



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 04:47 AM UTC

PDB ID : 7V2K / pdb_00007v2k
EMDB ID : EMD-31646
Title : Deactive state complex I from DQ-NADH dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-08-09
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

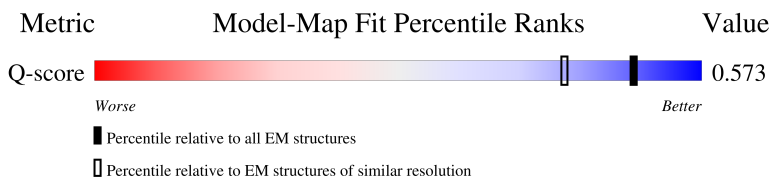
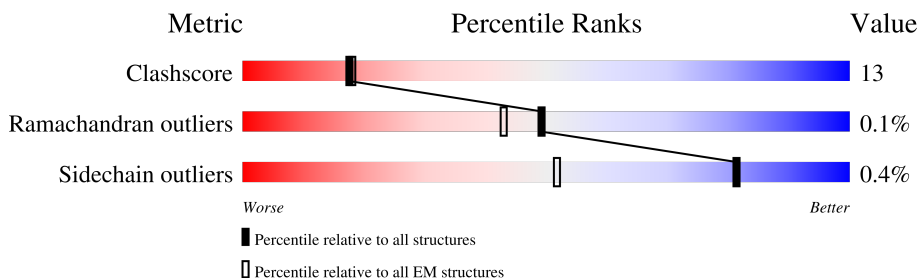
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



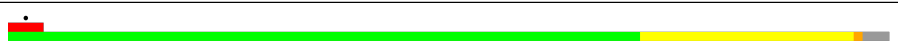
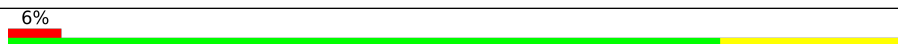
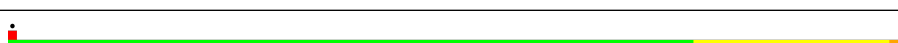
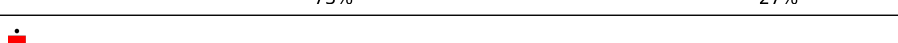
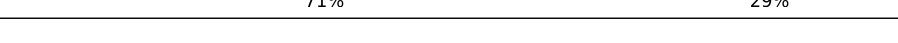
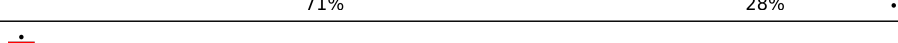
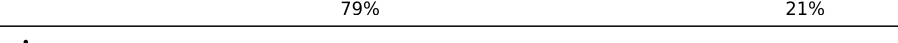
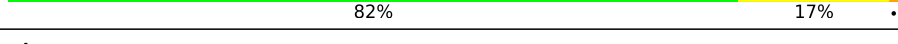
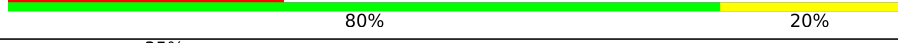
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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

Mol	Chain	Length	Quality of chain
1	A	431	 71% 28%
2	B	176	 72% 28%
3	C	156	 81% 18%
4	E	115	 74% 24%

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Mol	Chain	Length	Quality of chain
5	F	86	
6	G	88	
6	X	88	
7	H	112	
8	I	112	
9	J	341	
10	K	42	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	70	
23	Z	84	
24	a	140	
25	b	126	
26	c	156	
27	d	175	
28	e	107	

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Mol	Chain	Length	Quality of chain
29	f	42	
30	g	121	
31	h	105	
32	i	347	
33	j	113	
34	k	98	
35	l	603	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	131	
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	-
45	SF4	C	301	-	-	X	-
46	FMN	A	502	-	-	X	-
48	PEE	C	311	-	-	X	-
48	PEE	V	202	-	-	X	-
52	FES	M	803	-	-	X	-
54	CDL	a	201	-	-	X	-
54	CDL	l	712	-	-	X	-
54	CDL	n	102	-	-	X	-
56	UQ	s	403	-	-	X	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 66880 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3318	2095	591	612	20		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	86	Total	C	N	O	S	0	0
			691	434	129	126	2		

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

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
			695	448	103	139	5		

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

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

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	331	Total	C	N	O	S	0	0
			2615	1694	459	454	8		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	42	Total	C	N	O	S	0	0
			355	219	67	68	1		

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

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

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

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

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

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

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

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

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	419	Total	C	N	O	S	0	0
			3377	2162	578	613	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			567	364	104	94	5		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	70	Total	C	N	O	S	0	0
			600	393	98	108	1		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	103	Total	C	N	O	S	0	0
			879	573	158	147	1		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	42	Total	C	N	O	0	0
			342	225	58	59		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	99	Total	C	N	O	S	0	0
			800	545	118	132	5		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	603	Total	C	N	O	S	0	0
			4720	3118	739	814	49		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	129	Total	C	N	O	S	0	0
			919	614	137	160	8		

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

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

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

4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	o	128	Total	C	N	O	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	303	Total	C	N	O	S	0	0
			2394	1607	369	397	21		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			998	625	183	181	9		

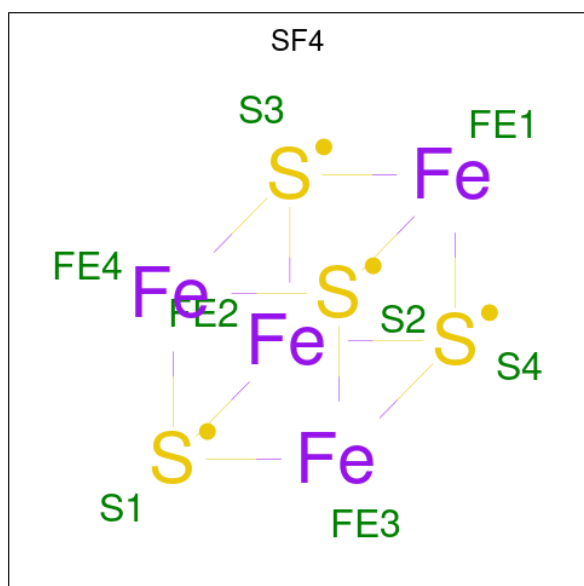
There is a discrepancy between the modelled and reference sequences:

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: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



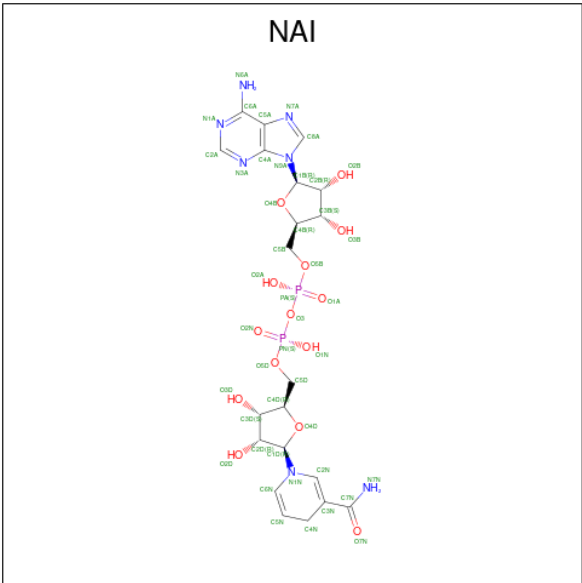
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

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



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

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



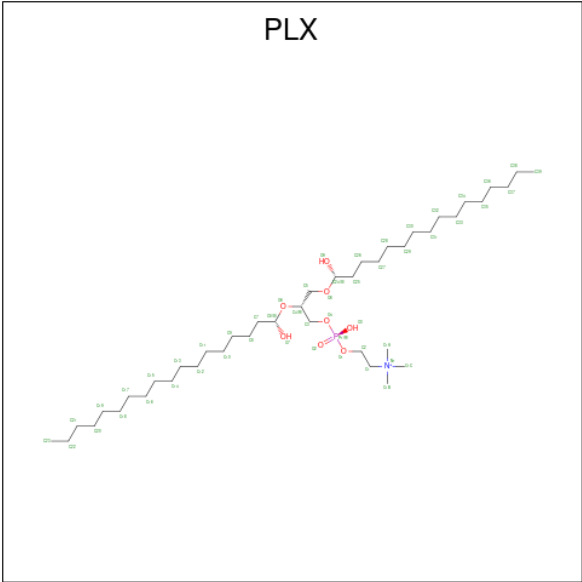
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

- 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).



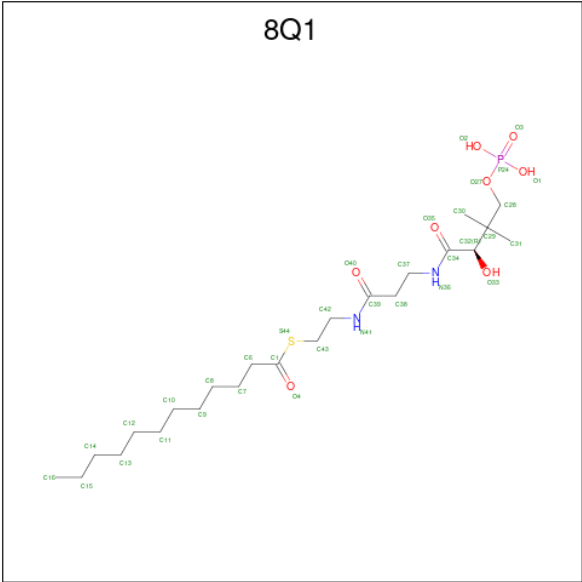
Mol	Chain	Residues	Atoms					AltConf
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	V	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	l	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	s	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).



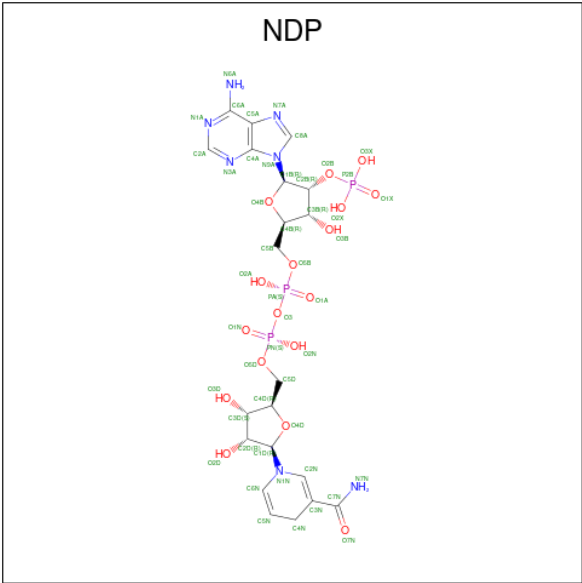
Mol	Chain	Residues	Atoms					AltConf
49	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	V	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	e	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	i	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	n	1	Total	C	N	O	P	0
			52	42	1	8	1	

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



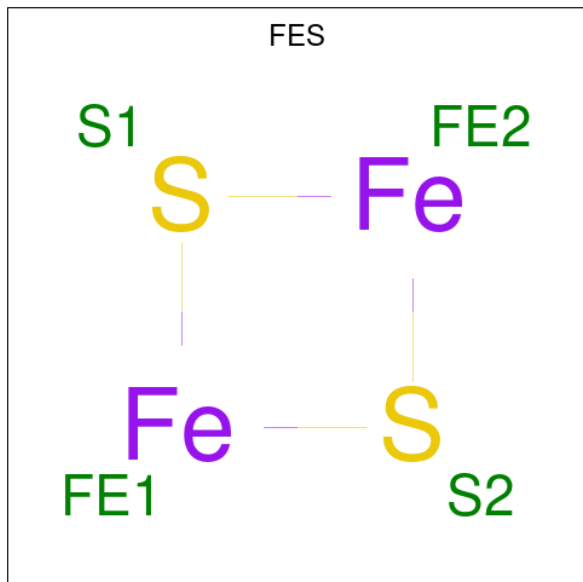
Mol	Chain	Residues	Atoms						AltConf
50	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
50	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

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



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

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

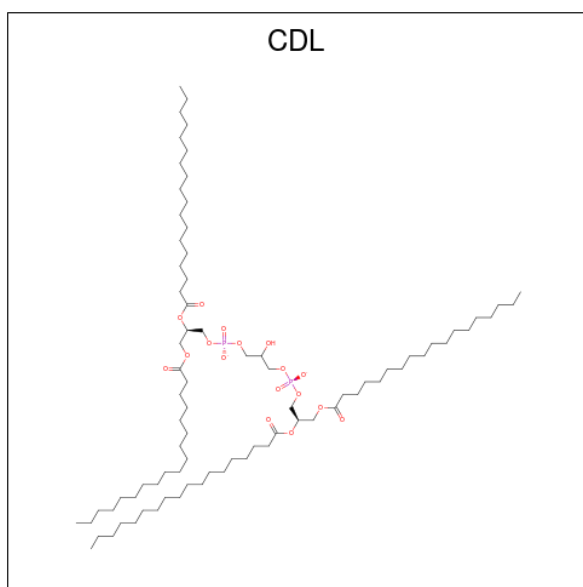


Mol	Chain	Residues	Atoms			AltConf
52	M	1	Total	Fe	S	0
			4	2	2	
52	O	1	Total	Fe	S	0
			4	2	2	

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

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

- Molecule 54 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

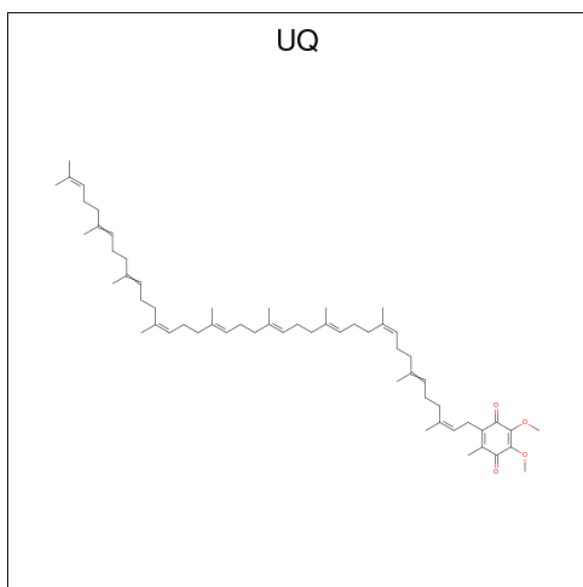


Mol	Chain	Residues	Atoms				AltConf
54	N	1	Total	C	O	P	0
			51	32	17	2	
54	a	1	Total	C	O	P	0
			91	72	17	2	
54	i	1	Total	C	O	P	0
			66	47	17	2	
54	l	1	Total	C	O	P	0
			99	80	17	2	
54	l	1	Total	C	O	P	0
			100	81	17	2	
54	n	1	Total	C	O	P	0
			78	59	17	2	
54	r	1	Total	C	O	P	0
			100	81	17	2	

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

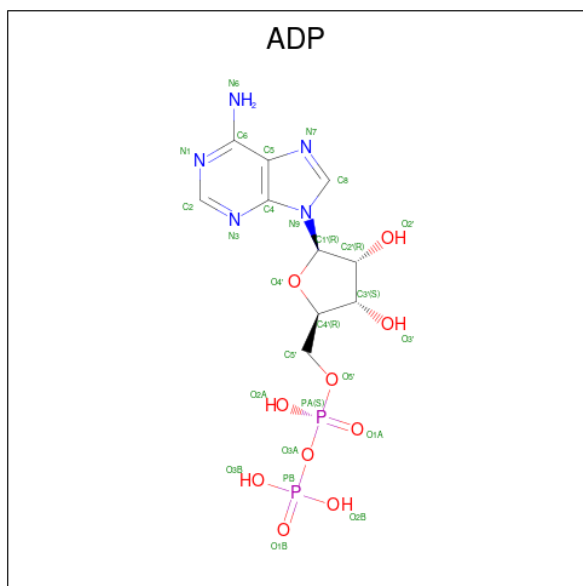
Mol	Chain	Residues	Atoms		AltConf
55	T	1	Total	Zn	0
			1	1	

- Molecule 56 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

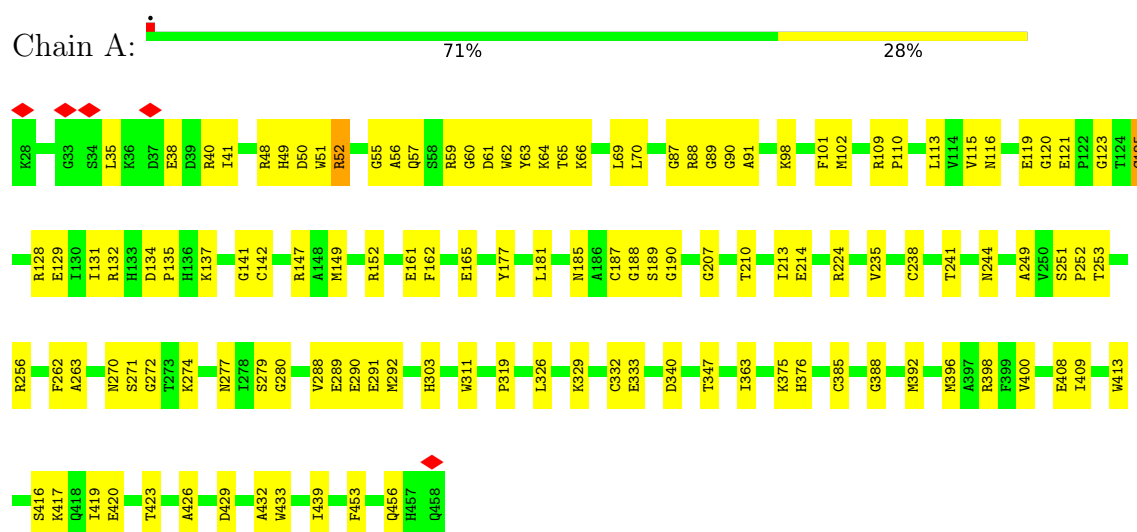


Mol	Chain	Residues	Atoms					AltConf
57	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

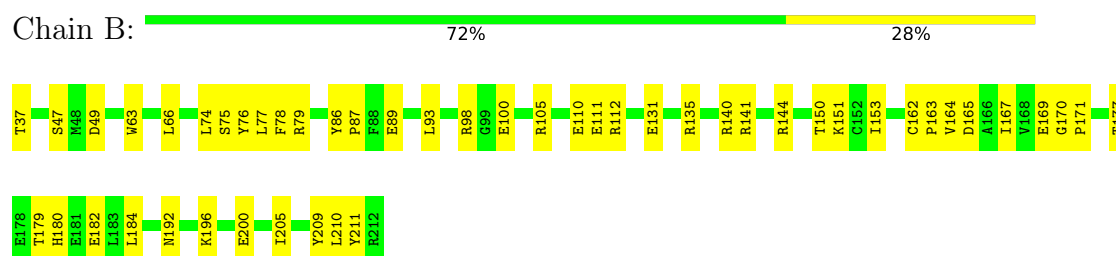
3 Residue-property plots

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

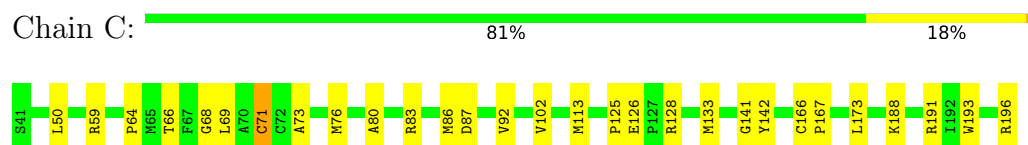
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



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

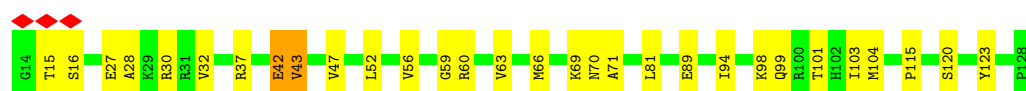


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



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

Chain E: 



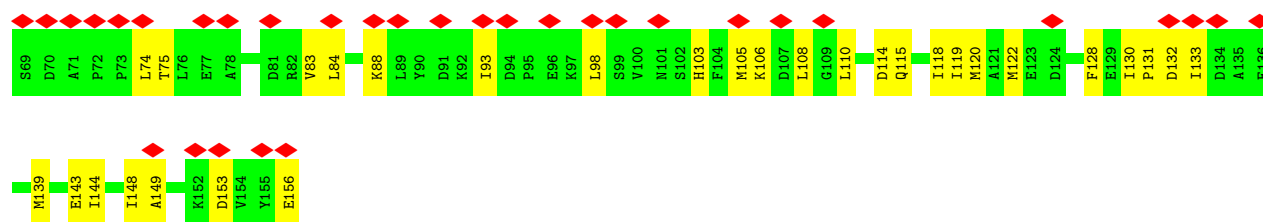
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain F: 



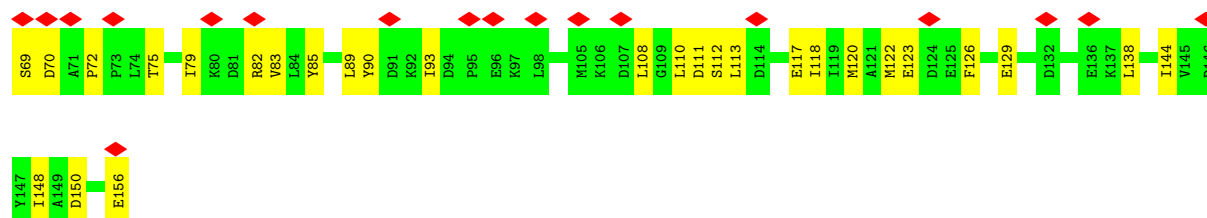
- Molecule 6: Acyl carrier protein, mitochondrial

Chain G: 



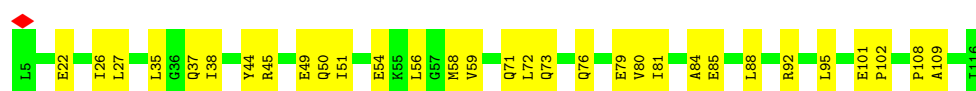
- Molecule 6: Acyl carrier protein, mitochondrial

Chain X: 



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

Chain H: 



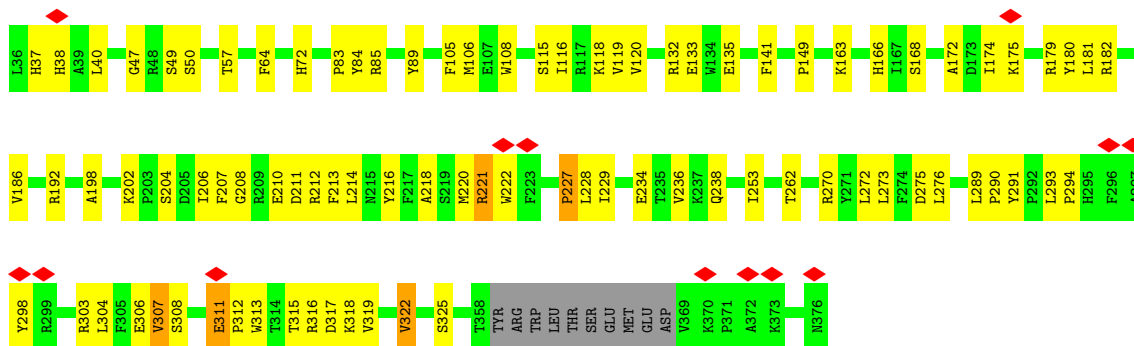
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain I: 





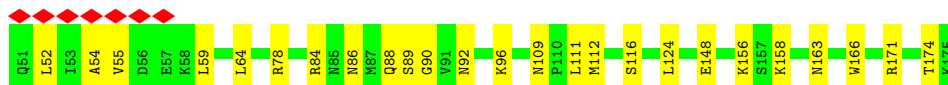
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



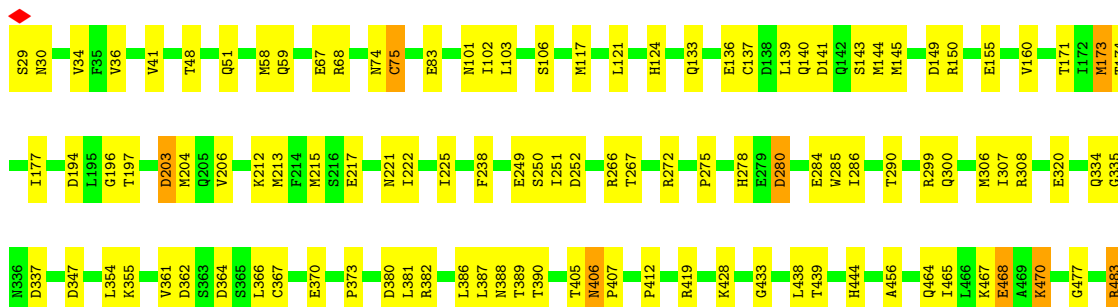
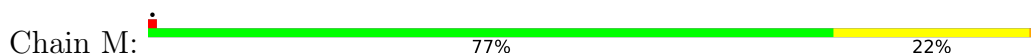
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

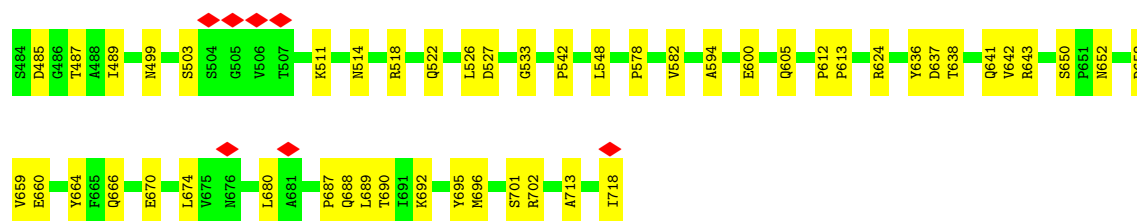


- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

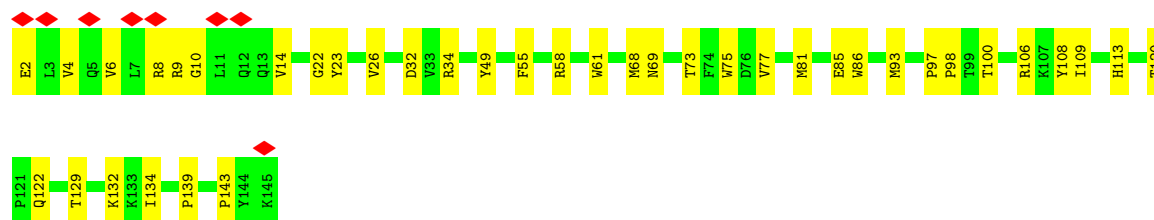
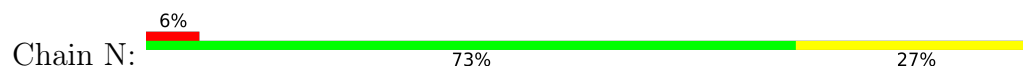


- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

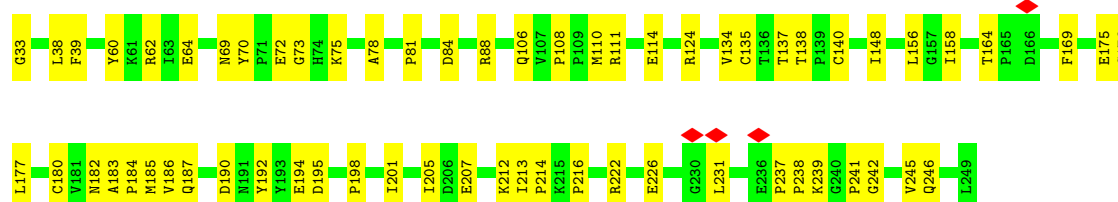




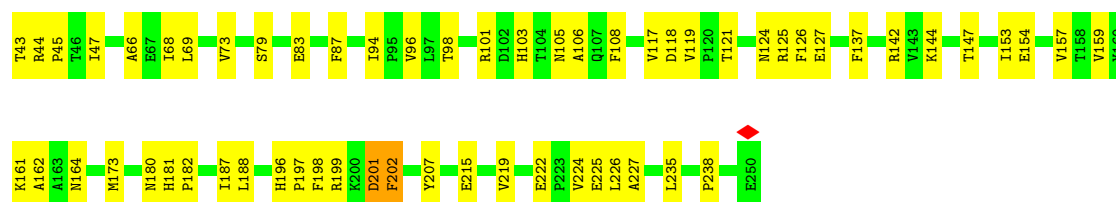
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



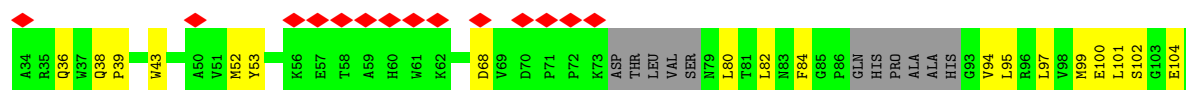
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

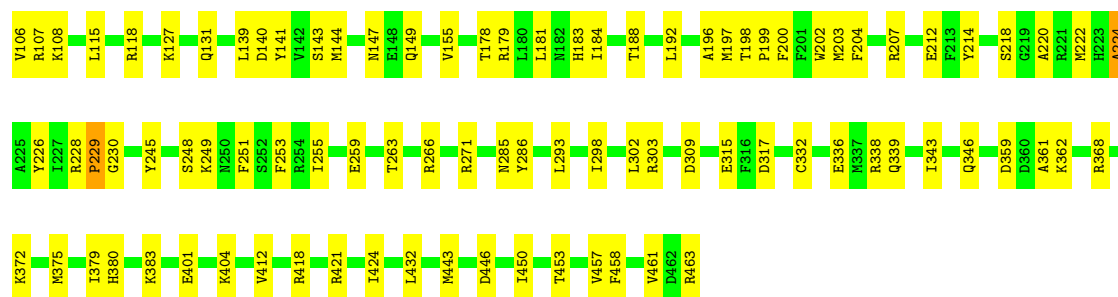


- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

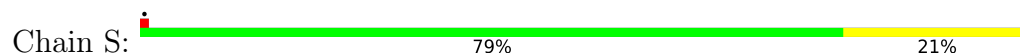


- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

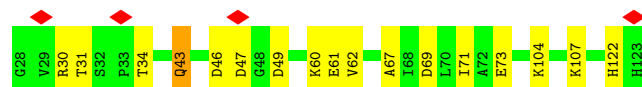
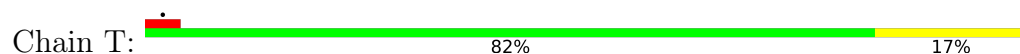




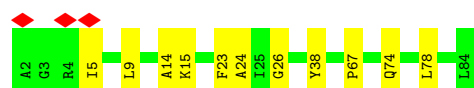
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



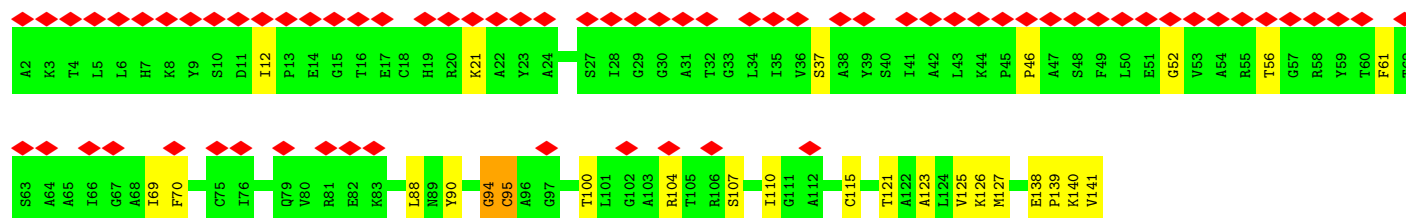
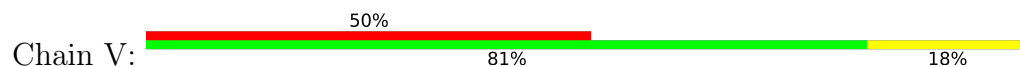
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



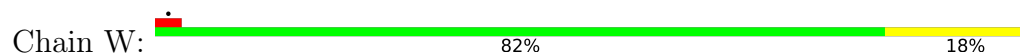
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



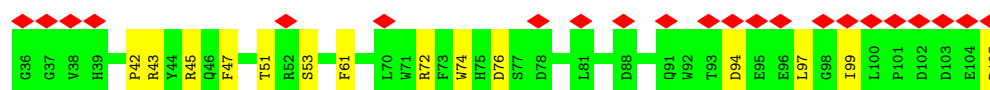
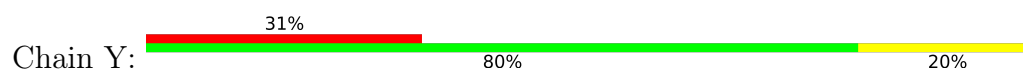
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



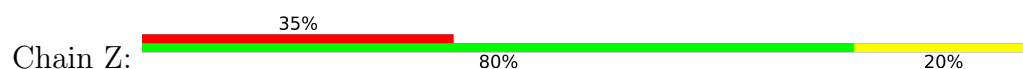
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



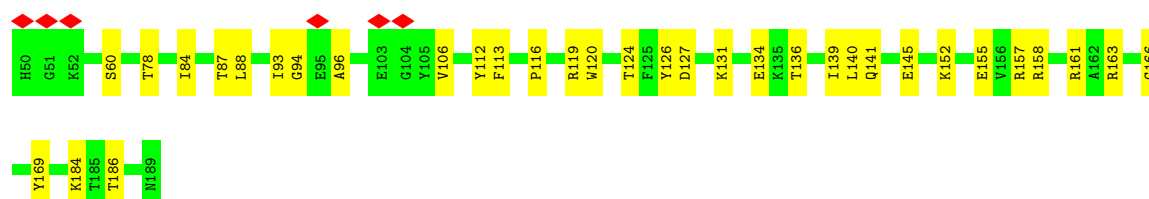
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



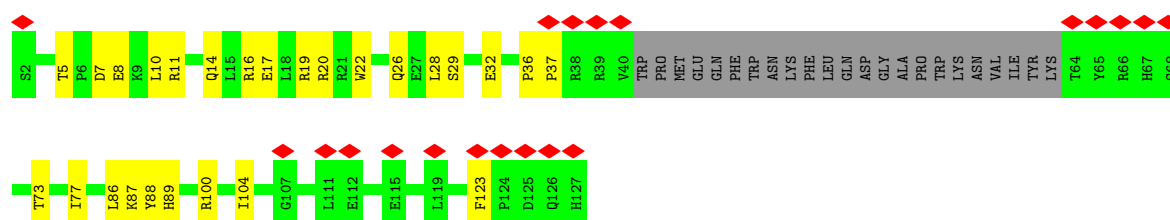
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



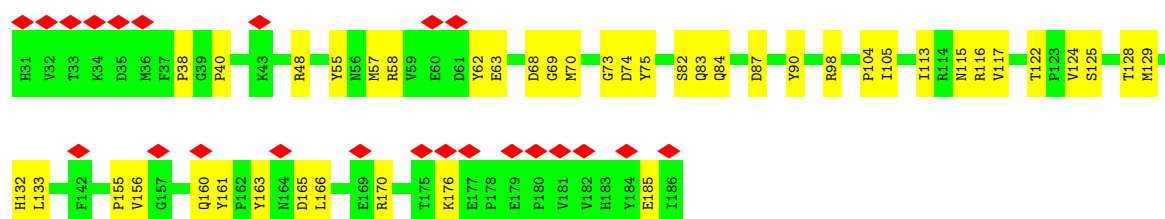
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



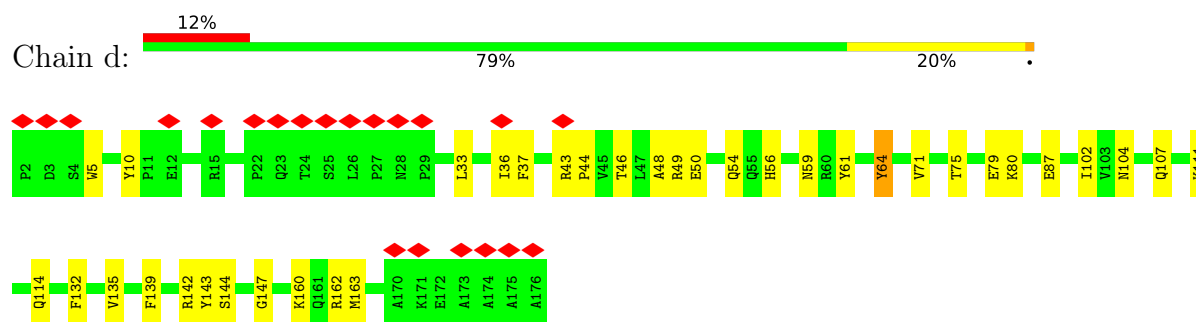
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



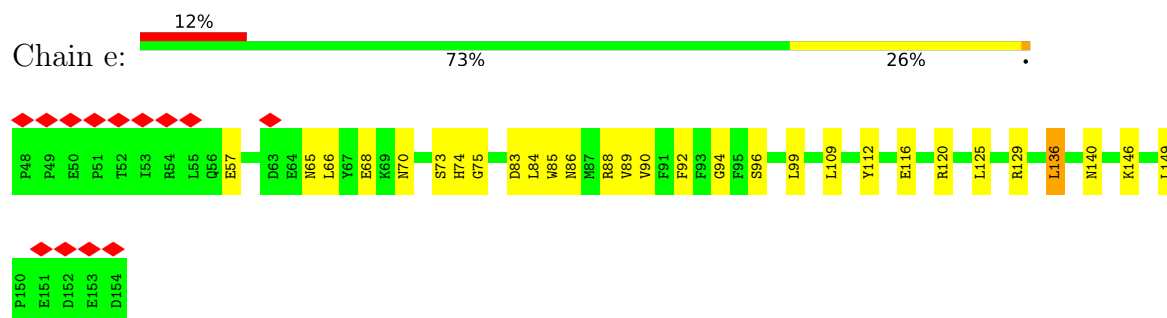
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



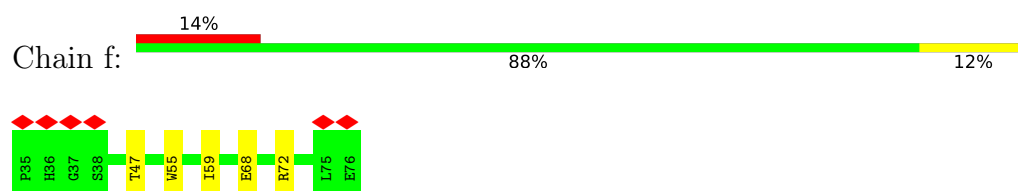
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



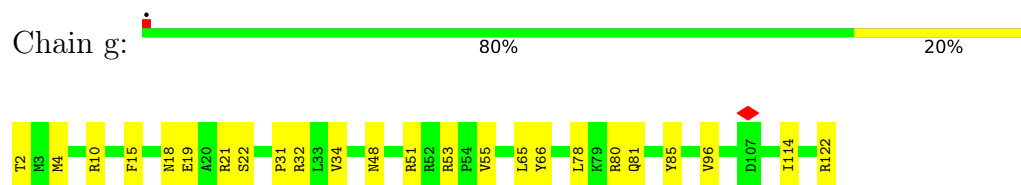
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



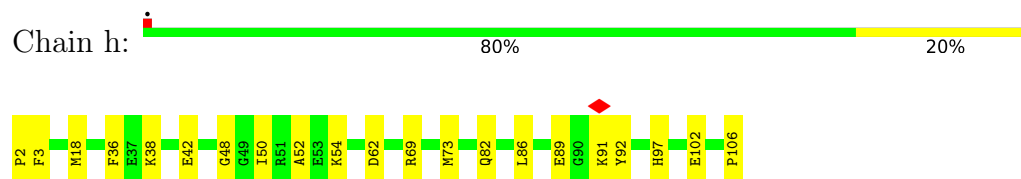
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



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

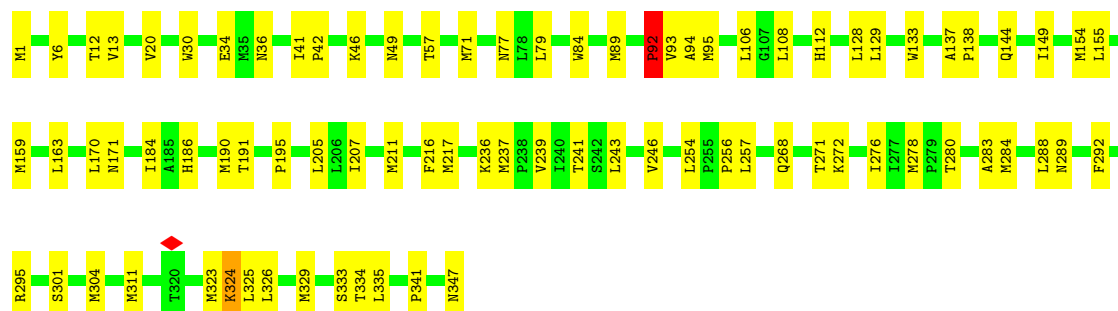


- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

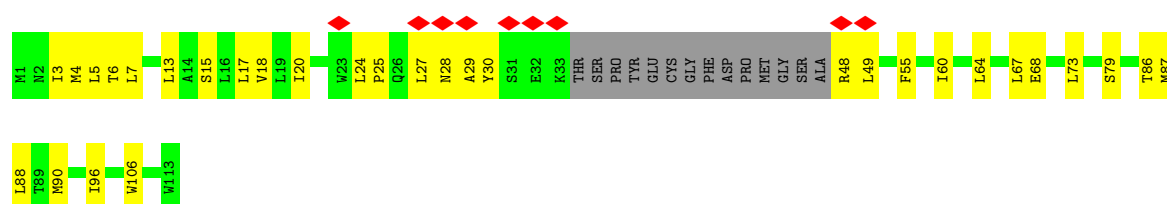


- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

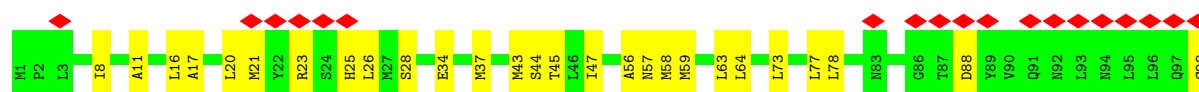


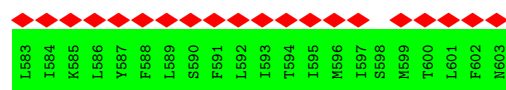


• Molecule 33: NADH-ubiquinone oxidoreductase chain 3

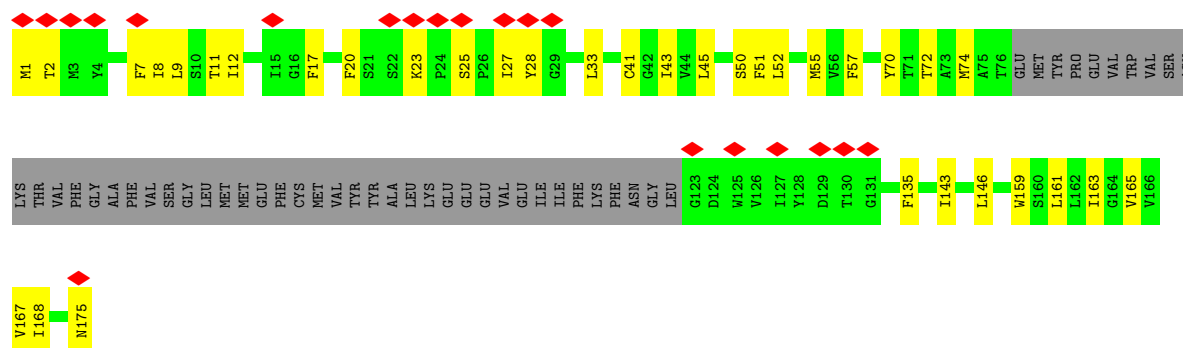


• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

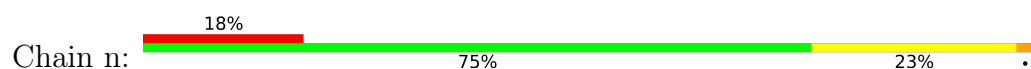




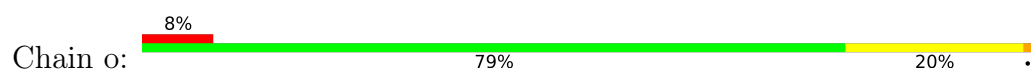
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6



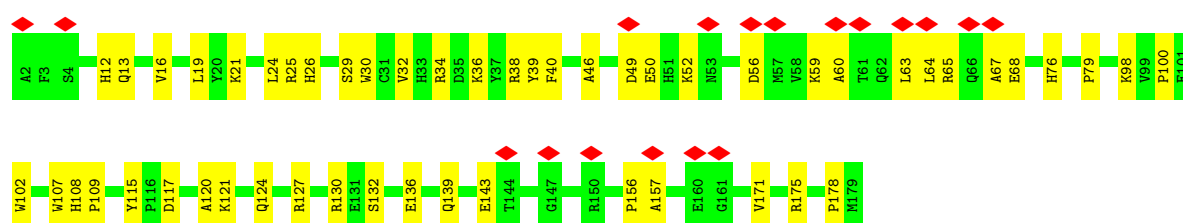
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



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

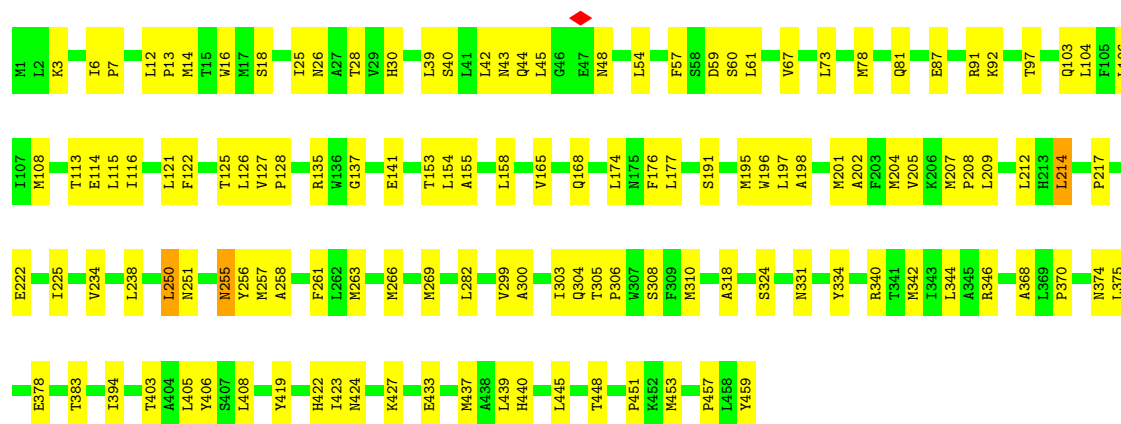


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

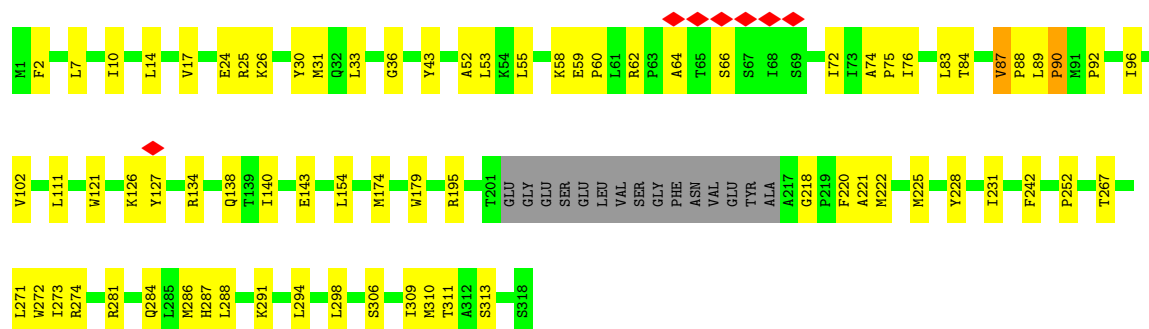


- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

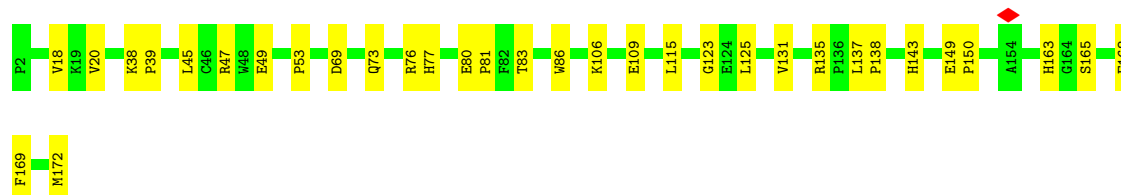
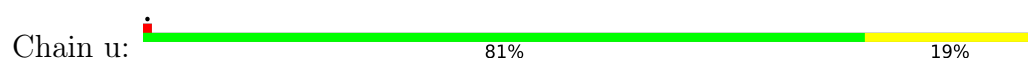




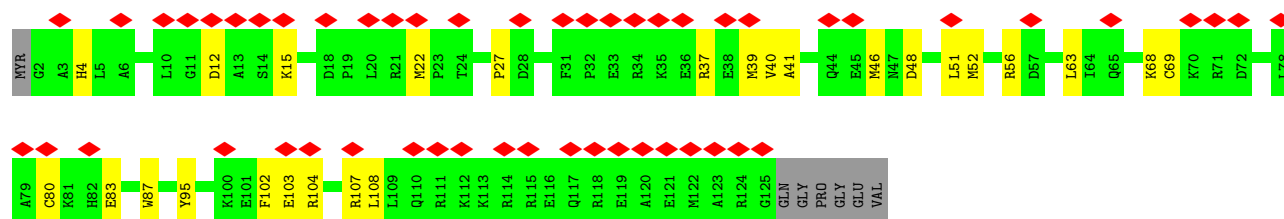
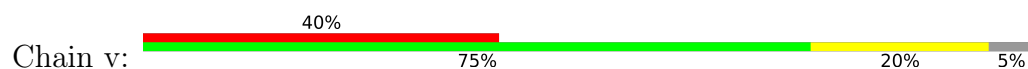
• Molecule 41: NADH-ubiquinone oxidoreductase chain 1



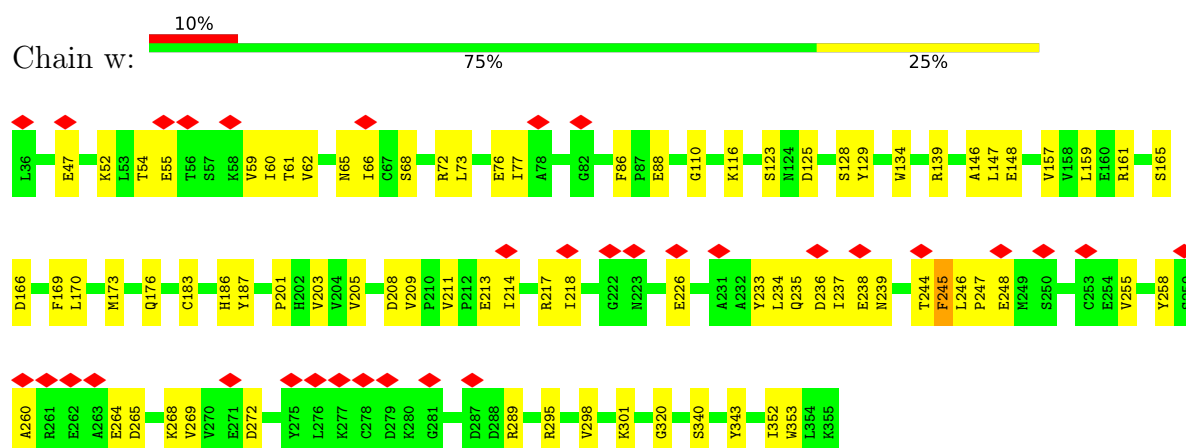
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



• 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	387112	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	0.229	Depositor
Minimum map value	-0.143	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0202	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.21	0/3393	0.51	1/4584 (0.0%)
2	B	0.19	0/1443	0.46	2/1952 (0.1%)
3	C	0.23	0/1279	0.54	0/1730
4	E	0.21	0/995	0.52	2/1340 (0.1%)
5	F	0.13	0/702	0.34	0/945
6	G	0.22	0/705	0.63	1/956 (0.1%)
6	X	0.13	0/707	0.34	0/958
7	H	0.17	0/929	0.49	0/1258
8	I	0.27	0/798	0.70	2/1079 (0.2%)
9	J	0.39	2/2684 (0.1%)	0.62	8/3638 (0.2%)
10	K	0.19	0/365	0.66	1/493 (0.2%)
11	L	0.16	0/1039	0.40	0/1403
12	M	0.25	0/5384	0.62	9/7295 (0.1%)
13	N	0.42	1/1245 (0.1%)	0.67	4/1694 (0.2%)
14	O	0.21	0/1711	0.61	4/2328 (0.2%)
15	P	0.25	0/1789	0.62	4/2436 (0.2%)
16	Q	0.20	0/3451	0.47	2/4672 (0.0%)
17	S	0.26	0/582	0.60	1/783 (0.1%)
18	T	0.16	0/755	0.36	0/1018
19	U	0.11	0/664	0.27	0/912
20	V	0.20	0/1042	0.51	3/1411 (0.2%)
21	W	0.14	0/1198	0.30	0/1617
22	Y	0.12	0/626	0.33	0/857
23	Z	0.10	0/695	0.28	0/939
24	a	0.18	0/1199	0.52	3/1623 (0.2%)
25	b	0.13	0/906	0.34	0/1232
26	c	0.16	0/1371	0.44	2/1875 (0.1%)
27	d	0.17	0/1494	0.48	3/2015 (0.1%)
28	e	0.16	0/916	0.48	1/1246 (0.1%)
29	f	0.12	0/350	0.25	0/473
30	g	0.11	0/1031	0.26	0/1394
31	h	0.15	0/889	0.41	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.17	0/2773	0.41	2/3768 (0.1%)
33	j	0.17	0/819	0.39	0/1117
34	k	0.20	0/759	0.46	0/1029
35	l	0.17	0/4845	0.42	0/6595
36	m	0.18	0/938	0.45	0/1271
37	n	0.21	0/491	0.55	1/663 (0.2%)
38	o	0.15	0/1092	0.51	2/1481 (0.1%)
39	p	0.19	0/1590	0.45	0/2155
40	r	0.20	0/3723	0.50	4/5078 (0.1%)
41	s	0.21	0/2464	0.48	2/3369 (0.1%)
42	u	0.16	0/1436	0.42	1/1938 (0.1%)
43	v	0.15	0/1022	0.44	0/1377
44	w	0.14	0/2642	0.42	1/3580 (0.0%)
All	All	0.21	3/66931 (0.0%)	0.49	66/90767 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	143	PRO	CG-CD	-13.40	1.05	1.50
9	J	210	GLU	C-N	12.70	1.50	1.33
9	J	234	GLU	C-N	11.22	1.48	1.33

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N	143	PRO	N-CD-CG	-18.08	76.08	103.20
13	N	143	PRO	CA-CB-CG	-10.99	83.61	104.50
12	M	173	MET	N-CA-C	9.89	123.09	111.71
38	o	53	ASP	CA-C-N	9.39	129.09	118.85
38	o	53	ASP	C-N-CA	9.39	129.09	118.85
27	d	144	SER	N-CA-C	8.28	120.31	111.28
1	A	120	GLY	N-CA-C	7.99	123.00	112.77
13	N	143	PRO	CA-N-CD	-7.97	100.84	112.00
15	P	196	HIS	CA-C-N	7.87	127.78	119.05
15	P	196	HIS	C-N-CA	7.87	127.78	119.05
9	J	308	SER	CA-C-N	7.51	127.38	119.05
9	J	308	SER	C-N-CA	7.51	127.38	119.05
2	B	162	CYS	CA-C-N	7.46	126.99	118.85
2	B	162	CYS	C-N-CA	7.46	126.99	118.85
13	N	143	PRO	CB-CG-CD	7.46	129.97	106.10
9	J	234	GLU	CA-C-N	-7.41	109.88	122.33
9	J	234	GLU	C-N-CA	-7.41	109.88	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	r	422	HIS	N-CA-C	7.37	119.39	111.36
40	r	250	LEU	N-CA-C	7.26	119.19	111.28
12	M	74	ASN	N-CA-C	7.24	119.25	111.36
8	I	44	GLY	CA-C-N	7.11	127.10	119.28
8	I	44	GLY	C-N-CA	7.11	127.10	119.28
20	V	95	CYS	CA-CB-SG	7.00	130.49	114.40
16	Q	224	ALA	N-CA-C	6.63	118.50	111.28
12	M	75	CYS	N-CA-C	6.56	118.43	111.28
27	d	143	TYR	N-CA-C	6.26	122.36	113.02
10	K	71	SER	N-CA-C	6.23	118.07	111.28
4	E	43	VAL	CB-CA-C	-6.14	107.84	114.35
20	V	94	GLY	CA-C-N	-6.14	112.41	122.54
20	V	94	GLY	C-N-CA	-6.14	112.41	122.54
15	P	202	PHE	CA-C-N	6.13	126.04	119.85
15	P	202	PHE	C-N-CA	6.13	126.04	119.85
27	d	142	ARG	N-CA-C	6.13	117.76	111.14
17	S	54	ILE	N-CA-C	6.12	116.90	110.72
37	n	16	LEU	N-CA-C	6.12	117.95	111.28
44	w	245	PHE	N-CA-C	5.96	117.44	111.07
12	M	406	ASN	CA-C-N	5.92	125.62	119.05
12	M	406	ASN	C-N-CA	5.92	125.62	119.05
26	c	68	ASP	CA-C-N	5.89	126.52	119.98
26	c	68	ASP	C-N-CA	5.89	126.52	119.98
24	a	166	GLY	CA-C-N	5.88	125.58	119.05
24	a	166	GLY	C-N-CA	5.88	125.58	119.05
40	r	214	LEU	N-CA-C	5.86	117.67	111.28
9	J	308	SER	N-CA-C	5.79	116.99	109.64
9	J	311	GLU	CA-C-N	5.78	125.68	119.85
9	J	311	GLU	C-N-CA	5.78	125.68	119.85
12	M	280	ASP	N-CA-C	5.72	117.51	111.28
32	i	92	PRO	CA-N-CD	-5.71	104.00	112.00
14	O	70	TYR	CA-C-N	5.67	125.62	119.78
14	O	70	TYR	C-N-CA	5.67	125.62	119.78
12	M	612	PRO	CA-C-N	5.52	125.43	119.85
12	M	612	PRO	C-N-CA	5.52	125.43	119.85
41	s	87	VAL	CA-C-N	5.49	124.84	118.85
41	s	87	VAL	C-N-CA	5.49	124.84	118.85
32	i	324	LYS	N-CA-C	5.46	117.23	111.28
24	a	163	ARG	N-CA-C	5.43	117.27	111.36
4	E	42	GLU	N-CA-C	5.38	118.06	111.82
14	O	237	PRO	CA-C-N	5.31	125.22	119.85
14	O	237	PRO	C-N-CA	5.31	125.22	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	133	ILE	N-CA-C	5.28	115.49	110.42
12	M	177	ILE	N-CA-C	5.21	117.19	112.29
40	r	258	ALA	N-CA-C	5.17	118.69	112.38
42	u	169	PHE	N-CA-C	5.15	119.55	113.16
28	e	136	LEU	CB-CA-C	-5.05	110.73	116.54
9	J	307	VAL	N-CA-C	5.03	117.33	111.05
16	Q	226	TYR	N-CA-C	5.00	116.81	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3318	0	3278	125	0
2	B	1412	0	1363	40	0
3	C	1248	0	1255	43	0
4	E	971	0	975	23	0
5	F	691	0	704	17	0
6	G	693	0	671	26	0
6	X	695	0	669	26	0
7	H	910	0	950	20	0
8	I	780	0	808	35	0
9	J	2615	0	2635	97	0
10	K	355	0	329	25	0
11	L	1016	0	1016	23	0
12	M	5296	0	5327	126	0
13	N	1204	0	1162	28	0
14	O	1671	0	1673	70	0
15	P	1738	0	1693	50	0
16	Q	3377	0	3319	104	0
17	S	567	0	565	14	0
18	T	741	0	702	15	0
19	U	643	0	642	10	0
20	V	1021	0	1027	27	0
21	W	1167	0	1155	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	Y	600	0	539	13	0
23	Z	674	0	643	15	0
24	a	1165	0	1174	43	0
25	b	879	0	899	25	0
26	c	1315	0	1208	40	0
27	d	1461	0	1429	40	0
28	e	890	0	837	27	0
29	f	342	0	341	7	0
30	g	1000	0	994	20	0
31	h	867	0	871	16	0
32	i	2710	0	2874	68	0
33	j	800	0	855	36	0
34	k	748	0	799	22	0
35	l	4720	0	4797	154	0
36	m	919	0	920	35	0
37	n	479	0	486	24	0
38	o	1062	0	1072	41	0
39	p	1534	0	1470	70	0
40	r	3631	0	3839	131	0
41	s	2394	0	2508	99	0
42	u	1398	0	1378	24	0
43	v	998	0	919	26	0
44	w	2582	0	2531	66	0
45	A	8	0	0	2	0
45	B	16	0	0	0	0
45	C	8	0	0	4	0
45	M	16	0	0	0	0
46	A	31	0	19	10	0
47	A	44	0	27	8	0
48	C	47	0	71	41	0
48	U	51	0	82	11	0
48	V	51	0	82	22	0
48	l	139	0	209	48	0
48	m	41	0	59	12	0
48	s	51	0	82	4	0
49	C	52	0	88	11	0
49	V	52	0	88	5	0
49	e	52	0	88	2	0
49	i	52	0	88	4	0
49	j	52	0	88	3	0
49	n	52	0	88	12	0
50	G	35	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	X	35	0	0	6	0
51	J	48	0	23	7	0
52	M	4	0	0	2	0
52	O	4	0	0	0	0
53	M	1	0	0	0	0
54	N	51	0	46	12	0
54	a	91	0	131	27	0
54	i	66	0	76	10	0
54	l	199	0	307	36	0
54	n	78	0	103	21	0
54	r	100	0	156	10	0
55	T	1	0	0	0	0
56	s	28	0	31	51	0
57	w	27	0	11	5	0
All	All	66880	0	67344	1806	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 13.

All (1806) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:19:LEU:CD2	39:p:64:LEU:CD1	1.75	1.56
12:M:405:THR:CG2	12:M:477:GLY:HA3	1.33	1.53
48:C:311:PEE:C45	56:s:403:UQ:H171	1.37	1.50
48:C:311:PEE:C47	56:s:403:UQ:H172	1.05	1.49
41:s:52:ALA:CB	56:s:403:UQ:H13	1.46	1.42
48:C:311:PEE:H77	56:s:403:UQ:C17	1.47	1.41
48:C:311:PEE:H82	56:s:403:UQ:C17	1.48	1.41
3:C:50:LEU:CD1	48:C:311:PEE:H25	1.48	1.41
39:p:19:LEU:HD22	39:p:64:LEU:CD1	1.31	1.40
38:o:23:TYR:CD2	39:p:65:ARG:HD2	1.57	1.38
48:C:311:PEE:C47	56:s:403:UQ:C17	1.99	1.38
39:p:19:LEU:CD2	39:p:64:LEU:HD12	1.40	1.35
48:C:311:PEE:C45	56:s:403:UQ:C17	2.02	1.31
37:n:13:VAL:CG1	40:r:14:MET:HG2	1.60	1.30
24:a:127:ASP:OD1	49:n:101:PLX:H1B3	1.31	1.29
12:M:405:THR:HG21	12:M:477:GLY:CA	1.63	1.28
26:c:128:THR:HG23	26:c:132:HIS:CE1	1.68	1.26
41:s:52:ALA:HB2	56:s:403:UQ:C13	1.67	1.23
48:C:311:PEE:C46	56:s:403:UQ:H172	1.67	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:128:THR:CG2	26:c:132:HIS:CE1	2.22	1.22
1:A:48:ARG:O	10:K:74:ARG:NH1	1.73	1.21
37:n:30:ARG:NE	54:n:102:CDL:OA4	1.72	1.21
41:s:25:ARG:HD3	56:s:403:UQ:CM2	1.69	1.20
3:C:50:LEU:HD13	48:C:311:PEE:C17	1.71	1.19
41:s:25:ARG:CD	56:s:403:UQ:HM21	1.71	1.19
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	1.77	1.17
39:p:19:LEU:HD23	39:p:64:LEU:CD1	1.56	1.16
3:C:50:LEU:HD13	48:C:311:PEE:H25	1.18	1.16
38:o:23:TYR:CE2	39:p:65:ARG:HD2	1.80	1.14
48:l:718:PEE:H36	48:l:718:PEE:H28	1.25	1.14
51:J:401:NDP:C4D	51:J:401:NDP:O4D	1.68	1.14
1:A:66:LYS:HE3	1:A:188:GLY:O	1.48	1.12
37:n:30:ARG:CD	54:n:102:CDL:OA4	1.99	1.11
48:C:311:PEE:H82	56:s:403:UQ:C18	1.81	1.10
48:C:311:PEE:H81	56:s:403:UQ:H172	1.31	1.10
9:J:133:GLU:OE2	9:J:212:ARG:HD2	1.48	1.10
3:C:92:VAL:HG21	56:s:403:UQ:HM31	1.19	1.10
54:l:712:CDL:H541	54:l:712:CDL:HA62	1.10	1.10
27:d:104:ASN:OD1	35:l:73:THR:O	1.69	1.09
1:A:48:ARG:HD3	10:K:70:ASN:O	1.53	1.08
39:p:19:LEU:HD22	39:p:64:LEU:HD11	1.31	1.08
26:c:128:THR:HG23	26:c:132:HIS:HE1	0.92	1.06
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.34	1.06
38:o:23:TYR:CD2	39:p:65:ARG:CD	2.38	1.05
3:C:166:CYS:SG	45:C:301:SF4:FE1	1.48	1.05
26:c:128:THR:CG2	26:c:132:HIS:HE1	1.64	1.05
38:o:23:TYR:CE2	39:p:65:ARG:CD	2.40	1.04
50:X:201:8Q1:C43	39:p:63:LEU:HB3	1.86	1.04
32:i:329:MET:HA	32:i:329:MET:HE2	1.37	1.04
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.38	1.03
41:s:25:ARG:HD3	56:s:403:UQ:HM21	1.08	1.03
20:V:141:VAL:CG2	24:a:157:ARG:HB3	1.88	1.03
22:Y:76:ASP:O	35:l:385:TYR:OH	1.77	1.03
39:p:19:LEU:HD23	39:p:64:LEU:HD13	1.07	1.03
3:C:50:LEU:CD1	48:C:311:PEE:C17	2.32	1.03
9:J:304:LEU:O	9:J:307:VAL:HG22	1.57	1.03
12:M:405:THR:CG2	12:M:477:GLY:CA	2.25	1.03
54:a:201:CDL:H211	54:a:201:CDL:H251	1.35	1.02
37:n:13:VAL:HG12	40:r:14:MET:HG2	1.42	1.02
1:A:89:GLY:CA	1:A:244:ASN:HD22	1.72	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLY:HA2	1:A:244:ASN:ND2	1.74	1.01
3:C:92:VAL:HG21	56:s:403:UQ:CM3	1.89	1.01
48:m:202:PEE:H25	48:m:202:PEE:H56	1.41	1.01
48:C:311:PEE:C46	56:s:403:UQ:C17	2.31	1.01
44:w:72:ARG:NH1	44:w:76:GLU:OE1	1.93	1.01
35:l:190:LEU:HD23	40:r:383:THR:HG21	1.43	1.00
54:l:712:CDL:H541	54:l:712:CDL:CA6	1.91	1.00
54:l:712:CDL:H862	54:l:712:CDL:C65	1.90	1.00
48:V:202:PEE:H3	40:r:191:SER:HB3	1.42	1.00
16:Q:84:PHE:HE2	16:Q:99:MET:SD	1.85	0.98
9:J:208:GLY:H	9:J:211:ASP:CG	1.71	0.98
37:n:30:ARG:HD3	54:n:102:CDL:OA4	1.58	0.98
48:V:202:PEE:H36	48:V:202:PEE:H79	1.45	0.98
41:s:87:VAL:HG23	41:s:88:PRO:HD3	1.43	0.98
9:J:236:VAL:HG22	9:J:325:SER:OG	1.62	0.97
24:a:127:ASP:OD1	49:n:101:PLX:C1B	2.11	0.97
10:K:76:LEU:HD22	10:K:76:LEU:H	1.28	0.97
44:w:72:ARG:HH11	44:w:76:GLU:CD	1.71	0.96
41:s:52:ALA:CB	56:s:403:UQ:C13	2.32	0.96
54:l:712:CDL:H422	40:r:448:THR:HG21	1.46	0.96
41:s:52:ALA:HB2	56:s:403:UQ:H13	0.97	0.96
18:T:46:ASP:OD1	18:T:49:ASP:HB2	1.64	0.95
9:J:207:PHE:HA	9:J:211:ASP:OD2	1.66	0.95
3:C:166:CYS:HG	45:C:301:SF4:FE1	0.79	0.95
54:l:712:CDL:H862	54:l:712:CDL:H652	1.45	0.95
10:K:75:ASN:O	10:K:78:HIS:ND1	2.00	0.94
35:l:534:HIS:ND1	48:l:719:PEE:H13	1.83	0.94
9:J:135:GLU:OE2	9:J:179:ARG:NH1	2.01	0.94
24:a:96:ALA:HB2	27:d:61:TYR:CE2	2.03	0.94
33:j:4:MET:SD	48:m:202:PEE:H21	2.08	0.94
1:A:50:ASP:O	1:A:59:ARG:NH2	2.02	0.93
10:K:75:ASN:O	10:K:78:HIS:CE1	2.21	0.93
16:Q:104:GLU:HG2	16:Q:443:MET:SD	2.08	0.93
41:s:84:THR:O	41:s:87:VAL:HG22	1.69	0.92
48:V:202:PEE:H21	48:V:202:PEE:H30	1.49	0.92
37:n:13:VAL:HG13	40:r:14:MET:HG2	1.48	0.92
9:J:180:TYR:HB2	9:J:317:ASP:OD2	1.68	0.92
1:A:89:GLY:HA2	1:A:244:ASN:HD22	1.26	0.91
9:J:236:VAL:CG2	9:J:325:SER:OG	2.18	0.91
3:C:92:VAL:CG2	56:s:403:UQ:HM31	2.00	0.91
54:n:102:CDL:C64	54:r:714:CDL:H431	1.99	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:324:SER:HG	40:r:440:HIS:HE2	1.18	0.91
41:s:25:ARG:HH21	56:s:403:UQ:CM2	1.84	0.91
20:V:95:CYS:HB2	20:V:115:CYS:HA	1.53	0.90
32:i:133:TRP:HE3	54:i:401:CDL:H391	1.35	0.90
3:C:50:LEU:HD11	48:C:311:PEE:H25	1.50	0.90
20:V:141:VAL:HG23	24:a:157:ARG:HB3	1.51	0.90
24:a:126:TYR:O	49:n:101:PLX:C1B	2.20	0.90
32:i:325:LEU:HD12	54:i:401:CDL:H121	1.53	0.90
1:A:256:ARG:HG2	14:O:245:VAL:HG22	1.54	0.89
20:V:141:VAL:O	24:a:169:TYR:OH	1.88	0.89
48:C:311:PEE:H82	56:s:403:UQ:H172	0.92	0.89
48:l:718:PEE:H28	48:l:718:PEE:C22	2.03	0.89
38:o:23:TYR:OH	39:p:68:GLU:OE1	1.89	0.89
39:p:19:LEU:CD2	39:p:64:LEU:HD11	1.94	0.88
12:M:117:MET:HE2	12:M:143:SER:HB2	1.56	0.88
39:p:16:VAL:HG12	39:p:64:LEU:HD22	1.55	0.88
38:o:23:TYR:HD2	39:p:65:ARG:NH1	1.72	0.87
41:s:24:GLU:OE2	41:s:228:TYR:OH	1.92	0.87
41:s:25:ARG:CG	56:s:403:UQ:HM21	2.04	0.87
12:M:405:THR:HG21	12:M:477:GLY:HA3	0.88	0.87
26:c:128:THR:HG22	26:c:132:HIS:CE1	2.07	0.87
49:n:101:PLX:H282	49:n:101:PLX:H322	1.56	0.86
44:w:169:PHE:CD2	57:w:401:ADP:N6	2.44	0.86
39:p:19:LEU:HD22	39:p:64:LEU:HD12	0.92	0.86
1:A:249:ALA:O	1:A:252:PRO:HD2	1.76	0.86
41:s:24:GLU:OE1	41:s:274:ARG:NH1	2.09	0.86
24:a:126:TYR:O	49:n:101:PLX:H1B2	1.75	0.85
24:a:145:GLU:OE1	42:u:163:HIS:NE2	2.08	0.85
41:s:25:ARG:NH2	56:s:403:UQ:O2	2.10	0.85
54:a:201:CDL:H521	48:l:720:PEE:C11	2.06	0.84
9:J:207:PHE:CD2	9:J:214:LEU:HD11	2.12	0.84
37:n:34:LYS:HZ1	54:n:102:CDL:HB22	1.41	0.84
48:m:202:PEE:H10	48:m:202:PEE:H2	1.60	0.84
35:l:562:LEU:HG	48:l:718:PEE:H32	1.60	0.84
44:w:65:ASN:HD21	44:w:238:GLU:HB2	1.43	0.83
46:A:502:FMN:N1	46:A:502:FMN:O3'	2.11	0.83
33:j:17:LEU:HD23	41:s:222:MET:HE1	1.58	0.83
8:I:3:SER:O	54:N:202:CDL:HA22	1.79	0.82
39:p:56:ASP:HB3	39:p:59:LYS:HB2	1.61	0.82
21:W:51:MET:HE2	41:s:311:THR:HB	1.59	0.82
41:s:52:ALA:CA	56:s:403:UQ:H13	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:a:201:CDL:H211	54:a:201:CDL:C25	2.09	0.82
12:M:405:THR:HG22	12:M:477:GLY:HA3	1.55	0.81
12:M:666:GLN:NE2	12:M:670:GLU:OE1	2.13	0.81
12:M:419:ARG:NH1	12:M:439:THR:O	2.13	0.81
40:r:116:ILE:HG12	40:r:174:LEU:CD1	2.10	0.81
9:J:318:LYS:O	9:J:322:VAL:HG12	1.81	0.81
16:Q:84:PHE:CE2	16:Q:99:MET:SD	2.72	0.81
27:d:114:GLN:CG	35:l:203:MET:HE2	2.11	0.81
54:l:712:CDL:C71	54:l:712:CDL:H751	2.11	0.81
1:A:50:ASP:O	1:A:55:GLY:HA3	1.80	0.80
8:I:24:LEU:HD23	8:I:28:TYR:HE2	1.44	0.80
25:b:100:ARG:HB2	35:l:60:GLU:HB2	1.62	0.80
26:c:128:THR:HG22	26:c:132:HIS:ND1	1.95	0.80
48:m:202:PEE:H10	48:m:202:PEE:C1	2.11	0.80
48:V:202:PEE:H79	48:V:202:PEE:C22	2.11	0.80
1:A:102:MET:CG	1:A:241:THR:OG1	2.29	0.80
38:o:23:TYR:HD2	39:p:65:ARG:CZ	1.92	0.80
44:w:246:LEU:HD12	44:w:255:VAL:HG11	1.63	0.80
9:J:135:GLU:OE2	9:J:141:PHE:CD2	2.34	0.80
48:C:311:PEE:H12	33:j:29:ALA:O	1.80	0.80
9:J:206:ILE:N	51:J:401:NDP:H71N	1.80	0.80
39:p:46:ALA:O	39:p:49:ASP:OD1	1.98	0.80
2:B:77:LEU:HD12	41:s:31:MET:HG3	1.63	0.80
26:c:62:TYR:OH	26:c:74:ASP:OD1	2.00	0.79
6:G:105:MET:HE1	6:G:139:MET:HG3	1.65	0.79
8:I:44:GLY:HA3	16:Q:359:ASP:OD2	1.81	0.79
15:P:154:GLU:OE2	15:P:180:ASN:ND2	2.16	0.79
27:d:162:ARG:NH2	28:e:140:ASN:OD1	2.13	0.79
41:s:87:VAL:CG2	41:s:88:PRO:HD3	2.12	0.79
26:c:128:THR:O	26:c:132:HIS:ND1	2.16	0.79
10:K:100:GLN:NE2	14:O:69:ASN:O	2.15	0.79
5:F:40:ARG:HH12	5:F:84:ALA:HB1	1.49	0.78
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.64	0.78
12:M:485:ASP:OD2	12:M:680:LEU:N	2.17	0.78
14:O:182:ASN:HB3	14:O:194:GLU:CB	2.12	0.78
1:A:61:ASP:OD1	1:A:137:LYS:HG2	1.83	0.77
4:E:71:ALA:HA	50:G:201:8Q1:O40	1.84	0.77
21:W:144:THR:HB	41:s:96:ILE:HG23	1.64	0.77
11:L:163:ASN:O	11:L:171:ARG:HA	1.84	0.77
48:C:311:PEE:C41	49:C:312:PLX:H192	2.14	0.77
12:M:405:THR:HG23	12:M:477:GLY:HA3	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:14:GLN:HE22	39:p:157:ALA:HB3	1.49	0.77
44:w:233:TYR:CZ	44:w:237:ILE:HD11	2.18	0.77
24:a:131:LYS:NZ	37:n:32:ASP:OD2	2.18	0.77
1:A:125:CYS:SG	1:A:277:ASN:ND2	2.58	0.76
9:J:207:PHE:CA	9:J:211:ASP:OD2	2.33	0.76
16:Q:97:LEU:HG	16:Q:99:MET:HE3	1.67	0.76
35:l:534:HIS:ND1	48:l:719:PEE:C11	2.49	0.76
35:l:562:LEU:HD21	48:l:718:PEE:H31	1.66	0.76
37:n:30:ARG:CZ	54:n:102:CDL:OA4	2.34	0.76
15:P:161:LYS:HD2	16:Q:286:TYR:CE1	2.21	0.76
54:a:201:CDL:H521	48:l:720:PEE:H13	1.67	0.76
48:C:311:PEE:H69	49:C:312:PLX:H192	1.67	0.75
28:e:125:LEU:HD21	28:e:129:ARG:CZ	2.16	0.75
5:F:68:ARG:NH2	12:M:364:ASP:OD1	2.20	0.75
44:w:246:LEU:CD1	44:w:255:VAL:HG11	2.17	0.75
13:N:129:THR:HA	18:T:43:GLN:HG2	1.68	0.75
9:J:49:SER:OG	15:P:225:GLU:HG2	1.85	0.75
16:Q:53:TYR:OH	48:l:718:PEE:C3	2.35	0.75
33:j:18:VAL:HA	41:s:222:MET:HE3	1.69	0.74
1:A:49:HIS:CE1	14:O:238:PRO:HG3	2.22	0.74
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.19	0.74
40:r:115:LEU:HD21	40:r:176:PHE:CE1	2.22	0.74
1:A:38:GLU:HB3	14:O:239:LYS:NZ	2.01	0.74
3:C:71:CYS:HB3	16:Q:141:TYR:HB2	1.69	0.74
1:A:102:MET:HG3	1:A:241:THR:OG1	1.88	0.74
3:C:126:GLU:O	9:J:89:TYR:OH	2.05	0.74
54:l:712:CDL:H751	54:l:712:CDL:H711	1.70	0.74
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.68	0.73
12:M:464:GLN:O	12:M:468:GLU:HG2	1.88	0.73
54:n:102:CDL:C82	54:r:714:CDL:H852	2.17	0.73
48:C:311:PEE:H16	33:j:27:LEU:HD13	1.70	0.73
48:l:720:PEE:O2P	48:l:720:PEE:N	2.21	0.73
1:A:141:GLY:HA2	1:A:252:PRO:HG3	1.69	0.73
16:Q:144:MET:HG2	16:Q:222:MET:O	1.88	0.73
35:l:71:LEU:HD12	40:r:310:MET:HE1	1.70	0.73
31:h:48:GLY:O	31:h:52:ALA:HB2	1.89	0.73
35:l:68:TRP:CE3	48:l:720:PEE:H47	2.23	0.73
41:s:52:ALA:HB1	56:s:403:UQ:H13	1.67	0.73
9:J:204:SER:OG	9:J:238:GLN:O	2.05	0.73
34:k:44:SER:HB2	34:k:59:MET:HE1	1.71	0.73
48:m:202:PEE:H56	48:m:202:PEE:C17	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:50:GLU:O	27:d:54:GLN:NE2	2.22	0.72
1:A:38:GLU:HB3	14:O:239:LYS:HZ3	1.55	0.72
6:G:103:HIS:HD2	6:G:106:LYS:HG2	1.54	0.72
20:V:141:VAL:CG2	24:a:157:ARG:CB	2.68	0.72
40:r:116:ILE:HG12	40:r:174:LEU:HD13	1.71	0.72
3:C:71:CYS:HB3	16:Q:141:TYR:CB	2.19	0.72
48:C:311:PEE:H77	56:s:403:UQ:C20	2.20	0.72
54:a:201:CDL:H732	54:a:201:CDL:H191	1.70	0.71
44:w:65:ASN:ND2	44:w:238:GLU:HB2	2.04	0.71
5:F:45:LYS:HE3	12:M:380:ASP:OD2	1.90	0.71
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.23	0.71
3:C:133:MET:SD	3:C:173:LEU:HD22	2.30	0.71
9:J:207:PHE:HD2	9:J:214:LEU:HD11	1.53	0.71
39:p:139:GLN:NE2	39:p:143:GLU:OE1	2.24	0.71
32:i:133:TRP:CE3	54:i:401:CDL:H391	2.24	0.71
32:i:329:MET:HA	32:i:329:MET:CE	2.20	0.71
24:a:127:ASP:OD1	49:n:101:PLX:H1C2	1.90	0.71
1:A:128:ARG:NH2	14:O:192:TYR:HD2	1.89	0.71
4:E:52:LEU:HD22	4:E:104:MET:HE3	1.70	0.71
38:o:23:TYR:CD2	39:p:65:ARG:NH1	2.57	0.71
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.72	0.71
6:G:139:MET:N	6:G:143:GLU:OE2	2.21	0.70
8:I:46:SER:O	8:I:52:ASN:ND2	2.23	0.70
15:P:44:ARG:HB3	15:P:45:PRO:HD3	1.74	0.70
27:d:114:GLN:HG3	35:l:203:MET:HE2	1.73	0.70
24:a:141:GLN:NE2	24:a:145:GLU:OE2	2.24	0.70
48:m:202:PEE:O4	48:m:202:PEE:H7	1.91	0.70
40:r:57:PHE:HD1	40:r:113:THR:HG22	1.57	0.70
34:k:8:ILE:HG21	34:k:43:MET:HB2	1.72	0.70
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.31	0.70
48:V:202:PEE:H78	40:r:201:MET:HE2	1.74	0.70
54:a:201:CDL:H322	48:l:720:PEE:H62	1.74	0.70
12:M:695:TYR:O	12:M:701:SER:OG	2.09	0.69
35:l:562:LEU:HG	48:l:718:PEE:C20	2.21	0.69
40:r:114:GLU:OE2	40:r:174:LEU:HB2	1.92	0.69
12:M:75:CYS:HG	52:M:803:FES:FE2	1.08	0.69
31:h:48:GLY:O	31:h:52:ALA:CB	2.40	0.69
41:s:25:ARG:HD3	56:s:403:UQ:HM22	1.72	0.69
11:L:86:ASN:OD1	12:M:275:PRO:O	2.11	0.69
48:V:202:PEE:H73	40:r:197:LEU:HD13	1.74	0.69
41:s:87:VAL:HG23	41:s:88:PRO:CD	2.20	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LYS:HE3	1:A:188:GLY:C	2.17	0.69
48:C:311:PEE:H76	56:s:403:UQ:C17	2.21	0.69
8:I:96:THR:HB	8:I:97:PRO:HD2	1.74	0.69
27:d:114:GLN:CG	35:l:203:MET:CE	2.71	0.69
1:A:49:HIS:CE1	14:O:238:PRO:CD	2.75	0.69
54:a:201:CDL:H532	48:l:720:PEE:H56	1.73	0.69
15:P:125:ARG:NH2	15:P:201:ASP:OD1	2.25	0.69
16:Q:53:TYR:OH	48:l:718:PEE:O3	2.10	0.69
9:J:133:GLU:OE2	9:J:212:ARG:NH2	2.25	0.69
9:J:238:GLN:HG2	9:J:270:ARG:HG2	1.75	0.69
40:r:87:GLU:O	40:r:92:LYS:NZ	2.26	0.69
48:V:202:PEE:C1	40:r:191:SER:HB3	2.20	0.69
48:C:311:PEE:H77	56:s:403:UQ:H203	1.73	0.69
8:I:8:ILE:HD11	54:N:202:CDL:H142	1.75	0.68
26:c:128:THR:CG2	26:c:132:HIS:ND1	2.54	0.68
38:o:23:TYR:CD2	39:p:65:ARG:CZ	2.75	0.68
40:r:104:LEU:HG	40:r:108:MET:HE2	1.73	0.68
6:X:82:ARG:HD2	6:X:126:PHE:HE1	1.58	0.68
9:J:206:ILE:H	51:J:401:NDP:H71N	1.40	0.68
9:J:220:MET:O	9:J:222:TRP:N	2.26	0.68
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.24	0.68
26:c:55:TYR:OH	26:c:74:ASP:O	2.03	0.68
35:l:60:GLU:OE1	35:l:83:ASP:HA	1.93	0.68
48:m:202:PEE:H53	48:m:202:PEE:H24	1.75	0.68
41:s:288:LEU:HD11	48:s:401:PEE:H7	1.73	0.68
19:U:26:GLY:HA3	48:U:101:PEE:H37	1.74	0.68
50:X:201:8Q1:C43	39:p:63:LEU:CB	2.67	0.68
1:A:123:GLY:N	14:O:180:CYS:SG	2.65	0.68
26:c:69:GLY:HA3	38:o:86:THR:HG21	1.75	0.68
10:K:76:LEU:HD22	10:K:76:LEU:N	2.07	0.68
39:p:16:VAL:CG1	39:p:64:LEU:HD22	2.23	0.68
12:M:75:CYS:SG	52:M:803:FES:FE2	1.85	0.68
40:r:257:MET:HA	40:r:257:MET:HE3	1.77	0.67
43:v:51:LEU:HD13	43:v:63:LEU:HD23	1.76	0.67
12:M:36:VAL:HG22	12:M:102:ILE:HD12	1.76	0.67
12:M:690:THR:HG23	12:M:692:LYS:HG2	1.76	0.67
32:i:207:ILE:HG22	32:i:211:MET:HE2	1.76	0.67
32:i:325:LEU:HD13	54:i:401:CDL:H132	1.77	0.67
9:J:212:ARG:O	9:J:216:TYR:CB	2.43	0.67
16:Q:36:GLN:HG3	40:r:137:GLY:O	1.94	0.67
16:Q:178:THR:OG1	16:Q:214:TYR:OH	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:114:GLN:HG2	35:l:203:MET:CE	2.24	0.67
38:o:23:TYR:CD2	39:p:65:ARG:NE	2.63	0.67
6:G:105:MET:HE1	6:G:139:MET:CG	2.25	0.67
12:M:467:LYS:HG3	12:M:503:SER:OG	1.95	0.67
18:T:104:LYS:HD2	18:T:107:LYS:HE3	1.77	0.67
3:C:166:CYS:SG	45:C:301:SF4:S2	2.93	0.67
6:G:83:VAL:HG13	6:G:122:MET:HE1	1.75	0.67
2:B:98:ARG:NH2	16:Q:224:ALA:O	2.26	0.66
37:n:47:ARG:NH1	37:n:53:GLU:OE1	2.27	0.66
44:w:169:PHE:CG	57:w:401:ADP:C6	2.83	0.66
54:l:712:CDL:H412	54:l:712:CDL:H602	1.77	0.66
1:A:123:GLY:CA	14:O:180:CYS:SG	2.83	0.66
1:A:152:ARG:NH2	10:K:99:PRO:O	2.27	0.66
12:M:335:GLY:HA2	12:M:362:ASP:O	1.96	0.66
27:d:111:LYS:NZ	35:l:200:GLN:OE1	2.24	0.66
41:s:87:VAL:N	41:s:88:PRO:HD2	2.10	0.66
33:j:25:PRO:HB2	41:s:60:PRO:HD3	1.77	0.66
1:A:90:GLY:HA3	47:A:503:NAI:H1D	1.77	0.66
1:A:123:GLY:HA2	14:O:180:CYS:SG	2.36	0.66
14:O:187:GLN:HG3	14:O:192:TYR:CE1	2.30	0.66
35:l:419:THR:HA	35:l:422:TYR:CE2	2.31	0.66
9:J:207:PHE:HD2	9:J:214:LEU:CD1	2.08	0.66
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.28	0.66
39:p:175:ARG:HH11	39:p:178:PRO:HA	1.61	0.66
31:h:89:GLU:OE1	31:h:91:LYS:NZ	2.29	0.65
26:c:116:ARG:HG2	48:l:719:PEE:H49	1.78	0.65
4:E:37:ARG:HG2	6:G:120:MET:HE2	1.78	0.65
32:i:155:LEU:HB3	32:i:278:MET:HE1	1.78	0.65
9:J:212:ARG:O	9:J:216:TYR:N	2.28	0.65
25:b:89:HIS:CE1	48:l:720:PEE:H50	2.32	0.65
32:i:77:ASN:HB2	32:i:89:MET:HE3	1.77	0.65
38:o:23:TYR:CE2	39:p:65:ARG:CG	2.79	0.65
54:l:712:CDL:HA62	54:l:712:CDL:C54	2.06	0.65
48:C:311:PEE:C45	56:s:403:UQ:H172	1.97	0.65
24:a:126:TYR:O	49:n:101:PLX:H1B3	1.95	0.65
16:Q:100:GLU:HG2	16:Q:108:LYS:HB3	1.78	0.65
43:v:12:ASP:HB3	43:v:15:LYS:HB2	1.78	0.65
40:r:204:MET:HG3	40:r:209:LEU:HB2	1.79	0.65
20:V:69:ILE:HG13	20:V:100:THR:HG21	1.79	0.64
41:s:221:ALA:O	41:s:225:MET:HG3	1.97	0.64
1:A:251:SER:OG	1:A:252:PRO:HD3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:59:ARG:NH1	49:C:312:PLX:O3	2.31	0.64
40:r:201:MET:HE1	40:r:212:LEU:HD11	1.79	0.64
19:U:23:PHE:CD2	48:U:101:PEE:H58	2.32	0.64
33:j:13:LEU:HD13	41:s:10:ILE:HD13	1.78	0.64
24:a:155:GLU:OE1	24:a:158:ARG:NH1	2.30	0.64
3:C:80:ALA:HB2	3:C:86:MET:HE3	1.79	0.64
11:L:89:SER:O	12:M:59:GLN:NE2	2.29	0.64
40:r:266:MET:HA	40:r:269:MET:HE3	1.80	0.64
29:f:72:ARG:NH2	30:g:18:ASN:OD1	2.31	0.64
32:i:89:MET:HG2	32:i:95:MET:HB2	1.80	0.64
54:N:202:CDL:C53	54:N:202:CDL:H742	2.27	0.64
14:O:175:GLU:OE1	14:O:175:GLU:HA	1.97	0.64
33:j:64:LEU:HD13	36:m:165:VAL:HG22	1.80	0.64
1:A:49:HIS:CE1	14:O:238:PRO:HD3	2.33	0.64
54:n:102:CDL:HB62	42:u:172:MET:HE2	1.80	0.64
41:s:288:LEU:CD1	48:s:401:PEE:H7	2.27	0.64
9:J:311:GLU:HG3	9:J:311:GLU:O	1.97	0.64
12:M:48:THR:OG1	12:M:51:GLN:HG3	1.97	0.64
13:N:32:ASP:OD2	13:N:58:ARG:NH2	2.30	0.64
16:Q:97:LEU:HG	16:Q:99:MET:CE	2.27	0.64
41:s:14:LEU:O	41:s:17:VAL:HG22	1.98	0.64
7:H:88:LEU:HD21	7:H:92:ARG:HH21	1.62	0.63
17:S:5:ILE:HG12	41:s:26:LYS:HG2	1.80	0.63
26:c:128:THR:C	26:c:132:HIS:HD1	2.06	0.63
27:d:56:HIS:O	27:d:59:ASN:O	2.16	0.63
35:l:562:LEU:CD2	48:l:718:PEE:H31	2.27	0.63
44:w:246:LEU:N	44:w:247:PRO:HD2	2.12	0.63
3:C:50:LEU:HD13	48:C:311:PEE:H26	1.72	0.63
9:J:83:PRO:HA	9:J:106:MET:O	1.98	0.63
54:a:201:CDL:H382	27:d:48:ALA:HB2	1.80	0.63
40:r:403:THR:HA	40:r:406:TYR:CE2	2.33	0.63
1:A:41:ILE:HG23	1:A:253:THR:HG21	1.79	0.63
7:H:54:GLU:O	7:H:58:MET:HG3	1.98	0.63
40:r:168:GLN:HB2	40:r:174:LEU:HG	1.81	0.63
2:B:177:THR:HG21	2:B:182:GLU:HB2	1.80	0.63
15:P:105:ASN:O	15:P:137:PHE:CE2	2.51	0.63
1:A:87:GLY:HA3	46:A:502:FMN:O2P	1.97	0.63
33:j:73:LEU:HD13	36:m:55:MET:HE1	1.80	0.63
8:I:3:SER:O	54:N:202:CDL:CA2	2.47	0.63
12:M:83:GLU:OE1	12:M:101:ASN:ND2	2.26	0.63
37:n:15:ILE:C	37:n:15:ILE:HD12	2.22	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:373:PRO:HB3	12:M:487:THR:HG22	1.81	0.63
41:s:281:ARG:HB2	41:s:284:GLN:HG3	1.80	0.63
1:A:409:ILE:HG23	1:A:439:ILE:HD12	1.80	0.63
15:P:164:ASN:OD1	15:P:181:HIS:CE1	2.51	0.63
14:O:182:ASN:CB	14:O:194:GLU:HG2	2.29	0.62
25:b:123:PHE:HD2	43:v:40:VAL:HG11	1.64	0.62
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.81	0.62
35:l:166:THR:CG2	48:l:719:PEE:H2	2.29	0.62
32:i:92:PRO:O	32:i:94:ALA:N	2.31	0.62
49:n:101:PLX:H322	49:n:101:PLX:C28	2.28	0.62
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.32	0.62
14:O:88:ARG:NH2	14:O:190:ASP:OD2	2.30	0.62
20:V:141:VAL:HG21	24:a:157:ARG:CB	2.29	0.62
2:B:184:LEU:HB3	11:L:112:MET:HE2	1.81	0.62
12:M:203:ASP:OD1	14:O:39:PHE:CE2	2.52	0.62
40:r:14:MET:HE2	40:r:30:HIS:HD2	1.62	0.62
11:L:90:GLY:HA3	15:P:238:PRO:HB2	1.79	0.62
20:V:95:CYS:HB2	20:V:115:CYS:CA	2.21	0.62
22:Y:51:THR:HG22	22:Y:53:SER:H	1.63	0.62
35:l:337:ALA:O	35:l:341:MET:HG2	1.99	0.62
34:k:23:ARG:HD3	36:m:23:LYS:HB2	1.81	0.62
35:l:107:TYR:HD2	35:l:108:MET:HE3	1.64	0.62
54:l:712:CDL:H422	40:r:448:THR:CG2	2.26	0.62
54:l:712:CDL:H612	54:l:712:CDL:H451	1.80	0.62
2:B:111:GLU:O	2:B:141:ARG:NH1	2.33	0.62
48:V:202:PEE:H36	48:V:202:PEE:H74	1.82	0.62
7:H:101:GLU:HB3	7:H:102:PRO:HD2	1.82	0.62
38:o:59:VAL:HG22	40:r:423:ILE:HG23	1.82	0.62
9:J:229:ILE:HD11	9:J:298:TYR:CG	2.35	0.61
12:M:389:THR:OG1	12:M:514:ASN:ND2	2.27	0.61
54:a:201:CDL:H322	48:l:720:PEE:C38	2.30	0.61
46:A:502:FMN:HO3'	46:A:502:FMN:C2	2.07	0.61
54:N:202:CDL:H742	54:N:202:CDL:H531	1.83	0.61
32:i:347:ASN:HB3	49:i:705:PLX:H301	1.80	0.61
54:n:102:CDL:HB62	42:u:172:MET:CE	2.29	0.61
9:J:192:ARG:NH1	9:J:198:ALA:O	2.33	0.61
9:J:213:PHE:HZ	9:J:276:LEU:HD21	1.65	0.61
6:X:69:SER:OG	6:X:70:ASP:N	2.31	0.61
25:b:86:LEU:HD11	35:l:9:LEU:HD12	1.82	0.61
9:J:236:VAL:HG23	9:J:325:SER:OG	2.00	0.61
12:M:308:ARG:NH2	12:M:578:PRO:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:98:CYS:HB2	35:l:580:GLN:HB2	1.83	0.61
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.83	0.61
1:A:256:ARG:CG	14:O:245:VAL:HG22	2.29	0.61
12:M:275:PRO:HB3	12:M:286:ILE:HG23	1.82	0.61
25:b:73:THR:HA	25:b:77:ILE:HD12	1.83	0.61
35:l:562:LEU:CG	48:l:718:PEE:H32	2.30	0.61
39:p:132:SER:OG	39:p:136:GLU:OE2	2.14	0.61
18:T:34:THR:OG1	18:T:47:ASP:OD1	2.15	0.61
21:W:134:LEU:HD21	36:m:2:THR:H	1.66	0.61
27:d:46:THR:O	27:d:50:GLU:HG2	2.01	0.61
35:l:286:LEU:HD22	35:l:411:MET:SD	2.40	0.61
1:A:89:GLY:O	47:A:503:NAI:H2N	2.01	0.60
3:C:66:THR:HG21	3:C:76:MET:HG2	1.83	0.60
24:a:96:ALA:HB2	27:d:61:TYR:CD2	2.36	0.60
34:k:25:HIS:O	34:k:28:SER:N	2.33	0.60
35:l:264:TYR:CD1	35:l:265:PRO:HD3	2.35	0.60
33:j:7:LEU:HD21	48:m:202:PEE:H59	1.82	0.60
41:s:24:GLU:HG3	41:s:271:LEU:HD22	1.83	0.60
40:r:196:TRP:CE3	40:r:257:MET:HG2	2.36	0.60
43:v:104:ARG:O	43:v:108:LEU:HG	2.01	0.60
44:w:165:SER:HB3	44:w:245:PHE:CE1	2.36	0.60
54:l:712:CDL:H862	54:l:712:CDL:H651	1.81	0.60
1:A:40:ARG:NH1	1:A:289:GLU:O	2.34	0.60
6:G:114:ASP:O	6:G:118:ILE:HG13	2.02	0.60
32:i:154:MET:HE2	32:i:191:THR:HB	1.84	0.60
32:i:217:MET:HB2	32:i:326:LEU:HD13	1.84	0.60
44:w:218:ILE:HG23	44:w:226:GLU:HG2	1.83	0.60
12:M:485:ASP:OD2	12:M:680:LEU:HG	2.02	0.60
30:g:34:VAL:HG21	54:n:102:CDL:OA7	2.01	0.60
5:F:89:ARG:O	5:F:93:ASN:ND2	2.29	0.60
48:V:202:PEE:H3	40:r:191:SER:CB	2.26	0.60
40:r:115:LEU:HD23	40:r:176:PHE:CZ	2.37	0.60
35:l:88:MET:HE1	35:l:468:ILE:HD13	1.84	0.60
41:s:102:VAL:HG11	41:s:154:LEU:HD11	1.84	0.60
3:C:69:LEU:HD23	16:Q:94:VAL:HG11	1.84	0.60
9:J:50:SER:OG	15:P:225:GLU:OE2	2.15	0.60
12:M:433:GLY:O	12:M:444:HIS:NE2	2.31	0.60
48:V:202:PEE:H80	48:V:202:PEE:H41	1.84	0.60
26:c:155:PRO:HG3	43:v:4:HIS:HD2	1.67	0.60
37:n:28:ASP:OD2	40:r:3:LYS:NZ	2.35	0.60
1:A:51:TRP:O	1:A:52:ARG:O	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:C:311:PEE:H68	49:C:312:PLX:H192	1.84	0.59
37:n:13:VAL:CG1	40:r:14:MET:CG	2.56	0.59
1:A:119:GLU:HA	1:A:119:GLU:OE2	2.01	0.59
12:M:34:VAL:HG23	12:M:41:VAL:HG13	1.82	0.59
15:P:173:MET:HB3	15:P:198:PHE:HB2	1.83	0.59
20:V:95:CYS:CB	20:V:115:CYS:HA	2.30	0.59
28:e:109:LEU:HD13	40:r:43:ASN:HB2	1.82	0.59
37:n:13:VAL:HG12	40:r:14:MET:CG	2.27	0.59
41:s:62:ARG:HD3	41:s:64:ALA:H	1.67	0.59
1:A:49:HIS:CE1	14:O:238:PRO:CG	2.84	0.59
9:J:212:ARG:O	9:J:216:TYR:HB2	2.01	0.59
12:M:367:CYS:HB3	12:M:533:GLY:O	2.02	0.59
16:Q:102:SER:OG	16:Q:107:ARG:NH1	2.36	0.59
35:l:302:VAL:HG13	35:l:339:LEU:HD23	1.85	0.59
41:s:287:HIS:CD2	41:s:291:LYS:HD2	2.37	0.59
6:X:138:LEU:HD13	6:X:144:ILE:HG12	1.84	0.59
24:a:112:TYR:CD2	27:d:64:TYR:O	2.56	0.59
32:i:329:MET:HE2	32:i:329:MET:CA	2.23	0.59
48:V:202:PEE:H79	48:V:202:PEE:C23	2.33	0.59
25:b:87:LYS:HG3	35:l:1:MET:HE2	1.85	0.59
38:o:23:TYR:CE2	39:p:65:ARG:NE	2.70	0.59
41:s:14:LEU:HA	41:s:17:VAL:HG22	1.83	0.59
9:J:132:ARG:NH2	51:J:401:NDP:O2X	2.35	0.59
35:l:370:THR:HA	35:l:431:PHE:CE2	2.38	0.59
2:B:98:ARG:HB3	2:B:169:GLU:CD	2.27	0.59
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	1.84	0.59
20:V:37:SER:HB3	20:V:56:THR:HG22	1.84	0.59
54:a:201:CDL:H761	54:a:201:CDL:H201	1.84	0.59
1:A:65:THR:HG22	1:A:69:LEU:HD23	1.85	0.59
2:B:78:PHE:O	8:I:12:ARG:NH2	2.35	0.59
3:C:83:ARG:NH1	16:Q:212:GLU:OE2	2.25	0.59
16:Q:52:MET:O	32:i:171:ASN:ND2	2.35	0.59
1:A:115:VAL:HG21	1:A:142:CYS:SG	2.42	0.59
7:H:37:GLN:HB2	7:H:95:LEU:HD11	1.84	0.59
31:h:69:ARG:O	31:h:73:MET:HG3	2.03	0.59
44:w:148:GLU:OE1	44:w:301:LYS:NZ	2.31	0.59
1:A:214:GLU:OE2	1:A:224:ARG:NH2	2.34	0.58
12:M:388:ASN:HB3	12:M:511:LYS:HE2	1.85	0.58
35:l:293:ILE:HD13	35:l:418:LEU:HD22	1.85	0.58
44:w:72:ARG:NH1	44:w:76:GLU:CD	2.48	0.58
2:B:177:THR:HG22	2:B:179:THR:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:76:LEU:O	10:K:79:HIS:HD2	1.86	0.58
16:Q:53:TYR:OH	48:l:718:PEE:H8	2.02	0.58
32:i:79:LEU:HB2	34:k:47:ILE:HD13	1.84	0.58
34:k:11:ALA:HB1	36:m:17:PHE:CD2	2.37	0.58
12:M:266:ARG:HG2	12:M:267:THR:HG23	1.85	0.58
24:a:127:ASP:OD1	49:n:101:PLX:C1C	2.51	0.58
26:c:128:THR:HG22	26:c:132:HIS:HD1	1.67	0.58
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.86	0.58
9:J:303:ARG:HB2	9:J:316:ARG:HD3	1.85	0.58
6:X:83:VAL:HG22	6:X:122:MET:HE1	1.86	0.58
32:i:239:VAL:HG23	54:r:714:CDL:H311	1.84	0.58
3:C:188:LYS:HD3	3:C:191:ARG:HD2	1.85	0.58
12:M:636:TYR:CD2	12:M:642:VAL:HG22	2.38	0.58
16:Q:140:ASP:OD2	16:Q:143:SER:OG	2.19	0.58
14:O:38:LEU:O	14:O:124:ARG:NH2	2.36	0.58
16:Q:218:SER:CB	16:Q:224:ALA:HB1	2.34	0.58
48:V:202:PEE:H14	32:i:276:ILE:HG21	1.86	0.58
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.86	0.58
41:s:87:VAL:CG2	41:s:88:PRO:CD	2.80	0.58
1:A:65:THR:O	1:A:69:LEU:HD23	2.04	0.58
48:C:311:PEE:H28	48:C:311:PEE:H20	1.86	0.58
26:c:160:GLN:OE1	43:v:37:ARG:NH1	2.36	0.58
1:A:48:ARG:HH12	14:O:231:LEU:HD11	1.69	0.58
1:A:48:ARG:NH2	14:O:226:GLU:OE2	2.36	0.58
49:C:312:PLX:H171	41:s:53:LEU:HD21	1.86	0.58
5:F:46:LYS:HE2	12:M:674:LEU:HD21	1.85	0.58
21:W:97:ILE:HG22	21:W:98:MET:HE2	1.84	0.58
6:X:120:MET:HE3	39:p:24:LEU:HD23	1.86	0.58
23:Z:36:LEU:HG	23:Z:41:LEU:HB2	1.86	0.58
3:C:193:TRP:HA	3:C:196:ARG:HG2	1.86	0.58
14:O:187:GLN:HG3	14:O:192:TYR:HE1	1.68	0.58
28:e:125:LEU:HD21	28:e:129:ARG:NE	2.17	0.58
39:p:50:GLU:OE1	39:p:50:GLU:HA	2.04	0.58
44:w:176:GLN:NE2	44:w:236:ASP:OD2	2.37	0.58
26:c:75:TYR:OH	26:c:105:ILE:O	2.12	0.57
32:i:41:ILE:HG13	34:k:73:LEU:HD21	1.86	0.57
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.39	0.57
1:A:210:THR:HB	1:A:224:ARG:HG2	1.87	0.57
48:U:101:PEE:H42	33:j:96:ILE:CD1	2.34	0.57
25:b:123:PHE:HB3	43:v:40:VAL:HG21	1.87	0.57
35:l:5:ALA:HB2	35:l:61:MET:SD	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:169:PHE:CG	57:w:401:ADP:N6	2.72	0.57
1:A:149:MET:SD	1:A:241:THR:HG21	2.45	0.57
15:P:125:ARG:HH22	15:P:201:ASP:CG	2.11	0.57
22:Y:94:ASP:HB3	22:Y:99:ILE:HB	1.86	0.57
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.86	0.57
8:I:12:ARG:HD3	8:I:20:LEU:HD22	1.86	0.57
12:M:136:GLU:OE2	12:M:272:ARG:NH2	2.37	0.57
24:a:134:GLU:OE1	37:n:57:TRP:NE1	2.28	0.57
54:i:401:CDL:H132	54:i:401:CDL:H171	1.85	0.57
35:l:534:HIS:CE1	48:l:719:PEE:H16	2.39	0.57
37:n:50:ARG:HB2	37:n:53:GLU:HB2	1.87	0.57
39:p:13:GLN:HA	39:p:16:VAL:HG22	1.86	0.57
44:w:68:SER:OG	44:w:209:VAL:HG21	2.05	0.57
22:Y:43:ARG:NH1	22:Y:47:PHE:O	2.37	0.57
27:d:107:GLN:OE1	35:l:194:ASN:ND2	2.36	0.57
35:l:250:SER:HB2	35:l:333:ALA:HA	1.84	0.57
41:s:10:ILE:HD11	41:s:83:LEU:HD13	1.85	0.57
10:K:88:ASP:O	10:K:92:GLU:HG3	2.05	0.57
33:j:60:ILE:HG21	36:m:168:ILE:HG21	1.87	0.57
3:C:133:MET:CE	3:C:173:LEU:HD22	2.35	0.57
10:K:77:GLN:OE1	10:K:77:GLN:N	2.37	0.57
37:n:34:LYS:HZ1	54:n:102:CDL:CB2	2.17	0.57
3:C:73:ALA:O	3:C:76:MET:HB3	2.05	0.57
2:B:93:LEU:O	8:I:34:ARG:NH2	2.38	0.57
8:I:44:GLY:CA	16:Q:359:ASP:OD2	2.52	0.57
16:Q:82:LEU:HD12	16:Q:101:LEU:HD11	1.86	0.57
16:Q:144:MET:HE3	16:Q:222:MET:O	2.05	0.57
34:k:26:LEU:HD22	34:k:78:LEU:HD13	1.87	0.57
35:l:496:MET:HA	35:l:499:MET:HE2	1.86	0.57
8:I:40:LYS:HB3	21:W:7:LYS:H	1.70	0.56
9:J:304:LEU:O	9:J:307:VAL:CG2	2.43	0.56
15:P:201:ASP:OD1	15:P:201:ASP:N	2.37	0.56
18:T:34:THR:HG1	18:T:47:ASP:CG	2.12	0.56
40:r:306:PRO:O	40:r:310:MET:HG3	2.05	0.56
3:C:50:LEU:HD12	48:C:311:PEE:H25	1.75	0.56
48:C:311:PEE:H64	49:C:312:PLX:H191	1.88	0.56
9:J:85:ARG:HD3	51:J:401:NDP:C2A	2.34	0.56
12:M:68:ARG:NH1	12:M:284:GLU:OE1	2.39	0.56
27:d:114:GLN:HG2	35:l:203:MET:HE2	1.82	0.56
48:l:718:PEE:C25	48:l:718:PEE:H34	2.35	0.56
44:w:59:VAL:HG13	44:w:201:PRO:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:139:ARG:NH1	44:w:166:ASP:OD2	2.39	0.56
7:H:44:TYR:HB2	15:P:68:ILE:HG23	1.87	0.56
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.87	0.56
25:b:5:THR:OG1	25:b:7:ASP:OD1	2.17	0.56
36:m:27:ILE:HD13	41:s:121:TRP:CZ3	2.40	0.56
6:X:83:VAL:HG13	6:X:122:MET:HE1	1.87	0.56
26:c:155:PRO:HG3	43:v:4:HIS:CD2	2.41	0.56
34:k:17:ALA:O	34:k:21:MET:HG3	2.05	0.56
44:w:47:GLU:OE2	44:w:52:LYS:NZ	2.34	0.56
6:G:84:LEU:O	6:G:88:LYS:HG2	2.04	0.56
8:I:24:LEU:HD23	8:I:28:TYR:CE2	2.32	0.56
39:p:16:VAL:HG12	39:p:64:LEU:CD2	2.33	0.56
41:s:220:PHE:CE2	56:s:403:UQ:HM52	2.41	0.56
6:G:115:GLN:O	6:G:119:ILE:HG12	2.05	0.56
12:M:307:ILE:HG22	12:M:582:VAL:HG22	1.87	0.56
24:a:152:LYS:HD3	30:g:96:VAL:HG21	1.87	0.56
25:b:104:ILE:HB	43:v:48:ASP:HB3	1.86	0.56
40:r:59:ASP:OD1	40:r:60:SER:N	2.39	0.56
44:w:268:LYS:NZ	44:w:272:ASP:OD2	2.35	0.56
6:G:105:MET:SD	6:G:139:MET:SD	3.03	0.56
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.38	0.56
15:P:44:ARG:HB3	15:P:45:PRO:CD	2.36	0.56
22:Y:72:ARG:NH1	22:Y:76:ASP:OD2	2.39	0.56
27:d:71:VAL:HG11	27:d:87:GLU:HB3	1.86	0.56
54:l:712:CDL:H742	54:l:712:CDL:H312	1.88	0.56
16:Q:68:ASP:O	32:i:49:ASN:ND2	2.38	0.56
35:l:366:MET:HB2	35:l:445:GLU:OE1	2.06	0.56
38:o:53:ASP:OD1	38:o:54:PRO:HD2	2.05	0.56
40:r:334:TYR:CD1	40:r:340:ARG:HB2	2.41	0.56
1:A:38:GLU:CB	14:O:239:LYS:HZ3	2.18	0.56
7:H:108:PRO:HG2	15:P:124:ASN:ND2	2.21	0.56
15:P:101:ARG:HE	15:P:159:VAL:HG13	1.70	0.56
32:i:71:MET:HE3	34:k:63:LEU:HD13	1.87	0.56
35:l:221:ALA:HA	35:l:226:GLN:HG2	1.88	0.56
35:l:258:PHE:O	35:l:262:ARG:HG2	2.06	0.56
43:v:51:LEU:O	43:v:52:MET:HG3	2.05	0.56
48:C:311:PEE:C45	56:s:403:UQ:H203	2.36	0.55
15:P:43:THR:HA	15:P:47:ILE:HD12	1.88	0.55
20:V:88:LEU:HD12	49:V:205:PLX:H24	1.86	0.55
19:U:24:ALA:HB2	48:U:101:PEE:H72	1.88	0.55
25:b:16:ARG:HG2	25:b:20:ARG:NH1	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:g:85:TYR:CZ	42:u:165:SER:HB2	2.41	0.55
35:l:559:GLU:OE2	40:r:214:LEU:HD13	2.05	0.55
39:p:19:LEU:CD2	39:p:64:LEU:HD13	1.76	0.55
7:H:72:LEU:HD13	7:H:80:VAL:HG11	1.89	0.55
14:O:134:VAL:HG22	14:O:186:VAL:CG1	2.37	0.55
27:d:33:LEU:HD12	27:d:36:ILE:HD11	1.89	0.55
35:l:562:LEU:CG	48:l:718:PEE:C20	2.85	0.55
40:r:196:TRP:CD2	40:r:257:MET:HG2	2.41	0.55
12:M:428:LYS:HE3	12:M:465:ILE:HD13	1.89	0.55
35:l:102:GLU:HG2	35:l:453:SER:HB3	1.88	0.55
6:X:118:ILE:O	6:X:122:MET:HG2	2.07	0.55
22:Y:99:ILE:HD11	43:v:107:ARG:HG3	1.89	0.55
35:l:375:ILE:HD12	35:l:458:LEU:HD11	1.87	0.55
1:A:125:CYS:H	1:A:277:ASN:HD22	1.54	0.55
9:J:220:MET:O	9:J:221:ARG:C	2.50	0.55
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.27	0.55
54:l:712:CDL:H652	54:l:712:CDL:C86	2.28	0.55
2:B:76:TYR:OH	41:s:33:LEU:HB2	2.07	0.55
16:Q:259:GLU:OE1	16:Q:338:ARG:NH2	2.34	0.55
17:S:55:SER:HA	17:S:64:LYS:HE2	1.87	0.55
24:a:106:VAL:HG13	37:n:50:ARG:HH21	1.72	0.55
31:h:38:LYS:HE2	31:h:42:GLU:OE2	2.07	0.55
35:l:391:SER:O	35:l:395:ILE:HG12	2.06	0.55
44:w:209:VAL:HG12	44:w:260:ALA:HB2	1.88	0.55
26:c:40:PRO:O	26:c:74:ASP:HB2	2.06	0.55
32:i:95:MET:HE2	32:i:149:ILE:HG22	1.88	0.55
35:l:72:GLN:NE2	40:r:459:TYR:O	2.39	0.55
44:w:72:ARG:NH2	44:w:264:GLU:HA	2.21	0.55
9:J:306:GLU:HG2	9:J:315:THR:HG22	1.89	0.55
11:L:156:LYS:HD2	12:M:67:GLU:HB3	1.87	0.55
14:O:140:CYS:SG	14:O:183:ALA:HB2	2.45	0.55
33:j:17:LEU:HA	33:j:20:ILE:HG12	1.89	0.55
48:C:311:PEE:H69	49:C:312:PLX:C19	2.36	0.54
8:I:70:MET:HE2	15:P:66:ALA:HB1	1.88	0.54
9:J:228:LEU:HD22	9:J:273:LEU:HD21	1.89	0.54
24:a:140:LEU:HD21	40:r:177:LEU:HB3	1.89	0.54
1:A:141:GLY:CA	1:A:252:PRO:HG3	2.34	0.54
10:K:75:ASN:ND2	10:K:78:HIS:CE1	2.75	0.54
10:K:76:LEU:O	10:K:77:GLN:C	2.47	0.54
12:M:518:ARG:HH12	12:M:687:PRO:HG3	1.73	0.54
14:O:198:PRO:O	14:O:201:ILE:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:214:LEU:O	40:r:217:PRO:HD2	2.07	0.54
4:E:59:GLY:O	4:E:63:VAL:HG23	2.08	0.54
9:J:227:PRO:HB3	9:J:291:TYR:CE1	2.42	0.54
22:Y:74:TRP:HB2	23:Z:78:PHE:HZ	1.72	0.54
35:l:16:THR:CG2	54:l:712:CDL:H841	2.37	0.54
49:n:101:PLX:H102	40:r:40:SER:HB3	1.89	0.54
41:s:25:ARG:HG3	56:s:403:UQ:HM21	1.85	0.54
48:C:311:PEE:C12	33:j:27:LEU:HD13	2.36	0.54
54:l:712:CDL:H621	54:l:712:CDL:H432	1.90	0.54
49:n:101:PLX:C28	49:n:101:PLX:C32	2.86	0.54
6:X:93:ILE:HD13	6:X:108:LEU:HD13	1.88	0.54
54:a:201:CDL:H521	48:l:720:PEE:H14	1.85	0.54
35:l:562:LEU:HB3	35:l:563:PRO:HD3	1.90	0.54
39:p:16:VAL:HA	39:p:64:LEU:HD22	1.88	0.54
35:l:123:LEU:CD1	54:l:712:CDL:OA7	2.55	0.54
35:l:245:ALA:O	35:l:249:SER:OG	2.26	0.54
48:m:202:PEE:C1	48:m:202:PEE:C4	2.86	0.54
12:M:252:ASP:OD2	12:M:290:THR:OG1	2.24	0.54
16:Q:184:ILE:HG12	16:Q:203:MET:HE3	1.90	0.54
32:i:280:THR:O	32:i:284:MET:HG2	2.08	0.54
9:J:293:LEU:HD23	9:J:298:TYR:HD1	1.71	0.54
13:N:4:VAL:O	13:N:8:ARG:HG2	2.08	0.54
16:Q:100:GLU:O	16:Q:100:GLU:HG3	2.08	0.54
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.89	0.54
36:m:25:SER:O	36:m:28:TYR:N	2.40	0.54
40:r:97:THR:HG21	54:r:714:CDL:H242	1.90	0.54
1:A:185:ASN:OD1	1:A:190:GLY:N	2.33	0.54
20:V:138:GLU:OE1	20:V:139:PRO:HD2	2.07	0.54
27:d:102:ILE:HD11	28:e:125:LEU:HD22	1.89	0.54
32:i:256:PRO:HB2	54:n:102:CDL:H612	1.90	0.54
9:J:208:GLY:N	9:J:211:ASP:CG	2.54	0.54
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.90	0.54
29:f:72:ARG:HH12	30:g:19:GLU:HA	1.73	0.54
33:j:15:SER:HA	41:s:76:ILE:HD12	1.88	0.54
35:l:272:LEU:O	35:l:276:MET:HG3	2.07	0.54
40:r:115:LEU:HD12	40:r:174:LEU:HD22	1.90	0.54
9:J:206:ILE:N	51:J:401:NDP:N7N	2.53	0.53
13:N:68:MET:HG2	13:N:69:ASN:H	1.72	0.53
14:O:60:TYR:O	14:O:64:GLU:HG2	2.08	0.53
14:O:201:ILE:O	14:O:205:ILE:HG12	2.08	0.53
54:a:201:CDL:HA61	54:a:201:CDL:OA7	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:559:GLU:O	35:l:563:PRO:HD2	2.08	0.53
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.90	0.53
24:a:139:ILE:HG23	40:r:54:LEU:HD23	1.90	0.53
27:d:160:LYS:NZ	30:g:114:ILE:O	2.39	0.53
35:l:227:PHE:O	35:l:230:HIS:ND1	2.40	0.53
44:w:73:LEU:HD12	44:w:73:LEU:O	2.07	0.53
28:e:65:ASN:ND2	40:r:427:LYS:HE2	2.23	0.53
35:l:511:LEU:HD12	39:p:39:TYR:HD2	1.73	0.53
40:r:346:ARG:O	40:r:419:TYR:HA	2.08	0.53
1:A:420:GLU:HG3	1:A:429:ASP:OD1	2.08	0.53
16:Q:82:LEU:HD12	16:Q:101:LEU:CD1	2.38	0.53
54:a:201:CDL:H541	48:l:720:PEE:C12	2.38	0.53
54:i:401:CDL:OA7	54:i:401:CDL:HA62	2.07	0.53
41:s:25:ARG:HH21	56:s:403:UQ:HM21	1.67	0.53
8:I:3:SER:O	54:N:202:CDL:H1	2.09	0.53
9:J:298:TYR:CD2	9:J:319:VAL:HB	2.44	0.53
16:Q:332:CYS:O	16:Q:336:GLU:HG3	2.08	0.53
20:V:70:PHE:HD1	20:V:94:GLY:HA2	1.74	0.53
28:e:92:PHE:O	28:e:96:SER:HB2	2.07	0.53
32:i:236:LYS:HB2	32:i:311:MET:HE2	1.90	0.53
35:l:37:LYS:HD3	35:l:98:TRP:HE1	1.73	0.53
1:A:116:ASN:ND2	1:A:207:GLY:O	2.41	0.53
8:I:2:ALA:HB2	8:I:24:LEU:HD21	1.90	0.53
20:V:138:GLU:OE1	20:V:139:PRO:CD	2.57	0.53
21:W:85:GLN:NE2	21:W:89:GLU:OE2	2.37	0.53
14:O:177:LEU:HD12	14:O:185:MET:HE1	1.91	0.53
15:P:69:LEU:HD22	15:P:96:VAL:HG22	1.91	0.53
39:p:120:ALA:O	39:p:124:GLN:HG3	2.09	0.53
40:r:14:MET:SD	40:r:26:ASN:HB3	2.48	0.53
44:w:66:ILE:HD12	44:w:234:LEU:CD2	2.39	0.53
1:A:263:ALA:HA	1:A:271:SER:HB2	1.91	0.53
33:j:79:SER:HA	33:j:87:MET:HE3	1.89	0.53
35:l:144:TRP:CE2	35:l:223:LYS:HG3	2.44	0.53
48:l:718:PEE:H34	48:l:718:PEE:H41	1.91	0.53
44:w:235:GLN:O	44:w:239:ASN:HB2	2.08	0.53
9:J:85:ARG:NH1	51:J:401:NDP:O2X	2.32	0.53
44:w:60:ILE:HG12	44:w:203:VAL:HB	1.91	0.53
2:B:47:SER:OG	2:B:49:ASP:OD1	2.23	0.52
4:E:28:ALA:O	4:E:32:VAL:HG23	2.09	0.52
8:I:24:LEU:CD2	8:I:28:TYR:HE2	2.18	0.52
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:84:GLN:O	26:c:98:ARG:NH1	2.42	0.52
1:A:177:TYR:HB3	10:K:96:PHE:HD2	1.72	0.52
12:M:405:THR:HG23	12:M:477:GLY:CA	2.32	0.52
54:a:201:CDL:H432	27:d:44:PRO:HB3	1.92	0.52
6:G:74:LEU:HD23	6:G:74:LEU:H	1.75	0.52
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.91	0.52
16:Q:39:PRO:HD2	32:i:304:MET:O	2.09	0.52
20:V:141:VAL:O	20:V:141:VAL:HG22	2.08	0.52
26:c:185:GLU:OE1	43:v:37:ARG:HG2	2.09	0.52
35:l:452:ASN:HA	35:l:455:LYS:HG2	1.92	0.52
3:C:92:VAL:CG2	56:s:403:UQ:CM3	2.74	0.52
4:E:66:MET:HA	4:E:69:LYS:HD3	1.91	0.52
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.91	0.52
14:O:110:MET:O	14:O:114:GLU:HG3	2.09	0.52
4:E:101:THR:OG1	15:P:219:VAL:O	2.23	0.52
54:a:201:CDL:C53	48:l:720:PEE:H56	2.40	0.52
32:i:84:TRP:HH2	34:k:59:MET:HE2	1.75	0.52
32:i:334:THR:HG21	54:r:714:CDL:H391	1.91	0.52
35:l:530:PRO:HA	35:l:534:HIS:HD2	1.74	0.52
11:L:109:ASN:ND2	11:L:111:LEU:O	2.43	0.52
13:N:6:VAL:HG12	13:N:9:ARG:NH2	2.24	0.52
16:Q:248:SER:OG	21:W:19:ILE:HD13	2.09	0.52
35:l:119:LYS:NZ	54:l:712:CDL:OA3	2.43	0.52
35:l:258:PHE:CE2	35:l:262:ARG:HD3	2.45	0.52
54:l:712:CDL:H452	40:r:445:LEU:HB3	1.91	0.52
41:s:52:ALA:HB1	56:s:403:UQ:H162	1.90	0.52
1:A:244:ASN:HB2	46:A:502:FMN:O1P	2.09	0.52
6:G:110:LEU:HD23	6:G:114:ASP:HB3	1.92	0.52
22:Y:97:LEU:HD12	43:v:104:ARG:HB2	1.91	0.52
1:A:388:GLY:HA3	1:A:419:ILE:HD11	1.92	0.52
2:B:163:PRO:O	16:Q:372:LYS:HE2	2.09	0.52
6:G:144:ILE:O	6:G:148:ILE:HG12	2.10	0.52
35:l:8:THR:HG23	35:l:82:MET:HE3	1.91	0.52
40:r:115:LEU:CD2	40:r:176:PHE:CZ	2.93	0.52
19:U:38:TYR:HB2	41:s:310:MET:O	2.09	0.51
27:d:37:PHE:CE2	35:l:3:PRO:HB3	2.45	0.51
35:l:144:TRP:CZ2	35:l:223:LYS:HG3	2.45	0.51
39:p:19:LEU:CB	39:p:64:LEU:HD11	2.40	0.51
39:p:100:PRO:HG3	40:r:419:TYR:CZ	2.44	0.51
40:r:114:GLU:OE1	40:r:116:ILE:N	2.43	0.51
40:r:204:MET:HE3	40:r:261:PHE:CD1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:C:311:PEE:H16	33:j:27:LEU:CD1	2.38	0.51
9:J:293:LEU:HD23	9:J:298:TYR:CD1	2.44	0.51
10:K:76:LEU:O	10:K:79:HIS:CD2	2.64	0.51
12:M:197:THR:HG21	12:M:204:MET:HE3	1.91	0.51
12:M:690:THR:HG21	12:M:692:LYS:HE3	1.91	0.51
32:i:128:LEU:HD12	32:i:216:PHE:HB3	1.93	0.51
35:l:526:LEU:HD12	35:l:530:PRO:HG2	1.93	0.51
1:A:375:LYS:HD3	1:A:376:HIS:CD2	2.45	0.51
12:M:171:THR:HG23	12:M:173:MET:SD	2.50	0.51
41:s:52:ALA:HB1	56:s:403:UQ:C13	2.31	0.51
44:w:66:ILE:HD12	44:w:234:LEU:HD23	1.92	0.51
3:C:125:PRO:HB2	41:s:58:LYS:HE3	1.93	0.51
35:l:81:LYS:HD3	35:l:262:ARG:HH22	1.75	0.51
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.43	0.51
44:w:170:LEU:HD22	44:w:187:TYR:CD1	2.46	0.51
3:C:71:CYS:HB3	16:Q:141:TYR:CG	2.45	0.51
7:H:51:ILE:HD11	8:I:94:ALA:HB3	1.92	0.51
10:K:109:ARG:NH2	14:O:106:GLN:O	2.34	0.51
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	1.91	0.51
23:Z:57:PHE:O	35:l:434:LYS:NZ	2.33	0.51
4:E:42:GLU:OE1	4:E:42:GLU:HA	2.09	0.51
4:E:70:ASN:O	50:G:201:8Q1:O40	2.28	0.51
19:U:14:ALA:O	19:U:15:LYS:HG2	2.11	0.51
35:l:9:LEU:HD11	35:l:63:ILE:HG21	1.92	0.51
40:r:433:GLU:O	40:r:437:MET:HG2	2.11	0.51
6:G:103:HIS:CD2	6:G:106:LYS:HG2	2.41	0.51
16:Q:249:LYS:HA	21:W:19:ILE:HG23	1.93	0.51
16:Q:315:GLU:O	16:Q:346:GLN:NE2	2.35	0.51
20:V:141:VAL:HG21	24:a:157:ARG:HB3	1.79	0.51
24:a:87:THR:HG22	54:a:201:CDL:H121	1.93	0.51
36:m:17:PHE:HA	36:m:20:PHE:CE1	2.46	0.51
41:s:14:LEU:O	41:s:17:VAL:CG2	2.57	0.51
7:H:76:GLN:O	7:H:79:GLU:HG2	2.11	0.51
9:J:236:VAL:HG12	9:J:272:LEU:HD23	1.93	0.51
12:M:160:VAL:H	12:M:174:THR:HG22	1.76	0.51
12:M:407:PRO:HD2	12:M:438:LEU:HD21	1.92	0.51
20:V:12:ILE:HB	20:V:21:LYS:HD3	1.92	0.51
25:b:32:GLU:HG3	39:p:115:TYR:HA	1.92	0.51
35:l:16:THR:CG2	54:l:712:CDL:H861	2.41	0.51
48:l:718:PEE:C22	48:l:718:PEE:C18	2.85	0.51
13:N:10:GLY:O	13:N:14:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:U:101:PEE:H2O	33:j:106:TRP:CE3	2.46	0.51
33:j:4:MET:SD	48:m:202:PEE:C15	2.91	0.51
33:j:5:LEU:HD23	41:s:2:PHE:HD2	1.76	0.51
36:m:9:LEU:HB3	36:m:43:ILE:HG12	1.93	0.51
54:n:102:CDL:H121	54:n:102:CDL:H762	1.92	0.51
39:p:100:PRO:HG3	40:r:419:TYR:CE1	2.46	0.51
40:r:207:MET:N	40:r:208:PRO:HA	2.26	0.51
40:r:255:ASN:OD1	40:r:255:ASN:N	2.43	0.51
48:C:311:PEE:H27	48:C:311:PEE:C34	2.41	0.50
12:M:278:HIS:CE1	12:M:280:ASP:HB2	2.46	0.50
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.45	0.50
26:c:38:PRO:HG2	38:o:71:ALA:HB2	1.92	0.50
36:m:57:PHE:CE1	41:s:111:LEU:HD11	2.46	0.50
38:o:23:TYR:CE2	39:p:65:ARG:HG3	2.45	0.50
1:A:270:ASN:ND2	1:A:340:ASP:OD2	2.37	0.50
9:J:227:PRO:HB2	9:J:298:TYR:HE1	1.77	0.50
10:K:76:LEU:N	10:K:76:LEU:HD13	2.26	0.50
14:O:134:VAL:HG22	14:O:186:VAL:HG12	1.92	0.50
26:c:70:MET:SD	38:o:86:THR:HG22	2.51	0.50
35:l:381:THR:HG21	35:l:498:PHE:CZ	2.46	0.50
14:O:207:GLU:HB3	14:O:212:LYS:HE3	1.92	0.50
19:U:78:LEU:HD12	42:u:123:GLY:HA3	1.93	0.50
6:X:82:ARG:HD2	6:X:126:PHE:CE1	2.42	0.50
54:l:712:CDL:C71	54:l:712:CDL:C75	2.87	0.50
1:A:288:VAL:HG21	1:A:303:HIS:CD2	2.47	0.50
1:A:311:TRP:NE1	1:A:333:GLU:OE2	2.31	0.50
46:A:502:FMN:O4'	46:A:502:FMN:O2'	2.27	0.50
5:F:37:ILE:HA	5:F:41:TYR:HB2	1.92	0.50
9:J:72:HIS:NE2	15:P:215:GLU:OE1	2.45	0.50
27:d:5:TRP:CZ3	27:d:10:TYR:HB2	2.46	0.50
27:d:147:GLY:HA2	38:o:129:TYR:CE2	2.47	0.50
30:g:4:MET:O	30:g:10:ARG:NH1	2.44	0.50
32:i:268:GLN:NE2	32:i:272:LYS:HE3	2.27	0.50
35:l:20:MET:HG2	54:l:712:CDL:H832	1.94	0.50
48:l:718:PEE:H10	48:l:718:PEE:H2	1.93	0.50
43:v:63:LEU:HD13	43:v:87:TRP:CE2	2.47	0.50
13:N:6:VAL:HB	54:N:202:CDL:OB7	2.12	0.50
13:N:97:PRO:HG2	13:N:100:THR:HG23	1.93	0.50
14:O:182:ASN:HB2	14:O:194:GLU:HG2	1.93	0.50
14:O:195:ASP:OD2	14:O:222:ARG:HD3	2.11	0.50
26:c:122:THR:OG1	26:c:124:VAL:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:211:MET:HG2	32:i:333:SER:HB2	1.94	0.50
44:w:258:TYR:CE2	44:w:269:VAL:HG22	2.45	0.50
7:H:108:PRO:HG2	15:P:124:ASN:HD22	1.76	0.50
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.92	0.50
48:V:202:PEE:H30	48:V:202:PEE:C15	2.32	0.50
48:l:718:PEE:H10	48:l:718:PEE:C1	2.42	0.50
38:o:57:LEU:O	38:o:57:LEU:HD23	2.11	0.50
38:o:127:ILE:O	38:o:127:ILE:HG22	2.10	0.50
43:v:46:MET:HE2	43:v:56:ARG:HG2	1.94	0.50
9:J:238:GLN:CG	9:J:270:ARG:HG2	2.42	0.50
25:b:29:SER:OG	25:b:32:GLU:OE1	2.28	0.50
32:i:325:LEU:CD1	54:i:401:CDL:H121	2.36	0.50
41:s:306:SER:O	41:s:310:MET:HG3	2.11	0.50
1:A:319:PRO:HG2	1:A:347:THR:HG21	1.94	0.50
28:e:66:LEU:HB3	28:e:73:SER:OG	2.12	0.50
31:h:18:MET:HE3	34:k:56:ALA:HA	1.94	0.50
40:r:87:GLU:OE2	40:r:91:ARG:HD2	2.11	0.50
40:r:168:GLN:OE1	42:u:168:PHE:CE1	2.65	0.50
41:s:7:LEU:HA	41:s:10:ILE:HG22	1.94	0.50
9:J:298:TYR:HD2	9:J:319:VAL:HB	1.75	0.50
11:L:124:LEU:HD21	15:P:201:ASP:O	2.12	0.50
12:M:624:ARG:NH2	12:M:637:ASP:OD1	2.37	0.50
14:O:148:ILE:CD1	14:O:184:PRO:CG	2.90	0.50
26:c:57:MET:HE2	26:c:104:PRO:HG3	1.94	0.50
40:r:12:LEU:HB2	40:r:13:PRO:HD3	1.94	0.50
8:I:39:PRO:HB2	8:I:41:LEU:HD13	1.94	0.49
48:V:202:PEE:O4	40:r:195:MET:HG3	2.11	0.49
35:l:83:ASP:CG	35:l:262:ARG:HH12	2.20	0.49
44:w:54:THR:O	44:w:55:GLU:HG3	2.12	0.49
4:E:103:ILE:HG22	4:E:104:MET:HE2	1.94	0.49
5:F:33:VAL:O	5:F:36:PHE:HB3	2.12	0.49
21:W:70:ALA:HB2	42:u:125:LEU:HD13	1.94	0.49
40:r:122:PHE:HE1	40:r:238:LEU:HB3	1.77	0.49
1:A:88:ARG:HD2	1:A:274:LYS:CD	2.42	0.49
9:J:207:PHE:HB2	9:J:211:ASP:OD2	2.12	0.49
9:J:303:ARG:HD3	9:J:303:ARG:C	2.37	0.49
28:e:129:ARG:NH1	28:e:136:LEU:O	2.40	0.49
32:i:323:MET:HE2	54:i:401:CDL:HA32	1.93	0.49
35:l:292:ALA:HB2	35:l:304:PHE:HB3	1.94	0.49
35:l:427:ILE:O	35:l:431:PHE:HB2	2.12	0.49
11:L:174:THR:HG23	14:O:111:ARG:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:456:ALA:O	12:M:499:ASN:ND2	2.46	0.49
15:P:87:PHE:CE1	15:P:144:LYS:HD2	2.47	0.49
23:Z:53:TYR:CE2	35:l:434:LYS:HG3	2.48	0.49
2:B:192:ASN:ND2	18:T:61:GLU:OE2	2.35	0.49
6:G:74:LEU:H	6:G:74:LEU:CD2	2.25	0.49
23:Z:79:VAL:HA	23:Z:82:VAL:HG12	1.95	0.49
35:l:557:TRP:O	35:l:561:ILE:HG12	2.13	0.49
48:l:719:PEE:C11	48:l:719:PEE:H7	2.43	0.49
36:m:57:PHE:HE1	41:s:111:LEU:HD11	1.77	0.49
39:p:12:HIS:HE1	39:p:60:ALA:O	1.95	0.49
1:A:66:LYS:CE	1:A:188:GLY:O	2.40	0.49
2:B:110:GLU:HG3	18:T:67:ALA:HB1	1.94	0.49
5:F:53:ILE:C	12:M:380:ASP:OD1	2.56	0.49
24:a:136:THR:HG21	40:r:48:ASN:HD22	1.77	0.49
39:p:19:LEU:HB2	39:p:64:LEU:HD11	1.94	0.49
1:A:185:ASN:O	1:A:187:CYS:N	2.46	0.49
14:O:140:CYS:SG	14:O:183:ALA:CB	3.01	0.49
16:Q:259:GLU:O	16:Q:263:THR:HG22	2.12	0.49
19:U:67:PRO:HA	19:U:74:GLN:HE21	1.77	0.49
6:X:111:ASP:OD2	39:p:52:LYS:HE3	2.11	0.49
6:X:113:LEU:O	6:X:117:GLU:HG3	2.13	0.49
22:Y:45:ARG:HG2	35:l:439:PRO:HB3	1.95	0.49
26:c:73:GLY:HA3	38:o:79:ASN:ND2	2.27	0.49
31:h:50:ILE:HG22	31:h:54:LYS:NZ	2.27	0.49
32:i:1:MET:HE3	32:i:46:LYS:HG2	1.94	0.49
32:i:20:VAL:HG11	32:i:137:ALA:HB1	1.95	0.49
32:i:271:THR:HG21	40:r:165:VAL:HG23	1.95	0.49
9:J:168:SER:O	9:J:202:LYS:HA	2.13	0.49
12:M:34:VAL:HG23	12:M:41:VAL:CG1	2.43	0.49
12:M:638:THR:O	12:M:642:VAL:HG23	2.13	0.49
16:Q:196:ALA:O	16:Q:197:MET:HG2	2.12	0.49
20:V:121:THR:O	20:V:125:VAL:HG23	2.12	0.49
26:c:58:ARG:HD2	38:o:35:GLU:HG3	1.92	0.49
35:l:72:GLN:NE2	35:l:72:GLN:N	2.60	0.49
48:l:719:PEE:H7	48:l:719:PEE:H14	1.94	0.49
44:w:88:GLU:OE2	44:w:161:ARG:NH1	2.46	0.49
44:w:146:ALA:HB1	44:w:157:VAL:HG21	1.94	0.49
1:A:125:CYS:O	1:A:129:GLU:HG2	2.12	0.49
2:B:74:LEU:HB2	41:s:272:TRP:CZ2	2.47	0.49
7:H:58:MET:HE2	7:H:71:GLN:HB3	1.94	0.49
21:W:144:THR:CB	41:s:96:ILE:HG23	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:79:ILE:O	6:X:83:VAL:HG23	2.13	0.49
23:Z:49:GLU:OE2	39:p:34:ARG:NH2	2.39	0.49
54:a:201:CDL:HB61	54:a:201:CDL:OB7	2.13	0.49
35:l:107:TYR:CD2	35:l:108:MET:HE3	2.46	0.49
42:u:80:GLU:HB2	42:u:81:PRO:HD3	1.95	0.49
4:E:27:GLU:HA	4:E:30:ARG:HG2	1.94	0.49
26:c:48:ARG:NH2	26:c:63:GLU:OE2	2.46	0.49
31:h:97:HIS:HA	31:h:102:GLU:HB3	1.95	0.49
32:i:112:HIS:HB2	32:i:184:ILE:HD13	1.95	0.49
32:i:283:ALA:HB1	40:r:158:LEU:HD13	1.94	0.49
44:w:129:TYR:CD1	44:w:183:CYS:HB3	2.48	0.49
1:A:413:TRP:O	1:A:416:SER:OG	2.25	0.48
9:J:207:PHE:HB2	9:J:214:LEU:HG	1.95	0.48
27:d:132:PHE:HA	27:d:135:VAL:HG12	1.95	0.48
33:j:3:ILE:HG21	48:m:202:PEE:H15	1.95	0.48
39:p:98:LYS:O	40:r:419:TYR:HE2	1.95	0.48
42:u:83:THR:HA	42:u:86:TRP:CD1	2.47	0.48
1:A:375:LYS:NZ	14:O:33:GLY:O	2.45	0.48
2:B:171:PRO:HB3	13:N:93:MET:HE1	1.95	0.48
9:J:313:TRP:CD1	9:J:313:TRP:H	2.31	0.48
25:b:11:ARG:HB2	39:p:156:PRO:HB3	1.95	0.48
31:h:2:PRO:HD2	49:i:705:PLX:H1C2	1.94	0.48
44:w:169:PHE:CD2	57:w:401:ADP:C6	3.01	0.48
4:E:16:SER:HA	11:L:54:ALA:HA	1.94	0.48
6:G:149:ALA:O	6:G:153:ASP:N	2.45	0.48
15:P:147:THR:HB	15:P:153:ILE:HD11	1.94	0.48
48:V:202:PEE:H36	48:V:202:PEE:C46	2.30	0.48
49:e:201:PLX:H382	40:r:67:VAL:HG12	1.95	0.48
40:r:115:LEU:CD2	40:r:176:PHE:CE1	2.93	0.48
12:M:650:SER:OG	12:M:652:ASN:OD1	2.31	0.48
16:Q:100:GLU:HG3	16:Q:107:ARG:HB2	1.94	0.48
24:a:136:THR:HG21	40:r:48:ASN:ND2	2.29	0.48
54:a:201:CDL:H541	48:l:720:PEE:H16	1.96	0.48
38:o:118:GLU:N	38:o:118:GLU:OE2	2.47	0.48
56:s:403:UQ:HM22	56:s:403:UQ:O3	2.12	0.48
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.49	0.48
6:G:75:THR:OG1	6:G:156:GLU:OE1	2.27	0.48
9:J:163:LYS:NZ	9:J:253:ILE:O	2.41	0.48
12:M:637:ASP:N	12:M:641:GLN:OE1	2.39	0.48
15:P:164:ASN:OD1	15:P:181:HIS:HE1	1.96	0.48
34:k:57:ASN:HB3	36:m:143:ILE:HG13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:233:LEU:HB3	35:l:234:PRO:HD3	1.95	0.48
43:v:27:PRO:O	43:v:104:ARG:NH2	2.46	0.48
1:A:57:GLN:O	14:O:241:PRO:HG3	2.13	0.48
14:O:78:ALA:C	14:O:81:PRO:HD2	2.39	0.48
16:Q:446:ASP:OD1	41:s:281:ARG:NH1	2.47	0.48
30:g:66:TYR:OH	32:i:324:LYS:NZ	2.36	0.48
33:j:68:GLU:HG3	36:m:161:LEU:HD13	1.96	0.48
36:m:25:SER:O	36:m:27:ILE:N	2.47	0.48
44:w:208:ASP:N	44:w:258:TYR:O	2.42	0.48
6:X:75:THR:OG1	6:X:156:GLU:O	2.23	0.48
1:A:256:ARG:O	14:O:246:GLN:OE1	2.31	0.48
3:C:113:MET:HE2	16:Q:115:LEU:HB3	1.95	0.48
9:J:38:HIS:NE2	13:N:132:LYS:HD2	2.29	0.48
12:M:284:GLU:HG2	12:M:284:GLU:O	2.14	0.48
12:M:485:ASP:CG	12:M:680:LEU:HG	2.39	0.48
24:a:112:TYR:HD2	27:d:64:TYR:O	1.96	0.48
33:j:30:TYR:CE2	41:s:59:GLU:HB2	2.49	0.48
49:j:203:PLX:H322	49:j:203:PLX:H351	1.58	0.48
34:k:37:MET:HE1	34:k:64:LEU:HD12	1.96	0.48
35:l:226:GLN:HG3	35:l:314:MET:HE1	1.96	0.48
38:o:29:THR:O	38:o:33:GLN:HG3	2.14	0.48
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.49	0.48
5:F:55:ILE:HD13	12:M:381:LEU:HD23	1.95	0.48
16:Q:461:VAL:O	16:Q:463:ARG:NH1	2.47	0.48
40:r:14:MET:HE2	40:r:30:HIS:CD2	2.46	0.48
40:r:61:LEU:HB2	40:r:457:PRO:HD3	1.96	0.48
7:H:56:LEU:HA	7:H:59:VAL:HG12	1.95	0.48
12:M:221:ASN:OD1	12:M:285:TRP:HB3	2.14	0.48
12:M:382:ARG:HG2	12:M:386:LEU:HD11	1.95	0.48
12:M:483:ARG:HD3	12:M:489:ILE:HD11	1.95	0.48
6:X:150:ASP:OD1	25:b:16:ARG:HG3	2.14	0.48
40:r:303:ILE:HG22	40:r:305:THR:HG23	1.94	0.48
41:s:220:PHE:CZ	56:s:403:UQ:HM51	2.49	0.48
44:w:169:PHE:CD1	57:w:401:ADP:C6	3.01	0.48
48:C:311:PEE:C12	33:j:27:LEU:CD1	2.92	0.47
9:J:47:GLY:HA3	15:P:225:GLU:OE1	2.14	0.47
11:L:78:ARG:NH2	11:L:148:GLU:OE1	2.40	0.47
32:i:79:LEU:HB2	34:k:47:ILE:CD1	2.43	0.47
34:k:58:MET:HE2	36:m:146:LEU:HA	1.95	0.47
36:m:27:ILE:HD13	41:s:121:TRP:HZ3	1.79	0.47
44:w:129:TYR:OH	44:w:186:HIS:ND1	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:SER:HB3	8:I:15:ALA:HB3	1.96	0.47
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.49	0.47
9:J:84:TYR:CE1	9:J:105:PHE:HB3	2.49	0.47
18:T:46:ASP:OD1	18:T:49:ASP:CB	2.51	0.47
35:l:42:TYR:HA	35:l:45:THR:HG22	1.96	0.47
35:l:359:MET:O	35:l:436:ARG:NH2	2.47	0.47
40:r:116:ILE:HG12	40:r:174:LEU:HD12	1.91	0.47
1:A:262:PHE:CZ	1:A:272:GLY:HA3	2.49	0.47
2:B:110:GLU:OE2	2:B:135:ARG:NH2	2.44	0.47
7:H:81:ILE:O	7:H:85:GLU:HG3	2.14	0.47
9:J:220:MET:C	9:J:222:TRP:N	2.71	0.47
10:K:76:LEU:HA	10:K:79:HIS:HD2	1.80	0.47
19:U:24:ALA:CB	48:U:101:PEE:H72	2.44	0.47
24:a:120:TRP:O	24:a:124:THR:HG22	2.14	0.47
35:l:190:LEU:CD2	40:r:383:THR:HG21	2.29	0.47
48:l:718:PEE:H37	48:l:718:PEE:H60	1.95	0.47
12:M:34:VAL:CG2	12:M:41:VAL:HG13	2.44	0.47
12:M:133:GLN:O	12:M:137:CYS:HB2	2.15	0.47
13:N:73:THR:HG22	13:N:77:VAL:HG12	1.96	0.47
18:T:30:ARG:HG2	18:T:31:THR:H	1.78	0.47
19:U:24:ALA:HB2	48:U:101:PEE:C43	2.45	0.47
25:b:10:LEU:O	25:b:14:GLN:HG3	2.14	0.47
35:l:398:ALA:O	35:l:402:SER:OG	2.27	0.47
35:l:512:LYS:O	39:p:36:LYS:NZ	2.47	0.47
39:p:117:ASP:O	39:p:121:LYS:HG3	2.14	0.47
41:s:218:GLY:O	41:s:222:MET:HG2	2.15	0.47
43:v:103:GLU:O	43:v:107:ARG:HG2	2.15	0.47
44:w:110:GLY:HA2	44:w:134:TRP:CD2	2.50	0.47
44:w:265:ASP:OD1	44:w:265:ASP:N	2.43	0.47
1:A:35:LEU:HD23	1:A:40:ARG:NH1	2.29	0.47
1:A:63:TYR:CZ	1:A:64:LYS:HE3	2.49	0.47
1:A:256:ARG:O	14:O:245:VAL:HA	2.15	0.47
12:M:124:HIS:HD2	16:Q:375:MET:HE2	1.79	0.47
54:a:201:CDL:H221	54:a:201:CDL:H791	1.96	0.47
35:l:76:LEU:HD21	35:l:196:TRP:HE3	1.79	0.47
35:l:213:LEU:HB3	35:l:273:VAL:HG11	1.97	0.47
37:n:54:GLU:N	37:n:54:GLU:OE2	2.48	0.47
1:A:177:TYR:HB3	10:K:96:PHE:CD2	2.48	0.47
47:A:503:NAI:H6N	47:A:503:NAI:H2D	1.71	0.47
26:c:165:ASP:OD1	26:c:170:ARG:NH2	2.47	0.47
36:m:45:LEU:HD23	36:m:50:SER:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:THR:HG22	1:A:69:LEU:CD2	2.43	0.47
9:J:313:TRP:CD1	9:J:313:TRP:N	2.81	0.47
12:M:306:MET:HE1	13:N:139:PRO:HG3	1.97	0.47
12:M:696:MET:SD	12:M:702:ARG:HA	2.54	0.47
13:N:73:THR:HG22	13:N:73:THR:O	2.14	0.47
14:O:182:ASN:HB3	14:O:194:GLU:CG	2.44	0.47
14:O:242:GLY:HA2	14:O:245:VAL:HG23	1.96	0.47
34:k:34:GLU:HA	34:k:37:MET:HG3	1.95	0.47
35:l:511:LEU:HD12	39:p:39:TYR:CD2	2.50	0.47
37:n:13:VAL:HG11	40:r:14:MET:HG2	1.81	0.47
38:o:113:GLU:O	38:o:117:GLN:HG2	2.14	0.47
1:A:50:ASP:C	1:A:59:ARG:NH2	2.71	0.47
49:C:312:PLX:H311	49:C:312:PLX:H281	1.61	0.47
5:F:55:ILE:O	5:F:56:ARG:NH1	2.48	0.47
6:G:88:LYS:NZ	6:G:98:LEU:HD11	2.30	0.47
9:J:272:LEU:HB2	9:J:275:ASP:OD1	2.15	0.47
16:Q:144:MET:HE3	16:Q:222:MET:HB2	1.97	0.47
20:V:107:SER:HB3	20:V:110:ILE:HG22	1.97	0.47
6:X:90:TYR:HE1	23:Z:44:PRO:HB2	1.79	0.47
50:X:201:8Q1:C30	39:p:52:LYS:HG3	2.45	0.47
28:e:90:VAL:HG22	40:r:28:THR:HG21	1.97	0.47
32:i:186:HIS:O	32:i:190:MET:HG3	2.15	0.47
44:w:72:ARG:C	44:w:72:ARG:HD2	2.40	0.47
48:C:311:PEE:H77	56:s:403:UQ:H171	0.54	0.47
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.50	0.47
8:I:3:SER:O	54:N:202:CDL:C1	2.62	0.47
9:J:37:HIS:O	9:J:40:LEU:N	2.38	0.47
11:L:78:ARG:NH1	12:M:249:GLU:OE1	2.42	0.47
20:V:70:PHE:CD1	20:V:94:GLY:HA2	2.50	0.47
6:X:123:GLU:HG2	6:X:129:GLU:HA	1.96	0.47
44:w:72:ARG:HD2	44:w:72:ARG:O	2.15	0.47
1:A:185:ASN:C	1:A:187:CYS:H	2.23	0.47
1:A:279:SER:OG	1:A:280:GLY:N	2.46	0.47
13:N:85:GLU:HB2	13:N:98:PRO:HB3	1.96	0.47
16:Q:155:VAL:HB	16:Q:229:PRO:HB3	1.98	0.47
49:j:203:PLX:H312	49:j:203:PLX:H282	1.79	0.47
38:o:23:TYR:CG	39:p:65:ARG:HD2	2.37	0.47
40:r:106:LEU:HD13	40:r:234:VAL:HG11	1.97	0.47
40:r:121:LEU:O	40:r:125:THR:HG23	2.14	0.47
12:M:140:GLN:HG2	16:Q:379:ILE:HG23	1.97	0.46
12:M:337:ASP:O	12:M:542:PRO:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:187:GLN:HG3	14:O:192:TYR:CD1	2.50	0.46
26:c:125:SER:O	26:c:129:MET:HG3	2.14	0.46
27:d:75:THR:OG1	28:e:146:LYS:HE3	2.14	0.46
29:f:47:THR:HG23	30:g:65:LEU:HD22	1.96	0.46
29:f:68:GLU:OE2	29:f:72:ARG:HG3	2.15	0.46
34:k:78:LEU:HD11	34:k:88:ASP:HB2	1.97	0.46
35:l:286:LEU:HD21	54:l:713:CDL:H812	1.96	0.46
35:l:496:MET:HE1	54:l:713:CDL:H622	1.97	0.46
40:r:340:ARG:HD2	40:r:340:ARG:O	2.15	0.46
1:A:87:GLY:CA	46:A:502:FMN:O2P	2.62	0.46
1:A:244:ASN:N	46:A:502:FMN:O1P	2.38	0.46
3:C:126:GLU:HB2	41:s:59:GLU:OE1	2.15	0.46
50:X:201:8Q1:O27	50:X:201:8Q1:O33	2.32	0.46
25:b:14:GLN:O	25:b:17:GLU:HG3	2.15	0.46
30:g:34:VAL:HG12	54:n:102:CDL:H771	1.97	0.46
44:w:244:THR:O	44:w:248:GLU:HG2	2.15	0.46
4:E:47:VAL:HA	4:E:52:LEU:HD12	1.96	0.46
12:M:194:ASP:OD2	12:M:212:LYS:HE3	2.15	0.46
16:Q:97:LEU:CG	16:Q:99:MET:HE3	2.44	0.46
20:V:141:VAL:HG23	24:a:157:ARG:CB	2.35	0.46
23:Z:21:GLN:O	23:Z:23:LYS:NZ	2.48	0.46
26:c:82:SER:OG	26:c:83:GLN:N	2.48	0.46
30:g:31:PRO:HD2	42:u:172:MET:HE1	1.97	0.46
35:l:55:MET:HE1	35:l:472:ILE:HG22	1.98	0.46
35:l:529:TYR:HB3	35:l:530:PRO:HD3	1.98	0.46
35:l:556:ILE:HD13	38:o:80:PHE:CD1	2.50	0.46
39:p:26:HIS:CD2	39:p:79:PRO:HB3	2.50	0.46
1:A:48:ARG:NH1	14:O:231:LEU:HD11	2.31	0.46
26:c:69:GLY:O	38:o:80:PHE:HA	2.14	0.46
37:n:34:LYS:NZ	54:n:102:CDL:HB22	2.19	0.46
1:A:134:ASP:N	1:A:135:PRO:HD3	2.30	0.46
1:A:161:GLU:OE1	1:A:161:GLU:N	2.49	0.46
3:C:167:PRO:HB3	45:C:301:SF4:S4	2.55	0.46
12:M:197:THR:HG22	12:M:206:VAL:HG22	1.97	0.46
12:M:658:ASP:OD1	12:M:660:GLU:HG2	2.16	0.46
40:r:16:TRP:NE1	40:r:97:THR:OG1	2.49	0.46
41:s:89:LEU:HA	41:s:90:PRO:HD3	1.82	0.46
1:A:70:LEU:HD21	1:A:189:SER:HA	1.98	0.46
26:c:176:LYS:HA	26:c:176:LYS:HD2	1.77	0.46
49:e:201:PLX:H121	49:e:201:PLX:H152	1.47	0.46
31:h:3:PHE:HB2	32:i:144:GLN:CD	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:127:THR:HG22	35:l:147:VAL:HG13	1.98	0.46
35:l:228:GLY:HA3	48:l:719:PEE:H38	1.98	0.46
38:o:59:VAL:HG11	40:r:344:LEU:HD21	1.97	0.46
44:w:213:GLU:O	44:w:217:ARG:HG3	2.15	0.46
4:E:115:PRO:HB2	4:E:120:SER:OG	2.16	0.46
5:F:42:VAL:HG21	12:M:670:GLU:HG3	1.98	0.46
7:H:35:LEU:HD13	7:H:49:GLU:HG3	1.97	0.46
16:Q:188:THR:HB	16:Q:200:PHE:HA	1.98	0.46
22:Y:72:ARG:HB3	35:l:385:TYR:CD1	2.51	0.46
27:d:79:GLU:OE1	27:d:80:LYS:HG2	2.15	0.46
32:i:46:LYS:HE2	32:i:46:LYS:HB3	1.80	0.46
35:l:370:THR:HA	35:l:431:PHE:CZ	2.51	0.46
1:A:417:LYS:HE2	1:A:417:LYS:HA	1.98	0.46
9:J:208:GLY:O	9:J:211:ASP:OD1	2.34	0.46
9:J:303:ARG:HD3	9:J:303:ARG:O	2.16	0.46
14:O:164:THR:HG22	14:O:169:PHE:H	1.81	0.46
15:P:125:ARG:HD3	15:P:126:PHE:CZ	2.51	0.46
48:V:202:PEE:H78	40:r:201:MET:CE	2.42	0.46
24:a:93:ILE:O	27:d:61:TYR:HE1	1.99	0.46
35:l:16:THR:HG21	54:l:712:CDL:H841	1.97	0.46
54:n:102:CDL:H201	54:n:102:CDL:H171	1.71	0.46
10:K:107:SER:HB3	10:K:110:HIS:ND1	2.31	0.46
16:Q:80:LEU:HD23	16:Q:80:LEU:H	1.81	0.46
21:W:128:ARG:HB3	21:W:132:GLU:OE2	2.16	0.46
21:W:134:LEU:HD21	36:m:2:THR:N	2.29	0.46
23:Z:13:LYS:HD2	23:Z:13:LYS:HA	1.78	0.46
26:c:163:TYR:OH	43:v:41:ALA:O	2.32	0.46
27:d:147:GLY:HA2	38:o:129:TYR:HE2	1.80	0.46
32:i:236:LYS:HG2	32:i:237:MET:HG3	1.98	0.46
15:P:161:LYS:CD	16:Q:286:TYR:CZ	2.99	0.46
42:u:73:GLN:HG2	42:u:76:ARG:HH21	1.81	0.46
3:C:86:MET:HG3	3:C:87:ASP:N	2.30	0.45
12:M:335:GLY:H	12:M:361:VAL:HG12	1.81	0.45
54:N:202:CDL:H521	17:S:3:PHE:CD1	2.52	0.45
24:a:87:THR:HG22	54:a:201:CDL:C12	2.46	0.45
26:c:87:ASP:OD2	26:c:90:TYR:N	2.50	0.45
54:n:102:CDL:C82	54:r:714:CDL:C85	2.92	0.45
40:r:205:VAL:O	40:r:208:PRO:HB3	2.17	0.45
41:s:55:LEU:HD12	56:s:403:UQ:C8	2.46	0.45
44:w:125:ASP:OD1	44:w:125:ASP:N	2.50	0.45
1:A:420:GLU:OE2	1:A:433:TRP:NE1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:THR:OG1	16:Q:317:ASP:OD1	2.29	0.45
3:C:76:MET:HE3	3:C:86:MET:HE1	1.96	0.45
54:N:202:CDL:H742	54:N:202:CDL:H532	1.98	0.45
14:O:78:ALA:O	14:O:81:PRO:HD2	2.16	0.45
14:O:164:THR:CG2	14:O:169:PHE:H	2.29	0.45
15:P:161:LYS:HG3	16:Q:285:ASN:HD22	1.80	0.45
21:W:62:ILE:O	21:W:66:GLU:HG2	2.16	0.45
35:l:81:LYS:HD3	35:l:262:ARG:NH2	2.32	0.45
35:l:570:GLN:HB2	48:l:718:PEE:H50	1.98	0.45
41:s:52:ALA:HA	56:s:403:UQ:H13	1.95	0.45
44:w:233:TYR:CE2	44:w:237:ILE:HD11	2.52	0.45
9:J:37:HIS:CE1	18:T:49:ASP:HA	2.51	0.45
10:K:109:ARG:NH1	14:O:108:PRO:HD3	2.32	0.45
14:O:137:THR:HG22	14:O:138:THR:H	1.80	0.45
35:l:49:VAL:HB	35:l:50:PRO:HD3	1.97	0.45
54:l:713:CDL:H622	54:l:713:CDL:H591	1.56	0.45
3:C:126:GLU:O	3:C:128:ARG:N	2.49	0.45
11:L:88:GLN:NE2	12:M:141:ASP:OD2	2.45	0.45
12:M:29:SER:OG	12:M:30:ASN:OD1	2.33	0.45
12:M:299:ARG:HG2	12:M:300:GLN:HG2	1.98	0.45
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.47	0.45
18:T:69:ASP:O	18:T:73:GLU:HG3	2.16	0.45
20:V:141:VAL:HG21	24:a:157:ARG:HB2	1.97	0.45
40:r:44:GLN:HG3	40:r:60:SER:HB3	1.99	0.45
41:s:52:ALA:HA	56:s:403:UQ:H112	1.98	0.45
41:s:273:ILE:HD11	48:s:401:PEE:H65	1.98	0.45
56:s:403:UQ:H151	56:s:403:UQ:H18	1.97	0.45
56:s:403:UQ:HM53	56:s:403:UQ:H72	1.73	0.45
1:A:38:GLU:HB3	14:O:239:LYS:HZ1	1.79	0.45
1:A:49:HIS:HE1	14:O:238:PRO:CD	2.27	0.45
1:A:270:ASN:O	1:A:292:MET:HG2	2.16	0.45
1:A:272:GLY:O	1:A:292:MET:HB2	2.16	0.45
3:C:71:CYS:HA	16:Q:141:TYR:CD1	2.52	0.45
9:J:208:GLY:H	9:J:211:ASP:CB	2.29	0.45
9:J:229:ILE:HD11	9:J:298:TYR:CB	2.46	0.45
16:Q:36:GLN:NE2	40:r:135:ARG:O	2.32	0.45
16:Q:127:LYS:HB3	16:Q:131:GLN:HB3	1.98	0.45
24:a:96:ALA:HB2	27:d:61:TYR:CZ	2.49	0.45
25:b:19:ARG:HA	39:p:171:VAL:HG13	1.99	0.45
28:e:70:ASN:O	28:e:73:SER:HB2	2.16	0.45
38:o:56:ARG:HB3	38:o:56:ARG:NH1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:116:ILE:HG13	42:u:168:PHE:CE1	2.52	0.45
40:r:300:ALA:O	40:r:308:SER:HB3	2.16	0.45
42:u:106:LYS:O	42:u:109:GLU:HG3	2.17	0.45
44:w:86:PHE:HB2	44:w:159:LEU:HD23	1.97	0.45
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.52	0.45
6:G:122:MET:HE3	6:G:144:ILE:HG21	1.99	0.45
16:Q:179:ARG:HG2	16:Q:183:HIS:CD2	2.51	0.45
18:T:122:HIS:ND1	18:T:122:HIS:O	2.50	0.45
25:b:28:LEU:HG	25:b:32:GLU:HG2	1.99	0.45
35:l:66:TRP:HZ3	48:l:720:PEE:H38	1.81	0.45
38:o:102:TYR:HB2	40:r:263:MET:HG3	1.98	0.45
40:r:225:ILE:HD13	40:r:331:ASN:HB2	1.99	0.45
41:s:267:THR:O	41:s:271:LEU:HG	2.16	0.45
9:J:293:LEU:HD12	9:J:294:PRO:CD	2.47	0.45
11:L:158:LYS:NZ	12:M:67:GLU:O	2.41	0.45
15:P:103:HIS:CD2	15:P:105:ASN:HB2	2.52	0.45
16:Q:375:MET:HE3	16:Q:379:ILE:HG13	1.98	0.45
27:d:162:ARG:HG2	27:d:162:ARG:HH11	1.82	0.45
1:A:121:GLU:HB2	47:A:503:NAI:C4N	2.29	0.45
12:M:370:GLU:HB2	12:M:522:GLN:OE1	2.16	0.45
15:P:119:VAL:HG12	15:P:121:THR:HG22	1.98	0.45
28:e:125:LEU:O	28:e:129:ARG:HG3	2.16	0.45
41:s:140:ILE:O	41:s:143:GLU:HG2	2.17	0.45
44:w:61:THR:HG22	44:w:159:LEU:HB2	1.99	0.45
47:A:503:NAI:O2N	47:A:503:NAI:H52A	2.17	0.45
49:C:312:PLX:H31	13:N:75:TRP:CE3	2.52	0.45
9:J:204:SER:OG	9:J:204:SER:O	2.32	0.45
11:L:116:SER:OG	15:P:227:ALA:O	2.19	0.45
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.81	0.45
21:W:93:GLU:OE1	31:h:92:TYR:OH	2.30	0.45
29:f:72:ARG:HD2	30:g:22:SER:HB3	1.99	0.45
35:l:237:MET:HB3	35:l:299:LYS:HE2	1.99	0.45
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.99	0.45
9:J:208:GLY:N	9:J:211:ASP:OD2	2.48	0.45
25:b:7:ASP:OD1	25:b:8:GLU:N	2.49	0.45
35:l:127:THR:HG21	35:l:146:GLY:HA3	1.99	0.45
35:l:257:VAL:HG13	35:l:317:ILE:HD11	1.99	0.45
40:r:14:MET:O	40:r:18:SER:OG	2.27	0.45
48:C:311:PEE:C41	49:C:312:PLX:C19	2.92	0.44
4:E:16:SER:HB3	11:L:52:LEU:HD12	1.99	0.44
11:L:92:ASN:HB3	15:P:238:PRO:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:126:PHE:CD2	6:X:148:ILE:HD13	2.51	0.44
26:c:161:TYR:HB3	26:c:166:LEU:HG	1.98	0.44
29:f:68:GLU:HG2	30:g:21:ARG:CZ	2.47	0.44
32:i:217:MET:CB	32:i:326:LEU:HD13	2.46	0.44
35:l:135:ASN:O	35:l:198:LEU:HG	2.15	0.44
35:l:529:TYR:CE2	35:l:533:MET:HG3	2.52	0.44
1:A:91:ALA:CB	47:A:503:NAI:H51A	2.47	0.44
8:I:23:LYS:NZ	16:Q:253:PHE:CE1	2.83	0.44
8:I:27:ARG:HE	8:I:27:ARG:HB2	1.47	0.44
9:J:207:PHE:CB	9:J:211:ASP:OD2	2.64	0.44
12:M:390:THR:HB	12:M:600:GLU:OE2	2.17	0.44
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.52	0.44
18:T:43:GLN:C	18:T:43:GLN:CD	2.85	0.44
35:l:142:ILE:HG12	40:r:370:PRO:HB2	1.98	0.44
35:l:383:MET:O	35:l:389:PHE:HB2	2.17	0.44
54:l:713:CDL:H421	54:l:713:CDL:H391	1.73	0.44
40:r:154:LEU:HD23	40:r:154:LEU:HA	1.87	0.44
2:B:79:ARG:NH2	8:I:20:LEU:HD21	2.33	0.44
2:B:151:LYS:HA	3:C:141:GLY:HA2	1.98	0.44
8:I:74:LYS:HD2	8:I:74:LYS:HA	1.79	0.44
9:J:64:PHE:CZ	9:J:211:ASP:HB3	2.53	0.44
9:J:132:ARG:HD3	9:J:132:ARG:HA	1.61	0.44
15:P:187:ILE:HG23	15:P:188:LEU:HG	2.00	0.44
50:X:201:8Q1:N36	50:X:201:8Q1:O40	2.49	0.44
32:i:106:LEU:HG	32:i:138:PRO:HB2	1.98	0.44
32:i:129:LEU:CD1	54:i:401:CDL:H341	2.47	0.44
32:i:334:THR:HG22	32:i:335:LEU:HG	1.99	0.44
35:l:72:GLN:NE2	35:l:72:GLN:H	2.16	0.44
35:l:530:PRO:O	35:l:534:HIS:HB2	2.18	0.44
40:r:78:MET:HE1	40:r:439:LEU:HD12	1.99	0.44
1:A:396:MET:O	1:A:400:VAL:HG23	2.17	0.44
7:H:73:GLN:HA	7:H:73:GLN:OE1	2.17	0.44
12:M:354:LEU:HD22	12:M:548:LEU:HD22	1.98	0.44
48:U:101:PEE:H42	33:j:96:ILE:HD12	2.00	0.44
35:l:83:ASP:OD2	35:l:262:ARG:NH1	2.51	0.44
54:n:102:CDL:H752	54:n:102:CDL:H781	1.63	0.44
43:v:39:MET:HE3	43:v:39:MET:HB3	1.76	0.44
1:A:119:GLU:HG3	1:A:119:GLU:O	2.18	0.44
9:J:57:THR:HG21	9:J:120:VAL:HG12	1.99	0.44
14:O:140:CYS:HA	14:O:183:ALA:HB1	1.97	0.44
15:P:94:ILE:O	15:P:98:THR:OG1	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:293:LEU:HD22	16:Q:298:ILE:HD12	2.00	0.44
17:S:4:GLU:OE1	41:s:30:TYR:OH	2.35	0.44
48:V:202:PEE:H69	49:V:205:PLX:H381	1.99	0.44
54:a:201:CDL:H761	54:a:201:CDL:C20	2.46	0.44
28:e:74:HIS:HB2	28:e:83:ASP:OD2	2.18	0.44
35:l:389:PHE:O	35:l:393:ASP:HB3	2.18	0.44
56:s:403:UQ:H103	56:s:403:UQ:H71	1.77	0.44
44:w:61:THR:HG22	44:w:159:LEU:HD12	2.00	0.44
44:w:62:VAL:HG22	44:w:205:VAL:HB	1.99	0.44
4:E:56:VAL:HG12	4:E:60:ARG:HD2	2.00	0.44
7:H:50:GLN:O	7:H:54:GLU:HG3	2.17	0.44
9:J:192:ARG:NH2	9:J:262:THR:OG1	2.51	0.44
12:M:250:SER:OG	12:M:251:ILE:N	2.50	0.44
12:M:355:LYS:HG3	12:M:366:LEU:HD13	1.99	0.44
15:P:161:LYS:HD2	16:Q:286:TYR:CZ	2.53	0.44
49:V:205:PLX:H331	49:V:205:PLX:H301	1.56	0.44
38:o:53:ASP:HA	38:o:54:PRO:HD3	1.63	0.44
44:w:213:GLU:OE1	44:w:217:ARG:HD2	2.17	0.44
1:A:98:LYS:HA	1:A:101:PHE:HD2	1.82	0.44
12:M:381:LEU:HD22	12:M:664:TYR:CD2	2.52	0.44
16:Q:102:SER:HB3	16:Q:107:ARG:HD2	1.99	0.44
35:l:130:ILE:HD11	54:l:712:CDL:H262	1.99	0.44
35:l:384:PRO:HA	35:l:389:PHE:CD1	2.52	0.44
39:p:30:TRP:NE1	39:p:76:HIS:HB2	2.33	0.44
16:Q:266:ARG:NH1	48:s:401:PEE:O1P	2.50	0.44
24:a:60:SER:HB3	39:p:107:TRP:HA	2.00	0.44
54:l:712:CDL:H722	54:l:712:CDL:H761	1.99	0.44
40:r:299:VAL:O	40:r:303:ILE:HG12	2.17	0.44
42:u:45:LEU:HD22	42:u:131:VAL:HB	1.99	0.44
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.99	0.44
3:C:64:PRO:HB3	3:C:102:VAL:HG13	2.00	0.44
10:K:76:LEU:HA	10:K:79:HIS:CD2	2.53	0.44
15:P:117:VAL:HB	15:P:127:GLU:HG2	1.98	0.44
48:V:202:PEE:H21	40:r:198:ALA:HB2	2.00	0.44
24:a:94:GLY:HA2	24:a:116:PRO:HG3	2.00	0.44
27:d:43:ARG:HB2	27:d:44:PRO:HD3	2.00	0.44
35:l:332:HIS:HA	35:l:335:PHE:CE2	2.53	0.44
36:m:70:TYR:CE1	36:m:74:MET:HE3	2.53	0.44
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.72	0.43
5:F:24:CYS:N	5:F:58:CYS:SG	2.91	0.43
10:K:88:ASP:OD1	14:O:62:ARG:NH2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:N:202:CDL:H711	41:s:43:TYR:OH	2.18	0.43
15:P:162:ALA:HB2	16:Q:286:TYR:C	2.43	0.43
28:e:85:TRP:O	28:e:89:VAL:HG22	2.17	0.43
30:g:2:THR:HG22	30:g:4:MET:HG3	2.00	0.43
31:h:36:PHE:CD1	31:h:62:ASP:HB3	2.53	0.43
34:k:45:THR:HG23	36:m:52:LEU:HD13	2.00	0.43
35:l:71:LEU:HD22	35:l:71:LEU:N	2.33	0.43
35:l:173:LEU:HD12	40:r:405:LEU:HD21	2.00	0.43
35:l:534:HIS:ND1	48:l:719:PEE:C10	2.81	0.43
41:s:220:PHE:HE2	56:s:403:UQ:HM52	1.84	0.43
8:I:40:LYS:HB3	21:W:6:VAL:HA	1.98	0.43
12:M:103:LEU:HB3	12:M:106:SER:HB2	1.99	0.43
12:M:117:MET:HE3	12:M:121:LEU:HG	1.99	0.43
13:N:14:VAL:HA	13:N:23:TYR:CD1	2.53	0.43
54:N:202:CDL:OA3	17:S:3:PHE:HE2	2.01	0.43
16:Q:220:ALA:HB3	16:Q:224:ALA:HA	2.00	0.43
35:l:331:MET:HE1	35:l:468:ILE:HD12	2.00	0.43
35:l:478:PRO:HD3	43:v:87:TRP:CH2	2.52	0.43
48:l:720:PEE:H60	48:l:720:PEE:H55	1.87	0.43
38:o:8:PRO:HG3	38:o:14:LEU:HD13	2.00	0.43
39:p:102:TRP:CH2	40:r:424:ASN:HA	2.53	0.43
40:r:202:ALA:O	40:r:205:VAL:HG12	2.18	0.43
41:s:14:LEU:C	41:s:17:VAL:HG22	2.42	0.43
41:s:72:ILE:O	41:s:76:ILE:HG12	2.18	0.43
41:s:92:PRO:HG3	41:s:252:PRO:CB	2.48	0.43
44:w:246:LEU:N	44:w:247:PRO:CD	2.80	0.43
2:B:171:PRO:HG3	2:B:200:GLU:HG2	2.00	0.43
6:G:128:PHE:HZ	6:G:148:ILE:CD1	2.30	0.43
16:Q:192:LEU:HD12	16:Q:197:MET:HA	1.99	0.43
32:i:170:LEU:HD11	32:i:288:LEU:HD22	2.00	0.43
32:i:243:LEU:HD23	54:r:714:CDL:H361	2.00	0.43
33:j:86:THR:O	33:j:90:MET:HG2	2.19	0.43
35:l:16:THR:HG23	54:l:712:CDL:H861	1.99	0.43
40:r:73:LEU:HD22	40:r:103:GLN:OE1	2.17	0.43
1:A:49:HIS:CB	1:A:59:ARG:HE	2.30	0.43
6:G:105:MET:HE1	6:G:139:MET:SD	2.57	0.43
7:H:38:ILE:O	7:H:45:ARG:NH1	2.48	0.43
9:J:116:ILE:O	9:J:120:VAL:HG22	2.19	0.43
9:J:182:ARG:O	9:J:186:VAL:HG23	2.19	0.43
10:K:79:HIS:ND1	14:O:216:PRO:HD2	2.33	0.43
12:M:58:MET:HG2	12:M:59:GLN:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:334:GLN:HA	12:M:361:VAL:CG1	2.48	0.43
12:M:406:ASN:ND2	12:M:688:GLN:O	2.46	0.43
15:P:197:PRO:HA	15:P:202:PHE:CD2	2.54	0.43
6:X:111:ASP:OD1	6:X:112:SER:N	2.50	0.43
22:Y:105:ASP:N	22:Y:105:ASP:OD1	2.49	0.43
32:i:190:MET:HE2	32:i:205:LEU:HA	2.00	0.43
54:l:713:CDL:H711	54:l:713:CDL:H742	1.66	0.43
36:m:8:ILE:H	36:m:8:ILE:HD12	1.83	0.43
42:u:69:ASP:O	42:u:73:GLN:HG3	2.18	0.43
48:C:311:PEE:C45	56:s:403:UQ:C16	2.91	0.43
9:J:311:GLU:HA	9:J:312:PRO:HD3	1.72	0.43
16:Q:101:LEU:HD22	16:Q:106:VAL:HG22	2.00	0.43
16:Q:245:TYR:O	16:Q:249:LYS:HG2	2.19	0.43
48:U:101:PEE:H64	48:U:101:PEE:H59	1.49	0.43
48:V:202:PEE:C22	48:V:202:PEE:H74	2.48	0.43
54:a:201:CDL:C25	54:a:201:CDL:C21	2.86	0.43
32:i:30:TRP:O	32:i:34:GLU:HG2	2.19	0.43
36:m:17:PHE:CD1	36:m:20:PHE:HE1	2.36	0.43
40:r:282:LEU:HG	40:r:342:MET:HG2	1.99	0.43
41:s:14:LEU:CA	41:s:17:VAL:HG22	2.48	0.43
9:J:319:VAL:O	9:J:322:VAL:HG13	2.18	0.43
12:M:347:ASP:HB3	12:M:594:ALA:HB1	2.00	0.43
12:M:382:ARG:HE	12:M:527:ASP:CG	2.27	0.43
54:a:201:CDL:H372	54:a:201:CDL:H341	1.86	0.43
32:i:57:THR:HA	34:k:77:LEU:HD13	1.99	0.43
39:p:108:HIS:CD2	39:p:109:PRO:HD2	2.54	0.43
44:w:128:SER:HB3	44:w:173:MET:CE	2.49	0.43
1:A:61:ASP:OD2	1:A:137:LYS:HG3	2.19	0.43
1:A:89:GLY:CA	1:A:244:ASN:ND2	2.46	0.43
1:A:131:ILE:O	1:A:135:PRO:HG3	2.18	0.43
1:A:392:MET:HE1	1:A:432:ALA:HA	2.01	0.43
5:F:53:ILE:N	12:M:380:ASP:OD1	2.52	0.43
17:S:48:MET:HE1	21:W:143:TYR:CZ	2.52	0.43
6:X:93:ILE:HD11	6:X:110:LEU:HD11	2.01	0.43
23:Z:75:PHE:O	23:Z:79:VAL:HG13	2.18	0.43
54:a:201:CDL:H592	48:l:720:PEE:H20	2.00	0.43
32:i:254:LEU:O	32:i:257:LEU:HB2	2.19	0.43
49:j:203:PLX:H342	49:j:203:PLX:H372	1.76	0.43
35:l:176:ARG:HA	35:l:179:ASP:HB2	2.00	0.43
35:l:551:SER:HA	35:l:555:LEU:HB2	2.00	0.43
44:w:258:TYR:HE2	44:w:269:VAL:HG22	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:130:ILE:HA	6:G:131:PRO:HD3	1.85	0.43
7:H:22:GLU:O	7:H:26:ILE:HG12	2.19	0.43
9:J:291:TYR:O	9:J:291:TYR:CD1	2.71	0.43
13:N:120:THR:HG22	13:N:122:GLN:H	1.83	0.43
14:O:185:MET:HB3	14:O:194:GLU:HA	2.01	0.43
16:Q:199:PRO:HA	16:Q:202:TRP:HB2	1.99	0.43
16:Q:303:ARG:HG3	16:Q:401:GLU:HB3	2.01	0.43
49:V:205:PLX:H22	49:V:205:PLX:H1C3	1.78	0.43
21:W:114:THR:OG1	42:u:143:HIS:ND1	2.42	0.43
6:X:72:PRO:HG2	22:Y:42:PRO:HG3	2.01	0.43
28:e:84:LEU:HG	28:e:88:ARG:HD2	2.00	0.43
32:i:170:LEU:O	32:i:295:ARG:NH2	2.39	0.43
33:j:30:TYR:HE2	41:s:59:GLU:HB2	1.84	0.43
54:l:712:CDL:H811	54:l:712:CDL:H851	2.00	0.43
48:l:718:PEE:H38	40:r:155:ALA:HB2	2.01	0.43
41:s:62:ARG:NH2	41:s:66:SER:O	2.52	0.43
1:A:326:LEU:HD22	1:A:363:ILE:HD11	2.01	0.43
2:B:196:LYS:HE3	13:N:113:HIS:CE1	2.54	0.43
49:V:205:PLX:H6	49:V:205:PLX:H51	1.31	0.43
21:W:128:ARG:NH1	31:h:102:GLU:OE2	2.36	0.43
25:b:16:ARG:HE	25:b:20:ARG:HH12	1.67	0.43
35:l:302:VAL:HG12	35:l:340:PHE:CZ	2.54	0.43
9:J:83:PRO:HG3	9:J:119:VAL:HG11	2.00	0.43
12:M:141:ASP:O	12:M:145:MET:HG2	2.18	0.43
48:V:202:PEE:H36	48:V:202:PEE:C44	2.48	0.43
28:e:94:GLY:O	28:e:99:LEU:HD23	2.19	0.43
32:i:13:VAL:HG13	32:i:36:ASN:ND2	2.34	0.43
34:k:16:LEU:O	34:k:20:LEU:HG	2.19	0.43
35:l:172:ILE:HG21	40:r:408:LEU:HD12	2.00	0.43
40:r:375:LEU:HA	40:r:378:GLU:HB3	1.99	0.43
41:s:87:VAL:N	41:s:88:PRO:CD	2.80	0.43
41:s:174:MET:HB3	41:s:242:PHE:HA	2.00	0.43
41:s:220:PHE:CE2	56:s:403:UQ:CM5	3.02	0.43
2:B:105:ARG:HD2	13:N:108:TYR:CG	2.54	0.42
4:E:81:LEU:HD23	11:L:64:LEU:HD13	2.00	0.42
17:S:66:LEU:O	17:S:68:ASN:N	2.51	0.42
54:a:201:CDL:H111	48:l:720:PEE:H61	2.01	0.42
26:c:113:ILE:C	26:c:115:ASN:H	2.27	0.42
26:c:156:VAL:HG11	43:v:95:TYR:CZ	2.54	0.42
33:j:90:MET:HE3	33:j:90:MET:HA	2.01	0.42
35:l:174:TYR:CD1	35:l:229:LEU:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:420:ALA:HB1	35:l:498:PHE:CD1	2.53	0.42
54:r:714:CDL:H161	54:r:714:CDL:H132	1.69	0.42
41:s:195:ARG:HD3	41:s:231:ILE:HD11	2.01	0.42
9:J:149:PRO:HB3	9:J:166:HIS:HE1	1.84	0.42
9:J:149:PRO:HB3	9:J:166:HIS:CE1	2.55	0.42
9:J:174:ILE:HG23	9:J:175:LYS:HG2	2.02	0.42
16:Q:198:THR:HB	16:Q:199:PRO:HD3	2.01	0.42
54:a:201:CDL:H201	54:a:201:CDL:C76	2.49	0.42
28:e:116:GLU:O	28:e:120:ARG:HG3	2.19	0.42
33:j:87:MET:SD	33:j:88:LEU:N	2.92	0.42
35:l:357:ARG:HG3	39:p:32:VAL:HG13	2.01	0.42
35:l:381:THR:HG21	35:l:498:PHE:CE1	2.54	0.42
36:m:20:PHE:CZ	36:m:33:LEU:HD13	2.54	0.42
36:m:51:PHE:O	36:m:55:MET:HG2	2.19	0.42
39:p:25:ARG:HD3	39:p:25:ARG:HA	1.91	0.42
41:s:294:LEU:O	41:s:298:LEU:HG	2.19	0.42
2:B:112:ARG:O	2:B:164:VAL:HG21	2.19	0.42
11:L:84:ARG:NH1	11:L:88:GLN:O	2.52	0.42
14:O:135:CYS:SG	14:O:176:CYS:HA	2.59	0.42
17:S:57:VAL:HG21	17:S:62:VAL:HG21	2.01	0.42
6:X:75:THR:O	6:X:79:ILE:HG13	2.20	0.42
27:d:139:PHE:CE1	38:o:127:ILE:CG2	3.03	0.42
28:e:125:LEU:HD21	28:e:129:ARG:NH2	2.34	0.42
49:i:705:PLX:H202	49:i:705:PLX:H393	2.01	0.42
40:r:12:LEU:HD22	40:r:97:THR:HG23	2.00	0.42
40:r:310:MET:HE3	40:r:459:TYR:HA	2.00	0.42
2:B:63:TRP:HB3	2:B:66:LEU:HD12	2.02	0.42
2:B:76:TYR:CE2	16:Q:202:TRP:NE1	2.86	0.42
9:J:303:ARG:C	9:J:303:ARG:CD	2.92	0.42
9:J:313:TRP:H	9:J:313:TRP:HD1	1.68	0.42
17:S:37:ARG:O	21:W:143:TYR:OH	2.28	0.42
26:c:117:VAL:HG23	35:l:535:ARG:HA	2.00	0.42
30:g:122:ARG:O	38:o:109:ARG:NH2	2.41	0.42
32:i:246:VAL:HG21	54:r:714:CDL:H362	2.02	0.42
35:l:289:ALA:O	35:l:293:ILE:HG23	2.20	0.42
54:n:102:CDL:H261	40:r:6:ILE:HD13	2.01	0.42
43:v:68:LYS:HB3	43:v:68:LYS:HE3	1.79	0.42
12:M:117:MET:HE1	12:M:139:LEU:HD12	2.01	0.42
25:b:89:HIS:CD2	48:l:720:PEE:H49	2.54	0.42
28:e:112:TYR:HB3	40:r:45:LEU:HG	2.01	0.42
31:h:82:GLN:O	31:h:86:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:55:PHE:CZ	41:s:134:ARG:HG2	2.54	0.42
35:l:445:GLU:O	35:l:447:ASN:N	2.53	0.42
36:m:72:THR:HG22	41:s:121:TRP:HH2	1.85	0.42
36:m:175:ASN:OD1	44:w:289:ARG:NH2	2.51	0.42
41:s:26:LYS:HA	41:s:36:GLY:HA3	2.02	0.42
42:u:38:LYS:HB3	42:u:39:PRO:HD3	2.01	0.42
48:C:311:PEE:H27	48:C:311:PEE:H55	2.01	0.42
8:I:18:ARG:NH2	21:W:24:ASN:O	2.53	0.42
15:P:106:ALA:HB1	15:P:108:PHE:CE1	2.55	0.42
48:V:202:PEE:H78	40:r:201:MET:SD	2.59	0.42
36:m:8:ILE:O	36:m:12:ILE:HG12	2.20	0.42
43:v:22:MET:HE1	43:v:102:PHE:HA	2.02	0.42
44:w:147:LEU:HD23	44:w:147:LEU:HA	1.91	0.42
7:H:108:PRO:O	7:H:109:ALA:C	2.63	0.42
13:N:2:GLU:HG3	13:N:4:VAL:HG22	2.01	0.42
16:Q:204:PHE:CD1	16:Q:207:ARG:HD3	2.54	0.42
54:a:201:CDL:H412	54:a:201:CDL:H381	1.91	0.42
32:i:6:TYR:CD1	32:i:46:LYS:HD2	2.55	0.42
48:l:720:PEE:O4	48:l:720:PEE:H3	2.20	0.42
36:m:7:PHE:O	36:m:11:THR:HG23	2.20	0.42
39:p:29:SER:HB3	39:p:76:HIS:CD2	2.55	0.42
1:A:263:ALA:O	1:A:271:SER:HB2	2.20	0.42
1:A:329:LYS:HA	1:A:332:CYS:SG	2.60	0.42
1:A:453:PHE:HA	1:A:456:GLN:HG2	2.01	0.42
4:E:15:THR:OG1	11:L:55:VAL:O	2.31	0.42
12:M:337:ASP:O	12:M:542:PRO:HB2	2.20	0.42
12:M:405:THR:CG2	12:M:477:GLY:N	2.78	0.42
16:Q:339:GLN:O	16:Q:343:ILE:HG13	2.20	0.42
24:a:93:ILE:O	27:d:61:TYR:CE1	2.73	0.42
28:e:86:ASN:ND2	40:r:81:GLN:HE22	2.18	0.42
30:g:32:ARG:HB2	30:g:78:LEU:HD11	2.01	0.42
35:l:323:HIS:ND1	35:l:475:MET:SD	2.92	0.42
35:l:407:TRP:O	35:l:411:MET:HG2	2.20	0.42
35:l:536:LEU:HB3	35:l:537:PRO:HD3	2.01	0.42
37:n:17:VAL:HG21	40:r:30:HIS:HB3	2.02	0.42
44:w:343:TYR:HA	44:w:352:ILE:HD12	2.01	0.42
8:I:14:TRP:O	21:W:28:ARG:NH2	2.52	0.42
12:M:347:ASP:OD1	12:M:347:ASP:N	2.51	0.42
17:S:41:PHE:HB3	36:m:135:PHE:C	2.45	0.42
24:a:113:PHE:HB2	24:a:119:ARG:HG2	2.02	0.42
27:d:163:MET:HG3	28:e:149:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:o:32:ALA:O	38:o:36:ARG:HG3	2.19	0.42
5:F:43:GLU:O	5:F:46:LYS:HB2	2.20	0.42
9:J:208:GLY:N	9:J:211:ASP:HB3	2.35	0.42
12:M:171:THR:CG2	12:M:173:MET:HG2	2.49	0.42
13:N:68:MET:SD	13:N:81:MET:HG2	2.60	0.42
15:P:118:ASP:OD1	15:P:125:ARG:HG2	2.20	0.42
16:Q:362:LYS:HE2	16:Q:380:HIS:HE1	1.84	0.42
16:Q:404:LYS:HE2	16:Q:457:VAL:CG2	2.50	0.42
20:V:52:GLY:O	20:V:56:THR:HG23	2.20	0.42
25:b:36:PRO:HA	25:b:37:PRO:HD3	1.93	0.42
30:g:15:PHE:O	30:g:80:ARG:NH1	2.52	0.42
35:l:69:MET:SD	40:r:451:PRO:HB2	2.60	0.42
35:l:309:GLN:O	35:l:313:MET:HG3	2.20	0.42
54:l:712:CDL:H461	40:r:445:LEU:O	2.20	0.42
39:p:127:ARG:HG2	39:p:130:ARG:NH2	2.35	0.42
40:r:126:LEU:HD13	40:r:153:THR:HG21	2.02	0.42
42:u:18:VAL:HG12	42:u:20:VAL:HG22	2.02	0.42
1:A:56:ALA:O	1:A:61:ASP:HB2	2.20	0.41
1:A:62:TRP:CD2	1:A:181:LEU:HD13	2.55	0.41
1:A:98:LYS:O	1:A:101:PHE:HB2	2.20	0.41
6:G:74:LEU:HD23	6:G:74:LEU:O	2.20	0.41
12:M:485:ASP:OD1	12:M:680:LEU:HG	2.20	0.41
20:V:123:ALA:O	20:V:127:MET:HG3	2.20	0.41
6:X:120:MET:CE	39:p:21:LYS:HG3	2.50	0.41
6:X:126:PHE:HD2	6:X:148:ILE:HD13	1.85	0.41
27:d:33:LEU:HD21	35:l:49:VAL:HG22	2.02	0.41
40:r:141:GLU:HB2	40:r:222:GLU:OE2	2.21	0.41
40:r:251:ASN:HD21	40:r:304:GLN:NE2	2.17	0.41
1:A:63:TYR:CE2	14:O:242:GLY:CA	3.03	0.41
1:A:134:ASP:OD2	1:A:137:LYS:HD3	2.20	0.41
8:I:40:LYS:O	8:I:41:LEU:O	2.38	0.41
12:M:144:MET:HG3	16:Q:383:LYS:HG3	2.02	0.41
13:N:85:GLU:HG2	13:N:86:TRP:H	1.85	0.41
16:Q:36:GLN:NE2	40:r:137:GLY:O	2.53	0.41
17:S:66:LEU:C	17:S:68:ASN:H	2.28	0.41
31:h:38:LYS:HE2	31:h:42:GLU:CD	2.44	0.41
33:j:24:LEU:HB3	33:j:25:PRO:HD3	2.02	0.41
54:l:712:CDL:H452	54:l:712:CDL:H421	1.89	0.41
36:m:159:TRP:CZ2	36:m:163:ILE:HD11	2.54	0.41
54:n:102:CDL:C82	54:r:714:CDL:C86	2.98	0.41
54:n:102:CDL:H741	54:n:102:CDL:H712	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:16:VAL:CA	39:p:64:LEU:HD22	2.50	0.41
42:u:47:ARG:NH2	42:u:53:PRO:HG3	2.35	0.41
2:B:76:TYR:O	2:B:79:ARG:HG2	2.21	0.41
4:E:43:VAL:O	4:E:47:VAL:HG23	2.20	0.41
7:H:27:LEU:HD13	7:H:84:ALA:HB3	2.01	0.41
14:O:75:LYS:HB2	14:O:75:LYS:HE3	1.69	0.41
18:T:60:LYS:HG2	18:T:62:VAL:HG23	2.02	0.41
20:V:61:PHE:HD2	20:V:104:ARG:HH12	1.68	0.41
24:a:184:LYS:C	24:a:186:THR:H	2.28	0.41
28:e:57:GLU:OE1	44:w:320:GLY:HA3	2.19	0.41
40:r:196:TRP:NE1	40:r:250:LEU:HB3	2.34	0.41
43:v:52:MET:O	43:v:56:ARG:HG3	2.20	0.41
2:B:210:LEU:HD12	8:I:38:PRO:HB3	2.01	0.41
4:E:89:GLU:OE1	4:E:98:LYS:NZ	2.42	0.41
12:M:196:GLY:HA3	14:O:110:MET:HE2	2.02	0.41
12:M:382:ARG:HG2	12:M:386:LEU:CD1	2.49	0.41
14:O:134:VAL:HG13	14:O:186:VAL:HG12	2.01	0.41
17:S:66:LEU:C	17:S:68:ASN:N	2.76	0.41
48:U:101:PEE:H67	48:U:101:PEE:H73	1.88	0.41
32:i:149:ILE:HD11	32:i:195:PRO:HG3	2.02	0.41
35:l:10:THR:O	35:l:14:ILE:HG23	2.20	0.41
54:l:712:CDL:H472	40:r:445:LEU:HB2	2.02	0.41
54:l:712:CDL:C42	40:r:448:THR:HG21	2.34	0.41
36:m:41:CYS:SG	36:m:57:PHE:HB2	2.60	0.41
37:n:39:ARG:HG3	37:n:57:TRP:CE2	2.55	0.41
40:r:122:PHE:CE1	40:r:238:LEU:HB3	2.55	0.41
40:r:127:VAL:HB	40:r:128:PRO:HD3	2.01	0.41
41:s:126:LYS:HG3	41:s:127:TYR:N	2.36	0.41
41:s:140:ILE:HA	41:s:143:GLU:HG2	2.03	0.41
1:A:109:ARG:HG2	11:L:166:TRP:CD1	2.56	0.41
1:A:113:LEU:HD13	1:A:149:MET:HE1	2.00	0.41
3:C:166:CYS:HA	3:C:167:PRO:HA	1.82	0.41
48:C:311:PEE:H1	33:j:28:ASN:CB	2.50	0.41
12:M:215:MET:HE3	12:M:215:MET:HB3	1.98	0.41
13:N:22:GLY:O	13:N:26:VAL:HG12	2.21	0.41
21:W:105:LYS:HE2	21:W:105:LYS:HB3	1.84	0.41
28:e:73:SER:O	28:e:75:GLY:N	2.54	0.41
49:i:705:PLX:H22	49:i:705:PLX:H1C3	1.82	0.41
33:j:88:LEU:HD13	41:s:309:ILE:HD12	2.02	0.41
38:o:56:ARG:HB3	38:o:56:ARG:HH11	1.84	0.41
39:p:36:LYS:NZ	39:p:40:PHE:HE2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:36:LYS:HZ1	39:p:40:PHE:HE2	1.68	0.41
44:w:211:VAL:HA	44:w:214:ILE:HG12	2.02	0.41
12:M:213:MET:HE1	12:M:713:ALA:O	2.21	0.41
12:M:468:GLU:HG2	12:M:468:GLU:H	1.67	0.41
16:Q:271:ARG:HD2	16:Q:271:ARG:HA	1.82	0.41
48:U:101:PEE:H22	48:U:101:PEE:H27	1.94	0.41
20:V:141:VAL:C	24:a:161:ARG:HH11	2.27	0.41
23:Z:11:HIS:ND1	23:Z:11:HIS:O	2.54	0.41
30:g:48:ASN:HB3	30:g:55:VAL:HA	2.03	0.41
35:l:89:PHE:HB2	35:l:326:PHE:HZ	1.86	0.41
39:p:38:ARG:HD2	39:p:38:ARG:HA	1.90	0.41
41:s:138:GLN:HA	41:s:286:MET:HE1	2.01	0.41
3:C:59:ARG:HH12	49:C:312:PLX:P1	2.44	0.41
8:I:17:GLY:C	8:I:18:ARG:HD2	2.45	0.41
8:I:107:SER:C	8:I:109:ASP:H	2.28	0.41
9:J:40:LEU:HD23	9:J:40:LEU:HA	1.86	0.41
9:J:289:LEU:HD22	9:J:289:LEU:N	2.36	0.41
54:i:401:CDL:H132	54:i:401:CDL:C17	2.45	0.41
48:m:202:PEE:H27	48:m:202:PEE:H22	1.75	0.41
40:r:39:LEU:HA	40:r:39:LEU:HD12	1.88	0.41
41:s:52:ALA:HB2	56:s:403:UQ:C14	2.44	0.41
43:v:80:CYS:HB3	43:v:83:GLU:OE1	2.20	0.41
44:w:116:LYS:NZ	44:w:123:SER:OG	2.54	0.41
1:A:60:GLY:HA2	14:O:241:PRO:HA	2.02	0.41
1:A:110:PRO:O	1:A:238:CYS:HB3	2.21	0.41
1:A:423:THR:HB	45:A:501:SF4:S4	2.60	0.41
1:A:426:ALA:HB3	46:A:502:FMN:HM81	2.02	0.41
12:M:470:LYS:HE3	12:M:470:LYS:HB3	1.72	0.41
17:S:55:SER:HA	17:S:64:LYS:CE	2.50	0.41
35:l:290:LEU:O	35:l:523:SER:OG	2.39	0.41
35:l:327:LEU:HD12	35:l:331:MET:HE3	2.02	0.41
35:l:393:ASP:O	35:l:397:GLU:HG3	2.20	0.41
40:r:42:LEU:HB3	40:r:453:MET:CE	2.51	0.41
40:r:318:ALA:HB1	40:r:374:ASN:CG	2.45	0.41
44:w:72:ARG:HH22	44:w:264:GLU:HA	1.85	0.41
1:A:213:ILE:HG23	1:A:235:VAL:HA	2.02	0.41
1:A:290:GLU:HG2	1:A:291:GLU:H	1.85	0.41
46:A:502:FMN:N5	47:A:503:NAI:H4N	2.36	0.41
2:B:110:GLU:HB2	18:T:71:ILE:HB	2.03	0.41
3:C:50:LEU:HD22	48:C:311:PEE:H59	2.03	0.41
5:F:18:GLU:OE1	5:F:68:ARG:NH1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:70:MET:HE1	15:P:73:VAL:HG12	2.03	0.41
9:J:83:PRO:HB2	9:J:108:TRP:CD1	2.55	0.41
9:J:172:ALA:HA	9:J:181:LEU:HB3	2.02	0.41
11:L:59:LEU:HD12	11:L:59:LEU:HA	1.95	0.41
12:M:605:GLN:OE1	12:M:643:ARG:NH1	2.54	0.41
12:M:658:ASP:OD1	12:M:659:VAL:N	2.54	0.41
14:O:213:ILE:HD12	14:O:214:PRO:HD2	2.03	0.41
15:P:161:LYS:CD	16:Q:286:TYR:CE1	3.00	0.41
16:Q:218:SER:OG	16:Q:224:ALA:CB	2.69	0.41
16:Q:432:LEU:HD12	16:Q:432:LEU:HA	1.94	0.41
16:Q:450:ILE:HA	16:Q:453:THR:HG22	2.03	0.41
21:W:128:ARG:HD3	21:W:132:GLU:OE2	2.21	0.41
6:X:89:LEU:HD23	23:Z:48:ASN:HA	2.02	0.41
50:X:201:8Q1:C10	39:p:67:ALA:HB1	2.51	0.41
22:Y:61:PHE:HE1	35:l:459:ILE:HD11	1.85	0.41
28:e:65:ASN:ND2	28:e:68:GLU:HG3	2.36	0.41
29:f:55:TRP:O	29:f:59:ILE:HG12	2.21	0.41
38:o:85:LYS:O	38:o:89:LEU:HD23	2.21	0.41
41:s:195:ARG:HH12	41:s:274:ARG:HH11	1.69	0.41
44:w:295:ARG:HA	44:w:298:VAL:HG22	2.02	0.41
44:w:340:SER:HB2	44:w:343:TYR:HD1	1.85	0.41
4:E:37:ARG:HH22	6:G:132:ASP:CG	2.29	0.41
9:J:218:ALA:O	9:J:221:ARG:HG2	2.21	0.41
13:N:55:PHE:CZ	13:N:58:ARG:HG3	2.55	0.41
15:P:162:ALA:HB2	16:Q:286:TYR:O	2.21	0.41
15:P:235:LEU:HD12	16:Q:418:ARG:HE	1.85	0.41
48:V:202:PEE:H74	48:V:202:PEE:H33	2.03	0.41
6:X:89:LEU:HD21	23:Z:22:TRP:CD1	2.56	0.41
24:a:84:ILE:O	24:a:88:LEU:HG	2.21	0.41
35:l:68:TRP:H	35:l:77:SER:HA	1.86	0.41
35:l:166:THR:HG21	48:l:719:PEE:H2	2.02	0.41
40:r:368:ALA:O	40:r:375:LEU:HD12	2.20	0.41
42:u:77:HIS:ND1	42:u:115:LEU:HD21	2.36	0.41
43:v:69:CYS:HB3	43:v:80:CYS:HB2	1.94	0.41
44:w:353:TRP:CD1	44:w:353:TRP:H	2.39	0.41
3:C:68:GLY:HA2	3:C:73:ALA:HB2	2.02	0.40
6:G:93:ILE:HD13	6:G:108:LEU:HD13	2.03	0.40
9:J:115:SER:HA	9:J:118:LYS:HG2	2.03	0.40
12:M:136:GLU:CD	12:M:272:ARG:HH22	2.28	0.40
12:M:613:PRO:HB3	13:N:134:ILE:HD13	2.03	0.40
12:M:718:ILE:HD12	12:M:718:ILE:HA	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.57	0.40
16:Q:404:LYS:HE2	16:Q:457:VAL:HB	2.03	0.40
17:S:31:ASN:ND2	17:S:60:TYR:OH	2.54	0.40
21:W:78:GLU:OE2	31:h:106:PRO:HB2	2.21	0.40
24:a:78:THR:HG21	28:e:96:SER:O	2.22	0.40
25:b:88:TYR:CE2	27:d:49:ARG:HB2	2.56	0.40
27:d:5:TRP:HZ3	27:d:10:TYR:HB2	1.85	0.40
32:i:149:ILE:HD12	32:i:154:MET:HG2	2.03	0.40
35:l:7:LEU:O	35:l:11:THR:HG23	2.21	0.40
35:l:88:MET:CE	35:l:468:ILE:HD13	2.51	0.40
35:l:248:HIS:HA	35:l:253:VAL:HG13	2.03	0.40
49:n:101:PLX:H22	49:n:101:PLX:H1A2	1.77	0.40
38:o:113:GLU:O	38:o:116:ILE:HG22	2.20	0.40
41:s:74:ALA:HB3	41:s:75:PRO:HD3	2.03	0.40
1:A:147:ARG:HA	1:A:147:ARG:HD2	1.91	0.40
1:A:290:GLU:HG2	1:A:291:GLU:N	2.36	0.40
2:B:100:GLU:O	2:B:170:GLY:N	2.49	0.40
2:B:150:THR:HG21	2:B:180:HIS:CD2	2.57	0.40
2:B:205:ILE:O	2:B:209:TYR:HB3	2.20	0.40
9:J:236:VAL:CG2	9:J:325:SER:HG	2.30	0.40
10:K:81:TYR:CD1	10:K:85:THR:HG21	2.57	0.40
12:M:522:GLN:O	12:M:526:LEU:HG	2.21	0.40
13:N:49:TYR:HB2	13:N:61:TRP:CE2	2.57	0.40
14:O:69:ASN:N	14:O:69:ASN:HD22	2.18	0.40
15:P:157:VAL:HG11	15:P:182:PRO:HD3	2.03	0.40
16:Q:251:PHE:O	16:Q:255:ILE:HG13	2.21	0.40
21:W:87:LEU:HD23	21:W:87:LEU:HA	1.94	0.40
30:g:51:ARG:HD3	30:g:53:ARG:NH1	2.36	0.40
32:i:159:MET:HE3	32:i:163:LEU:HG	2.03	0.40
33:j:67:LEU:HD23	33:j:67:LEU:HA	1.92	0.40
40:r:394:ILE:H	40:r:394:ILE:HD12	1.86	0.40
1:A:51:TRP:C	1:A:52:ARG:O	2.63	0.40
5:F:19:ILE:HD12	5:F:51:LEU:HD21	2.02	0.40
12:M:689:LEU:HD12	12:M:689:LEU:HA	1.85	0.40
16:Q:228:ARG:C	16:Q:230:GLY:H	2.29	0.40
2:B:153:ILE:CG2	3:C:142:TYR:HB2	2.51	0.40
5:F:23:LEU:O	5:F:57:GLU:HA	2.21	0.40
8:I:66:PRO:HB3	15:P:79:SER:HA	2.02	0.40
9:J:228:LEU:HD22	9:J:273:LEU:CD2	2.49	0.40
14:O:84:ASP:O	14:O:88:ARG:HG3	2.21	0.40
16:Q:139:LEU:HD13	16:Q:424:ILE:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:143:SER:O	16:Q:147:ASN:OD1	2.39	0.40
21:W:51:MET:HA	41:s:313:SER:HB2	2.03	0.40
26:c:133:LEU:HD13	35:l:527:GLY:O	2.22	0.40
30:g:81:GLN:NE2	32:i:341:PRO:HB2	2.35	0.40
32:i:12:THR:HG21	36:m:163:ILE:HG21	2.03	0.40
32:i:241:THR:HB	32:i:301:SER:HB3	2.02	0.40
33:j:48:ARG:HB2	33:j:49:LEU:H	1.66	0.40
48:l:720:PEE:H4	48:l:720:PEE:P	2.44	0.40
44:w:165:SER:HB3	44:w:245:PHE:CD1	2.57	0.40
4:E:37:ARG:HG2	6:G:120:MET:CE	2.50	0.40
11:L:96:LYS:HA	11:L:96:LYS:HD3	1.87	0.40
14:O:156:LEU:HB3	14:O:158:ILE:HG12	2.03	0.40
15:P:207:TYR:C	15:P:224:VAL:HG23	2.47	0.40
16:Q:38:GLN:OE1	16:Q:38:GLN:HA	2.22	0.40
19:U:5:ILE:O	19:U:9:LEU:HD23	2.21	0.40
20:V:90:TYR:CZ	20:V:126:LYS:HD3	2.57	0.40
21:W:130:ASN:HB3	36:m:1:MET:H3	1.86	0.40
23:Z:18:ASP:OD1	23:Z:18:ASP:N	2.46	0.40
25:b:22:TRP:O	25:b:26:GLN:HG2	2.22	0.40
27:d:114:GLN:HB2	35:l:203:MET:HE3	2.03	0.40
37:n:17:VAL:HG13	40:r:7:PRO:HB3	2.04	0.40
42:u:83:THR:HA	42:u:86:TRP:NE1	2.36	0.40
42:u:149:GLU:CD	42:u:150:PRO:HD2	2.47	0.40
44:w:77:ILE:HD11	44:w:269:VAL:HG11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	429/431 (100%)	412 (96%)	16 (4%)	1 (0%)	43 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	174/176 (99%)	174 (100%)	0	0	100	100
3	C	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
4	E	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
5	F	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
6	G	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
6	X	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
7	H	110/112 (98%)	104 (94%)	6 (6%)	0	100	100
8	I	93/112 (83%)	82 (88%)	10 (11%)	1 (1%)	11	29
9	J	327/341 (96%)	311 (95%)	13 (4%)	3 (1%)	14	35
10	K	40/42 (95%)	38 (95%)	2 (5%)	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	669 (97%)	19 (3%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	208 (97%)	6 (3%)	1 (0%)	24	48
15	P	206/208 (99%)	196 (95%)	10 (5%)	0	100	100
16	Q	412/430 (96%)	399 (97%)	12 (3%)	1 (0%)	43	68
17	S	68/70 (97%)	63 (93%)	5 (7%)	0	100	100
18	T	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
19	U	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
20	V	138/140 (99%)	130 (94%)	7 (5%)	1 (1%)	18	41
21	W	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
22	Y	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
23	Z	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
24	a	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
25	b	99/126 (79%)	93 (94%)	6 (6%)	0	100	100
26	c	154/156 (99%)	145 (94%)	9 (6%)	0	100	100
27	d	173/175 (99%)	172 (99%)	1 (1%)	0	100	100
28	e	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
29	f	40/42 (95%)	38 (95%)	2 (5%)	0	100	100
30	g	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
31	h	103/105 (98%)	99 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	i	345/347 (99%)	330 (96%)	13 (4%)	2 (1%)	21	44
33	j	95/113 (84%)	89 (94%)	6 (6%)	0	100	100
34	k	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
35	l	601/603 (100%)	578 (96%)	23 (4%)	0	100	100
36	m	125/175 (71%)	112 (90%)	13 (10%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
39	p	176/178 (99%)	167 (95%)	9 (5%)	0	100	100
40	r	457/459 (100%)	444 (97%)	13 (3%)	0	100	100
41	s	299/318 (94%)	289 (97%)	9 (3%)	1 (0%)	36	60
42	u	169/171 (99%)	164 (97%)	5 (3%)	0	100	100
43	v	122/131 (93%)	113 (93%)	9 (7%)	0	100	100
44	w	318/320 (99%)	304 (96%)	14 (4%)	0	100	100
All	All	8067/8315 (97%)	7757 (96%)	299 (4%)	11 (0%)	49	73

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
9	J	221	ARG
32	i	93	VAL
14	O	73	GLY
32	i	92	PRO
8	I	41	LEU
9	J	290	PRO
41	s	90	PRO
9	J	227	PRO
20	V	46	PRO
16	Q	229	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/345 (100%)	344 (100%)	1 (0%)	86	94
2	B	151/151 (100%)	150 (99%)	1 (1%)	76	90
3	C	132/132 (100%)	131 (99%)	1 (1%)	73	88
4	E	107/107 (100%)	105 (98%)	2 (2%)	50	77
5	F	76/76 (100%)	76 (100%)	0	100	100
6	G	76/81 (94%)	76 (100%)	0	100	100
6	X	75/81 (93%)	75 (100%)	0	100	100
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	85 (98%)	2 (2%)	44	73
9	J	278/295 (94%)	277 (100%)	1 (0%)	84	93
10	K	41/41 (100%)	40 (98%)	1 (2%)	43	72
11	L	113/113 (100%)	113 (100%)	0	100	100
12	M	580/580 (100%)	576 (99%)	4 (1%)	76	90
13	N	130/130 (100%)	130 (100%)	0	100	100
14	O	183/183 (100%)	182 (100%)	1 (0%)	81	92
15	P	190/190 (100%)	186 (98%)	4 (2%)	47	75
16	Q	361/370 (98%)	361 (100%)	0	100	100
17	S	58/58 (100%)	58 (100%)	0	100	100
18	T	79/79 (100%)	78 (99%)	1 (1%)	61	83
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	100 (99%)	1 (1%)	68	86
21	W	122/123 (99%)	122 (100%)	0	100	100
22	Y	63/63 (100%)	63 (100%)	0	100	100
23	Z	65/65 (100%)	65 (100%)	0	100	100
24	a	122/122 (100%)	122 (100%)	0	100	100
25	b	98/119 (82%)	98 (100%)	0	100	100
26	c	141/141 (100%)	141 (100%)	0	100	100
27	d	155/155 (100%)	154 (99%)	1 (1%)	78	91
28	e	99/99 (100%)	99 (100%)	0	100	100
29	f	35/38 (92%)	35 (100%)	0	100	100
30	g	108/108 (100%)	108 (100%)	0	100	100
31	h	93/93 (100%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	i	311/311 (100%)	311 (100%)	0	100	100
33	j	88/99 (89%)	88 (100%)	0	100	100
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	518/537 (96%)	514 (99%)	4 (1%)	73	88
36	m	91/141 (64%)	91 (100%)	0	100	100
37	n	53/53 (100%)	52 (98%)	1 (2%)	50	77
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%)	408 (100%)	2 (0%)	81	92
41	s	263/275 (96%)	263 (100%)	0	100	100
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	98/115 (85%)	98 (100%)	0	100	100
44	w	281/283 (99%)	281 (100%)	0	100	100
All	All	7055/7238 (98%)	7027 (100%)	28 (0%)	81	93

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	CYS
2	B	167	ILE
3	C	71	CYS
4	E	94	ILE
4	E	99	GLN
8	I	27	ARG
8	I	95	VAL
9	J	322	VAL
10	K	76	LEU
12	M	203	ASP
12	M	468	GLU
12	M	470	LYS
12	M	483	ARG
14	O	72	GLU
15	P	199	ARG
15	P	201	ASP
15	P	222	GLU
15	P	226	LEU
18	T	43	GLN

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Mol	Chain	Res	Type
20	V	140	LYS
27	d	64	TYR
35	l	70	THR
35	l	71	LEU
35	l	72	GLN
35	l	387	THR
37	n	15	ILE
40	r	255	ASN
40	r	256	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	57	GLN
1	A	277	ASN
1	A	393	ASN
1	A	436	GLN
3	C	111	ASN
4	E	58	GLN
4	E	70	ASN
4	E	95	ASN
4	E	126	HIS
5	F	62	GLN
5	F	80	ASN
6	G	103	HIS
6	G	142	GLN
7	H	83	GLN
9	J	122	HIS
9	J	154	GLN
9	J	295	HIS
10	K	79	HIS
10	K	100	GLN
11	L	86	ASN
12	M	278	HIS
12	M	388	ASN
12	M	464	GLN
13	N	12	GLN
13	N	17	HIS
14	O	41	HIS
14	O	69	ASN
15	P	105	ASN

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Mol	Chain	Res	Type
15	P	124	ASN
16	Q	160	ASN
16	Q	190	HIS
16	Q	234	GLN
16	Q	285	ASN
16	Q	380	HIS
17	S	31	ASN
17	S	40	HIS
17	S	46	ASN
18	T	120	GLN
20	V	134	GLN
24	a	170	GLN
25	b	13	GLN
25	b	14	GLN
26	c	154	GLN
26	c	183	HIS
27	d	54	GLN
27	d	55	GLN
28	e	132	ASN
29	f	61	GLN
30	g	119	HIS
31	h	82	GLN
32	i	91	ASN
32	i	144	GLN
32	i	310	ASN
34	k	50	ASN
34	k	57	ASN
35	l	34	ASN
35	l	67	HIS
35	l	72	GLN
35	l	165	ASN
35	l	309	GLN
37	n	3	ASN
38	o	52	ASN
38	o	79	ASN
39	p	75	GLN
39	p	141	GLN
40	r	81	GLN
40	r	168	GLN
40	r	175	ASN
40	r	251	ASN
40	r	415	GLN

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Mol	Chain	Res	Type
41	s	124	ASN
41	s	250	HIS
41	s	287	HIS
42	u	30	HIS
43	v	4	HIS
43	v	84	GLN
44	w	37	GLN
44	w	92	HIS
44	w	124	ASN
44	w	132	GLN
44	w	142	GLN
44	w	176	GLN
44	w	329	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	2MR	Q	118	16	10,12,13	2.00	1 (10%)	5,13,15	6.10	3 (60%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.70	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	12.42	130.86	119.48
16	Q	118	2MR	CD-NE-CZ	4.33	131.50	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.32	130.77	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.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 2 are monoatomic - leaving 36 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	$\# Z > 2$
49	PLX	V	205	-	51,51,51	1.20	5 (9%)	53,59,59	0.63	1 (1%)
48	PEE	s	401	-	50,50,50	1.18	6 (12%)	53,55,55	0.99	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	CDL	l	712	-	98,98,99	0.93	4 (4%)	104,110,111	1.15	6 (5%)
49	PLX	e	201	-	51,51,51	1.21	4 (7%)	53,59,59	0.60	1 (1%)
45	SF4	B	302	2	0,12,12	-	-	-	-	-
49	PLX	C	312	-	51,51,51	1.21	4 (7%)	53,59,59	0.62	1 (1%)
48	PEE	l	718	-	46,46,50	1.22	6 (13%)	49,51,55	1.02	3 (6%)
49	PLX	n	101	-	51,51,51	0.61	0	53,59,59	0.70	1 (1%)
45	SF4	A	501	1	0,12,12	-	-	-	-	-
50	8Q1	G	201	-	32,34,34	2.34	7 (21%)	39,43,43	1.77	11 (28%)
54	CDL	N	202	-	50,50,99	1.29	4 (8%)	56,62,111	1.28	5 (8%)
45	SF4	C	301	3	0,12,12	-	-	-	-	-
51	NDP	J	401	-	51,52,52	4.25	25 (49%)	71,80,80	2.22	13 (18%)
48	PEE	l	719	-	45,45,50	1.25	6 (13%)	48,50,55	1.01	2 (4%)
52	FES	O	301	14	0,4,4	-	-	-	-	-
49	PLX	i	705	-	51,51,51	1.20	4 (7%)	53,59,59	0.62	1 (1%)
50	8Q1	X	201	-	32,34,34	2.27	7 (21%)	39,43,43	1.68	9 (23%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-
54	CDL	n	102	-	77,77,99	1.03	4 (5%)	83,89,111	1.14	6 (7%)
48	PEE	V	202	-	50,50,50	1.18	6 (12%)	53,55,55	1.02	2 (3%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
54	CDL	a	201	-	90,90,99	0.97	4 (4%)	96,102,111	1.07	6 (6%)
46	FMN	A	502	-	33,33,33	1.44	6 (18%)	48,50,50	1.27	7 (14%)
48	PEE	m	202	-	40,40,50	1.16	5 (12%)	43,45,55	0.99	2 (4%)
47	NAI	A	503	-	47,48,48	4.00	22 (46%)	64,73,73	1.70	12 (18%)
52	FES	M	803	12	0,4,4	-	-	-	-	-
56	UQ	s	403	-	28,28,63	3.31	7 (25%)	36,37,79	2.71	11 (30%)
54	CDL	i	401	-	65,65,99	1.14	4 (6%)	71,77,111	1.21	5 (7%)
48	PEE	C	311	-	46,46,50	1.24	6 (13%)	49,51,55	0.97	2 (4%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
49	PLX	j	203	-	51,51,51	1.22	5 (9%)	53,59,59	0.60	1 (1%)
48	PEE	l	720	-	45,45,50	1.24	6 (13%)	48,50,55	1.02	2 (4%)
54	CDL	r	714	-	99,99,99	1.12	9 (9%)	105,111,111	0.86	4 (3%)
54	CDL	l	713	-	99,99,99	1.12	9 (9%)	105,111,111	0.86	4 (3%)
57	ADP	w	401	-	28,29,29	3.17	9 (32%)	43,45,45	1.91	9 (20%)
48	PEE	U	101	-	50,50,50	1.17	6 (12%)	53,55,55	0.99	2 (3%)

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
49	PLX	V	205	-	-	28/55/55/55	-
48	PEE	s	401	-	-	27/54/54/54	-
54	CDL	l	712	-	-	37/109/109/110	-
49	PLX	e	201	-	-	30/55/55/55	-
45	SF4	B	302	2	-	-	0/6/5/5
49	PLX	C	312	-	-	26/55/55/55	-
48	PEE	l	718	-	-	22/50/50/54	-
49	PLX	n	101	-	-	13/55/55/55	-
54	CDL	N	202	-	-	20/61/61/110	-
50	8Q1	G	201	-	-	20/41/41/41	-
45	SF4	A	501	1	-	-	0/6/5/5
45	SF4	C	301	3	-	-	0/6/5/5
51	NDP	J	401	-	-	4/34/77/77	0/5/5/5
48	PEE	l	719	-	-	26/49/49/54	-
52	FES	O	301	14	-	-	0/1/1/1
49	PLX	i	705	-	-	25/55/55/55	-
50	8Q1	X	201	-	-	22/41/41/41	-
54	CDL	n	102	-	-	26/88/88/110	-
45	SF4	M	801	12	-	-	0/6/5/5
48	PEE	V	202	-	-	26/54/54/54	-
45	SF4	M	802	12	-	-	0/6/5/5
54	CDL	a	201	-	-	27/101/101/110	-
46	FMN	A	502	-	-	7/18/18/18	0/3/3/3
48	PEE	m	202	-	-	20/44/44/54	-
47	NAI	A	503	-	-	8/29/72/72	0/5/5/5
52	FES	M	803	12	-	-	0/1/1/1
56	UQ	s	403	-	-	8/21/45/87	0/1/1/1
54	CDL	i	401	-	-	25/76/76/110	-
48	PEE	C	311	-	-	24/50/50/54	-
45	SF4	B	301	2	-	-	0/6/5/5
49	PLX	j	203	-	-	30/55/55/55	-
48	PEE	l	720	-	-	26/49/49/54	-
54	CDL	r	714	-	-	61/110/110/110	-
54	CDL	l	713	-	-	62/110/110/110	-
57	ADP	w	401	-	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PEE	U	101	-	-	25/54/54/54	-

All (190) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	J	401	NDP	C3B-C2B	-12.94	1.24	1.53
51	J	401	NDP	O4D-C4D	10.73	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.44	1.26	1.53
51	J	401	NDP	C3D-C4D	-10.08	1.27	1.53
56	s	403	UQ	C13-C14	9.58	1.55	1.33
56	s	403	UQ	C8-C9	9.28	1.54	1.33
47	A	503	NAI	O4B-C1B	9.26	1.63	1.42
57	w	401	ADP	C3'-C4'	-8.97	1.30	1.53
47	A	503	NAI	O4B-C4B	-8.38	1.26	1.45
50	G	201	8Q1	P24-O27	8.11	1.85	1.60
51	J	401	NDP	O4B-C4B	-8.08	1.27	1.45
56	s	403	UQ	C18-C19	7.81	1.55	1.32
47	A	503	NAI	C2D-C1D	-7.79	1.29	1.53
57	w	401	ADP	O4'-C4'	7.67	1.62	1.45
50	X	201	8Q1	P24-O27	7.62	1.84	1.60
51	J	401	NDP	C2N-C3N	7.44	1.55	1.35
47	A	503	NAI	C2B-C1B	-7.44	1.30	1.53
51	J	401	NDP	C6N-C5N	7.24	1.55	1.33
47	A	503	NAI	O4D-C4D	6.87	1.60	1.45
57	w	401	ADP	PA-O3A	6.51	1.66	1.59
51	J	401	NDP	PN-O3	6.20	1.66	1.59
50	G	201	8Q1	C28-C29	6.17	1.62	1.52
47	A	503	NAI	PA-O3	6.09	1.66	1.59
47	A	503	NAI	C2D-C3D	5.86	1.69	1.53
51	J	401	NDP	C6A-N6A	5.66	1.48	1.34
51	J	401	NDP	P2B-O2B	5.58	1.69	1.59
50	X	201	8Q1	C28-C29	5.56	1.61	1.52
51	J	401	NDP	PA-O3	5.47	1.65	1.59
57	w	401	ADP	C6-N6	5.46	1.48	1.34
47	A	503	NAI	PN-O3	5.45	1.65	1.59
47	A	503	NAI	O4D-C1D	5.42	1.54	1.42
51	J	401	NDP	C3B-C4B	5.33	1.66	1.53
47	A	503	NAI	C4N-C3N	-5.31	1.40	1.50
47	A	503	NAI	C7N-N7N	5.24	1.48	1.33
51	J	401	NDP	O4D-C1D	-5.12	1.30	1.42
46	A	502	FMN	C9A-C5A	5.05	1.49	1.41
47	A	503	NAI	C6A-N6A	5.04	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	J	401	NDP	C6N-N1N	4.99	1.49	1.37
51	J	401	NDP	C1B-N9A	-4.69	1.33	1.46
51	J	401	NDP	O4B-C1B	4.59	1.52	1.42
57	w	401	ADP	O4'-C1'	-4.55	1.31	1.42
47	A	503	NAI	O2B-C2B	4.35	1.53	1.43
54	N	202	CDL	OB8-CB7	4.34	1.46	1.33
54	l	712	CDL	OA8-CA7	4.32	1.46	1.33
54	l	712	CDL	OB8-CB7	4.28	1.45	1.33
54	N	202	CDL	OA8-CA7	4.28	1.45	1.33
54	i	401	CDL	OB8-CB7	4.28	1.45	1.33
54	a	201	CDL	OB8-CB7	4.28	1.45	1.33
54	a	201	CDL	OA8-CA7	4.27	1.45	1.33
54	i	401	CDL	OA8-CA7	4.27	1.45	1.33
54	n	102	CDL	OA8-CA7	4.22	1.45	1.33
54	n	102	CDL	OB8-CB7	4.20	1.45	1.33
54	i	401	CDL	OB6-CB5	4.17	1.46	1.34
54	N	202	CDL	OA6-CA5	4.16	1.46	1.34
54	i	401	CDL	OA6-CA5	4.15	1.46	1.34
54	l	712	CDL	OB6-CB5	4.14	1.46	1.34
54	a	201	CDL	OB6-CB5	4.07	1.45	1.34
54	a	201	CDL	OA6-CA5	4.06	1.45	1.34
54	n	102	CDL	OB6-CB5	4.06	1.45	1.34
54	N	202	CDL	OB6-CB5	4.05	1.45	1.34
54	n	102	CDL	OA6-CA5	4.00	1.45	1.34
54	l	712	CDL	OA6-CA5	4.00	1.45	1.34
51	J	401	NDP	O2D-C2D	-3.99	1.33	1.43
50	X	201	8Q1	C1-S44	3.97	1.85	1.76
50	G	201	8Q1	C1-S44	3.97	1.85	1.76
48	C	311	PEE	C18-C19	3.83	1.53	1.31
48	s	401	PEE	C18-C19	3.83	1.53	1.31
48	l	719	PEE	C18-C19	3.83	1.53	1.31
51	J	401	NDP	C7N-N7N	3.82	1.44	1.33
48	m	202	PEE	C18-C19	3.82	1.53	1.31
48	l	720	PEE	C18-C19	3.81	1.53	1.31
48	C	311	PEE	C39-C38	3.79	1.53	1.31
48	U	101	PEE	C18-C19	3.79	1.53	1.31
48	l	718	PEE	C18-C19	3.78	1.53	1.31
48	V	202	PEE	C18-C19	3.78	1.53	1.31
48	l	719	PEE	C39-C38	3.73	1.52	1.31
48	l	718	PEE	C39-C38	3.72	1.52	1.31
48	V	202	PEE	C39-C38	3.71	1.52	1.31
48	l	720	PEE	C39-C38	3.71	1.52	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	s	401	PEE	C39-C38	3.70	1.52	1.31
48	U	101	PEE	C39-C38	3.70	1.52	1.31
47	A	503	NAI	C7N-C3N	3.57	1.56	1.48
54	l	713	CDL	OA8-CA7	3.49	1.43	1.33
50	X	201	8Q1	C6-C1	3.46	1.54	1.50
54	r	714	CDL	OA8-CA7	3.46	1.43	1.33
50	G	201	8Q1	C34-N36	3.44	1.41	1.33
50	X	201	8Q1	O27-C28	-3.43	1.32	1.43
47	A	503	NAI	C4N-C5N	-3.40	1.40	1.49
46	A	502	FMN	C8-C7	3.31	1.48	1.40
51	J	401	NDP	C8A-N9A	-3.30	1.31	1.37
57	w	401	ADP	C8-N9	-3.29	1.32	1.37
50	G	201	8Q1	O27-C28	-3.27	1.33	1.43
50	X	201	8Q1	C34-N36	3.19	1.41	1.33
51	J	401	NDP	C5A-N7A	-3.07	1.33	1.39
57	w	401	ADP	O2'-C2'	-3.07	1.35	1.43
57	w	401	ADP	O3'-C3'	3.04	1.50	1.43
54	r	714	CDL	OB6-CB5	3.03	1.42	1.34
54	l	713	CDL	OB8-CB7	3.03	1.42	1.33
54	r	714	CDL	OB8-CB7	3.01	1.42	1.33
54	l	713	CDL	OB6-CB5	2.99	1.42	1.34
54	l	713	CDL	OA6-CA5	2.99	1.42	1.34
54	r	714	CDL	OA6-CA5	2.97	1.42	1.34
51	J	401	NDP	C7N-C3N	2.95	1.55	1.48
49	C	312	PLX	O6-C4	-2.93	1.40	1.44
51	J	401	NDP	O3D-C3D	2.92	1.50	1.43
49	i	705	PLX	O6-C4	-2.84	1.41	1.44
49	j	203	PLX	O6-C4	-2.80	1.41	1.44
47	A	503	NAI	C8A-N9A	-2.79	1.32	1.37
50	X	201	8Q1	C39-N41	2.77	1.40	1.33
49	e	201	PLX	O6-C4	-2.77	1.41	1.44
46	A	502	FMN	C4-N3	-2.76	1.33	1.38
50	G	201	8Q1	C6-C1	2.76	1.53	1.50
56	s	403	UQ	C6-C1	2.74	1.54	1.46
50	G	201	8Q1	C39-N41	2.68	1.39	1.33
48	l	718	PEE	O2-C2	-2.68	1.40	1.46
51	J	401	NDP	O2B-C2B	2.67	1.53	1.44
48	C	311	PEE	O3-C30	2.66	1.41	1.33
48	s	401	PEE	O2-C2	-2.62	1.40	1.46
48	V	202	PEE	O2-C2	-2.61	1.40	1.46
48	l	719	PEE	O2-C2	-2.57	1.40	1.46
48	U	101	PEE	O2-C2	-2.57	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	l	713	CDL	OA6-CA4	-2.53	1.40	1.46
48	C	311	PEE	O2-C2	-2.53	1.40	1.46
48	l	720	PEE	O2-C2	-2.52	1.40	1.46
48	l	718	PEE	O3-C30	2.51	1.40	1.33
54	r	714	CDL	OA6-CA4	-2.51	1.40	1.46
48	l	720	PEE	O3-C30	2.49	1.40	1.33
48	m	202	PEE	O2-C2	-2.48	1.40	1.46
48	l	719	PEE	O3-C30	2.43	1.40	1.33
48	s	401	PEE	O3-C30	2.41	1.40	1.33
47	A	503	NAI	C6N-C5N	2.40	1.40	1.33
49	V	205	PLX	C7-C6	2.39	1.55	1.50
51	J	401	NDP	C2D-C3D	2.39	1.59	1.53
49	j	203	PLX	C7-C6	2.38	1.55	1.50
49	e	201	PLX	C7-C6	2.37	1.55	1.50
49	i	705	PLX	C7-C6	2.37	1.55	1.50
47	A	503	NAI	O3B-C3B	-2.36	1.37	1.43
57	w	401	ADP	C5-N7	-2.36	1.34	1.39
48	V	202	PEE	O3-C3	-2.35	1.39	1.45
48	U	101	PEE	O3-C30	2.35	1.40	1.33
48	m	202	PEE	O3-C30	2.33	1.40	1.33
49	C	312	PLX	C7-C6	2.31	1.55	1.50
54	l	713	CDL	OB6-CB4	-2.30	1.41	1.46
47	A	503	NAI	PN-O5D	2.30	1.68	1.59
48	l	720	PEE	O2-C10	2.30	1.40	1.34
54	l	713	CDL	PB2-OB2	2.29	1.68	1.59
48	V	202	PEE	O3-C30	2.28	1.40	1.33
48	m	202	PEE	O2-C10	2.28	1.40	1.34
48	C	311	PEE	O2-C10	2.28	1.40	1.34
49	V	205	PLX	O6-C4	-2.28	1.41	1.44
54	r	714	CDL	OB6-CB4	-2.26	1.41	1.46
54	r	714	CDL	PB2-OB5	2.25	1.68	1.59
48	U	101	PEE	O2-C10	2.25	1.40	1.34
51	J	401	NDP	O7N-C7N	-2.24	1.19	1.24
54	r	714	CDL	PB2-OB2	2.24	1.68	1.59
54	l	713	CDL	PB2-OB5	2.23	1.68	1.59
48	l	719	PEE	O2-C10	2.23	1.40	1.34
48	V	202	PEE	O2-C10	2.23	1.40	1.34
49	V	205	PLX	P1-O4	2.22	1.68	1.59
47	A	503	NAI	C5B-C4B	2.21	1.58	1.51
46	A	502	FMN	C5A-N5	-2.21	1.35	1.39
48	m	202	PEE	O3-C3	-2.21	1.40	1.45
49	j	203	PLX	P1-O4	2.19	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	l	719	PEE	O3-C3	-2.19	1.40	1.45
56	s	403	UQ	C7-C8	2.18	1.54	1.50
49	i	705	PLX	P1-O4	2.17	1.67	1.59
49	C	312	PLX	P1-O4	2.17	1.67	1.59
48	s	401	PEE	O2-C10	2.17	1.40	1.34
49	e	201	PLX	P1-O4	2.16	1.67	1.59
48	U	101	PEE	O3-C3	-2.16	1.40	1.45
49	V	205	PLX	P1-O1	2.14	1.67	1.59
48	l	720	PEE	O3-C3	-2.14	1.40	1.45
49	j	203	PLX	P1-O1	2.14	1.67	1.59
48	l	718	PEE	O2-C10	2.13	1.40	1.34
56	s	403	UQ	O3-CM3	-2.12	1.40	1.45
47	A	503	NAI	C5A-N7A	-2.12	1.35	1.39
48	s	401	PEE	O3-C3	-2.12	1.40	1.45
56	s	403	UQ	O4-C4	-2.10	1.18	1.23
46	A	502	FMN	C2-N3	-2.09	1.34	1.39
46	A	502	FMN	C4A-N5	2.08	1.35	1.30
49	C	312	PLX	P1-O1	2.07	1.67	1.59
49	e	201	PLX	P1-O1	2.06	1.67	1.59
48	l	718	PEE	O3-C3	-2.04	1.40	1.45
54	l	713	CDL	C11-CA5	2.04	1.56	1.50
54	r	714	CDL	C11-CA5	2.03	1.56	1.50
49	j	203	PLX	C1-C2	2.01	1.57	1.51
49	V	205	PLX	C25-C24	2.01	1.54	1.50
51	J	401	NDP	PA-O5B	2.01	1.67	1.59
49	i	705	PLX	P1-O1	2.01	1.67	1.59
48	C	311	PEE	O3-C3	-2.00	1.40	1.45

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	s	403	UQ	C7-C8-C9	-8.63	111.96	126.83
51	J	401	NDP	C3N-C2N-N1N	-8.14	111.25	123.20
56	s	403	UQ	C12-C13-C14	-6.46	112.83	127.62
51	J	401	NDP	C6N-N1N-C2N	-6.42	112.45	119.32
51	J	401	NDP	C1D-N1N-C2N	-6.40	110.60	121.14
51	J	401	NDP	C5A-C4A-N3A	-5.59	119.02	126.72
51	J	401	NDP	C1D-N1N-C6N	-5.52	109.11	120.77
57	w	401	ADP	C5-C4-N3	-5.47	119.18	126.72
47	A	503	NAI	C5A-C4A-N3A	-5.42	119.25	126.72
50	G	201	8Q1	C6-C1-S44	5.14	119.53	113.40
54	l	712	CDL	OA6-CA5-C11	4.85	121.98	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	w	401	ADP	N3-C2-N1	-4.54	121.71	128.58
56	s	403	UQ	C17-C18-C19	-4.51	112.62	127.64
47	A	503	NAI	N3A-C2A-N1A	-4.42	121.89	128.58
56	s	403	UQ	C10-C9-C8	-4.36	112.43	123.63
50	X	201	8Q1	C6-C1-S44	4.33	118.57	113.40
54	i	401	CDL	OA6-CA5-C11	4.31	120.81	111.48
54	n	102	CDL	OA6-CA5-C11	4.31	120.81	111.48
56	s	403	UQ	C15-C14-C13	-4.28	112.63	123.63
57	w	401	ADP	N3-C4-N9	4.26	134.42	127.17
48	V	202	PEE	O2-C10-C11	4.20	120.56	111.48
51	J	401	NDP	N3A-C2A-N1A	-4.17	122.27	128.58
56	s	403	UQ	C11-C9-C8	-4.11	111.94	121.17
48	s	401	PEE	O2-C10-C11	4.04	120.21	111.48
48	l	719	PEE	O2-C10-C11	4.02	120.17	111.48
54	a	201	CDL	OB6-CB5-C51	4.02	120.17	111.48
48	l	718	PEE	O2-C10-C11	4.01	120.16	111.48
54	l	713	CDL	OA6-CA5-C11	4.01	120.16	111.48
54	N	202	CDL	OB6-CB5-C51	4.01	120.16	111.48
48	m	202	PEE	O2-C10-C11	4.00	120.13	111.48
48	l	720	PEE	O2-C10-C11	3.99	120.11	111.48
51	J	401	NDP	N3A-C4A-N9A	3.98	133.94	127.17
54	N	202	CDL	OA6-CA5-C11	3.97	120.06	111.48
54	i	401	CDL	OB6-CB5-C51	3.95	120.03	111.48
54	r	714	CDL	OB6-CB5-C51	3.95	120.02	111.48
48	C	311	PEE	O2-C10-C11	3.94	120.00	111.48
48	U	101	PEE	O2-C10-C11	3.92	119.97	111.48
50	X	201	8Q1	C43-S44-C1	3.90	113.37	101.84
54	l	713	CDL	OB6-CB5-C51	3.88	119.88	111.48
56	s	403	UQ	C16-C14-C13	-3.86	112.51	121.17
47	A	503	NAI	N3A-C4A-N9A	3.85	133.72	127.17
54	r	714	CDL	OA6-CA5-C11	3.85	119.80	111.48
54	l	712	CDL	OB6-CB5-C51	3.83	119.77	111.48
54	n	102	CDL	OB6-CB5-C51	3.79	119.68	111.48
54	l	712	CDL	CA4-OA6-CA5	-3.77	108.76	117.80
54	a	201	CDL	OA6-CA5-C11	3.75	119.59	111.48
50	G	201	8Q1	C43-S44-C1	3.73	112.87	101.84
47	A	503	NAI	C2A-N3A-C4A	3.68	120.82	111.83
51	J	401	NDP	C2A-N3A-C4A	3.65	120.75	111.83
57	w	401	ADP	C2-N3-C4	3.56	120.52	111.83
50	X	201	8Q1	O35-C34-N36	-3.55	115.47	122.98
57	w	401	ADP	N9-C8-N7	-3.52	108.94	113.94
47	A	503	NAI	C4A-C5A-N7A	-3.47	106.62	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	A	503	NAI	C5A-N7A-C8A	3.41	108.81	103.45
47	A	503	NAI	N9A-C8A-N7A	-3.33	109.20	113.94
56	s	403	UQ	C20-C19-C18	-3.30	112.74	122.66
50	G	201	8Q1	O35-C34-N36	-3.29	116.01	122.98
51	J	401	NDP	N9A-C8A-N7A	-3.26	109.31	113.94
51	J	401	NDP	C4A-C5A-N7A	-3.23	106.89	110.58
56	s	403	UQ	C21-C19-C18	-3.23	112.97	122.66
57	w	401	ADP	C5-N7-C8	3.21	108.49	103.45
47	A	503	NAI	C4D-O4D-C1D	-3.19	102.42	109.47
57	w	401	ADP	C4-N9-C8	3.14	109.03	105.74
51	J	401	NDP	C5A-N7A-C8A	3.09	108.31	103.45
54	a	201	CDL	OB8-CB7-C71	3.03	121.08	111.83
57	w	401	ADP	C4-C5-N7	-3.02	107.13	110.58
54	i	401	CDL	OA8-CA7-C31	2.98	120.91	111.83
56	s	403	UQ	C7-C6-C5	-2.97	119.80	124.89
48	s	401	PEE	O3-C30-C31	2.96	120.87	111.83
54	l	712	CDL	OB8-CB7-C71	2.93	120.78	111.83
54	a	201	CDL	OA8-CA7-C31	2.90	120.66	111.83
50	X	201	8Q1	O2-P24-O27	-2.89	99.13	106.67
48	l	719	PEE	O3-C30-C31	2.85	120.53	111.83
56	s	403	UQ	CM5-C5-C6	-2.81	119.83	124.45
48	V	202	PEE	O3-C30-C31	2.80	120.39	111.83
54	l	712	CDL	OA8-CA7-C31	2.80	120.37	111.83
54	n	102	CDL	OA8-CA7-C31	2.79	120.33	111.83
47	A	503	NAI	C3D-C2D-C1D	2.76	106.69	101.46
50	G	201	8Q1	O2-P24-O27	-2.76	99.48	106.67
46	A	502	FMN	C4-C4A-N5	2.72	121.96	118.21
54	l	713	CDL	OB8-CB7-C71	2.71	120.09	111.83
48	U	101	PEE	O3-C30-C31	2.71	120.09	111.83
54	N	202	CDL	OB8-CB7-C71	2.70	120.08	111.83
48	l	720	PEE	O3-C30-C31	2.68	120.01	111.83
54	N	202	CDL	OA8-CA7-C31	2.68	120.00	111.83
48	l	718	PEE	O3-C30-C31	2.66	119.93	111.83
54	n	102	CDL	OB8-CB7-C71	2.66	119.93	111.83
50	G	201	8Q1	O4-C1-C6	-2.65	120.92	123.98
54	l	713	CDL	OA8-CA7-C31	2.64	119.87	111.83
54	r	714	CDL	OB8-CB7-C71	2.63	119.86	111.83
54	r	714	CDL	OA8-CA7-C31	2.63	119.85	111.83
47	A	503	NAI	C2D-C3D-C4D	2.63	107.69	102.61
50	G	201	8Q1	C32-C34-N36	2.62	121.45	116.48
48	C	311	PEE	O3-C30-C31	2.61	119.81	111.83
51	J	401	NDP	C4A-N9A-C8A	2.59	108.45	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	G	201	8Q1	O40-C39-N41	-2.56	118.00	123.03
49	i	705	PLX	C1A-N1-C1	2.56	120.10	109.91
48	m	202	PEE	O3-C30-C31	2.55	119.60	111.83
54	i	401	CDL	OB8-CB7-C71	2.51	119.49	111.83
50	X	201	8Q1	O40-C39-N41	-2.50	118.13	123.03
46	A	502	FMN	C4A-C10-N1	-2.48	118.50	124.59
49	e	201	PLX	C1A-N1-C1	2.48	119.76	109.91
47	A	503	NAI	C4A-N9A-C8A	2.47	108.33	105.74
50	G	201	8Q1	O4-C1-S44	-2.47	119.55	122.68
54	a	201	CDL	CB4-OB6-CB5	-2.46	111.91	117.80
49	V	205	PLX	C1A-N1-C1	2.42	119.53	109.91
54	n	102	CDL	CA4-OA6-CA5	-2.40	112.04	117.80
54	l	712	CDL	OA6-CA5-OA7	-2.39	118.11	123.70
49	j	203	PLX	C1A-N1-C1	2.37	119.34	109.91
50	G	201	8Q1	C37-C38-C39	2.36	116.33	112.39
50	X	201	8Q1	C32-C34-N36	2.34	120.93	116.48
49	C	312	PLX	C1A-N1-C1	2.34	119.21	109.91
50	X	201	8Q1	O1-P24-O2	2.30	116.43	107.80
54	n	102	CDL	OA6-CA5-OA7	-2.28	118.37	123.70
50	G	201	8Q1	O1-P24-O2	2.27	116.32	107.80
50	X	201	8Q1	O4-C1-S44	-2.23	119.84	122.68
46	A	502	FMN	O4-C4-C4A	-2.22	120.66	126.53
49	n	101	PLX	C2-C1-N1	-2.21	108.73	115.82
51	J	401	NDP	C2B-C1B-N9A	-2.19	110.16	113.75
50	G	201	8Q1	O27-P24-O3	-2.14	100.65	106.44
46	A	502	FMN	C4A-C4-N3	2.14	118.70	113.25
54	i	401	CDL	CA4-OA6-CA5	-2.11	112.74	117.80
46	A	502	FMN	C10-N1-C2	2.10	121.39	116.85
54	N	202	CDL	CB4-OB6-CB5	-2.09	112.79	117.80
47	A	503	NAI	C6N-N1N-C2N	2.08	121.54	119.32
50	X	201	8Q1	O4-C1-C6	-2.07	121.59	123.98
57	w	401	ADP	C4'-O4'-C1'	-2.06	104.91	109.47
46	A	502	FMN	C4-N3-C2	-2.02	122.06	125.64
48	l	718	PEE	C2-O2-C10	-2.01	112.98	117.80
46	A	502	FMN	C4A-C10-N10	2.01	119.35	116.48
54	a	201	CDL	OB6-CB5-OB7	-2.00	119.03	123.70

There are no chirality outliers.

All (678) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C1'-C2'-C3'-O3'
46	A	502	FMN	C1'-C2'-C3'-C4'
48	C	311	PEE	C1-O3P-P-O2P
48	C	311	PEE	C1-O3P-P-O1P
48	C	311	PEE	C1-O3P-P-O4P
48	U	101	PEE	C19-C20-C21-C22
48	U	101	PEE	C11-C10-O2-C2
48	U	101	PEE	C4-O4P-P-O3P
48	U	101	PEE	C4-O4P-P-O2P
48	V	202	PEE	C11-C10-O2-C2
48	V	202	PEE	C4-O4P-P-O3P
48	V	202	PEE	C4-O4P-P-O1P
48	l	718	PEE	C4-O4P-P-O3P
48	l	718	PEE	C4-O4P-P-O2P
48	l	718	PEE	C4-O4P-P-O1P
48	l	719	PEE	C11-C10-O2-C2
48	l	719	PEE	C4-O4P-P-O3P
48	l	719	PEE	C4-O4P-P-O2P
48	l	719	PEE	C4-O4P-P-O1P
48	m	202	PEE	C11-C10-O2-C2
48	m	202	PEE	C4-O4P-P-O3P
48	m	202	PEE	C4-O4P-P-O2P
48	m	202	PEE	C4-O4P-P-O1P
48	m	202	PEE	O4P-C4-C5-N
48	s	401	PEE	O4P-C4-C5-N
49	C	312	PLX	O4-C3-C4-O6
49	C	312	PLX	C3-O4-P1-O1
49	C	312	PLX	C3-O4-P1-O2
49	C	312	PLX	C3-O4-P1-O3
49	C	312	PLX	C2-O1-P1-O4
49	C	312	PLX	C2-O1-P1-O2
49	C	312	PLX	N1-C1-C2-O1
49	V	205	PLX	O7-C6-O6-C4
49	V	205	PLX	C5-C4-O6-C6
49	V	205	PLX	C3-O4-P1-O1
49	V	205	PLX	C3-O4-P1-O2
49	V	205	PLX	O9-C24-O8-C5
49	V	205	PLX	O9-C24-C25-C26
49	e	201	PLX	O7-C6-O6-C4
49	e	201	PLX	C2-O1-P1-O4
49	e	201	PLX	C2-O1-P1-O2

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Mol	Chain	Res	Type	Atoms
49	e	201	PLX	C2-O1-P1-O3
49	e	201	PLX	O9-C24-O8-C5
49	e	201	PLX	O9-C24-C25-C26
49	i	705	PLX	O7-C6-O6-C4
49	i	705	PLX	C25-C24-O8-C5
49	j	203	PLX	O7-C6-C7-C8
49	j	203	PLX	C7-C6-O6-C4
49	j	203	PLX	O7-C6-O6-C4
49	j	203	PLX	O9-C24-C25-C26
49	n	101	PLX	C3-O4-P1-O1
49	n	101	PLX	C2-O1-P1-O4
50	G	201	8Q1	O4-C1-S44-C43
50	G	201	8Q1	C6-C1-S44-C43
50	G	201	8Q1	C28-C29-C32-C34
50	G	201	8Q1	C28-C29-C32-O33
50	G	201	8Q1	C30-C29-C32-C34
50	G	201	8Q1	C30-C29-C32-O33
50	G	201	8Q1	C31-C29-C32-C34
50	G	201	8Q1	C31-C29-C32-O33
50	G	201	8Q1	N36-C37-C38-C39
50	G	201	8Q1	C42-C43-S44-C1
50	G	201	8Q1	C28-O27-P24-O3
50	G	201	8Q1	C28-O27-P24-O2
50	X	201	8Q1	C1-C6-C7-C8
50	X	201	8Q1	O4-C1-S44-C43
50	X	201	8Q1	C6-C1-S44-C43
50	X	201	8Q1	C28-C29-C32-C34
50	X	201	8Q1	C28-C29-C32-O33
50	X	201	8Q1	C30-C29-C32-C34
50	X	201	8Q1	C30-C29-C32-O33
50	X	201	8Q1	C31-C29-C32-C34
50	X	201	8Q1	C31-C29-C32-O33
50	X	201	8Q1	C29-C32-C34-N36
50	X	201	8Q1	C29-C32-C34-O35
50	X	201	8Q1	O33-C32-C34-N36
50	X	201	8Q1	N36-C37-C38-C39
50	X	201	8Q1	C42-C43-S44-C1
54	N	202	CDL	O1-C1-CB2-OB2
54	N	202	CDL	CA2-C1-CB2-OB2
54	N	202	CDL	CA2-OA2-PA1-OA4
54	N	202	CDL	CA2-OA2-PA1-OA5
54	N	202	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
54	N	202	CDL	CA3-OA5-PA1-OA4
54	N	202	CDL	CA6-CA4-OA6-CA5
54	N	202	CDL	C11-CA5-OA6-CA4
54	N	202	CDL	CB2-OB2-PB2-OB4
54	N	202	CDL	CB2-OB2-PB2-OB5
54	a	201	CDL	CA2-OA2-PA1-OA3
54	a	201	CDL	CA2-OA2-PA1-OA4
54	a	201	CDL	CA2-OA2-PA1-OA5
54	a	201	CDL	CA3-OA5-PA1-OA2
54	a	201	CDL	CA3-OA5-PA1-OA4
54	a	201	CDL	CB2-OB2-PB2-OB3
54	a	201	CDL	CB2-OB2-PB2-OB5
54	i	401	CDL	CB2-C1-CA2-OA2
54	i	401	CDL	O1-C1-CB2-OB2
54	i	401	CDL	CA2-OA2-PA1-OA4
54	i	401	CDL	CA2-OA2-PA1-OA5
54	i	401	CDL	CA3-OA5-PA1-OA2
54	i	401	CDL	CA3-OA5-PA1-OA4
54	i	401	CDL	CB2-OB2-PB2-OB5
54	i	401	CDL	CB3-OB5-PB2-OB3
54	i	401	CDL	OB6-CB4-CB6-OB8
54	l	712	CDL	O1-C1-CB2-OB2
54	l	712	CDL	CA2-C1-CB2-OB2
54	l	712	CDL	CA2-OA2-PA1-OA5
54	l	712	CDL	CA3-OA5-PA1-OA2
54	l	712	CDL	CA3-OA5-PA1-OA3
54	l	712	CDL	CB2-OB2-PB2-OB4
54	l	712	CDL	CB2-OB2-PB2-OB5
54	l	713	CDL	O1-C1-CB2-OB2
54	l	713	CDL	CA2-OA2-PA1-OA4
54	l	713	CDL	CA2-OA2-PA1-OA5
54	l	713	CDL	CA3-OA5-PA1-OA2
54	l	713	CDL	CA3-OA5-PA1-OA4
54	l	713	CDL	OA6-CA4-CA6-OA8
54	l	713	CDL	CB2-OB2-PB2-OB4
54	l	713	CDL	CB2-OB2-PB2-OB5
54	l	713	CDL	CB3-OB5-PB2-OB2
54	l	713	CDL	CB3-OB5-PB2-OB3
54	l	713	CDL	OB6-CB4-CB6-OB8
54	n	102	CDL	CA2-OA2-PA1-OA4
54	n	102	CDL	CA2-OA2-PA1-OA5
54	n	102	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
54	n	102	CDL	CA3-OA5-PA1-OA3
54	n	102	CDL	CA3-OA5-PA1-OA4
54	n	102	CDL	CB2-OB2-PB2-OB4
54	n	102	CDL	CB2-OB2-PB2-OB5
54	n	102	CDL	CB3-OB5-PB2-OB3
54	r	714	CDL	CA3-OA5-PA1-OA2
54	r	714	CDL	OA6-CA4-CA6-OA8
54	r	714	CDL	CB3-OB5-PB2-OB3
56	s	403	UQ	C7-C8-C9-C10
56	s	403	UQ	C7-C8-C9-C11
57	w	401	ADP	C5'-O5'-PA-O2A
48	U	101	PEE	O4-C10-O2-C2
48	V	202	PEE	O4-C10-O2-C2
48	m	202	PEE	O4-C10-O2-C2
54	N	202	CDL	OA7-CA5-OA6-CA4
54	N	202	CDL	OB7-CB5-OB6-CB4
54	r	714	CDL	OB7-CB5-OB6-CB4
56	s	403	UQ	C17-C18-C19-C21
48	m	202	PEE	C31-C30-O3-C3
54	r	714	CDL	C71-CB7-OB8-CB6
54	N	202	CDL	C51-CB5-OB6-CB4
54	r	714	CDL	C51-CB5-OB6-CB4
56	s	403	UQ	C12-C11-C9-C10
48	V	202	PEE	C17-C18-C19-C20
56	s	403	UQ	C12-C13-C14-C16
54	r	714	CDL	OB9-CB7-OB8-CB6
48	l	719	PEE	O4-C10-O2-C2
54	N	202	CDL	O1-C1-CA2-OA2
54	n	102	CDL	O1-C1-CA2-OA2
48	l	720	PEE	C31-C30-O3-C3
54	l	712	CDL	C31-CA7-OA8-CA6
54	l	713	CDL	C71-CB7-OB8-CB6
48	m	202	PEE	O5-C30-O3-C3
48	l	718	PEE	C11-C10-O2-C2
48	l	720	PEE	O5-C30-O3-C3
54	l	712	CDL	OA9-CA7-OA8-CA6
56	s	403	UQ	C12-C11-C9-C8
48	l	718	PEE	O4-C10-O2-C2
54	l	713	CDL	OB9-CB7-OB8-CB6
54	l	713	CDL	C11-C12-C13-C14
48	U	101	PEE	C17-C18-C19-C20
48	l	720	PEE	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
49	C	312	PLX	C28-C29-C30-C31
49	e	201	PLX	C12-C13-C14-C15
49	i	705	PLX	C7-C8-C9-C10
54	i	401	CDL	CA2-C1-CB2-OB2
54	l	713	CDL	CA2-C1-CB2-OB2
48	l	719	PEE	C31-C30-O3-C3
54	i	401	CDL	C31-CA7-OA8-CA6
49	V	205	PLX	C9-C10-C11-C12
49	j	203	PLX	C28-C29-C30-C31
49	V	205	PLX	C30-C31-C32-C33
54	l	713	CDL	C59-C60-C61-C62
54	i	401	CDL	O1-C1-CA2-OA2
48	l	719	PEE	O5-C30-O3-C3
54	i	401	CDL	OA9-CA7-OA8-CA6
54	l	713	CDL	C54-C55-C56-C57
48	U	101	PEE	C30-C31-C32-C33
48	l	720	PEE	C10-C11-C12-C13
51	J	401	NDP	O4D-C4D-C5D-O5D
48	V	202	PEE	C41-C42-C43-C44
49	e	201	PLX	C2-C1-N1-C1A
54	l	713	CDL	CB7-C71-C72-C73
54	r	714	CDL	CA7-C31-C32-C33
48	V	202	PEE	C10-C11-C12-C13
54	r	714	CDL	CB7-C71-C72-C73
49	V	205	PLX	C11-C12-C13-C14
49	j	203	PLX	C15-C16-C17-C18
54	l	713	CDL	C35-C36-C37-C38
48	l	719	PEE	C37-C38-C39-C40
48	s	401	PEE	C37-C38-C39-C40
54	l	713	CDL	C39-C40-C41-C42
48	C	311	PEE	C11-C10-O2-C2
51	J	401	NDP	C2D-C1D-N1N-C6N
48	C	311	PEE	O4-C10-O2-C2
48	U	101	PEE	C31-C30-O3-C3
48	V	202	PEE	C31-C30-O3-C3
49	j	203	PLX	C32-C33-C34-C35
49	e	201	PLX	C2-C1-N1-C1C
49	i	705	PLX	C12-C13-C14-C15
54	r	714	CDL	C74-C75-C76-C77
54	l	712	CDL	CB7-C71-C72-C73
54	a	201	CDL	O1-C1-CA2-OA2
48	s	401	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
48	m	202	PEE	C13-C14-C15-C16
54	l	712	CDL	C72-C73-C74-C75
54	l	712	CDL	C20-C21-C22-C23
54	n	102	CDL	C11-CA5-OA6-CA4
48	m	202	PEE	C31-C32-C33-C34
48	m	202	PEE	C22-C23-C24-C25
54	l	713	CDL	C71-C72-C73-C74
54	l	713	CDL	C37-C38-C39-C40
54	l	713	CDL	C60-C61-C62-C63
54	r	714	CDL	C56-C57-C58-C59
49	V	205	PLX	C27-C28-C29-C30
49	e	201	PLX	C25-C26-C27-C28
54	r	714	CDL	C14-C15-C16-C17
54	r	714	CDL	C55-C56-C57-C58
49	i	705	PLX	C33-C34-C35-C36
50	G	201	8Q1	C12-C13-C14-C15
50	G	201	8Q1	C11-C12-C13-C14
49	C	312	PLX	O7-C6-C7-C8
48	C	311	PEE	C32-C33-C34-C35
48	C	311	PEE	C42-C43-C44-C45
48	U	101	PEE	C40-C41-C42-C43
49	e	201	PLX	C13-C14-C15-C16
49	i	705	PLX	C28-C29-C30-C31
49	i	705	PLX	C32-C33-C34-C35
49	C	312	PLX	C17-C18-C19-C20
49	e	201	PLX	C28-C29-C30-C31
49	i	705	PLX	C30-C31-C32-C33
49	j	203	PLX	C12-C13-C14-C15
50	G	201	8Q1	C10-C11-C12-C13
49	j	203	PLX	C27-C28-C29-C30
48	V	202	PEE	C13-C14-C15-C16
54	r	714	CDL	C73-C74-C75-C76
48	l	720	PEE	C11-C10-O2-C2
49	e	201	PLX	C29-C30-C31-C32
54	l	713	CDL	C73-C74-C75-C76
48	U	101	PEE	O5-C30-O3-C3
48	l	720	PEE	C2-C3-O3-C30
49	j	203	PLX	C10-C11-C12-C13
49	i	705	PLX	C10-C11-C12-C13
49	i	705	PLX	C11-C10-C9-C8
49	j	203	PLX	C34-C35-C36-C37
48	l	719	PEE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
48	l	719	PEE	C31-C32-C33-C34
49	j	203	PLX	C7-C8-C9-C10
46	A	502	FMN	O2'-C2'-C3'-O3'
49	C	312	PLX	C7-C8-C9-C10
54	i	401	CDL	C36-C37-C38-C39
54	r	714	CDL	C71-C72-C73-C74
48	V	202	PEE	O5-C30-O3-C3
48	l	720	PEE	C13-C14-C15-C16
54	r	714	CDL	C43-C44-C45-C46
48	l	720	PEE	C22-C23-C24-C25
48	V	202	PEE	C11-C12-C13-C14
54	i	401	CDL	C33-C34-C35-C36
54	l	713	CDL	C75-C76-C77-C78
54	n	102	CDL	C54-C55-C56-C57
48	l	720	PEE	C31-C32-C33-C34
54	l	712	CDL	C75-C76-C77-C78
54	l	712	CDL	C11-CA5-OA6-CA4
48	U	101	PEE	C38-C39-C40-C41
46	A	502	FMN	O2'-C2'-C3'-C4'
48	V	202	PEE	C19-C20-C21-C22
54	r	714	CDL	C13-C14-C15-C16
54	r	714	CDL	C75-C76-C77-C78
49	e	201	PLX	C33-C34-C35-C36
48	s	401	PEE	C30-C31-C32-C33
54	l	713	CDL	CB5-C51-C52-C53
54	r	714	CDL	C12-C13-C14-C15
48	s	401	PEE	O5-C30-O3-C3
48	l	720	PEE	O4-C10-O2-C2
54	l	712	CDL	OA7-CA5-OA6-CA4
54	n	102	CDL	OA7-CA5-OA6-CA4
48	s	401	PEE	C34-C35-C36-C37
49	e	201	PLX	C14-C15-C16-C17
54	i	401	CDL	C11-C12-C13-C14
54	r	714	CDL	C52-C53-C54-C55
54	l	713	CDL	C56-C57-C58-C59
54	n	102	CDL	C75-C76-C77-C78
49	C	312	PLX	C11-C12-C13-C14
49	e	201	PLX	C30-C31-C32-C33
49	V	205	PLX	C13-C14-C15-C16
54	l	713	CDL	C55-C56-C57-C58
54	a	201	CDL	C51-CB5-OB6-CB4
49	V	205	PLX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
48	U	101	PEE	C23-C24-C25-C26
49	j	203	PLX	C25-C26-C27-C28
54	l	712	CDL	C73-C74-C75-C76
54	l	713	CDL	C77-C78-C79-C80
48	V	202	PEE	C22-C23-C24-C25
49	e	201	PLX	C2-C1-N1-C1B
48	l	718	PEE	C34-C35-C36-C37
49	i	705	PLX	C9-C10-C11-C12
49	i	705	PLX	C27-C28-C29-C30
54	l	712	CDL	OA5-CA3-CA4-OA6
48	l	720	PEE	C14-C15-C16-C17
49	V	205	PLX	C12-C13-C14-C15
49	V	205	PLX	C33-C34-C35-C36
54	l	713	CDL	C52-C53-C54-C55
49	V	205	PLX	C16-C17-C18-C19
49	C	312	PLX	C13-C14-C15-C16
49	C	312	PLX	C33-C34-C35-C36
54	r	714	CDL	C32-C33-C34-C35
54	r	714	CDL	C59-C60-C61-C62
49	j	203	PLX	C14-C15-C16-C17
54	n	102	CDL	C53-C54-C55-C56
54	r	714	CDL	O1-C1-CA2-OA2
49	e	201	PLX	C16-C17-C18-C19
49	V	205	PLX	C31-C32-C33-C34
49	i	705	PLX	C25-C26-C27-C28
49	j	203	PLX	C9-C10-C11-C12
49	V	205	PLX	C15-C16-C17-C18
54	r	714	CDL	C41-C42-C43-C44
48	s	401	PEE	C33-C34-C35-C36
49	V	205	PLX	C14-C15-C16-C17
54	l	713	CDL	C62-C63-C64-C65
48	U	101	PEE	C36-C37-C38-C39
54	l	713	CDL	C40-C41-C42-C43
48	s	401	PEE	C35-C36-C37-C38
48	l	718	PEE	C31-C32-C33-C34
54	l	712	CDL	OA5-CA3-CA4-CA6
54	a	201	CDL	OB7-CB5-OB6-CB4
48	l	720	PEE	C32-C33-C34-C35
49	e	201	PLX	C31-C32-C33-C34
49	e	201	PLX	C11-C12-C13-C14
49	n	101	PLX	C10-C11-C12-C13
54	r	714	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
48	l	720	PEE	C1-C2-C3-O3
49	V	205	PLX	C3-C4-C5-O8
49	e	201	PLX	C3-C4-C5-O8
54	i	401	CDL	CB3-CB4-CB6-OB8
54	a	201	CDL	C31-C32-C33-C34
48	C	311	PEE	C15-C16-C17-C18
48	s	401	PEE	C15-C16-C17-C18
54	l	713	CDL	C53-C54-C55-C56
54	N	202	CDL	CB5-C51-C52-C53
48	l	718	PEE	C22-C23-C24-C25
49	C	312	PLX	C15-C16-C17-C18
48	s	401	PEE	C13-C14-C15-C16
48	V	202	PEE	C12-C13-C14-C15
49	C	312	PLX	C31-C32-C33-C34
48	U	101	PEE	C42-C43-C44-C45
48	s	401	PEE	C23-C24-C25-C26
49	e	201	PLX	C9-C10-C11-C12
48	l	720	PEE	C33-C34-C35-C36
54	r	714	CDL	C62-C63-C64-C65
48	s	401	PEE	C17-C18-C19-C20
48	s	401	PEE	C32-C33-C34-C35
49	C	312	PLX	C9-C10-C11-C12
54	a	201	CDL	CB2-C1-CA2-OA2
51	J	401	NDP	C3D-C4D-C5D-O5D
54	r	714	CDL	CA5-C11-C12-C13
54	i	401	CDL	C35-C36-C37-C38
54	r	714	CDL	C17-C18-C19-C20
49	C	312	PLX	C30-C31-C32-C33
49	i	705	PLX	C19-C20-C21-C22
54	l	713	CDL	C72-C73-C74-C75
48	m	202	PEE	O2-C2-C3-O3
54	r	714	CDL	OB6-CB4-CB6-OB8
54	l	713	CDL	C64-C65-C66-C67
54	l	712	CDL	C36-C37-C38-C39
54	l	713	CDL	C14-C15-C16-C17
54	l	712	CDL	C52-C53-C54-C55
48	s	401	PEE	C14-C15-C16-C17
48	U	101	PEE	C32-C33-C34-C35
49	e	201	PLX	C27-C28-C29-C30
48	l	718	PEE	C24-C25-C26-C27
54	l	712	CDL	CB5-C51-C52-C53
54	a	201	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
54	i	401	CDL	C13-C14-C15-C16
54	a	201	CDL	C71-C72-C73-C74
50	G	201	8Q1	C9-C10-C11-C12
54	r	714	CDL	C23-C24-C25-C26
49	j	203	PLX	C26-C27-C28-C29
54	r	714	CDL	C72-C73-C74-C75
49	i	705	PLX	C20-C21-C22-C23
48	l	718	PEE	O3P-C1-C2-C3
49	C	312	PLX	O4-C3-C4-C5
48	s	401	PEE	C11-C10-O2-C2
50	X	201	8Q1	C13-C14-C15-C16
49	C	312	PLX	C16-C17-C18-C19
50	X	201	8Q1	C9-C10-C11-C12
50	G	201	8Q1	C29-C32-C34-N36
48	C	311	PEE	C14-C15-C16-C17
49	e	201	PLX	C7-C8-C9-C10
48	V	202	PEE	C36-C37-C38-C39
48	s	401	PEE	C21-C22-C23-C24
49	i	705	PLX	C14-C15-C16-C17
54	r	714	CDL	C82-C83-C84-C85
48	s	401	PEE	C10-C11-C12-C13
48	C	311	PEE	C1-C2-C3-O3
48	l	718	PEE	C1-C2-C3-O3
49	j	203	PLX	C3-C4-C5-O8
54	l	713	CDL	CA3-CA4-CA6-OA8
54	l	713	CDL	CB3-CB4-CB6-OB8
54	r	714	CDL	CB3-CB4-CB6-OB8
48	l	720	PEE	C23-C24-C25-C26
54	r	714	CDL	C60-C61-C62-C63
48	V	202	PEE	C30-C31-C32-C33
48	m	202	PEE	C11-C12-C13-C14
49	j	203	PLX	C19-C20-C21-C22
48	C	311	PEE	C41-C42-C43-C44
48	l	719	PEE	C13-C14-C15-C16
54	l	712	CDL	C35-C36-C37-C38
48	U	101	PEE	C43-C44-C45-C46
48	l	720	PEE	C34-C35-C36-C37
54	r	714	CDL	C64-C65-C66-C67
50	X	201	8Q1	O4-C1-C6-C7
50	X	201	8Q1	S44-C1-C6-C7
47	A	503	NAI	PN-O3-PA-O5B
54	r	714	CDL	C80-C81-C82-C83

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Mol	Chain	Res	Type	Atoms
48	U	101	PEE	C41-C42-C43-C44
48	l	720	PEE	C16-C17-C18-C19
54	l	712	CDL	C81-C82-C83-C84
54	n	102	CDL	CB2-C1-CA2-OA2
48	l	718	PEE	C11-C12-C13-C14
49	i	705	PLX	O4-C3-C4-C5
54	l	713	CDL	OA5-CA3-CA4-CA6
48	l	718	PEE	C18-C19-C20-C21
54	i	401	CDL	C71-C72-C73-C74
48	m	202	PEE	C3-C2-O2-C10
49	j	203	PLX	C31-C32-C33-C34
48	C	311	PEE	C13-C14-C15-C16
48	l	719	PEE	C32-C33-C34-C35
56	s	403	UQ	C1-C2-O2-CM2
50	X	201	8Q1	C11-C12-C13-C14
54	l	713	CDL	C58-C59-C60-C61
48	s	401	PEE	O4-C10-O2-C2
48	l	718	PEE	O3P-C1-C2-O2
48	l	719	PEE	O3P-C1-C2-O2
48	m	202	PEE	O3P-C1-C2-O2
54	a	201	CDL	OA5-CA3-CA4-OA6
48	s	401	PEE	C1-C2-C3-O3
54	r	714	CDL	CA3-CA4-CA6-OA8
48	l	720	PEE	C5-C4-O4P-P
48	C	311	PEE	C37-C38-C39-C40
48	C	311	PEE	C39-C40-C41-C42
48	l	720	PEE	O2-C2-C3-O3
49	j	203	PLX	O6-C4-C5-O8
49	j	203	PLX	C33-C34-C35-C36
50	X	201	8Q1	C7-C8-C9-C10
48	l	718	PEE	C32-C33-C34-C35
48	s	401	PEE	C24-C25-C26-C27
48	s	401	PEE	C20-C21-C22-C23
49	C	312	PLX	C25-C26-C27-C28
51	J	401	NDP	O4D-C1D-N1N-C6N
47	A	503	NAI	C3D-C4D-C5D-O5D
49	n	101	PLX	N1-C1-C2-O1
49	i	705	PLX	C13-C14-C15-C16
48	l	718	PEE	C21-C22-C23-C24
48	U	101	PEE	C37-C38-C39-C40
54	r	714	CDL	C51-C52-C53-C54
49	j	203	PLX	C25-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
54	a	201	CDL	C71-CB7-OB8-CB6
48	s	401	PEE	C39-C40-C41-C42
48	m	202	PEE	O3P-C1-C2-C3
54	r	714	CDL	C78-C79-C80-C81
48	V	202	PEE	C24-C25-C26-C27
49	j	203	PLX	O6-C6-C7-C8
49	n	101	PLX	O6-C6-C7-C8
48	s	401	PEE	O3P-C1-C2-O2
49	i	705	PLX	O4-C3-C4-O6
54	l	713	CDL	OA5-CA3-CA4-OA6
49	j	203	PLX	C13-C14-C15-C16
48	l	720	PEE	C18-C19-C20-C21
49	C	312	PLX	C27-C28-C29-C30
54	n	102	CDL	CB7-C71-C72-C73
48	C	311	PEE	O2-C2-C3-O3
48	l	718	PEE	O2-C2-C3-O3
49	V	205	PLX	O6-C4-C5-O8
48	C	311	PEE	C10-C11-C12-C13
48	m	202	PEE	C1-C2-C3-O3
47	A	503	NAI	C2D-C1D-N1N-C2N
54	i	401	CDL	C14-C15-C16-C17
48	V	202	PEE	C23-C24-C25-C26
54	r	714	CDL	C76-C77-C78-C79
54	l	712	CDL	C51-C52-C53-C54
54	l	713	CDL	C33-C34-C35-C36
46	A	502	FMN	C2'-C1'-N10-C10
47	A	503	NAI	C5B-O5B-PA-O1A
48	U	101	PEE	C1-O3P-P-O2P
48	U	101	PEE	C1-O3P-P-O4P
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	l	719	PEE	C1-O3P-P-O2P
48	l	719	PEE	O4P-C4-C5-N
49	C	312	PLX	C2-O1-P1-O3
49	V	205	PLX	C2-O1-P1-O4
49	V	205	PLX	C2-O1-P1-O3
49	i	705	PLX	C3-O4-P1-O2
49	i	705	PLX	C2-O1-P1-O2
49	n	101	PLX	C3-O4-P1-O2
49	n	101	PLX	C2-O1-P1-O2
54	a	201	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
54	a	201	CDL	CB3-OB5-PB2-OB3
54	i	401	CDL	CB2-OB2-PB2-OB3
54	l	712	CDL	CA2-OA2-PA1-OA3
54	l	712	CDL	CA3-OA5-PA1-OA4
54	l	712	CDL	CB2-OB2-PB2-OB3
54	l	713	CDL	CA2-OA2-PA1-OA3
54	l	713	CDL	CB2-OB2-PB2-OB3
54	n	102	CDL	CB3-OB5-PB2-OB2
54	n	102	CDL	CB3-OB5-PB2-OB4
54	r	714	CDL	CA2-OA2-PA1-OA3
54	r	714	CDL	CA3-OA5-PA1-OA3
54	r	714	CDL	CB2-OB2-PB2-OB3
54	r	714	CDL	CB2-OB2-PB2-OB4
54	r	714	CDL	CB2-OB2-PB2-OB5
54	r	714	CDL	CB3-OB5-PB2-OB2
57	w	401	ADP	C5'-O5'-PA-O1A
57	w	401	ADP	C5'-O5'-PA-O3A
54	r	714	CDL	C42-C43-C44-C45
54	l	712	CDL	C37-C38-C39-C40
54	r	714	CDL	CB4-CB3-OB5-PB2
54	N	202	CDL	OA9-CA7-OA8-CA6
54	r	714	CDL	C20-C21-C22-C23
54	l	713	CDL	C12-C13-C14-C15
54	r	714	CDL	C39-C40-C41-C42
49	e	201	PLX	C36-C37-C38-C39
48	C	311	PEE	C20-C21-C22-C23
54	l	713	CDL	C44-C45-C46-C47
48	l	718	PEE	C38-C39-C40-C41
48	l	719	PEE	C30-C31-C32-C33
54	l	713	CDL	C34-C35-C36-C37
48	l	719	PEE	C1-C2-O2-C10
48	l	719	PEE	C3-C2-O2-C10
54	a	201	CDL	CA6-CA4-OA6-CA5
54	l	712	CDL	CA6-CA4-OA6-CA5
49	j	203	PLX	C30-C31-C32-C33
49	V	205	PLX	C10-C11-C12-C13
48	s	401	PEE	O3P-C1-C2-C3
49	j	203	PLX	O4-C3-C4-C5
54	N	202	CDL	C11-C12-C13-C14
49	j	203	PLX	O4-C3-C4-O6
54	a	201	CDL	OB9-CB7-OB8-CB6
54	l	713	CDL	C57-C58-C59-C60

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Mol	Chain	Res	Type	Atoms
54	N	202	CDL	C31-CA7-OA8-CA6
54	l	712	CDL	CA4-CA3-OA5-PA1
48	s	401	PEE	O2-C2-C3-O3
49	e	201	PLX	O6-C4-C5-O8
54	l	713	CDL	O1-C1-CA2-OA2
48	C	311	PEE	C11-C12-C13-C14
48	C	311	PEE	C38-C39-C40-C41
49	V	205	PLX	C4-C5-O8-C24
49	n	101	PLX	O7-C6-C7-C8
54	r	714	CDL	C44-C45-C46-C47
49	e	201	PLX	O8-C24-C25-C26
54	l	713	CDL	C63-C64-C65-C66
47	A	503	NAI	C2D-C1D-N1N-C6N
54	r	714	CDL	C81-C82-C83-C84
48	l	718	PEE	C10-C11-C12-C13
48	m	202	PEE	C18-C19-C20-C21
48	C	311	PEE	C33-C34-C35-C36
54	r	714	CDL	C83-C84-C85-C86
54	r	714	CDL	C15-C16-C17-C18
54	r	714	CDL	C54-C55-C56-C57
49	i	705	PLX	C15-C16-C17-C18
54	r	714	CDL	C63-C64-C65-C66
49	V	205	PLX	C29-C30-C31-C32
54	l	712	CDL	C24-C25-C26-C27
47	A	503	NAI	O4D-C1D-N1N-C2N
48	l	720	PEE	C38-C39-C40-C41
54	r	714	CDL	CB2-C1-CA2-OA2
54	l	712	CDL	C76-C77-C78-C79
49	j	203	PLX	C11-C12-C13-C14
54	i	401	CDL	CA6-CA4-OA6-CA5
54	n	102	CDL	CA6-CA4-OA6-CA5
48	C	311	PEE	C30-C31-C32-C33
48	U	101	PEE	C24-C25-C26-C27
49	n	101	PLX	C13-C14-C15-C16
54	l	713	CDL	C32-C33-C34-C35
48	l	720	PEE	C36-C37-C38-C39
54	N	202	CDL	OB6-CB4-CB6-OB8
54	l	712	CDL	OA6-CA4-CA6-OA8
49	e	201	PLX	C26-C27-C28-C29
54	l	713	CDL	C17-C18-C19-C20
49	C	312	PLX	C36-C37-C38-C39
47	A	503	NAI	C2N-C3N-C7N-N7N

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Mol	Chain	Res	Type	Atoms
48	m	202	PEE	O3-C30-C31-C32
48	l	718	PEE	C35-C36-C37-C38
54	a	201	CDL	CA2-C1-CB2-OB2
54	l	713	CDL	C13-C14-C15-C16
54	n	102	CDL	C78-C79-C80-C81
48	V	202	PEE	C16-C17-C18-C19
49	V	205	PLX	O8-C24-C25-C26
54	l	713	CDL	C15-C16-C17-C18
49	n	101	PLX	C33-C34-C35-C36
48	V	202	PEE	C44-C45-C46-C47
49	V	205	PLX	C7-C8-C9-C10
50	G	201	8Q1	C1-C6-C7-C8
48	l	718	PEE	C2-C1-O3P-P
54	a	201	CDL	CA4-CA3-OA5-PA1
54	l	712	CDL	C56-C57-C58-C59
54	l	713	CDL	C31-C32-C33-C34
48	V	202	PEE	C18-C19-C20-C21
54	N	202	CDL	CB2-C1-CA2-OA2
49	e	201	PLX	C24-C25-C26-C27
48	l	719	PEE	O3P-C1-C2-C3
54	a	201	CDL	OA5-CA3-CA4-CA6
48	l	719	PEE	O2-C2-C3-O3
48	s	401	PEE	C36-C37-C38-C39
48	l	719	PEE	C14-C15-C16-C17
48	U	101	PEE	C12-C13-C14-C15
54	n	102	CDL	C18-C19-C20-C21
50	G	201	8Q1	C28-O27-P24-O1
54	n	102	CDL	C12-C13-C14-C15
49	e	201	PLX	C10-C11-C12-C13
48	l	719	PEE	C36-C37-C38-C39
48	l	719	PEE	C16-C17-C18-C19
48	s	401	PEE	C31-C32-C33-C34
54	i	401	CDL	OA5-CA3-CA4-OA6
50	X	201	8Q1	C6-C7-C8-C9
48	l	718	PEE	C36-C37-C38-C39
54	r	714	CDL	C40-C41-C42-C43
48	l	719	PEE	C18-C19-C20-C21
54	a	201	CDL	C72-C73-C74-C75
54	i	401	CDL	OA5-CA3-CA4-CA6
48	l	720	PEE	O2-C10-C11-C12
48	C	311	PEE	C16-C17-C18-C19
48	U	101	PEE	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
54	r	714	CDL	C1-CB2-OB2-PB2
54	n	102	CDL	C12-C11-CA5-OA6
54	a	201	CDL	O1-C1-CB2-OB2
48	V	202	PEE	C31-C32-C33-C34
54	l	712	CDL	C74-C75-C76-C77
54	l	713	CDL	OB7-CB5-OB6-CB4
49	n	101	PLX	O4-C3-C4-O6
50	G	201	8Q1	C29-C32-C34-O35
56	s	403	UQ	C13-C14-C16-C17
54	a	201	CDL	C58-C59-C60-C61
54	l	712	CDL	C71-C72-C73-C74
48	C	311	PEE	O3-C30-C31-C32
48	l	719	PEE	C1-C2-C3-O3
49	V	205	PLX	C26-C27-C28-C29
50	X	201	8Q1	N41-C42-C43-S44
54	r	714	CDL	C33-C34-C35-C36
54	l	713	CDL	C32-C31-CA7-OA8
48	l	720	PEE	O3-C30-C31-C32
47	A	503	NAI	O4D-C1D-N1N-C6N
49	i	705	PLX	C35-C36-C37-C38
48	V	202	PEE	O3P-C1-C2-C3
54	n	102	CDL	C14-C15-C16-C17
54	l	713	CDL	C82-C83-C84-C85
54	n	102	CDL	CA5-C11-C12-C13
49	n	101	PLX	C7-C8-C9-C10
48	C	311	PEE	O5-C30-C31-C32
49	i	705	PLX	O8-C24-C25-C26
49	j	203	PLX	O8-C24-C25-C26
54	a	201	CDL	CA5-C11-C12-C13
54	l	713	CDL	C41-C42-C43-C44
48	l	719	PEE	C34-C35-C36-C37
49	i	705	PLX	O9-C24-O8-C5
49	n	101	PLX	O9-C24-O8-C5
54	n	102	CDL	C12-C11-CA5-OA7
49	j	203	PLX	C4-C5-O8-C24
48	l	720	PEE	O4-C10-C11-C12
48	m	202	PEE	C23-C24-C25-C26
49	C	312	PLX	C18-C19-C20-C21
49	C	312	PLX	C11-C10-C9-C8
54	l	712	CDL	C72-C71-CB7-OB8
54	l	713	CDL	C12-C11-CA5-OA6
54	r	714	CDL	C52-C51-CB5-OB6

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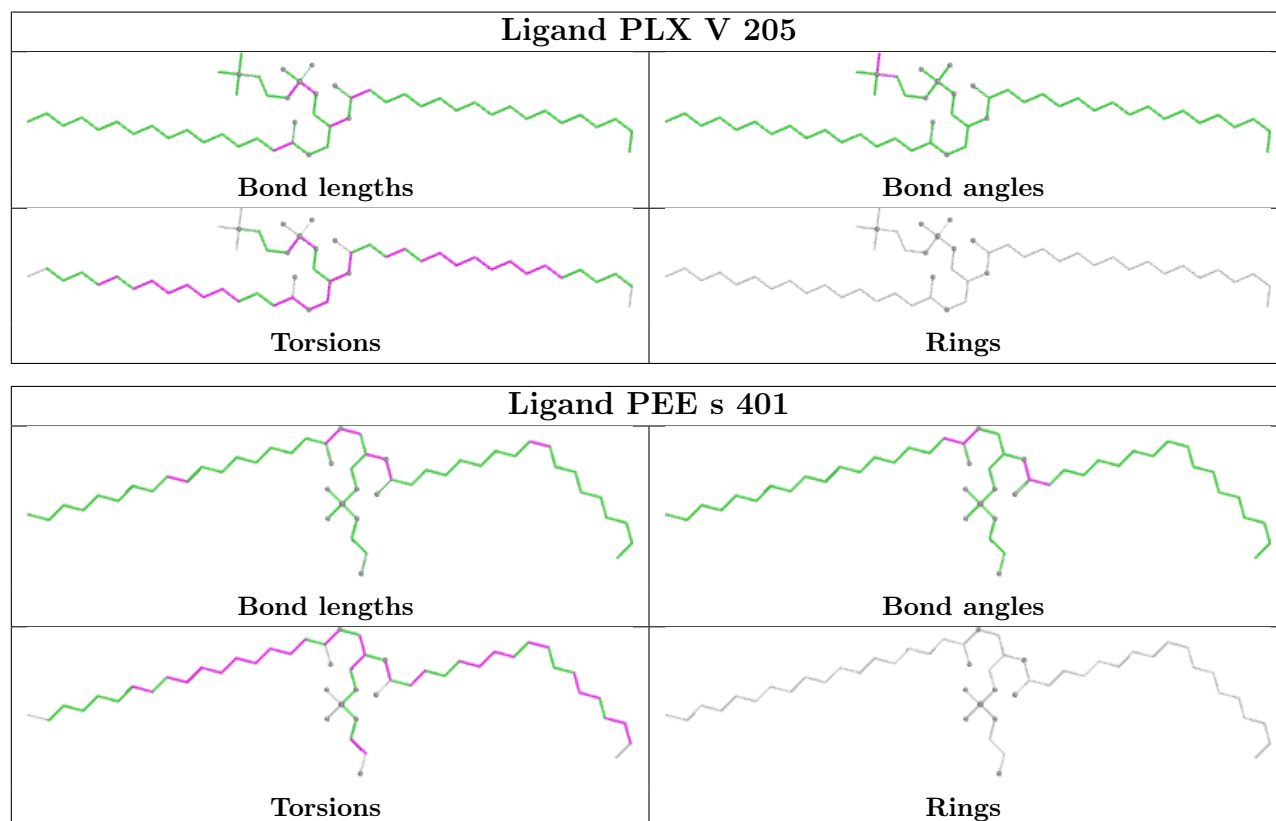
Mol	Chain	Res	Type	Atoms
48	U	101	PEE	O3-C30-C31-C32
54	l	713	CDL	C32-C31-CA7-OA9
54	l	713	CDL	C51-CB5-OB6-CB4
48	U	101	PEE	O2-C10-C11-C12
48	l	720	PEE	O5-C30-C31-C32

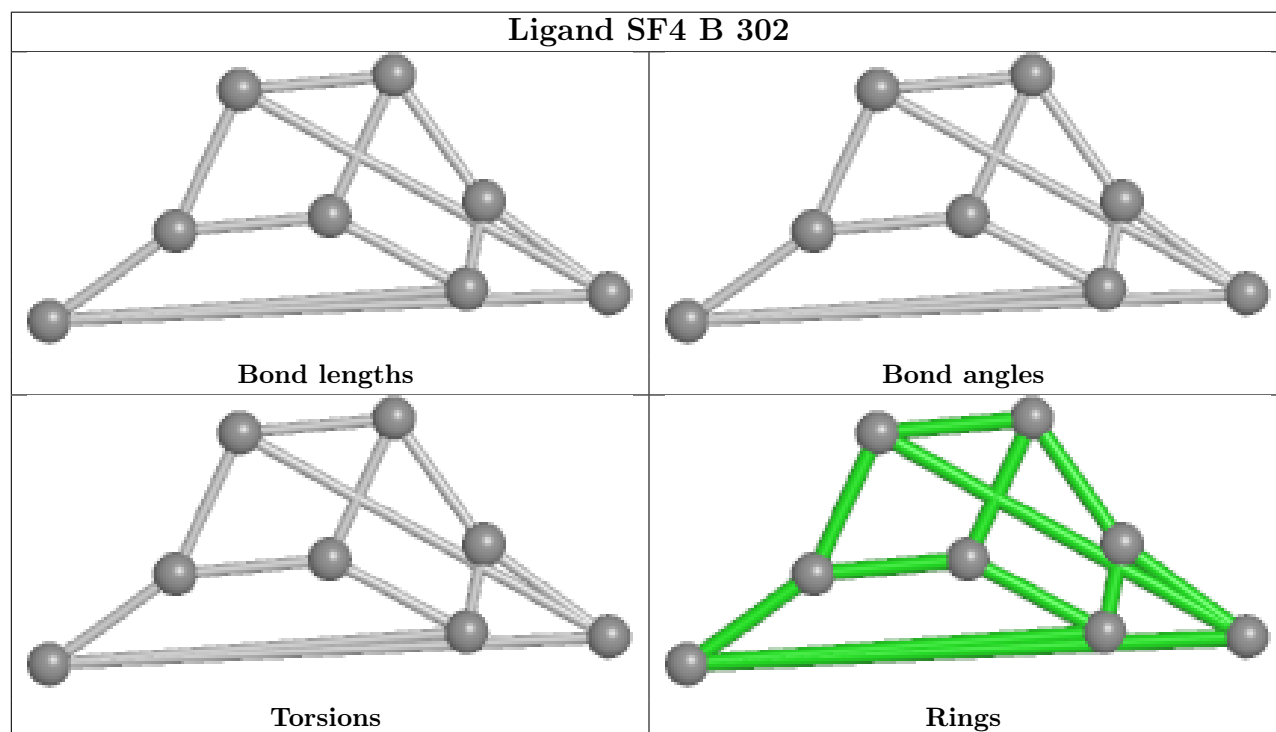
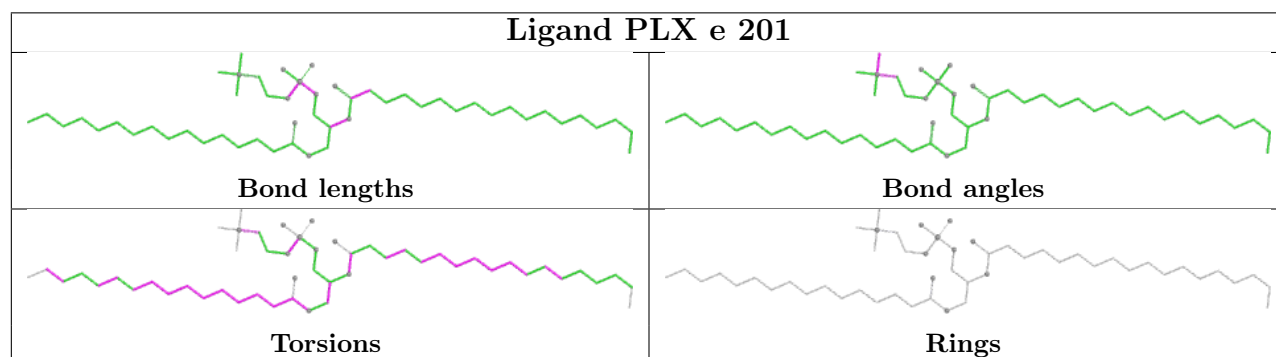
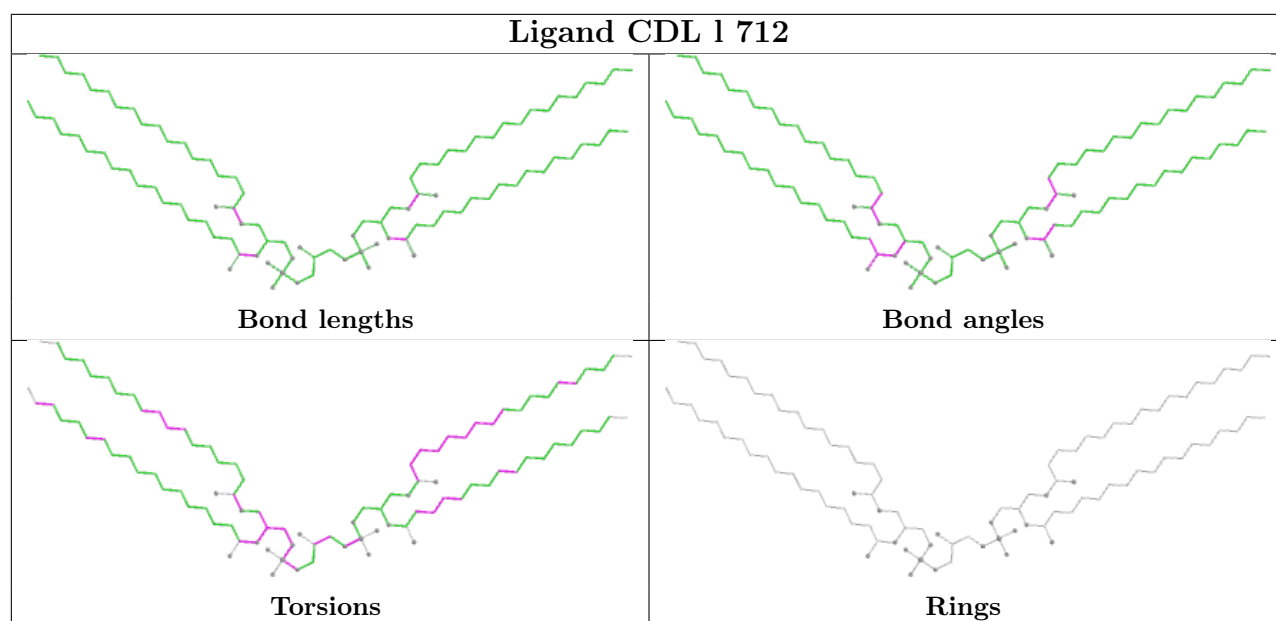
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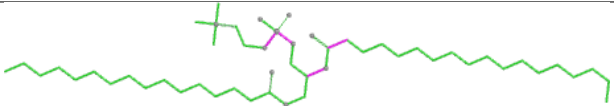
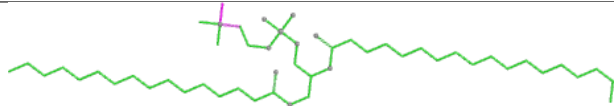
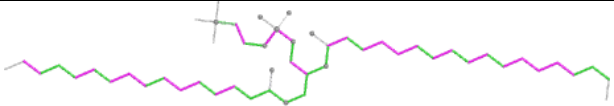
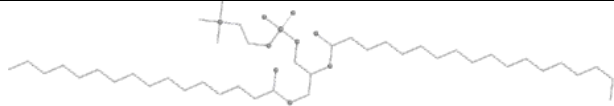
31 monomers are involved in 347 short contacts:

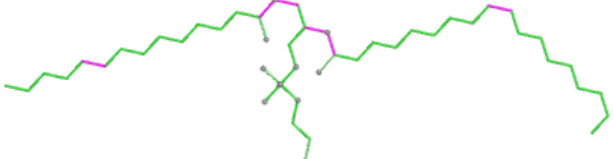
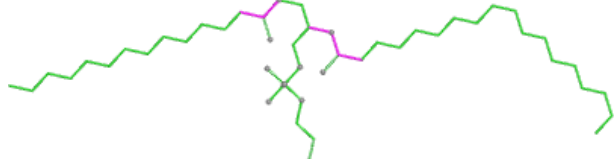
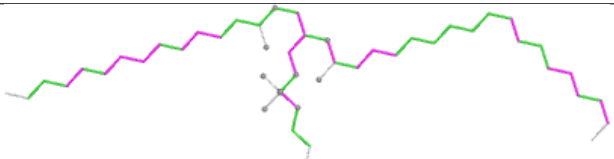
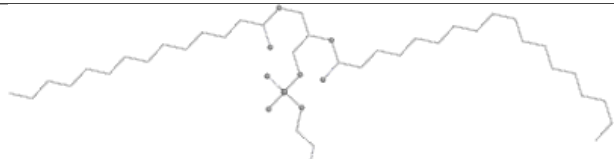
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	V	205	PLX	5	0
48	s	401	PEE	4	0
54	l	712	CDL	31	0
49	e	201	PLX	2	0
49	C	312	PLX	11	0
48	l	718	PEE	19	0
49	n	101	PLX	12	0
45	A	501	SF4	2	0
50	G	201	8Q1	2	0
54	N	202	CDL	12	0
45	C	301	SF4	4	0
51	J	401	NDP	7	0
48	l	719	PEE	10	0
49	i	705	PLX	4	0
50	X	201	8Q1	6	0
54	n	102	CDL	21	0
48	V	202	PEE	22	0
54	a	201	CDL	27	0
46	A	502	FMN	10	0
48	m	202	PEE	12	0
47	A	503	NAI	8	0
52	M	803	FES	2	0
56	s	403	UQ	51	0
54	i	401	CDL	10	0
48	C	311	PEE	41	0
49	j	203	PLX	3	0
48	l	720	PEE	19	0
54	r	714	CDL	10	0
54	l	713	CDL	5	0
57	w	401	ADP	5	0
48	U	101	PEE	11	0

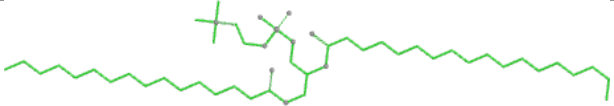
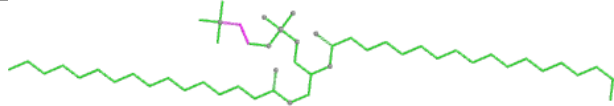
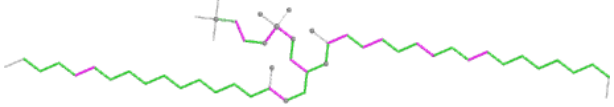
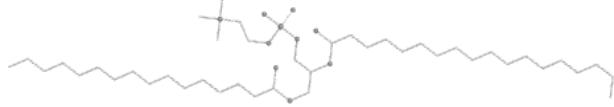
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

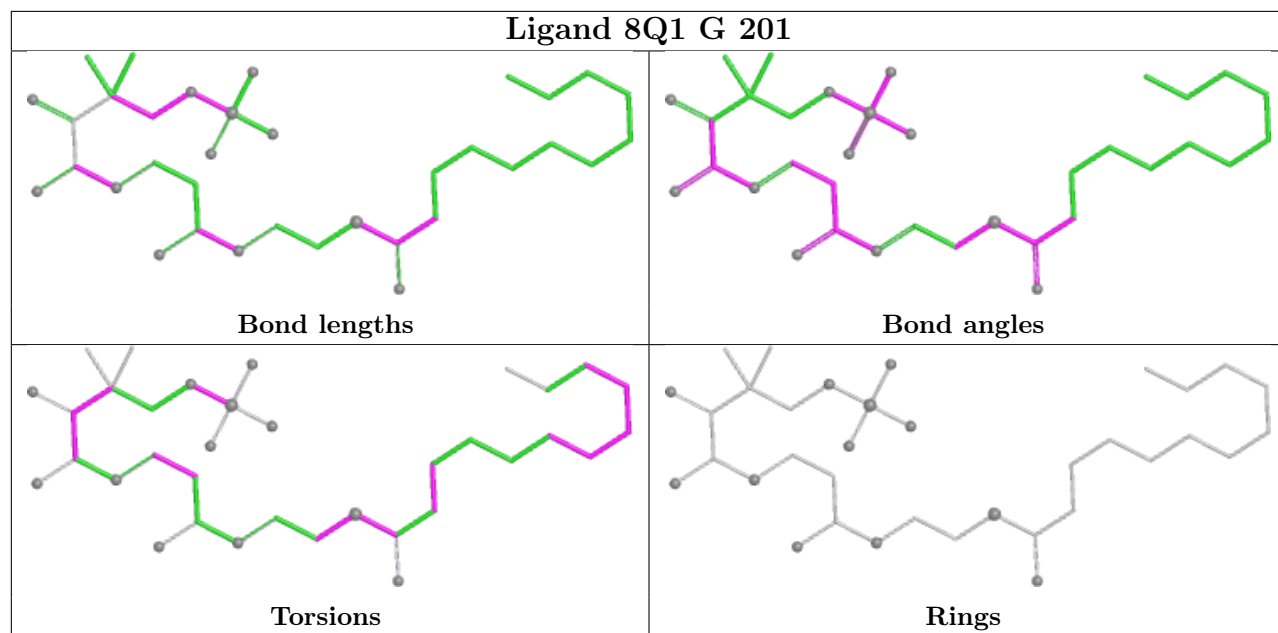
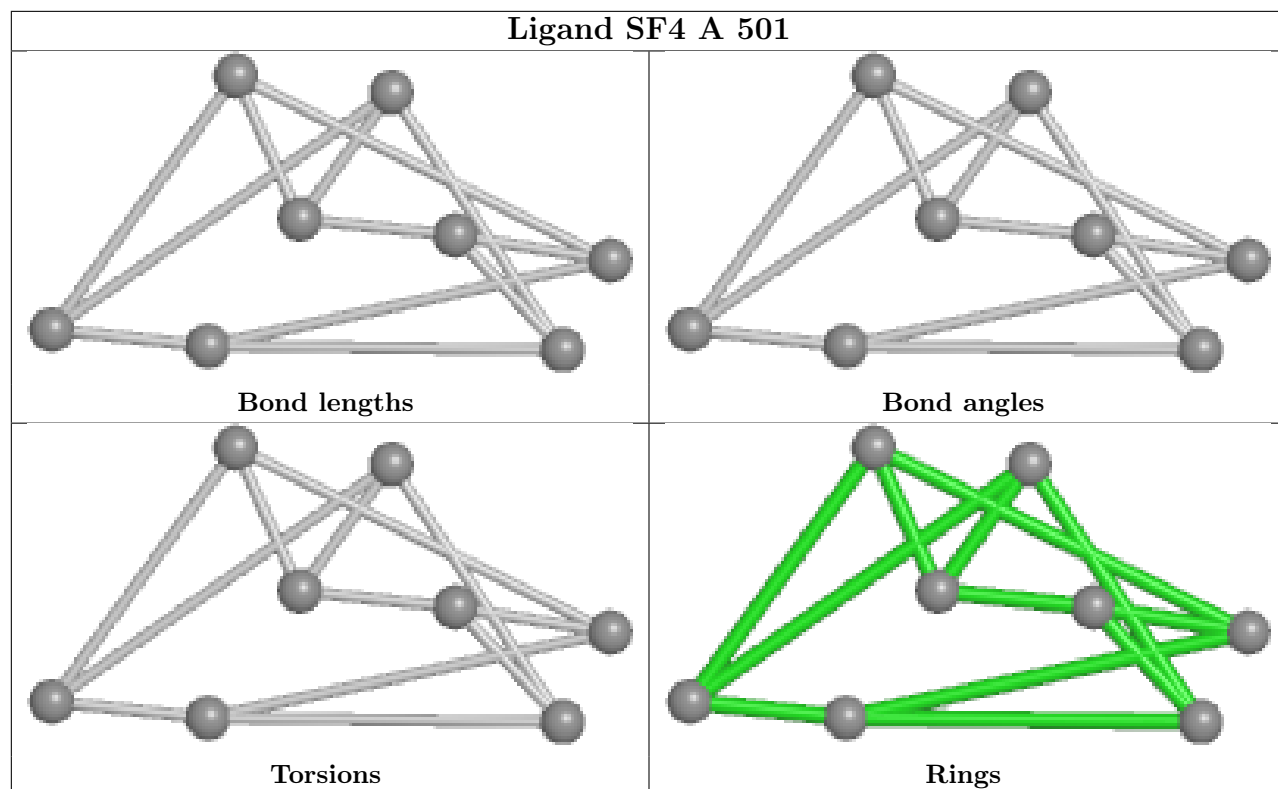


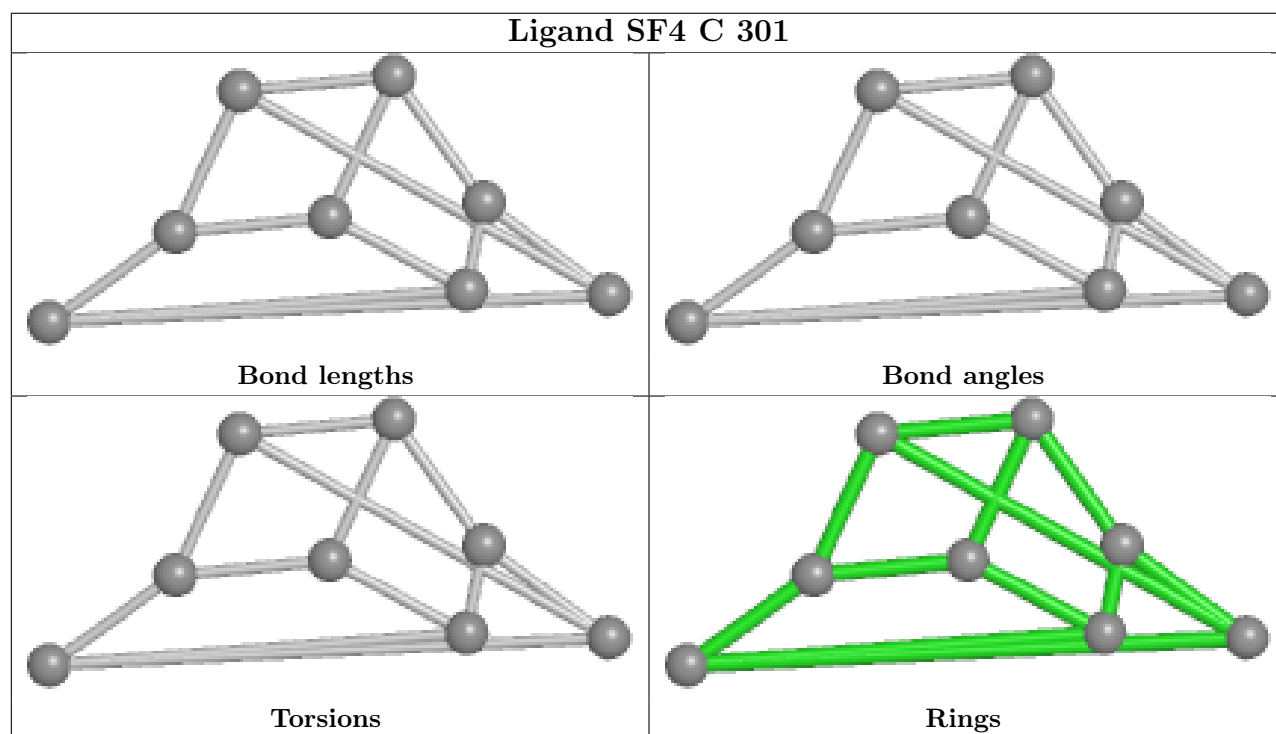
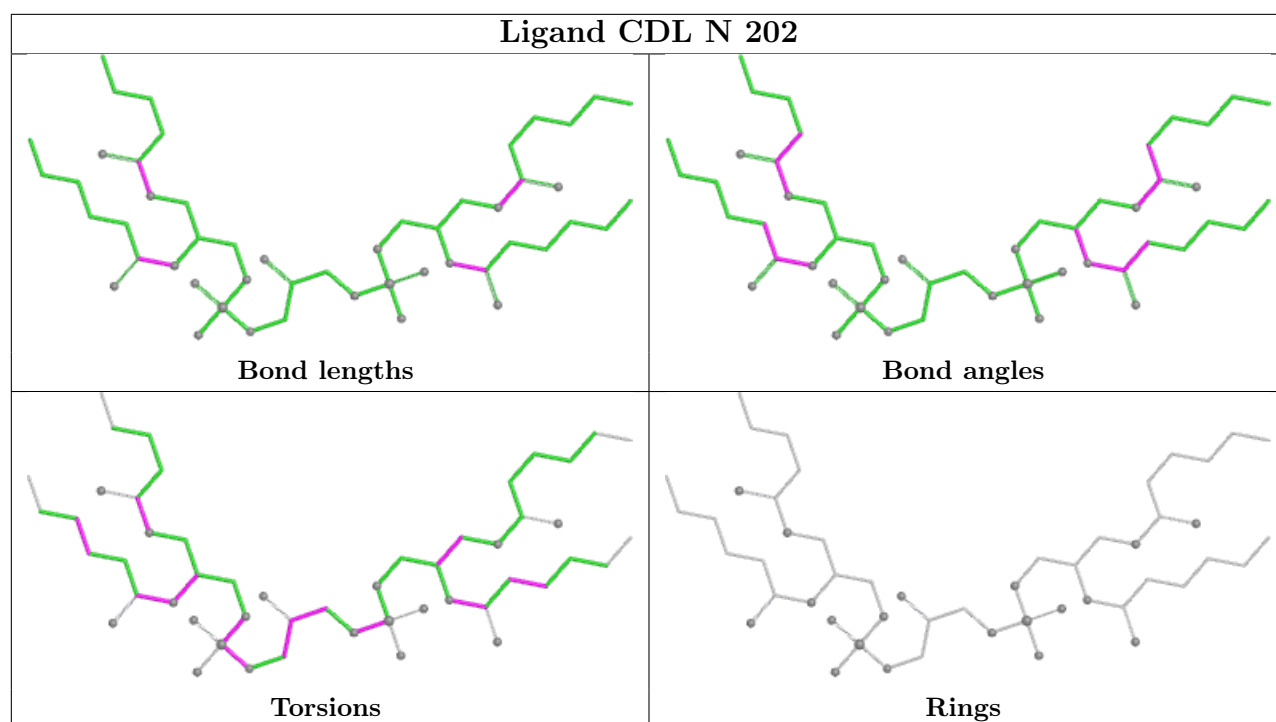


Ligand PLX C 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

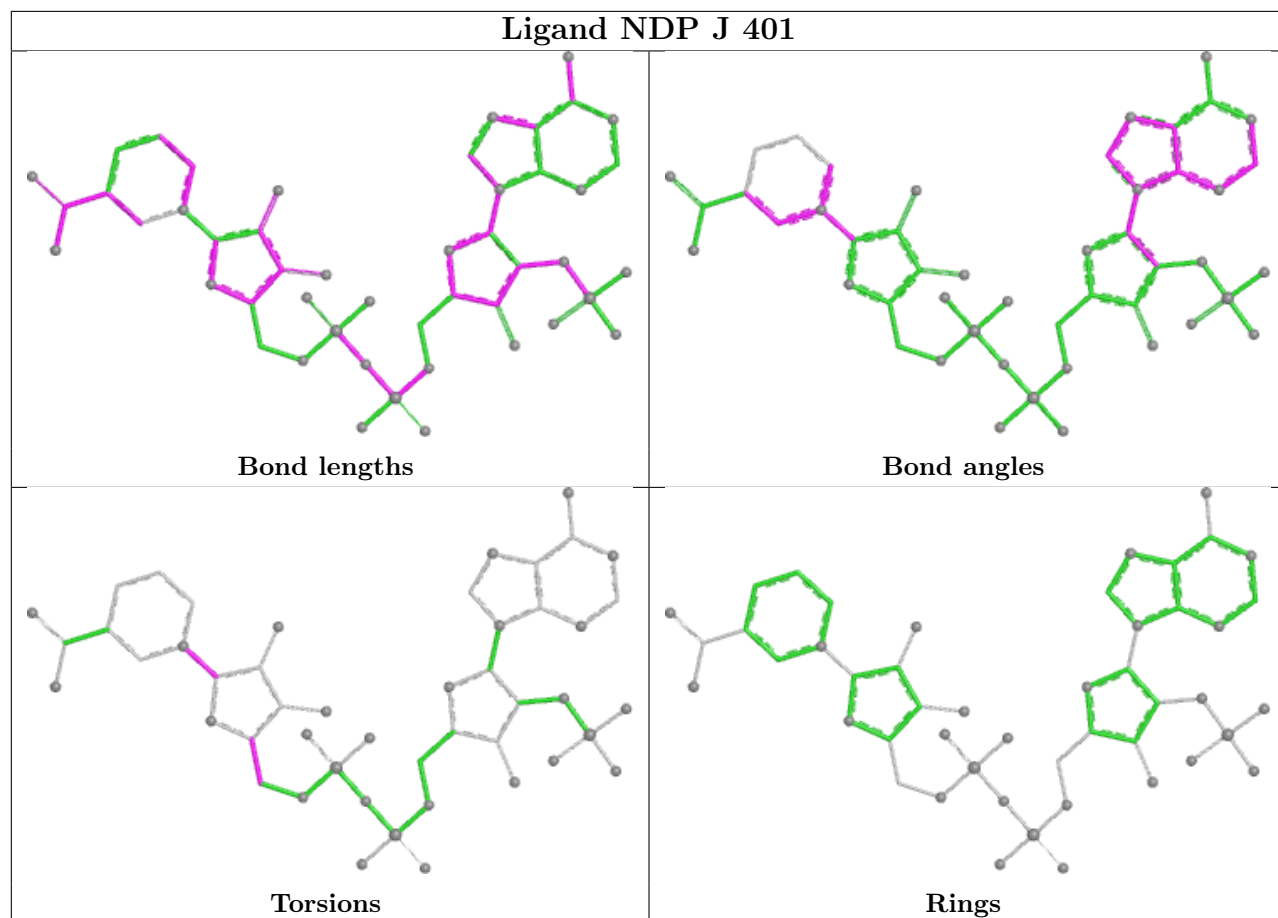
Ligand PEE l 718	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PLX n 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

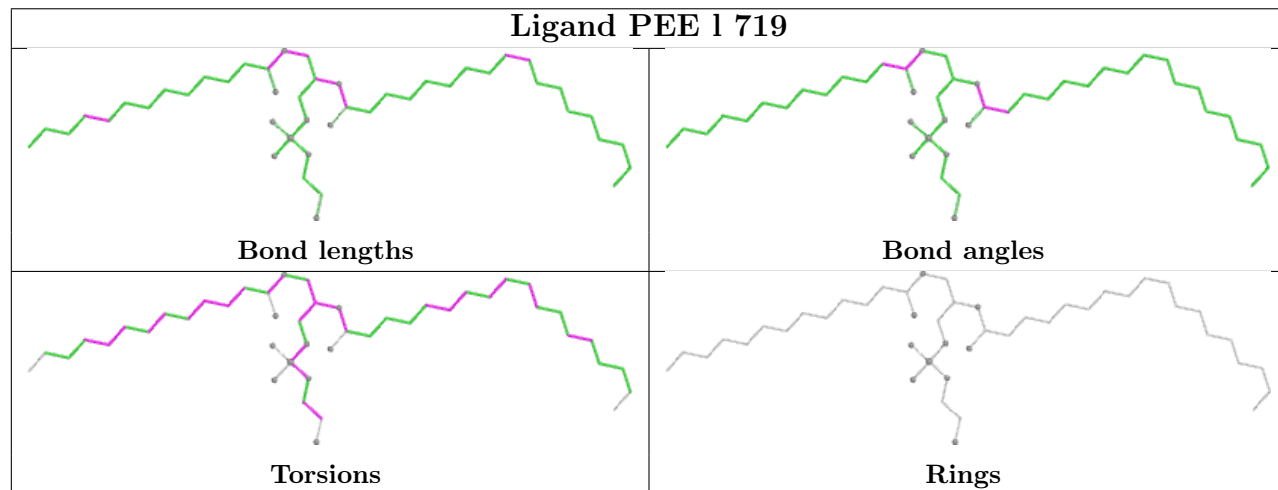


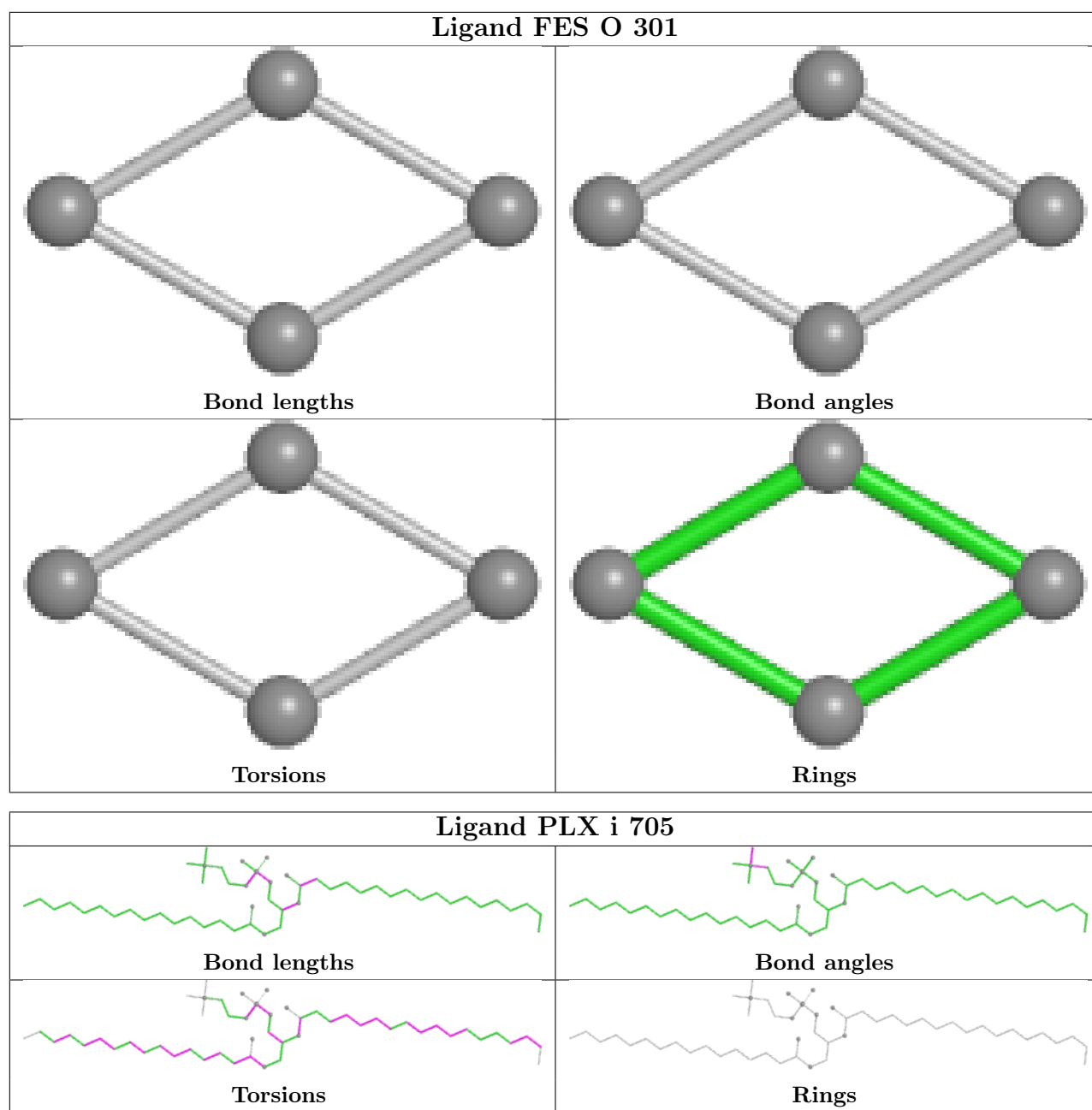


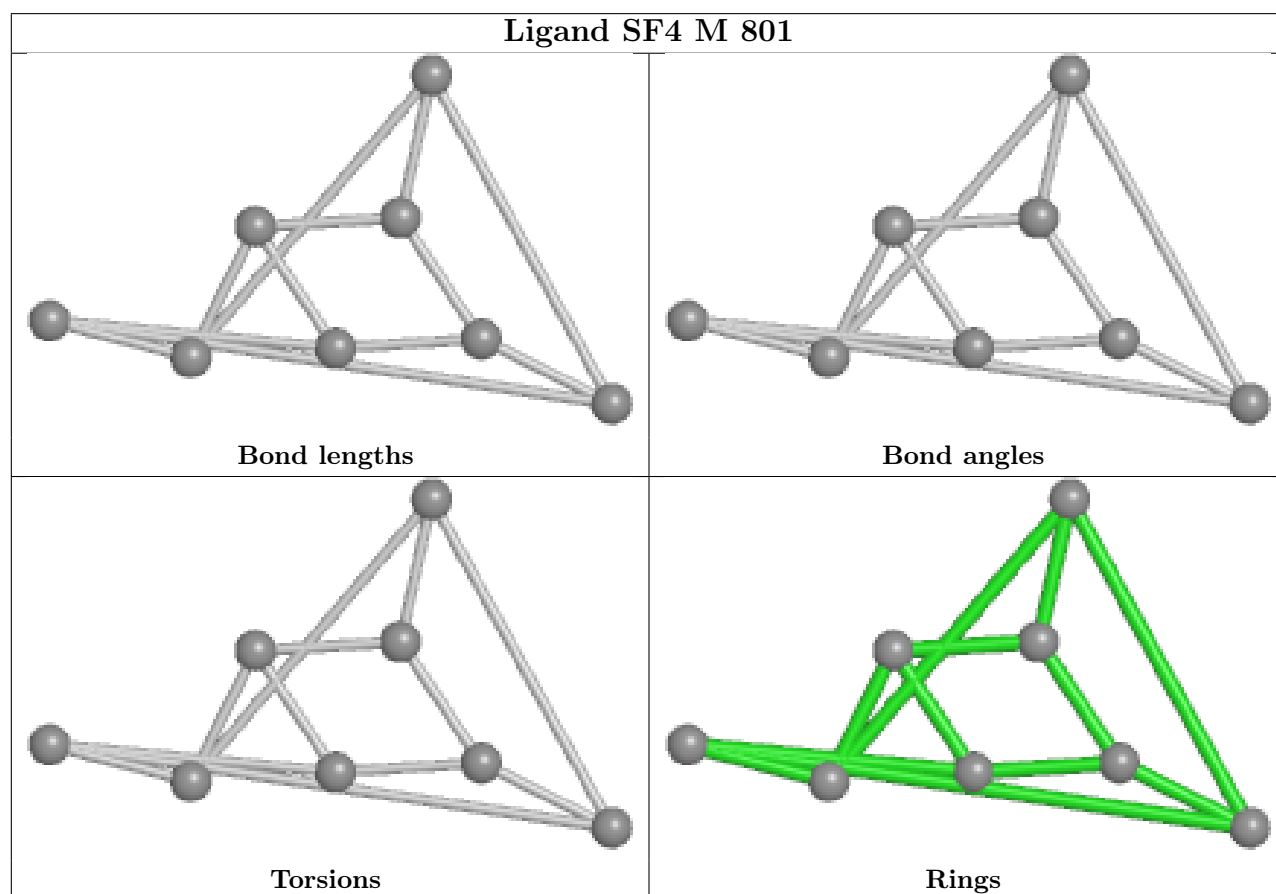
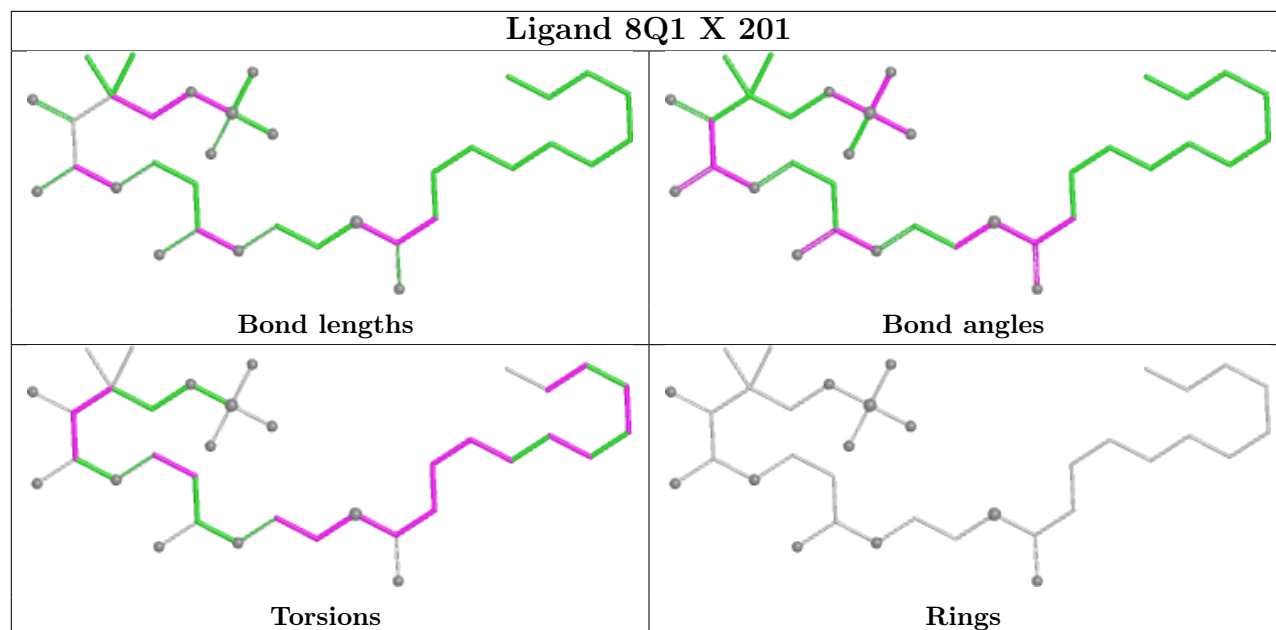
Ligand NDP J 401

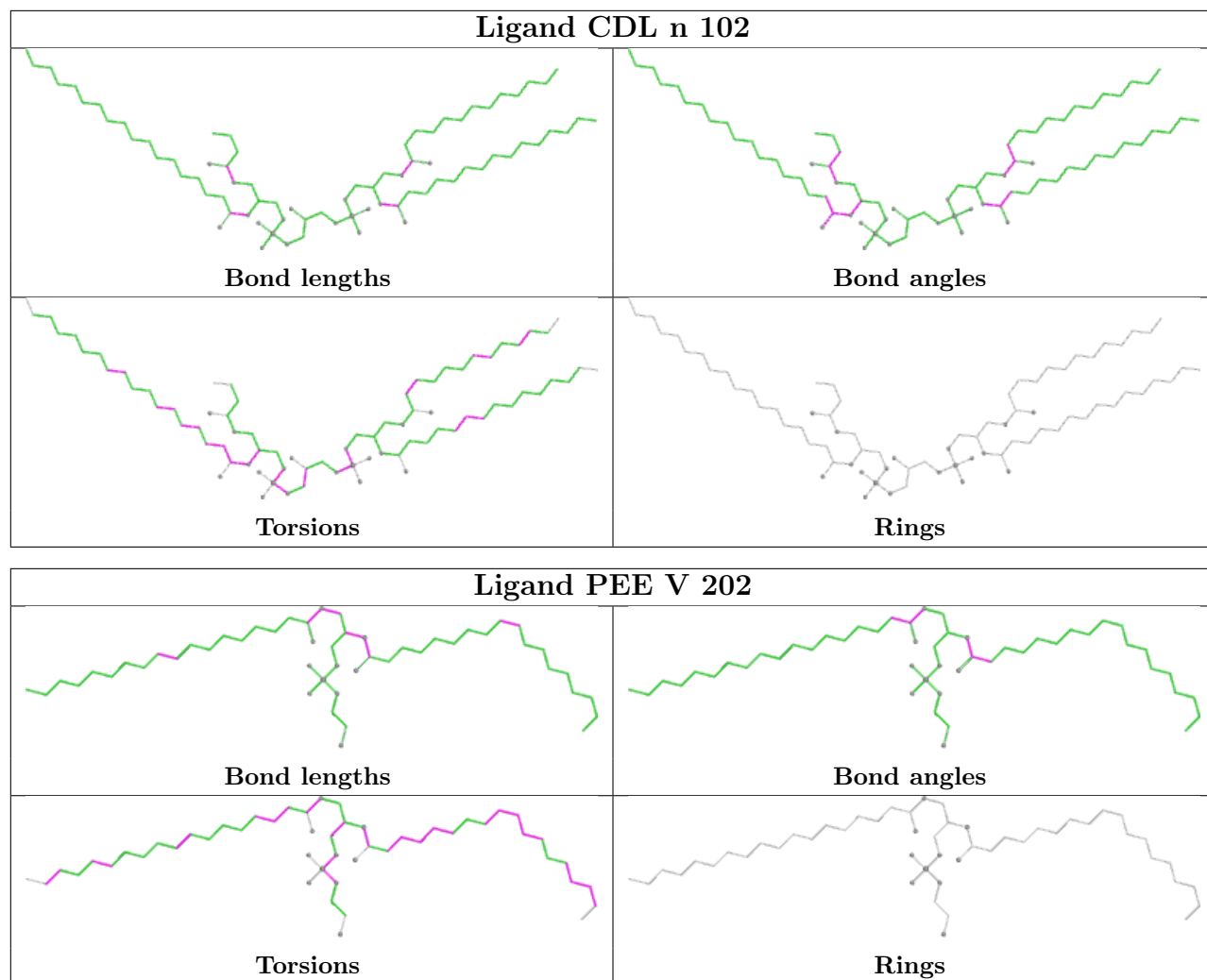


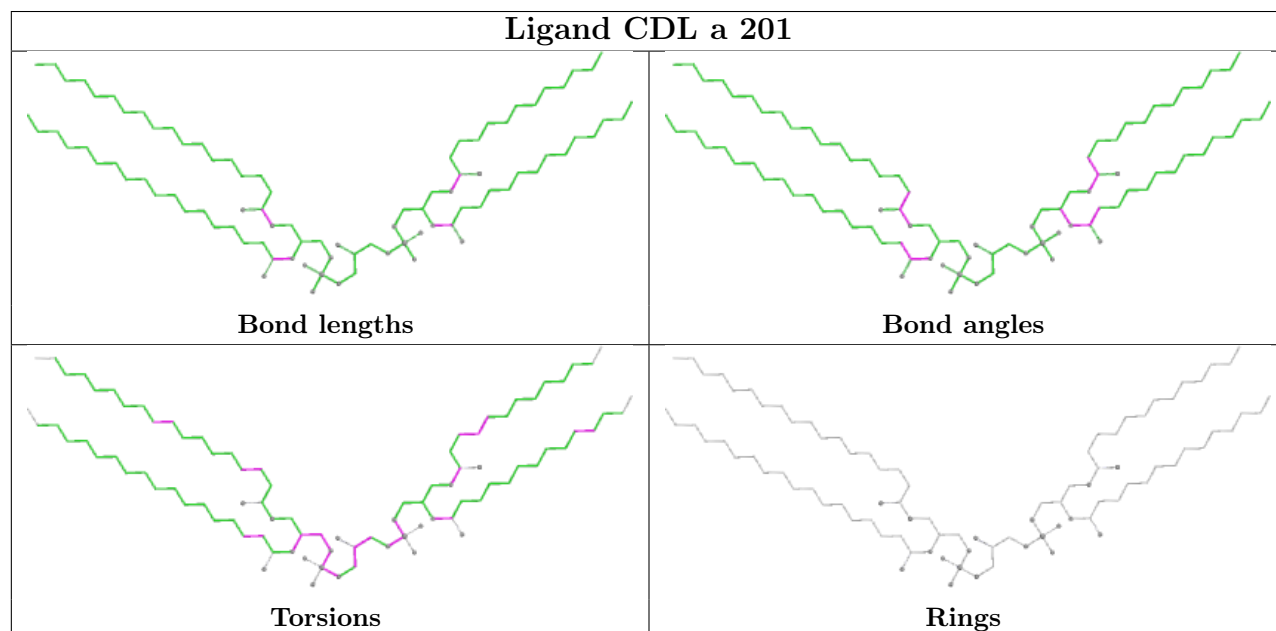
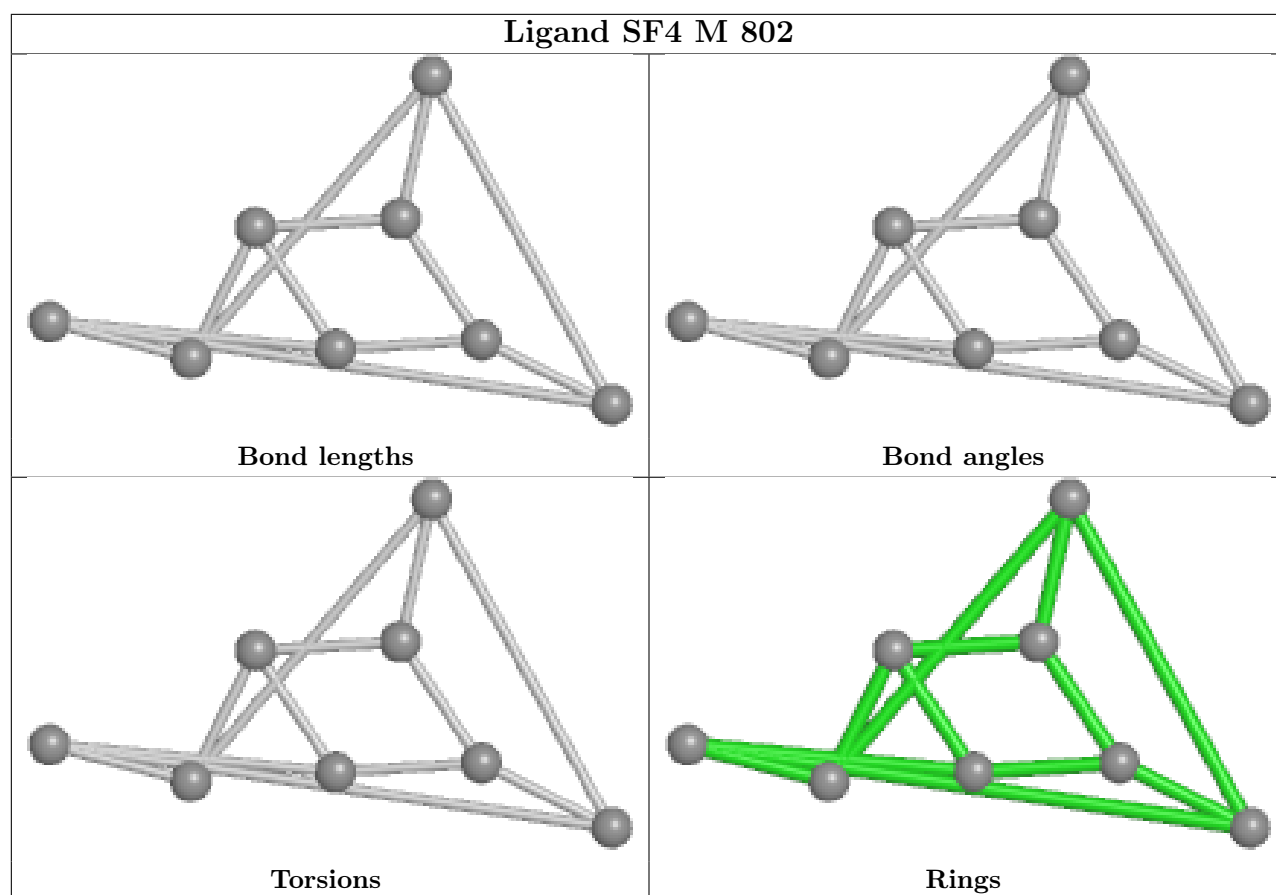
Ligand PEE 1 719

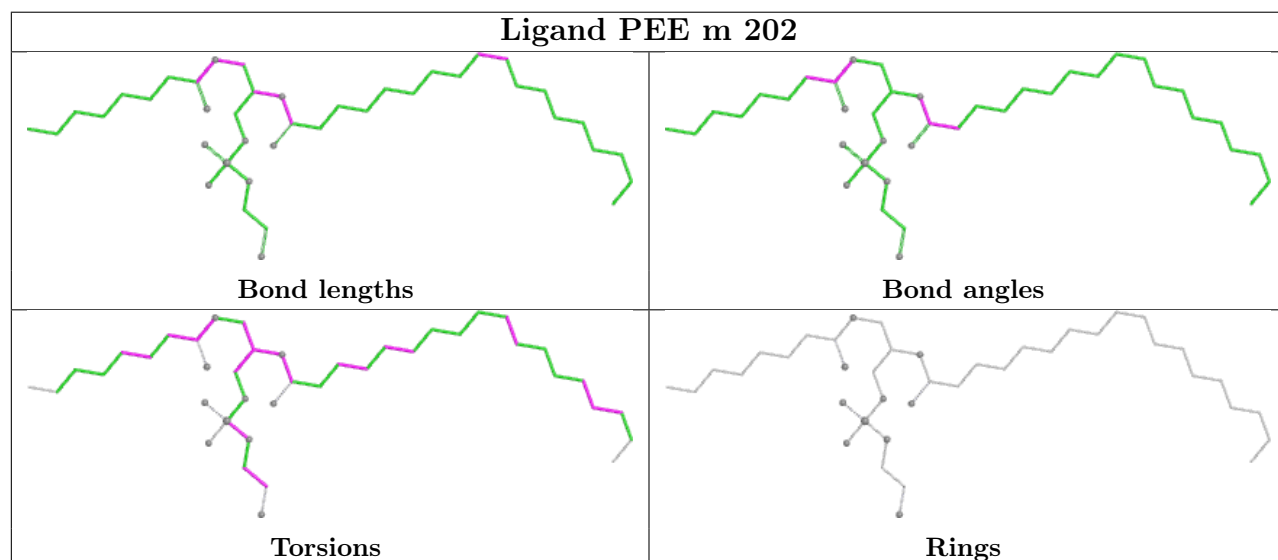
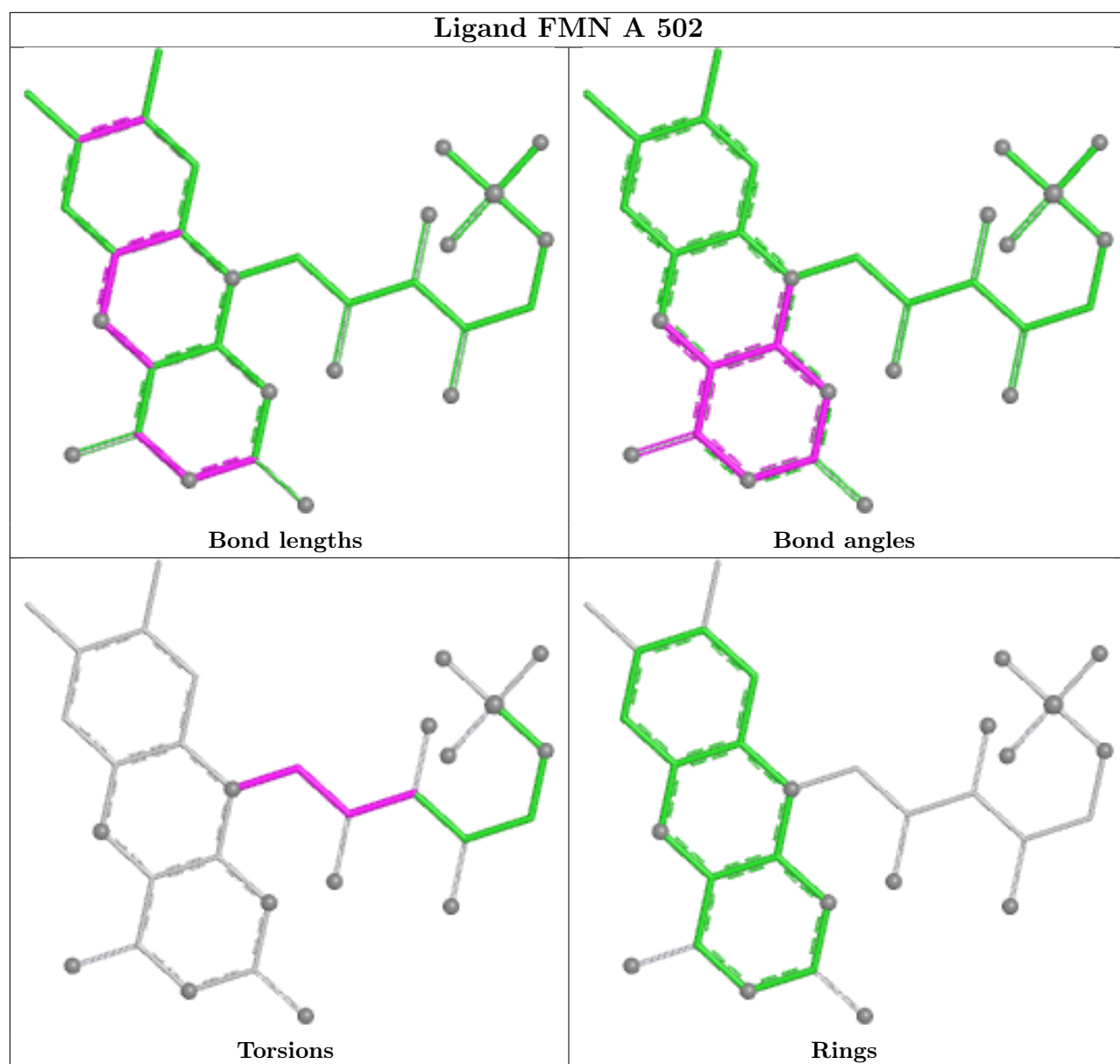


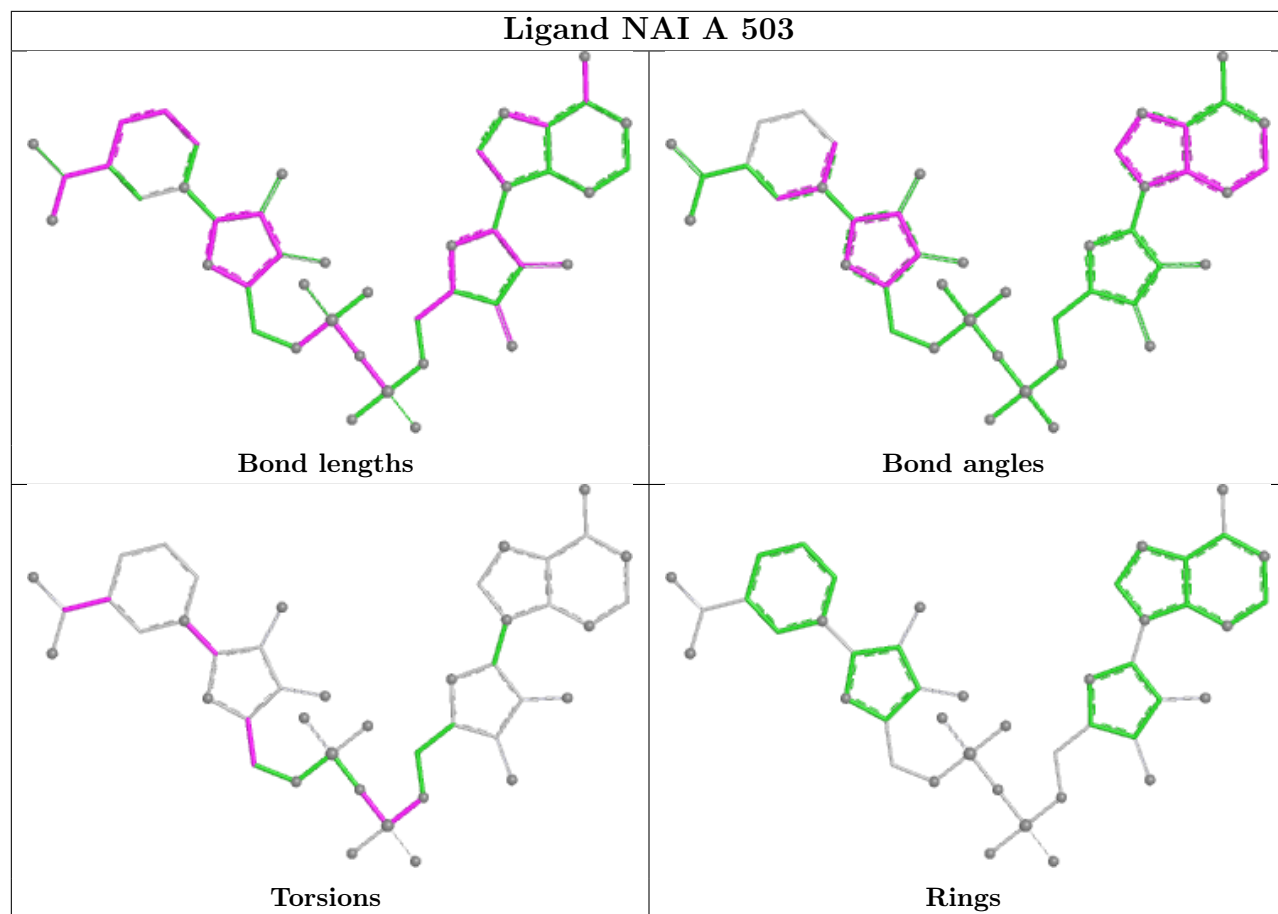


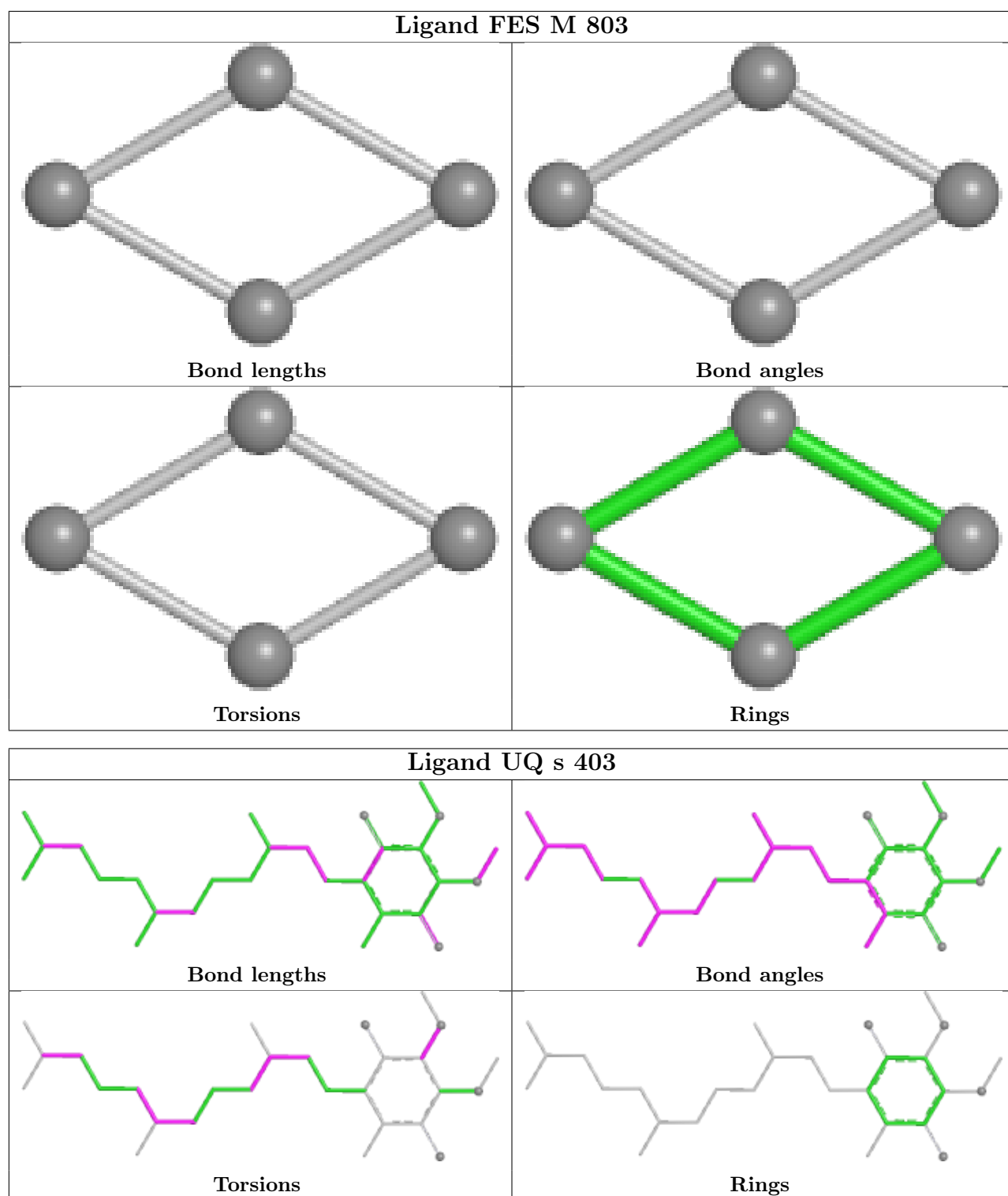


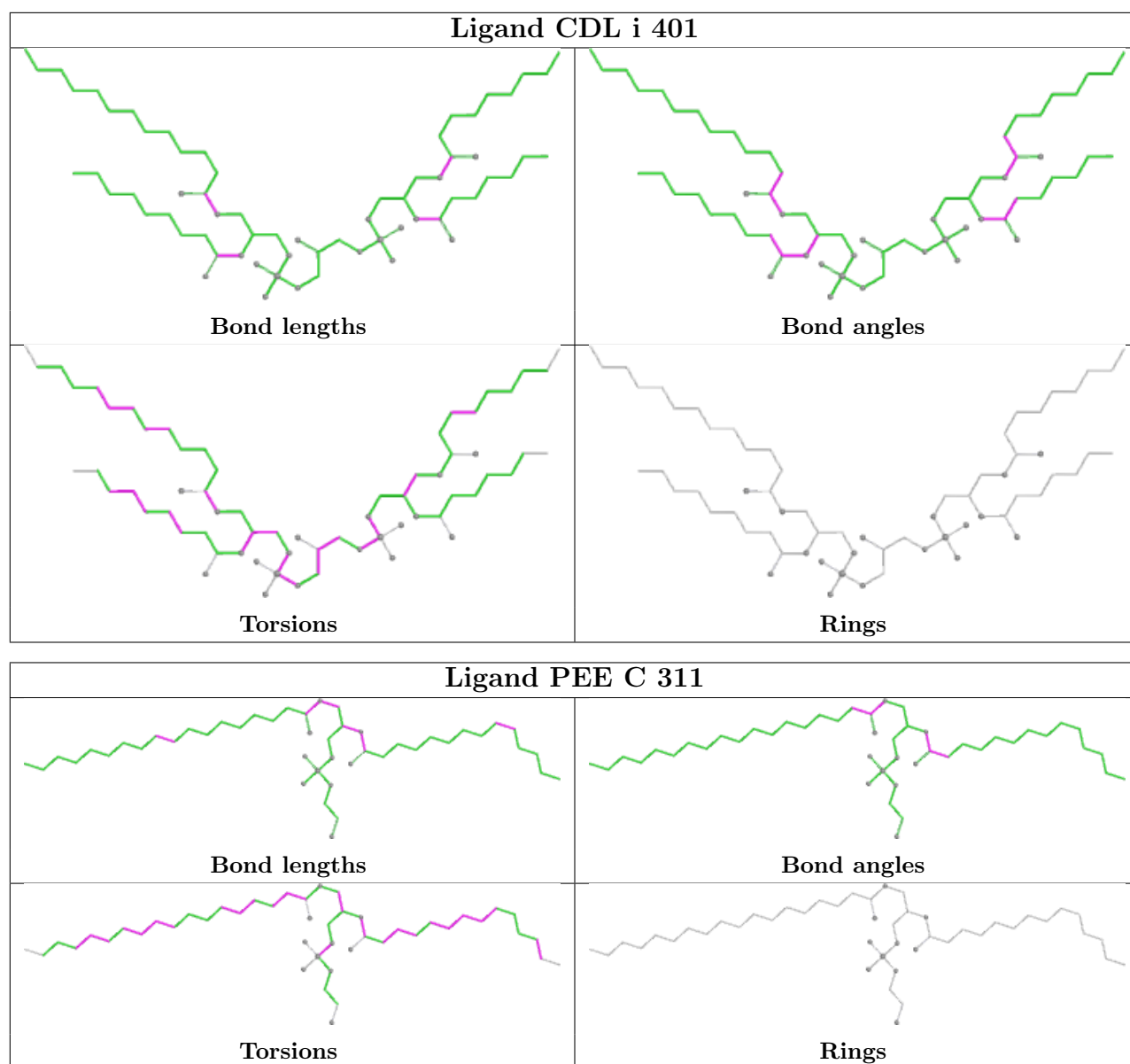


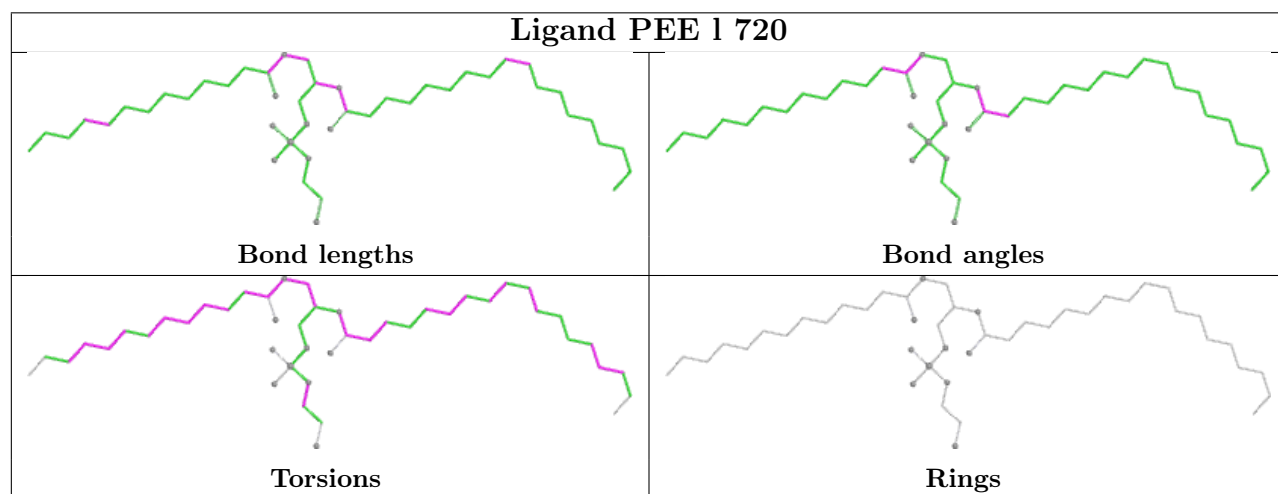
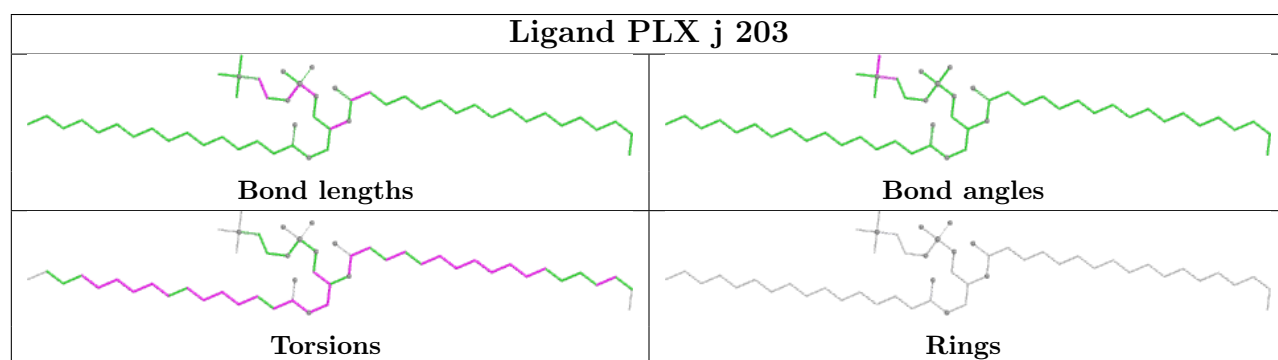
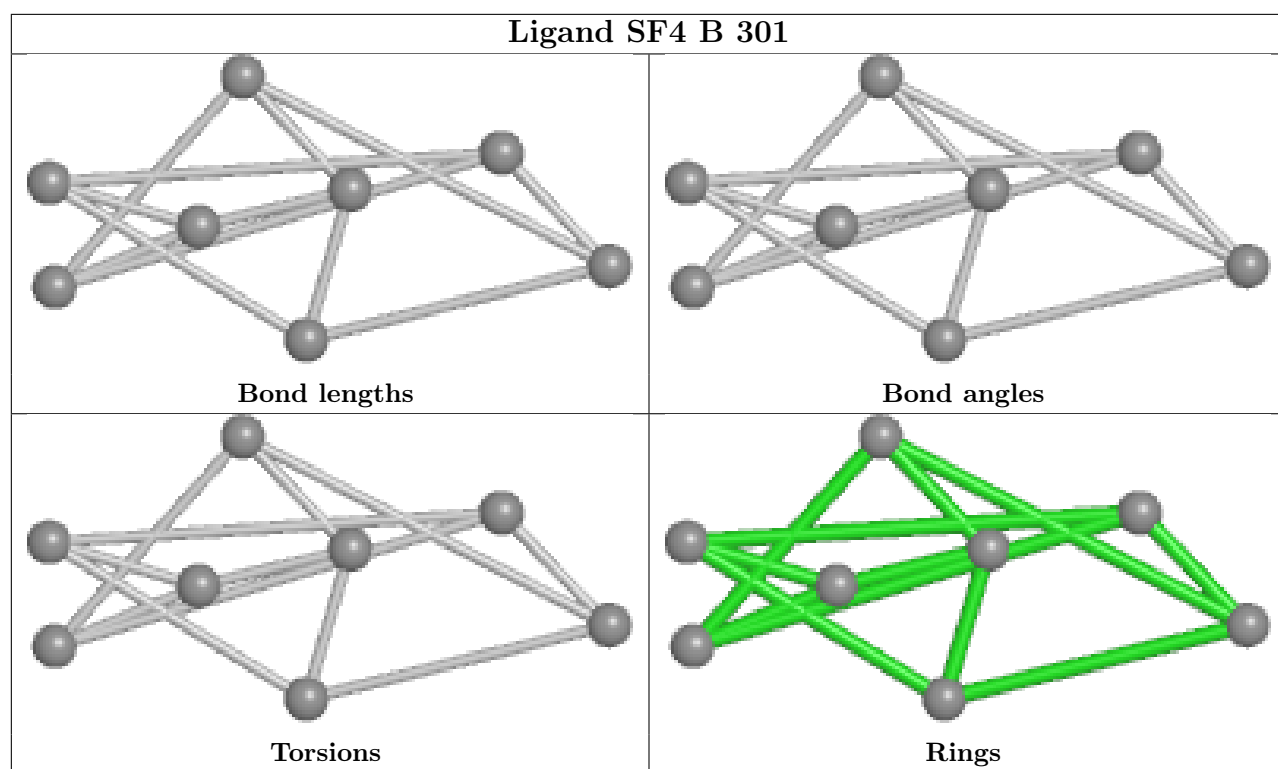


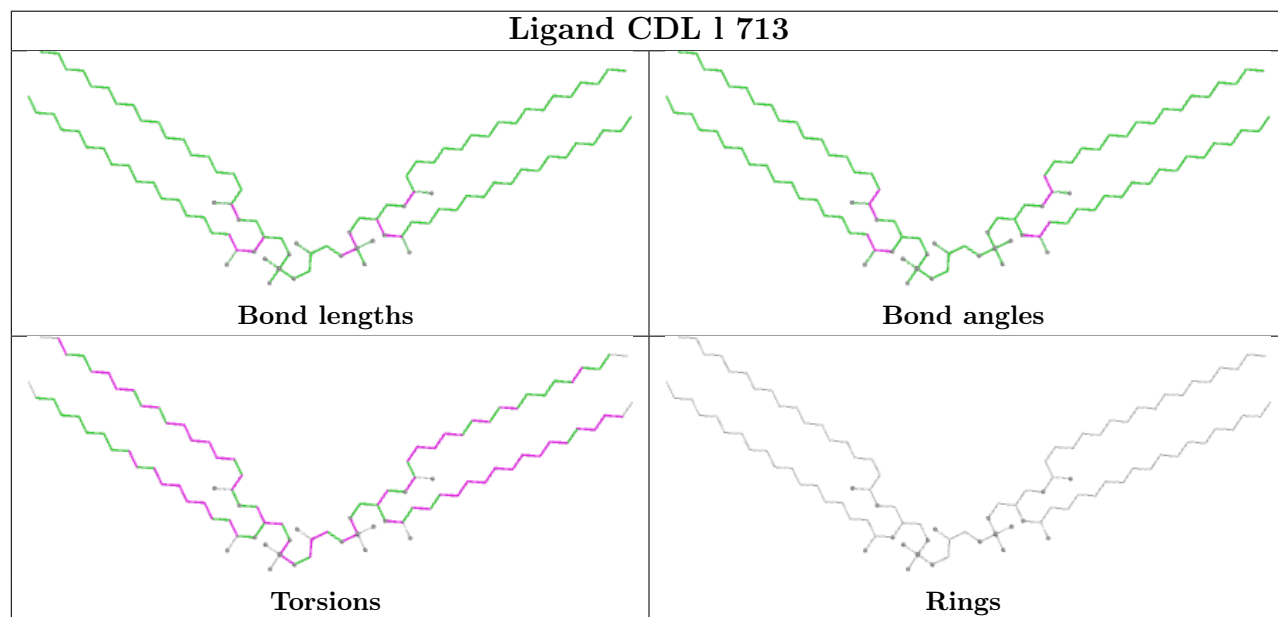
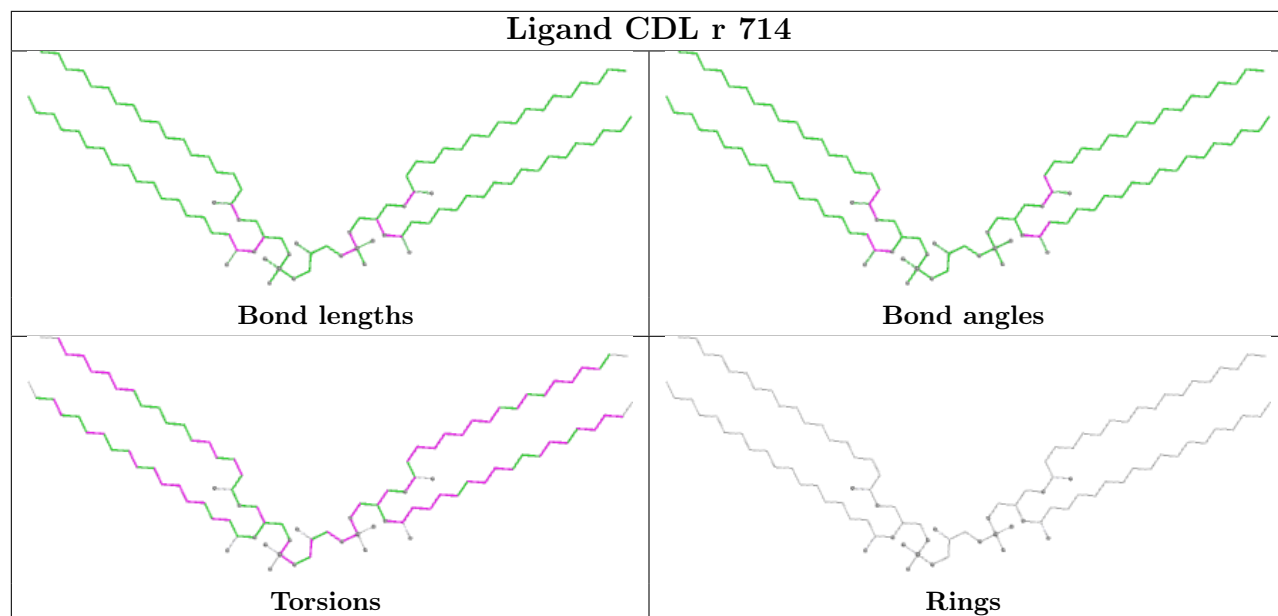


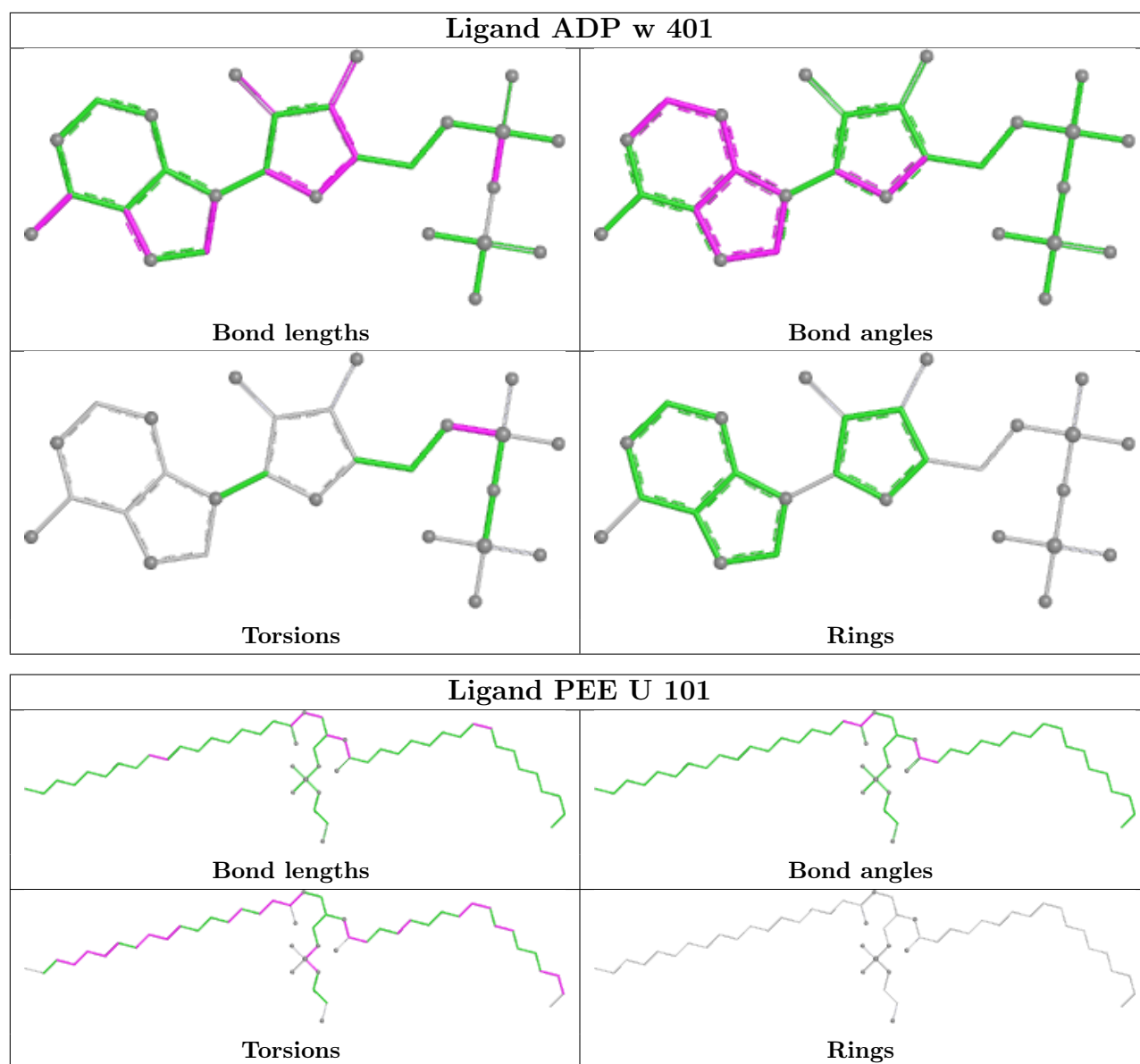












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

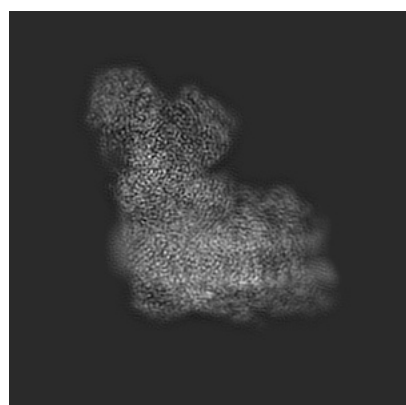
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31646. These allow visual inspection of the internal detail of the map and identification of artifacts.

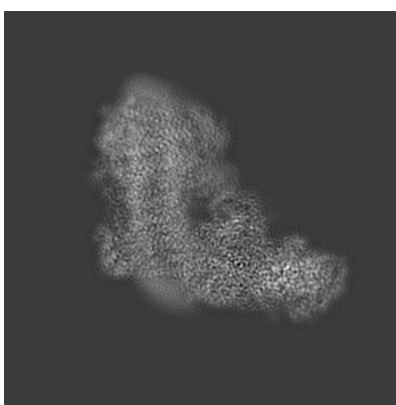
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

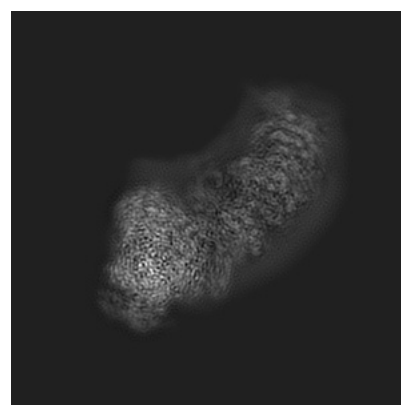
6.1.1 Primary map



X



Y

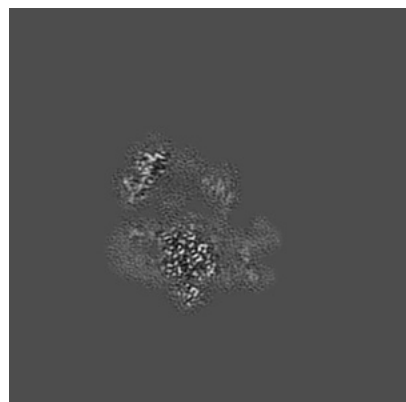


Z

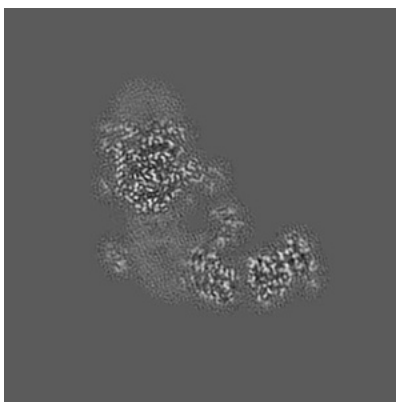
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

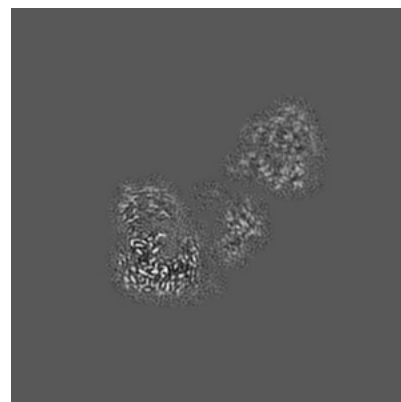
6.2.1 Primary map



X Index: 155



Y Index: 155

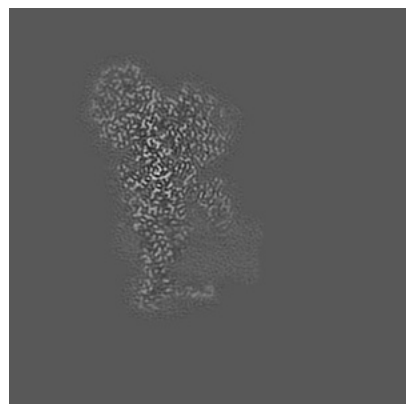


Z Index: 155

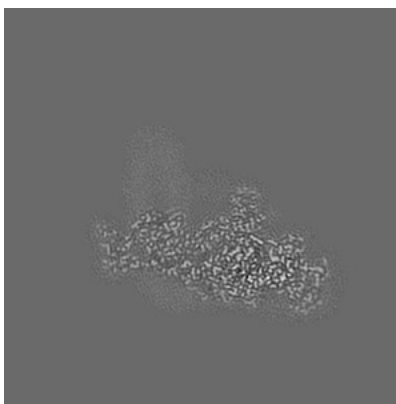
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

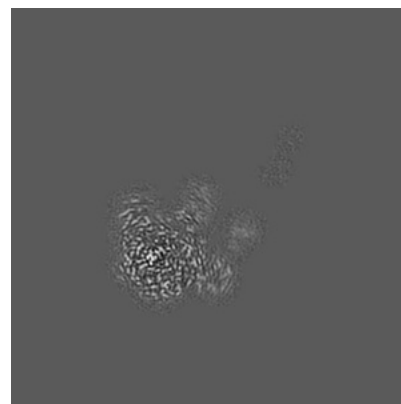
6.3.1 Primary map



X Index: 108



Y Index: 111

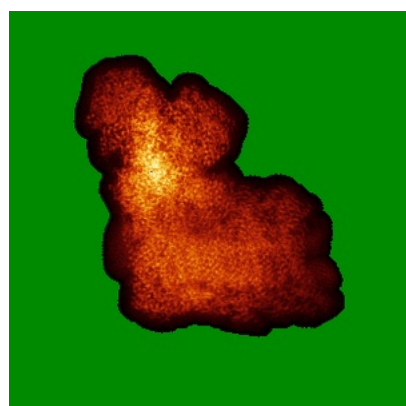


Z Index: 178

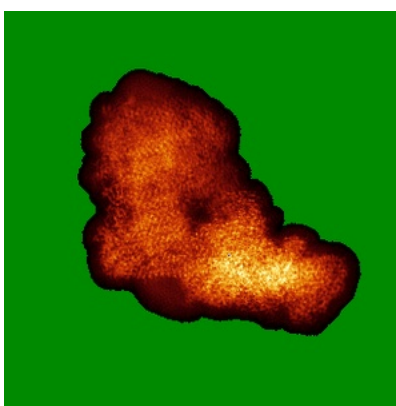
The images above show the largest variance slices of the map in three orthogonal directions.

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

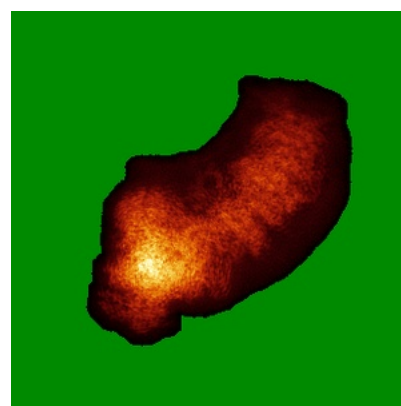
6.4.1 Primary map



X



Y

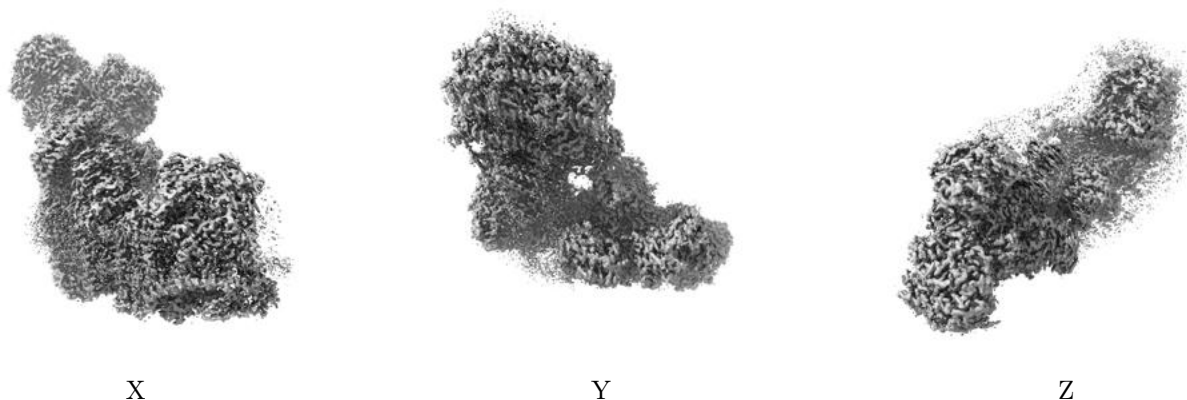


Z

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 0.0202. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

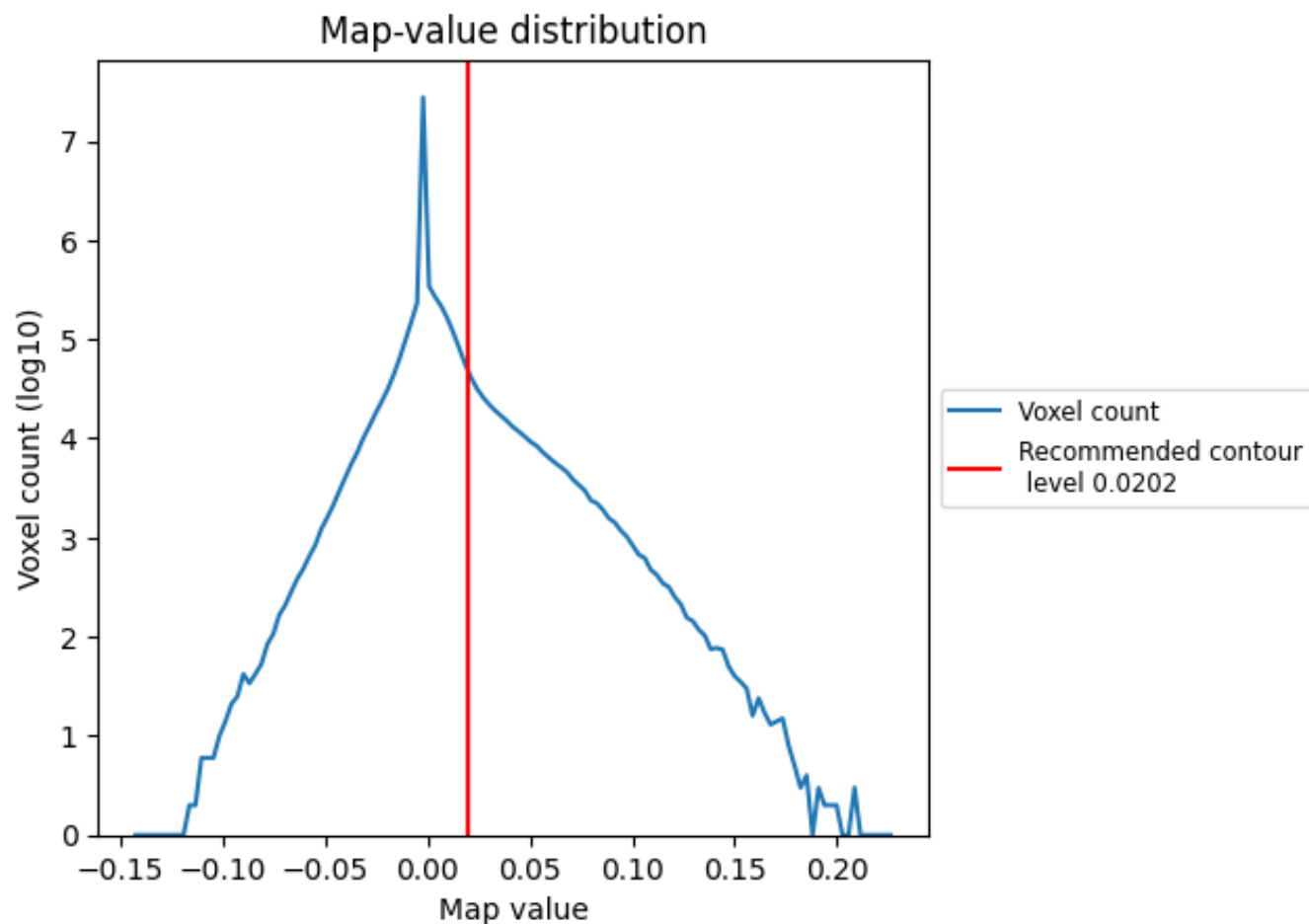
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

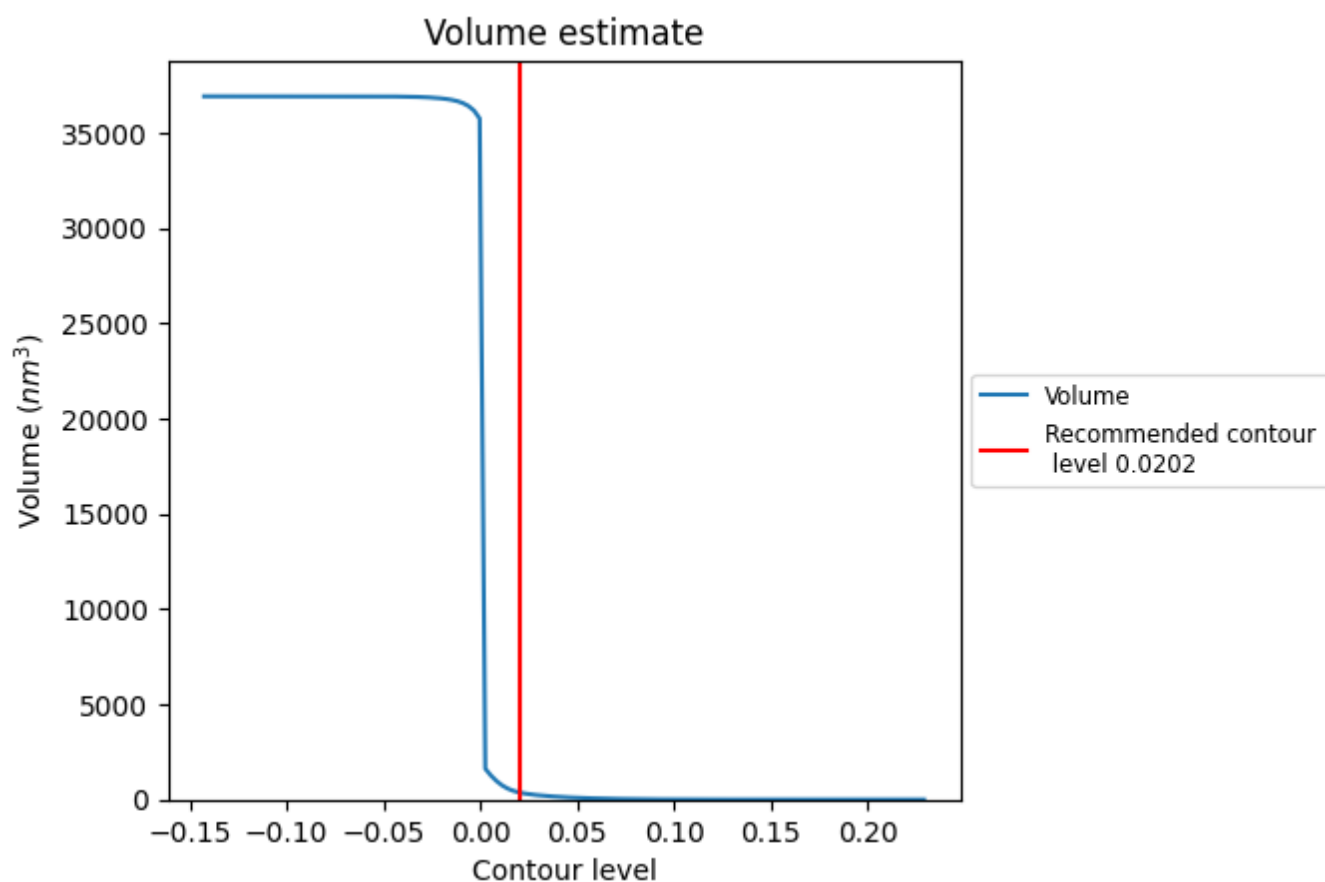
This section contains the results of statistical analysis of the map.

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.

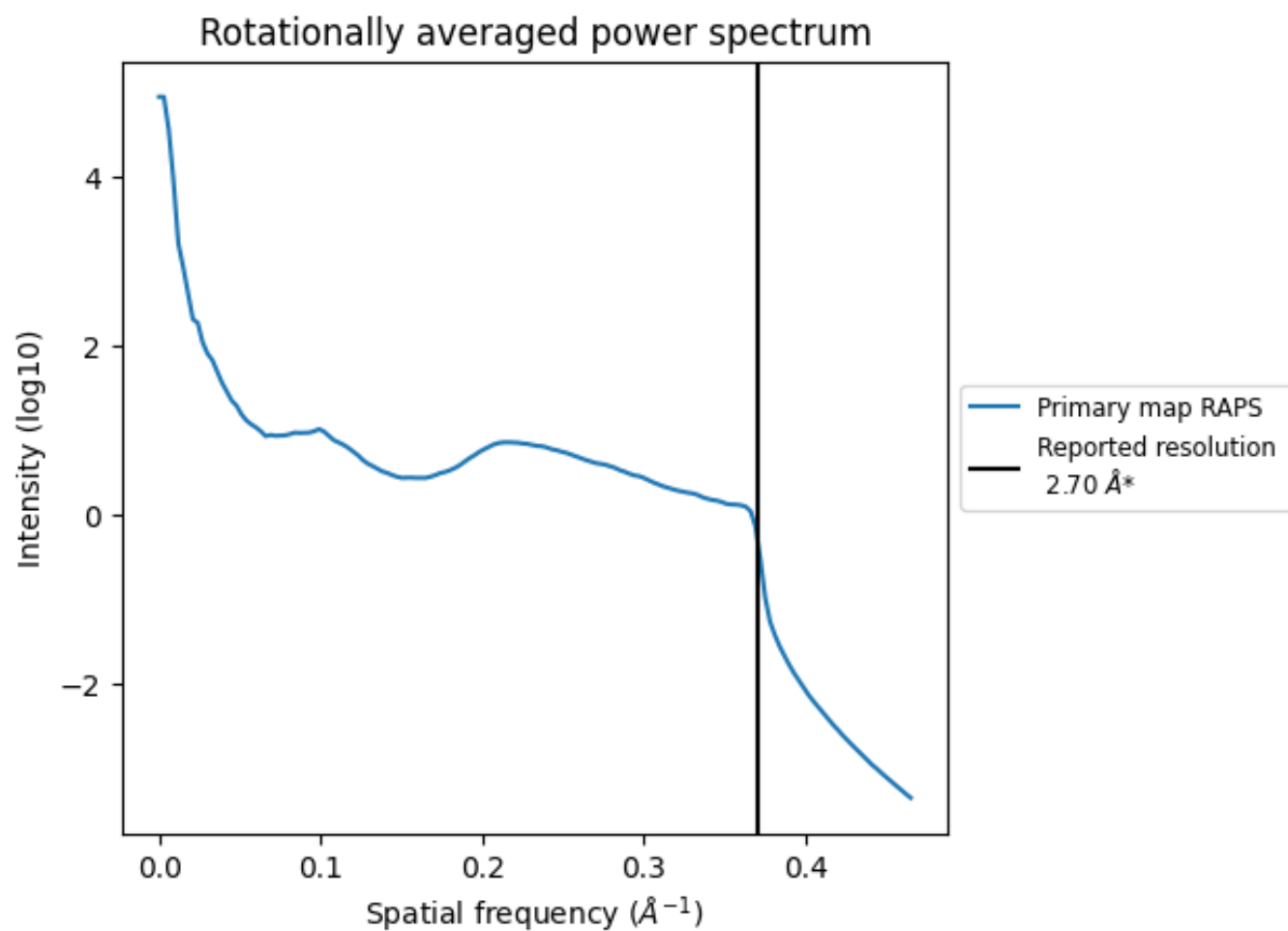
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 371 nm³; this corresponds to an approximate mass of 335 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

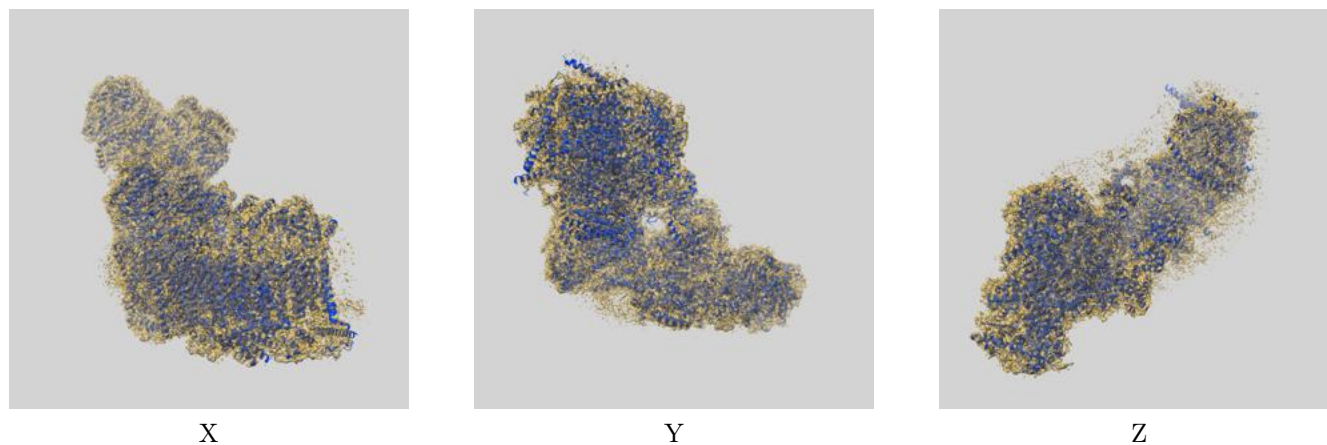
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

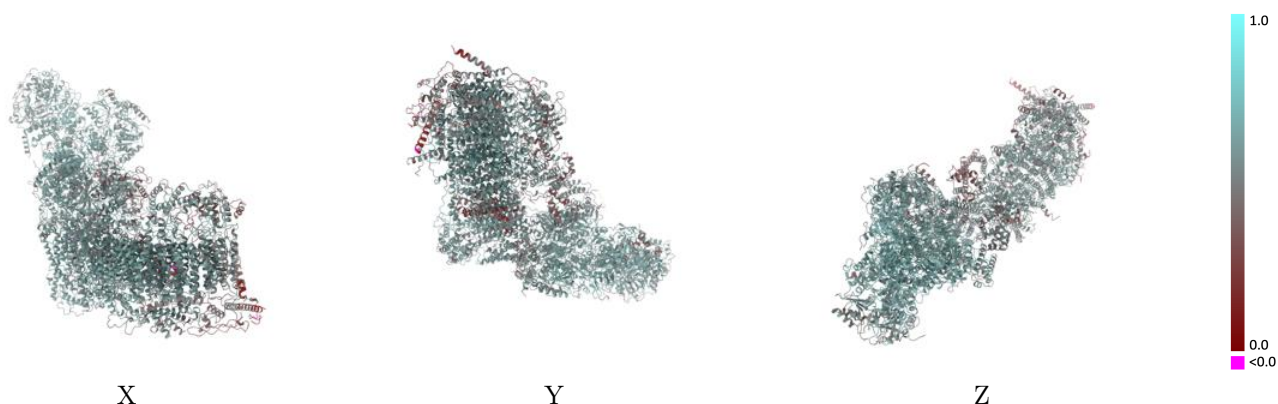
This section contains information regarding the fit between EMDB map EMD-31646 and PDB model 7V2K. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



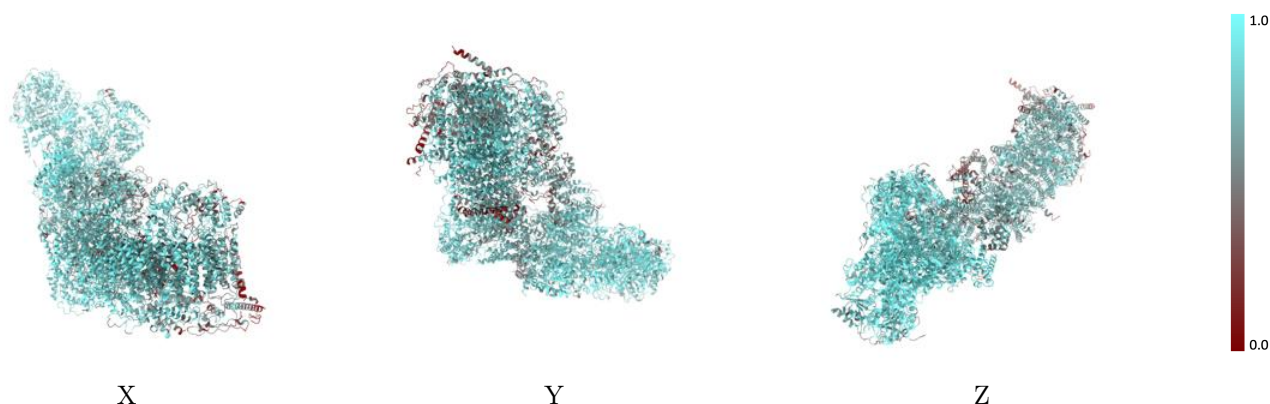
The images above show the 3D surface view of the map at the recommended contour level 0.0202 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



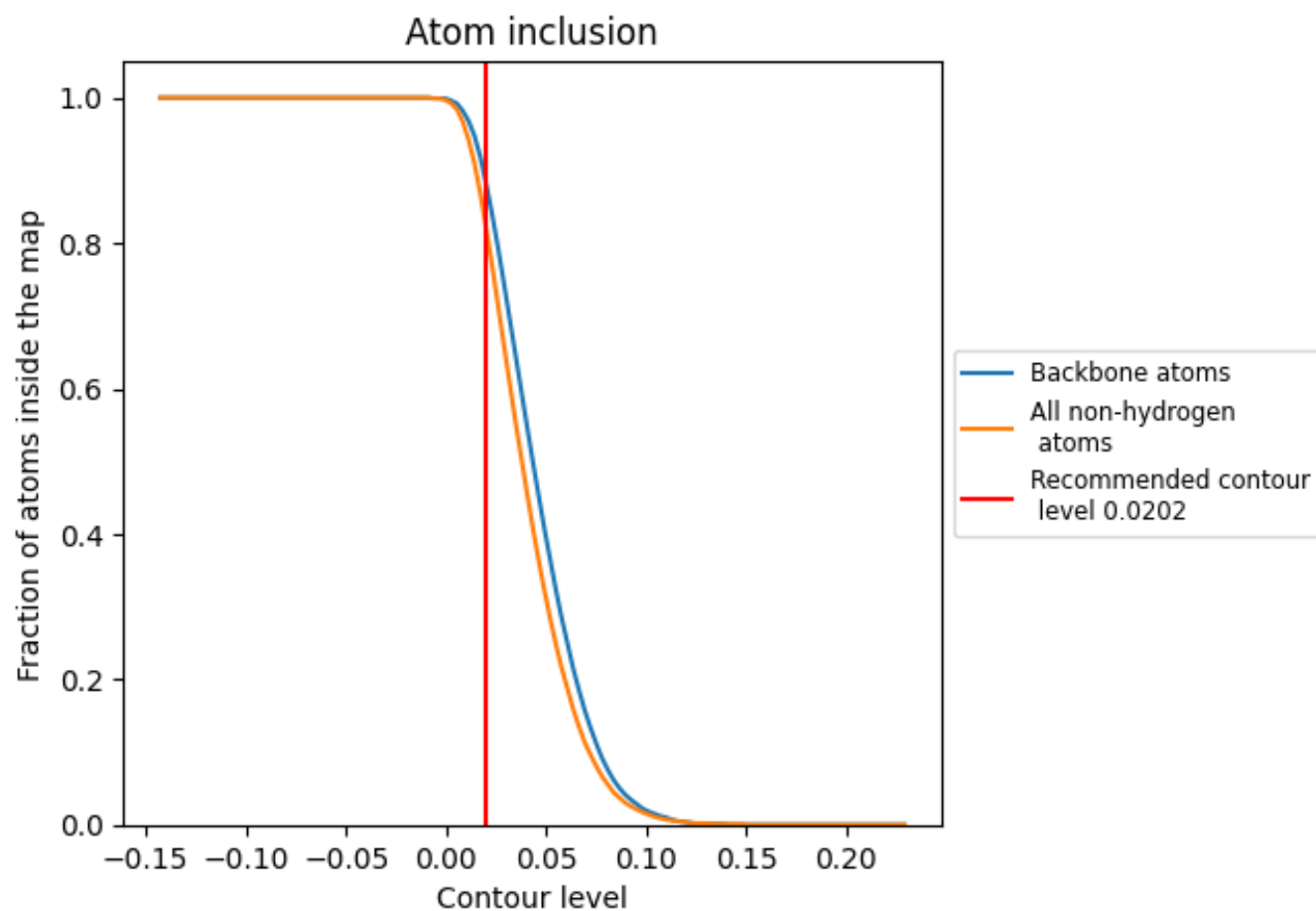
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0202).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 82% 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 (0.0202) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8180	 0.5730
A	 0.8870	 0.5920
B	 0.9640	 0.6520
C	 0.9230	 0.6320
E	 0.8520	 0.5820
F	 0.8110	 0.5270
G	 0.5290	 0.3950
H	 0.8600	 0.5560
I	 0.8180	 0.5830
J	 0.8290	 0.5700
K	 0.8050	 0.5440
L	 0.9040	 0.6240
M	 0.9260	 0.6220
N	 0.8410	 0.6050
O	 0.8260	 0.5580
P	 0.9570	 0.6430
Q	 0.9190	 0.6360
S	 0.9260	 0.6170
T	 0.8660	 0.6130
U	 0.8600	 0.5990
V	 0.4250	 0.4060
W	 0.8890	 0.6020
X	 0.6240	 0.4860
Y	 0.5370	 0.4200
Z	 0.5170	 0.4080
a	 0.8090	 0.5780
b	 0.6370	 0.4670
c	 0.7050	 0.5170
d	 0.7220	 0.5230
e	 0.7040	 0.5290
f	 0.7130	 0.5160
g	 0.8810	 0.5990
h	 0.8750	 0.6000
i	 0.9110	 0.6230
j	 0.7810	 0.5490



Continued on next page...

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Chain	Atom inclusion	Q-score
k	 0.7320	 0.5450
l	 0.7540	 0.5590
m	 0.7510	 0.5530
n	 0.6570	 0.5290
o	 0.7430	 0.5300
p	 0.7160	 0.5260
r	 0.9000	 0.6170
s	 0.9110	 0.6150
u	 0.8880	 0.5940
v	 0.5210	 0.4060
w	 0.7050	 0.5210