL	OA8-CA7	3.39	1.43	1.33
52	o	201	CDL	OA8-CA7	3.37	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	A	502	FMN	C4A-N5	3.33	1.38	1.30
47	A	503	NAI	C4N-C5N	-3.33	1.40	1.49
53	J	401	NDP	C8A-N9A	-3.22	1.32	1.37
52	V	201	CDL	OA6-CA5	3.15	1.43	1.34
58	w	401	ADP	O2'-C2'	-3.14	1.35	1.43
52	k	101	CDL	OA6-CA5	3.10	1.43	1.34
53	J	401	NDP	C5A-N7A	-3.07	1.33	1.39
52	i	401	CDL	OB6-CB5	3.07	1.42	1.34
52	l	701	CDL	OB6-CB5	3.06	1.42	1.34
52	i	401	CDL	OB8-CB7	3.06	1.42	1.33
52	I	201	CDL	OB8-CB7	3.05	1.42	1.33
52	r	502	CDL	OB6-CB5	3.05	1.42	1.34
52	l	701	CDL	OB8-CB7	3.05	1.42	1.33
53	J	401	NDP	C7N-C3N	3.04	1.55	1.48
52	a	201	CDL	OB6-CB5	3.03	1.42	1.34
52	s	401	CDL	OB6-CB5	3.02	1.42	1.34
52	a	201	CDL	OB8-CB7	3.02	1.42	1.33
52	r	502	CDL	OB8-CB7	3.01	1.42	1.33
52	o	201	CDL	OA6-CA5	3.01	1.42	1.34
52	I	201	CDL	OB6-CB5	3.01	1.42	1.34
52	g	202	CDL	OB6-CB5	3.00	1.42	1.34
52	k	101	CDL	OB8-CB7	3.00	1.42	1.33
52	u	201	CDL	OB6-CB5	2.99	1.42	1.34
52	I	201	CDL	OA6-CA5	2.98	1.42	1.34
52	u	201	CDL	OB8-CB7	2.98	1.42	1.33
52	i	401	CDL	OA6-CA5	2.98	1.42	1.34
58	w	401	ADP	O3'-C3'	2.98	1.50	1.43
52	V	201	CDL	OB8-CB7	2.97	1.42	1.33
52	k	101	CDL	OB6-CB5	2.96	1.42	1.34
52	o	201	CDL	OB6-CB5	2.96	1.42	1.34
52	s	401	CDL	OB8-CB7	2.95	1.42	1.33
52	l	701	CDL	OA6-CA5	2.95	1.42	1.34
52	g	202	CDL	OB8-CB7	2.95	1.41	1.33
52	s	401	CDL	OA6-CA5	2.94	1.42	1.34
52	V	201	CDL	OB6-CB5	2.93	1.42	1.34
52	o	201	CDL	OB8-CB7	2.93	1.41	1.33
52	u	201	CDL	OA6-CA5	2.93	1.42	1.34
52	a	201	CDL	OA6-CA5	2.93	1.42	1.34
53	J	401	NDP	O3D-C3D	2.89	1.50	1.43
52	g	202	CDL	OA6-CA5	2.87	1.42	1.34
52	r	502	CDL	OA6-CA5	2.83	1.42	1.34
49	a	202	PLX	O6-C4	-2.82	1.41	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	J	402	UQ	C6-C1	2.80	1.54	1.46
49	e	201	PLX	O6-C4	-2.79	1.41	1.44
54	s	402	UQ	C6-C1	2.75	1.54	1.46
47	A	503	NAI	C8A-N9A	-2.73	1.32	1.37
49	g	201	PLX	O6-C4	-2.72	1.41	1.44
49	j	203	PLX	O6-C4	-2.72	1.41	1.44
49	C	303	PLX	O6-C4	-2.68	1.41	1.44
48	C	302	PEE	O2-C2	-2.66	1.40	1.46
49	J	403	PLX	O6-C4	-2.65	1.41	1.44
52	a	201	CDL	OA6-CA4	-2.61	1.40	1.46
52	g	202	CDL	OA6-CA4	-2.60	1.40	1.46
48	W	201	PEE	O2-C2	-2.60	1.40	1.46
48	l	702	PEE	O2-C2	-2.59	1.40	1.46
48	j	201	PEE	O2-C2	-2.57	1.40	1.46
52	u	201	CDL	OA6-CA4	-2.57	1.40	1.46
48	B	303	PEE	O2-C2	-2.57	1.40	1.46
52	o	201	CDL	OA6-CA4	-2.56	1.40	1.46
52	s	401	CDL	OA6-CA4	-2.56	1.40	1.46
48	V	202	PEE	O3-C30	2.55	1.40	1.33
52	r	502	CDL	OA6-CA4	-2.54	1.40	1.46
52	I	201	CDL	OA6-CA4	-2.53	1.40	1.46
48	r	501	PEE	O2-C2	-2.52	1.40	1.46
53	J	401	NDP	O2B-C2B	2.51	1.52	1.44
48	j	202	PEE	O2-C2	-2.51	1.40	1.46
48	l	703	PEE	O2-C2	-2.51	1.40	1.46
48	j	202	PEE	O3-C30	2.49	1.40	1.33
46	A	502	FMN	C10-N1	2.49	1.38	1.33
52	i	401	CDL	OA6-CA4	-2.49	1.40	1.46
48	j	201	PEE	O3-C30	2.46	1.40	1.33
49	e	201	PLX	C7-C6	2.45	1.55	1.50
48	W	201	PEE	O3-C30	2.45	1.40	1.33
52	l	701	CDL	OA6-CA4	-2.44	1.40	1.46
48	B	303	PEE	O3-C30	2.44	1.40	1.33
48	V	202	PEE	O2-C2	-2.44	1.40	1.46
51	G	201	8Q1	C1-S44	2.43	1.82	1.76
48	l	703	PEE	O3-C30	2.42	1.40	1.33
58	w	401	ADP	C5-N7	-2.42	1.34	1.39
47	A	503	NAI	PN-O5D	2.41	1.68	1.59
48	C	302	PEE	O3-C30	2.41	1.40	1.33
48	l	702	PEE	O3-C30	2.41	1.40	1.33
47	A	503	NAI	C6N-C5N	2.41	1.40	1.33
49	C	303	PLX	C7-C6	2.40	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	J	401	NDP	C2D-C3D	2.40	1.59	1.53
52	k	101	CDL	OB6-CB4	-2.39	1.41	1.46
49	j	203	PLX	C7-C6	2.39	1.55	1.50
52	V	201	CDL	OB6-CB4	-2.38	1.41	1.46
51	X	201	8Q1	C1-S44	2.37	1.81	1.76
54	s	402	UQ	C7-C8	2.37	1.54	1.50
51	G	201	8Q1	O40-C39	-2.37	1.18	1.23
49	J	403	PLX	C7-C6	2.36	1.55	1.50
49	g	201	PLX	C7-C6	2.36	1.55	1.50
48	r	501	PEE	O3-C30	2.35	1.40	1.33
48	V	202	PEE	O2-C10	2.35	1.40	1.34
47	A	503	NAI	O3B-C3B	-2.34	1.37	1.43
48	W	201	PEE	O2-C10	2.34	1.40	1.34
47	A	503	NAI	C5B-C4B	2.34	1.58	1.51
49	a	202	PLX	C7-C6	2.34	1.55	1.50
51	G	201	8Q1	O35-C34	-2.33	1.18	1.23
52	l	701	CDL	OB6-CB4	-2.33	1.41	1.46
52	o	201	CDL	OB6-CB4	-2.33	1.41	1.46
48	l	703	PEE	O2-C10	2.32	1.40	1.34
51	X	201	8Q1	O35-C34	-2.32	1.19	1.23
52	I	201	CDL	OB6-CB4	-2.32	1.41	1.46
51	X	201	8Q1	O40-C39	-2.31	1.18	1.23
52	u	201	CDL	OB6-CB4	-2.31	1.41	1.46
52	s	401	CDL	OB6-CB4	-2.31	1.41	1.46
52	V	201	CDL	PB2-OB2	2.30	1.68	1.59
52	k	101	CDL	OA6-CA4	-2.30	1.41	1.46
50	C	304	DCQ	O4-C4M	-2.30	1.40	1.45
48	B	303	PEE	O2-C10	2.29	1.40	1.34
50	C	304	DCQ	C6-C5	2.27	1.52	1.46
52	k	101	CDL	PB2-OB2	2.26	1.68	1.59
52	r	502	CDL	OB6-CB4	-2.26	1.41	1.46
52	g	202	CDL	PB2-OB2	2.26	1.68	1.59
52	u	201	CDL	PB2-OB2	2.26	1.68	1.59
48	j	202	PEE	O2-C10	2.26	1.40	1.34
52	o	201	CDL	PB2-OB2	2.25	1.68	1.59
52	a	201	CDL	OB6-CB4	-2.25	1.41	1.46
52	i	401	CDL	PB2-OB5	2.25	1.68	1.59
48	C	302	PEE	O2-C10	2.25	1.40	1.34
52	i	401	CDL	PB2-OB2	2.25	1.68	1.59
48	r	501	PEE	O2-C10	2.25	1.40	1.34
48	l	702	PEE	O2-C10	2.25	1.40	1.34
52	I	201	CDL	PB2-OB2	2.24	1.68	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	C	304	DCQ	O3-C3M	-2.24	1.40	1.45
52	l	701	CDL	PB2-OB2	2.24	1.68	1.59
48	C	302	PEE	O3-C3	-2.24	1.40	1.45
52	r	502	CDL	PB2-OB5	2.24	1.68	1.59
52	i	401	CDL	OB6-CB4	-2.23	1.41	1.46
52	I	201	CDL	PB2-OB5	2.23	1.68	1.59
52	V	201	CDL	PB2-OB5	2.23	1.68	1.59
48	l	702	PEE	O3-C3	-2.22	1.40	1.45
48	r	501	PEE	O3-C3	-2.22	1.40	1.45
54	J	402	UQ	C7-C8	2.22	1.54	1.50
52	g	202	CDL	OB6-CB4	-2.22	1.41	1.46
52	r	502	CDL	PB2-OB2	2.22	1.68	1.59
48	j	201	PEE	O2-C10	2.22	1.40	1.34
52	g	202	CDL	PB2-OB5	2.21	1.68	1.59
52	o	201	CDL	PB2-OB5	2.21	1.68	1.59
52	s	401	CDL	PB2-OB2	2.20	1.68	1.59
49	g	201	PLX	P1-O4	2.19	1.68	1.59
48	W	201	PEE	O3-C3	-2.19	1.40	1.45
49	a	202	PLX	P1-O4	2.19	1.68	1.59
52	s	401	CDL	PB2-OB5	2.19	1.68	1.59
52	u	201	CDL	PB2-OB5	2.18	1.67	1.59
48	B	303	PEE	O3-C3	-2.18	1.40	1.45
52	a	201	CDL	PB2-OB2	2.18	1.67	1.59
52	k	101	CDL	PB2-OB5	2.17	1.67	1.59
48	j	201	PEE	O3-C3	-2.17	1.40	1.45
49	e	201	PLX	P1-O4	2.16	1.67	1.59
49	j	203	PLX	P1-O4	2.16	1.67	1.59
53	J	401	NDP	PA-O5B	2.16	1.67	1.59
51	G	201	8Q1	C6-C1	2.16	1.53	1.50
52	a	201	CDL	PB2-OB5	2.15	1.67	1.59
49	C	303	PLX	P1-O4	2.15	1.67	1.59
53	J	401	NDP	O7N-C7N	-2.15	1.19	1.24
49	J	403	PLX	P1-O4	2.14	1.67	1.59
48	j	202	PEE	O3-C3	-2.14	1.40	1.45
52	l	701	CDL	PB2-OB5	2.14	1.67	1.59
54	s	402	UQ	O4-C4	-2.13	1.18	1.23
48	V	202	PEE	O3-C3	-2.13	1.40	1.45
51	X	201	8Q1	C6-C1	2.13	1.53	1.50
48	l	703	PEE	O3-C3	-2.13	1.40	1.45
52	V	201	CDL	OA6-CA4	-2.10	1.41	1.46
47	A	503	NAI	C5A-N7A	-2.10	1.35	1.39
54	s	402	UQ	O3-CM3	-2.10	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	j	203	PLX	P1-O1	2.09	1.67	1.59
54	J	402	UQ	O4-C4	-2.09	1.18	1.23
52	V	201	CDL	C11-CA5	2.09	1.56	1.50
49	a	202	PLX	P1-O1	2.08	1.67	1.59
54	J	402	UQ	O3-CM3	-2.08	1.40	1.45
49	g	201	PLX	P1-O1	2.06	1.67	1.59
49	J	403	PLX	P1-O1	2.06	1.67	1.59
49	C	303	PLX	P1-O1	2.05	1.67	1.59
54	J	402	UQ	C21-C19	2.05	1.55	1.51
49	e	201	PLX	P1-O1	2.02	1.67	1.59

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	J	401	NDP	C3N-C2N-N1N	-9.28	109.58	123.20
54	s	402	UQ	C7-C8-C9	-7.79	113.42	126.83
54	J	402	UQ	C7-C8-C9	-7.63	113.69	126.83
51	G	201	8Q1	C6-C1-S44	6.72	121.42	113.40
53	J	401	NDP	C6N-N1N-C2N	-6.48	112.39	119.32
54	J	402	UQ	C17-C18-C19	-6.45	112.87	127.62
54	s	402	UQ	C22-C23-C24	-6.45	112.87	127.62
54	J	402	UQ	C12-C13-C14	-6.44	112.89	127.62
54	s	402	UQ	C17-C18-C19	-6.28	113.26	127.62
54	s	402	UQ	C12-C13-C14	-6.11	113.64	127.62
51	X	201	8Q1	C6-C1-S44	5.91	120.45	113.40
53	J	401	NDP	C1D-N1N-C2N	-5.76	111.65	121.14
53	J	401	NDP	C5A-C4A-N3A	-5.68	118.90	126.72
47	A	503	NAI	C5A-C4A-N3A	-5.44	119.22	126.72
58	w	401	ADP	C5-C4-N3	-5.40	119.28	126.72
58	w	401	ADP	N3-C2-N1	-4.67	121.51	128.58
54	J	402	UQ	C10-C9-C8	-4.67	111.64	123.63
53	J	401	NDP	C1D-N1N-C6N	-4.66	110.91	120.77
47	A	503	NAI	N3A-C2A-N1A	-4.47	121.82	128.58
54	s	402	UQ	C10-C9-C8	-4.43	112.24	123.63
54	s	402	UQ	C27-C28-C29	-4.34	113.19	127.64
58	w	401	ADP	N3-C4-N9	4.30	134.49	127.17
54	s	402	UQ	C25-C24-C23	-4.28	112.63	123.63
54	J	402	UQ	C15-C14-C13	-4.27	112.67	123.63
54	J	402	UQ	C22-C23-C24	-4.23	113.53	127.64
52	l	701	CDL	OA6-CA5-C11	4.15	120.45	111.48
54	J	402	UQ	C20-C19-C18	-4.15	112.98	123.63
52	s	401	CDL	OA6-CA5-C11	4.14	120.44	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	B	303	PEE	O2-C10-C11	4.13	120.41	111.48
52	g	202	CDL	OA6-CA5-C11	4.12	120.40	111.48
52	r	502	CDL	OA6-CA5-C11	4.12	120.40	111.48
48	j	202	PEE	O2-C10-C11	4.11	120.38	111.48
52	r	502	CDL	OB6-CB5-C51	4.11	120.36	111.48
53	J	401	NDP	N3A-C2A-N1A	-4.06	122.43	128.58
52	V	201	CDL	OA6-CA5-C11	4.04	120.23	111.48
52	o	201	CDL	OA6-CA5-C11	4.03	120.20	111.48
52	o	201	CDL	OB6-CB5-C51	4.03	120.20	111.48
52	g	202	CDL	OB6-CB5-C51	4.03	120.19	111.48
53	J	401	NDP	N3A-C4A-N9A	4.02	134.01	127.17
52	k	101	CDL	OB6-CB5-C51	4.00	120.14	111.48
52	u	201	CDL	OA6-CA5-C11	3.98	120.08	111.48
48	V	202	PEE	O2-C10-C11	3.98	120.08	111.48
51	G	201	8Q1	O4-C1-C6	-3.97	119.40	123.98
48	r	501	PEE	O2-C10-C11	3.96	120.06	111.48
52	I	201	CDL	OA6-CA5-C11	3.95	120.03	111.48
52	a	201	CDL	OB6-CB5-C51	3.94	120.02	111.48
48	l	703	PEE	O2-C10-C11	3.93	119.99	111.48
52	V	201	CDL	OB6-CB5-C51	3.92	119.97	111.48
52	u	201	CDL	OB6-CB5-C51	3.92	119.97	111.48
54	s	402	UQ	C20-C19-C18	-3.92	113.56	123.63
52	I	201	CDL	OB6-CB5-C51	3.91	119.93	111.48
48	l	702	PEE	O2-C10-C11	3.91	119.93	111.48
54	J	402	UQ	C16-C14-C13	-3.90	112.42	121.17
48	C	302	PEE	O2-C10-C11	3.90	119.91	111.48
52	i	401	CDL	OB6-CB5-C51	3.89	119.90	111.48
52	i	401	CDL	OA6-CA5-C11	3.89	119.89	111.48
47	A	503	NAI	N3A-C4A-N9A	3.86	133.73	127.17
48	j	201	PEE	O2-C10-C11	3.85	119.81	111.48
54	s	402	UQ	C26-C24-C23	-3.85	112.53	121.17
52	s	401	CDL	OB6-CB5-C51	3.84	119.78	111.48
48	W	201	PEE	O2-C10-C11	3.83	119.78	111.48
52	a	201	CDL	OA6-CA5-C11	3.82	119.74	111.48
54	J	402	UQ	C11-C9-C8	-3.76	112.72	121.17
54	s	402	UQ	C11-C9-C8	-3.76	112.73	121.17
54	s	402	UQ	C16-C14-C13	-3.75	112.75	121.17
54	s	402	UQ	C15-C14-C13	-3.74	114.03	123.63
52	k	101	CDL	OA6-CA5-C11	3.73	119.55	111.48
47	A	503	NAI	C2A-N3A-C4A	3.70	120.88	111.83
51	X	201	8Q1	O4-C1-C6	-3.69	119.72	123.98
52	l	701	CDL	OB6-CB5-C51	3.68	119.44	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	s	402	UQ	C21-C19-C18	-3.62	113.04	121.17
53	J	401	NDP	C2A-N3A-C4A	3.62	120.67	111.83
58	w	401	ADP	C2-N3-C4	3.58	120.58	111.83
58	w	401	ADP	N9-C8-N7	-3.57	108.87	113.94
54	J	402	UQ	C21-C19-C18	-3.48	113.35	121.17
47	A	503	NAI	C3D-C2D-C1D	3.46	108.00	101.46
51	G	201	8Q1	C37-C38-C39	3.42	118.09	112.39
47	A	503	NAI	C4A-C5A-N7A	-3.37	106.73	110.58
47	A	503	NAI	C5A-N7A-C8A	3.35	108.72	103.45
58	w	401	ADP	C4-N9-C8	3.32	109.23	105.74
46	A	502	FMN	C4-N3-C2	-3.30	119.78	125.64
47	A	503	NAI	N9A-C8A-N7A	-3.29	109.27	113.94
54	s	402	UQ	C30-C29-C28	-3.28	112.80	122.66
53	J	401	NDP	C4A-C5A-N7A	-3.27	106.84	110.58
54	J	402	UQ	C26-C24-C23	-3.18	113.12	122.66
58	w	401	ADP	C5-N7-C8	3.17	108.43	103.45
54	J	402	UQ	C25-C24-C23	-3.16	113.16	122.66
54	s	402	UQ	C31-C29-C28	-3.16	113.18	122.66
53	J	401	NDP	C5A-N7A-C8A	3.10	108.33	103.45
53	J	401	NDP	N9A-C8A-N7A	-3.09	109.55	113.94
51	X	201	8Q1	C37-C38-C39	3.04	117.46	112.39
54	J	402	UQ	C7-C6-C5	-3.00	119.74	124.89
47	A	503	NAI	C2D-C3D-C4D	3.00	108.40	102.61
48	B	303	PEE	O3-C30-C31	2.96	120.87	111.83
58	w	401	ADP	C4-C5-N7	-2.92	107.24	110.58
52	I	201	CDL	OB8-CB7-C71	2.85	120.53	111.83
52	g	202	CDL	OB8-CB7-C71	2.85	120.51	111.83
52	i	401	CDL	OA8-CA7-C31	2.85	120.51	111.83
48	l	703	PEE	O3-C30-C31	2.84	120.50	111.83
52	u	201	CDL	OA8-CA7-C31	2.83	119.75	111.15
52	a	201	CDL	OB8-CB7-C71	2.83	120.46	111.83
52	u	201	CDL	OB8-CB7-C71	2.82	120.44	111.83
52	o	201	CDL	OB8-CB7-C71	2.82	120.44	111.83
52	k	101	CDL	OA8-CA7-C31	2.81	120.39	111.83
52	r	502	CDL	OA8-CA7-C31	2.79	120.36	111.83
48	l	702	PEE	O3-C30-C31	2.78	120.31	111.83
48	r	501	PEE	O3-C30-C31	2.77	120.29	111.83
48	V	202	PEE	O3-C30-C31	2.77	120.28	111.83
52	l	701	CDL	OB8-CB7-C71	2.76	120.26	111.83
48	W	201	PEE	O3-C30-C31	2.76	120.24	111.83
51	G	201	8Q1	O4-C1-S44	-2.75	119.18	122.68
52	r	502	CDL	OB8-CB7-C71	2.72	120.14	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	s	401	CDL	OB8-CB7-C71	2.70	120.07	111.83
52	V	201	CDL	OB8-CB7-C71	2.70	120.07	111.83
52	s	401	CDL	OA8-CA7-C31	2.69	120.05	111.83
48	j	201	PEE	O3-C30-C31	2.69	120.03	111.83
48	j	202	PEE	O3-C30-C31	2.69	120.02	111.83
52	a	201	CDL	OA8-CA7-C31	2.69	120.02	111.83
54	J	402	UQ	CM5-C5-C6	-2.68	120.04	124.45
46	A	502	FMN	C4A-C4-N3	2.68	120.08	113.25
52	l	701	CDL	OA8-CA7-C31	2.67	119.96	111.83
52	k	101	CDL	OB8-CB7-C71	2.66	119.96	111.83
52	g	202	CDL	OA8-CA7-C31	2.66	119.93	111.83
52	i	401	CDL	OB8-CB7-C71	2.63	119.86	111.83
48	C	302	PEE	O3-C30-C31	2.60	119.77	111.83
52	I	201	CDL	OA8-CA7-C31	2.59	119.75	111.83
49	a	202	PLX	C1A-N1-C1	2.54	120.02	109.91
46	A	502	FMN	C5A-C9A-N10	2.54	120.27	117.97
52	V	201	CDL	OA8-CA7-C31	2.54	119.58	111.83
50	C	304	DCQ	C1M-C1-C6	-2.53	120.29	124.45
52	o	201	CDL	OA8-CA7-C31	2.53	119.56	111.83
46	A	502	FMN	O4-C4-C4A	-2.50	119.94	126.53
49	g	201	PLX	C1A-N1-C1	2.47	119.74	109.91
49	j	203	PLX	C1A-N1-C1	2.42	119.54	109.91
51	X	201	8Q1	C38-C39-N41	2.41	120.73	116.34
53	J	401	NDP	C2B-C1B-N9A	-2.40	109.80	113.75
46	A	502	FMN	C4A-C10-N10	2.39	119.91	116.48
58	w	401	ADP	C4'-O4'-C1'	-2.39	104.19	109.47
47	A	503	NAI	C4A-N9A-C8A	2.38	108.24	105.74
49	J	403	PLX	C1A-N1-C1	2.36	119.31	109.91
53	J	401	NDP	C4A-N9A-C8A	2.34	108.19	105.74
48	V	202	PEE	C20-C19-C18	-2.33	112.39	126.42
49	C	303	PLX	C1A-N1-C1	2.31	119.10	109.91
54	s	402	UQ	C7-C6-C5	-2.31	120.93	124.89
46	A	502	FMN	C9A-C5A-N5	-2.28	120.04	122.45
46	A	502	FMN	C4A-C10-N1	-2.27	119.02	124.59
52	s	401	CDL	CA4-OA6-CA5	-2.27	112.37	117.80
51	X	201	8Q1	O4-C1-S44	-2.24	119.83	122.68
51	X	201	8Q1	C43-S44-C1	2.22	108.39	101.84
49	e	201	PLX	C1A-N1-C1	2.21	118.71	109.91
47	A	503	NAI	C4D-O4D-C1D	-2.21	104.58	109.47
46	A	502	FMN	C10-C4A-N5	-2.21	120.30	124.81
54	s	402	UQ	CM5-C5-C6	-2.17	120.88	124.45
51	G	201	8Q1	C43-S44-C1	2.16	108.23	101.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	r	502	CDL	CA4-OA6-CA5	-2.15	112.64	117.80
51	X	201	8Q1	C42-N41-C39	-2.11	118.89	122.82
51	X	201	8Q1	C32-C34-N36	2.09	120.45	116.48
47	A	503	NAI	C3B-C2B-C1B	2.01	105.27	101.46

There are no chirality outliers.

All (1056) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C3'-C4'-C5'-O5'
46	A	502	FMN	O4'-C4'-C5'-O5'
46	A	502	FMN	C5'-O5'-P-O1P
47	A	503	NAI	PN-O3-PA-O5B
48	C	302	PEE	C1-O3P-P-O1P
48	V	202	PEE	C11-C10-O2-C2
48	V	202	PEE	C1-O3P-P-O2P
48	V	202	PEE	C1-O3P-P-O1P
48	V	202	PEE	C1-O3P-P-O4P
48	j	201	PEE	C1-O3P-P-O1P
48	j	201	PEE	C4-O4P-P-O1P
48	j	202	PEE	C1-O3P-P-O2P
48	j	202	PEE	C4-O4P-P-O3P
48	j	202	PEE	C4-O4P-P-O2P
48	j	202	PEE	C4-O4P-P-O1P
48	j	202	PEE	O4P-C4-C5-N
48	l	702	PEE	C11-C10-O2-C2
48	l	702	PEE	O3P-C1-C2-O2
48	l	702	PEE	C1-O3P-P-O1P
48	l	702	PEE	C1-O3P-P-O4P
48	l	702	PEE	C4-O4P-P-O3P
48	l	703	PEE	C11-C10-O2-C2
48	r	501	PEE	C1-O3P-P-O2P
49	C	303	PLX	O7-C6-C7-C8
49	C	303	PLX	O6-C6-C7-C8
49	C	303	PLX	O6-C4-C5-O8
49	C	303	PLX	C2-O1-P1-O4
49	C	303	PLX	C2-O1-P1-O2
49	C	303	PLX	O9-C24-O8-C5
49	J	403	PLX	O7-C6-C7-C8
49	J	403	PLX	O7-C6-O6-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	J	403	PLX	C3-O4-P1-O1
49	J	403	PLX	C3-O4-P1-O3
49	J	403	PLX	C25-C24-O8-C5
49	J	403	PLX	O9-C24-C25-C26
49	a	202	PLX	O7-C6-O6-C4
49	a	202	PLX	O9-C24-C25-C26
49	e	201	PLX	O7-C6-O6-C4
49	e	201	PLX	C3-O4-P1-O1
49	e	201	PLX	C3-O4-P1-O2
49	e	201	PLX	C3-O4-P1-O3
49	e	201	PLX	C2-O1-P1-O4
49	e	201	PLX	C2-O1-P1-O2
49	e	201	PLX	C25-C24-O8-C5
49	e	201	PLX	O9-C24-C25-C26
49	g	201	PLX	C3-O4-P1-O1
49	g	201	PLX	C3-O4-P1-O2
49	g	201	PLX	C3-O4-P1-O3
49	g	201	PLX	C2-O1-P1-O4
49	g	201	PLX	C2-O1-P1-O2
49	g	201	PLX	C2-O1-P1-O3
49	g	201	PLX	O9-C24-O8-C5
49	j	203	PLX	O7-C6-C7-C8
49	j	203	PLX	O7-C6-O6-C4
49	j	203	PLX	C3-O4-P1-O1
49	j	203	PLX	C3-O4-P1-O2
49	j	203	PLX	C3-O4-P1-O3
49	j	203	PLX	O9-C24-O8-C5
49	j	203	PLX	O9-C24-C25-C26
51	G	201	8Q1	O4-C1-S44-C43
51	G	201	8Q1	C6-C1-S44-C43
51	G	201	8Q1	O27-C28-C29-C30
51	G	201	8Q1	O27-C28-C29-C31
51	G	201	8Q1	O27-C28-C29-C32
51	G	201	8Q1	N41-C42-C43-S44
51	G	201	8Q1	C42-C43-S44-C1
51	G	201	8Q1	C28-O27-P24-O3
51	G	201	8Q1	C28-O27-P24-O2
51	G	201	8Q1	C28-O27-P24-O1
51	X	201	8Q1	C42-C43-S44-C1
51	X	201	8Q1	C28-O27-P24-O2
52	I	201	CDL	CA2-OA2-PA1-OA4
52	I	201	CDL	CA2-OA2-PA1-OA5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	I	201	CDL	OA5-CA3-CA4-OA6
52	I	201	CDL	CB2-OB2-PB2-OB3
52	I	201	CDL	CB2-OB2-PB2-OB4
52	I	201	CDL	CB2-OB2-PB2-OB5
52	I	201	CDL	CB3-OB5-PB2-OB2
52	I	201	CDL	CB3-OB5-PB2-OB3
52	I	201	CDL	CB3-OB5-PB2-OB4
52	I	201	CDL	C51-CB5-OB6-CB4
52	V	201	CDL	CA3-OA5-PA1-OA2
52	V	201	CDL	CA3-OA5-PA1-OA3
52	V	201	CDL	CA3-OA5-PA1-OA4
52	V	201	CDL	C11-CA5-OA6-CA4
52	V	201	CDL	CB2-OB2-PB2-OB3
52	V	201	CDL	CB2-OB2-PB2-OB4
52	V	201	CDL	CB2-OB2-PB2-OB5
52	V	201	CDL	CB3-OB5-PB2-OB2
52	V	201	CDL	CB3-OB5-PB2-OB3
52	V	201	CDL	CB3-OB5-PB2-OB4
52	a	201	CDL	CA2-OA2-PA1-OA3
52	a	201	CDL	CA2-OA2-PA1-OA4
52	a	201	CDL	CA2-OA2-PA1-OA5
52	a	201	CDL	CB2-OB2-PB2-OB3
52	a	201	CDL	CB2-OB2-PB2-OB4
52	a	201	CDL	CB2-OB2-PB2-OB5
52	g	202	CDL	CA2-OA2-PA1-OA3
52	g	202	CDL	CA2-OA2-PA1-OA5
52	g	202	CDL	CA3-OA5-PA1-OA3
52	g	202	CDL	CB2-OB2-PB2-OB3
52	g	202	CDL	CB2-OB2-PB2-OB4
52	g	202	CDL	CB2-OB2-PB2-OB5
52	g	202	CDL	CB3-OB5-PB2-OB2
52	g	202	CDL	CB3-OB5-PB2-OB3
52	i	401	CDL	CA2-C1-CB2-OB2
52	i	401	CDL	CA3-OA5-PA1-OA2
52	i	401	CDL	CA3-OA5-PA1-OA4
52	i	401	CDL	C31-CA7-OA8-CA6
52	i	401	CDL	CB3-OB5-PB2-OB3
52	k	101	CDL	CA2-C1-CB2-OB2
52	k	101	CDL	CA2-OA2-PA1-OA3
52	k	101	CDL	CA3-OA5-PA1-OA2
52	k	101	CDL	CA3-OA5-PA1-OA4
52	k	101	CDL	OA5-CA3-CA4-OA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	k	101	CDL	CB2-OB2-PB2-OB4
52	k	101	CDL	CB2-OB2-PB2-OB5
52	k	101	CDL	CB3-OB5-PB2-OB3
52	l	701	CDL	O1-C1-CA2-OA2
52	l	701	CDL	CB2-OB2-PB2-OB3
52	l	701	CDL	CB2-OB2-PB2-OB4
52	l	701	CDL	CB2-OB2-PB2-OB5
52	l	701	CDL	OB6-CB4-CB6-OB8
52	o	201	CDL	CA2-OA2-PA1-OA5
52	o	201	CDL	CB2-OB2-PB2-OB3
52	o	201	CDL	C51-CB5-OB6-CB4
52	r	502	CDL	CB2-C1-CA2-OA2
52	r	502	CDL	CA2-C1-CB2-OB2
52	r	502	CDL	OA5-CA3-CA4-OA6
52	r	502	CDL	OA9-CA7-OA8-CA6
52	r	502	CDL	C31-CA7-OA8-CA6
52	r	502	CDL	CB2-OB2-PB2-OB3
52	r	502	CDL	CB2-OB2-PB2-OB4
52	r	502	CDL	CB2-OB2-PB2-OB5
52	r	502	CDL	CB3-OB5-PB2-OB2
52	r	502	CDL	CB3-OB5-PB2-OB3
52	r	502	CDL	CB3-OB5-PB2-OB4
52	s	401	CDL	CA2-OA2-PA1-OA3
52	s	401	CDL	CA2-OA2-PA1-OA4
52	s	401	CDL	CA2-OA2-PA1-OA5
52	s	401	CDL	OA9-CA7-OA8-CA6
52	s	401	CDL	C31-CA7-OA8-CA6
52	s	401	CDL	CB3-OB5-PB2-OB2
52	s	401	CDL	CB3-OB5-PB2-OB3
52	u	201	CDL	O1-C1-CA2-OA2
52	u	201	CDL	CB2-C1-CA2-OA2
52	u	201	CDL	CA3-OA5-PA1-OA4
52	u	201	CDL	CB3-OB5-PB2-OB2
52	u	201	CDL	CB3-OB5-PB2-OB3
52	u	201	CDL	CB3-OB5-PB2-OB4
53	J	401	NDP	O4D-C1D-N1N-C6N
54	J	402	UQ	C7-C8-C9-C11
54	J	402	UQ	C12-C13-C14-C15
54	J	402	UQ	C12-C13-C14-C16
54	J	402	UQ	C16-C17-C18-C19
54	J	402	UQ	C17-C18-C19-C21
54	s	402	UQ	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	s	402	UQ	C22-C23-C24-C26
52	i	401	CDL	OA9-CA7-OA8-CA6
54	J	402	UQ	C22-C23-C24-C25
54	J	402	UQ	C22-C23-C24-C26
48	V	202	PEE	O4-C10-O2-C2
48	l	702	PEE	O4-C10-O2-C2
48	l	703	PEE	O4-C10-O2-C2
52	V	201	CDL	OA7-CA5-OA6-CA4
52	g	202	CDL	OB7-CB5-OB6-CB4
52	o	201	CDL	OB7-CB5-OB6-CB4
52	s	401	CDL	OB7-CB5-OB6-CB4
52	g	202	CDL	C51-CB5-OB6-CB4
52	s	401	CDL	C51-CB5-OB6-CB4
54	J	402	UQ	C12-C11-C9-C8
54	s	402	UQ	C18-C19-C21-C22
54	s	402	UQ	C23-C24-C26-C27
50	C	304	DCQ	C6-C7-C8-C9
52	V	201	CDL	C71-CB7-OB8-CB6
54	J	402	UQ	C7-C8-C9-C10
54	J	402	UQ	C17-C18-C19-C20
48	l	703	PEE	C37-C38-C39-C40
54	s	402	UQ	C7-C8-C9-C11
54	s	402	UQ	C17-C18-C19-C21
52	I	201	CDL	OB7-CB5-OB6-CB4
52	I	201	CDL	O1-C1-CA2-OA2
52	g	202	CDL	O1-C1-CA2-OA2
52	i	401	CDL	O1-C1-CB2-OB2
52	k	101	CDL	O1-C1-CB2-OB2
52	l	701	CDL	O1-C1-CB2-OB2
52	s	401	CDL	O1-C1-CA2-OA2
48	l	702	PEE	C31-C30-O3-C3
48	r	501	PEE	C11-C10-O2-C2
52	k	101	CDL	C11-CA5-OA6-CA4
54	J	402	UQ	C12-C11-C9-C10
54	J	402	UQ	C13-C14-C16-C17
52	V	201	CDL	OB9-CB7-OB8-CB6
52	k	101	CDL	OA7-CA5-OA6-CA4
54	J	402	UQ	C14-C16-C17-C18
49	g	201	PLX	C7-C8-C9-C10
52	l	701	CDL	C35-C36-C37-C38
48	j	201	PEE	C31-C30-O3-C3
48	V	202	PEE	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	W	201	PEE	C17-C18-C19-C20
48	j	201	PEE	C17-C18-C19-C20
48	l	702	PEE	O5-C30-O3-C3
48	j	201	PEE	C11-C10-O2-C2
52	u	201	CDL	C71-C72-C73-C74
52	I	201	CDL	CB2-C1-CA2-OA2
52	a	201	CDL	CA2-C1-CB2-OB2
52	k	101	CDL	CB2-C1-CA2-OA2
52	l	701	CDL	CB2-C1-CA2-OA2
52	s	401	CDL	CA2-C1-CB2-OB2
52	g	202	CDL	C71-CB7-OB8-CB6
52	l	701	CDL	C71-CB7-OB8-CB6
52	o	201	CDL	C31-CA7-OA8-CA6
52	r	502	CDL	C71-CB7-OB8-CB6
49	j	203	PLX	C13-C14-C15-C16
52	l	701	CDL	C71-C72-C73-C74
49	g	201	PLX	C9-C10-C11-C12
49	j	203	PLX	C28-C29-C30-C31
52	V	201	CDL	C32-C33-C34-C35
52	k	101	CDL	C62-C63-C64-C65
49	g	201	PLX	C2-C1-N1-C1A
52	V	201	CDL	C59-C60-C61-C62
52	o	201	CDL	C17-C18-C19-C20
52	r	502	CDL	CB5-C51-C52-C53
52	I	201	CDL	O1-C1-CB2-OB2
52	r	502	CDL	O1-C1-CB2-OB2
52	u	201	CDL	O1-C1-CB2-OB2
52	o	201	CDL	C33-C34-C35-C36
49	J	403	PLX	C11-C10-C9-C8
52	u	201	CDL	C55-C56-C57-C58
52	o	201	CDL	OA9-CA7-OA8-CA6
48	r	501	PEE	O4-C10-O2-C2
52	V	201	CDL	OB5-CB3-CB4-OB6
48	j	202	PEE	C31-C30-O3-C3
52	V	201	CDL	C62-C63-C64-C65
48	B	303	PEE	C11-C12-C13-C14
52	i	401	CDL	CA5-C11-C12-C13
52	k	101	CDL	CA7-C31-C32-C33
58	w	401	ADP	O4'-C4'-C5'-O5'
52	V	201	CDL	C31-CA7-OA8-CA6
49	J	403	PLX	C29-C30-C31-C32
52	g	202	CDL	C74-C75-C76-C77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	J	403	PLX	C13-C14-C15-C16
54	s	402	UQ	C27-C28-C29-C31
54	s	402	UQ	C14-C16-C17-C18
49	g	201	PLX	C2-C1-N1-C1B
52	g	202	CDL	CB5-C51-C52-C53
52	l	701	CDL	CA7-C31-C32-C33
52	u	201	CDL	CB5-C51-C52-C53
52	l	701	CDL	OB9-CB7-OB8-CB6
48	V	202	PEE	C30-C31-C32-C33
52	I	201	CDL	CB5-C51-C52-C53
52	i	401	CDL	CB7-C71-C72-C73
52	l	701	CDL	CB7-C71-C72-C73
52	g	202	CDL	OB9-CB7-OB8-CB6
52	r	502	CDL	OB9-CB7-OB8-CB6
52	l	701	CDL	C31-C32-C33-C34
52	V	201	CDL	O1-C1-CB2-OB2
52	a	201	CDL	O1-C1-CA2-OA2
52	i	401	CDL	O1-C1-CA2-OA2
52	o	201	CDL	O1-C1-CB2-OB2
52	r	502	CDL	O1-C1-CA2-OA2
52	s	401	CDL	O1-C1-CB2-OB2
48	W	201	PEE	C31-C30-O3-C3
48	j	201	PEE	O5-C30-O3-C3
52	I	201	CDL	CA7-C31-C32-C33
48	j	201	PEE	O4-C10-O2-C2
52	k	101	CDL	C51-CB5-OB6-CB4
48	j	202	PEE	O5-C30-O3-C3
48	j	201	PEE	C30-C31-C32-C33
52	g	202	CDL	C76-C77-C78-C79
52	r	502	CDL	C34-C35-C36-C37
49	j	203	PLX	C32-C33-C34-C35
52	l	701	CDL	C33-C34-C35-C36
52	a	201	CDL	CB2-C1-CA2-OA2
52	i	401	CDL	CB2-C1-CA2-OA2
52	o	201	CDL	CA2-C1-CB2-OB2
52	s	401	CDL	CB2-C1-CA2-OA2
52	a	201	CDL	C71-CB7-OB8-CB6
52	r	502	CDL	C32-C33-C34-C35
52	r	502	CDL	C58-C59-C60-C61
52	u	201	CDL	C75-C76-C77-C78
52	k	101	CDL	C60-C61-C62-C63
52	a	201	CDL	C36-C37-C38-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	J	403	PLX	O8-C24-C25-C26
49	j	203	PLX	O6-C6-C7-C8
48	j	202	PEE	C11-C10-O2-C2
52	V	201	CDL	OA9-CA7-OA8-CA6
48	j	202	PEE	O4-C10-O2-C2
52	k	101	CDL	OB7-CB5-OB6-CB4
48	B	303	PEE	C17-C18-C19-C20
52	a	201	CDL	O1-C1-CB2-OB2
52	k	101	CDL	O1-C1-CA2-OA2
52	o	201	CDL	C76-C77-C78-C79
48	B	303	PEE	C34-C35-C36-C37
52	V	201	CDL	C53-C54-C55-C56
52	a	201	CDL	CB7-C71-C72-C73
52	k	101	CDL	C43-C44-C45-C46
48	W	201	PEE	O5-C30-O3-C3
52	r	502	CDL	CB7-C71-C72-C73
52	s	401	CDL	C14-C15-C16-C17
52	i	401	CDL	OB6-CB4-CB6-OB8
52	I	201	CDL	C31-CA7-OA8-CA6
52	V	201	CDL	C51-C52-C53-C54
48	j	201	PEE	C21-C22-C23-C24
49	J	403	PLX	C10-C11-C12-C13
49	g	201	PLX	C12-C13-C14-C15
52	s	401	CDL	C71-C72-C73-C74
48	W	201	PEE	C12-C13-C14-C15
48	r	501	PEE	C11-C12-C13-C14
52	V	201	CDL	C12-C13-C14-C15
52	i	401	CDL	C59-C60-C61-C62
52	i	401	CDL	C81-C82-C83-C84
52	k	101	CDL	C14-C15-C16-C17
52	r	502	CDL	C74-C75-C76-C77
52	s	401	CDL	C12-C13-C14-C15
52	s	401	CDL	C18-C19-C20-C21
52	s	401	CDL	C52-C53-C54-C55
52	i	401	CDL	C34-C35-C36-C37
52	k	101	CDL	C73-C74-C75-C76
52	o	201	CDL	C32-C33-C34-C35
52	r	502	CDL	C52-C53-C54-C55
52	s	401	CDL	C19-C20-C21-C22
48	C	302	PEE	C13-C14-C15-C16
48	j	202	PEE	C23-C24-C25-C26
49	C	303	PLX	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	g	201	PLX	C30-C31-C32-C33
52	a	201	CDL	C21-C22-C23-C24
52	g	202	CDL	C33-C34-C35-C36
52	r	502	CDL	C14-C15-C16-C17
52	r	502	CDL	C35-C36-C37-C38
52	s	401	CDL	C31-C32-C33-C34
52	u	201	CDL	C54-C55-C56-C57
48	V	202	PEE	C11-C12-C13-C14
49	C	303	PLX	C27-C28-C29-C30
52	o	201	CDL	C59-C60-C61-C62
52	k	101	CDL	CB5-C51-C52-C53
52	s	401	CDL	CB7-C71-C72-C73
48	j	202	PEE	C13-C14-C15-C16
49	J	403	PLX	C11-C12-C13-C14
49	a	202	PLX	C31-C32-C33-C34
49	j	203	PLX	C12-C13-C14-C15
48	B	303	PEE	C11-C10-O2-C2
52	l	701	CDL	C21-C22-C23-C24
49	g	201	PLX	C33-C34-C35-C36
52	g	202	CDL	C43-C44-C45-C46
52	r	502	CDL	C36-C37-C38-C39
52	u	201	CDL	C52-C53-C54-C55
52	o	201	CDL	CA7-C31-C32-C33
48	V	202	PEE	C32-C33-C34-C35
48	l	702	PEE	C32-C33-C34-C35
49	g	201	PLX	C13-C14-C15-C16
52	g	202	CDL	C34-C35-C36-C37
52	g	202	CDL	C59-C60-C61-C62
52	u	201	CDL	C74-C75-C76-C77
52	V	201	CDL	C72-C73-C74-C75
52	a	201	CDL	OB9-CB7-OB8-CB6
49	e	201	PLX	C27-C28-C29-C30
52	r	502	CDL	C56-C57-C58-C59
52	r	502	CDL	C71-C72-C73-C74
52	s	401	CDL	C82-C83-C84-C85
49	a	202	PLX	C10-C11-C12-C13
52	l	701	CDL	C15-C16-C17-C18
52	s	401	CDL	C37-C38-C39-C40
52	V	201	CDL	CA2-C1-CB2-OB2
52	g	202	CDL	CB2-C1-CA2-OA2
48	B	303	PEE	C31-C30-O3-C3
52	I	201	CDL	CA3-CA4-CA6-OA8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	B	303	PEE	C23-C24-C25-C26
48	r	501	PEE	C31-C32-C33-C34
49	g	201	PLX	C32-C33-C34-C35
52	V	201	CDL	C31-C32-C33-C34
52	V	201	CDL	C37-C38-C39-C40
52	r	502	CDL	C62-C63-C64-C65
52	s	401	CDL	C15-C16-C17-C18
49	g	201	PLX	C27-C28-C29-C30
49	j	203	PLX	C27-C28-C29-C30
49	j	203	PLX	C29-C30-C31-C32
52	a	201	CDL	C35-C36-C37-C38
52	a	201	CDL	C60-C61-C62-C63
52	a	201	CDL	C62-C63-C64-C65
52	k	101	CDL	C55-C56-C57-C58
52	o	201	CDL	C13-C14-C15-C16
52	s	401	CDL	C75-C76-C77-C78
48	W	201	PEE	C13-C14-C15-C16
49	C	303	PLX	C13-C14-C15-C16
49	J	403	PLX	C32-C33-C34-C35
52	V	201	CDL	C52-C53-C54-C55
52	k	101	CDL	C35-C36-C37-C38
52	k	101	CDL	C78-C79-C80-C81
52	l	701	CDL	C55-C56-C57-C58
48	C	302	PEE	C11-C12-C13-C14
48	V	202	PEE	C33-C34-C35-C36
52	k	101	CDL	C39-C40-C41-C42
49	g	201	PLX	C2-C1-N1-C1C
49	J	403	PLX	C30-C31-C32-C33
49	a	202	PLX	C14-C15-C16-C17
49	a	202	PLX	C9-C10-C11-C12
52	g	202	CDL	C41-C42-C43-C44
52	a	201	CDL	CB5-C51-C52-C53
48	C	302	PEE	C42-C43-C44-C45
49	e	201	PLX	C13-C14-C15-C16
52	s	401	CDL	C73-C74-C75-C76
48	B	303	PEE	C35-C36-C37-C38
48	j	201	PEE	C37-C38-C39-C40
49	C	303	PLX	C10-C11-C12-C13
49	J	403	PLX	C7-C8-C9-C10
52	k	101	CDL	C56-C57-C58-C59
52	o	201	CDL	C11-C12-C13-C14
51	G	201	8Q1	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	l	701	CDL	C73-C74-C75-C76
48	W	201	PEE	C22-C23-C24-C25
49	g	201	PLX	C28-C29-C30-C31
52	I	201	CDL	OA9-CA7-OA8-CA6
49	J	403	PLX	C12-C13-C14-C15
52	k	101	CDL	C51-C52-C53-C54
53	J	401	NDP	C2D-C1D-N1N-C2N
49	J	403	PLX	C9-C10-C11-C12
49	j	203	PLX	C7-C8-C9-C10
49	j	203	PLX	C33-C34-C35-C36
52	k	101	CDL	C37-C38-C39-C40
51	X	201	8Q1	C12-C13-C14-C15
52	a	201	CDL	C12-C13-C14-C15
52	g	202	CDL	C75-C76-C77-C78
52	o	201	CDL	C56-C57-C58-C59
52	o	201	CDL	C73-C74-C75-C76
48	j	202	PEE	C11-C12-C13-C14
52	l	701	CDL	C59-C60-C61-C62
52	r	502	CDL	C78-C79-C80-C81
52	s	401	CDL	C35-C36-C37-C38
48	B	303	PEE	C20-C21-C22-C23
48	C	302	PEE	C41-C42-C43-C44
52	o	201	CDL	C41-C42-C43-C44
52	r	502	CDL	C31-C32-C33-C34
49	a	202	PLX	C12-C13-C14-C15
49	j	203	PLX	C25-C26-C27-C28
48	r	501	PEE	C33-C34-C35-C36
49	e	201	PLX	C25-C26-C27-C28
49	j	203	PLX	C11-C12-C13-C14
48	l	702	PEE	C23-C24-C25-C26
49	C	303	PLX	C11-C12-C13-C14
49	C	303	PLX	C9-C10-C11-C12
52	o	201	CDL	C55-C56-C57-C58
52	r	502	CDL	C11-C12-C13-C14
52	r	502	CDL	C75-C76-C77-C78
52	s	401	CDL	C32-C33-C34-C35
48	r	501	PEE	C41-C42-C43-C44
52	V	201	CDL	C51-CB5-OB6-CB4
52	a	201	CDL	C11-CA5-OA6-CA4
52	a	201	CDL	C51-CB5-OB6-CB4
52	s	401	CDL	C11-CA5-OA6-CA4
48	W	201	PEE	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	k	101	CDL	C64-C65-C66-C67
52	V	201	CDL	OB7-CB5-OB6-CB4
52	s	401	CDL	OA7-CA5-OA6-CA4
49	J	403	PLX	C34-C35-C36-C37
49	j	203	PLX	C14-C15-C16-C17
52	k	101	CDL	C81-C82-C83-C84
48	j	202	PEE	C14-C15-C16-C17
52	l	701	CDL	C11-C12-C13-C14
48	B	303	PEE	O5-C30-O3-C3
49	J	403	PLX	C27-C28-C29-C30
49	e	201	PLX	C11-C10-C9-C8
52	g	202	CDL	C73-C74-C75-C76
49	C	303	PLX	C28-C29-C30-C31
52	i	401	CDL	C76-C77-C78-C79
48	B	303	PEE	O4-C10-O2-C2
52	r	502	CDL	OB5-CB3-CB4-OB6
51	G	201	8Q1	C12-C13-C14-C15
52	g	202	CDL	C13-C14-C15-C16
52	s	401	CDL	C54-C55-C56-C57
48	C	302	PEE	C12-C13-C14-C15
52	g	202	CDL	C82-C83-C84-C85
54	s	402	UQ	C27-C28-C29-C30
52	k	101	CDL	C18-C19-C20-C21
52	s	401	CDL	C83-C84-C85-C86
52	r	502	CDL	OA6-CA4-CA6-OA8
52	s	401	CDL	OB6-CB4-CB6-OB8
52	u	201	CDL	OA6-CA4-CA6-OA8
49	a	202	PLX	C13-C14-C15-C16
52	V	201	CDL	C75-C76-C77-C78
52	g	202	CDL	C55-C56-C57-C58
52	s	401	CDL	C33-C34-C35-C36
48	j	201	PEE	C36-C37-C38-C39
48	C	302	PEE	C34-C35-C36-C37
48	l	703	PEE	C32-C33-C34-C35
52	V	201	CDL	C42-C43-C44-C45
52	r	502	CDL	C73-C74-C75-C76
52	g	202	CDL	C71-C72-C73-C74
52	o	201	CDL	C52-C53-C54-C55
52	u	201	CDL	C73-C74-C75-C76
52	l	701	CDL	CA2-C1-CB2-OB2
52	o	201	CDL	CB2-C1-CA2-OA2
51	G	201	8Q1	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	k	101	CDL	C17-C18-C19-C20
52	k	101	CDL	C75-C76-C77-C78
52	l	701	CDL	C75-C76-C77-C78
52	i	401	CDL	C52-C53-C54-C55
52	s	401	CDL	C60-C61-C62-C63
52	i	401	CDL	C14-C15-C16-C17
48	C	302	PEE	C11-C10-O2-C2
49	a	202	PLX	C7-C8-C9-C10
49	a	202	PLX	C34-C35-C36-C37
48	l	703	PEE	C20-C21-C22-C23
49	C	303	PLX	C25-C26-C27-C28
52	k	101	CDL	C76-C77-C78-C79
52	o	201	CDL	C62-C63-C64-C65
52	o	201	CDL	C83-C84-C85-C86
48	r	501	PEE	C30-C31-C32-C33
52	a	201	CDL	C37-C38-C39-C40
52	i	401	CDL	C55-C56-C57-C58
49	g	201	PLX	C31-C32-C33-C34
52	k	101	CDL	C52-C53-C54-C55
52	r	502	CDL	C51-C52-C53-C54
52	g	202	CDL	C37-C38-C39-C40
52	g	202	CDL	C56-C57-C58-C59
52	k	101	CDL	C34-C35-C36-C37
52	I	201	CDL	OA5-CA3-CA4-CA6
52	V	201	CDL	OB5-CB3-CB4-CB6
48	B	303	PEE	C13-C14-C15-C16
48	C	302	PEE	C32-C33-C34-C35
49	j	203	PLX	C9-C10-C11-C12
52	i	401	CDL	C75-C76-C77-C78
52	o	201	CDL	C75-C76-C77-C78
52	s	401	CDL	C55-C56-C57-C58
48	l	702	PEE	C30-C31-C32-C33
49	C	303	PLX	C26-C27-C28-C29
48	V	202	PEE	C31-C30-O3-C3
49	a	202	PLX	C11-C12-C13-C14
52	a	201	CDL	C32-C33-C34-C35
52	l	701	CDL	C51-C52-C53-C54
52	i	401	CDL	C37-C38-C39-C40
48	C	302	PEE	C1-C2-C3-O3
48	V	202	PEE	C1-C2-C3-O3
48	W	201	PEE	C1-C2-C3-O3
48	j	202	PEE	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	r	501	PEE	C1-C2-C3-O3
49	C	303	PLX	C3-C4-C5-O8
49	a	202	PLX	C3-C4-C5-O8
52	V	201	CDL	CA3-CA4-CA6-OA8
52	l	701	CDL	CB3-CB4-CB6-OB8
52	s	401	CDL	CB3-CB4-CB6-OB8
52	g	202	CDL	C12-C13-C14-C15
52	r	502	CDL	C37-C38-C39-C40
49	e	201	PLX	C30-C31-C32-C33
52	k	101	CDL	C53-C54-C55-C56
52	k	101	CDL	C71-C72-C73-C74
52	i	401	CDL	C71-CB7-OB8-CB6
50	C	304	DCQ	C7-C8-C9-C10
52	g	202	CDL	C32-C33-C34-C35
52	k	101	CDL	C38-C39-C40-C41
52	l	701	CDL	C72-C73-C74-C75
52	V	201	CDL	C33-C34-C35-C36
49	g	201	PLX	C25-C26-C27-C28
52	V	201	CDL	CA5-C11-C12-C13
52	r	502	CDL	C16-C17-C18-C19
52	r	502	CDL	C55-C56-C57-C58
52	a	201	CDL	OA7-CA5-OA6-CA4
52	o	201	CDL	C12-C13-C14-C15
48	V	202	PEE	C39-C40-C41-C42
48	j	202	PEE	C12-C13-C14-C15
52	i	401	CDL	C73-C74-C75-C76
52	k	101	CDL	C15-C16-C17-C18
52	i	401	CDL	C35-C36-C37-C38
48	l	703	PEE	C31-C30-O3-C3
52	k	101	CDL	CA6-CA4-OA6-CA5
48	C	302	PEE	C19-C20-C21-C22
48	C	302	PEE	C15-C16-C17-C18
52	g	202	CDL	C14-C15-C16-C17
52	g	202	CDL	CB7-C71-C72-C73
48	r	501	PEE	C17-C18-C19-C20
49	J	403	PLX	C25-C26-C27-C28
49	J	403	PLX	C28-C29-C30-C31
52	g	202	CDL	C62-C63-C64-C65
48	r	501	PEE	O3P-C1-C2-O2
52	a	201	CDL	OA5-CA3-CA4-OA6
48	j	201	PEE	C43-C44-C45-C46
52	V	201	CDL	C74-C75-C76-C77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	V	202	PEE	C34-C35-C36-C37
52	g	202	CDL	C15-C16-C17-C18
48	r	501	PEE	C14-C15-C16-C17
52	o	201	CDL	C74-C75-C76-C77
52	r	502	CDL	OB6-CB4-CB6-OB8
52	V	201	CDL	C55-C56-C57-C58
52	k	101	CDL	C84-C85-C86-C87
48	j	201	PEE	C41-C42-C43-C44
49	a	202	PLX	C16-C17-C18-C19
48	j	201	PEE	C22-C23-C24-C25
48	B	303	PEE	C38-C39-C40-C41
52	a	201	CDL	OB7-CB5-OB6-CB4
48	j	201	PEE	C19-C20-C21-C22
52	I	201	CDL	C52-C53-C54-C55
52	i	401	CDL	C71-C72-C73-C74
49	C	303	PLX	C33-C34-C35-C36
52	i	401	CDL	C11-CA5-OA6-CA4
49	g	201	PLX	C11-C12-C13-C14
49	j	203	PLX	C30-C31-C32-C33
52	a	201	CDL	C84-C85-C86-C87
48	l	702	PEE	C24-C25-C26-C27
52	r	502	CDL	C81-C82-C83-C84
52	g	202	CDL	C58-C59-C60-C61
52	k	101	CDL	C41-C42-C43-C44
52	k	101	CDL	C54-C55-C56-C57
52	V	201	CDL	C43-C44-C45-C46
52	i	401	CDL	C54-C55-C56-C57
52	l	701	CDL	C36-C37-C38-C39
48	V	202	PEE	O5-C30-O3-C3
49	a	202	PLX	C28-C29-C30-C31
49	a	202	PLX	C29-C30-C31-C32
52	o	201	CDL	C19-C20-C21-C22
48	l	703	PEE	C31-C32-C33-C34
49	a	202	PLX	C11-C10-C9-C8
52	k	101	CDL	C61-C62-C63-C64
48	l	702	PEE	O3P-C1-C2-C3
52	i	401	CDL	OB5-CB3-CB4-CB6
52	k	101	CDL	OA5-CA3-CA4-CA6
52	l	701	CDL	OA5-CA3-CA4-CA6
52	r	502	CDL	OB5-CB3-CB4-CB6
52	o	201	CDL	O1-C1-CA2-OA2
58	w	401	ADP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	l	701	CDL	C14-C15-C16-C17
52	a	201	CDL	C34-C35-C36-C37
52	g	202	CDL	C81-C82-C83-C84
52	i	401	CDL	OB9-CB7-OB8-CB6
52	i	401	CDL	C77-C78-C79-C80
52	k	101	CDL	C33-C34-C35-C36
52	o	201	CDL	C51-C52-C53-C54
52	i	401	CDL	CA7-C31-C32-C33
52	s	401	CDL	CA5-C11-C12-C13
52	l	701	CDL	C24-C25-C26-C27
52	s	401	CDL	C40-C41-C42-C43
48	j	201	PEE	C44-C45-C46-C47
52	g	202	CDL	C64-C65-C66-C67
52	l	701	CDL	C64-C65-C66-C67
52	r	502	CDL	C82-C83-C84-C85
48	l	702	PEE	C1-C2-C3-O3
49	e	201	PLX	C3-C4-C5-O8
52	i	401	CDL	CA3-CA4-CA6-OA8
52	i	401	CDL	CB3-CB4-CB6-OB8
52	r	502	CDL	CA3-CA4-CA6-OA8
52	r	502	CDL	CB3-CB4-CB6-OB8
52	u	201	CDL	CA3-CA4-CA6-OA8
48	W	201	PEE	C23-C24-C25-C26
52	o	201	CDL	C37-C38-C39-C40
48	l	703	PEE	C14-C15-C16-C17
48	l	703	PEE	C12-C13-C14-C15
52	V	201	CDL	C71-C72-C73-C74
48	W	201	PEE	C31-C32-C33-C34
52	u	201	CDL	C51-C52-C53-C54
52	o	201	CDL	C60-C61-C62-C63
48	j	202	PEE	O3P-C1-C2-O2
48	l	702	PEE	C14-C15-C16-C17
49	e	201	PLX	C10-C11-C12-C13
48	l	703	PEE	O5-C30-O3-C3
48	W	201	PEE	C15-C16-C17-C18
52	i	401	CDL	C1-CB2-OB2-PB2
49	a	202	PLX	C27-C28-C29-C30
52	a	201	CDL	C14-C15-C16-C17
48	W	201	PEE	O2-C2-C3-O3
48	r	501	PEE	O2-C2-C3-O3
49	J	403	PLX	O6-C4-C5-O8
49	e	201	PLX	O6-C4-C5-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	s	401	CDL	OA6-CA4-CA6-OA8
52	g	202	CDL	C60-C61-C62-C63
52	g	202	CDL	C84-C85-C86-C87
52	r	502	CDL	C39-C40-C41-C42
49	J	403	PLX	O6-C6-C7-C8
49	a	202	PLX	O8-C24-C25-C26
49	j	203	PLX	O8-C24-C25-C26
48	l	702	PEE	C13-C14-C15-C16
49	e	201	PLX	C17-C18-C19-C20
52	a	201	CDL	CA5-C11-C12-C13
52	i	401	CDL	CB5-C51-C52-C53
52	s	401	CDL	CA7-C31-C32-C33
52	l	701	CDL	C74-C75-C76-C77
52	g	202	CDL	C53-C54-C55-C56
52	k	101	CDL	C63-C64-C65-C66
49	g	201	PLX	C10-C11-C12-C13
52	o	201	CDL	C77-C78-C79-C80
52	a	201	CDL	C82-C83-C84-C85
48	j	202	PEE	C24-C25-C26-C27
49	J	403	PLX	O4-C3-C4-C5
52	i	401	CDL	OA5-CA3-CA4-CA6
52	r	502	CDL	OA5-CA3-CA4-CA6
48	r	501	PEE	C36-C37-C38-C39
48	B	303	PEE	C44-C45-C46-C47
52	i	401	CDL	C64-C65-C66-C67
49	e	201	PLX	C31-C32-C33-C34
52	k	101	CDL	C19-C20-C21-C22
50	C	304	DCQ	C10-C11-C12-C13
52	k	101	CDL	C44-C45-C46-C47
52	i	401	CDL	C56-C57-C58-C59
48	r	501	PEE	C24-C25-C26-C27
46	A	502	FMN	C5'-O5'-P-O2P
49	a	202	PLX	C25-C26-C27-C28
48	C	302	PEE	O4-C10-O2-C2
49	e	201	PLX	C11-C12-C13-C14
49	j	203	PLX	C10-C11-C12-C13
52	o	201	CDL	C84-C85-C86-C87
49	e	201	PLX	C26-C27-C28-C29
52	k	101	CDL	C13-C14-C15-C16
48	j	202	PEE	C19-C20-C21-C22
49	C	303	PLX	C12-C13-C14-C15
48	W	201	PEE	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	a	201	CDL	C38-C39-C40-C41
48	B	303	PEE	O3P-C1-C2-O2
52	i	401	CDL	OA5-CA3-CA4-OA6
52	i	401	CDL	OB5-CB3-CB4-OB6
52	V	201	CDL	C39-C40-C41-C42
48	j	201	PEE	C34-C35-C36-C37
48	l	703	PEE	C1-C2-C3-O3
49	J	403	PLX	C3-C4-C5-O8
48	B	303	PEE	C31-C32-C33-C34
49	J	403	PLX	C1-C2-O1-P1
48	C	302	PEE	O2-C2-C3-O3
48	V	202	PEE	O2-C2-C3-O3
48	l	702	PEE	O2-C2-C3-O3
49	a	202	PLX	O6-C4-C5-O8
52	V	201	CDL	OA6-CA4-CA6-OA8
52	i	401	CDL	OA6-CA4-CA6-OA8
52	o	201	CDL	OB6-CB4-CB6-OB8
52	i	401	CDL	OA7-CA5-OA6-CA4
48	l	702	PEE	C43-C44-C45-C46
52	l	701	CDL	C12-C13-C14-C15
52	l	701	CDL	C32-C33-C34-C35
49	J	403	PLX	C7-C6-O6-C4
49	j	203	PLX	C7-C6-O6-C4
52	a	201	CDL	C71-C72-C73-C74
52	s	401	CDL	OB9-CB7-OB8-CB6
52	r	502	CDL	C11-CA5-OA6-CA4
47	A	503	NAI	C3D-C4D-C5D-O5D
52	s	401	CDL	C71-CB7-OB8-CB6
52	g	202	CDL	C17-C18-C19-C20
52	s	401	CDL	C84-C85-C86-C87
49	C	303	PLX	N1-C1-C2-O1
49	J	403	PLX	N1-C1-C2-O1
49	g	201	PLX	C14-C15-C16-C17
48	C	302	PEE	C44-C45-C46-C47
49	a	202	PLX	C25-C24-O8-C5
49	j	203	PLX	C25-C24-O8-C5
52	r	502	CDL	C54-C55-C56-C57
48	B	303	PEE	O3P-C1-C2-C3
48	j	202	PEE	O3P-C1-C2-C3
48	r	501	PEE	O3P-C1-C2-C3
52	a	201	CDL	OA5-CA3-CA4-CA6
49	e	201	PLX	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	g	202	CDL	C1-CB2-OB2-PB2
52	k	101	CDL	CA4-CA3-OA5-PA1
52	s	401	CDL	C34-C35-C36-C37
49	e	201	PLX	O8-C24-C25-C26
49	J	403	PLX	O4-C3-C4-O6
49	g	201	PLX	O4-C3-C4-O6
52	a	201	CDL	OB5-CB3-CB4-OB6
52	l	701	CDL	OA5-CA3-CA4-OA6
52	r	502	CDL	C22-C23-C24-C25
52	r	502	CDL	C51-CB5-OB6-CB4
51	X	201	8Q1	C11-C10-C9-C8
48	B	303	PEE	C10-C11-C12-C13
48	V	202	PEE	C10-C11-C12-C13
48	j	202	PEE	O2-C2-C3-O3
48	l	703	PEE	O2-C2-C3-O3
52	I	201	CDL	OA6-CA4-CA6-OA8
48	l	702	PEE	C34-C35-C36-C37
52	I	201	CDL	CA2-C1-CB2-OB2
52	s	401	CDL	C17-C18-C19-C20
52	s	401	CDL	CA3-CA4-CA6-OA8
49	J	403	PLX	C26-C27-C28-C29
52	r	502	CDL	C63-C64-C65-C66
49	C	303	PLX	C16-C17-C18-C19
49	C	303	PLX	C31-C32-C33-C34
48	B	303	PEE	C18-C19-C20-C21
48	l	703	PEE	C38-C39-C40-C41
52	k	101	CDL	OB9-CB7-OB8-CB6
52	o	201	CDL	C54-C55-C56-C57
49	g	201	PLX	C6-C7-C8-C9
52	V	201	CDL	C19-C20-C21-C22
48	C	302	PEE	C1-O3P-P-O2P
48	C	302	PEE	C1-O3P-P-O4P
48	C	302	PEE	C4-O4P-P-O2P
48	j	201	PEE	C1-O3P-P-O2P
48	j	201	PEE	C1-O3P-P-O4P
48	j	202	PEE	C1-O3P-P-O1P
48	j	202	PEE	C1-O3P-P-O4P
48	l	702	PEE	C4-O4P-P-O2P
48	l	703	PEE	C1-O3P-P-O2P
48	l	703	PEE	C1-O3P-P-O1P
48	l	703	PEE	C1-O3P-P-O4P
48	r	501	PEE	C1-O3P-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	r	501	PEE	C1-O3P-P-O4P
49	C	303	PLX	C3-O4-P1-O2
49	C	303	PLX	C2-O1-P1-O3
49	J	403	PLX	C3-C4-O6-C6
49	J	403	PLX	C5-C4-O6-C6
49	J	403	PLX	C3-O4-P1-O2
49	a	202	PLX	C3-O4-P1-O1
49	a	202	PLX	C3-O4-P1-O2
49	a	202	PLX	C3-O4-P1-O3
49	e	201	PLX	C3-C4-O6-C6
49	e	201	PLX	C5-C4-O6-C6
49	j	203	PLX	C2-O1-P1-O2
52	I	201	CDL	CA3-OA5-PA1-OA2
52	I	201	CDL	CA3-OA5-PA1-OA3
52	I	201	CDL	CA3-OA5-PA1-OA4
52	a	201	CDL	CB3-OB5-PB2-OB3
52	g	202	CDL	CA2-OA2-PA1-OA4
52	g	202	CDL	CB3-OB5-PB2-OB4
52	i	401	CDL	CA2-OA2-PA1-OA3
52	i	401	CDL	CA2-OA2-PA1-OA4
52	i	401	CDL	CA2-OA2-PA1-OA5
52	i	401	CDL	CB3-OB5-PB2-OB2
52	i	401	CDL	CB3-OB5-PB2-OB4
52	l	701	CDL	CA3-OA5-PA1-OA2
52	l	701	CDL	CA3-OA5-PA1-OA3
52	l	701	CDL	CB3-OB5-PB2-OB2
52	l	701	CDL	CB3-OB5-PB2-OB3
52	l	701	CDL	CB3-OB5-PB2-OB4
52	o	201	CDL	CA3-OA5-PA1-OA2
52	o	201	CDL	CA3-OA5-PA1-OA3
52	o	201	CDL	CA3-OA5-PA1-OA4
52	o	201	CDL	CB2-OB2-PB2-OB4
52	o	201	CDL	CB2-OB2-PB2-OB5
52	s	401	CDL	CB2-OB2-PB2-OB3
52	s	401	CDL	CB2-OB2-PB2-OB4
52	s	401	CDL	CB2-OB2-PB2-OB5
52	u	201	CDL	CA3-OA5-PA1-OA2
52	u	201	CDL	CA3-OA5-PA1-OA3
48	r	501	PEE	C20-C21-C22-C23
52	o	201	CDL	C15-C16-C17-C18
52	V	201	CDL	C1-CB2-OB2-PB2
52	r	502	CDL	OA7-CA5-OA6-CA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	e	201	PLX	C15-C16-C17-C18
53	J	401	NDP	O4D-C1D-N1N-C2N
52	i	401	CDL	C51-C52-C53-C54
52	V	201	CDL	C64-C65-C66-C67
52	u	201	CDL	C72-C71-CB7-OB8
52	r	502	CDL	C44-C45-C46-C47
47	A	503	NAI	C2D-C1D-N1N-C2N
52	V	201	CDL	CA6-CA4-OA6-CA5
52	o	201	CDL	C24-C25-C26-C27
52	V	201	CDL	CA7-C31-C32-C33
52	l	701	CDL	C53-C54-C55-C56
49	g	201	PLX	O4-C3-C4-C5
52	u	201	CDL	CA2-C1-CB2-OB2
49	e	201	PLX	O4-C3-C4-O6
48	j	202	PEE	C34-C35-C36-C37
49	e	201	PLX	C7-C8-C9-C10
52	a	201	CDL	C18-C19-C20-C21
52	r	502	CDL	C20-C21-C22-C23
52	o	201	CDL	OB9-CB7-OB8-CB6
48	l	702	PEE	C31-C32-C33-C34
52	o	201	CDL	C61-C62-C63-C64
52	l	701	CDL	C78-C79-C80-C81
52	r	502	CDL	OB7-CB5-OB6-CB4
48	j	201	PEE	C24-C25-C26-C27
49	J	403	PLX	C33-C34-C35-C36
49	e	201	PLX	C29-C30-C31-C32
52	I	201	CDL	OB6-CB4-CB6-OB8
52	o	201	CDL	C57-C58-C59-C60
52	k	101	CDL	C71-CB7-OB8-CB6
48	l	703	PEE	C30-C31-C32-C33
48	r	501	PEE	C44-C45-C46-C47
48	l	702	PEE	C44-C45-C46-C47
48	j	202	PEE	C15-C16-C17-C18
52	a	201	CDL	C54-C55-C56-C57
52	o	201	CDL	C72-C73-C74-C75
52	i	401	CDL	C15-C16-C17-C18
52	s	401	CDL	C81-C82-C83-C84
48	l	702	PEE	C38-C39-C40-C41
49	C	303	PLX	C7-C8-C9-C10
49	C	303	PLX	C24-C25-C26-C27
52	r	502	CDL	C59-C60-C61-C62
52	o	201	CDL	C71-CB7-OB8-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	C	303	PLX	C35-C36-C37-C38
52	u	201	CDL	C72-C73-C74-C75
52	g	202	CDL	C79-C80-C81-C82
52	a	201	CDL	C58-C59-C60-C61
52	a	201	CDL	C31-C32-C33-C34
48	l	703	PEE	C13-C14-C15-C16
52	o	201	CDL	C21-C22-C23-C24
52	a	201	CDL	OB5-CB3-CB4-CB6
49	J	403	PLX	C24-C25-C26-C27
49	a	202	PLX	C2-C1-N1-C1A
48	l	703	PEE	C18-C19-C20-C21
52	V	201	CDL	C58-C59-C60-C61
48	l	702	PEE	C15-C16-C17-C18
52	a	201	CDL	C55-C56-C57-C58
52	a	201	CDL	C57-C58-C59-C60
52	o	201	CDL	C34-C35-C36-C37
47	A	503	NAI	O4D-C1D-N1N-C2N
52	V	201	CDL	CA4-CA3-OA5-PA1
52	k	101	CDL	C1-CA2-OA2-PA1
52	l	701	CDL	CA4-CA3-OA5-PA1
48	V	202	PEE	C35-C36-C37-C38
49	C	303	PLX	C11-C10-C9-C8
49	e	201	PLX	C28-C29-C30-C31
52	g	202	CDL	C20-C21-C22-C23
49	g	201	PLX	C36-C37-C38-C39
49	J	403	PLX	C31-C32-C33-C34
52	s	401	CDL	C56-C57-C58-C59
48	l	703	PEE	C34-C35-C36-C37
54	J	402	UQ	C19-C21-C22-C23
52	s	401	CDL	C74-C75-C76-C77
52	V	201	CDL	C44-C45-C46-C47
49	e	201	PLX	C9-C10-C11-C12
52	s	401	CDL	C39-C40-C41-C42
52	g	202	CDL	C11-CA5-OA6-CA4
48	r	501	PEE	C38-C39-C40-C41
52	s	401	CDL	CB4-CB3-OB5-PB2
52	V	201	CDL	C40-C41-C42-C43
48	V	202	PEE	C13-C14-C15-C16
52	l	701	CDL	C77-C78-C79-C80
52	u	201	CDL	OA5-CA3-CA4-CA6
52	k	101	CDL	C21-C22-C23-C24
48	B	303	PEE	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	u	201	CDL	OB6-CB4-CB6-OB8
49	j	203	PLX	C24-C25-C26-C27
53	J	401	NDP	O4D-C4D-C5D-O5D
48	l	702	PEE	C42-C43-C44-C45
49	e	201	PLX	C18-C19-C20-C21
52	g	202	CDL	OA7-CA5-OA6-CA4
52	o	201	CDL	C44-C45-C46-C47
52	l	701	CDL	C16-C17-C18-C19
49	g	201	PLX	O6-C6-C7-C8
49	g	201	PLX	C11-C10-C9-C8
49	a	202	PLX	C15-C16-C17-C18
49	e	201	PLX	C16-C17-C18-C19
52	k	101	CDL	C82-C83-C84-C85
52	a	201	CDL	C11-C12-C13-C14
52	i	401	CDL	C38-C39-C40-C41
48	B	303	PEE	C2-C1-O3P-P
49	C	303	PLX	C29-C30-C31-C32
46	A	502	FMN	O3'-C3'-C4'-C5'
52	o	201	CDL	CB3-CB4-CB6-OB8
49	C	303	PLX	O9-C24-C25-C26
49	j	203	PLX	O4-C3-C4-O6
52	l	701	CDL	OB5-CB3-CB4-OB6
52	s	401	CDL	OA5-CA3-CA4-OA6
52	k	101	CDL	C52-C51-CB5-OB6
52	k	101	CDL	C11-C12-C13-C14
49	j	203	PLX	C15-C16-C17-C18
52	s	401	CDL	C38-C39-C40-C41
48	V	202	PEE	C16-C17-C18-C19
48	l	702	PEE	C16-C17-C18-C19
46	A	502	FMN	O3'-C3'-C4'-O4'
49	e	201	PLX	C32-C33-C34-C35
52	l	701	CDL	OB5-CB3-CB4-CB6
48	C	302	PEE	C38-C39-C40-C41
48	W	201	PEE	C16-C17-C18-C19
48	l	702	PEE	C36-C37-C38-C39
48	r	501	PEE	C34-C35-C36-C37
52	V	201	CDL	C56-C57-C58-C59
48	B	303	PEE	C16-C17-C18-C19
54	s	402	UQ	C12-C13-C14-C16
48	B	303	PEE	C12-C13-C14-C15
52	a	201	CDL	C39-C40-C41-C42
48	B	303	PEE	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	V	202	PEE	C14-C15-C16-C17
52	l	701	CDL	C12-C11-CA5-OA6
49	J	403	PLX	C20-C21-C22-C23
48	C	302	PEE	C18-C19-C20-C21
52	l	701	CDL	C23-C24-C25-C26
52	V	201	CDL	C34-C35-C36-C37
52	u	201	CDL	C56-C57-C58-C59
48	j	201	PEE	C38-C39-C40-C41
47	A	503	NAI	C2D-C1D-N1N-C6N
48	V	202	PEE	C2-C1-O3P-P
52	r	502	CDL	C21-C22-C23-C24
52	o	201	CDL	OA5-CA3-CA4-OA6
52	u	201	CDL	OB5-CB3-CB4-OB6
46	A	502	FMN	C2'-C3'-C4'-O4'
52	g	202	CDL	C54-C55-C56-C57
49	j	203	PLX	C34-C35-C36-C37
52	V	201	CDL	C76-C77-C78-C79
48	V	202	PEE	C38-C39-C40-C41
48	j	201	PEE	C16-C17-C18-C19
52	i	401	CDL	C63-C64-C65-C66
52	g	202	CDL	C52-C51-CB5-OB6
49	e	201	PLX	O4-C3-C4-C5
49	a	202	PLX	C2-C1-N1-C1C
52	o	201	CDL	C78-C79-C80-C81
48	B	303	PEE	C22-C23-C24-C25
52	g	202	CDL	C72-C71-CB7-OB8
48	j	202	PEE	C18-C19-C20-C21
48	j	202	PEE	C16-C17-C18-C19
52	s	401	CDL	C61-C62-C63-C64
52	a	201	CDL	C32-C31-CA7-OA8
52	i	401	CDL	C12-C11-CA5-OA6
52	u	201	CDL	C52-C51-CB5-OB6
48	j	201	PEE	C23-C24-C25-C26
49	a	202	PLX	C2-C1-N1-C1B
48	C	302	PEE	C35-C36-C37-C38
52	u	201	CDL	C53-C54-C55-C56
48	j	201	PEE	O2-C10-C11-C12
52	I	201	CDL	C72-C71-CB7-OB8
49	g	201	PLX	O7-C6-C7-C8
48	C	302	PEE	O3-C30-C31-C32
48	r	501	PEE	C40-C41-C42-C43
49	e	201	PLX	C24-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	r	502	CDL	CA4-CA3-OA5-PA1
48	l	703	PEE	O2-C10-C11-C12
52	r	502	CDL	C72-C71-CB7-OB8
52	I	201	CDL	CB3-CB4-CB6-OB8
49	C	303	PLX	C25-C24-O8-C5
50	C	304	DCQ	C2-C3-O3-C3M
52	s	401	CDL	C12-C11-CA5-OA6
52	g	202	CDL	OB6-CB4-CB6-OB8
47	A	503	NAI	O4D-C1D-N1N-C6N
52	a	201	CDL	C33-C34-C35-C36
52	V	201	CDL	C22-C23-C24-C25
48	l	702	PEE	O2-C10-C11-C12
52	l	701	CDL	C32-C31-CA7-OA8
52	V	201	CDL	C12-C11-CA5-OA6
52	g	202	CDL	C16-C17-C18-C19
52	V	201	CDL	C20-C21-C22-C23
49	e	201	PLX	C14-C15-C16-C17
52	i	401	CDL	C36-C37-C38-C39
49	a	202	PLX	C30-C31-C32-C33
47	A	503	NAI	O4D-C4D-C5D-O5D
53	J	401	NDP	O4B-C4B-C5B-O5B
48	j	201	PEE	O4-C10-C11-C12
52	V	201	CDL	C36-C37-C38-C39
49	e	201	PLX	C2-C1-N1-C1B
49	j	203	PLX	C26-C27-C28-C29
49	j	203	PLX	C16-C17-C18-C19
49	J	403	PLX	O9-C24-O8-C5
49	e	201	PLX	O9-C24-O8-C5
52	g	202	CDL	C52-C53-C54-C55
52	V	201	CDL	C78-C79-C80-C81
52	s	401	CDL	C12-C11-CA5-OA7
52	k	101	CDL	C16-C17-C18-C19
49	g	201	PLX	C4-C5-O8-C24
52	g	202	CDL	C57-C58-C59-C60
52	g	202	CDL	C52-C51-CB5-OB7
52	I	201	CDL	CA5-C11-C12-C13
48	V	202	PEE	C31-C32-C33-C34
52	a	201	CDL	C19-C20-C21-C22
52	g	202	CDL	C77-C78-C79-C80
52	a	201	CDL	C83-C84-C85-C86
51	G	201	8Q1	O33-C32-C34-N36
48	C	302	PEE	O5-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	l	701	CDL	C32-C31-CA7-OA9
52	r	502	CDL	C72-C71-CB7-OB9
48	l	702	PEE	O4-C10-C11-C12
52	I	201	CDL	C72-C71-CB7-OB9
52	V	201	CDL	C12-C11-CA5-OA7
52	a	201	CDL	C32-C31-CA7-OA9
52	V	201	CDL	C73-C74-C75-C76
52	I	201	CDL	C12-C11-CA5-OA6
48	l	703	PEE	O4-C10-C11-C12
52	u	201	CDL	C52-C51-CB5-OB7
48	r	501	PEE	O5-C30-O3-C3
52	a	201	CDL	C74-C75-C76-C77
52	l	701	CDL	C56-C57-C58-C59
52	l	701	CDL	C52-C51-CB5-OB6
52	r	502	CDL	C24-C25-C26-C27

There are no ring outliers.

35 monomers are involved in 136 short contacts:

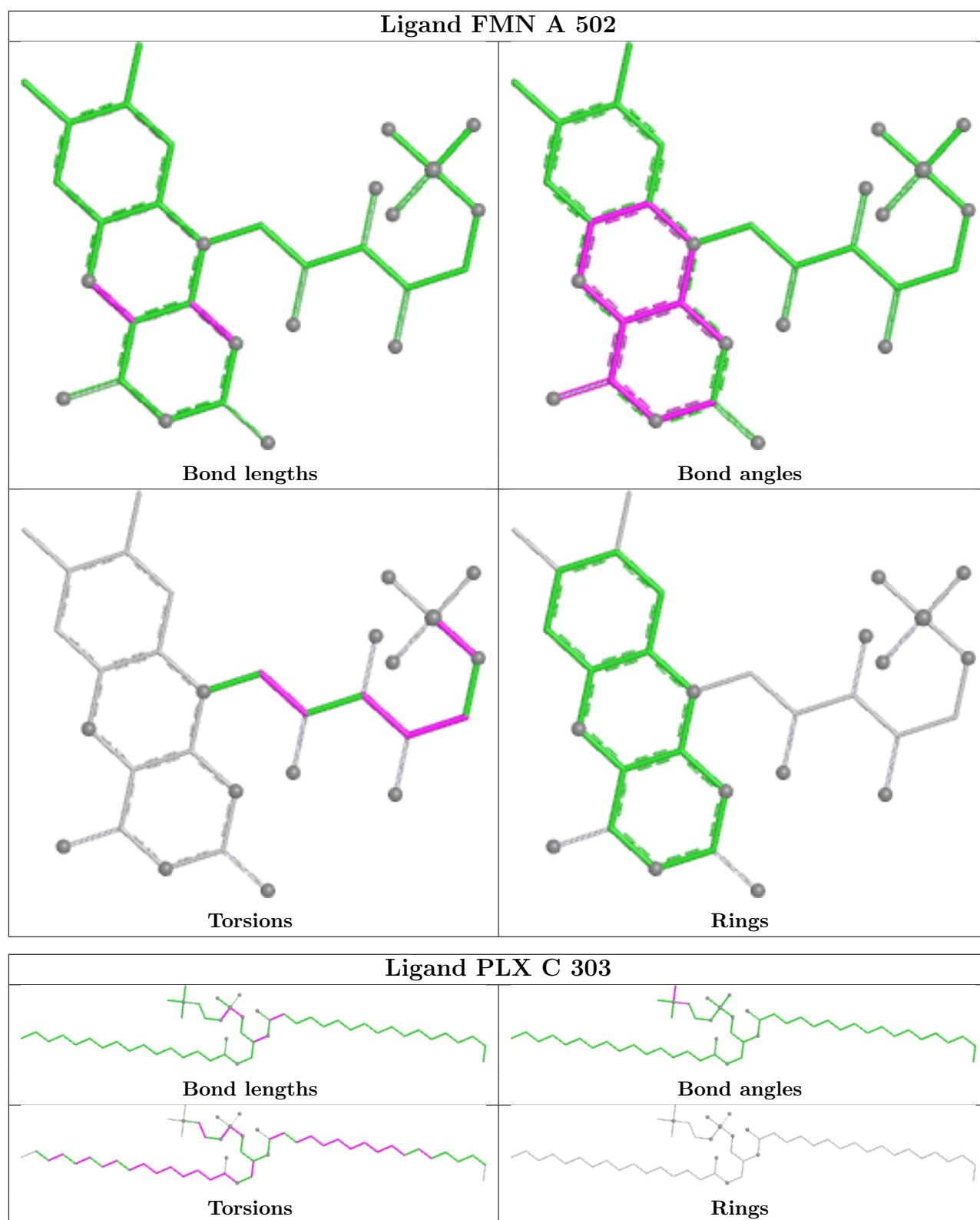
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	A	502	FMN	5	0
49	C	303	PLX	4	0
49	j	203	PLX	3	0
54	s	402	UQ	5	0
52	I	201	CDL	1	0
53	J	401	NDP	2	0
48	l	703	PEE	3	0
49	e	201	PLX	2	0
52	o	201	CDL	10	0
52	k	101	CDL	7	0
52	a	201	CDL	5	0
48	j	201	PEE	5	0
48	W	201	PEE	1	0
49	g	201	PLX	6	0
52	g	202	CDL	7	0
52	s	401	CDL	7	0
52	l	701	CDL	6	0
47	A	503	NAI	6	0
58	w	401	ADP	1	0
54	J	402	UQ	2	0
48	B	303	PEE	4	0
52	i	401	CDL	2	0

Continued on next page...

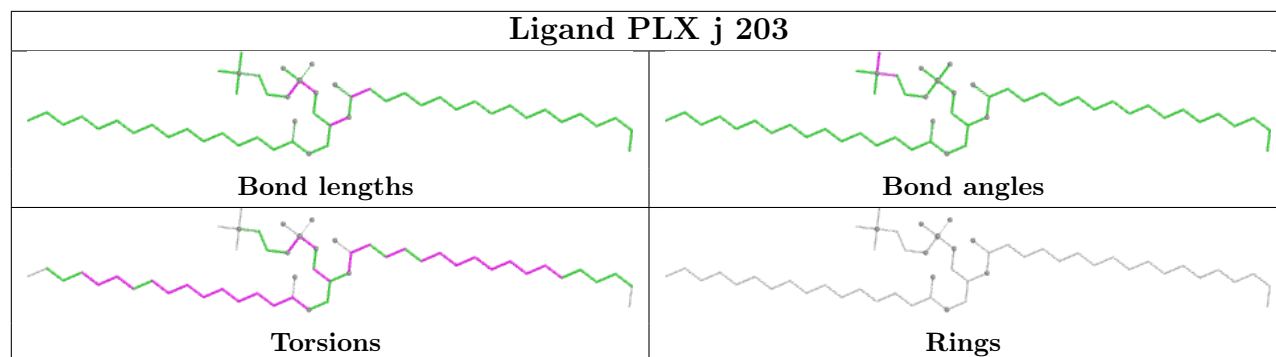
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	V	201	CDL	7	0
45	A	501	SF4	2	0
48	V	202	PEE	2	0
48	j	202	PEE	4	0
52	r	502	CDL	9	0
52	u	201	CDL	4	0
49	a	202	PLX	1	0
50	C	304	DCQ	4	0
48	C	302	PEE	1	0
48	r	501	PEE	3	0
51	X	201	8Q1	3	0
49	J	403	PLX	5	0
45	C	301	SF4	1	0

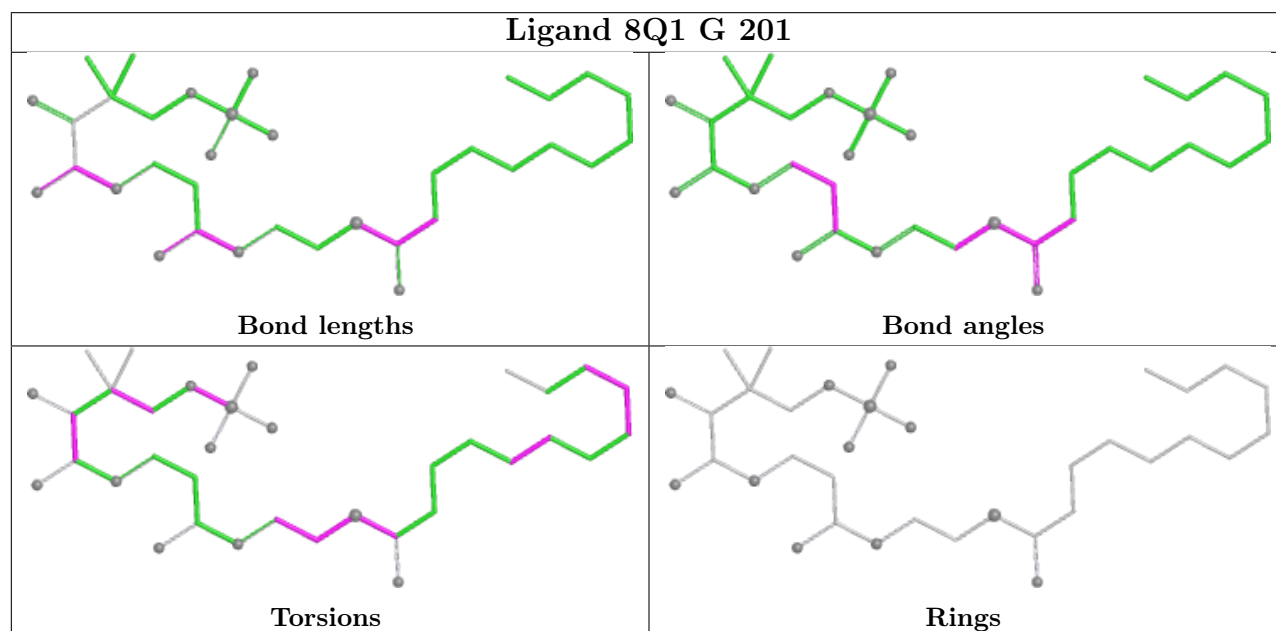
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



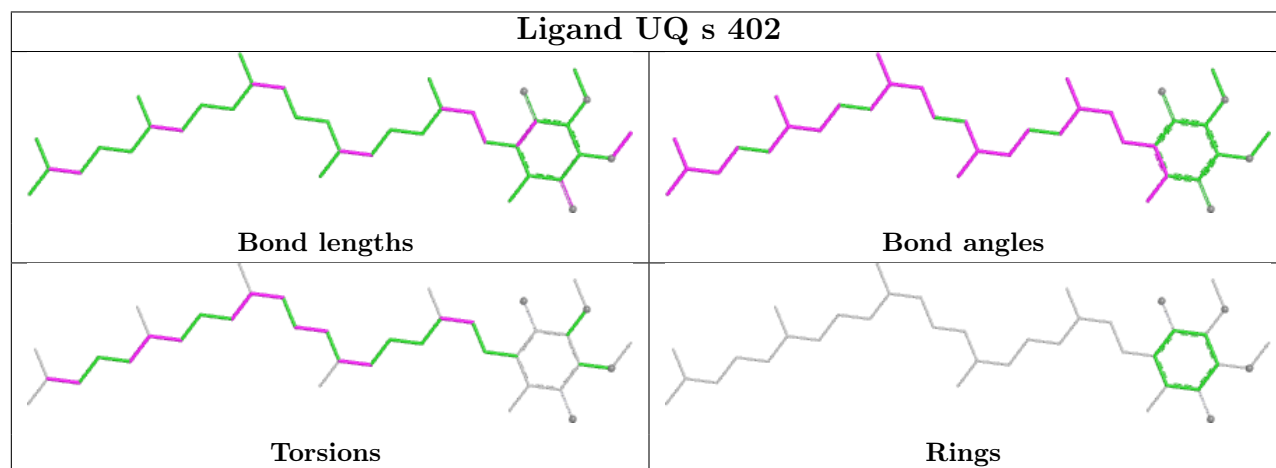
Ligand PLX j 203

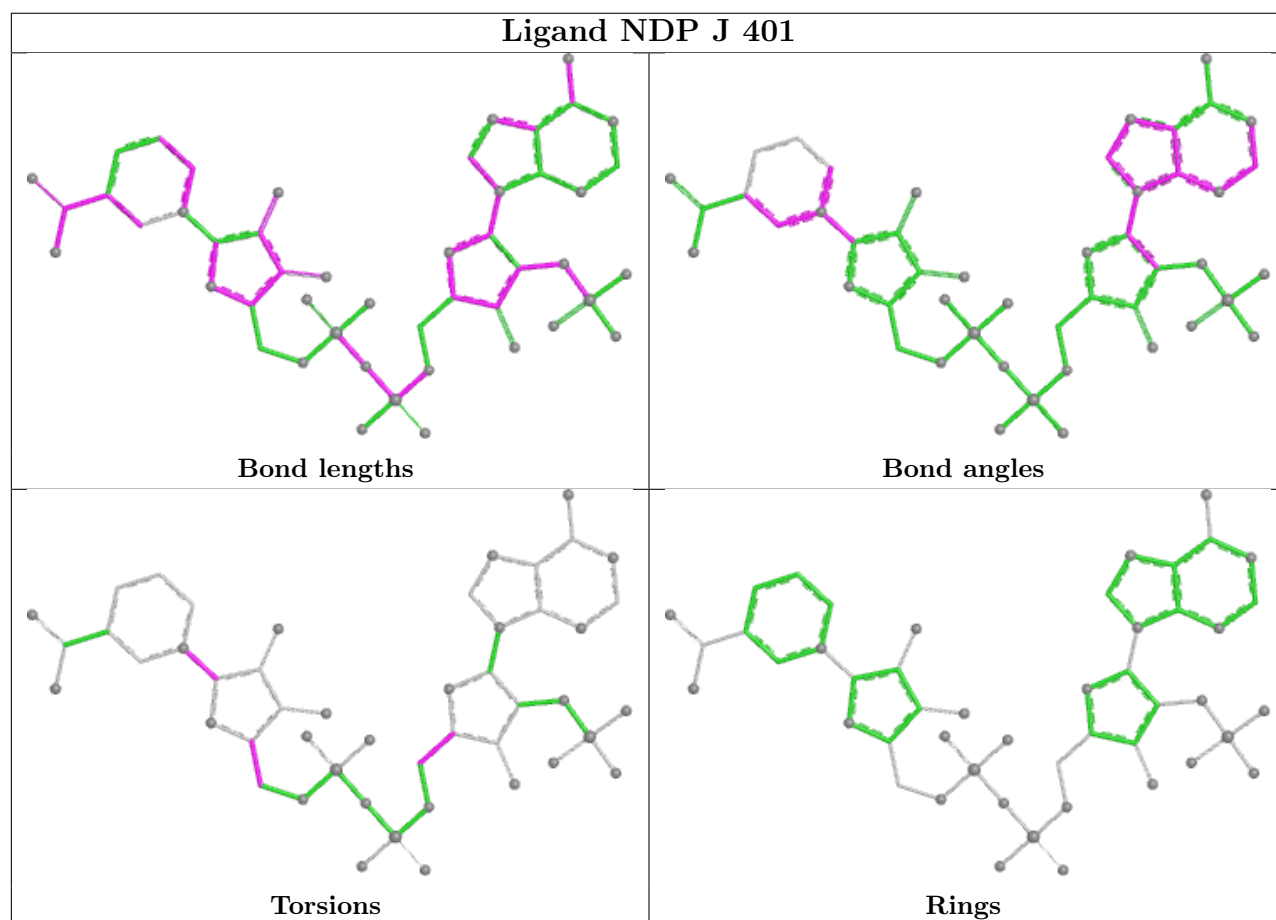
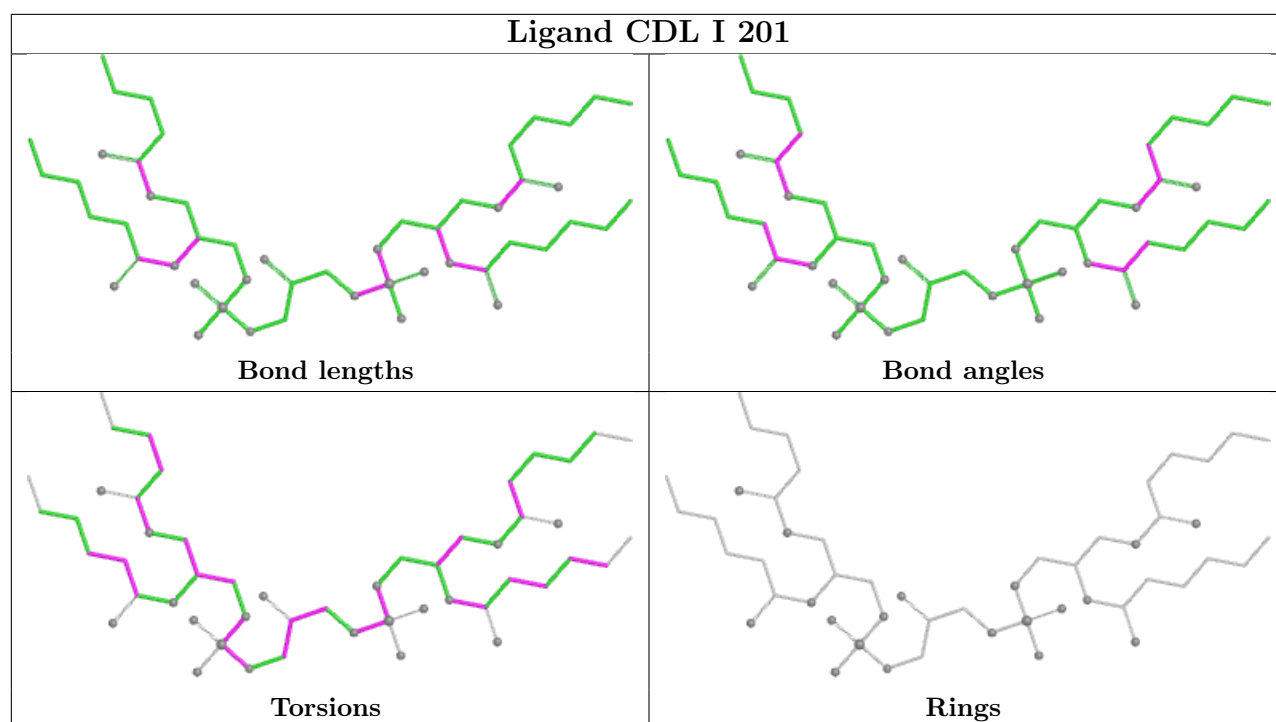


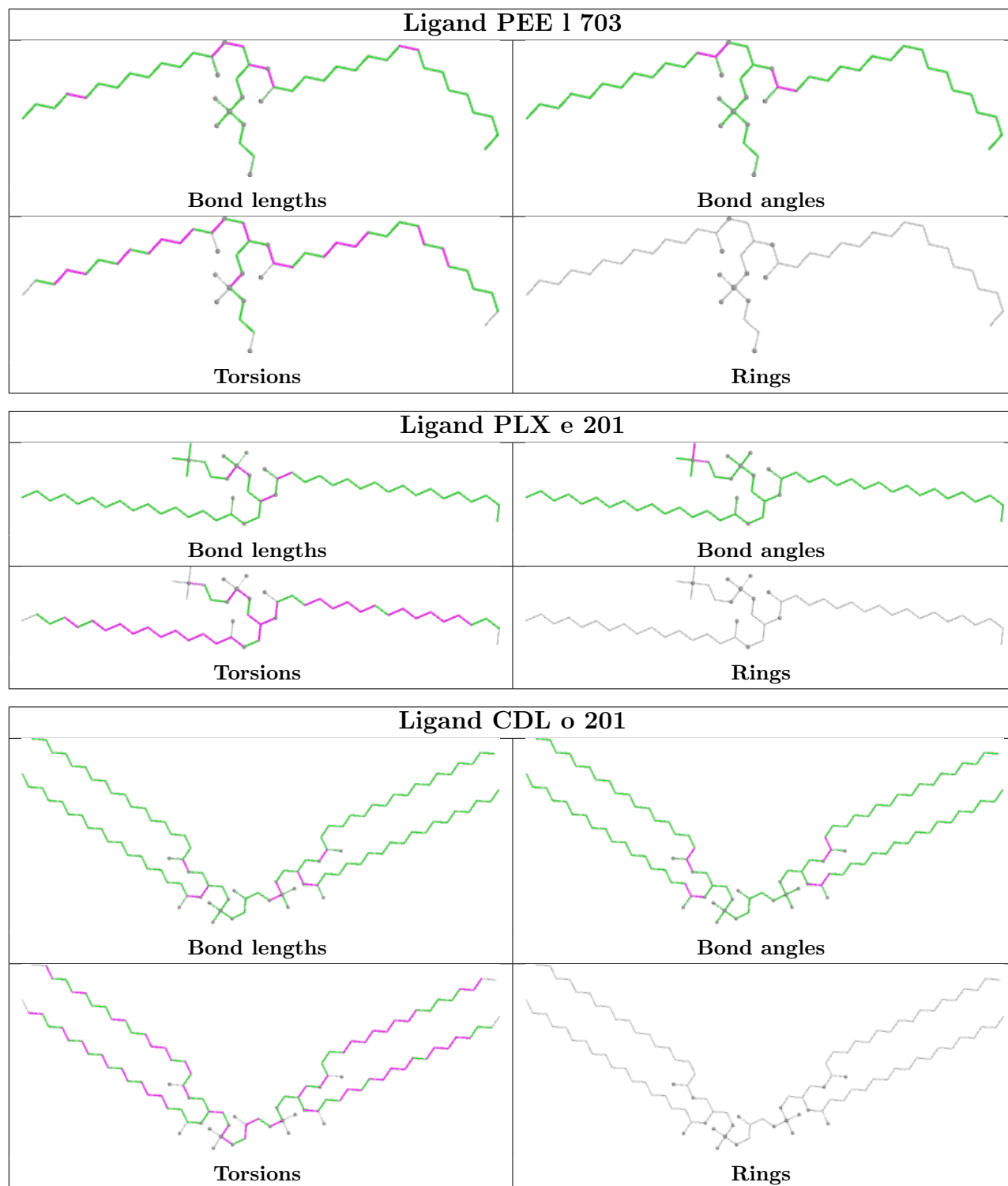
Ligand 8Q1 G 201

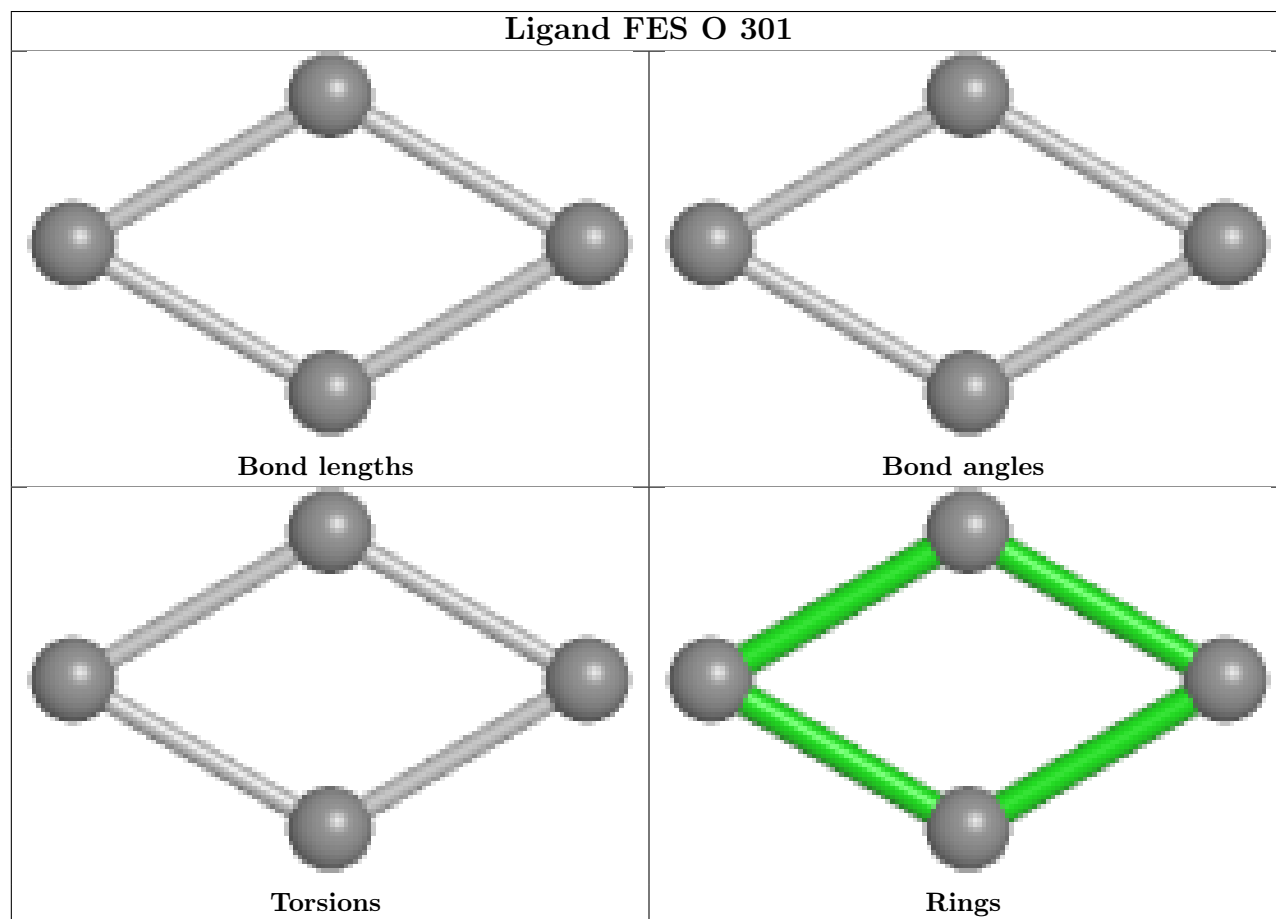
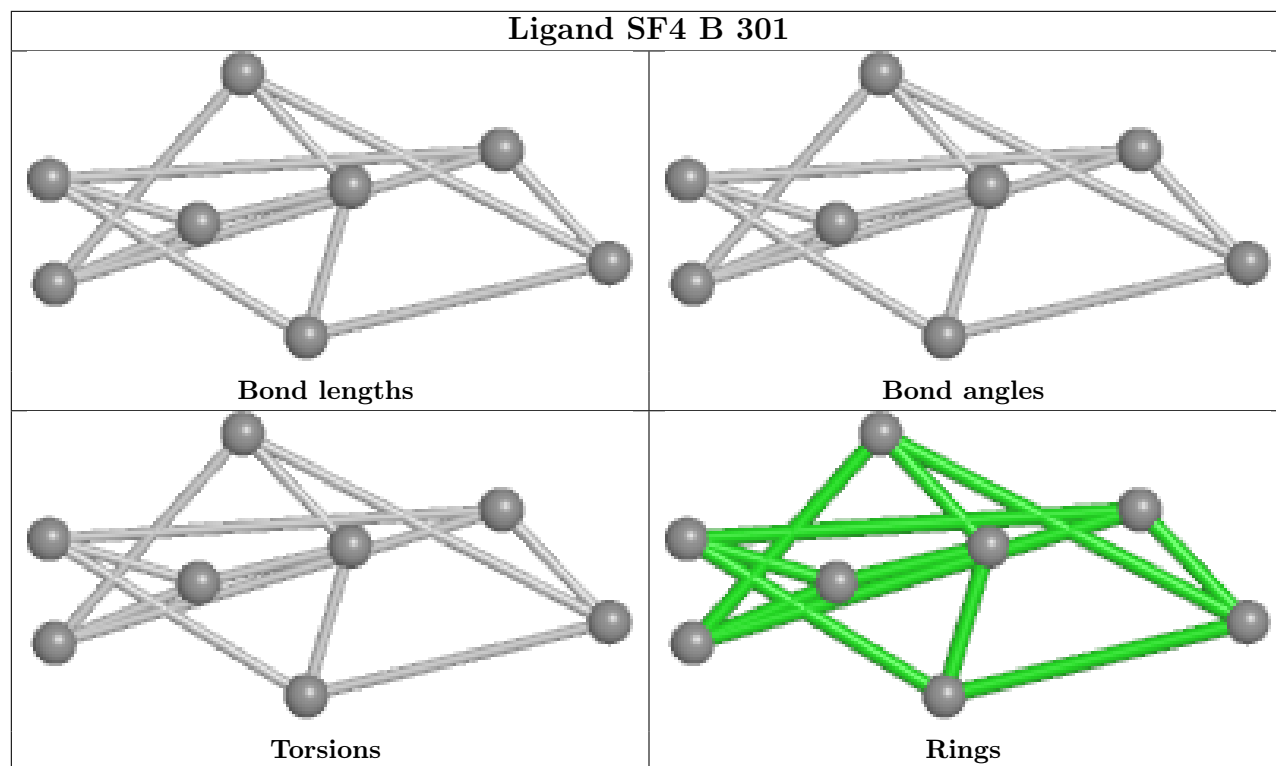


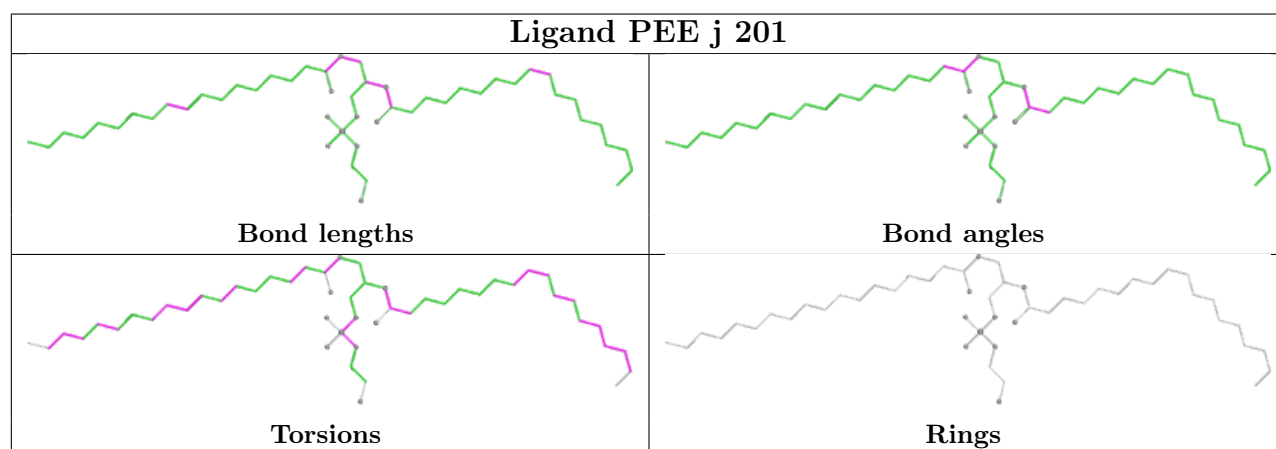
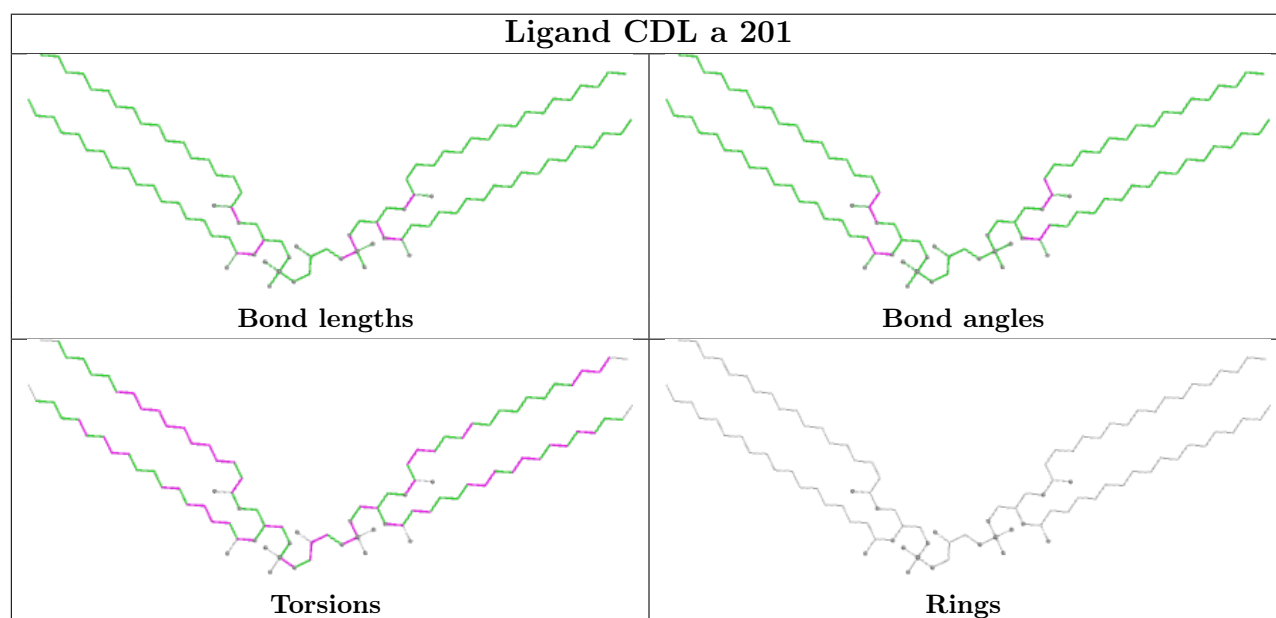
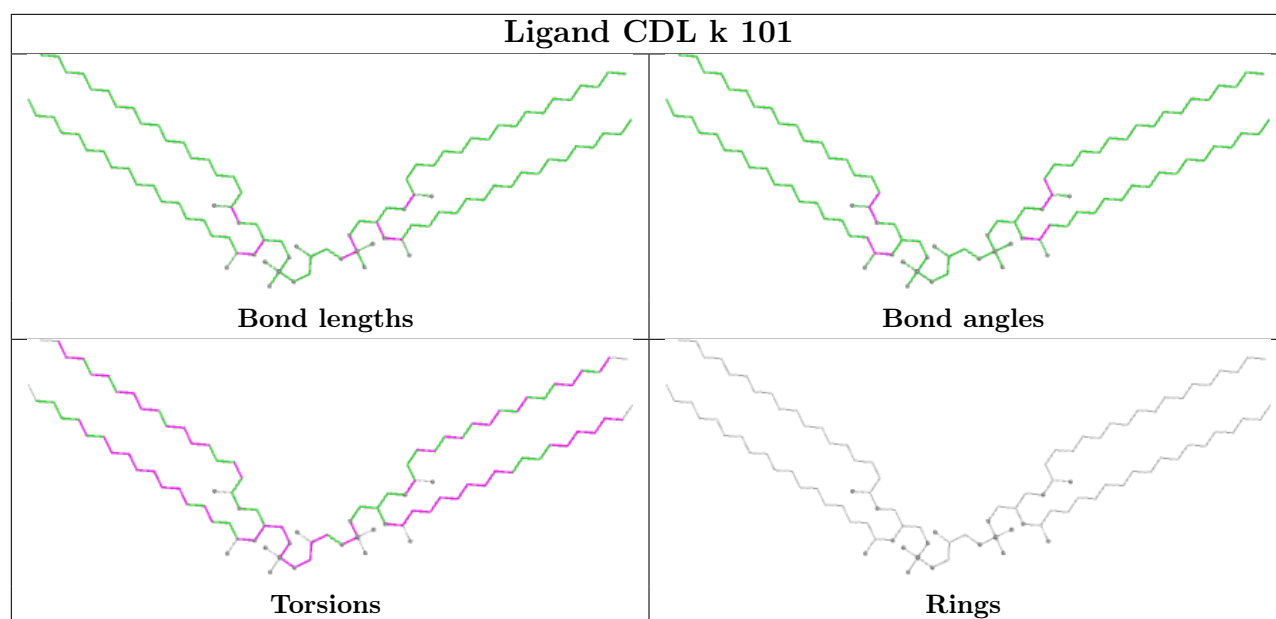
Ligand UQ s 402

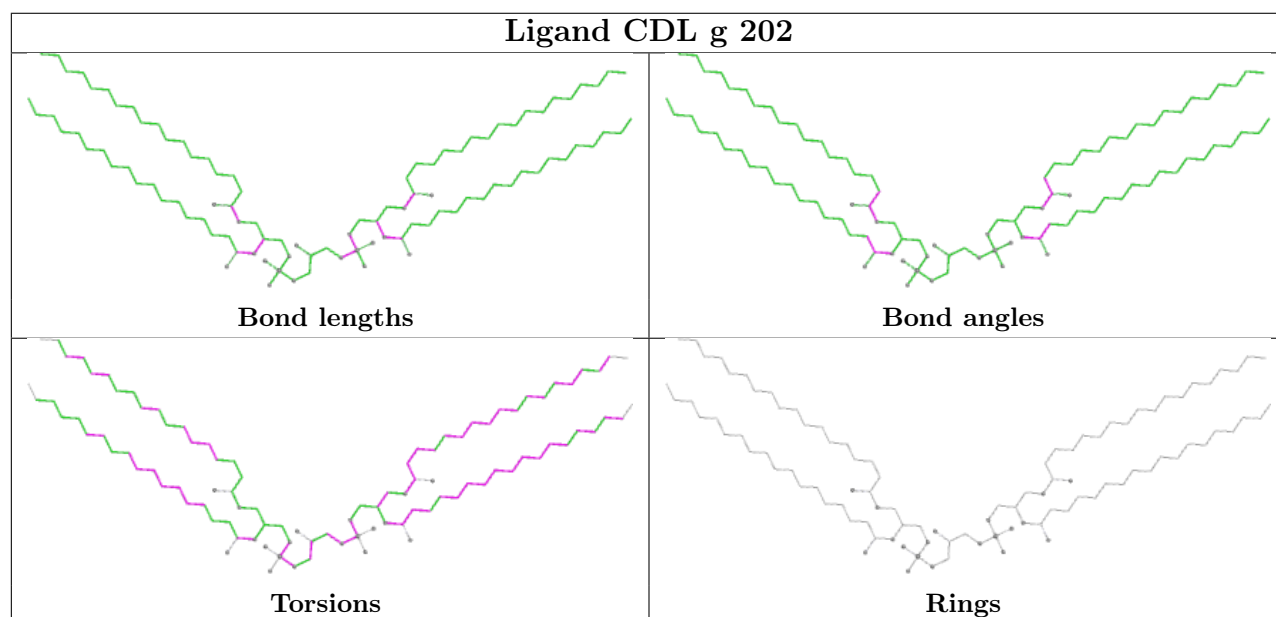
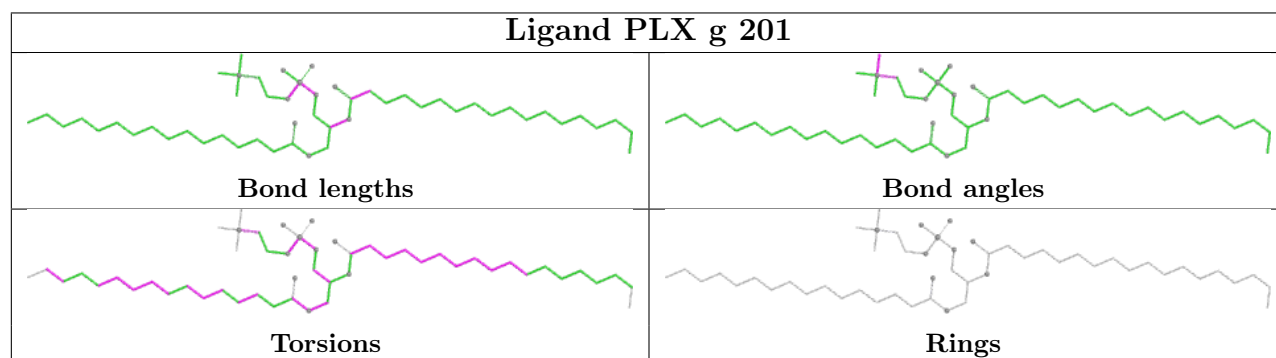
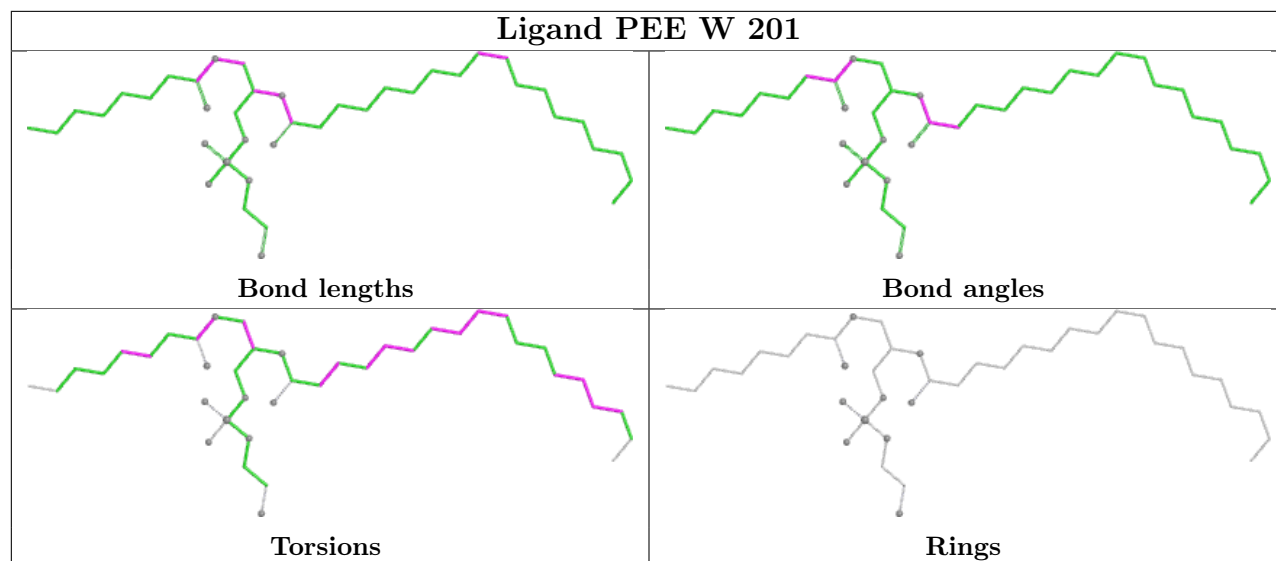


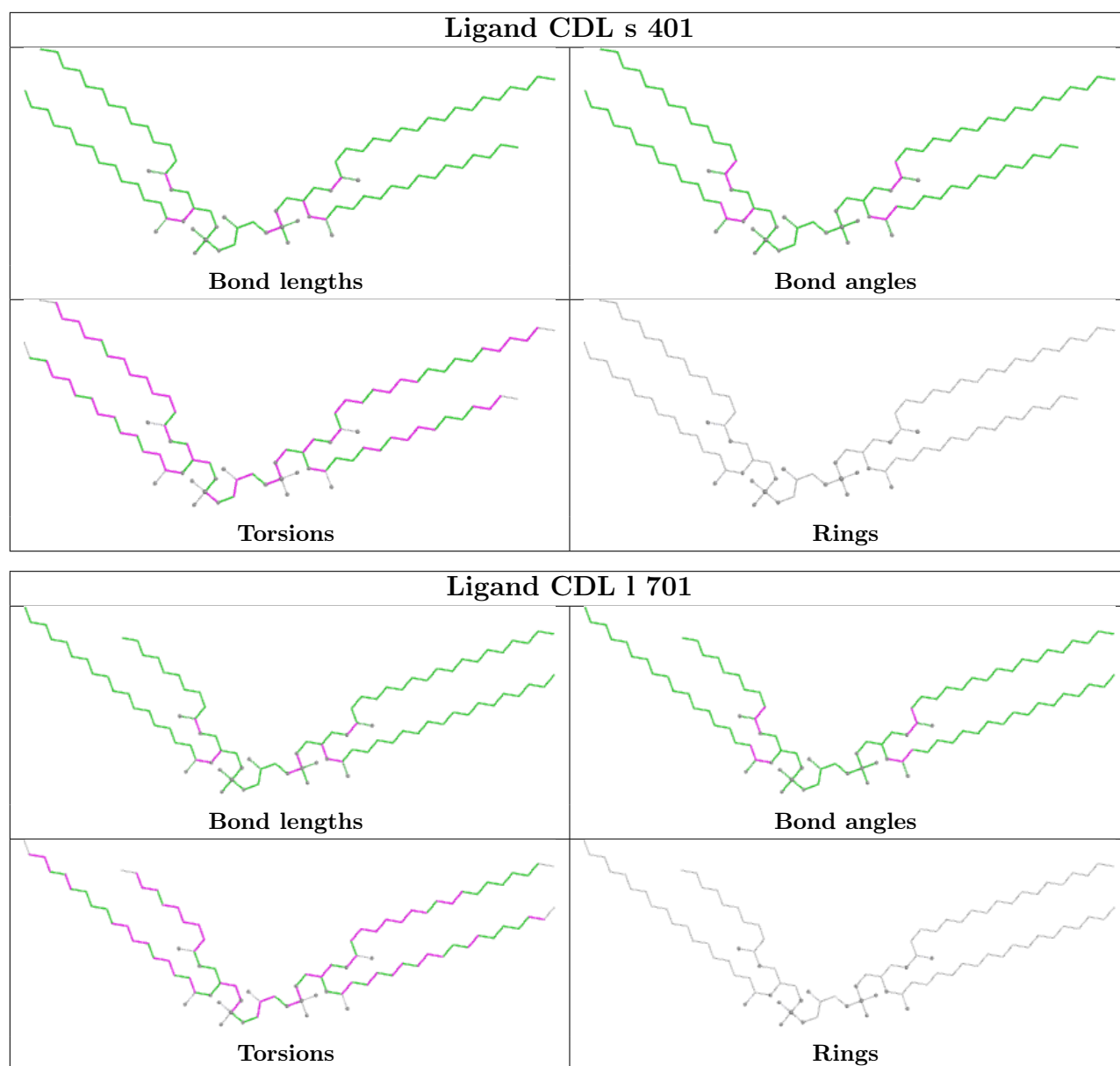




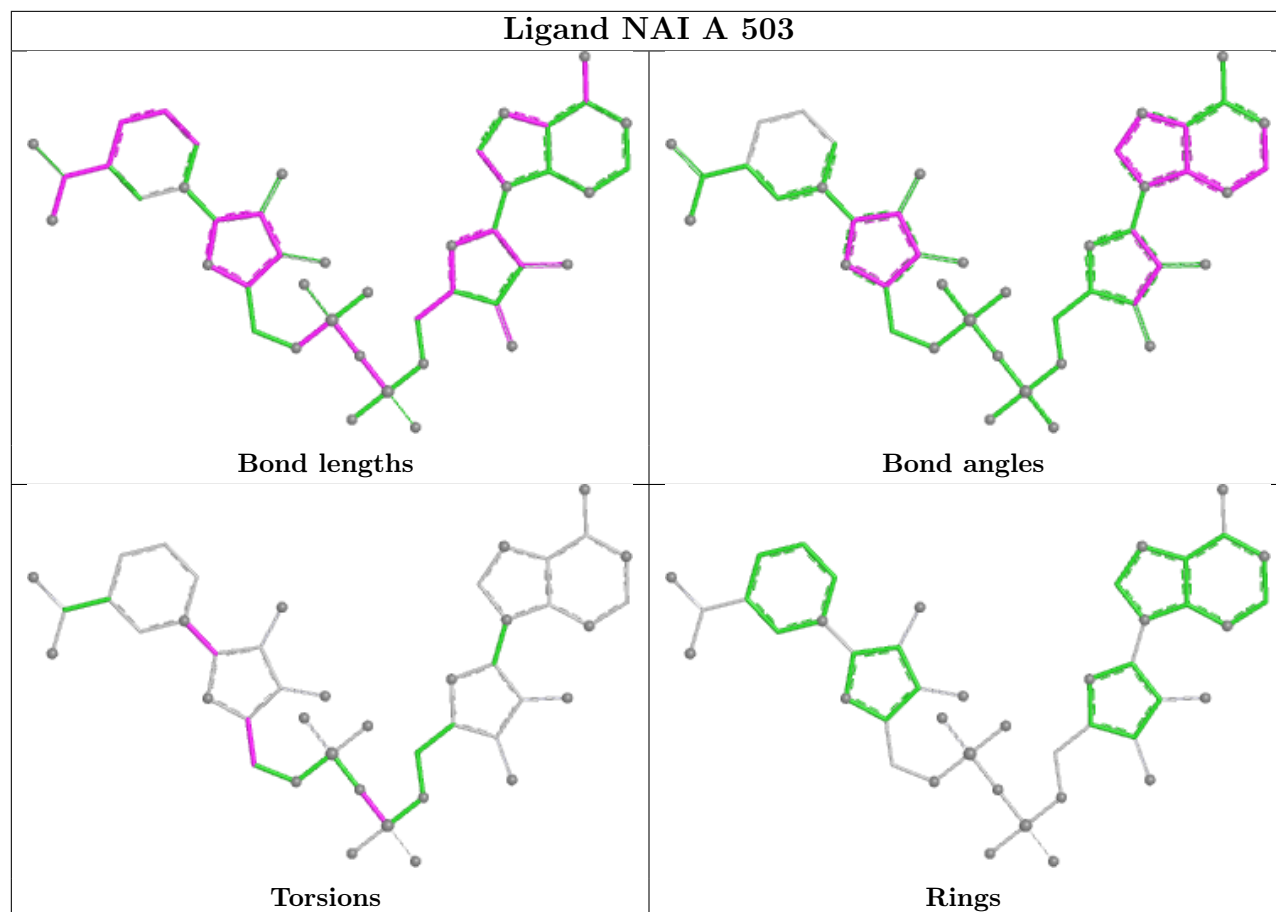




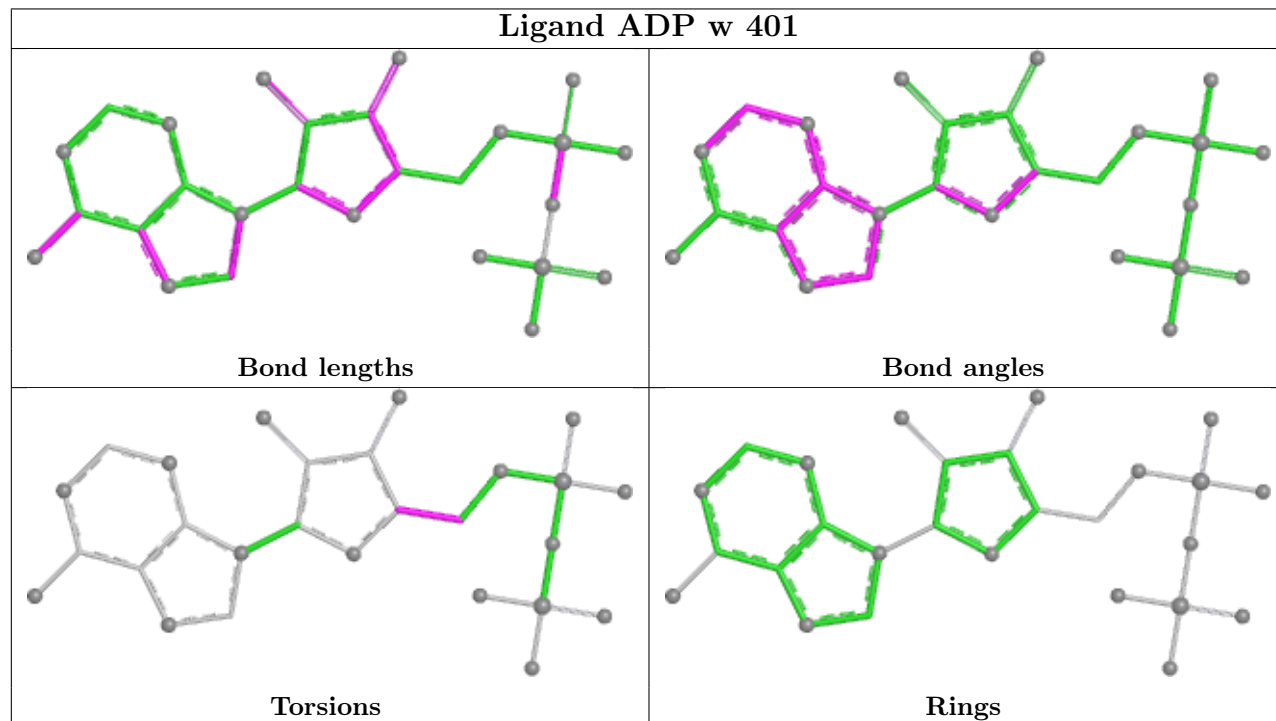


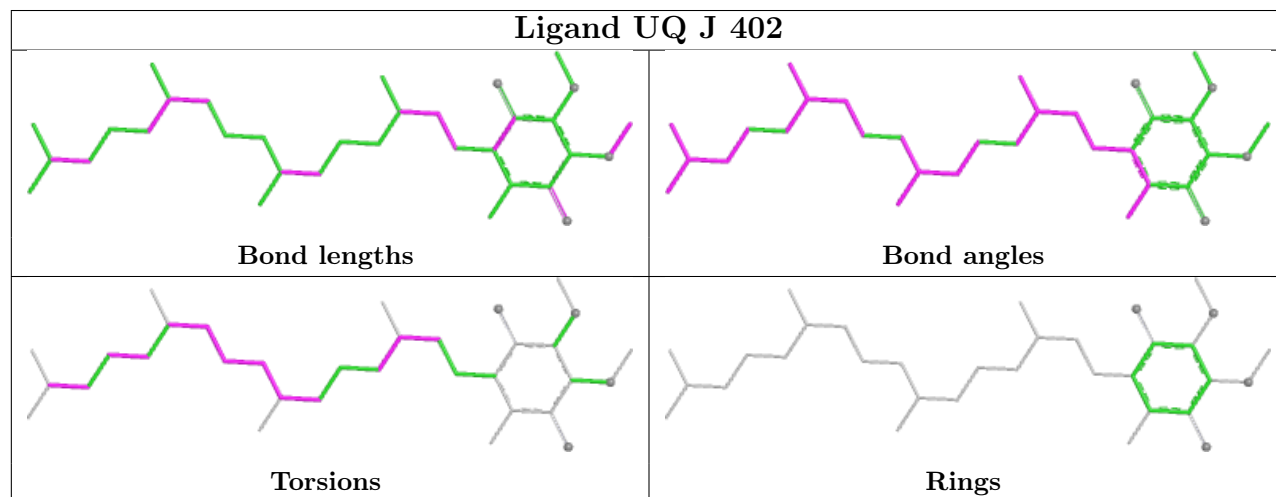
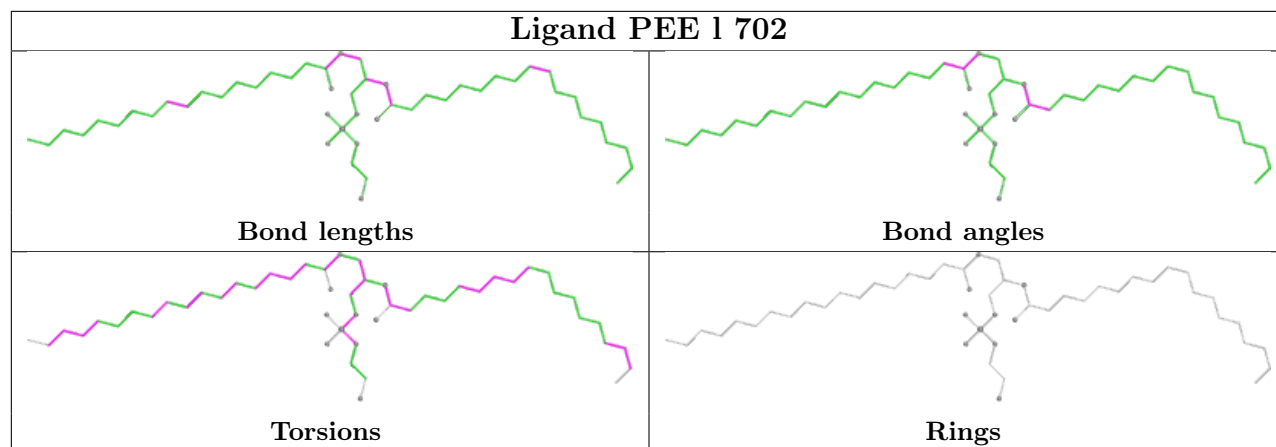


Ligand NAI A 503

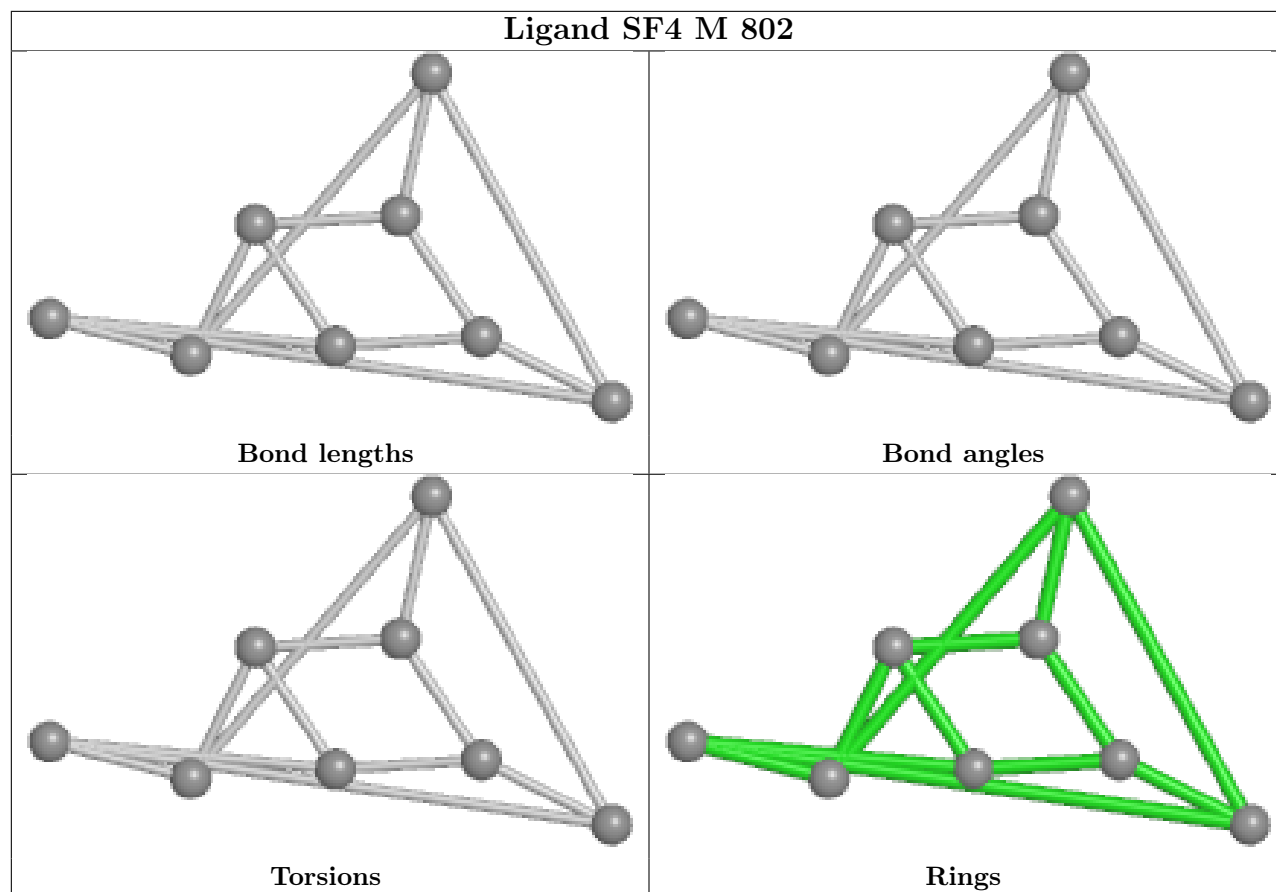


Ligand ADP w 401

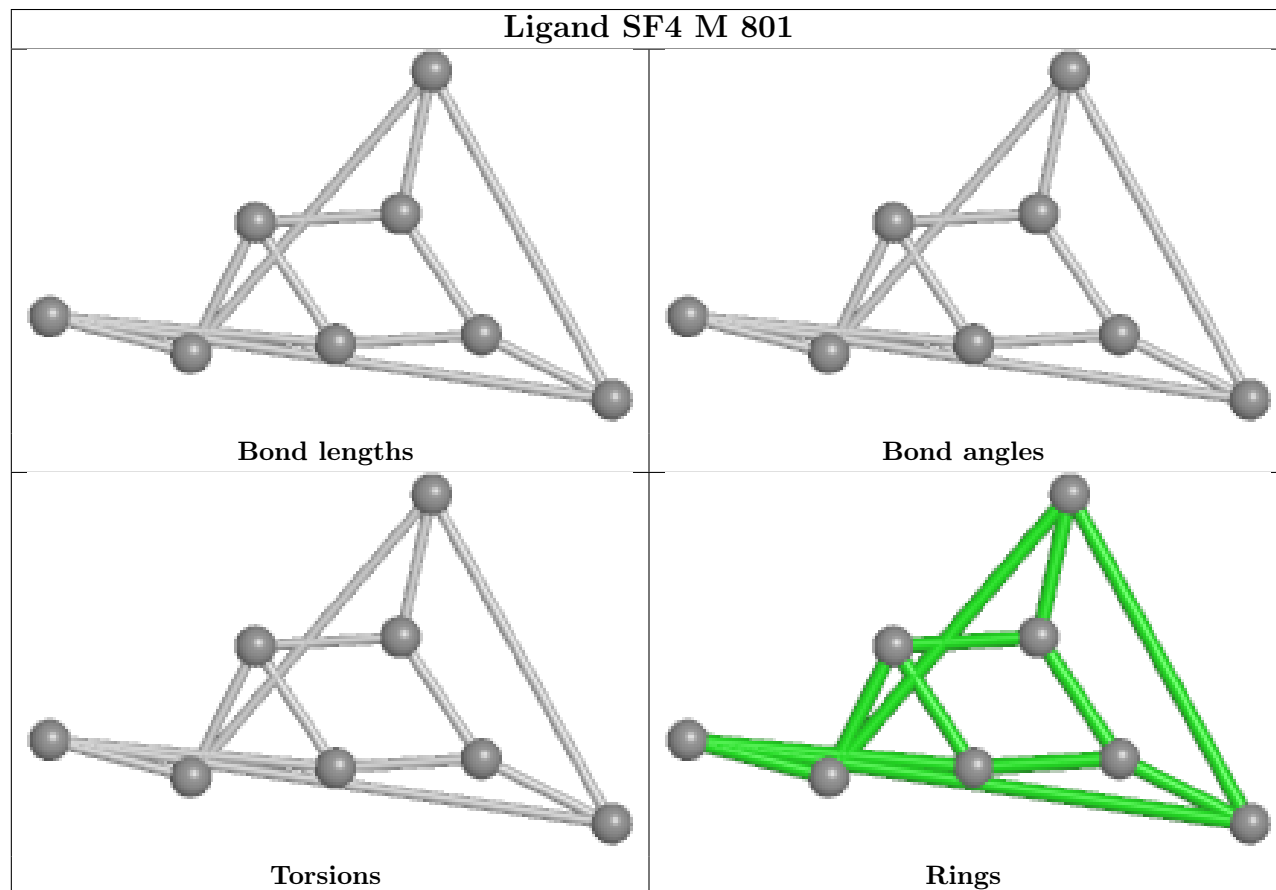


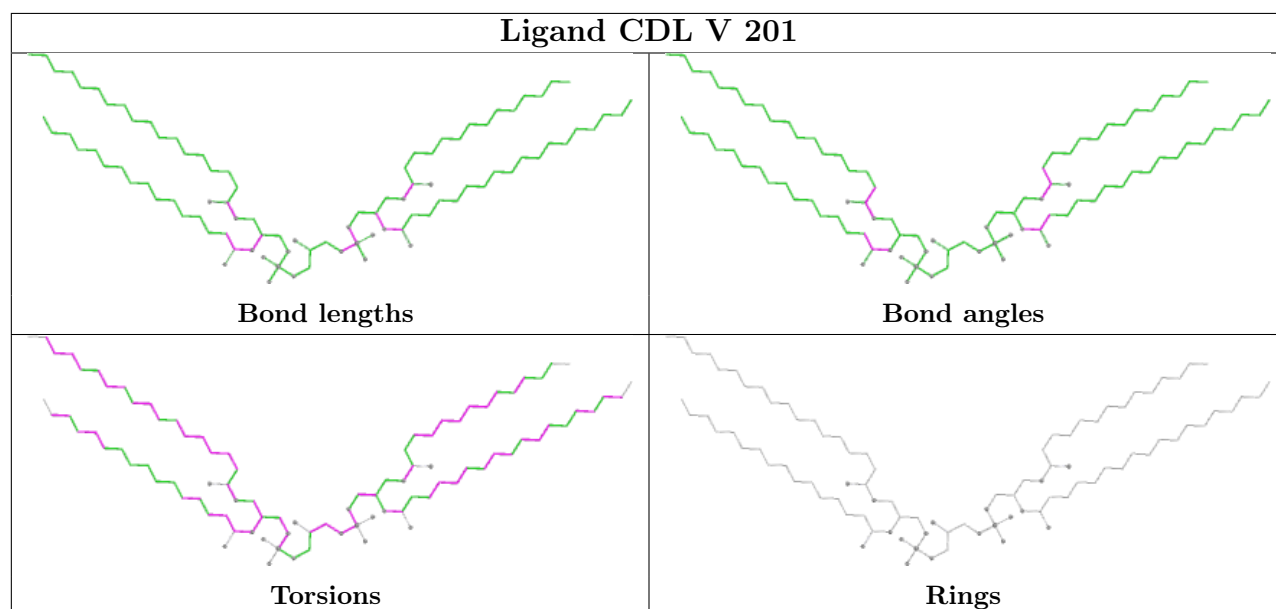
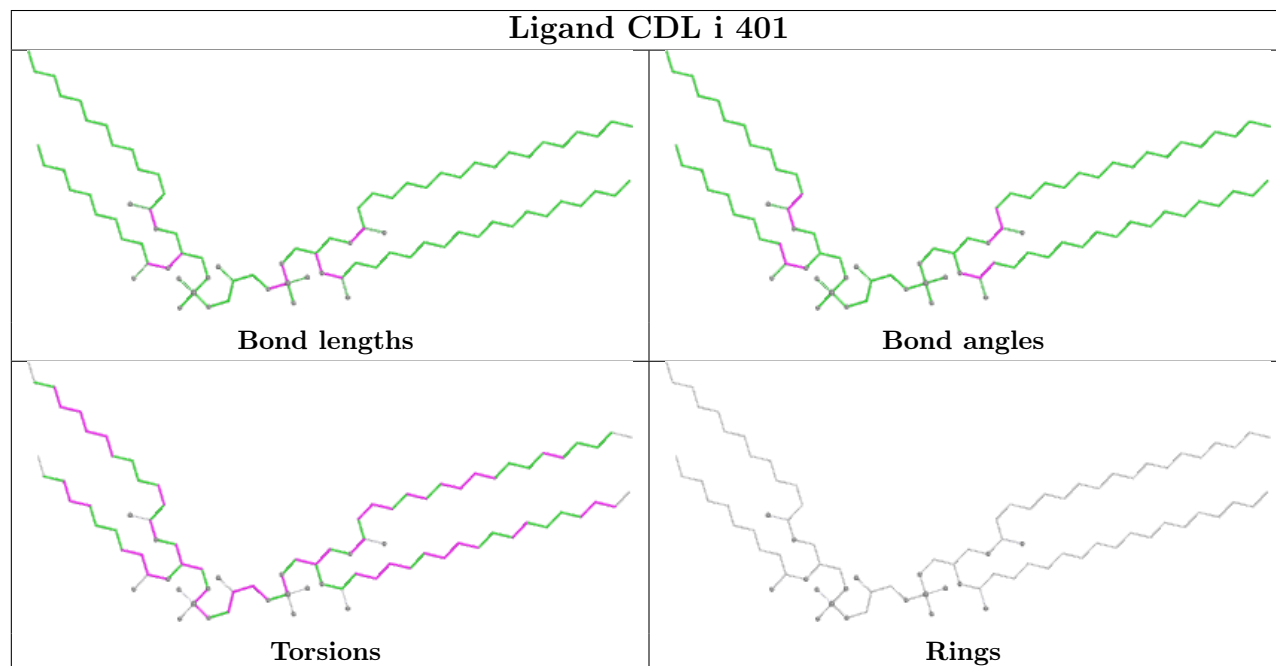
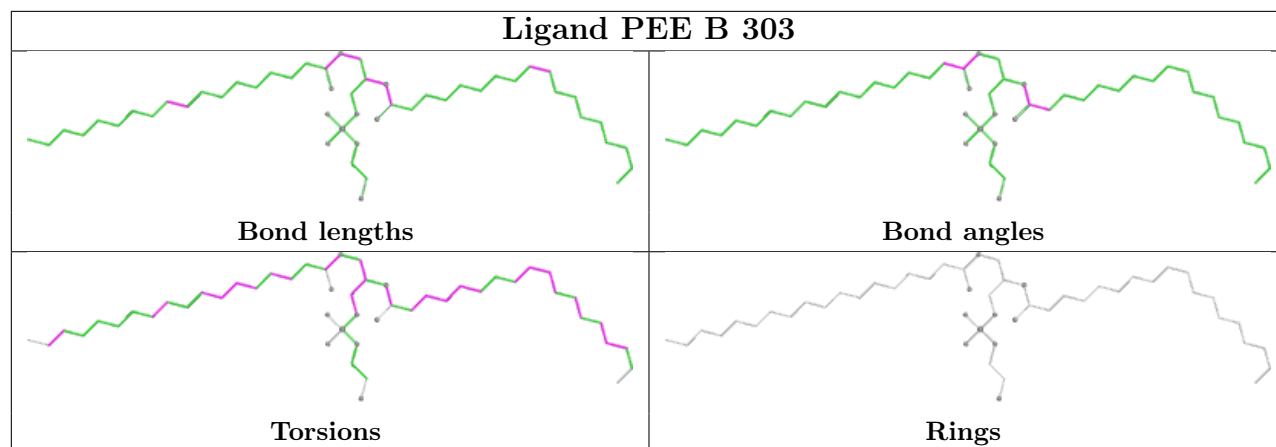


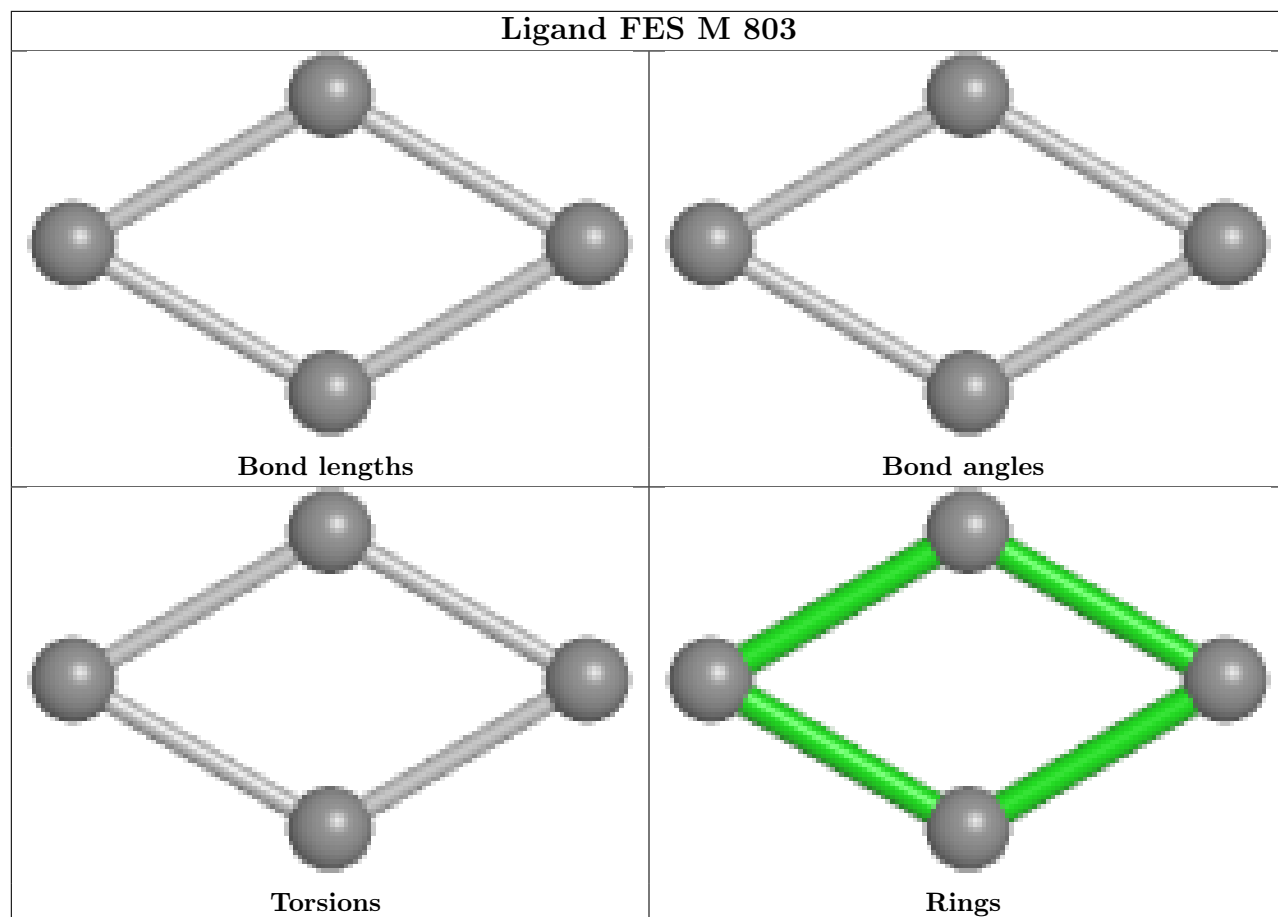
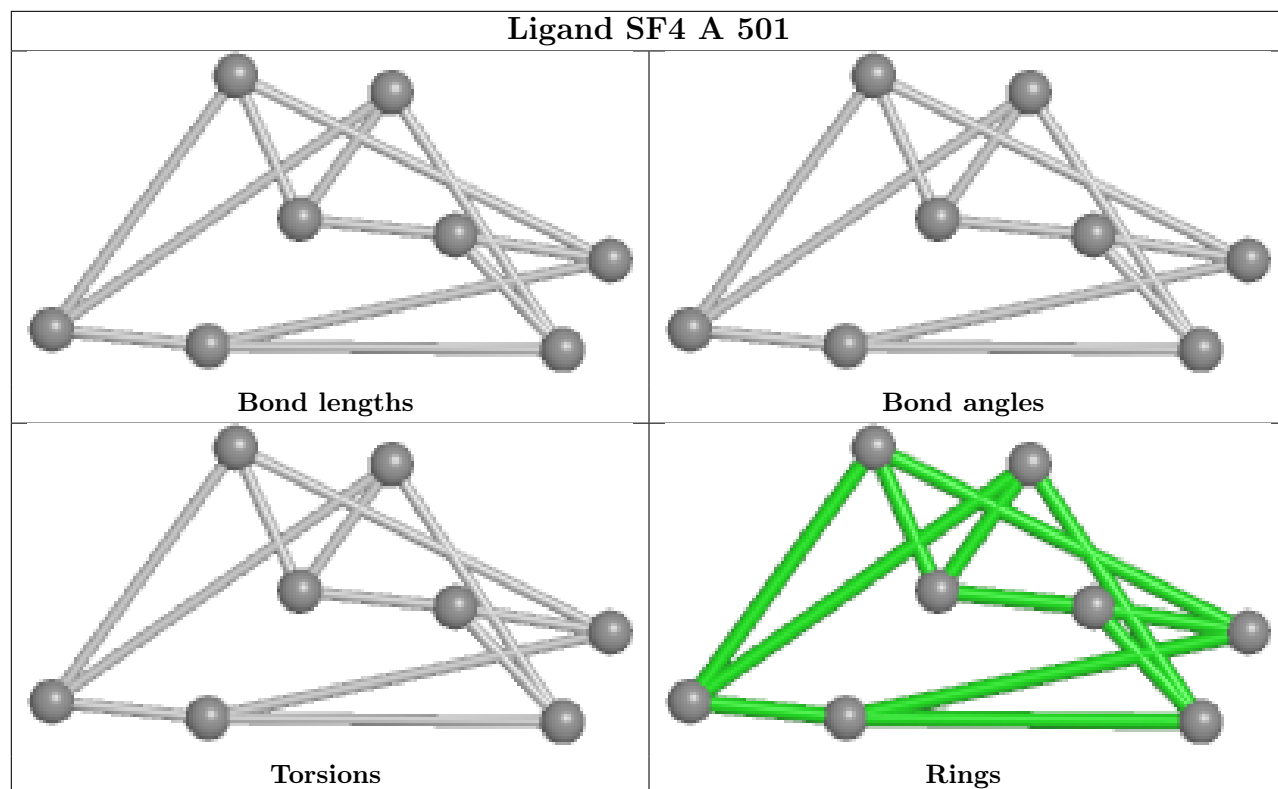
Ligand SF4 M 802

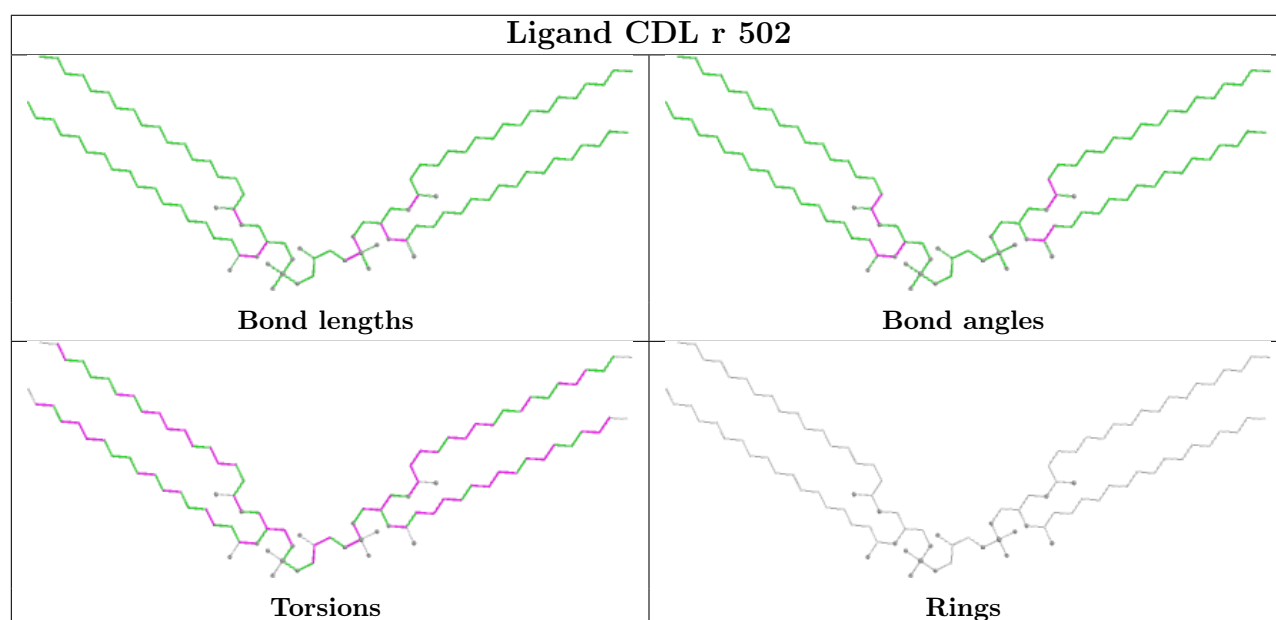
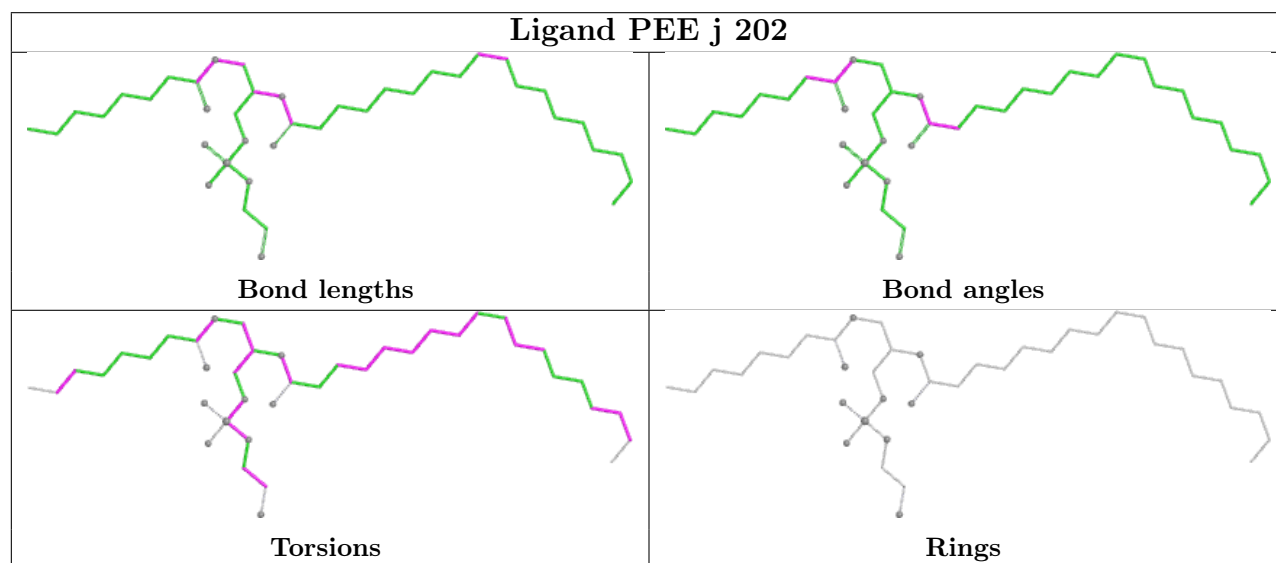
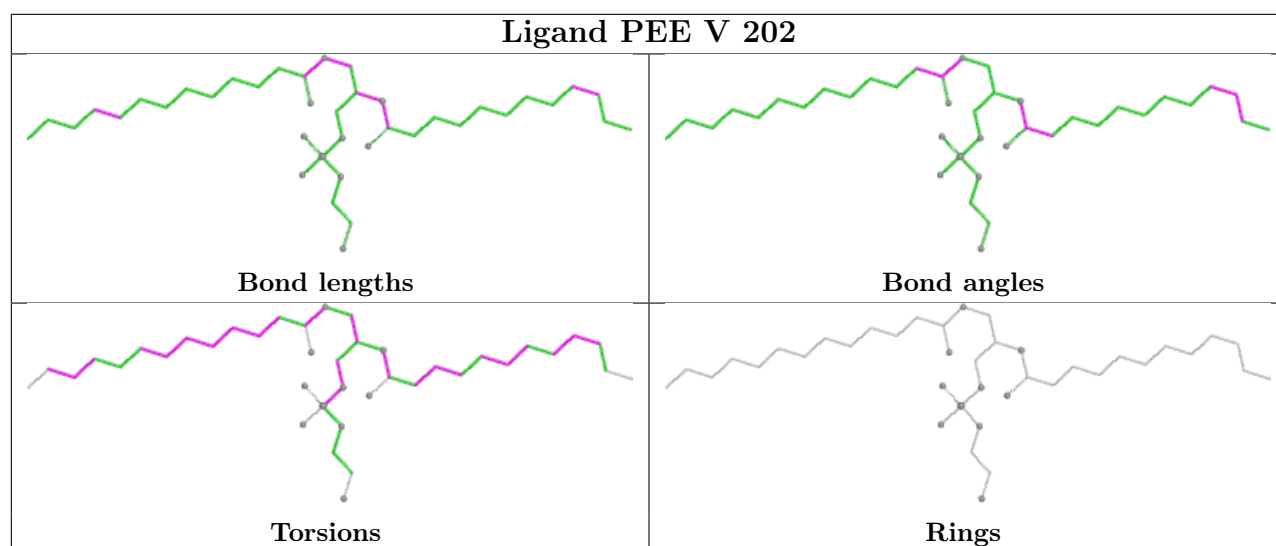


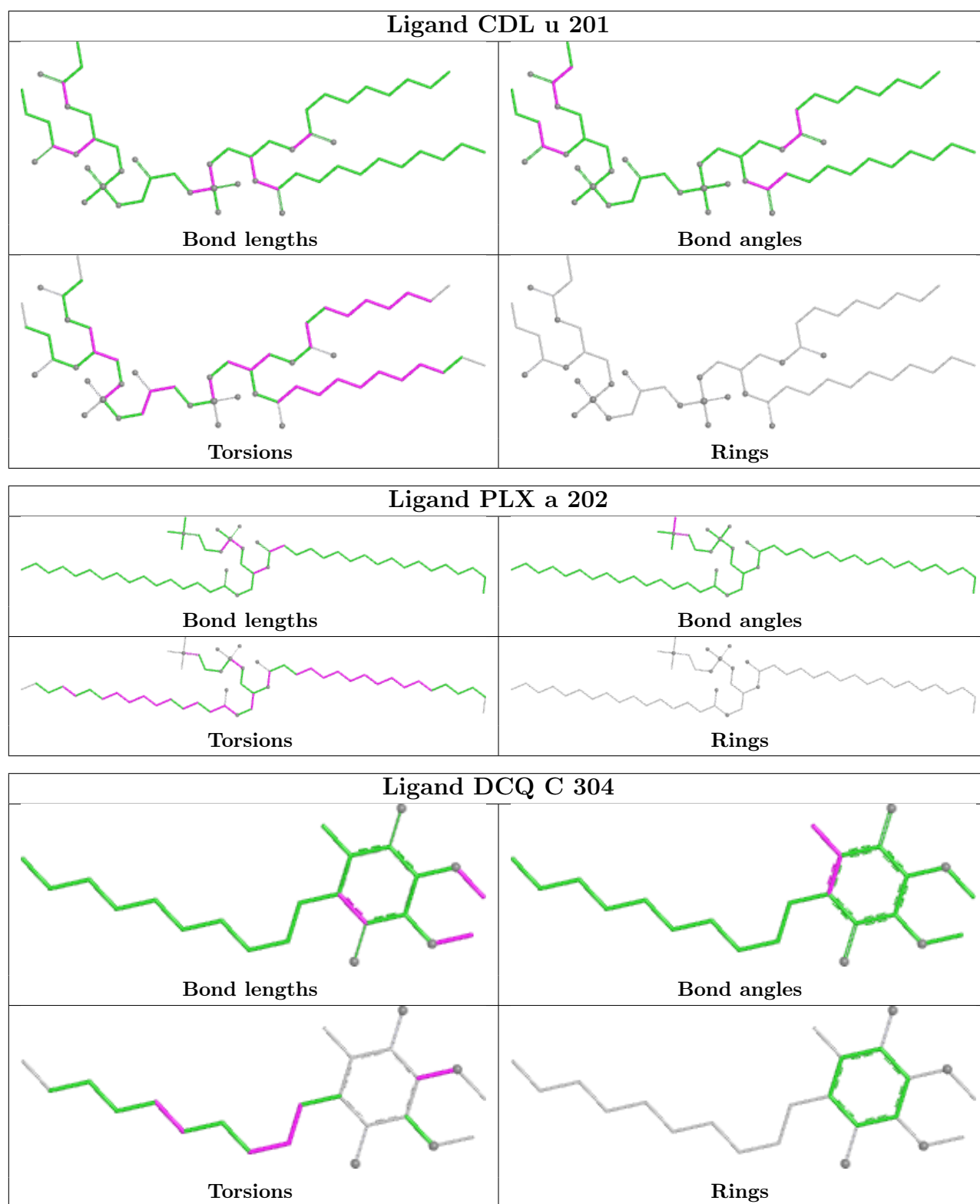
Ligand SF4 M 801

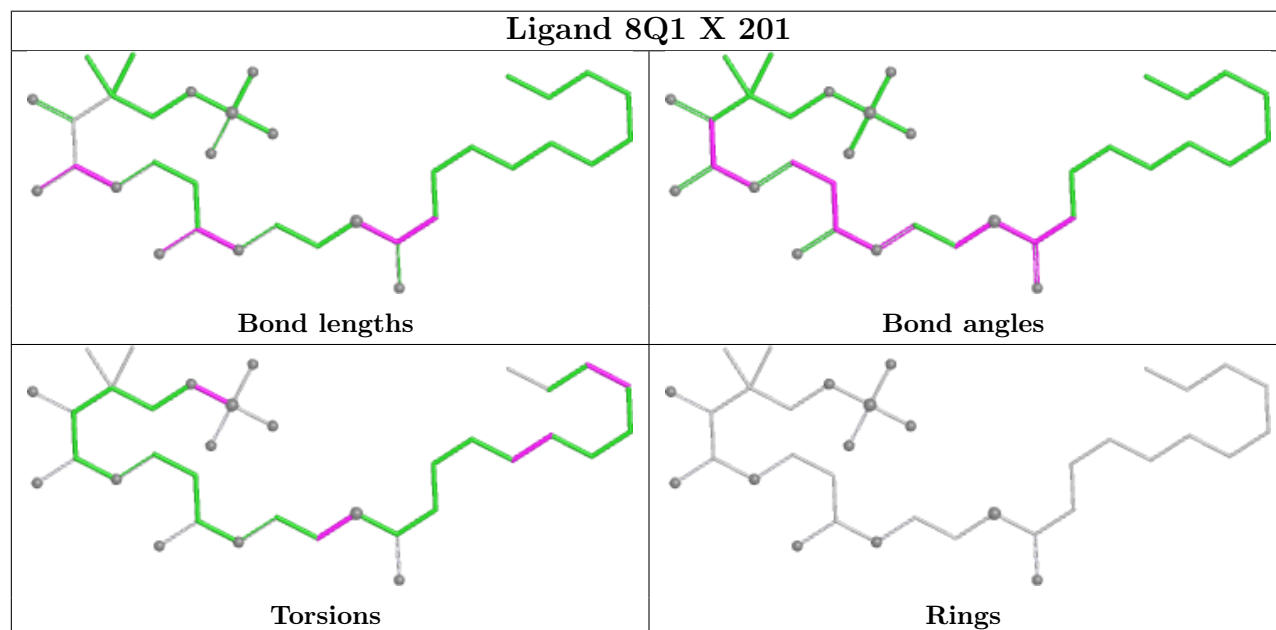
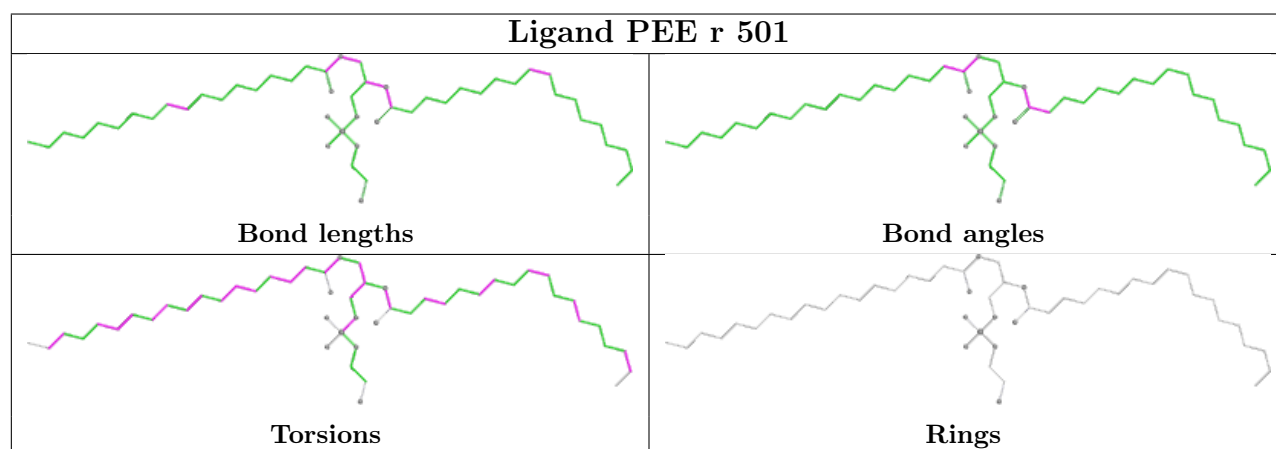
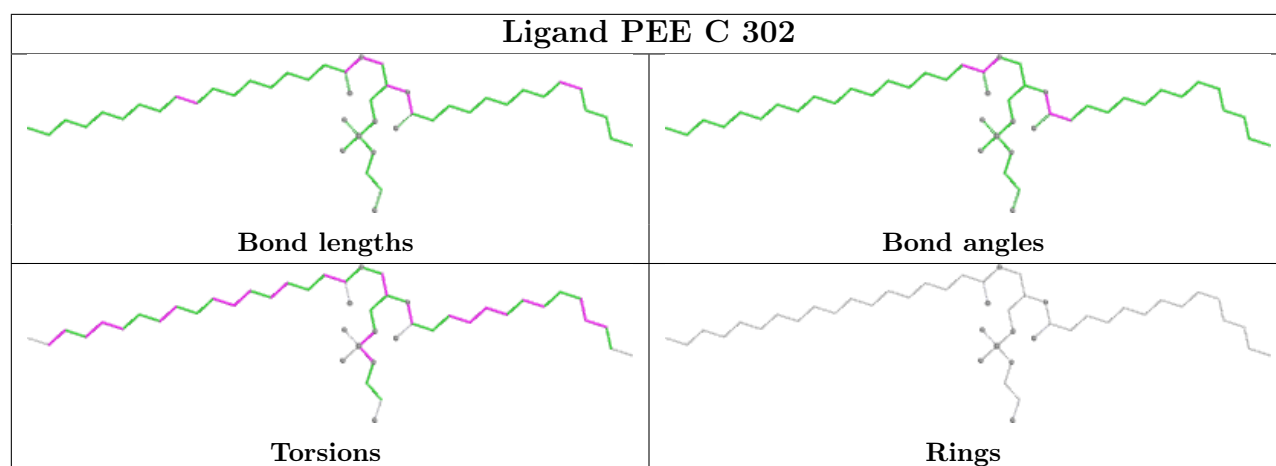


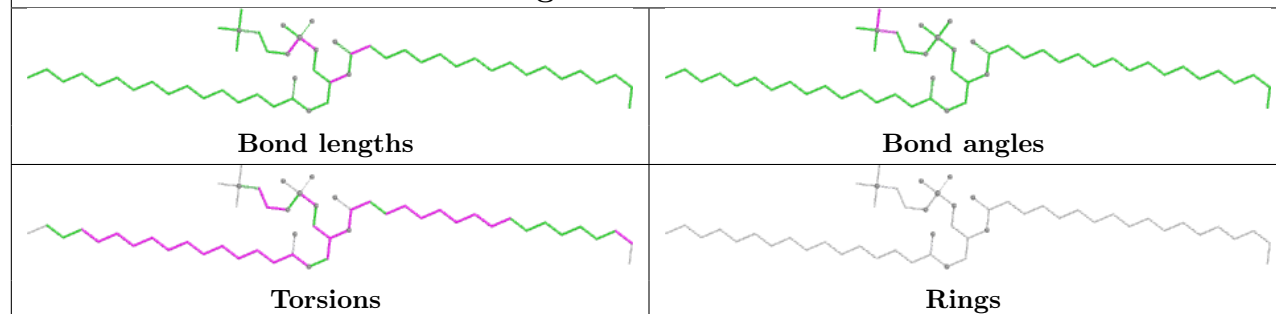
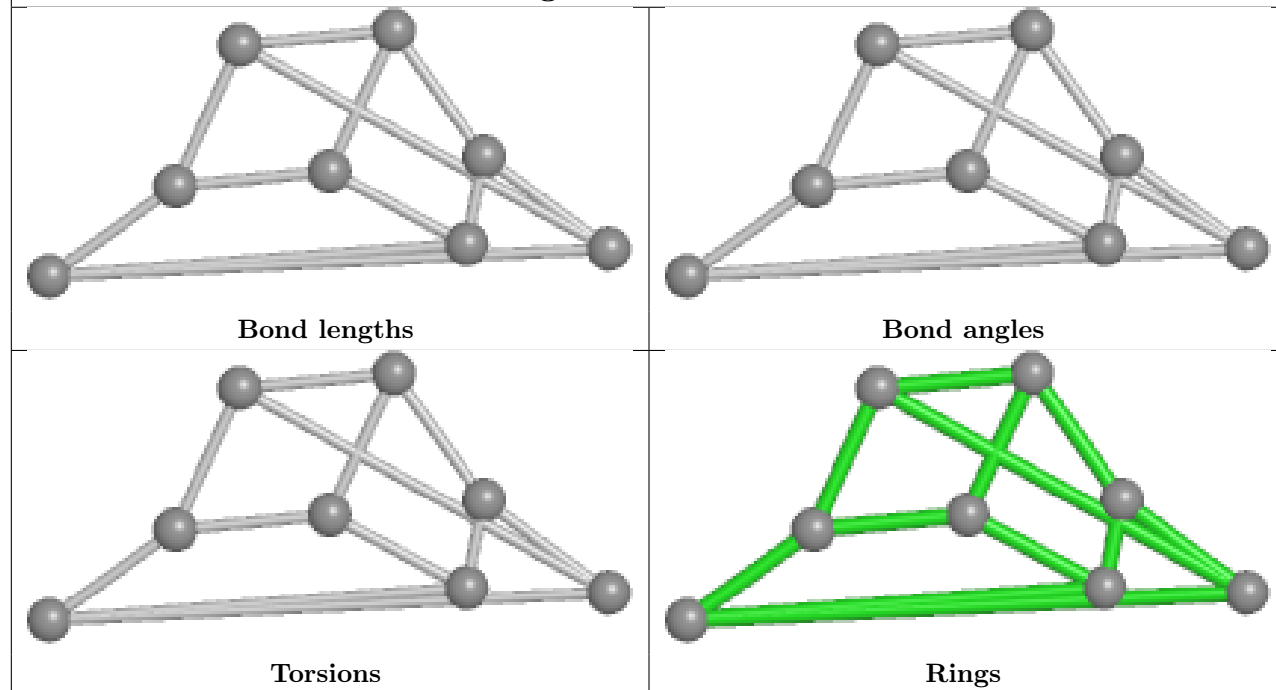


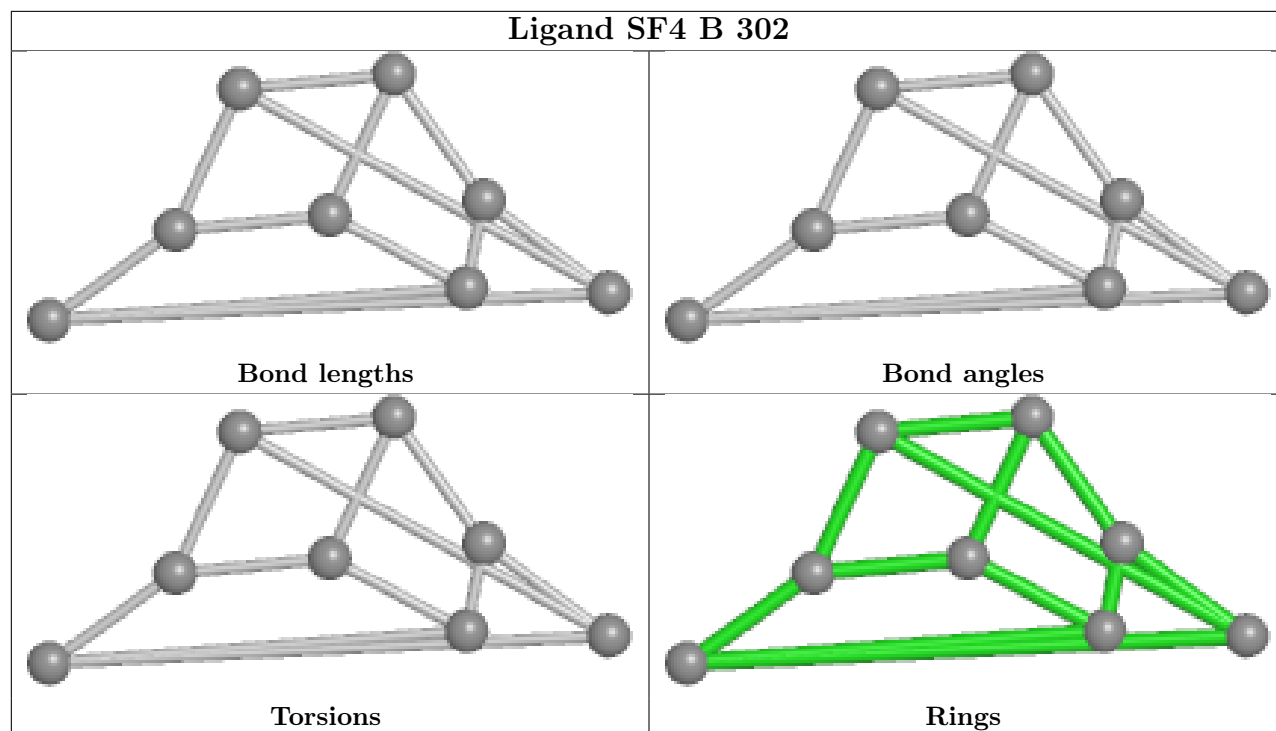








Ligand PLX J 403**Ligand SF4 C 301**



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.

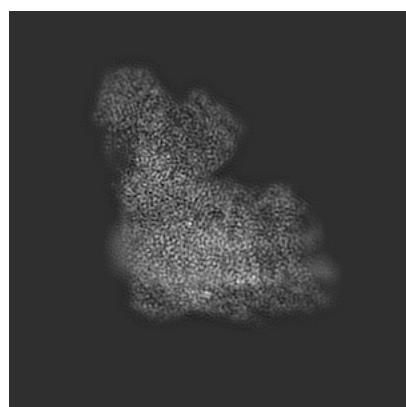
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32266. These allow visual inspection of the internal detail of the map and identification of artifacts.

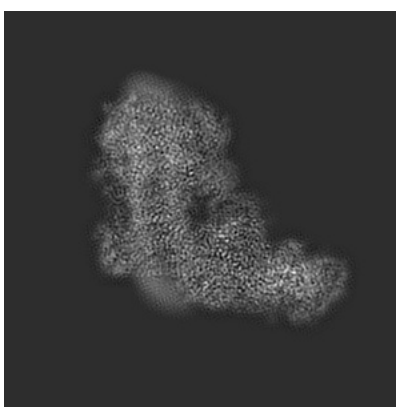
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

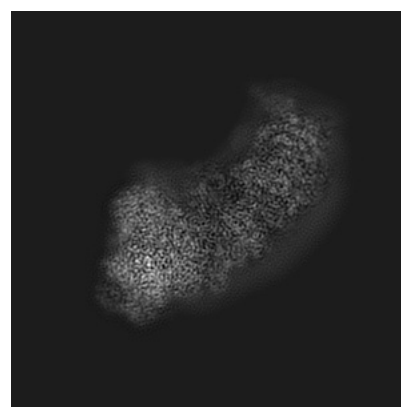
6.1.1 Primary map



X



Y

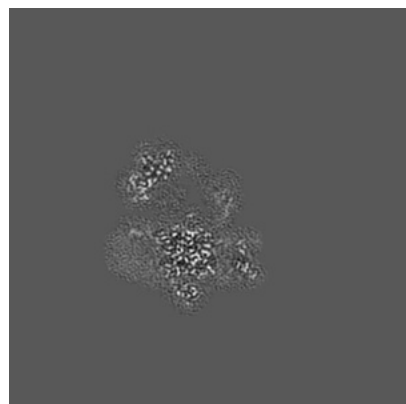


Z

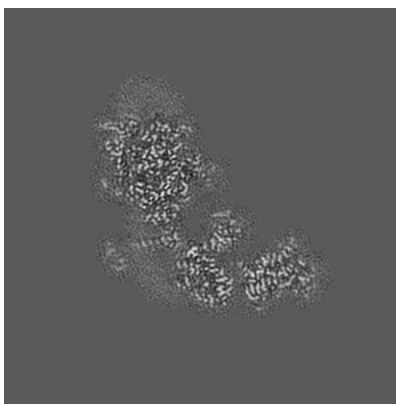
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

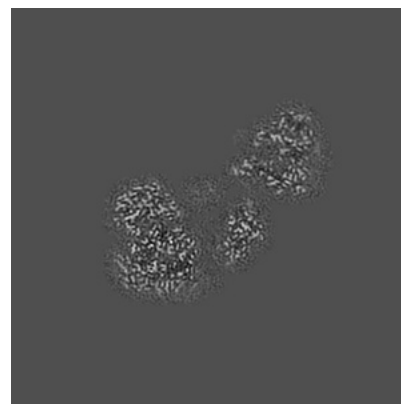
6.2.1 Primary map



X Index: 155



Y Index: 155

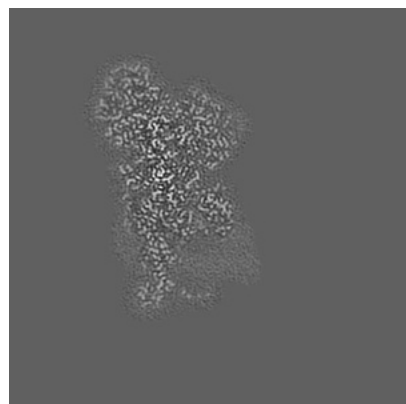


Z Index: 155

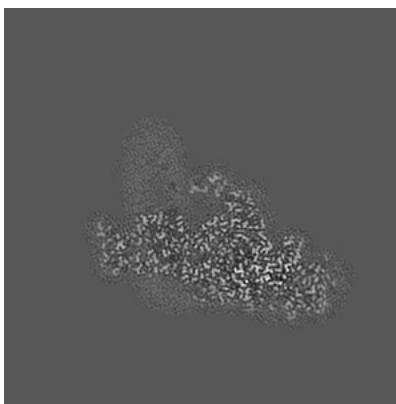
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

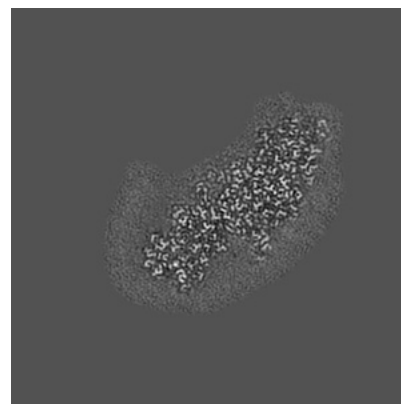
6.3.1 Primary map



X Index: 106



Y Index: 112

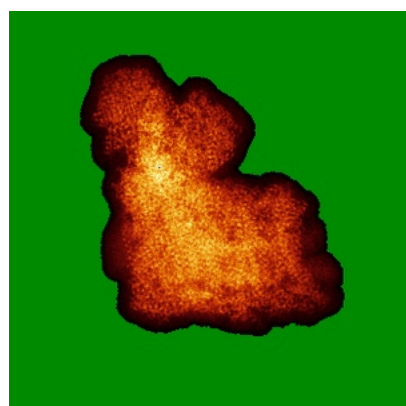


Z Index: 126

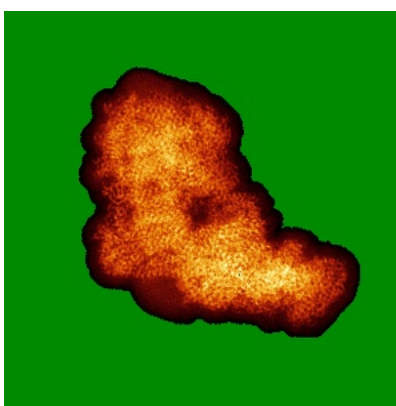
The images above show the largest variance slices of the map in three orthogonal directions.

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

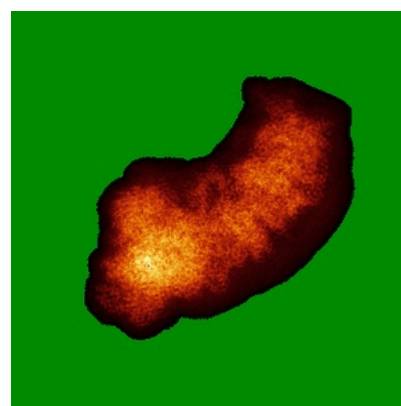
6.4.1 Primary map



X



Y

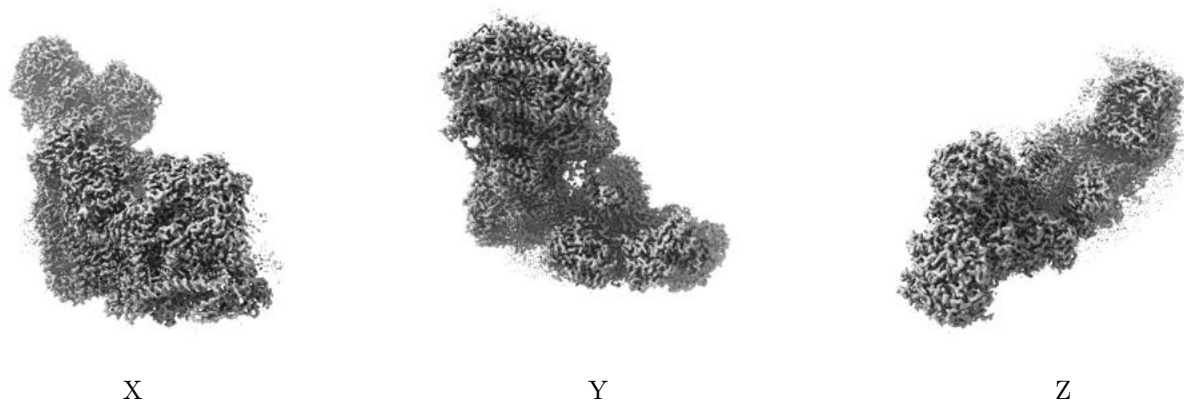


Z

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 0.0265. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

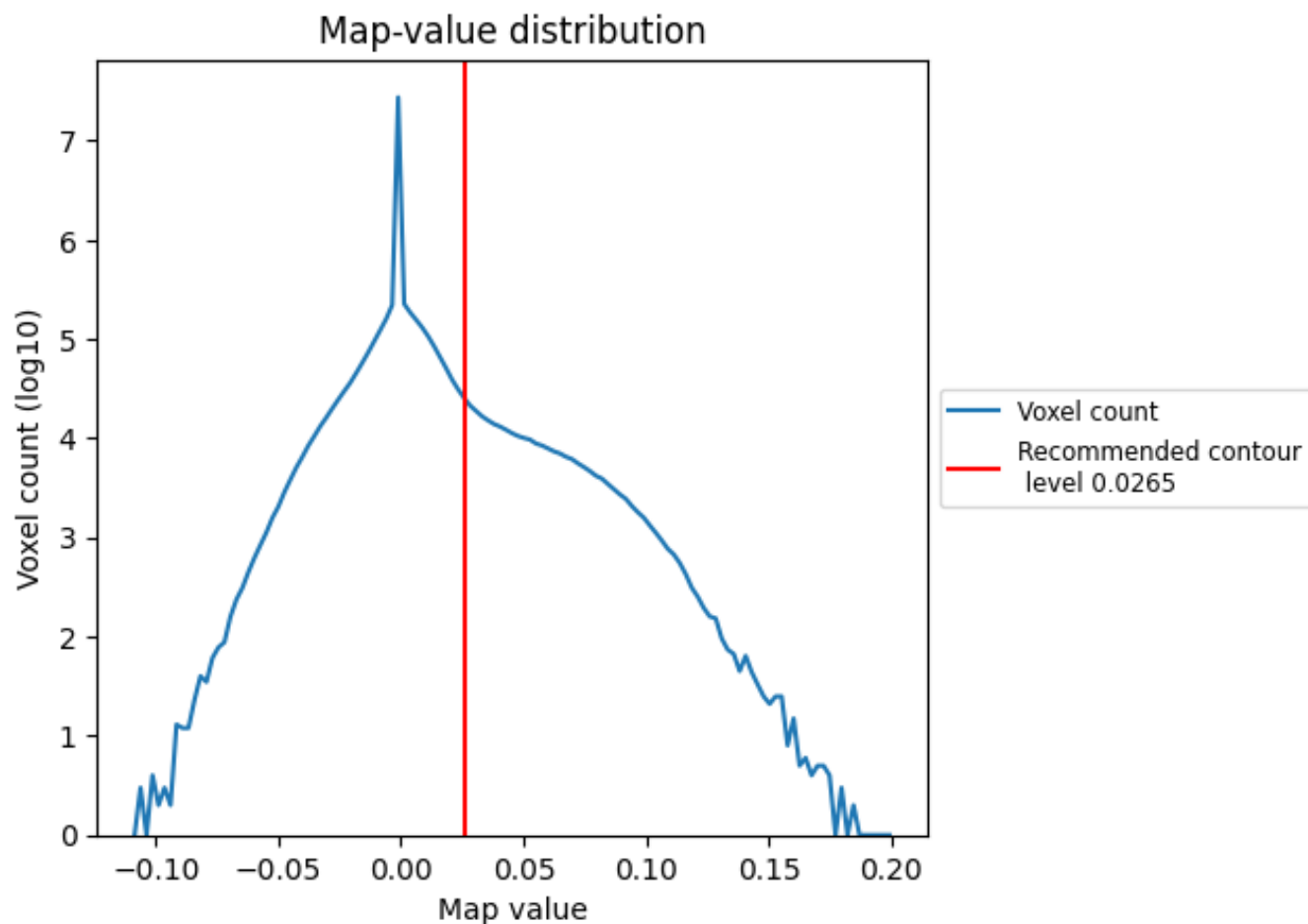
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

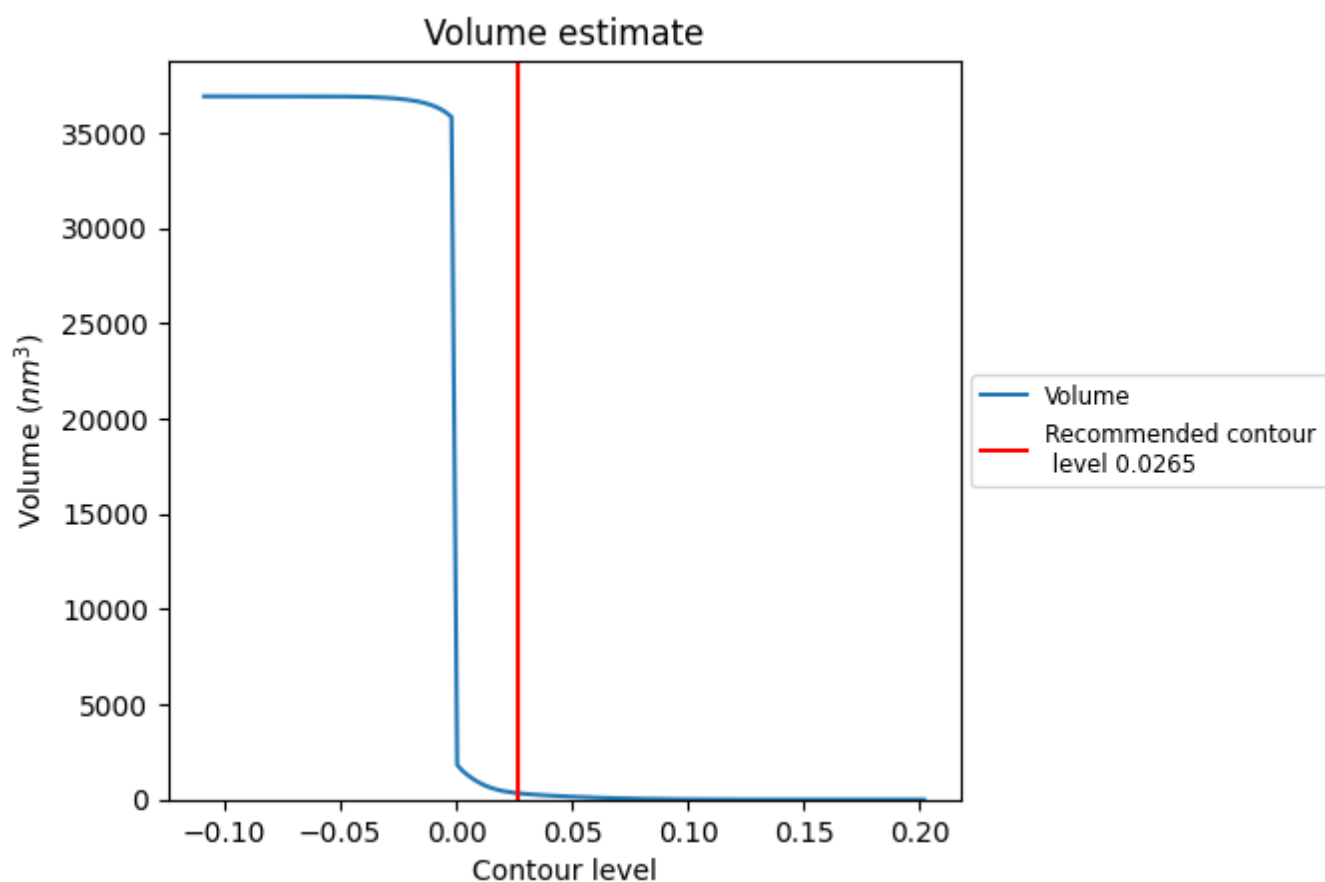
This section contains the results of statistical analysis of the map.

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.

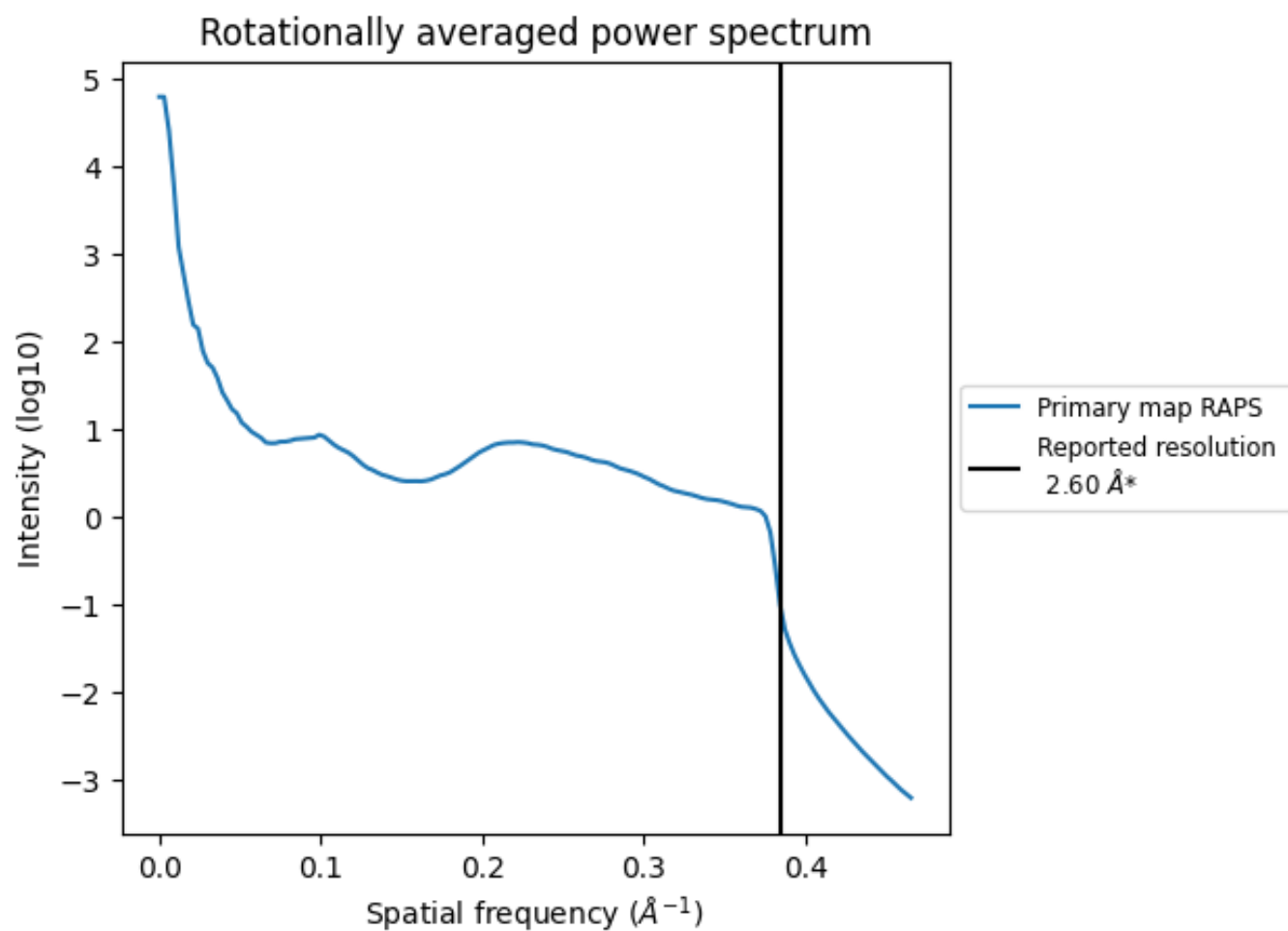
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 337 nm^3 ; this corresponds to an approximate mass of 305 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 0.385 Å⁻¹

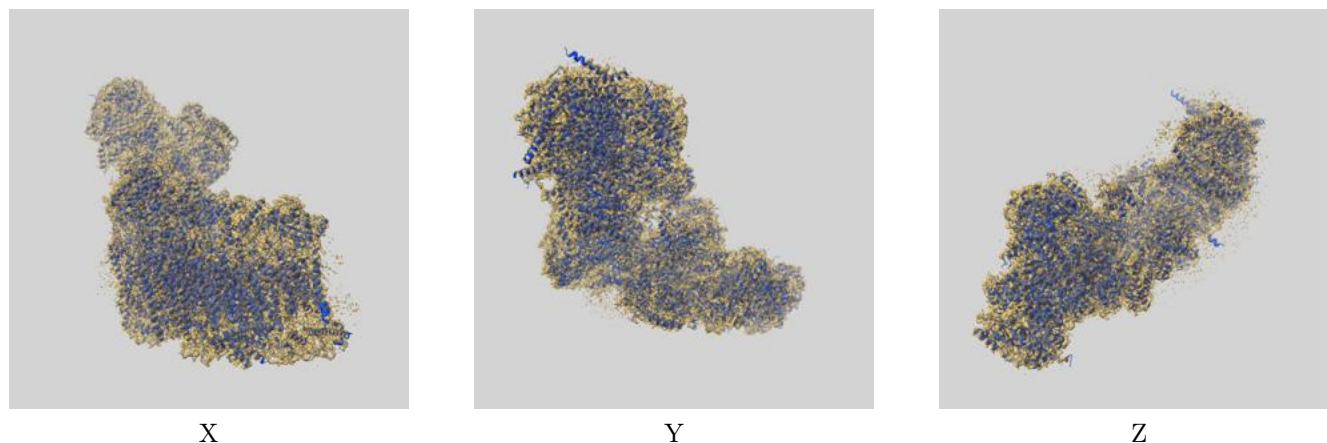
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

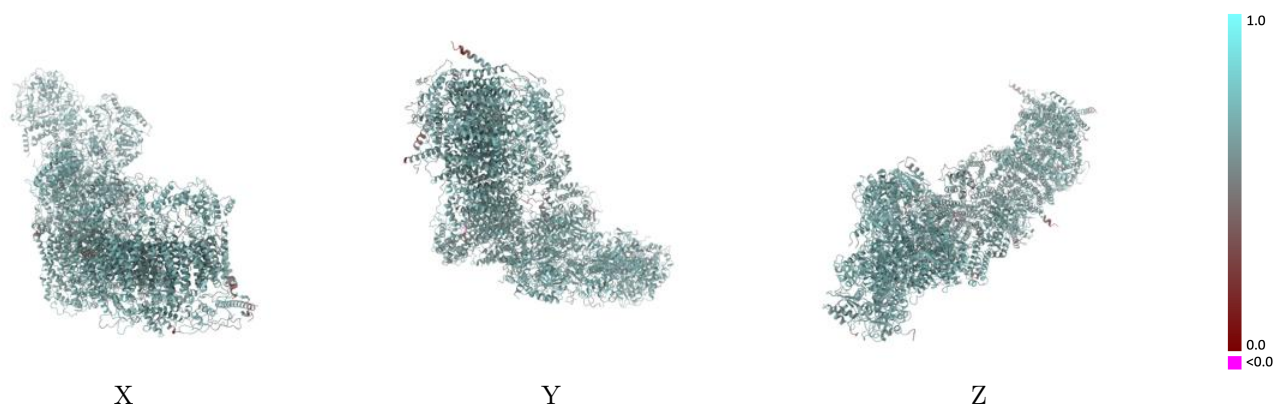
This section contains information regarding the fit between EMDB map EMD-32266 and PDB model 7W2U. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



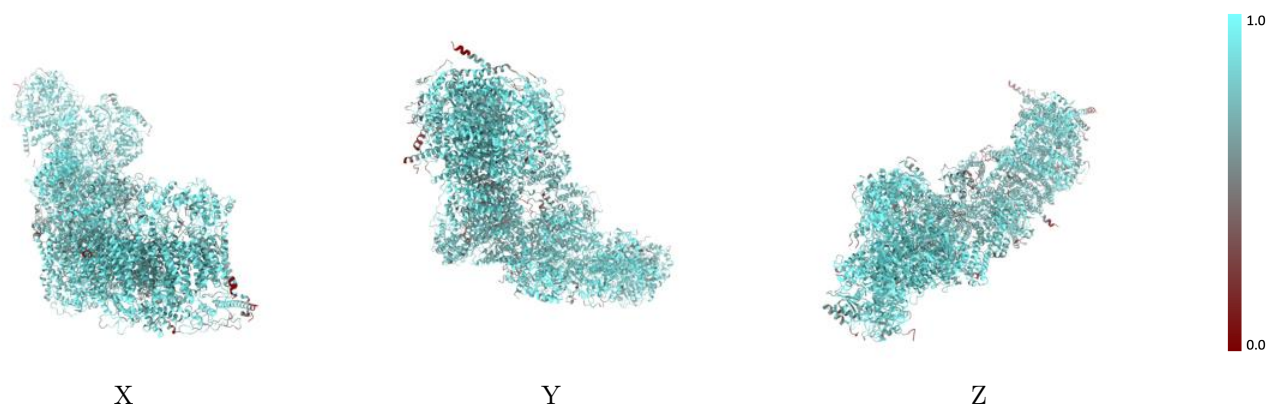
The images above show the 3D surface view of the map at the recommended contour level 0.0265 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



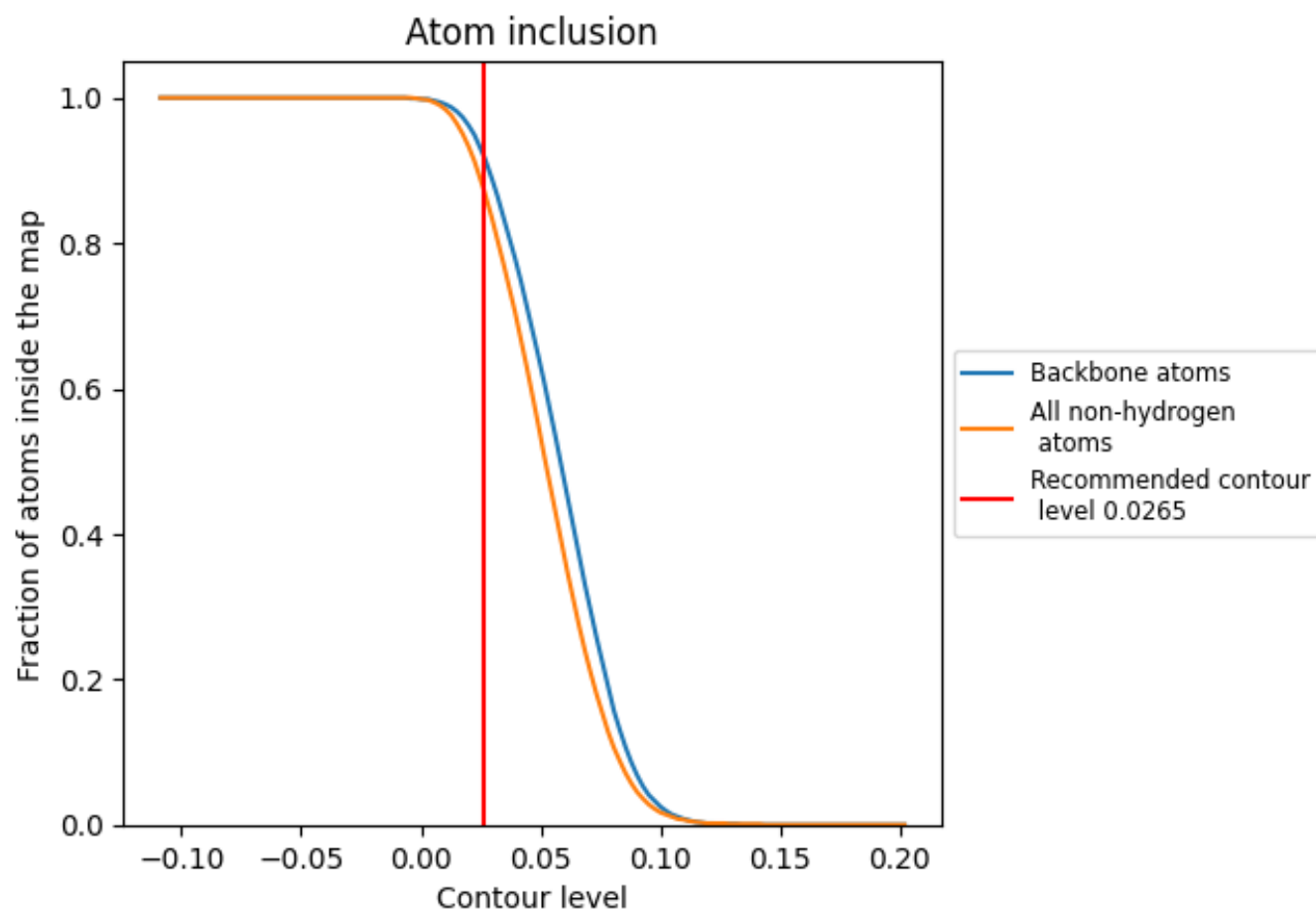
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0265).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 87% 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 (0.0265) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8710	 0.6380
A	 0.8640	 0.6320
B	 0.9510	 0.6740
C	 0.9350	 0.6710
E	 0.8910	 0.6470
F	 0.7760	 0.5890
G	 0.6210	 0.5170
H	 0.8900	 0.6420
I	 0.7490	 0.6030
J	 0.8950	 0.6480
K	 0.7520	 0.5940
L	 0.8950	 0.6530
M	 0.9130	 0.6530
N	 0.7850	 0.6300
O	 0.8080	 0.6160
P	 0.9630	 0.6780
Q	 0.9520	 0.6730
S	 0.9170	 0.6460
T	 0.8200	 0.6350
U	 0.8470	 0.6230
V	 0.7660	 0.6130
W	 0.8540	 0.6260
X	 0.8260	 0.6180
Y	 0.7100	 0.5770
Z	 0.6530	 0.5490
a	 0.8500	 0.6370
b	 0.7910	 0.5980
c	 0.8460	 0.6320
d	 0.8060	 0.6140
e	 0.7980	 0.6110
f	 0.6950	 0.5650
g	 0.8530	 0.6320
h	 0.8760	 0.6300
i	 0.9410	 0.6630
j	 0.8680	 0.6470



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	 0.8890	 0.6470
l	 0.8960	 0.6450
m	 0.8330	 0.6120
n	 0.7560	 0.5840
o	 0.8190	 0.6220
p	 0.8630	 0.6320
r	 0.9390	 0.6580
s	 0.9360	 0.6590
u	 0.8530	 0.6300
v	 0.7730	 0.5870
w	 0.8570	 0.6320