



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 10:34 PM JST

PDB ID : 7V30 / pdb_00007v30
EMDB ID : EMD-31648
Title : Deactive state complex I from Q1-NADH dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-08-10
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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

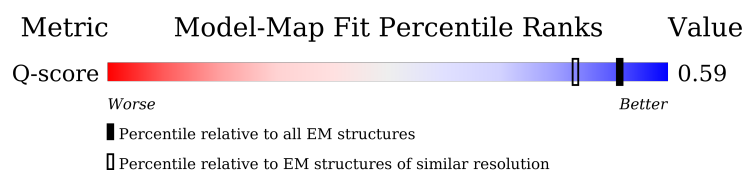
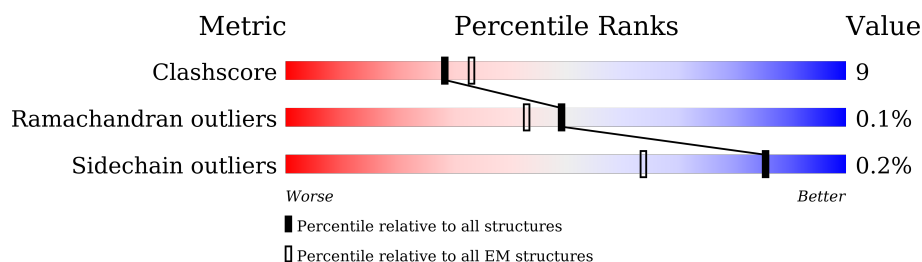
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	
2	B	176	
3	C	156	
4	E	115	

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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	-
54	CDL	a	201	-	-	X	-
57	ADP	w	401	-	-	X	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 66820 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
			696	449	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	297	Total	C	N	O	S	0	0
			2359	1514	421	416	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
			1173	755	203	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
			597	392	98	106	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
			4782	3172	740	819	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	129	Total	C	N	O	S	0	0
			948	636	138	166	8		

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

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

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

4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	o	128	Total	C	N	O	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
			1028	642	195	182	9		

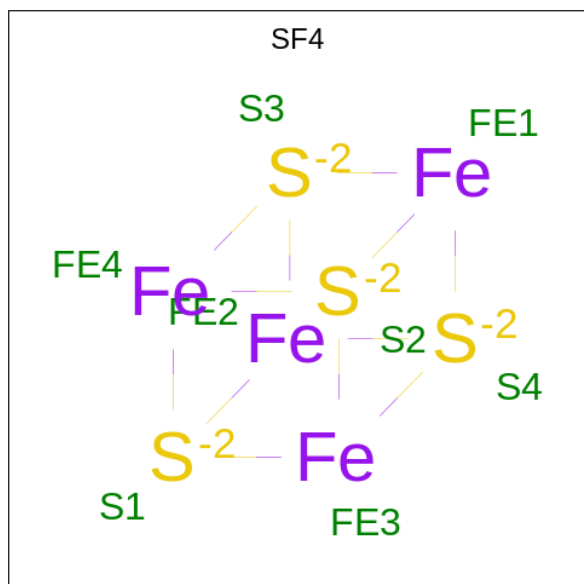
There is a discrepancy between the modelled and reference sequences:

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

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

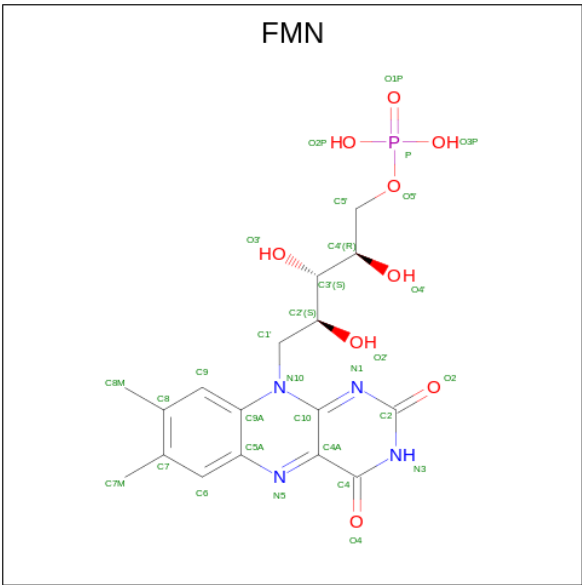
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2582	1643	438	491	10		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



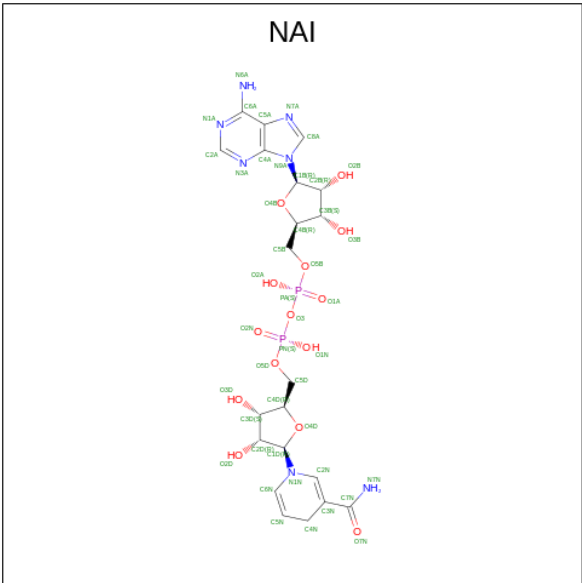
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- 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).



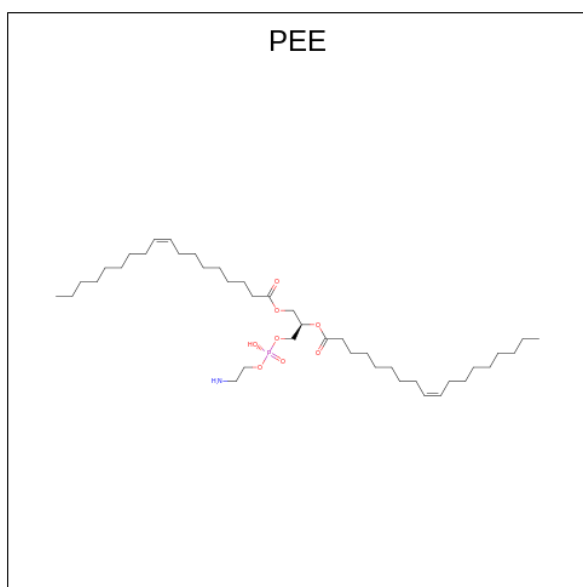
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



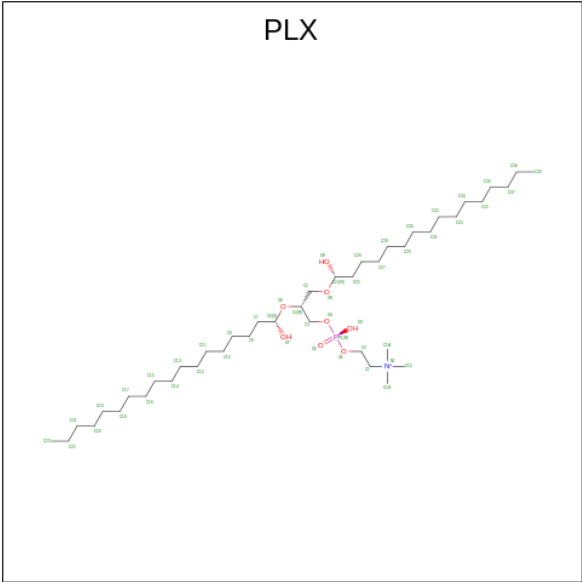
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 48 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P) (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-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



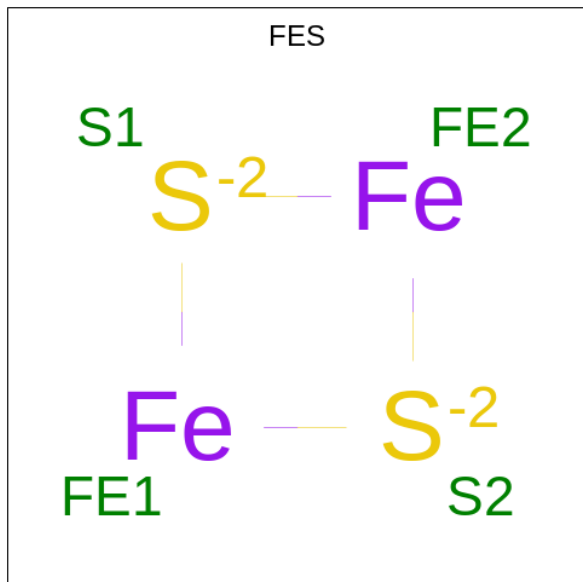
Mol	Chain	Residues	Atoms						AltCon
50	G	1	Total 35	C 23	N 2	O 8	P 1	S 1	0
50	X	1	Total 35	C 23	N 2	O 8	P 1	S 1	0

- Molecule 51 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



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

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

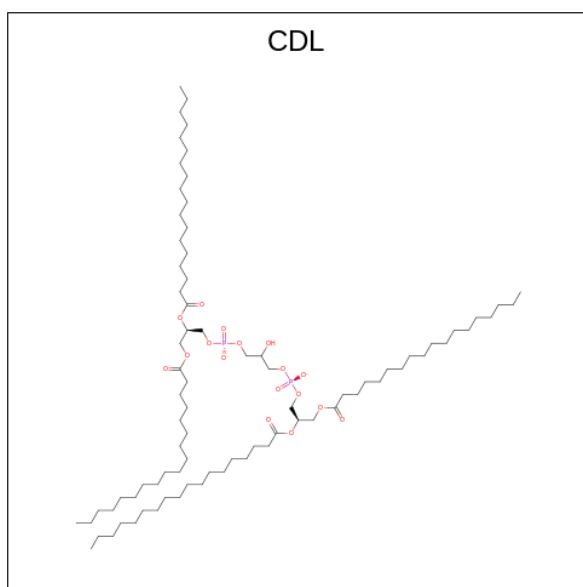


Mol	Chain	Residues	Atoms			AltConf
52	M	1	Total	Fe	S	0
			4	2	2	
52	O	1	Total	Fe	S	0
			4	2	2	

- 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).

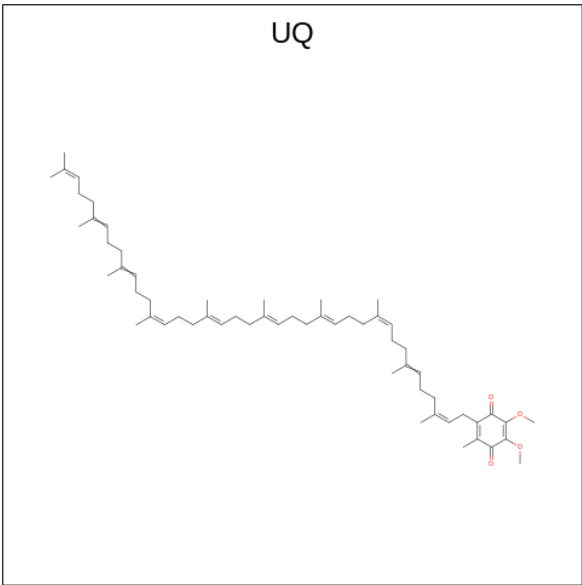


Mol	Chain	Residues	Atoms				AltConf
54	N	1	Total	C	O	P	0
			51	32	17	2	
54	V	1	Total	C	O	P	0
			71	52	17	2	
54	a	1	Total	C	O	P	0
			91	72	17	2	
54	i	1	Total	C	O	P	0
			66	47	17	2	
54	l	1	Total	C	O	P	0
			99	80	17	2	
54	l	1	Total	C	O	P	0
			100	81	17	2	
54	n	1	Total	C	O	P	0
			78	59	17	2	
54	r	1	Total	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).

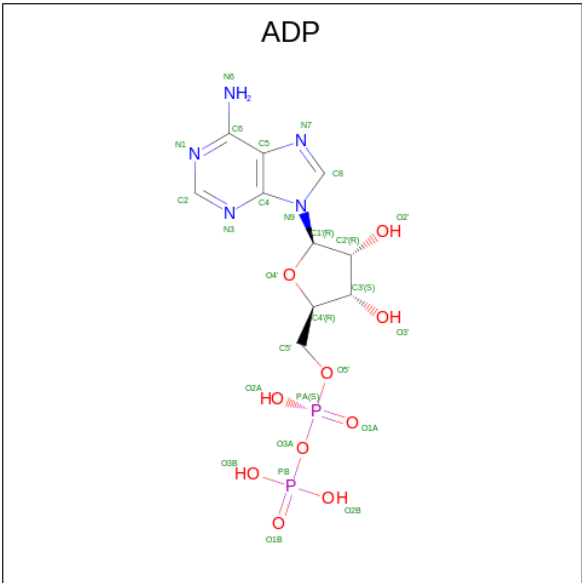
Mol	Chain	Residues	Atoms		AltConf
55	T	1	Total	Zn	0
			1	1	

- 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).

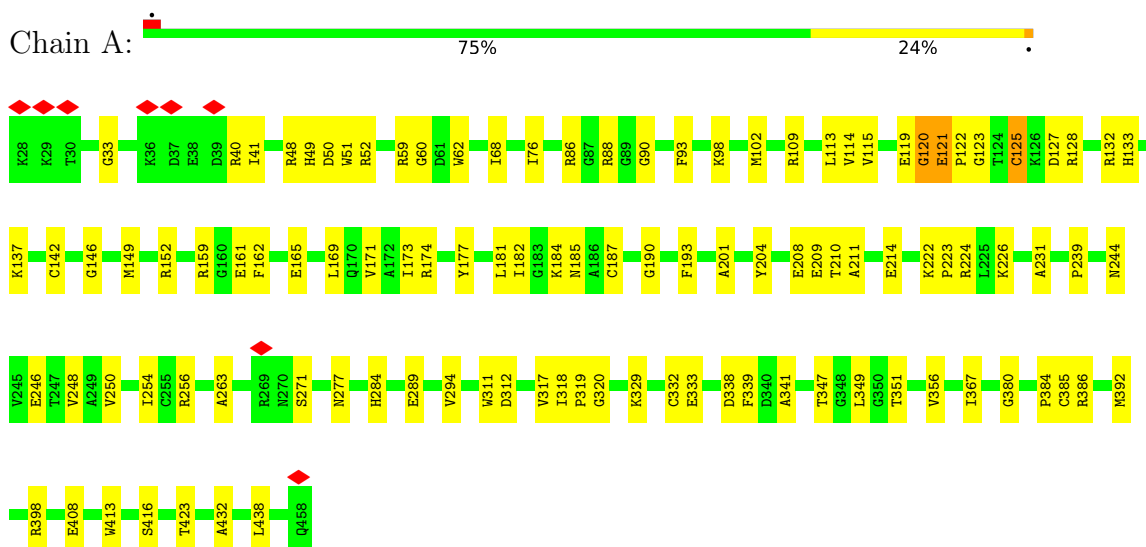


Mol	Chain	Residues	Atoms					AltConf
57	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

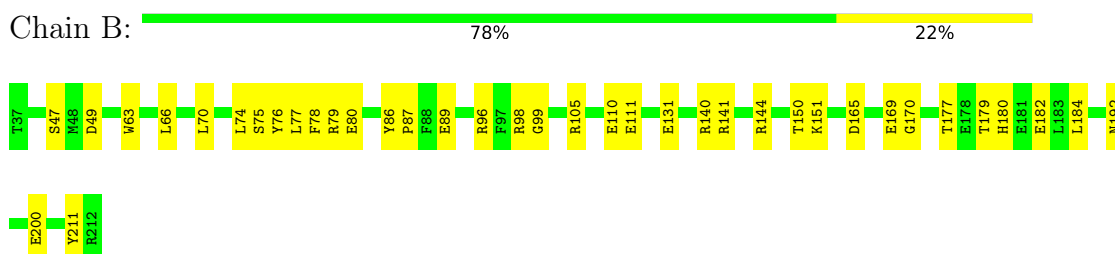
3 Residue-property plots

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.

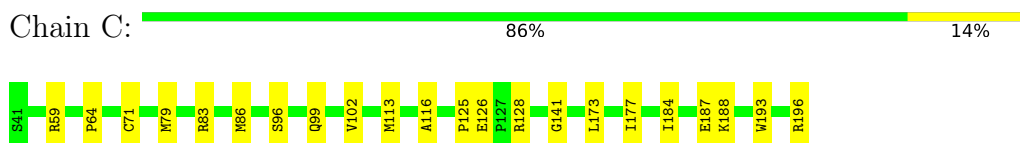
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



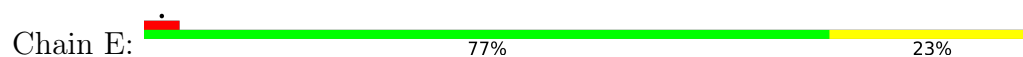
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



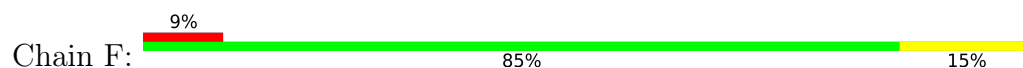
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



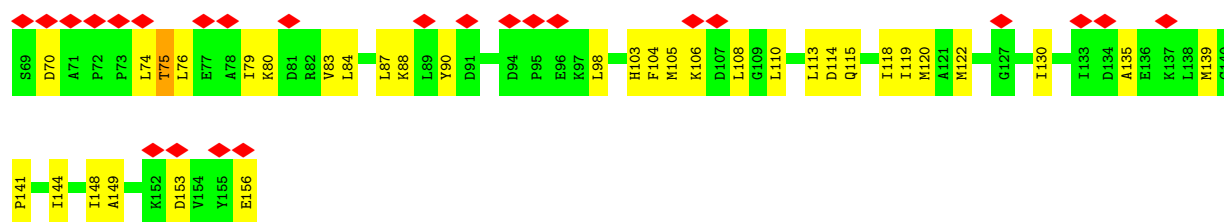
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



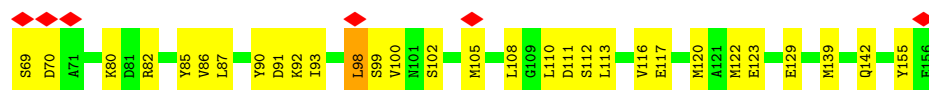
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



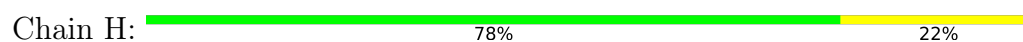
- Molecule 6: Acyl carrier protein, mitochondrial



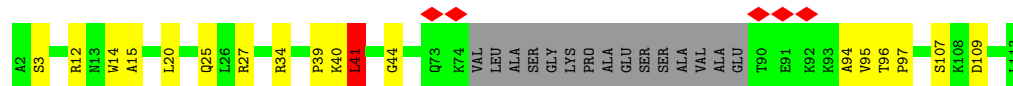
- Molecule 6: Acyl carrier protein, mitochondrial



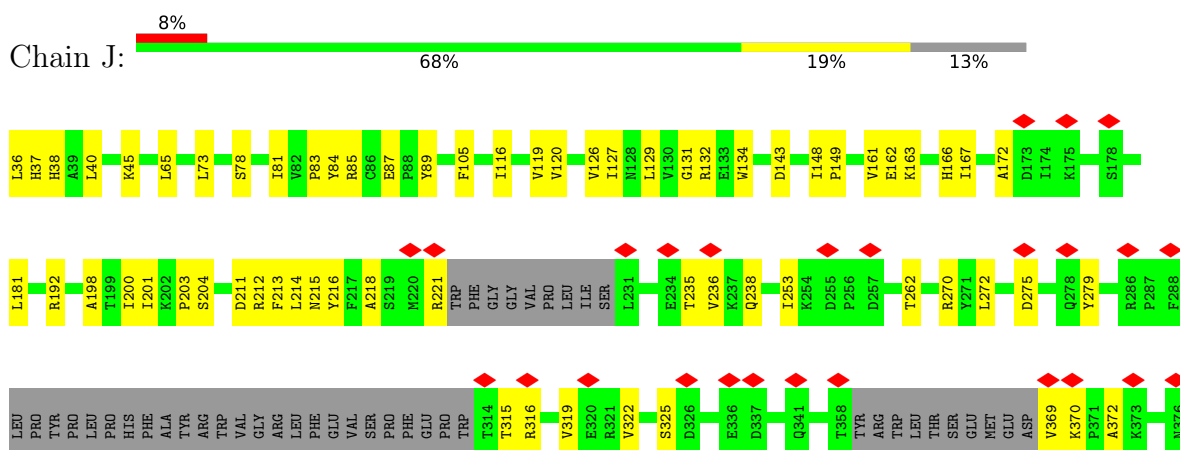
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



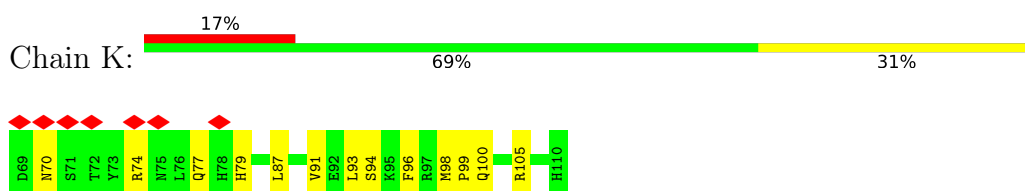
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



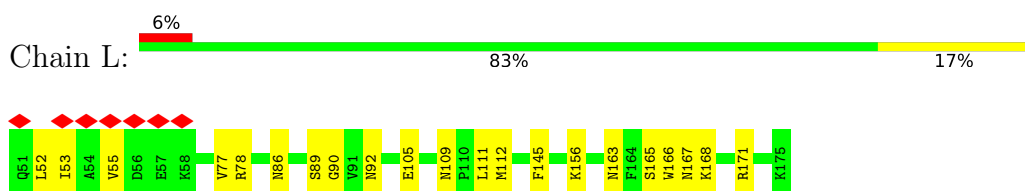
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



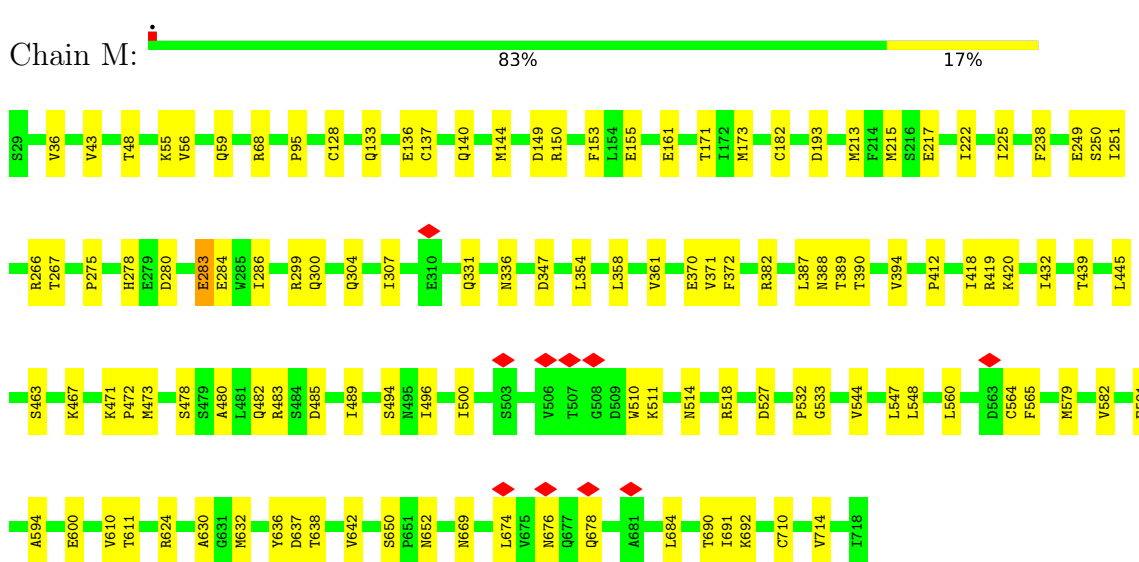
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



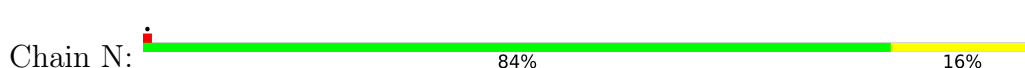
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



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

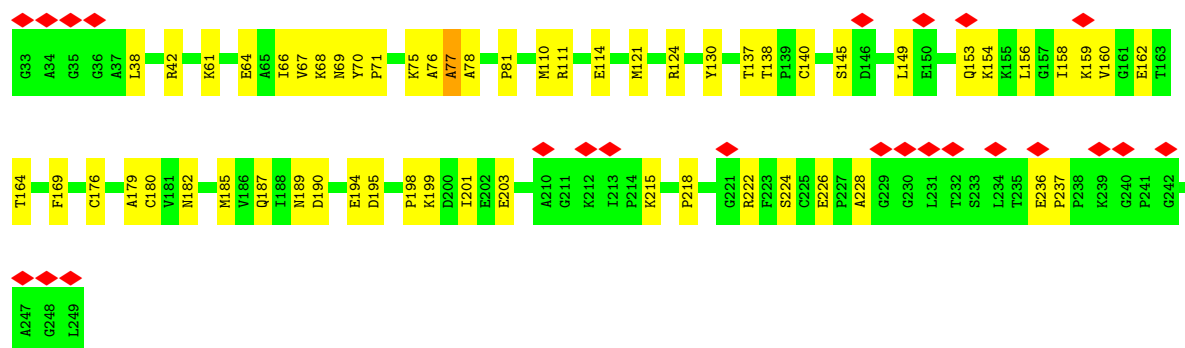
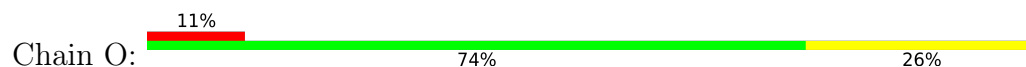


- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

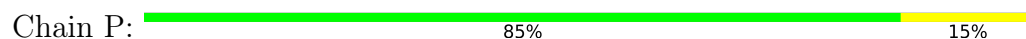




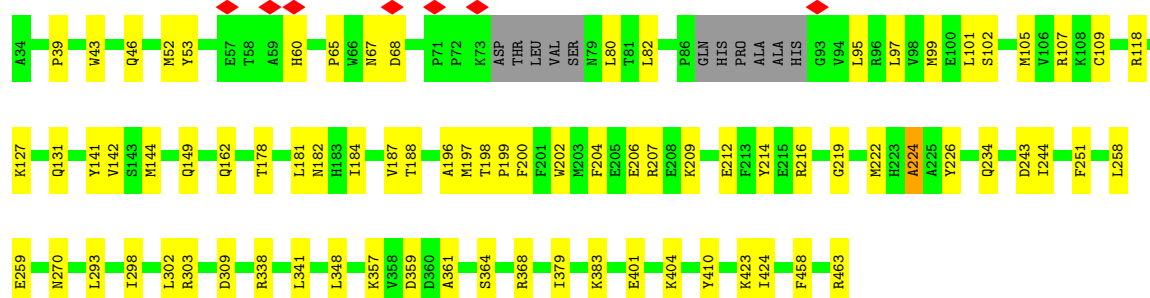
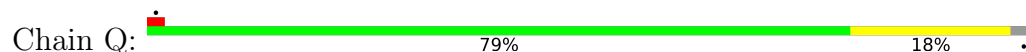
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



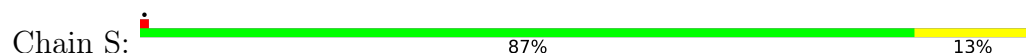
- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



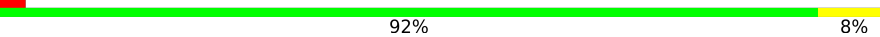
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



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



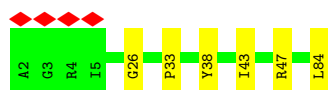
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T:  92% 8%



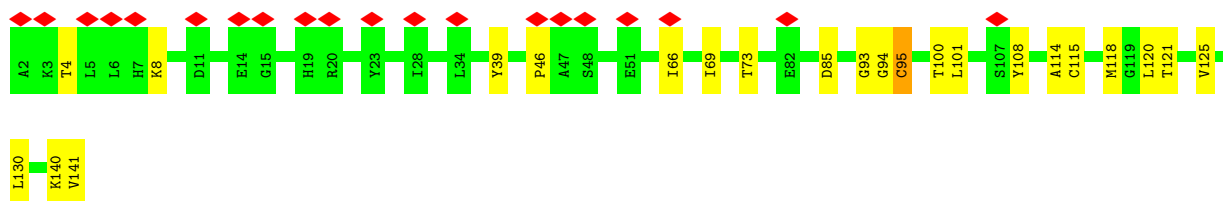
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:  5% 93% 7%



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

Chain V:  14% 84% 16%



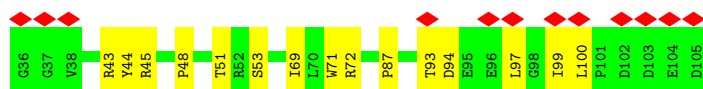
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:  80% 20%



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

Chain Y:  17% 79% 21%



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

Chain Z:  20% 89% 11%



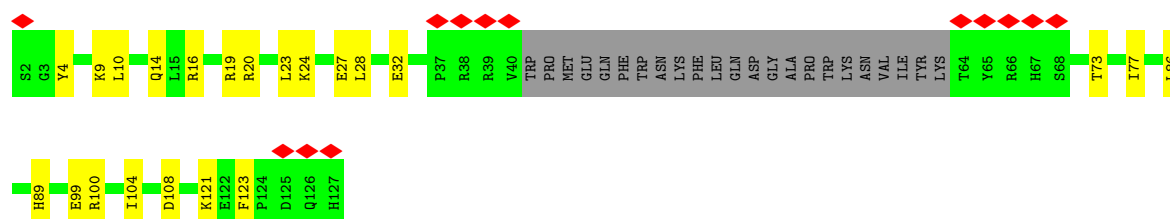
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a: 



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

Chain b: 



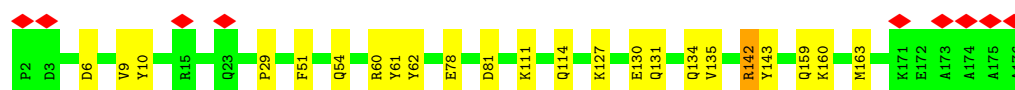
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c: 



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

Chain d: 

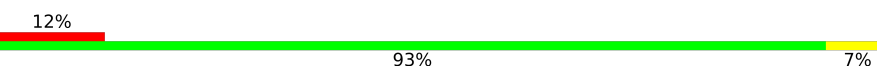


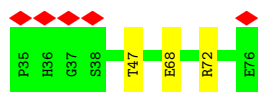
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e: 

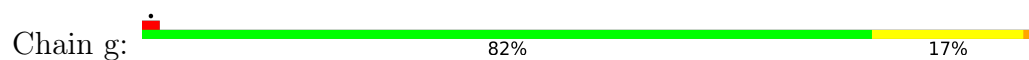


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

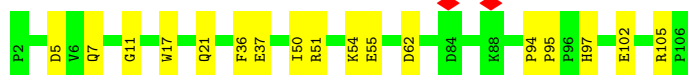
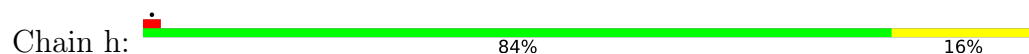
Chain f: 



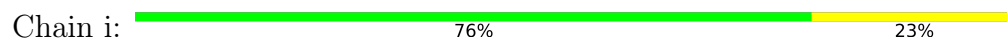
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



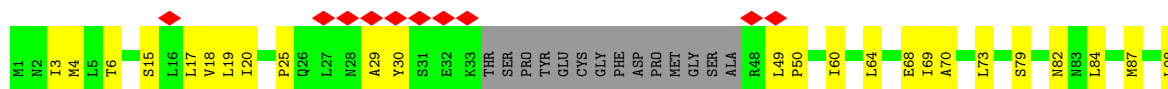
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



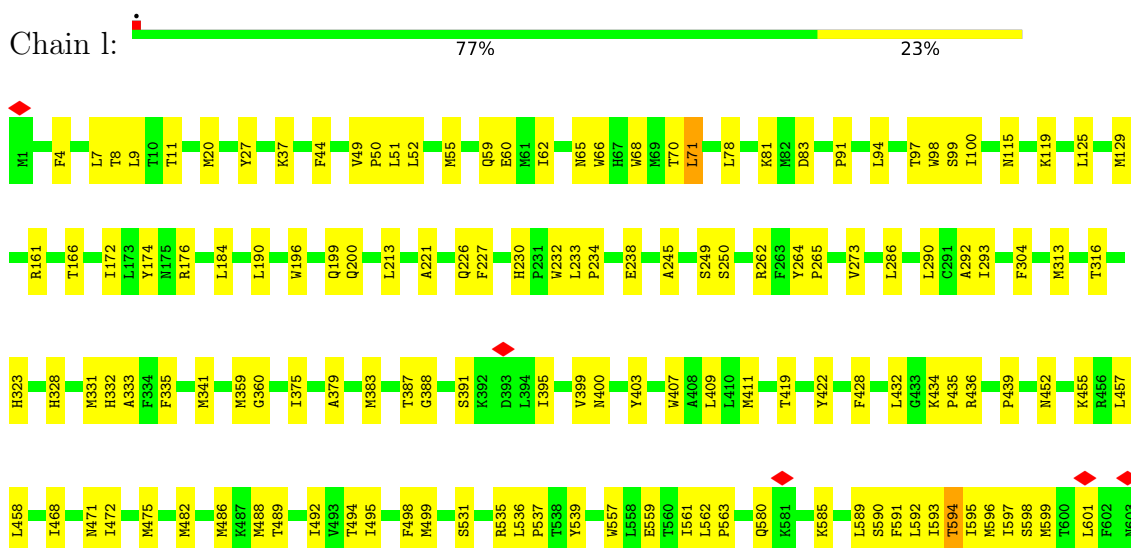
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3



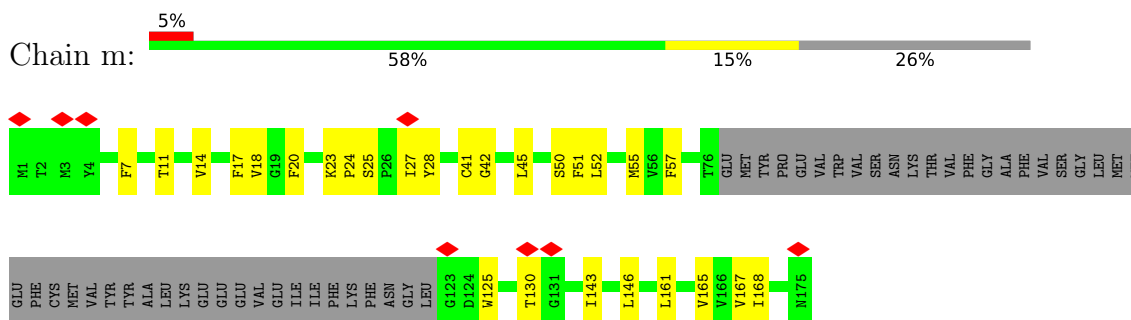
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L



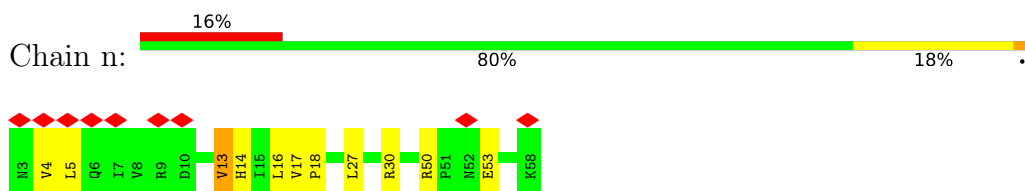
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5



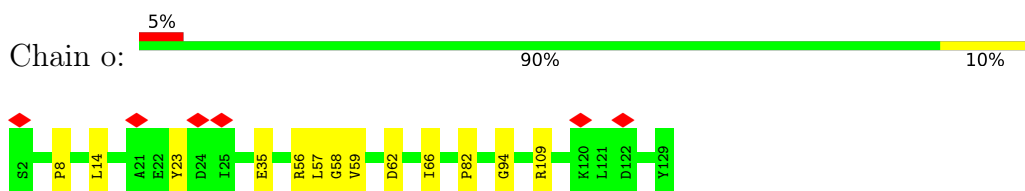
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6



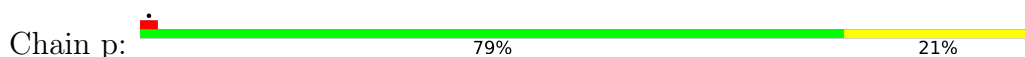
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

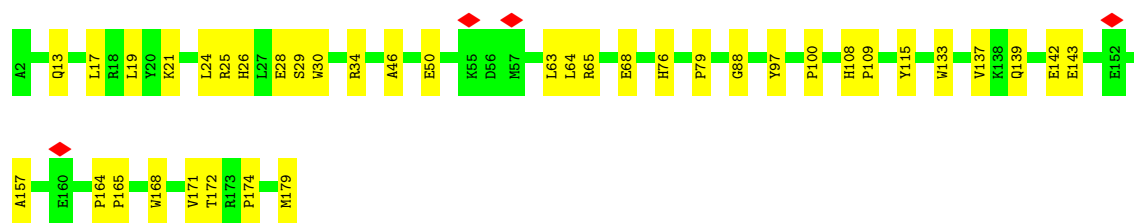


- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



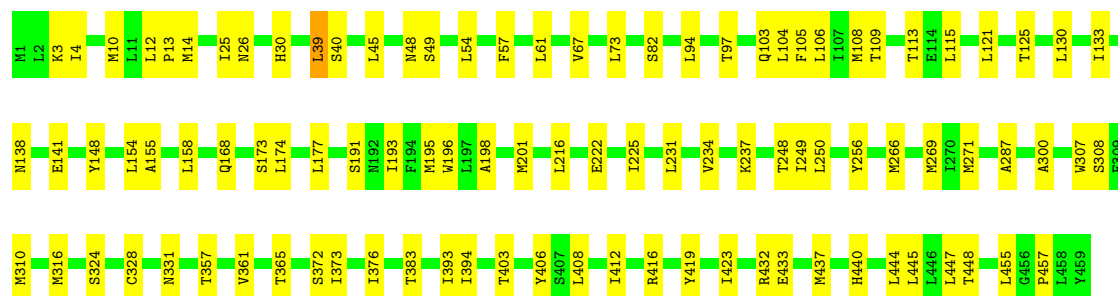
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9





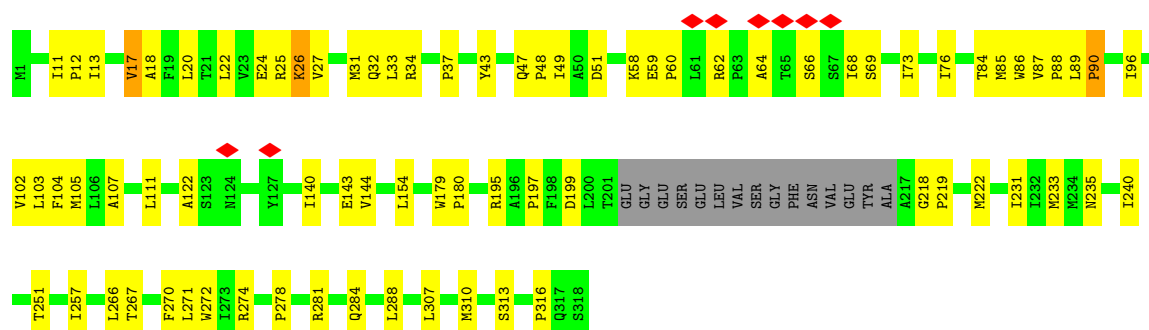
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r: 79% 21%



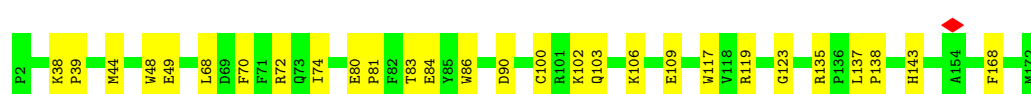
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s: 71% 24% 5%



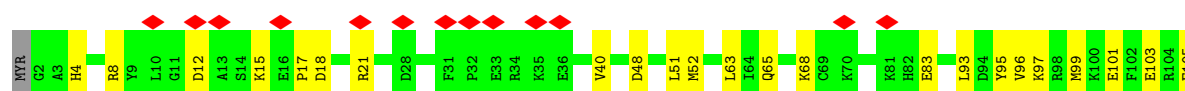
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u: 84% 16%



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

Chain v: 18% 74% 21% 5%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	209056	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	0.212	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0239	Depositor
Map size (Å)	333.7616, 333.7616, 333.7616	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.18	0/3393	0.48	6/4584 (0.1%)
2	B	0.15	0/1443	0.34	0/1952
3	C	0.13	0/1279	0.33	0/1730
4	E	0.12	0/995	0.31	0/1340
5	F	0.11	0/702	0.34	0/945
6	G	0.15	0/705	0.39	0/956
6	X	0.16	0/708	0.45	0/959
7	H	0.12	0/929	0.32	0/1258
8	I	0.21	0/798	0.54	2/1079 (0.2%)
9	J	0.12	0/2411	0.33	0/3254
10	K	0.09	0/365	0.30	0/493
11	L	0.13	0/1039	0.31	0/1403
12	M	0.14	0/5384	0.34	1/7295 (0.0%)
13	N	0.28	1/1245 (0.1%)	0.49	3/1694 (0.2%)
14	O	0.16	0/1711	0.43	0/2328
15	P	0.14	0/1789	0.40	1/2436 (0.0%)
16	Q	0.17	0/3451	0.40	1/4672 (0.0%)
17	S	0.16	0/582	0.39	0/783
18	T	0.09	0/755	0.27	0/1018
19	U	0.11	0/664	0.33	0/912
20	V	0.19	0/1042	0.47	3/1411 (0.2%)
21	W	0.13	0/1204	0.30	0/1624
22	Y	0.13	0/623	0.30	0/853
23	Z	0.10	0/695	0.27	0/939
24	a	0.13	0/1199	0.33	0/1623
25	b	0.17	0/906	0.36	0/1232
26	c	0.17	0/1371	0.34	0/1875
27	d	0.17	0/1494	0.39	2/2015 (0.1%)
28	e	0.18	0/916	0.48	1/1246 (0.1%)
29	f	0.13	0/350	0.31	0/473
30	g	0.16	0/1031	0.49	4/1394 (0.3%)
31	h	0.11	0/889	0.29	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.17	0/2773	0.38	0/3768
33	j	0.16	0/819	0.37	0/1117
34	k	0.14	0/759	0.38	0/1029
35	l	0.18	0/4911	0.40	1/6679 (0.0%)
36	m	0.15	0/970	0.37	0/1316
37	n	0.21	0/491	0.66	1/663 (0.2%)
38	o	0.12	0/1092	0.32	0/1481
39	p	0.13	0/1590	0.31	0/2155
40	r	0.18	0/3723	0.44	0/5078
41	s	0.24	0/2464	0.54	4/3369 (0.1%)
42	u	0.13	0/1436	0.36	0/1938
43	v	0.14	0/1052	0.44	0/1411
44	w	0.14	0/2642	0.39	1/3580 (0.0%)
All	All	0.16	1/66790 (0.0%)	0.40	31/90550 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	143	PRO	CG-CD	-8.16	1.23	1.50

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N	143	PRO	N-CD-CG	-11.44	86.05	103.20
13	N	143	PRO	CA-N-CD	-8.28	100.40	112.00
44	w	243	LYS	N-CA-C	7.87	119.94	111.36
1	A	120	GLY	N-CA-C	7.38	121.59	112.73
1	A	318	ILE	CA-C-N	7.33	126.83	118.85
1	A	318	ILE	C-N-CA	7.33	126.83	118.85
30	g	11	VAL	CA-C-N	7.12	127.12	119.28
30	g	11	VAL	C-N-CA	7.12	127.12	119.28
37	n	16	LEU	N-CA-C	6.96	118.87	111.28
35	l	68	TRP	N-CA-C	6.78	118.46	111.14
20	V	95	CYS	CA-CB-SG	6.42	129.17	114.40
16	Q	224	ALA	N-CA-C	6.39	118.25	111.28
20	V	94	GLY	CA-C-N	-6.19	112.33	122.54
20	V	94	GLY	C-N-CA	-6.19	112.33	122.54
13	N	143	PRO	CA-CB-CG	-6.16	92.81	104.50
1	A	121	GLU	N-CA-C	6.05	117.32	109.64
27	d	142	ARG	N-CA-C	6.01	117.63	111.14
27	d	143	TYR	N-CA-C	5.74	122.22	113.61
1	A	121	GLU	CA-C-N	5.57	125.33	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	GLU	C-N-CA	5.57	125.33	119.76
15	P	52	ASP	N-CA-C	5.41	117.25	111.36
8	I	41	LEU	CA-C-N	5.38	125.14	119.76
8	I	41	LEU	C-N-CA	5.38	125.14	119.76
41	s	86	TRP	N-CA-C	5.08	117.71	111.82
28	e	136	LEU	CB-CA-C	-5.07	110.71	116.54
41	s	218	GLY	CA-C-N	5.05	124.65	119.05
41	s	218	GLY	C-N-CA	5.05	124.65	119.05
12	M	173	MET	N-CA-C	5.01	118.49	112.38
30	g	7	ARG	CA-C-N	5.00	124.93	119.78
30	g	7	ARG	C-N-CA	5.00	124.93	119.78
41	s	219	PRO	N-CA-C	-5.00	106.58	113.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3318	0	3280	95	0
2	B	1412	0	1363	36	0
3	C	1248	0	1254	16	0
4	E	971	0	975	20	0
5	F	691	0	704	9	0
6	G	693	0	671	27	0
6	X	696	0	680	33	0
7	H	910	0	950	16	0
8	I	780	0	808	18	0
9	J	2359	0	2402	40	0
10	K	355	0	329	15	0
11	L	1016	0	1016	18	0
12	M	5296	0	5326	78	0
13	N	1204	0	1162	14	0
14	O	1671	0	1673	48	0
15	P	1738	0	1693	22	0
16	Q	3377	0	3319	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	S	567	0	565	8	0
18	T	741	0	702	7	0
19	U	643	0	642	6	0
20	V	1021	0	1027	20	0
21	W	1173	0	1166	23	0
22	Y	597	0	537	11	0
23	Z	674	0	643	11	0
24	a	1165	0	1174	23	0
25	b	879	0	899	27	0
26	c	1315	0	1208	26	0
27	d	1461	0	1429	17	0
28	e	890	0	837	16	0
29	f	342	0	341	3	0
30	g	1000	0	994	23	0
31	h	867	0	871	13	0
32	i	2710	0	2874	84	0
33	j	800	0	855	26	0
34	k	748	0	799	22	0
35	l	4782	0	4929	117	0
36	m	948	0	960	24	0
37	n	479	0	486	11	0
38	o	1062	0	1072	11	0
39	p	1534	0	1470	29	0
40	r	3631	0	3839	77	0
41	s	2394	0	2508	77	0
42	u	1398	0	1378	22	0
43	v	1028	0	980	23	0
44	w	2582	0	2531	68	0
45	A	8	0	0	2	0
45	B	16	0	0	0	0
45	C	8	0	0	0	0
45	M	16	0	0	0	0
46	A	31	0	19	4	0
47	A	44	0	27	4	0
48	C	47	0	71	5	0
48	U	51	0	82	4	0
48	V	51	0	82	11	0
48	l	139	0	209	35	0
48	m	41	0	59	13	0
48	s	51	0	82	3	0
49	C	52	0	88	4	0
49	V	52	0	88	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	e	52	0	88	8	0
49	i	52	0	88	6	0
49	j	52	0	88	3	0
49	n	52	0	88	7	0
50	G	35	0	0	2	0
50	X	35	0	0	1	0
51	J	48	0	23	3	0
52	M	4	0	0	0	0
52	O	4	0	0	0	0
53	M	1	0	0	0	0
54	N	51	0	46	4	0
54	V	71	0	92	14	0
54	a	91	0	132	26	0
54	i	66	0	76	11	0
54	l	199	0	307	16	0
54	n	78	0	103	12	0
54	r	100	0	156	14	0
55	T	1	0	0	0	0
56	s	28	0	31	8	0
57	w	27	0	11	10	0
All	All	66820	0	67457	1272	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (1272) 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)
54:n:102:CDL:C82	54:r:714:CDL:H852	1.45	1.43
37:n:30:ARG:NE	54:n:102:CDL:OA4	1.70	1.23
1:A:48:ARG:HD2	10:K:70:ASN:O	1.41	1.21
6:X:93:ILE:CG2	6:X:108:LEU:HD23	1.71	1.20
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.19
30:g:7:ARG:NH1	30:g:91:ASP:OD2	1.79	1.16
6:X:93:ILE:HG23	6:X:108:LEU:HD23	1.23	1.15
51:J:401:NDP:O4D	51:J:401:NDP:C4D	1.68	1.15
54:a:201:CDL:H521	48:l:720:PEE:H14	1.26	1.10
25:b:100:ARG:HB3	35:l:60:GLU:HB2	1.32	1.10
37:n:13:VAL:HG13	40:r:14:MET:HG2	1.31	1.10
30:g:7:ARG:HH12	30:g:91:ASP:CG	1.64	1.06
25:b:100:ARG:CB	35:l:60:GLU:HB2	1.85	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:n:102:CDL:C82	54:r:714:CDL:C85	2.34	1.05
54:a:201:CDL:H521	48:l:720:PEE:C11	1.88	1.03
44:w:72:ARG:HH21	44:w:75:ARG:HB3	1.20	1.02
26:c:106:HIS:HD2	26:c:108:ASP:H	1.02	1.01
44:w:72:ARG:NH2	44:w:75:ARG:HB3	1.74	1.01
24:a:169:TYR:HH	30:g:2:THR:N	1.59	1.00
41:s:25:ARG:HD3	56:s:403:UQ:HM21	1.43	1.00
20:V:95:CYS:HB2	20:V:115:CYS:HA	1.44	0.98
41:s:13:ILE:O	41:s:17:VAL:HG13	1.64	0.97
1:A:123:GLY:N	14:O:180:CYS:SG	2.37	0.96
33:j:4:MET:HE2	48:m:202:PEE:H19	1.48	0.96
1:A:50:ASP:O	1:A:59:ARG:NH2	1.99	0.95
24:a:95:GLU:OE2	54:a:201:CDL:O1	1.84	0.94
32:i:220:ILE:HG22	32:i:323:MET:HE1	1.48	0.94
37:n:13:VAL:CG1	40:r:14:MET:HG2	2.00	0.92
48:l:718:PEE:H37	48:l:718:PEE:H60	1.51	0.92
6:X:93:ILE:CG2	6:X:108:LEU:CD2	2.48	0.92
48:m:202:PEE:H10	48:m:202:PEE:H2	1.53	0.91
44:w:169:PHE:CG	57:w:401:ADP:N6	2.39	0.91
41:s:87:VAL:HG23	41:s:88:PRO:HD3	1.53	0.90
6:X:123:GLU:HG2	6:X:129:GLU:HA	1.53	0.90
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.51	0.89
26:c:116:ARG:HG2	48:l:719:PEE:H49	1.51	0.89
35:l:119:LYS:NZ	54:l:712:CDL:OA3	2.05	0.89
35:l:590:SER:O	35:l:594:THR:HG22	1.71	0.89
6:X:93:ILE:HG21	6:X:108:LEU:HD23	1.57	0.86
6:X:93:ILE:HG21	6:X:108:LEU:CD2	2.06	0.85
20:V:108:TYR:HE2	54:V:203:CDL:H112	1.39	0.85
25:b:99:GLU:OE2	35:l:59:GLN:OE1	1.93	0.85
44:w:67:CYS:SG	44:w:218:ILE:HD13	2.16	0.84
20:V:66:ILE:HD11	20:V:101:LEU:HD13	1.59	0.84
32:i:220:ILE:HG22	32:i:323:MET:CE	2.07	0.84
24:a:127:ASP:OD1	49:n:101:PLX:H12	1.77	0.84
16:Q:82:LEU:CD1	16:Q:101:LEU:HD22	2.08	0.84
22:Y:69:ILE:HD13	35:l:383:MET:HE2	1.60	0.83
6:G:74:LEU:H	6:G:74:LEU:HD23	1.44	0.83
48:m:202:PEE:H52	41:s:104:PHE:HE1	1.43	0.82
27:d:130:GLU:OE2	27:d:134:GLN:NE2	2.12	0.82
25:b:99:GLU:OE2	35:l:59:GLN:CD	2.22	0.82
26:c:106:HIS:CD2	26:c:108:ASP:H	1.94	0.82
1:A:48:ARG:CD	10:K:70:ASN:O	2.26	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:98:LEU:HD12	6:X:98:LEU:O	1.79	0.81
54:a:201:CDL:H191	54:a:201:CDL:H732	1.62	0.81
30:g:7:ARG:NH1	30:g:91:ASP:CG	2.30	0.81
1:A:209:GLU:OE2	1:A:226:LYS:NZ	2.11	0.81
35:l:591:PHE:HA	35:l:594:THR:CG2	2.11	0.81
16:Q:82:LEU:HD12	16:Q:101:LEU:HD22	1.60	0.80
48:m:202:PEE:H52	41:s:104:PHE:CE1	2.16	0.80
20:V:108:TYR:HE2	54:V:203:CDL:C11	1.94	0.80
11:L:156:LYS:HE2	12:M:68:ARG:HE	1.46	0.80
54:V:203:CDL:OB7	54:V:203:CDL:H1	1.83	0.79
16:Q:105:MET:HB2	16:Q:107:ARG:HH12	1.48	0.79
32:i:133:TRP:HE3	54:i:401:CDL:H391	1.49	0.78
48:l:718:PEE:H28	48:l:718:PEE:C22	2.14	0.78
1:A:125:CYS:SG	1:A:277:ASN:ND2	2.57	0.78
35:l:190:LEU:HD23	40:r:383:THR:HG21	1.65	0.77
44:w:67:CYS:C	44:w:214:ILE:HD11	2.08	0.77
32:i:320:THR:HG21	44:w:300:ASN:HA	1.66	0.76
54:a:201:CDL:H251	54:a:201:CDL:H211	1.66	0.76
32:i:320:THR:CG2	44:w:300:ASN:HA	2.15	0.76
40:r:57:PHE:HD1	40:r:113:THR:HG22	1.48	0.76
44:w:169:PHE:CD2	57:w:401:ADP:N6	2.53	0.76
22:Y:100:LEU:HB2	43:v:111:ARG:HH12	1.51	0.76
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.20	0.75
20:V:69:ILE:HG13	20:V:100:THR:HG21	1.68	0.75
41:s:87:VAL:CG2	41:s:88:PRO:HD3	2.16	0.75
1:A:320:GLY:O	1:A:351:THR:HG22	1.85	0.75
1:A:33:GLY:HA2	1:A:294:VAL:HG12	1.69	0.75
12:M:299:ARG:HG2	12:M:300:GLN:HG2	1.69	0.75
54:a:201:CDL:H761	54:a:201:CDL:H201	1.67	0.75
32:i:95:MET:HE2	32:i:149:ILE:HA	1.68	0.74
6:G:119:ILE:HD13	6:G:135:ALA:HB1	1.68	0.74
41:s:89:LEU:HD23	41:s:105:MET:HE1	1.69	0.74
35:l:592:LEU:O	35:l:596:MET:HG3	1.88	0.74
48:l:718:PEE:C25	48:l:718:PEE:H34	2.17	0.74
48:m:202:PEE:H10	48:m:202:PEE:C1	2.16	0.74
13:N:6:VAL:HG12	13:N:9:ARG:HH21	1.51	0.74
35:l:591:PHE:O	35:l:594:THR:HG23	1.87	0.73
25:b:99:GLU:OE2	35:l:59:GLN:NE2	2.21	0.73
38:o:23:TYR:OH	39:p:68:GLU:OE1	2.06	0.73
41:s:88:PRO:HG2	41:s:105:MET:HE2	1.70	0.73
16:Q:102:SER:OG	16:Q:107:ARG:NH1	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:97:MET:HE3	35:l:599:MET:HE1	1.70	0.73
35:l:419:THR:HA	35:l:422:TYR:CE2	2.24	0.73
1:A:52:ARG:HG3	1:A:52:ARG:HH11	1.51	0.73
3:C:126:GLU:O	9:J:89:TYR:OH	2.06	0.73
32:i:91:ASN:OD1	32:i:92:PRO:HD2	1.89	0.73
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.71	0.72
34:k:22:TYR:O	35:l:585:LYS:NZ	2.17	0.72
32:i:97:MET:CE	35:l:599:MET:HE1	2.19	0.72
25:b:123:PHE:HB3	43:v:40:VAL:HG21	1.71	0.72
1:A:121:GLU:HG3	1:A:122:PRO:HD2	1.71	0.72
54:a:201:CDL:H201	54:a:201:CDL:H772	1.71	0.72
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.71	0.72
48:l:718:PEE:H28	48:l:718:PEE:H36	1.70	0.71
16:Q:68:ASP:O	32:i:49:ASN:ND2	2.23	0.71
44:w:72:ARG:NH2	44:w:75:ARG:CB	2.53	0.71
34:k:57:ASN:HB3	36:m:143:ILE:HG13	1.71	0.71
6:G:74:LEU:HD12	6:G:79:ILE:HD11	1.71	0.71
4:E:29:LYS:NZ	50:G:201:8Q1:O35	2.23	0.71
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.71	0.71
41:s:24:GLU:OE2	41:s:274:ARG:NH1	2.23	0.71
44:w:38:TYR:HH	44:w:292:HIS:HD1	1.36	0.71
5:F:46:LYS:HE2	12:M:674:LEU:HD21	1.73	0.71
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.71	0.70
40:r:104:LEU:HG	40:r:108:MET:HE2	1.72	0.70
14:O:182:ASN:ND2	14:O:194:GLU:OE1	2.25	0.70
40:r:14:MET:HE2	40:r:30:HIS:HD2	1.57	0.70
25:b:14:GLN:HE22	39:p:157:ALA:HB3	1.54	0.70
24:a:152:LYS:HD3	30:g:96:VAL:HG21	1.74	0.70
48:l:718:PEE:H34	48:l:718:PEE:H41	1.72	0.70
40:r:403:THR:HA	40:r:406:TYR:CE2	2.27	0.70
54:V:203:CDL:H831	38:o:94:GLY:HA3	1.73	0.69
1:A:52:ARG:HG3	1:A:52:ARG:NH1	2.06	0.69
12:M:485:ASP:O	12:M:489:ILE:HG12	1.93	0.69
48:V:202:PEE:H3	40:r:191:SER:HB3	1.74	0.69
39:p:19:LEU:HD12	39:p:68:GLU:HG3	1.73	0.69
39:p:139:GLN:NE2	39:p:143:GLU:OE1	2.25	0.69
9:J:83:PRO:HG3	9:J:119:VAL:HG11	1.74	0.69
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.33	0.69
16:Q:99:MET:CE	16:Q:109:CYS:SG	2.81	0.69
54:a:201:CDL:H322	48:l:720:PEE:H62	1.75	0.68
1:A:119:GLU:CD	1:A:127:ASP:HB2	2.17	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.76	0.68
35:l:495:ILE:HG22	35:l:499:MET:HE2	1.73	0.68
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.26	0.68
37:n:30:ARG:CD	54:n:102:CDL:OA4	2.41	0.68
49:n:101:PLX:H1A2	49:n:101:PLX:O3	1.94	0.68
43:v:103:GLU:OE2	43:v:106:ARG:NH2	2.26	0.68
27:d:127:LYS:NZ	27:d:131:GLN:OE1	2.27	0.67
44:w:169:PHE:CB	57:w:401:ADP:N6	2.57	0.67
6:X:93:ILE:HG23	6:X:108:LEU:CD2	2.12	0.67
36:m:42:GLY:HA2	48:m:202:PEE:H23	1.76	0.67
1:A:119:GLU:OE2	1:A:127:ASP:HB2	1.93	0.67
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.27	0.67
32:i:95:MET:HE2	32:i:149:ILE:CA	2.23	0.67
34:k:98:CYS:HB2	35:l:580:GLN:HB2	1.76	0.67
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.28	0.67
44:w:176:GLN:NE2	44:w:236:ASP:OD2	2.28	0.67
35:l:250:SER:HB2	35:l:333:ALA:HA	1.76	0.67
35:l:391:SER:O	35:l:395:ILE:HG12	1.95	0.67
32:i:320:THR:HG21	44:w:300:ASN:CA	2.24	0.67
39:p:19:LEU:HD13	39:p:64:LEU:HD12	1.76	0.67
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.78	0.66
20:V:95:CYS:HB2	20:V:115:CYS:CA	2.16	0.66
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.27	0.66
6:X:92:LYS:HG2	6:X:110:LEU:HD21	1.76	0.66
1:A:86:ARG:NE	1:A:339:PHE:CD2	2.64	0.66
25:b:100:ARG:HB2	35:l:60:GLU:HB2	1.74	0.66
1:A:41:ILE:O	1:A:137:LYS:NZ	2.29	0.66
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.26	0.66
25:b:108:ASP:OD1	43:v:68:LYS:NZ	2.29	0.66
30:g:12:PRO:O	49:i:705:PLX:O2	2.13	0.66
3:C:71:CYS:HB3	16:Q:141:TYR:CG	2.30	0.65
32:i:329:MET:HE3	54:i:401:CDL:H131	1.78	0.65
41:s:51:ASP:HB3	56:s:403:UQ:H8	1.78	0.65
9:J:131:GLY:O	51:J:401:NDP:H51A	1.97	0.65
20:V:108:TYR:CE2	54:V:203:CDL:C11	2.79	0.65
41:s:62:ARG:HH21	41:s:68:ILE:HB	1.62	0.65
7:H:38:ILE:O	7:H:45:ARG:NH1	2.26	0.65
41:s:89:LEU:CD2	41:s:105:MET:HE1	2.26	0.65
54:a:201:CDL:H761	54:a:201:CDL:C19	2.25	0.65
33:j:3:ILE:CG2	48:m:202:PEE:H13	2.26	0.65
4:E:62:LYS:HD2	4:E:66:MET:HE2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:94:GLU:OE2	21:W:104:TRP:NE1	2.27	0.65
54:a:201:CDL:H761	54:a:201:CDL:C20	2.27	0.65
1:A:48:ARG:O	10:K:74:ARG:NH1	2.29	0.65
5:F:40:ARG:HH12	5:F:84:ALA:HB1	1.62	0.65
21:W:85:GLN:OE1	31:h:105:ARG:NH1	2.26	0.65
41:s:235:ASN:HD21	41:s:270:PHE:HE2	1.41	0.65
44:w:72:ARG:HH21	44:w:75:ARG:CB	2.04	0.64
48:V:202:PEE:C1	40:r:191:SER:HB3	2.27	0.64
48:V:202:PEE:H33	48:V:202:PEE:H71	1.79	0.64
2:B:47:SER:OG	2:B:49:ASP:OD1	2.16	0.64
54:a:201:CDL:H201	54:a:201:CDL:C76	2.27	0.64
16:Q:53:TYR:OH	48:l:718:PEE:O2P	2.08	0.64
14:O:198:PRO:O	14:O:201:ILE:HG22	1.98	0.64
33:j:68:GLU:HG2	36:m:161:LEU:HD13	1.80	0.64
49:n:101:PLX:H81	40:r:40:SER:CB	2.28	0.64
1:A:123:GLY:CA	14:O:180:CYS:SG	2.85	0.63
24:a:106:VAL:HG13	37:n:50:ARG:HH21	1.63	0.63
25:b:28:LEU:HG	25:b:32:GLU:HG2	1.79	0.63
48:l:718:PEE:H36	48:l:718:PEE:C18	2.27	0.63
9:J:369:VAL:HG12	9:J:370:LYS:HG2	1.80	0.63
25:b:16:ARG:HD3	25:b:20:ARG:HH12	1.64	0.63
49:e:201:PLX:H1C3	48:l:720:PEE:O2P	1.97	0.63
3:C:59:ARG:NH1	49:C:312:PLX:O3	2.29	0.63
14:O:76:ALA:O	14:O:78:ALA:N	2.32	0.63
44:w:63:ASP:O	44:w:206:TYR:HD1	1.82	0.63
32:i:95:MET:CE	32:i:149:ILE:HG22	2.28	0.63
12:M:370:GLU:OE2	12:M:518:ARG:NH2	2.32	0.63
9:J:218:ALA:O	9:J:221:ARG:NH1	2.31	0.63
6:G:75:THR:OG1	6:G:156:GLU:OE1	2.16	0.63
8:I:44:GLY:HA3	16:Q:359:ASP:OD2	1.99	0.62
32:i:133:TRP:CE3	54:i:401:CDL:H391	2.34	0.62
32:i:211:MET:HG2	32:i:333:SER:HB2	1.81	0.62
34:k:44:SER:HB2	34:k:59:MET:HE1	1.81	0.62
41:s:62:ARG:HD3	41:s:64:ALA:H	1.64	0.62
14:O:38:LEU:O	14:O:124:ARG:NH2	2.31	0.62
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.81	0.62
41:s:25:ARG:CD	56:s:403:UQ:HM21	2.25	0.62
32:i:7:THR:HG22	32:i:11:MET:HE2	1.79	0.62
32:i:268:GLN:HE22	32:i:272:LYS:HE3	1.65	0.62
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.32	0.62
24:a:154:LEU:HD21	32:i:272:LYS:HE2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:a:201:CDL:H521	48:l:720:PEE:H13	1.79	0.62
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.34	0.62
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.32	0.62
54:a:201:CDL:H712	54:a:201:CDL:H172	1.81	0.62
31:h:50:ILE:HG22	31:h:54:LYS:HE2	1.82	0.62
44:w:241:TYR:O	44:w:246:LEU:HD23	2.00	0.62
48:C:311:PEE:H82	56:s:403:UQ:H172	1.82	0.62
36:m:7:PHE:O	36:m:11:THR:HG23	1.98	0.62
4:E:104:MET:HE2	4:E:104:MET:HA	1.82	0.62
15:P:44:ARG:HB3	15:P:45:PRO:HD3	1.82	0.62
41:s:235:ASN:ND2	41:s:270:PHE:HE2	1.97	0.62
54:a:201:CDL:H201	54:a:201:CDL:C77	2.30	0.62
48:l:720:PEE:O1P	48:l:720:PEE:H8	1.99	0.62
54:r:714:CDL:H612	54:r:714:CDL:H662	1.82	0.62
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.81	0.61
26:c:117:VAL:HG21	35:l:539:TYR:HB2	1.81	0.61
41:s:20:LEU:HD12	41:s:20:LEU:O	2.00	0.61
9:J:211:ASP:O	9:J:215:ASN:ND2	2.33	0.61
28:e:128:TYR:CE1	28:e:132:ASN:ND2	2.68	0.61
30:g:7:ARG:NH1	30:g:91:ASP:OD1	2.27	0.61
41:s:84:THR:O	41:s:87:VAL:HG22	2.01	0.61
44:w:67:CYS:O	44:w:214:ILE:HD11	2.00	0.61
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.81	0.61
54:V:203:CDL:H721	54:V:203:CDL:H561	1.80	0.61
41:s:87:VAL:N	41:s:88:PRO:HD2	2.15	0.61
1:A:123:GLY:HA2	14:O:180:CYS:CB	2.29	0.61
42:u:80:GLU:HG2	42:u:81:PRO:HD3	1.83	0.61
25:b:86:LEU:HD11	35:l:9:LEU:HD12	1.83	0.61
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.33	0.60
16:Q:99:MET:HE2	16:Q:109:CYS:SG	2.40	0.60
44:w:125:ASP:O	44:w:130:ARG:NH2	2.34	0.60
32:i:334:THR:HG21	54:r:714:CDL:H391	1.83	0.60
1:A:210:THR:HB	1:A:224:ARG:HG2	1.83	0.60
32:i:95:MET:HE2	32:i:149:ILE:N	2.16	0.60
33:j:64:LEU:HD13	36:m:165:VAL:HG22	1.82	0.60
13:N:120:THR:HG22	13:N:122:GLN:H	1.65	0.60
22:Y:51:THR:HG22	22:Y:53:SER:H	1.67	0.60
27:d:111:LYS:NZ	35:l:200:GLN:OE1	2.29	0.60
54:n:102:CDL:H811	54:n:102:CDL:H242	1.84	0.60
15:P:147:THR:HB	15:P:153:ILE:HD11	1.84	0.60
14:O:195:ASP:OD2	14:O:222:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:146:ALA:HB1	44:w:157:VAL:HG21	1.84	0.60
2:B:111:GLU:O	2:B:141:ARG:NH1	2.35	0.60
16:Q:82:LEU:HD11	16:Q:101:LEU:HD22	1.84	0.60
6:X:98:LEU:HD12	6:X:98:LEU:C	2.26	0.60
26:c:58:ARG:NE	38:o:35:GLU:OE2	2.29	0.60
35:l:245:ALA:O	35:l:249:SER:OG	2.18	0.60
35:l:161:ARG:NH1	35:l:238:GLU:OE1	2.35	0.59
11:L:90:GLY:HA3	15:P:238:PRO:HB2	1.82	0.59
11:L:168:LYS:HE2	11:L:168:LYS:HA	1.84	0.59
24:a:168:TRP:CD2	30:g:2:THR:HG23	2.36	0.59
28:e:132:ASN:HB2	28:e:134:LEU:HD23	1.84	0.59
32:i:220:ILE:CG2	32:i:323:MET:HE1	2.28	0.59
33:j:18:VAL:HG22	41:s:222:MET:HG3	1.82	0.59
15:P:68:ILE:HG22	15:P:69:LEU:HD12	1.84	0.59
2:B:177:THR:HG21	2:B:182:GLU:HB2	1.83	0.59
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.84	0.59
8:I:40:LYS:HB3	21:W:7:LYS:H	1.66	0.59
33:j:3:ILE:HG21	48:m:202:PEE:H13	1.83	0.59
34:k:23:ARG:HG2	36:m:23:LYS:HE2	1.84	0.59
41:s:102:VAL:HG11	41:s:154:LEU:HD11	1.84	0.59
44:w:123:SER:OG	44:w:125:ASP:OD1	2.19	0.59
27:d:9:VAL:HG11	28:e:123:GLU:HG2	1.83	0.59
40:r:266:MET:HA	40:r:269:MET:HE3	1.85	0.59
33:j:70:ALA:HA	33:j:73:LEU:HD12	1.85	0.59
41:s:87:VAL:HG23	41:s:88:PRO:CD	2.29	0.59
12:M:161:GLU:OE1	14:O:42:ARG:NH2	2.35	0.59
35:l:591:PHE:O	35:l:594:THR:CG2	2.51	0.59
1:A:185:ASN:ND2	1:A:187:CYS:O	2.35	0.59
1:A:319:PRO:CG	1:A:347:THR:HG21	2.33	0.59
4:E:15:THR:OG1	11:L:55:VAL:O	2.20	0.59
10:K:100:GLN:HB3	14:O:71:PRO:HA	1.85	0.59
32:i:96:THR:O	32:i:100:MET:HG2	2.03	0.58
35:l:27:TYR:O	35:l:115:ASN:ND2	2.35	0.58
35:l:591:PHE:HA	35:l:594:THR:HG22	1.85	0.58
11:L:109:ASN:ND2	11:L:111:LEU:O	2.35	0.58
20:V:108:TYR:HB2	54:V:203:CDL:HB32	1.84	0.58
21:W:85:GLN:O	21:W:89:GLU:HG3	2.03	0.58
41:s:288:LEU:CD1	48:s:401:PEE:H7	2.33	0.58
44:w:118:TYR:OH	57:w:401:ADP:O2'	2.21	0.58
23:Z:21:GLN:O	23:Z:23:LYS:NZ	2.35	0.58
1:A:88:ARG:HG2	1:A:246:GLU:HG2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:THR:HG22	2:B:179:THR:H	1.68	0.58
6:G:115:GLN:HE22	6:G:119:ILE:HD11	1.68	0.58
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.86	0.58
54:V:203:CDL:H712	54:V:203:CDL:H521	1.86	0.58
32:i:347:ASN:HB3	49:i:705:PLX:H301	1.86	0.58
1:A:119:GLU:OE2	1:A:127:ASP:N	2.35	0.58
1:A:317:VAL:HG23	1:A:356:VAL:HG12	1.86	0.58
14:O:76:ALA:C	14:O:78:ALA:H	2.12	0.58
15:P:154:GLU:OE2	15:P:180:ASN:ND2	2.34	0.58
26:c:62:TYR:OH	26:c:74:ASP:OD1	2.21	0.58
28:e:112:TYR:HB3	40:r:45:LEU:HG	1.85	0.58
43:v:51:LEU:O	43:v:52:MET:HG3	2.04	0.58
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.17	0.58
16:Q:97:LEU:HG	16:Q:99:MET:HE3	1.85	0.58
1:A:115:VAL:HG21	1:A:142:CYS:SG	2.44	0.58
44:w:67:CYS:SG	44:w:218:ILE:CD1	2.89	0.58
1:A:60:GLY:O	1:A:256:ARG:NH1	2.37	0.57
12:M:624:ARG:NH2	12:M:637:ASP:OD1	2.35	0.57
28:e:116:GLU:O	28:e:120:ARG:HG3	2.04	0.57
37:n:50:ARG:HB2	37:n:53:GLU:HB2	1.86	0.57
8:I:12:ARG:HD3	8:I:20:LEU:HD22	1.84	0.57
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.86	0.57
35:l:559:GLU:O	35:l:563:PRO:HD2	2.04	0.57
1:A:40:ARG:NH1	1:A:289:GLU:O	2.37	0.57
12:M:419:ARG:NH1	12:M:439:THR:O	2.37	0.57
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.39	0.57
21:W:68:ARG:O	21:W:72:MET:HG3	2.04	0.57
54:i:401:CDL:H171	54:i:401:CDL:H132	1.85	0.57
36:m:41:CYS:SG	36:m:57:PHE:HB2	2.45	0.57
12:M:636:TYR:CD2	12:M:642:VAL:HG22	2.39	0.57
32:i:268:GLN:HG3	42:u:168:PHE:HZ	1.68	0.57
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.40	0.57
14:O:76:ALA:C	14:O:78:ALA:N	2.63	0.57
15:P:104:THR:O	15:P:107:GLN:NE2	2.37	0.57
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.35	0.57
20:V:95:CYS:CB	20:V:115:CYS:HA	2.28	0.57
31:h:97:HIS:HA	31:h:102:GLU:HB3	1.87	0.57
28:e:152:ASP:OD1	28:e:153:GLU:N	2.37	0.57
32:i:11:MET:HE1	54:i:401:CDL:H771	1.87	0.57
44:w:42:ALA:HB1	44:w:47:GLU:HG3	1.86	0.57
35:l:593:ILE:HA	35:l:596:MET:HE2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:66:ILE:O	44:w:214:ILE:HG12	2.04	0.57
1:A:152:ARG:NH2	10:K:99:PRO:O	2.37	0.56
49:n:101:PLX:H322	49:n:101:PLX:H282	1.87	0.56
6:X:93:ILE:HD11	6:X:110:LEU:HD11	1.87	0.56
1:A:128:ARG:NH2	14:O:194:GLU:OE2	2.37	0.56
21:W:27:ARG:NH1	21:W:29:GLY:HA2	2.21	0.56
25:b:121:LYS:HE2	43:v:40:VAL:HA	1.87	0.56
32:i:220:ILE:CG2	32:i:323:MET:CE	2.82	0.56
48:m:202:PEE:H2	48:m:202:PEE:C4	2.31	0.56
41:s:281:ARG:HB2	41:s:284:GLN:HG3	1.86	0.56
44:w:65:ASN:OD1	44:w:66:ILE:N	2.39	0.56
54:a:201:CDL:H541	48:l:720:PEE:H16	1.86	0.56
34:k:37:MET:HE1	34:k:64:LEU:HD12	1.88	0.56
54:n:102:CDL:C82	54:r:714:CDL:C86	2.84	0.56
11:L:165:SER:OG	11:L:168:LYS:HB2	2.05	0.56
17:S:5:ILE:HG23	41:s:26:LYS:HB3	1.88	0.56
48:V:202:PEE:H74	48:V:202:PEE:C22	2.35	0.56
25:b:4:TYR:HB2	25:b:9:LYS:HE3	1.87	0.56
25:b:123:PHE:HD2	43:v:40:VAL:HG11	1.69	0.56
22:Y:45:ARG:HG2	35:l:439:PRO:HB3	1.88	0.56
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.86	0.56
39:p:28:GLU:OE2	39:p:34:ARG:NH1	2.36	0.56
19:U:47:ARG:HD3	33:j:82:ASN:ND2	2.21	0.56
49:n:101:PLX:H282	49:n:101:PLX:C32	2.36	0.56
9:J:192:ARG:NH2	9:J:262:THR:OG1	2.39	0.56
54:a:201:CDL:OA7	54:a:201:CDL:HA61	2.05	0.56
32:i:207:ILE:HG22	32:i:211:MET:HE2	1.88	0.56
32:i:284:MET:O	48:l:718:PEE:H67	2.06	0.56
37:n:27:LEU:HD11	54:n:102:CDL:H112	1.88	0.56
49:n:101:PLX:H81	40:r:40:SER:HB3	1.87	0.56
27:d:159:GLN:O	27:d:163:MET:HG3	2.04	0.56
35:l:99:SER:HB3	35:l:341:MET:HE1	1.88	0.56
12:M:676:ASN:O	12:M:678:GLN:NE2	2.37	0.55
24:a:87:THR:O	24:a:91:VAL:HG23	2.07	0.55
54:l:712:CDL:H842	54:l:712:CDL:H651	1.89	0.55
6:X:69:SER:OG	6:X:70:ASP:N	2.38	0.55
26:c:100:ASN:HB2	26:c:103:GLU:HG3	1.89	0.55
26:c:127:ASN:O	26:c:131:LYS:HG3	2.06	0.55
32:i:267:ILE:HG12	32:i:279:PRO:HB3	1.86	0.55
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.87	0.55
5:F:42:VAL:O	5:F:46:LYS:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:N:202:CDL:H711	41:s:43:TYR:OH	2.06	0.55
29:f:68:GLU:OE2	29:f:72:ARG:HD2	2.07	0.55
30:g:12:PRO:HB3	31:h:5:ASP:HB3	1.88	0.55
32:i:95:MET:CE	32:i:149:ILE:HA	2.37	0.55
32:i:268:GLN:NE2	32:i:272:LYS:HE3	2.20	0.55
35:l:227:PHE:O	35:l:230:HIS:ND1	2.37	0.55
13:N:69:ASN:OD1	13:N:112:ASN:ND2	2.38	0.55
24:a:97:GLU:OE2	27:d:60:ARG:NH1	2.40	0.55
36:m:57:PHE:CZ	41:s:111:LEU:HD11	2.42	0.55
1:A:121:GLU:HG3	1:A:122:PRO:CD	2.37	0.55
9:J:127:ILE:HD11	9:J:253:ILE:HD11	1.87	0.55
32:i:155:LEU:HD22	32:i:278:MET:HE1	1.87	0.55
35:l:488:MET:HE2	35:l:488:MET:HA	1.88	0.55
46:A:502:FMN:N5	47:A:503:NAI:H4N	2.22	0.55
4:E:37:ARG:O	4:E:41:ARG:HG2	2.07	0.55
5:F:24:CYS:N	5:F:58:CYS:SG	2.80	0.55
35:l:66:TRP:CD1	48:l:720:PEE:H3	2.42	0.55
54:l:712:CDL:H581	54:l:712:CDL:H851	1.89	0.55
41:s:88:PRO:HG2	41:s:105:MET:CE	2.37	0.55
54:a:201:CDL:H732	54:a:201:CDL:C19	2.35	0.55
43:v:103:GLU:O	43:v:107:ARG:HG2	2.07	0.55
7:H:35:LEU:HD11	7:H:48:THR:HG22	1.88	0.55
12:M:388:ASN:HB3	12:M:511:LYS:HE2	1.89	0.55
12:M:480:ALA:O	12:M:483:ARG:HG2	2.07	0.55
26:c:106:HIS:HD2	26:c:108:ASP:N	1.87	0.55
35:l:557:TRP:O	35:l:561:ILE:HG12	2.07	0.55
41:s:69:SER:O	41:s:73:ILE:HG12	2.07	0.55
39:p:13:GLN:HE22	39:p:17:LEU:HD11	1.71	0.54
16:Q:46:GLN:HB3	48:l:718:PEE:H6	1.72	0.54
34:k:2:PRO:HD2	34:k:5:TYR:CD2	2.42	0.54
7:H:94:MET:HE2	7:H:99:PRO:HG3	1.90	0.54
16:Q:105:MET:HB2	16:Q:107:ARG:NH1	2.18	0.54
6:G:74:LEU:H	6:G:74:LEU:CD2	2.16	0.54
21:W:66:GLU:OE2	42:u:123:GLY:N	2.30	0.54
24:a:169:TYR:OH	30:g:2:THR:N	2.33	0.54
1:A:109:ARG:HG2	11:L:166:TRP:CD1	2.42	0.54
7:H:76:GLN:O	7:H:79:GLU:HG2	2.07	0.54
15:P:43:THR:HA	15:P:47:ILE:HD12	1.89	0.54
25:b:104:ILE:HB	43:v:48:ASP:HB3	1.88	0.54
35:l:323:HIS:ND1	35:l:475:MET:SD	2.81	0.54
41:s:85:MET:HB3	41:s:233:MET:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:204:SER:OG	9:J:238:GLN:O	2.23	0.54
18:T:34:THR:OG1	18:T:47:ASP:OD1	2.26	0.54
35:l:221:ALA:HA	35:l:226:GLN:HG2	1.88	0.54
44:w:66:ILE:O	44:w:214:ILE:CG1	2.56	0.54
44:w:258:TYR:CE2	44:w:269:VAL:HG22	2.42	0.54
14:O:110:MET:O	14:O:114:GLU:HG3	2.08	0.54
17:S:34:LYS:NZ	42:u:90:ASP:OD2	2.32	0.54
6:X:99:SER:O	6:X:102:SER:OG	2.16	0.54
32:i:97:MET:CE	35:l:599:MET:CE	2.85	0.54
54:i:401:CDL:OA7	54:i:401:CDL:HA62	2.07	0.54
33:j:73:LEU:HD13	36:m:55:MET:HE1	1.90	0.54
48:m:202:PEE:C1	48:m:202:PEE:C4	2.85	0.54
3:C:184:ILE:O	3:C:187:GLU:HG2	2.08	0.54
54:N:202:CDL:C34	54:N:202:CDL:CA7	2.86	0.54
12:M:472:PRO:O	12:M:510:TRP:NE1	2.32	0.54
6:X:105:MET:HG2	6:X:139:MET:HE1	1.89	0.54
30:g:73:PHE:HE2	49:i:705:PLX:H392	1.72	0.54
37:n:14:HIS:CE1	40:r:26:ASN:OD1	2.61	0.54
38:o:56:ARG:NH1	38:o:58:GLY:O	2.41	0.54
44:w:67:CYS:O	44:w:214:ILE:CD1	2.56	0.54
3:C:83:ARG:NH1	16:Q:212:GLU:OE2	2.24	0.53
13:N:32:ASP:OD2	13:N:58:ARG:NH2	2.41	0.53
26:c:155:PRO:HG3	43:v:4:HIS:CE1	2.43	0.53
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.90	0.53
54:i:401:CDL:HB31	44:w:40:PRO:CB	2.38	0.53
35:l:407:TRP:O	35:l:411:MET:HG2	2.08	0.53
9:J:73:LEU:O	9:J:78:SER:OG	2.24	0.53
16:Q:259:GLU:OE1	16:Q:338:ARG:NH2	2.37	0.53
54:a:201:CDL:H191	54:a:201:CDL:H761	1.89	0.53
35:l:331:MET:SD	35:l:387:THR:HG23	2.48	0.53
41:s:49:ILE:HD12	41:s:49:ILE:N	2.23	0.53
43:v:95:TYR:O	43:v:99:MET:HG3	2.08	0.53
1:A:90:GLY:HA3	47:A:503:NAI:H1D	1.90	0.53
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.91	0.53
26:c:156:VAL:HG12	43:v:99:MET:HG2	1.90	0.53
35:l:591:PHE:CA	35:l:594:THR:HG22	2.38	0.53
42:u:100:CYS:HB2	42:u:103:GLN:OE1	2.08	0.53
26:c:55:TYR:OH	26:c:74:ASP:O	2.21	0.53
7:H:35:LEU:HD13	7:H:49:GLU:HG3	1.91	0.53
12:M:361:VAL:HB	12:M:632:MET:HE1	1.90	0.53
35:l:290:LEU:O	35:l:293:ILE:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:97:THR:HG21	54:r:714:CDL:H242	1.89	0.53
7:H:44:TYR:HB2	15:P:68:ILE:HG23	1.89	0.53
15:P:44:ARG:HB3	15:P:45:PRO:CD	2.39	0.53
49:e:201:PLX:C1C	48:l:720:PEE:O2P	2.56	0.53
40:r:61:LEU:HB2	40:r:457:PRO:HD3	1.91	0.53
54:r:714:CDL:H742	54:r:714:CDL:H271	1.90	0.53
9:J:192:ARG:NH1	9:J:198:ALA:O	2.41	0.53
54:a:201:CDL:H172	54:a:201:CDL:C71	2.39	0.53
33:j:60:ILE:HG21	36:m:168:ILE:HG21	1.90	0.53
35:l:375:ILE:HD12	35:l:458:LEU:HD11	1.90	0.53
17:S:52:ARG:NH1	17:S:58:ASN:OD1	2.41	0.53
35:l:428:PHE:HA	35:l:432:LEU:HD12	1.91	0.53
12:M:336:ASN:O	12:M:336:ASN:ND2	2.42	0.53
29:f:47:THR:HG23	30:g:65:LEU:HD22	1.91	0.53
30:g:122:ARG:O	38:o:109:ARG:NH2	2.25	0.53
1:A:102:MET:HG2	1:A:149:MET:HB3	1.90	0.52
12:M:275:PRO:HB3	12:M:286:ILE:HG23	1.91	0.52
25:b:89:HIS:CD2	48:l:720:PEE:H49	2.45	0.52
48:l:718:PEE:H34	48:l:718:PEE:H42	1.90	0.52
21:W:63:GLU:OE1	42:u:119:ARG:NH2	2.42	0.52
22:Y:43:ARG:HG3	22:Y:48:PRO:HA	1.91	0.52
33:j:30:TYR:HE2	41:s:59:GLU:HB2	1.74	0.52
41:s:87:VAL:CG2	41:s:88:PRO:CD	2.85	0.52
44:w:59:VAL:HG13	44:w:201:PRO:HA	1.91	0.52
14:O:70:TYR:HB3	14:O:71:PRO:HD2	1.91	0.52
41:s:24:GLU:HG3	41:s:271:LEU:HD22	1.91	0.52
44:w:125:ASP:OD1	44:w:125:ASP:N	2.42	0.52
11:L:163:ASN:O	11:L:171:ARG:HA	2.09	0.52
16:Q:144:MET:HE3	16:Q:222:MET:HB2	1.90	0.52
32:i:54:GLU:HG2	34:k:96:LEU:HD12	1.91	0.52
44:w:169:PHE:HB2	57:w:401:ADP:HN62	1.74	0.52
3:C:71:CYS:HB3	16:Q:141:TYR:CB	2.40	0.52
12:M:283:GLU:OE2	12:M:420:LYS:NZ	2.39	0.52
1:A:311:TRP:NE1	1:A:333:GLU:OE2	2.34	0.52
13:N:10:GLY:O	13:N:14:VAL:HG23	2.10	0.52
32:i:326:LEU:N	32:i:327:PRO:CD	2.72	0.52
48:C:311:PEE:C5	33:j:29:ALA:O	2.58	0.52
4:E:25:MET:O	4:E:29:LYS:HG3	2.10	0.52
11:L:105:GLU:HA	12:M:611:THR:HG21	1.92	0.52
14:O:218:PRO:HG3	14:O:224:SER:H	1.75	0.52
20:V:140:LYS:HG2	20:V:141:VAL:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:166:THR:CG2	48:l:719:PEE:H2	2.40	0.52
36:m:57:PHE:HD1	41:s:107:ALA:HB1	1.75	0.52
44:w:169:PHE:CG	57:w:401:ADP:C6	2.98	0.52
4:E:40:TYR:HD2	6:G:120:MET:SD	2.32	0.52
6:X:90:TYR:HE1	23:Z:44:PRO:HB2	1.75	0.52
26:c:57:MET:HE2	26:c:104:PRO:HG3	1.91	0.52
44:w:169:PHE:CB	57:w:401:ADP:HN62	2.22	0.52
1:A:392:MET:HE1	1:A:432:ALA:HA	1.91	0.51
4:E:114:ARG:HD3	4:E:115:PRO:HD2	1.92	0.51
8:I:27:ARG:NH1	16:Q:212:GLU:OE1	2.43	0.51
12:M:36:VAL:HB	12:M:56:VAL:HG21	1.93	0.51
12:M:278:HIS:CE1	12:M:280:ASP:HB2	2.45	0.51
30:g:51:ARG:NE	32:i:322:GLN:HB3	2.26	0.51
41:s:62:ARG:HH11	41:s:64:ALA:HA	1.75	0.51
4:E:56:VAL:HG12	4:E:60:ARG:HD2	1.91	0.51
6:G:84:LEU:O	6:G:88:LYS:HG2	2.10	0.51
36:m:25:SER:O	36:m:28:TYR:N	2.42	0.51
44:w:66:ILE:HG23	57:w:401:ADP:O2A	2.11	0.51
1:A:51:TRP:HH2	1:A:171:VAL:CG1	2.22	0.51
9:J:85:ARG:NH2	51:J:401:NDP:O2X	2.43	0.51
9:J:162:GLU:HG2	9:J:163:LYS:HG3	1.92	0.51
40:r:237:LYS:NZ	40:r:316:MET:O	2.43	0.51
44:w:242:LYS:HA	44:w:246:LEU:HD23	1.92	0.51
3:C:113:MET:HE3	3:C:116:ALA:HB3	1.92	0.51
54:a:201:CDL:H211	54:a:201:CDL:C25	2.39	0.51
26:c:142:PHE:HD1	26:c:143:MET:HE2	1.75	0.51
28:e:151:GLU:HG3	28:e:153:GLU:HG3	1.92	0.51
34:k:17:ALA:O	34:k:21:MET:HG2	2.11	0.51
44:w:72:ARG:HE	44:w:72:ARG:C	2.17	0.51
1:A:244:ASN:N	46:A:502:FMN:O1P	2.40	0.51
3:C:188:LYS:N	9:J:87:GLU:OE1	2.29	0.51
4:E:17:VAL:HG23	11:L:53:ILE:HD13	1.93	0.51
4:E:43:VAL:HG11	4:E:60:ARG:HG3	1.91	0.51
42:u:102:LYS:O	42:u:106:LYS:HG2	2.11	0.51
6:G:74:LEU:HD23	6:G:74:LEU:N	2.19	0.51
12:M:494:SER:OG	12:M:669:ASN:OD1	2.28	0.51
16:Q:206:GLU:OE2	16:Q:209:LYS:NZ	2.44	0.51
26:c:153:TYR:HB3	35:l:403:TYR:HD1	1.75	0.51
49:e:201:PLX:H122	54:l:712:CDL:H652	1.92	0.51
35:l:83:ASP:OD2	35:l:262:ARG:NH1	2.43	0.51
1:A:185:ASN:OD1	1:A:190:GLY:N	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:141:VAL:O	24:a:169:TYR:OH	2.28	0.51
22:Y:94:ASP:HB3	22:Y:99:ILE:HB	1.92	0.51
44:w:76:GLU:OE2	44:w:76:GLU:HA	2.11	0.51
1:A:123:GLY:HA2	14:O:180:CYS:SG	2.50	0.51
1:A:132:ARG:HG3	1:A:133:HIS:CD2	2.46	0.51
6:X:120:MET:HG2	39:p:21:LYS:HZ3	1.75	0.51
27:d:29:PRO:HG2	35:l:52:LEU:HD21	1.93	0.51
35:l:286:LEU:HD22	35:l:411:MET:SD	2.50	0.51
32:i:128:LEU:HD12	32:i:216:PHE:HB3	1.93	0.51
34:k:30:LEU:O	34:k:34:GLU:HG2	2.11	0.51
40:r:433:GLU:O	40:r:437:MET:HG2	2.11	0.51
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.93	0.50
24:a:120:TRP:O	24:a:124:THR:HG22	2.12	0.50
27:d:10:TYR:OH	28:e:123:GLU:OE1	2.27	0.50
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.92	0.50
48:l:718:PEE:C25	48:l:718:PEE:C21	2.86	0.50
1:A:367:ILE:HG13	1:A:438:LEU:HD13	1.93	0.50
12:M:691:ILE:HG23	12:M:714:VAL:HG11	1.92	0.50
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	1.92	0.50
26:c:122:THR:OG1	26:c:124:VAL:O	2.27	0.50
33:j:30:TYR:CE2	41:s:59:GLU:HB2	2.47	0.50
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.47	0.50
43:v:18:ASP:HB3	43:v:21:ARG:HG2	1.92	0.50
2:B:98:ARG:HB3	2:B:169:GLU:CD	2.37	0.50
12:M:389:THR:O	12:M:390:THR:OG1	2.25	0.50
22:Y:99:ILE:HD11	43:v:107:ARG:HG3	1.94	0.50
54:l:712:CDL:H452	40:r:445:LEU:HB3	1.93	0.50
18:T:46:ASP:OD1	18:T:49:ASP:HB2	2.12	0.50
54:V:203:CDL:HB61	38:o:82:PRO:HB2	1.92	0.50
32:i:326:LEU:HB3	32:i:327:PRO:HD3	1.94	0.50
35:l:591:PHE:CA	35:l:594:THR:CG2	2.86	0.50
41:s:195:ARG:HD3	41:s:231:ILE:HD11	1.93	0.50
44:w:110:GLY:HA2	44:w:134:TRP:CD2	2.47	0.50
41:s:288:LEU:HD11	48:s:401:PEE:H7	1.92	0.50
44:w:66:ILE:HA	57:w:401:ADP:O2A	2.12	0.50
2:B:76:TYR:OH	41:s:33:LEU:HB2	2.12	0.50
16:Q:303:ARG:HG3	16:Q:401:GLU:HB3	1.94	0.50
6:X:120:MET:HE1	39:p:24:LEU:HB3	1.94	0.50
34:k:26:LEU:HD12	34:k:29:SER:HB2	1.93	0.50
1:A:284:HIS:CE1	14:O:228:ALA:HB3	2.46	0.50
9:J:116:ILE:O	9:J:120:VAL:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:250:SER:OG	12:M:251:ILE:N	2.45	0.50
12:M:307:ILE:HG22	12:M:582:VAL:HG22	1.93	0.50
14:O:61:LYS:O	14:O:64:GLU:HG3	2.12	0.50
16:Q:52:MET:HE1	48:I:718:PEE:N	2.27	0.50
48:V:202:PEE:H14	32:i:276:ILE:HG21	1.93	0.50
6:X:113:LEU:O	6:X:117:GLU:HG3	2.12	0.50
24:a:96:ALA:HB2	27:d:61:TYR:CE2	2.47	0.50
32:i:268:GLN:HG3	42:u:168:PHE:CZ	2.47	0.50
33:j:25:PRO:HB2	41:s:60:PRO:HD3	1.93	0.50
34:k:20:LEU:HB2	35:l:592:LEU:HD12	1.93	0.50
44:w:169:PHE:HB2	57:w:401:ADP:N6	2.27	0.50
1:A:68:ILE:HG22	1:A:76:ILE:HD11	1.94	0.50
2:B:74:LEU:HB2	41:s:272:TRP:CZ2	2.46	0.50
3:C:125:PRO:HB2	41:s:58:LYS:HE3	1.94	0.50
21:W:144:THR:HB	41:s:96:ILE:HG23	1.94	0.50
40:r:12:LEU:HB2	40:r:13:PRO:HD3	1.94	0.50
35:l:591:PHE:O	35:l:595:ILE:HG13	2.12	0.49
48:m:202:PEE:O4	48:m:202:PEE:H7	2.08	0.49
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.94	0.49
1:A:214:GLU:HG3	1:A:222:LYS:O	2.13	0.49
12:M:463:SER:O	12:M:467:LYS:HG3	2.12	0.49
24:a:99:ALA:HB2	27:d:62:TYR:HD2	1.77	0.49
39:p:29:SER:HB3	39:p:76:HIS:HD2	1.77	0.49
6:G:90:TYR:OH	6:G:114:ASP:OD1	2.23	0.49
9:J:275:ASP:OD1	9:J:275:ASP:N	2.45	0.49
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.47	0.49
41:s:32:GLN:OE1	41:s:34:ARG:NH2	2.43	0.49
48:C:311:PEE:H12	33:j:29:ALA:O	2.11	0.49
9:J:65:LEU:HD23	9:J:129:LEU:HD22	1.94	0.49
10:K:79:HIS:CE1	14:O:215:LYS:HB2	2.48	0.49
15:P:213:ASP:HB3	15:P:216:VAL:HG22	1.94	0.49
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.48	0.49
16:Q:251:PHE:HB3	16:Q:341:LEU:HD11	1.93	0.49
32:i:20:VAL:HG11	32:i:137:ALA:HB1	1.94	0.49
35:l:591:PHE:HA	35:l:594:THR:HG21	1.91	0.49
2:B:78:PHE:O	8:I:12:ARG:NH2	2.44	0.49
36:m:23:LYS:N	36:m:24:PRO:HD3	2.28	0.49
36:m:25:SER:O	36:m:27:ILE:N	2.45	0.49
41:s:47:GLN:HB3	41:s:48:PRO:HD3	1.93	0.49
44:w:98:THR:OG1	44:w:337:ARG:NH2	2.41	0.49
1:A:177:TYR:CD1	10:K:96:PHE:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:e:201:PLX:H212	54:l:712:CDL:H801	1.95	0.49
44:w:116:LYS:NZ	44:w:123:SER:OG	2.46	0.49
10:K:91:VAL:O	10:K:94:SER:OG	2.24	0.49
42:u:83:THR:HA	42:u:86:TRP:NE1	2.28	0.49
1:A:319:PRO:HG2	1:A:347:THR:HG21	1.94	0.49
17:S:43:TYR:CZ	21:W:68:ARG:HG3	2.48	0.49
54:V:203:CDL:CB6	38:o:82:PRO:HB2	2.43	0.49
6:G:104:PHE:HA	6:G:108:LEU:HD12	1.94	0.49
6:G:149:ALA:O	6:G:153:ASP:N	2.45	0.49
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.93	0.49
12:M:382:ARG:NH2	12:M:527:ASP:OD2	2.46	0.49
32:i:170:LEU:O	32:i:295:ARG:NH2	2.34	0.49
40:r:248:THR:HG23	40:r:249:ILE:HG23	1.94	0.49
41:s:66:SER:HB2	41:s:122:ALA:O	2.13	0.49
35:l:331:MET:HE1	35:l:468:ILE:HD12	1.93	0.48
42:u:74:ILE:HD11	42:u:117:TRP:HZ3	1.78	0.48
44:w:72:ARG:NH2	44:w:75:ARG:CG	2.75	0.48
44:w:214:ILE:O	44:w:218:ILE:HG12	2.13	0.48
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.95	0.48
6:G:144:ILE:O	6:G:148:ILE:HG12	2.14	0.48
8:I:39:PRO:HB2	8:I:41:LEU:HD13	1.95	0.48
20:V:39:TYR:OH	35:l:597:ILE:HD12	2.13	0.48
32:i:97:MET:HE2	35:l:599:MET:CE	2.44	0.48
37:n:17:VAL:HB	37:n:18:PRO:HD3	1.93	0.48
12:M:153:PHE:CZ	12:M:155:GLU:HB2	2.48	0.48
12:M:358:LEU:HA	12:M:361:VAL:HG12	1.96	0.48
23:Z:33:GLN:HE22	23:Z:42:ARG:HA	1.77	0.48
32:i:95:MET:HE3	32:i:149:ILE:HG22	1.95	0.48
35:l:129:MET:HA	35:l:129:MET:HE2	1.96	0.48
54:V:203:CDL:H873	49:V:205:PLX:H222	1.94	0.48
32:i:153:LEU:O	32:i:157:MET:HG3	2.12	0.48
1:A:173:ILE:HG23	1:A:182:ILE:HD11	1.95	0.48
7:H:23:ARG:HG2	7:H:81:ILE:HD13	1.94	0.48
14:O:199:LYS:NZ	14:O:203:GLU:OE2	2.39	0.48
14:O:222:ARG:HD3	14:O:226:GLU:O	2.13	0.48
33:j:17:LEU:HA	33:j:20:ILE:HG12	1.96	0.48
35:l:161:ARG:NH2	39:p:88:GLY:O	2.47	0.48
54:l:712:CDL:H601	54:l:712:CDL:H772	1.94	0.48
1:A:210:THR:O	1:A:214:GLU:HG2	2.13	0.48
48:C:311:PEE:H69	49:C:312:PLX:H192	1.94	0.48
12:M:128:CYS:SG	12:M:140:GLN:NE2	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:108:TYR:CE2	54:V:203:CDL:CA5	2.96	0.48
6:X:111:ASP:OD1	6:X:112:SER:N	2.43	0.48
50:X:201:8Q1:N36	50:X:201:8Q1:O40	2.45	0.48
35:l:494:THR:HG22	35:l:498:PHE:CE2	2.49	0.48
12:M:483:ARG:HD3	12:M:684:LEU:CD2	2.43	0.48
14:O:156:LEU:HB3	14:O:158:ILE:HG12	1.95	0.48
1:A:319:PRO:HG3	1:A:347:THR:HG21	1.96	0.48
10:K:105:ARG:NH1	11:L:167:ASN:O	2.47	0.48
12:M:193:ASP:OD1	14:O:111:ARG:NH2	2.40	0.48
54:a:201:CDL:H211	54:a:201:CDL:H182	1.72	0.48
35:l:71:LEU:N	35:l:71:LEU:HD22	2.29	0.48
44:w:129:TYR:OH	44:w:186:HIS:ND1	2.30	0.48
8:I:34:ARG:N	13:N:95:ASP:OD2	2.46	0.48
12:M:144:MET:HG3	16:Q:383:LYS:HG3	1.95	0.48
32:i:106:LEU:HG	32:i:138:PRO:HB2	1.96	0.48
1:A:201:ALA:HB1	14:O:121:MET:HB2	1.96	0.48
12:M:68:ARG:NH1	12:M:284:GLU:HB2	2.29	0.48
16:Q:102:SER:HG	16:Q:107:ARG:NH1	2.11	0.48
35:l:452:ASN:HA	35:l:455:LYS:HG2	1.96	0.48
20:V:108:TYR:CE2	54:V:203:CDL:H112	2.32	0.47
38:o:57:LEU:HD23	38:o:57:LEU:O	2.14	0.47
38:o:59:VAL:HG22	40:r:423:ILE:HG23	1.95	0.47
44:w:166:ASP:OD1	44:w:187:TYR:OH	2.22	0.47
44:w:258:TYR:HE2	44:w:269:VAL:HG22	1.79	0.47
12:M:390:THR:HA	12:M:600:GLU:HG2	1.96	0.47
12:M:394:VAL:HG22	12:M:473:MET:HE1	1.97	0.47
16:Q:244:ILE:HG22	16:Q:348:LEU:HD11	1.96	0.47
48:V:202:PEE:H74	48:V:202:PEE:H36	1.96	0.47
24:a:155:GLU:OE2	24:a:158:ARG:NH2	2.40	0.47
32:i:254:LEU:HD21	40:r:154:LEU:HD11	1.96	0.47
54:l:713:CDL:H382	54:l:713:CDL:H351	1.65	0.47
6:G:118:ILE:O	6:G:122:MET:HG2	2.14	0.47
16:Q:196:ALA:O	16:Q:197:MET:HG2	2.13	0.47
49:e:201:PLX:H121	49:e:201:PLX:H152	1.51	0.47
32:i:89:MET:O	32:i:90:PHE:HB2	2.13	0.47
54:n:102:CDL:H581	54:n:102:CDL:H542	1.95	0.47
40:r:300:ALA:O	40:r:308:SER:HB3	2.14	0.47
7:H:51:ILE:HD11	8:I:94:ALA:HB3	1.95	0.47
14:O:149:LEU:O	14:O:153:GLN:HG2	2.14	0.47
54:a:201:CDL:C52	48:l:720:PEE:H14	2.19	0.47
40:r:14:MET:HE2	40:r:30:HIS:CD2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:47:GLN:N	41:s:48:PRO:CD	2.77	0.47
6:G:110:LEU:HD23	6:G:114:ASP:HB3	1.97	0.47
9:J:37:HIS:CE1	18:T:49:ASP:HA	2.50	0.47
9:J:129:LEU:HD23	9:J:167:ILE:HG13	1.97	0.47
14:O:130:TYR:HA	14:O:189:ASN:ND2	2.29	0.47
16:Q:226:TYR:OH	16:Q:234:GLN:O	2.19	0.47
21:W:114:THR:OG1	42:u:143:HIS:ND1	2.42	0.47
8:I:14:TRP:O	21:W:28:ARG:NH2	2.48	0.47
14:O:140:CYS:O	14:O:145:SER:OG	2.27	0.47
6:X:91:ASP:OD2	23:Z:42:ARG:NE	2.45	0.47
25:b:73:THR:HA	25:b:77:ILE:HD12	1.96	0.47
40:r:307:TRP:HA	40:r:310:MET:HE2	1.97	0.47
1:A:123:GLY:HA2	14:O:180:CYS:HB3	1.95	0.47
4:E:28:ALA:HB1	4:E:79:VAL:HG11	1.96	0.47
4:E:98:LYS:HB3	4:E:102:HIS:HB2	1.96	0.47
15:P:45:PRO:O	16:Q:162:GLN:NE2	2.46	0.47
30:g:4:MET:CE	30:g:84:MET:HE3	2.45	0.47
35:l:395:ILE:O	35:l:399:VAL:HG23	2.14	0.47
40:r:412:ILE:HA	40:r:416:ARG:HG3	1.96	0.47
41:s:27:VAL:HG13	41:s:31:MET:HE3	1.97	0.47
21:W:57:ARG:HB3	41:s:316:PRO:HG3	1.96	0.47
35:l:172:ILE:HG21	40:r:408:LEU:HD12	1.97	0.47
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.97	0.47
39:p:100:PRO:HG3	40:r:419:TYR:CE1	2.49	0.47
41:s:88:PRO:HB2	41:s:105:MET:HE3	1.96	0.47
2:B:80:GLU:HG3	17:S:1:MET:SD	2.55	0.47
6:G:103:HIS:ND1	6:G:106:LYS:HG2	2.30	0.47
9:J:172:ALA:HA	9:J:181:LEU:HB3	1.96	0.47
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.97	0.47
12:M:354:LEU:HD22	12:M:548:LEU:HD22	1.97	0.47
12:M:547:LEU:HD11	12:M:579:MET:HE2	1.96	0.47
32:i:329:MET:HE3	54:i:401:CDL:C13	2.44	0.47
1:A:52:ARG:HH11	1:A:52:ARG:CG	2.22	0.46
2:B:200:GLU:HG3	13:N:88:ARG:HB2	1.97	0.46
8:I:3:SER:O	54:N:202:CDL:HA22	2.14	0.46
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.97	0.46
21:W:140:PHE:O	48:m:202:PEE:H11	2.14	0.46
32:i:237:MET:HE1	32:i:319:HIS:NE2	2.30	0.46
54:l:713:CDL:H673	54:l:713:CDL:H452	1.96	0.46
36:m:45:LEU:HD23	36:m:50:SER:HA	1.97	0.46
44:w:181:LYS:O	44:w:185:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:C:311:PEE:H27	48:C:311:PEE:H58	1.97	0.46
14:O:222:ARG:HD2	14:O:222:ARG:O	2.15	0.46
19:U:38:TYR:HB2	41:s:310:MET:O	2.15	0.46
25:b:19:ARG:HA	39:p:171:VAL:HG13	1.98	0.46
25:b:121:LYS:O	25:b:121:LYS:HG2	2.15	0.46
32:i:170:LEU:HD11	32:i:288:LEU:HD22	1.96	0.46
39:p:29:SER:HB3	39:p:76:HIS:CD2	2.51	0.46
11:L:78:ARG:NH2	12:M:249:GLU:OE1	2.36	0.46
24:a:166:GLY:O	24:a:170:GLN:NE2	2.49	0.46
25:b:32:GLU:HG3	39:p:115:TYR:HA	1.97	0.46
35:l:190:LEU:HD21	40:r:307:TRP:CH2	2.51	0.46
37:n:17:VAL:N	37:n:18:PRO:CD	2.77	0.46
40:r:115:LEU:HD12	40:r:174:LEU:HD22	1.97	0.46
41:s:90:PRO:HD2	41:s:240:ILE:HD13	1.96	0.46
43:v:106:ARG:O	43:v:110:GLN:HG2	2.16	0.46
44:w:165:SER:HB3	44:w:245:PHE:CE1	2.51	0.46
9:J:143:ASP:O	9:J:148:ILE:HG12	2.16	0.46
14:O:130:TYR:HA	14:O:189:ASN:HD21	1.81	0.46
40:r:193:ILE:HD11	40:r:256:TYR:OH	2.15	0.46
43:v:17:PRO:HB3	43:v:105:GLU:OE1	2.15	0.46
12:M:213:MET:HB3	12:M:215:MET:HE2	1.97	0.46
54:a:201:CDL:H541	48:l:720:PEE:C12	2.45	0.46
39:p:168:TRP:O	39:p:172:THR:OG1	2.25	0.46
41:s:18:ALA:HB2	56:s:403:UQ:H151	1.97	0.46
42:u:44:MET:O	42:u:48:TRP:HE3	1.99	0.46
8:I:40:LYS:HG2	21:W:5:LYS:O	2.16	0.46
16:Q:410:TYR:HB3	16:Q:423:LYS:HB3	1.97	0.46
32:i:146:SER:O	32:i:149:ILE:HG12	2.16	0.46
34:k:34:GLU:HA	34:k:37:MET:HG3	1.96	0.46
35:l:7:LEU:O	35:l:11:THR:HG23	2.16	0.46
1:A:250:VAL:O	1:A:254:ILE:HG12	2.15	0.46
2:B:76:TYR:HA	2:B:79:ARG:HE	1.80	0.46
12:M:68:ARG:HH12	12:M:284:GLU:HB2	1.80	0.46
27:d:114:GLN:OE1	35:l:199:GLN:HG3	2.15	0.46
34:k:38:LEU:O	34:k:42:ILE:HG12	2.15	0.46
56:s:403:UQ:HM53	56:s:403:UQ:H72	1.73	0.46
44:w:139:ARG:NH1	44:w:166:ASP:OD2	2.48	0.46
3:C:193:TRP:HA	3:C:196:ARG:HG2	1.98	0.46
9:J:236:VAL:HG12	9:J:272:LEU:HD22	1.97	0.46
12:M:591:GLU:HG2	12:M:610:VAL:HG23	1.98	0.46
12:M:710:CYS:O	12:M:714:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:49:ASP:OD2	18:T:51:ARG:HB2	2.15	0.46
27:d:51:PHE:O	27:d:54:GLN:HG2	2.16	0.46
49:j:203:PLX:H342	49:j:203:PLX:H372	1.65	0.46
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.51	0.46
5:F:41:TYR:CE1	5:F:55:ILE:HD11	2.50	0.46
28:e:74:HIS:HB2	28:e:83:ASP:OD2	2.15	0.46
35:l:313:MET:HG3	35:l:328:HIS:HD2	1.79	0.46
40:r:3:LYS:HG3	40:r:4:ILE:HD12	1.96	0.46
6:G:103:HIS:CE1	6:G:105:MET:HB2	2.50	0.46
17:S:17:PHE:CE1	41:s:257:ILE:HA	2.51	0.46
6:X:86:VAL:HB	6:X:122:MET:HE1	1.97	0.46
32:i:95:MET:CE	32:i:149:ILE:CG2	2.94	0.46
39:p:97:TYR:HB3	39:p:179:MET:HE3	1.98	0.46
9:J:36:LEU:HB3	12:M:304:GLN:NE2	2.31	0.45
13:N:44:TYR:HH	13:N:113:HIS:H	1.60	0.45
54:N:202:CDL:H312	54:N:202:CDL:H541	1.99	0.45
6:X:98:LEU:C	6:X:98:LEU:CD1	2.89	0.45
54:r:714:CDL:H362	54:r:714:CDL:H392	1.63	0.45
7:H:83:GLN:NE2	15:P:107:GLN:OE1	2.49	0.45
12:M:43:VAL:HG12	12:M:55:LYS:HD3	1.98	0.45
16:Q:80:LEU:HD23	16:Q:80:LEU:H	1.80	0.45
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.50	0.45
27:d:142:ARG:NE	28:e:138:GLU:O	2.43	0.45
48:l:718:PEE:H19	40:r:148:TYR:CE1	2.52	0.45
44:w:72:ARG:HA	44:w:72:ARG:NE	2.31	0.45
12:M:638:THR:O	12:M:642:VAL:HG23	2.16	0.45
16:Q:99:MET:HE2	16:Q:99:MET:HB3	1.83	0.45
26:c:118:ASP:O	35:l:535:ARG:HD3	2.17	0.45
36:m:14:VAL:O	36:m:18:VAL:HG23	2.16	0.45
1:A:185:ASN:C	1:A:187:CYS:H	2.25	0.45
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.75	0.45
2:B:184:LEU:HD23	11:L:112:MET:HG3	1.98	0.45
3:C:79:MET:HE3	3:C:86:MET:HE2	1.97	0.45
11:L:89:SER:O	12:M:59:GLN:NE2	2.42	0.45
14:O:153:GLN:HE22	14:O:160:VAL:HA	1.82	0.45
25:b:32:GLU:HG3	39:p:115:TYR:HD1	1.82	0.45
35:l:100:ILE:HD13	35:l:341:MET:HE3	1.98	0.45
2:B:179:THR:OG1	2:B:182:GLU:OE2	2.35	0.45
7:H:54:GLU:O	7:H:58:MET:HG3	2.16	0.45
9:J:84:TYR:CE2	9:J:105:PHE:HB3	2.52	0.45
16:Q:198:THR:HB	16:Q:199:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:82:ARG:HD3	22:Y:44:TYR:CE1	2.52	0.45
26:c:165:ASP:OD1	26:c:170:ARG:NH2	2.50	0.45
43:v:12:ASP:HB3	43:v:15:LYS:HB2	1.98	0.45
1:A:93:PHE:CE1	1:A:98:LYS:HG3	2.52	0.45
31:h:51:ARG:O	31:h:55:GLU:HG3	2.16	0.45
48:l:718:PEE:H28	48:l:718:PEE:H35	1.93	0.45
54:n:102:CDL:H521	54:n:102:CDL:H551	1.68	0.45
1:A:159:ARG:NH2	14:O:176:CYS:O	2.44	0.45
16:Q:53:TYR:HE1	48:l:718:PEE:H2	1.82	0.45
31:h:21:GLN:HB2	31:h:37:GLU:OE1	2.16	0.45
35:l:561:ILE:HG22	35:l:562:LEU:HD12	1.98	0.45
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.99	0.45
20:V:73:THR:HB	20:V:93:GLY:HA2	1.98	0.45
25:b:99:GLU:CG	35:l:59:GLN:OE1	2.65	0.45
39:p:26:HIS:CD2	39:p:79:PRO:HB3	2.51	0.45
44:w:88:GLU:OE2	44:w:161:ARG:NH1	2.50	0.45
2:B:192:ASN:ND2	18:T:61:GLU:OE2	2.41	0.45
24:a:139:ILE:HG23	40:r:54:LEU:HD23	1.98	0.45
33:j:15:SER:HA	41:s:76:ILE:HD12	1.98	0.45
49:n:101:PLX:C32	49:n:101:PLX:C28	2.94	0.45
54:n:102:CDL:H752	54:n:102:CDL:H781	1.59	0.45
40:r:445:LEU:O	40:r:448:THR:HG22	2.16	0.45
1:A:120:GLY:HA3	1:A:204:TYR:HD1	1.81	0.45
1:A:338:ASP:OD1	1:A:341:ALA:HB3	2.17	0.45
2:B:75:SER:HB3	8:I:15:ALA:HB3	1.99	0.45
4:E:16:SER:HB3	11:L:52:LEU:HD12	1.99	0.45
48:U:101:PEE:H35	48:U:101:PEE:H30	1.54	0.45
26:c:153:TYR:OH	43:v:8:ARG:NH1	2.37	0.45
35:l:83:ASP:CG	35:l:262:ARG:HH12	2.25	0.45
54:r:714:CDL:H832	54:r:714:CDL:H862	1.68	0.45
1:A:51:TRP:CE3	1:A:51:TRP:O	2.70	0.44
1:A:113:LEU:HD23	1:A:113:LEU:C	2.43	0.44
1:A:263:ALA:HA	1:A:271:SER:OG	2.17	0.44
4:E:68:MET:HE1	50:G:201:8Q1:C30	2.47	0.44
6:G:88:LYS:HD3	6:G:98:LEU:HD21	1.99	0.44
11:L:92:ASN:HB3	15:P:238:PRO:HA	2.00	0.44
19:U:33:PRO:HA	41:s:310:MET:HG2	1.98	0.44
6:X:93:ILE:HG21	6:X:108:LEU:HD21	1.95	0.44
22:Y:71:TRP:CD1	22:Y:72:ARG:HH21	2.36	0.44
26:c:81:ARG:HD3	26:c:85:GLU:OE1	2.17	0.44
30:g:83:TYR:CZ	30:g:87:LEU:HD11	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:80:GLU:O	42:u:84:GLU:HG3	2.16	0.44
1:A:51:TRP:HH2	1:A:171:VAL:HG11	1.82	0.44
12:M:560:LEU:HD23	12:M:564:CYS:SG	2.56	0.44
13:N:68:MET:HG2	13:N:69:ASN:H	1.82	0.44
14:O:187:GLN:NE2	14:O:190:ASP:H	2.15	0.44
16:Q:293:LEU:HD22	16:Q:298:ILE:HD12	1.99	0.44
48:V:202:PEE:H79	40:r:201:MET:HE2	1.99	0.44
49:V:205:PLX:H22	49:V:205:PLX:H1C3	1.78	0.44
35:l:184:LEU:HB2	40:r:393:ILE:HG12	1.99	0.44
42:u:83:THR:HA	42:u:86:TRP:CD1	2.52	0.44
12:M:48:THR:HA	12:M:95:PRO:HA	1.99	0.44
12:M:544:VAL:HG23	12:M:565:PHE:HB3	1.99	0.44
14:O:75:LYS:HE3	14:O:75:LYS:HB2	1.83	0.44
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.52	0.44
49:e:201:PLX:H382	40:r:67:VAL:HG12	1.98	0.44
32:i:283:ALA:HB1	40:r:158:LEU:HD22	1.98	0.44
35:l:233:LEU:HB3	35:l:234:PRO:HD3	1.98	0.44
54:l:713:CDL:H622	54:l:713:CDL:H591	1.64	0.44
40:r:138:ASN:C	40:r:138:ASN:HD22	2.26	0.44
44:w:67:CYS:HB2	44:w:218:ILE:HD11	1.98	0.44
44:w:353:TRP:H	44:w:353:TRP:CD1	2.35	0.44
12:M:650:SER:OG	12:M:652:ASN:OD1	2.35	0.44
14:O:137:THR:HG22	14:O:138:THR:H	1.82	0.44
35:l:531:SER:O	35:l:535:ARG:HG3	2.18	0.44
39:p:30:TRP:NE1	39:p:76:HIS:HB2	2.33	0.44
40:r:216:LEU:HD23	40:r:287:ALA:HB1	1.99	0.44
1:A:146:GLY:HA3	1:A:193:PHE:CE1	2.53	0.44
9:J:213:PHE:HD2	9:J:214:LEU:HD12	1.82	0.44
32:i:112:HIS:HB2	32:i:184:ILE:HD13	1.99	0.44
33:j:79:SER:HA	33:j:87:MET:HE3	1.99	0.44
54:l:713:CDL:H391	54:l:713:CDL:H421	1.69	0.44
1:A:231:ALA:O	1:A:239:PRO:HB3	2.18	0.44
1:A:380:GLY:O	1:A:386:ARG:NH1	2.50	0.44
2:B:77:LEU:HD12	41:s:31:MET:HG3	1.99	0.44
24:a:79:GLY:HA3	54:a:201:CDL:H222	2.00	0.44
34:k:25:HIS:O	34:k:28:SER:N	2.49	0.44
34:k:48:ILE:HD11	34:k:59:MET:HE3	1.98	0.44
35:l:37:LYS:HD3	35:l:98:TRP:HE1	1.83	0.44
54:l:712:CDL:H582	54:l:712:CDL:H551	1.57	0.44
40:r:48:ASN:OD1	40:r:49:SER:N	2.46	0.44
12:M:133:GLN:O	12:M:137:CYS:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:51:MET:HA	41:s:313:SER:HB2	2.00	0.44
33:j:3:ILE:HG22	48:m:202:PEE:H13	1.98	0.44
40:r:324:SER:HG	40:r:440:HIS:CD2	2.35	0.44
16:Q:182:ASN:OD1	16:Q:404:LYS:NZ	2.51	0.44
20:V:4:THR:O	20:V:8:LYS:HD3	2.17	0.44
54:a:201:CDL:OB7	48:l:720:PEE:H14	2.18	0.44
35:l:4:PHE:O	35:l:8:THR:HG23	2.18	0.44
54:l:712:CDL:H582	54:l:712:CDL:H791	2.00	0.44
39:p:108:HIS:CD2	39:p:109:PRO:HD2	2.53	0.44
54:r:714:CDL:H802	54:r:714:CDL:H831	1.88	0.44
3:C:64:PRO:HB3	3:C:102:VAL:HG13	1.99	0.44
4:E:93:THR:HG23	4:E:103:ILE:HD11	2.00	0.44
9:J:235:THR:HG23	9:J:325:SER:HA	1.99	0.44
28:e:102:GLY:HA3	40:r:39:LEU:CD2	2.47	0.44
1:A:62:TRP:CD2	1:A:181:LEU:HD13	2.53	0.43
1:A:185:ASN:O	1:A:187:CYS:N	2.51	0.43
5:F:17:ARG:HB2	5:F:68:ARG:HE	1.83	0.43
12:M:133:GLN:HG3	12:M:136:GLU:HG3	2.00	0.43
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.48	0.43
6:X:113:LEU:O	6:X:116:VAL:HG12	2.18	0.43
35:l:65:ASN:OD1	35:l:66:TRP:N	2.48	0.43
35:l:341:MET:SD	35:l:457:LEU:HD12	2.58	0.43
40:r:121:LEU:O	40:r:125:THR:HG23	2.18	0.43
41:s:26:LYS:HE2	41:s:37:PRO:O	2.18	0.43
1:A:49:HIS:HA	10:K:74:ARG:HD2	2.00	0.43
28:e:137:MET:HE3	28:e:137:MET:HB2	1.87	0.43
35:l:359:MET:O	35:l:436:ARG:NH2	2.51	0.43
39:p:63:LEU:O	39:p:64:LEU:HB3	2.18	0.43
1:A:125:CYS:H	1:A:277:ASN:HD22	1.66	0.43
2:B:76:TYR:HE1	8:I:25:GLN:HE22	1.65	0.43
4:E:36:TYR:CE2	6:G:113:LEU:HD13	2.53	0.43
6:G:70:ASP:H	16:Q:60:HIS:HE1	1.65	0.43
12:M:266:ARG:HG2	12:M:267:THR:HG23	2.01	0.43
19:U:26:GLY:HA3	48:U:101:PEE:H37	2.00	0.43
32:i:232:HIS:HB3	32:i:311:MET:HE1	1.99	0.43
35:l:44:PHE:HB2	35:l:94:LEU:HB3	2.00	0.43
35:l:601:LEU:HD12	35:l:601:LEU:O	2.18	0.43
12:M:278:HIS:HE1	12:M:280:ASP:HB2	1.83	0.43
12:M:347:ASP:HB3	12:M:594:ALA:HB1	2.00	0.43
12:M:690:THR:HG23	12:M:692:LYS:HG2	2.00	0.43
14:O:159:LYS:HB2	14:O:162:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:122:HIS:O	18:T:122:HIS:ND1	2.51	0.43
35:l:174:TYR:CD2	35:l:232:TRP:HB3	2.53	0.43
35:l:400:ASN:ND2	35:l:489:THR:HG21	2.34	0.43
40:r:373:ILE:HD11	40:r:444:LEU:HD23	2.00	0.43
40:r:373:ILE:HA	40:r:376:ILE:HD12	2.00	0.43
2:B:151:LYS:HA	3:C:141:GLY:HA2	2.00	0.43
6:G:83:VAL:O	6:G:87:LEU:HD23	2.18	0.43
16:Q:270:ASN:HB3	41:s:284:GLN:NE2	2.34	0.43
48:U:101:PEE:H67	48:U:101:PEE:H73	1.76	0.43
48:V:202:PEE:H21	40:r:198:ALA:HB2	1.99	0.43
27:d:6:ASP:OD2	28:e:127:LYS:HE3	2.18	0.43
32:i:190:MET:HE2	32:i:205:LEU:HA	2.00	0.43
49:i:705:PLX:H101	49:i:705:PLX:H72	1.73	0.43
35:l:55:MET:HE2	35:l:471:ASN:HB3	2.00	0.43
40:r:94:LEU:HD13	54:r:714:CDL:H142	1.99	0.43
41:s:13:ILE:O	41:s:17:VAL:CG1	2.52	0.43
43:v:51:LEU:HD13	43:v:63:LEU:HD23	1.99	0.43
43:v:93:LEU:HA	43:v:96:VAL:HG12	2.00	0.43
1:A:115:VAL:HG22	1:A:248:VAL:HG21	2.01	0.43
7:H:22:GLU:O	7:H:26:ILE:HG12	2.18	0.43
16:Q:102:SER:OG	16:Q:102:SER:O	2.35	0.43
16:Q:198:THR:HG22	16:Q:202:TRP:CE2	2.53	0.43
26:c:176:LYS:HD2	26:c:176:LYS:HA	1.73	0.43
32:i:258:SER:OG	32:i:336:VAL:HG22	2.18	0.43
54:i:401:CDL:H132	54:i:401:CDL:C17	2.45	0.43
2:B:105:ARG:HD2	13:N:108:TYR:CG	2.54	0.43
5:F:23:LEU:HD13	5:F:33:VAL:HG12	2.01	0.43
15:P:103:HIS:CD2	15:P:105:ASN:HB2	2.53	0.43
21:W:30:LEU:HB3	21:W:35:MET:HE3	2.01	0.43
54:a:201:CDL:H512	48:l:720:PEE:H52	2.00	0.43
49:e:201:PLX:H211	35:l:20:MET:HA	2.00	0.43
30:g:11:VAL:HA	30:g:12:PRO:HD3	1.78	0.43
30:g:110:THR:O	30:g:114:ILE:HG13	2.18	0.43
32:i:97:MET:HE2	35:l:599:MET:HE1	2.01	0.43
40:r:106:LEU:HD13	40:r:234:VAL:HG11	2.01	0.43
40:r:133:ILE:HD11	40:r:231:LEU:HD11	2.00	0.43
15:P:211:ARG:NH2	15:P:222:GLU:OE2	2.45	0.43
49:V:205:PLX:H301	49:V:205:PLX:H331	1.70	0.43
23:Z:18:ASP:OD1	23:Z:18:ASP:N	2.49	0.43
31:h:36:PHE:CD1	31:h:62:ASP:HB3	2.54	0.43
33:j:69:ILE:HD11	41:s:144:VAL:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:468:ILE:O	35:l:472:ILE:HG12	2.19	0.43
37:n:4:VAL:HG12	37:n:5:LEU:HD22	2.01	0.43
40:r:10:MET:HE1	54:r:714:CDL:H632	1.99	0.43
1:A:312:ASP:OD1	1:A:329:LYS:NZ	2.52	0.43
6:G:103:HIS:CD2	6:G:139:MET:HG3	2.53	0.43
9:J:132:ARG:HD2	9:J:134:TRP:CE2	2.54	0.43
12:M:478:SER:O	12:M:482:GLN:HG2	2.18	0.43
13:N:85:GLU:HB2	13:N:98:PRO:HB3	2.01	0.43
14:O:236:GLU:HG2	14:O:237:PRO:HD2	2.01	0.43
15:P:125:ARG:HD3	15:P:126:PHE:CZ	2.54	0.43
48:V:202:PEE:O4	40:r:195:MET:HB2	2.19	0.43
44:w:343:TYR:HA	44:w:352:ILE:HD12	2.00	0.43
8:I:40:LYS:HB3	21:W:7:LYS:N	2.31	0.43
8:I:96:THR:HB	8:I:97:PRO:HD2	2.00	0.43
15:P:125:ARG:HH22	15:P:201:ASP:CG	2.26	0.43
20:V:120:LEU:HD21	49:V:205:PLX:H332	2.01	0.43
6:X:129:GLU:OE2	26:c:89:TRP:HZ2	2.02	0.43
32:i:294:MET:CE	40:r:130:LEU:HD21	2.49	0.43
32:i:294:MET:HE1	40:r:130:LEU:HD21	2.01	0.43
35:l:213:LEU:HB3	35:l:273:VAL:HG11	2.01	0.43
40:r:310:MET:HB3	40:r:455:LEU:HD22	2.01	0.43
1:A:86:ARG:NE	1:A:339:PHE:CE2	2.85	0.42
1:A:184:LYS:HA	10:K:98:MET:HE1	2.01	0.42
2:B:150:THR:HG21	2:B:180:HIS:CD2	2.54	0.42
6:G:75:THR:O	6:G:76:LEU:C	2.62	0.42
9:J:238:GLN:NE2	9:J:270:ARG:HG2	2.34	0.42
14:O:67:VAL:HG13	14:O:75:LYS:HG3	2.01	0.42
19:U:43:ILE:O	19:U:47:ARG:HG2	2.19	0.42
6:X:80:LYS:HB3	6:X:80:LYS:HE3	1.77	0.42
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.42	0.42
23:Z:57:PHE:CG	35:l:435:PRO:HG3	2.54	0.42
31:h:21:GLN:HG2	34:k:53:PHE:HD1	1.83	0.42
40:r:141:GLU:HB2	40:r:222:GLU:OE2	2.19	0.42
54:r:714:CDL:H741	54:r:714:CDL:H772	1.75	0.42
44:w:350:LYS:HD3	44:w:350:LYS:HA	1.80	0.42
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.54	0.42
12:M:394:VAL:HG11	12:M:418:ILE:HG12	2.00	0.42
12:M:471:LYS:HB3	12:M:510:TRP:CZ2	2.54	0.42
42:u:80:GLU:CG	42:u:81:PRO:HD3	2.46	0.42
1:A:119:GLU:OE2	1:A:127:ASP:CB	2.65	0.42
2:B:76:TYR:CE2	16:Q:202:TRP:NE1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:88:LYS:NZ	6:G:98:LEU:HD11	2.33	0.42
7:H:58:MET:CE	7:H:71:GLN:HG2	2.49	0.42
12:M:371:VAL:HG22	12:M:533:GLY:HA2	2.01	0.42
26:c:110:ASP:OD1	26:c:110:ASP:N	2.52	0.42
32:i:91:ASN:ND2	32:i:93:VAL:HG23	2.34	0.42
40:r:357:THR:O	40:r:361:VAL:HG23	2.18	0.42
16:Q:198:THR:HG22	16:Q:202:TRP:NE1	2.35	0.42
48:V:202:PEE:H33	48:V:202:PEE:C42	2.48	0.42
32:i:31:ILE:HD11	34:k:62:ILE:HG21	2.00	0.42
48:l:718:PEE:H38	40:r:155:ALA:HB2	2.01	0.42
40:r:365:THR:HG21	40:r:444:LEU:HD13	1.99	0.42
44:w:271:GLU:HG2	44:w:275:TYR:CE2	2.54	0.42
2:B:70:LEU:HD11	48:s:401:PEE:H65	2.02	0.42
12:M:182:CYS:HA	12:M:225:ILE:HD11	2.02	0.42
14:O:68:LYS:HE3	14:O:68:LYS:HB2	1.88	0.42
25:b:24:LYS:NZ	25:b:27:GLU:OE1	2.37	0.42
31:h:17:TRP:CD1	31:h:17:TRP:H	2.37	0.42
32:i:325:LEU:O	32:i:329:MET:HG2	2.19	0.42
36:m:51:PHE:O	36:m:55:MET:HG2	2.19	0.42
56:s:403:UQ:H72	56:s:403:UQ:H111	1.89	0.42
43:v:97:LYS:O	43:v:101:GLU:HG2	2.20	0.42
7:H:37:GLN:HB2	7:H:95:LEU:HD11	2.01	0.42
10:K:100:GLN:NE2	14:O:69:ASN:O	2.52	0.42
35:l:379:ALA:O	35:l:388:GLY:HA3	2.19	0.42
39:p:133:TRP:O	39:p:137:VAL:HG23	2.20	0.42
40:r:57:PHE:CE1	40:r:113:THR:HA	2.55	0.42
40:r:73:LEU:HD22	40:r:103:GLN:OE1	2.18	0.42
2:B:99:GLY:HA3	2:B:170:GLY:O	2.19	0.42
6:X:155:TYR:CE1	25:b:23:LEU:HB3	2.55	0.42
30:g:36:MET:HE1	49:i:705:PLX:H382	2.02	0.42
54:i:401:CDL:OB4	44:w:40:PRO:HG3	2.20	0.42
35:l:488:MET:O	35:l:492:ILE:HG12	2.20	0.42
41:s:179:TRP:CG	41:s:180:PRO:HD3	2.55	0.42
44:w:170:LEU:HD22	44:w:187:TYR:CD1	2.54	0.42
1:A:317:VAL:CG2	1:A:356:VAL:HG12	2.49	0.42
2:B:99:GLY:CA	2:B:170:GLY:O	2.68	0.42
4:E:23:ARG:NH1	11:L:53:ILE:HG13	2.33	0.42
9:J:126:VAL:HG23	9:J:161:VAL:HG11	2.01	0.42
12:M:140:GLN:HG2	16:Q:379:ILE:HG23	2.02	0.42
12:M:483:ARG:CD	12:M:684:LEU:HD23	2.49	0.42
12:M:496:ILE:O	12:M:500:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:117:VAL:HB	15:P:127:GLU:HG2	2.01	0.42
16:Q:187:VAL:HG11	16:Q:258:LEU:HD21	2.01	0.42
21:W:98:MET:HE3	21:W:101:VAL:HG21	2.02	0.42
26:c:113:ILE:C	26:c:115:ASN:H	2.27	0.42
49:e:201:PLX:H371	40:r:447:LEU:HD11	2.01	0.42
40:r:168:GLN:HB2	40:r:174:LEU:HG	2.02	0.42
40:r:328:CYS:HB3	40:r:437:MET:HE1	2.01	0.42
10:K:87:LEU:HD22	14:O:66:ILE:HD11	2.02	0.42
17:S:39:ALA:HA	17:S:44:GLN:HG3	2.02	0.42
6:X:100:VAL:HG12	6:X:142:GLN:HB2	2.02	0.42
25:b:99:GLU:CD	35:l:59:GLN:OE1	2.61	0.42
32:i:342:ALA:HB3	49:i:705:PLX:H332	2.00	0.42
41:s:251:THR:HG23	41:s:251:THR:O	2.20	0.42
3:C:126:GLU:O	3:C:128:ARG:N	2.52	0.42
9:J:315:THR:C	9:J:316:ARG:HD2	2.45	0.42
23:Z:49:GLU:OE2	39:p:34:ARG:NH2	2.47	0.42
33:j:49:LEU:N	33:j:50:PRO:HD2	2.34	0.42
39:p:46:ALA:O	39:p:50:GLU:HG3	2.20	0.42
40:r:225:ILE:HD13	40:r:331:ASN:HB2	2.00	0.42
1:A:339:PHE:CE1	1:A:349:LEU:HD23	2.55	0.41
7:H:27:LEU:HD13	7:H:84:ALA:HB3	2.02	0.41
16:Q:178:THR:OG1	16:Q:214:TYR:OH	2.22	0.41
20:V:121:THR:O	20:V:125:VAL:HG23	2.20	0.41
24:a:140:LEU:HD21	40:r:177:LEU:HB3	2.02	0.41
26:c:96:ASP:OD1	26:c:96:ASP:N	2.52	0.41
29:f:72:ARG:HE	30:g:22:SER:HB2	1.85	0.41
31:h:21:GLN:HA	34:k:53:PHE:CE1	2.55	0.41
41:s:235:ASN:ND2	41:s:266:LEU:HB3	2.34	0.41
42:u:38:LYS:HB3	42:u:39:PRO:HD3	2.01	0.41
44:w:72:ARG:NE	44:w:72:ARG:CA	2.82	0.41
2:B:98:ARG:NH2	16:Q:224:ALA:O	2.46	0.41
5:F:17:ARG:CB	5:F:68:ARG:HE	2.33	0.41
31:h:7:GLN:O	31:h:11:GLY:N	2.53	0.41
33:j:84:LEU:HD23	33:j:84:LEU:HA	1.86	0.41
49:j:203:PLX:H312	49:j:203:PLX:H282	1.82	0.41
35:l:316:THR:OG1	35:l:395:ILE:HD12	2.20	0.41
35:l:482:MET:HE2	35:l:482:MET:HB3	1.88	0.41
41:s:197:PRO:HB3	41:s:278:PRO:O	2.19	0.41
9:J:201:ILE:HG22	9:J:203:PRO:HD3	2.02	0.41
9:J:204:SER:OG	9:J:204:SER:O	2.33	0.41
16:Q:65:PRO:HB2	16:Q:67:ASN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:341:LEU:HD23	16:Q:341:LEU:HA	1.95	0.41
20:V:85:ASP:HB3	20:V:130:LEU:HD21	2.01	0.41
6:X:87:LEU:HD23	6:X:87:LEU:HA	1.93	0.41
24:a:78:THR:HG21	28:e:96:SER:O	2.20	0.41
32:i:261:MET:HE2	32:i:340:THR:OG1	2.20	0.41
54:l:712:CDL:H432	54:l:712:CDL:H621	2.02	0.41
39:p:25:ARG:HD3	39:p:25:ARG:HA	1.94	0.41
43:v:65:GLN:HG2	43:v:83:GLU:HG2	2.02	0.41
4:E:114:ARG:NH2	9:J:45:LYS:HG2	2.35	0.41
7:H:58:MET:HE3	7:H:71:GLN:HG2	2.01	0.41
14:O:76:ALA:O	14:O:77:ALA:C	2.64	0.41
16:Q:142:VAL:HG12	16:Q:182:ASN:HA	2.02	0.41
48:U:101:PEE:H20	33:j:106:TRP:CE3	2.55	0.41
32:i:254:LEU:O	32:i:257:LEU:HB2	2.21	0.41
35:l:62:ILE:HD13	35:l:81:LYS:HA	2.03	0.41
48:l:718:PEE:C22	48:l:718:PEE:C18	2.86	0.41
41:s:11:ILE:HB	41:s:12:PRO:HD3	2.02	0.41
14:O:164:THR:CG2	14:O:169:PHE:H	2.33	0.41
16:Q:82:LEU:HD12	16:Q:101:LEU:CD2	2.41	0.41
48:V:202:PEE:C46	40:r:201:MET:HE2	2.50	0.41
22:Y:93:THR:O	22:Y:97:LEU:HD23	2.21	0.41
23:Z:23:LYS:HE2	23:Z:23:LYS:HB2	1.87	0.41
30:g:51:ARG:HE	32:i:322:GLN:HB3	1.84	0.41
32:i:261:MET:HB3	32:i:262:PRO:HD3	2.02	0.41
35:l:49:VAL:HB	35:l:50:PRO:HD3	2.02	0.41
36:m:55:MET:HE3	41:s:103:LEU:HD21	2.01	0.41
40:r:394:ILE:H	40:r:394:ILE:HD12	1.85	0.41
41:s:49:ILE:N	41:s:49:ILE:CD1	2.83	0.41
42:u:68:LEU:O	42:u:72:ARG:HG3	2.21	0.41
2:B:79:ARG:NH2	8:I:20:LEU:HD21	2.35	0.41
3:C:96:SER:HB3	3:C:99:GLN:NE2	2.36	0.41
15:P:115:THR:HB	16:Q:423:LYS:HE3	2.02	0.41
16:Q:357:LYS:HD3	16:Q:364:SER:HB3	2.03	0.41
21:W:36:PHE:O	21:W:40:ILE:HG12	2.21	0.41
30:g:106:LYS:HE2	30:g:107:ASP:O	2.20	0.41
31:h:94:PRO:HA	31:h:95:PRO:HD3	1.93	0.41
32:i:26:TRP:HB3	32:i:74:ILE:HD13	2.02	0.41
32:i:100:MET:HE2	35:l:598:SER:OG	2.20	0.41
32:i:320:THR:HG23	44:w:300:ASN:HA	1.99	0.41
32:i:324:LYS:HD2	32:i:324:LYS:HA	1.91	0.41
33:j:68:GLU:OE1	33:j:98:LEU:HD13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:63:LEU:C	39:p:65:ARG:H	2.27	0.41
41:s:267:THR:O	41:s:271:LEU:HG	2.20	0.41
44:w:72:ARG:HH22	44:w:75:ARG:HG2	1.85	0.41
6:G:141:PRO:HA	6:G:144:ILE:HD12	2.02	0.41
22:Y:87:PRO:HG3	43:v:96:VAL:HG23	2.02	0.41
33:j:15:SER:O	33:j:19:LEU:HD13	2.20	0.41
54:n:102:CDL:C82	54:r:714:CDL:H861	2.50	0.41
44:w:223:ASN:O	44:w:227:MET:HG2	2.21	0.41
1:A:113:LEU:HD23	1:A:114:VAL:N	2.35	0.41
1:A:161:GLU:OE1	1:A:161:GLU:N	2.50	0.41
12:M:483:ARG:HD3	12:M:684:LEU:HD23	2.02	0.41
14:O:66:ILE:HG21	14:O:81:PRO:HB2	2.02	0.41
19:U:84:LEU:HD23	19:U:84:LEU:HA	1.92	0.41
32:i:237:MET:HG3	32:i:237:MET:O	2.21	0.41
35:l:66:TRP:NE1	48:l:720:PEE:H3	2.36	0.41
35:l:332:HIS:HA	35:l:335:PHE:CZ	2.56	0.41
40:r:271:MET:HE2	40:r:271:MET:HA	2.02	0.41
1:A:169:LEU:O	1:A:173:ILE:HG13	2.21	0.41
2:B:110:GLU:HG3	18:T:67:ALA:HB1	2.03	0.41
49:C:312:PLX:H21	49:C:312:PLX:H1C3	1.66	0.41
49:C:312:PLX:H311	49:C:312:PLX:H281	1.68	0.41
6:G:130:ILE:HG22	6:G:135:ALA:HB2	2.03	0.41
8:I:107:SER:C	8:I:109:ASP:H	2.28	0.41
9:J:212:ARG:O	9:J:216:TYR:HB3	2.20	0.41
9:J:319:VAL:HA	9:J:322:VAL:HG12	2.03	0.41
12:M:372:PHE:H	12:M:532:PRO:HB2	1.84	0.41
14:O:154:LYS:HE3	14:O:154:LYS:HB2	1.72	0.41
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	2.03	0.41
17:S:17:PHE:HE1	41:s:257:ILE:HA	1.86	0.41
54:V:203:CDL:OB9	54:V:203:CDL:H731	2.20	0.41
21:W:90:ASN:ND2	21:W:123:GLU:O	2.54	0.41
6:X:99:SER:O	6:X:100:VAL:C	2.62	0.41
24:a:147:ALA:HB2	40:r:173:SER:HB2	2.03	0.41
24:a:170:GLN:O	30:g:6:GLY:HA3	2.21	0.41
25:b:10:LEU:O	25:b:14:GLN:HG3	2.21	0.41
32:i:40:MET:HE1	32:i:129:LEU:HD23	2.02	0.41
32:i:98:MET:HE2	32:i:98:MET:HB2	1.93	0.41
32:i:186:HIS:O	32:i:190:MET:HG3	2.20	0.41
32:i:222:SER:O	32:i:224:ALA:N	2.53	0.41
49:j:203:PLX:H322	49:j:203:PLX:H351	1.87	0.41
35:l:51:LEU:HD22	35:l:91:PRO:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:589:LEU:O	35:l:593:ILE:HG13	2.21	0.41
35:l:591:PHE:C	35:l:594:THR:HG22	2.46	0.41
35:l:591:PHE:C	35:l:594:THR:CG2	2.94	0.41
40:r:82:SER:HB3	40:r:432:ARG:NH2	2.36	0.41
41:s:140:ILE:O	41:s:143:GLU:HG2	2.20	0.41
41:s:307:LEU:HA	41:s:310:MET:HE3	2.02	0.41
44:w:147:LEU:HD23	44:w:147:LEU:HA	1.90	0.41
1:A:51:TRP:O	1:A:51:TRP:HE3	2.03	0.41
5:F:16:LEU:HD12	5:F:16:LEU:HA	1.92	0.41
21:W:119:PRO:O	36:m:130:THR:OG1	2.36	0.41
6:X:91:ASP:OD2	23:Z:42:ARG:NH2	2.52	0.41
54:l:712:CDL:H381	40:r:372:SER:HB3	2.02	0.41
38:o:8:PRO:HG3	38:o:14:LEU:HD13	2.02	0.41
42:u:106:LYS:O	42:u:109:GLU:HG3	2.20	0.41
44:w:180:ARG:NH1	44:w:316:GLU:OE2	2.48	0.41
1:A:423:THR:HB	45:A:501:SF4:S4	2.61	0.40
12:M:331:GLN:HE21	12:M:630:ALA:HA	1.86	0.40
16:Q:188:THR:HB	16:Q:200:PHE:HA	2.03	0.40
20:V:114:ALA:O	20:V:118:MET:HG3	2.21	0.40
27:d:131:GLN:O	27:d:135:VAL:HG23	2.22	0.40
34:k:58:MET:HG2	36:m:146:LEU:HB2	2.03	0.40
35:l:360:GLY:HA3	35:l:435:PRO:HA	2.03	0.40
41:s:87:VAL:N	41:s:88:PRO:CD	2.84	0.40
44:w:66:ILE:O	44:w:214:ILE:HD11	2.21	0.40
1:A:329:LYS:HA	1:A:332:CYS:SG	2.61	0.40
2:B:96:ARG:O	16:Q:219:GLY:HA3	2.21	0.40
2:B:99:GLY:O	2:B:169:GLU:CG	2.69	0.40
6:G:76:LEU:HB3	6:G:80:LYS:NZ	2.36	0.40
9:J:166:HIS:HB3	9:J:200:ILE:HD13	2.02	0.40
11:L:77:VAL:HG23	11:L:145:PHE:HB3	2.02	0.40
14:O:179:ALA:HB3	14:O:185:MET:HG2	2.04	0.40
21:W:133:ILE:HD13	36:m:125:TRP:CH2	2.56	0.40
24:a:187:PRO:HA	42:u:48:TRP:CD1	2.56	0.40
34:k:45:THR:HG23	36:m:52:LEU:HD13	2.03	0.40
35:l:190:LEU:HD22	35:l:196:TRP:CZ2	2.55	0.40
35:l:292:ALA:HB2	35:l:304:PHE:HB3	2.02	0.40
54:n:102:CDL:H252	54:n:102:CDL:H221	1.57	0.40
40:r:105:PHE:O	40:r:109:THR:OG1	2.31	0.40
1:A:211:ALA:HB2	1:A:223:PRO:HG3	2.02	0.40
4:E:41:ARG:O	4:E:44:PRO:HD2	2.21	0.40
7:H:82:LEU:HA	7:H:85:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:37:HIS:O	9:J:40:LEU:N	2.41	0.40
12:M:432:ILE:HD11	12:M:445:LEU:HD12	2.02	0.40
13:N:3:LEU:O	13:N:6:VAL:HG22	2.21	0.40
16:Q:127:LYS:HB3	16:Q:131:GLN:HB3	2.03	0.40
26:c:84:GLN:O	26:c:98:ARG:NH1	2.55	0.40
27:d:78:GLU:HB2	27:d:81:ASP:HB2	2.02	0.40
35:l:78:LEU:HD11	54:l:712:CDL:H272	2.02	0.40
35:l:400:ASN:HA	35:l:409:LEU:HD11	2.04	0.40
35:l:486:MET:HE3	35:l:486:MET:HB2	1.98	0.40
39:p:139:GLN:O	39:p:142:GLU:HG2	2.21	0.40
39:p:164:PRO:HA	39:p:165:PRO:HD3	1.97	0.40
42:u:70:PHE:O	42:u:74:ILE:HG12	2.22	0.40
1:A:52:ARG:NH1	10:K:77:GLN:HE21	2.19	0.40
1:A:413:TRP:O	1:A:416:SER:OG	2.33	0.40
3:C:173:LEU:O	3:C:177:ILE:HG12	2.21	0.40
9:J:148:ILE:HB	9:J:149:PRO:HD3	2.03	0.40
16:Q:216:ARG:HH12	16:Q:243:ASP:CG	2.27	0.40
23:Z:57:PHE:O	35:l:434:LYS:NZ	2.38	0.40
31:h:21:GLN:HA	34:k:53:PHE:CD1	2.56	0.40
32:i:95:MET:HE2	32:i:148:SER:C	2.46	0.40
38:o:62:ASP:O	38:o:66:ILE:HG12	2.22	0.40
41:s:199:ASP:OD1	41:s:199:ASP:N	2.54	0.40
9:J:81:ILE:O	9:J:83:PRO:HD3	2.22	0.40
16:Q:52:MET:HE1	48:l:718:PEE:H5	1.84	0.40
27:d:160:LYS:NZ	28:e:147:ILE:HG23	2.36	0.40
32:i:220:ILE:CG2	32:i:323:MET:HE2	2.52	0.40
54:i:401:CDL:HB31	44:w:40:PRO:HB2	2.03	0.40
35:l:176:ARG:HA	35:l:176:ARG:HD2	1.92	0.40
56:s:403:UQ:H203	56:s:403:UQ:H171	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	415 (97%)	14 (3%)	0	100	100
2	B	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
3	C	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
4	E	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
5	F	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
6	G	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
6	X	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
7	H	110/112 (98%)	103 (94%)	7 (6%)	0	100	100
8	I	93/112 (83%)	81 (87%)	11 (12%)	1 (1%)	11	29
9	J	289/341 (85%)	278 (96%)	10 (4%)	1 (0%)	36	60
10	K	40/42 (95%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	668 (97%)	19 (3%)	1 (0%)	48	73
13	N	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
14	O	215/217 (99%)	203 (94%)	11 (5%)	1 (0%)	24	48
15	P	206/208 (99%)	197 (96%)	9 (4%)	0	100	100
16	Q	412/430 (96%)	400 (97%)	12 (3%)	0	100	100
17	S	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
18	T	94/96 (98%)	89 (95%)	5 (5%)	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%)	136 (97%)	4 (3%)	0	100	100
22	Y	68/70 (97%)	63 (93%)	5 (7%)	0	100	100
23	Z	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
24	a	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
25	b	99/126 (79%)	94 (95%)	5 (5%)	0	100	100
26	c	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
27	d	173/175 (99%)	172 (99%)	1 (1%)	0	100	100
28	e	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
29	f	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
30	g	119/121 (98%)	115 (97%)	3 (2%)	1 (1%)	16	37
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%)	338 (98%)	7 (2%)	0	100	100
33	j	95/113 (84%)	90 (95%)	5 (5%)	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%)	8 (4%)	1 (1%)	21	44
40	r	457/459 (100%)	445 (97%)	12 (3%)	0	100	100
41	s	299/318 (94%)	288 (96%)	10 (3%)	1 (0%)	36	60
42	u	169/171 (99%)	161 (95%)	8 (5%)	0	100	100
43	v	122/131 (93%)	112 (92%)	10 (8%)	0	100	100
44	w	318/320 (99%)	303 (95%)	15 (5%)	0	100	100
All	All	8029/8315 (97%)	7720 (96%)	301 (4%)	8 (0%)	49	73

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	O	77	ALA
8	I	41	LEU
12	M	283	GLU
30	g	3	MET
9	J	38	HIS
20	V	46	PRO
39	p	174	PRO
41	s	90	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%)	151 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	76/76 (100%)	76 (100%)	0	100	100
6	G	76/81 (94%)	75 (99%)	1 (1%)	61	83
6	X	77/81 (95%)	76 (99%)	1 (1%)	61	83
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	86 (99%)	1 (1%)	65	85
9	J	255/295 (86%)	255 (100%)	0	100	100
10	K	41/41 (100%)	41 (100%)	0	100	100
11	L	113/113 (100%)	112 (99%)	1 (1%)	70	87
12	M	580/580 (100%)	579 (100%)	1 (0%)	87	95
13	N	130/130 (100%)	130 (100%)	0	100	100
14	O	183/183 (100%)	183 (100%)	0	100	100
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	361/370 (98%)	361 (100%)	0	100	100
17	S	58/58 (100%)	58 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	101 (100%)	0	100	100
21	W	123/123 (100%)	123 (100%)	0	100	100
22	Y	62/63 (98%)	62 (100%)	0	100	100
23	Z	65/65 (100%)	65 (100%)	0	100	100
24	a	122/122 (100%)	122 (100%)	0	100	100
25	b	98/119 (82%)	98 (100%)	0	100	100
26	c	141/141 (100%)	141 (100%)	0	100	100
27	d	155/155 (100%)	155 (100%)	0	100	100
28	e	99/99 (100%)	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%)	310 (100%)	1 (0%)	86	94
33	j	88/99 (89%)	88 (100%)	0	100	100
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	536/537 (100%)	533 (99%)	3 (1%)	78	91
36	m	98/141 (70%)	98 (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%)	409 (100%)	1 (0%)	87	95
41	s	263/275 (96%)	260 (99%)	3 (1%)	65	85
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	104/115 (90%)	104 (100%)	0	100	100
44	w	281/283 (99%)	281 (100%)	0	100	100
All	All	7065/7238 (98%)	7050 (100%)	15 (0%)	85	95

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	CYS
6	G	75	THR
8	I	95	VAL
11	L	86	ASN
12	M	171	THR
6	X	98	LEU
32	i	93	VAL
35	l	70	THR
35	l	71	LEU
35	l	594	THR
37	n	13	VAL
40	r	39	LEU
41	s	17	VAL
41	s	22	LEU
41	s	26	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	ASN
1	A	277	ASN
1	A	393	ASN
1	A	457	HIS
3	C	111	ASN
6	G	115	GLN
7	H	37	GLN
7	H	83	GLN
8	I	25	GLN
9	J	128	ASN
9	J	238	GLN
9	J	356	HIS
10	K	100	GLN
12	M	278	HIS
12	M	304	GLN
12	M	388	ASN
13	N	123	GLN
14	O	41	HIS
14	O	69	ASN
14	O	189	ASN
15	P	75	GLN
15	P	77	GLN
15	P	131	ASN
15	P	196	HIS
16	Q	160	ASN
16	Q	234	GLN
16	Q	339	GLN
18	T	63	ASN
20	V	129	GLN
22	Y	83	HIS
25	b	13	GLN
25	b	14	GLN
25	b	89	HIS
26	c	106	HIS
26	c	132	HIS
26	c	164	ASN
27	d	124	ASN
29	f	61	GLN
30	g	119	HIS
32	i	310	ASN
34	k	50	ASN
35	l	34	ASN
35	l	165	ASN

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Mol	Chain	Res	Type
35	l	192	HIS
35	l	270	ASN
35	l	274	GLN
35	l	354	GLN
35	l	447	ASN
35	l	471	ASN
36	m	46	ASN
37	n	3	ASN
37	n	6	GLN
37	n	14	HIS
38	o	52	ASN
39	p	13	GLN
40	r	30	HIS
40	r	180	HIS
40	r	251	ASN
40	r	366	ASN
40	r	390	ASN
40	r	399	ASN
41	s	235	ASN
42	u	64	ASN
42	u	151	ASN
43	v	47	ASN
43	v	84	GLN
43	v	85	HIS
44	w	92	HIS
44	w	286	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	2MR	Q	118	16	10,12,13	1.98	1 (10%)	5,13,15	6.05	3 (60%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	2MR	Q	118	16	-	3/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.69	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	12.32	130.78	119.48
16	Q	118	2MR	CD-NE-CZ	4.52	131.87	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.09	130.70	123.86

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 39 ligands modelled in this entry, 2 are monoatomic - leaving 37 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
45	SF4	C	301	3	0,12,12	-	-	-		
49	PLX	i	705	-	51,51,51	1.14	3 (5%)	55,59,59	0.59	1 (1%)
54	CDL	N	202	-	50,50,99	1.28	4 (8%)	56,62,111	1.33	7 (12%)
54	CDL	n	102	-	77,77,99	1.02	4 (5%)	83,89,111	1.11	4 (4%)
50	8Q1	X	201	6	31,34,34	2.14	6 (19%)	40,43,43	1.66	10 (25%)
50	8Q1	G	201	6	31,34,34	2.11	6 (19%)	40,43,43	1.74	12 (30%)
48	PEE	l	719	-	45,45,50	1.22	6 (13%)	48,50,55	0.99	2 (4%)
54	CDL	l	712	-	98,98,99	1.09	8 (8%)	104,110,111	0.88	4 (3%)
48	PEE	s	401	-	50,50,50	1.16	6 (12%)	53,55,55	0.98	2 (3%)
49	PLX	V	205	-	51,51,51	1.14	4 (7%)	55,59,59	0.61	1 (1%)
52	FES	M	803	12	0,4,4	-	-	-		
54	CDL	l	713	-	99,99,99	1.09	9 (9%)	105,111,111	0.85	4 (3%)
45	SF4	M	802	12	0,12,12	-	-	-		
48	PEE	U	101	-	50,50,50	1.15	6 (12%)	53,55,55	0.96	2 (3%)
49	PLX	n	101	-	51,51,51	0.62	0	55,59,59	0.69	0
51	NDP	J	401	-	49,52,52	4.37	22 (44%)	66,80,80	2.18	14 (21%)
45	SF4	A	501	1	0,12,12	-	-	-		
47	NAI	A	503	-	45,48,48	3.90	20 (44%)	60,73,73	1.81	12 (20%)
54	CDL	i	401	-	65,65,99	1.14	4 (6%)	71,77,111	1.19	5 (7%)
48	PEE	m	202	-	40,40,50	1.14	5 (12%)	43,45,55	0.97	2 (4%)
49	PLX	j	203	-	51,51,51	1.15	4 (7%)	55,59,59	0.59	1 (1%)
49	PLX	C	312	-	51,51,51	1.15	4 (7%)	55,59,59	0.60	1 (1%)
48	PEE	C	311	-	46,46,50	1.21	5 (10%)	49,51,55	0.94	2 (4%)
45	SF4	M	801	12	0,12,12	-	-	-		
49	PLX	e	201	-	51,51,51	1.14	4 (7%)	55,59,59	0.61	1 (1%)
57	ADP	w	401	-	27,29,29	2.97	8 (29%)	42,45,45	1.98	9 (21%)
54	CDL	a	201	-	90,90,99	0.96	4 (4%)	96,102,111	1.07	5 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	UQ	s	403	-	28,28,63	3.27	8 (28%)	34,37,79	2.76	10 (29%)
45	SF4	B	302	2	0,12,12	-	-	-	-	-
48	PEE	l	718	-	46,46,50	1.20	6 (13%)	49,51,55	1.01	2 (4%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
54	CDL	r	714	-	99,99,99	1.09	9 (9%)	105,111,111	0.86	4 (3%)
52	FES	O	301	14	0,4,4	-	-	-	-	-
48	PEE	l	720	-	45,45,50	1.22	6 (13%)	48,50,55	0.98	2 (4%)
46	FMN	A	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.19	8 (16%)
48	PEE	V	202	-	50,50,50	1.15	6 (12%)	53,55,55	1.01	2 (3%)
54	CDL	V	203	-	70,70,99	1.08	4 (5%)	76,82,111	1.14	7 (9%)

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
45	SF4	C	301	3	-	-	0/6/5/5
49	PLX	i	705	-	-	27/55/55/55	-
54	CDL	N	202	-	-	26/61/61/110	-
54	CDL	n	102	-	-	27/88/88/110	-
50	8Q1	X	201	6	-	26/41/41/41	-
50	8Q1	G	201	6	-	15/41/41/41	-
48	PEE	l	719	-	-	21/49/49/54	-
54	CDL	l	712	-	-	57/109/109/110	-
48	PEE	s	401	-	-	25/54/54/54	-
49	PLX	V	205	-	-	26/55/55/55	-
52	FES	M	803	12	-	-	0/1/1/1
54	CDL	l	713	-	-	57/110/110/110	-
48	PEE	U	101	-	-	26/54/54/54	-
45	SF4	M	802	12	-	-	0/6/5/5
49	PLX	n	101	-	-	17/55/55/55	-
51	NDP	J	401	-	-	8/34/77/77	0/4/5/5
45	SF4	A	501	1	-	-	0/6/5/5
47	NAI	A	503	-	-	6/29/72/72	0/5/5/5
54	CDL	i	401	-	-	26/76/76/110	-
48	PEE	m	202	-	-	22/44/44/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	PLX	j	203	-	-	26/55/55/55	-
49	PLX	C	312	-	-	25/55/55/55	-
48	PEE	C	311	-	-	21/50/50/54	-
49	PLX	e	201	-	-	34/55/55/55	-
45	SF4	M	801	12	-	-	0/6/5/5
57	ADP	w	401	-	-	4/16/32/32	0/3/3/3
54	CDL	a	201	-	-	26/101/101/110	-
56	UQ	s	403	-	-	8/21/45/87	0/1/1/1
48	PEE	l	718	-	-	19/50/50/54	-
54	CDL	r	714	-	-	66/110/110/110	-
45	SF4	B	301	2	-	-	0/6/5/5
45	SF4	B	302	2	-	-	0/6/5/5
52	FES	O	301	14	-	-	0/1/1/1
48	PEE	l	720	-	-	24/49/49/54	-
46	FMN	A	502	-	-	4/18/18/18	0/3/3/3
48	PEE	V	202	-	-	24/54/54/54	-
54	CDL	V	203	-	-	45/81/81/110	-

All (183) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	J	401	NDP	C3B-C2B	-12.44	1.25	1.52
51	J	401	NDP	C6N-C5N	12.40	1.55	1.33
51	J	401	NDP	O4D-C4D	10.65	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.44	1.26	1.53
51	J	401	NDP	C3D-C4D	-9.98	1.27	1.53
56	s	403	UQ	C13-C14	9.30	1.55	1.33
47	A	503	NAI	O4B-C1B	9.12	1.63	1.42
56	s	403	UQ	C8-C9	8.96	1.54	1.33
57	w	401	ADP	C3'-C4'	-8.92	1.30	1.53
56	s	403	UQ	C18-C19	8.25	1.56	1.32
47	A	503	NAI	O4B-C4B	-8.22	1.26	1.45
51	J	401	NDP	O4B-C4B	-8.09	1.26	1.45
50	G	201	8Q1	P24-O27	8.00	1.86	1.60
50	X	201	8Q1	P24-O27	7.82	1.85	1.60
57	w	401	ADP	O4'-C4'	7.74	1.62	1.45
47	A	503	NAI	C2D-C1D	-7.57	1.29	1.53
51	J	401	NDP	C2N-C3N	7.49	1.55	1.34
47	A	503	NAI	C2B-C1B	-7.28	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	O4D-C4D	6.93	1.60	1.45
47	A	503	NAI	C2D-C3D	5.84	1.69	1.53
51	J	401	NDP	C6A-N6A	5.83	1.48	1.34
47	A	503	NAI	C7N-N7N	5.72	1.48	1.33
57	w	401	ADP	C6-N6	5.56	1.48	1.34
51	J	401	NDP	P2B-O2B	5.55	1.69	1.59
47	A	503	NAI	O4D-C1D	5.40	1.54	1.42
51	J	401	NDP	C3B-C4B	5.28	1.66	1.53
47	A	503	NAI	C6A-N6A	5.20	1.47	1.34
47	A	503	NAI	C4N-C3N	-5.09	1.39	1.49
51	J	401	NDP	C6N-N1N	4.97	1.49	1.37
51	J	401	NDP	O4D-C1D	-4.91	1.30	1.42
51	J	401	NDP	C1B-N9A	-4.56	1.33	1.46
47	A	503	NAI	O2B-C2B	4.50	1.53	1.43
51	J	401	NDP	O4B-C1B	4.49	1.52	1.42
57	w	401	ADP	O4'-C1'	-4.38	1.31	1.42
54	N	202	CDL	OB8-CB7	4.29	1.45	1.33
54	i	401	CDL	OA8-CA7	4.27	1.45	1.33
54	V	203	CDL	OA8-CA7	4.27	1.45	1.33
54	i	401	CDL	OB8-CB7	4.27	1.45	1.33
54	n	102	CDL	OA8-CA7	4.24	1.45	1.33
54	a	201	CDL	OB8-CB7	4.24	1.45	1.33
54	N	202	CDL	OA8-CA7	4.22	1.45	1.33
54	V	203	CDL	OB8-CB7	4.21	1.45	1.33
51	J	401	NDP	O2D-C2D	-4.19	1.33	1.43
50	G	201	8Q1	C1-S44	4.18	1.86	1.76
54	N	202	CDL	OA6-CA5	4.18	1.46	1.34
54	a	201	CDL	OA8-CA7	4.18	1.45	1.33
54	i	401	CDL	OA6-CA5	4.17	1.46	1.34
54	a	201	CDL	OB6-CB5	4.17	1.46	1.34
54	n	102	CDL	OB8-CB7	4.16	1.45	1.33
54	i	401	CDL	OB6-CB5	4.16	1.46	1.34
51	J	401	NDP	C7N-N7N	4.14	1.44	1.33
54	V	203	CDL	OA6-CA5	4.10	1.45	1.34
54	n	102	CDL	OA6-CA5	4.08	1.45	1.34
54	V	203	CDL	OB6-CB5	4.00	1.45	1.34
54	a	201	CDL	OA6-CA5	3.99	1.45	1.34
46	A	502	FMN	C4A-N5	3.98	1.38	1.30
50	X	201	8Q1	C1-S44	3.94	1.85	1.76
54	N	202	CDL	OB6-CB5	3.93	1.45	1.34
54	n	102	CDL	OB6-CB5	3.91	1.45	1.34
47	A	503	NAI	C6N-C5N	3.90	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	s	401	PEE	C18-C19	3.75	1.53	1.31
48	C	311	PEE	C18-C19	3.74	1.53	1.31
48	l	720	PEE	C18-C19	3.73	1.53	1.31
48	m	202	PEE	C18-C19	3.73	1.53	1.31
48	l	719	PEE	C18-C19	3.72	1.53	1.31
48	U	101	PEE	C18-C19	3.69	1.53	1.31
48	l	718	PEE	C18-C19	3.69	1.53	1.31
48	V	202	PEE	C18-C19	3.68	1.53	1.31
48	C	311	PEE	C39-C38	3.65	1.52	1.31
48	V	202	PEE	C39-C38	3.64	1.52	1.31
48	l	720	PEE	C39-C38	3.63	1.52	1.31
48	l	719	PEE	C39-C38	3.63	1.52	1.31
48	U	101	PEE	C39-C38	3.63	1.52	1.31
48	s	401	PEE	C39-C38	3.63	1.52	1.31
48	l	718	PEE	C39-C38	3.62	1.52	1.31
50	X	201	8Q1	C34-N36	3.62	1.41	1.33
47	A	503	NAI	C7N-C3N	3.58	1.56	1.48
54	l	713	CDL	OA8-CA7	3.45	1.43	1.33
54	r	714	CDL	OA8-CA7	3.43	1.43	1.33
54	l	712	CDL	OA8-CA7	3.42	1.43	1.33
47	A	503	NAI	C4N-C5N	-3.33	1.40	1.48
50	X	201	8Q1	C6-C1	3.33	1.54	1.50
50	G	201	8Q1	C34-N36	3.30	1.40	1.33
50	G	201	8Q1	O27-C28	-3.30	1.33	1.43
57	w	401	ADP	O2'-C2'	-3.28	1.35	1.43
50	X	201	8Q1	O27-C28	-3.27	1.33	1.43
50	X	201	8Q1	C39-N41	3.21	1.40	1.33
57	w	401	ADP	C8-N9	-3.17	1.31	1.37
51	J	401	NDP	O3D-C3D	3.14	1.50	1.43
57	w	401	ADP	O3'-C3'	3.13	1.50	1.43
51	J	401	NDP	C8A-N9A	-3.04	1.32	1.37
51	J	401	NDP	C5A-N7A	-3.02	1.33	1.39
54	l	713	CDL	OB6-CB5	3.01	1.42	1.34
54	l	712	CDL	OB6-CB5	3.00	1.42	1.34
54	l	713	CDL	OB8-CB7	3.00	1.42	1.33
54	r	714	CDL	OB8-CB7	3.00	1.42	1.33
54	l	713	CDL	OA6-CA5	2.99	1.42	1.34
54	r	714	CDL	OA6-CA5	2.98	1.42	1.34
54	r	714	CDL	OB6-CB5	2.97	1.42	1.34
54	l	712	CDL	OB8-CB7	2.96	1.42	1.33
50	G	201	8Q1	C39-N41	2.95	1.40	1.33
51	J	401	NDP	C7N-C3N	2.92	1.54	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	G	201	8Q1	C6-C1	2.88	1.53	1.50
54	l	712	CDL	OA6-CA5	2.87	1.42	1.34
49	C	312	PLX	O6-C4	-2.75	1.40	1.44
49	i	705	PLX	O6-C4	-2.72	1.41	1.44
49	e	201	PLX	O6-C4	-2.64	1.41	1.44
56	s	403	UQ	C6-C1	2.61	1.54	1.46
47	A	503	NAI	C8A-N9A	-2.59	1.32	1.37
49	j	203	PLX	O6-C4	-2.57	1.41	1.44
48	s	401	PEE	O2-C2	-2.54	1.40	1.46
48	C	311	PEE	O3-C30	2.54	1.40	1.33
48	l	719	PEE	O2-C2	-2.53	1.40	1.46
51	J	401	NDP	O2B-C2B	2.52	1.53	1.44
48	l	718	PEE	O3-C30	2.48	1.40	1.33
47	A	503	NAI	O3B-C3B	-2.47	1.37	1.43
48	C	311	PEE	O2-C2	-2.44	1.40	1.46
48	l	718	PEE	O2-C2	-2.44	1.40	1.46
48	l	720	PEE	O3-C30	2.43	1.40	1.33
46	A	502	FMN	C10-N1	2.43	1.38	1.33
48	U	101	PEE	O2-C2	-2.43	1.40	1.46
48	V	202	PEE	O2-C2	-2.40	1.40	1.46
49	j	203	PLX	C7-C6	2.40	1.55	1.50
54	r	714	CDL	OA6-CA4	-2.39	1.40	1.46
54	l	712	CDL	OA6-CA4	-2.39	1.40	1.46
49	V	205	PLX	C7-C6	2.39	1.55	1.50
48	m	202	PEE	O2-C2	-2.39	1.40	1.46
48	l	719	PEE	O3-C30	2.38	1.40	1.33
54	l	713	CDL	OA6-CA4	-2.36	1.40	1.46
48	l	720	PEE	O2-C2	-2.36	1.40	1.46
48	U	101	PEE	O3-C30	2.36	1.40	1.33
48	s	401	PEE	O3-C30	2.35	1.40	1.33
49	i	705	PLX	C7-C6	2.34	1.55	1.50
48	V	202	PEE	O3-C30	2.32	1.40	1.33
47	A	503	NAI	PN-O5D	2.28	1.68	1.59
48	l	720	PEE	O2-C10	2.27	1.40	1.34
49	C	312	PLX	C7-C6	2.27	1.55	1.50
48	U	101	PEE	O2-C10	2.27	1.40	1.34
51	J	401	NDP	C2D-C3D	2.26	1.59	1.53
47	A	503	NAI	C5B-C4B	2.26	1.58	1.51
49	e	201	PLX	C7-C6	2.25	1.55	1.50
48	m	202	PEE	O3-C30	2.25	1.39	1.33
48	l	718	PEE	O2-C10	2.25	1.40	1.34
57	w	401	ADP	C5-N7	-2.24	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	V	205	PLX	O6-C4	-2.24	1.41	1.44
48	C	311	PEE	O2-C10	2.24	1.40	1.34
48	V	202	PEE	O3-C3	-2.23	1.40	1.45
48	m	202	PEE	O2-C10	2.23	1.40	1.34
56	s	403	UQ	O4-C4	-2.22	1.18	1.23
48	l	719	PEE	O3-C3	-2.22	1.40	1.45
48	U	101	PEE	O3-C3	-2.22	1.40	1.45
54	r	714	CDL	PB2-OB2	2.21	1.68	1.59
51	J	401	NDP	O7N-C7N	-2.21	1.19	1.24
54	l	712	CDL	OB6-CB4	-2.20	1.41	1.46
54	l	712	CDL	PB2-OB2	2.20	1.68	1.59
54	r	714	CDL	PB2-OB5	2.20	1.68	1.59
54	l	713	CDL	OB6-CB4	-2.19	1.41	1.46
48	m	202	PEE	O3-C3	-2.19	1.40	1.45
54	l	712	CDL	PB2-OB5	2.19	1.68	1.59
56	s	403	UQ	C7-C8	2.18	1.53	1.50
49	j	203	PLX	P1-O4	2.17	1.68	1.59
54	l	713	CDL	PB2-OB2	2.17	1.68	1.59
48	l	720	PEE	O3-C3	-2.17	1.40	1.45
54	l	713	CDL	PB2-OB5	2.16	1.68	1.59
49	V	205	PLX	P1-O4	2.15	1.68	1.59
48	s	401	PEE	O2-C10	2.14	1.40	1.34
48	V	202	PEE	O2-C10	2.14	1.40	1.34
48	s	401	PEE	O3-C3	-2.14	1.40	1.45
54	r	714	CDL	OB6-CB4	-2.14	1.41	1.46
49	C	312	PLX	P1-O4	2.12	1.67	1.59
49	i	705	PLX	P1-O4	2.11	1.67	1.59
49	e	201	PLX	P1-O4	2.10	1.67	1.59
48	l	718	PEE	O3-C3	-2.10	1.40	1.45
56	s	403	UQ	O1-C1	-2.09	1.18	1.23
49	j	203	PLX	P1-O1	2.09	1.67	1.59
47	A	503	NAI	C5A-N7A	-2.07	1.35	1.39
49	V	205	PLX	P1-O1	2.04	1.67	1.59
54	l	713	CDL	C11-CA5	2.03	1.56	1.50
49	C	312	PLX	P1-O1	2.03	1.67	1.59
49	e	201	PLX	P1-O1	2.02	1.67	1.59
48	l	719	PEE	O2-C10	2.01	1.40	1.34
56	s	403	UQ	O3-CM3	-2.01	1.40	1.45
54	r	714	CDL	C11-CA5	2.00	1.56	1.50

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	s	403	UQ	C7-C8-C9	-9.45	111.06	126.79
51	J	401	NDP	C3N-C2N-N1N	-8.13	111.49	123.10
51	J	401	NDP	C1D-N1N-C2N	-6.25	110.70	121.11
47	A	503	NAI	C5A-C4A-N3A	-5.88	119.08	126.75
56	s	403	UQ	C12-C13-C14	-5.86	113.56	127.66
51	J	401	NDP	C5A-C4A-N3A	-5.80	119.18	126.75
57	w	401	ADP	C5-C4-N3	-5.79	119.19	126.75
51	J	401	NDP	C1D-N1N-C6N	-5.61	108.75	120.83
50	G	201	8Q1	C6-C1-S44	5.08	119.37	113.46
56	s	403	UQ	C11-C9-C8	-4.75	111.50	121.12
50	X	201	8Q1	C6-C1-S44	4.52	118.72	113.46
57	w	401	ADP	N3-C4-N9	4.49	134.47	127.08
57	w	401	ADP	N3-C2-N1	-4.43	121.67	128.60
56	s	403	UQ	C10-C9-C8	-4.40	112.38	123.68
47	A	503	NAI	N3A-C2A-N1A	-4.38	121.75	128.60
54	i	401	CDL	OA6-CA5-C11	4.32	120.81	111.50
54	n	102	CDL	OA6-CA5-C11	4.31	120.80	111.50
54	N	202	CDL	OA6-CA5-C11	4.29	120.75	111.50
54	V	203	CDL	OB6-CB5-C51	4.24	120.65	111.50
48	V	202	PEE	O2-C10-C11	4.14	120.43	111.50
56	s	403	UQ	C16-C14-C13	-4.13	112.76	121.12
54	a	201	CDL	OB6-CB5-C51	4.12	120.38	111.50
48	l	718	PEE	O2-C10-C11	4.11	120.36	111.50
47	A	503	NAI	N3A-C4A-N9A	4.10	133.84	127.08
54	l	713	CDL	OA6-CA5-C11	4.08	120.30	111.50
54	N	202	CDL	OB6-CB5-C51	4.08	120.30	111.50
56	s	403	UQ	C17-C18-C19	-4.08	113.82	127.75
51	J	401	NDP	N3A-C2A-N1A	-4.08	122.23	128.60
51	J	401	NDP	N3A-C4A-N9A	4.05	133.75	127.08
48	s	401	PEE	O2-C10-C11	3.99	120.10	111.50
54	r	714	CDL	OA6-CA5-C11	3.99	120.09	111.50
54	r	714	CDL	OB6-CB5-C51	3.97	120.05	111.50
54	l	712	CDL	OA6-CA5-C11	3.96	120.05	111.50
56	s	403	UQ	C15-C14-C13	-3.95	113.54	123.68
54	i	401	CDL	OB6-CB5-C51	3.94	120.00	111.50
47	A	503	NAI	C2A-N3A-C4A	3.93	121.04	111.75
48	m	202	PEE	O2-C10-C11	3.93	119.96	111.50
54	l	712	CDL	OB6-CB5-C51	3.92	119.94	111.50
54	n	102	CDL	OB6-CB5-C51	3.91	119.93	111.50
48	C	311	PEE	O2-C10-C11	3.87	119.84	111.50
48	U	101	PEE	O2-C10-C11	3.86	119.81	111.50
54	l	713	CDL	OB6-CB5-C51	3.80	119.70	111.50
48	l	720	PEE	O2-C10-C11	3.80	119.69	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	w	401	ADP	C2-N3-C4	3.73	120.56	111.75
48	l	719	PEE	O2-C10-C11	3.73	119.54	111.50
51	J	401	NDP	C2A-N3A-C4A	3.73	120.56	111.75
47	A	503	NAI	C5A-N7A-C8A	3.66	108.70	103.51
54	a	201	CDL	OA6-CA5-C11	3.62	119.31	111.50
57	w	401	ADP	N9-C8-N7	-3.61	108.98	113.91
47	A	503	NAI	C3D-C2D-C1D	3.52	108.11	101.43
50	G	201	8Q1	O35-C34-N36	-3.48	115.52	122.99
50	X	201	8Q1	C43-S44-C1	3.48	112.69	101.87
57	w	401	ADP	C5-N7-C8	3.44	108.40	103.51
54	V	203	CDL	OA6-CA5-C11	3.38	120.23	110.80
56	s	403	UQ	C21-C19-C18	-3.35	112.95	122.65
50	G	201	8Q1	C43-S44-C1	3.35	112.30	101.87
47	A	503	NAI	N9A-C8A-N7A	-3.34	109.34	113.91
51	J	401	NDP	C5A-N7A-C8A	3.30	108.19	103.51
51	J	401	NDP	N9A-C8A-N7A	-3.21	109.53	113.91
47	A	503	NAI	C4A-C5A-N7A	-3.20	106.72	110.62
50	X	201	8Q1	O35-C34-N36	-3.17	116.18	122.99
57	w	401	ADP	C4-N9-C8	3.09	109.08	105.73
56	s	403	UQ	C20-C19-C18	-3.03	113.88	122.65
48	s	401	PEE	O3-C30-C31	3.00	121.32	111.91
51	J	401	NDP	C4A-C5A-N7A	-2.99	106.98	110.62
47	A	503	NAI	C4D-O4D-C1D	-2.98	102.89	109.47
54	a	201	CDL	OB8-CB7-C71	2.98	121.24	111.91
48	l	719	PEE	O3-C30-C31	2.92	121.06	111.91
54	i	401	CDL	OA8-CA7-C31	2.87	120.91	111.91
54	N	202	CDL	OA8-CA7-C31	2.86	120.89	111.91
56	s	403	UQ	CM5-C5-C6	-2.86	119.73	124.40
47	A	503	NAI	PN-O3-PA	-2.86	123.02	132.83
50	G	201	8Q1	C32-C34-N36	2.82	122.19	116.58
54	a	201	CDL	OA8-CA7-C31	2.80	120.70	111.91
57	w	401	ADP	C4-C5-N7	-2.80	107.21	110.62
46	A	502	FMN	C4-N3-C2	-2.79	120.49	125.64
48	V	202	PEE	O3-C30-C31	2.78	120.64	111.91
54	N	202	CDL	OB8-CB7-C71	2.77	120.62	111.91
54	n	102	CDL	OA8-CA7-C31	2.75	120.53	111.91
54	V	203	CDL	OB8-CB7-C71	2.74	120.51	111.91
50	X	201	8Q1	O2-P24-O27	-2.68	99.59	106.73
54	V	203	CDL	OA8-CA7-C31	2.66	120.25	111.91
50	G	201	8Q1	O2-P24-O27	-2.65	99.67	106.73
54	l	712	CDL	OB8-CB7-C71	2.64	120.20	111.91
57	w	401	ADP	PA-O3A-PB	-2.62	123.84	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	l	712	CDL	OA8-CA7-C31	2.60	120.07	111.91
48	l	720	PEE	O3-C30-C31	2.58	120.01	111.91
50	G	201	8Q1	O4-C1-C6	-2.58	120.94	123.99
54	r	714	CDL	OA8-CA7-C31	2.55	119.92	111.91
48	U	101	PEE	O3-C30-C31	2.54	119.88	111.91
54	n	102	CDL	OB8-CB7-C71	2.54	119.88	111.91
54	r	714	CDL	OB8-CB7-C71	2.54	119.88	111.91
54	l	713	CDL	OB8-CB7-C71	2.53	119.85	111.91
48	l	718	PEE	O3-C30-C31	2.53	119.85	111.91
54	N	202	CDL	CB4-OB6-CB5	-2.51	111.61	117.79
46	A	502	FMN	C4A-C4-N3	2.50	119.54	113.19
46	A	502	FMN	C4A-C10-N10	2.50	120.13	116.48
51	J	401	NDP	C2B-C1B-N9A	-2.49	109.33	113.53
49	e	201	PLX	C1A-N1-C1	2.49	120.11	109.92
49	i	705	PLX	C1A-N1-C1	2.49	120.08	109.92
54	N	202	CDL	CA6-CA4-CA3	-2.47	105.95	111.79
54	l	713	CDL	OA8-CA7-C31	2.47	119.65	111.91
48	C	311	PEE	O3-C30-C31	2.45	119.59	111.91
51	J	401	NDP	PN-O3-PA	-2.42	124.53	132.83
54	i	401	CDL	OB8-CB7-C71	2.41	119.47	111.91
50	X	201	8Q1	C32-C34-N36	2.40	121.36	116.58
48	m	202	PEE	O3-C30-C31	2.40	119.43	111.91
49	V	205	PLX	C1A-N1-C1	2.39	119.70	109.92
46	A	502	FMN	C10-C4A-N5	-2.37	119.83	124.86
49	j	203	PLX	C1A-N1-C1	2.34	119.47	109.92
50	X	201	8Q1	O1-P24-O2	2.33	116.56	107.64
54	V	203	CDL	CB4-OB6-CB5	-2.32	112.08	117.79
51	J	401	NDP	C4A-N9A-C8A	2.32	108.24	105.73
50	G	201	8Q1	O1-P24-O2	2.31	116.48	107.64
50	G	201	8Q1	O40-C39-N41	-2.31	118.66	123.01
50	X	201	8Q1	O4-C1-S44	-2.28	119.66	122.61
49	C	312	PLX	C1A-N1-C1	2.27	119.20	109.92
46	A	502	FMN	C9A-C5A-N5	-2.26	119.97	122.43
50	G	201	8Q1	O4-C1-S44	-2.25	119.69	122.61
54	V	203	CDL	CA4-OA6-CA5	-2.25	112.26	117.79
47	A	503	NAI	C4A-N9A-C8A	2.24	108.16	105.73
47	A	503	NAI	C2D-C3D-C4D	2.24	106.99	102.64
50	X	201	8Q1	C37-C38-C39	2.23	116.07	112.36
50	X	201	8Q1	O40-C39-N41	-2.21	118.84	123.01
50	G	201	8Q1	O27-P24-O3	-2.20	100.30	106.47
54	a	201	CDL	CB4-OB6-CB5	-2.20	112.37	117.79
50	G	201	8Q1	C37-C38-C39	2.15	115.94	112.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	G	201	8Q1	C38-C39-N41	2.12	119.99	116.42
51	J	401	NDP	C2B-C3B-C4B	2.09	106.53	101.99
54	N	202	CDL	OB6-CB5-OB7	-2.08	118.66	123.70
54	V	203	CDL	OB6-CB5-OB7	-2.06	118.72	123.70
46	A	502	FMN	C4A-C10-N1	-2.04	119.99	124.73
46	A	502	FMN	O4-C4-C4A	-2.04	121.19	126.60
54	i	401	CDL	CA4-OA6-CA5	-2.04	112.78	117.79
46	A	502	FMN	C5A-C9A-N10	2.02	120.04	117.95
50	X	201	8Q1	O4-C1-C6	-2.01	121.62	123.99

There are no chirality outliers.

All (738) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
47	A	503	NAI	C5B-O5B-PA-O1A
47	A	503	NAI	C3D-C4D-C5D-O5D
48	C	311	PEE	C1-O3P-P-O1P
48	U	101	PEE	C19-C20-C21-C22
48	U	101	PEE	C17-C18-C19-C20
48	U	101	PEE	C1-O3P-P-O2P
48	U	101	PEE	C1-O3P-P-O1P
48	U	101	PEE	O4P-C4-C5-N
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	718	PEE	C11-C10-O2-C2
48	l	719	PEE	C11-C10-O2-C2
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
49	C	312	PLX	O7-C6-C7-C8
49	C	312	PLX	C3-O4-P1-O2
49	C	312	PLX	C3-O4-P1-O3
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-O2
49	V	205	PLX	O9-C24-C25-C26
49	e	201	PLX	O7-C6-O6-C4

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Mol	Chain	Res	Type	Atoms
49	e	201	PLX	C3-O4-P1-O1
49	e	201	PLX	C3-O4-P1-O2
49	e	201	PLX	C2-O1-P1-O4
49	e	201	PLX	C2-O1-P1-O2
49	e	201	PLX	C2-O1-P1-O3
49	e	201	PLX	C25-C24-O8-C5
49	e	201	PLX	O9-C24-C25-C26
49	i	705	PLX	O7-C6-O6-C4
49	i	705	PLX	C2-O1-P1-O2
49	i	705	PLX	O9-C24-O8-C5
49	j	203	PLX	O7-C6-C7-C8
49	n	101	PLX	C3-O4-P1-O1
49	n	101	PLX	C3-O4-P1-O2
49	n	101	PLX	C3-O4-P1-O3
50	G	201	8Q1	O27-C28-C29-C32
50	G	201	8Q1	N36-C37-C38-C39
50	G	201	8Q1	N41-C42-C43-S44
50	G	201	8Q1	C28-O27-P24-O1
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	N36-C37-C38-C39
50	X	201	8Q1	C28-O27-P24-O3
50	X	201	8Q1	C28-O27-P24-O2
50	X	201	8Q1	C28-O27-P24-O1
51	J	401	NDP	C5B-O5B-PA-O1A
51	J	401	NDP	C5B-O5B-PA-O3
51	J	401	NDP	C2N-C3N-C7N-N7N
54	N	202	CDL	CA2-OA2-PA1-OA3
54	N	202	CDL	CA2-OA2-PA1-OA4
54	N	202	CDL	CA3-OA5-PA1-OA4
54	N	202	CDL	CB2-OB2-PB2-OB3
54	N	202	CDL	CB2-OB2-PB2-OB4
54	N	202	CDL	CB2-OB2-PB2-OB5
54	N	202	CDL	CB3-OB5-PB2-OB4
54	V	203	CDL	CA2-OA2-PA1-OA4
54	V	203	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
54	V	203	CDL	CB3-OB5-PB2-OB4
54	a	201	CDL	CA2-OA2-PA1-OA3
54	a	201	CDL	CA2-OA2-PA1-OA4
54	a	201	CDL	CA3-OA5-PA1-OA2
54	a	201	CDL	CB2-OB2-PB2-OB3
54	a	201	CDL	CB3-OB5-PB2-OB3
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	CA3-OA5-PA1-OA2
54	i	401	CDL	CB3-OB5-PB2-OB3
54	i	401	CDL	OB6-CB4-CB6-OB8
54	l	712	CDL	CA2-OA2-PA1-OA3
54	l	712	CDL	CA2-OA2-PA1-OA4
54	l	712	CDL	CB2-OB2-PB2-OB3
54	l	712	CDL	CB2-OB2-PB2-OB4
54	l	712	CDL	CB3-OB5-PB2-OB3
54	l	713	CDL	CA2-OA2-PA1-OA4
54	l	713	CDL	CB2-OB2-PB2-OB3
54	l	713	CDL	CB2-OB2-PB2-OB4
54	l	713	CDL	CB2-OB2-PB2-OB5
54	l	713	CDL	CB3-OB5-PB2-OB3
54	l	713	CDL	OB6-CB4-CB6-OB8
54	n	102	CDL	CA2-OA2-PA1-OA3
54	n	102	CDL	CA2-OA2-PA1-OA4
54	n	102	CDL	CA2-OA2-PA1-OA5
54	n	102	CDL	CA3-OA5-PA1-OA4
54	n	102	CDL	CB2-OB2-PB2-OB3
54	n	102	CDL	CB2-OB2-PB2-OB4
54	n	102	CDL	CB2-OB2-PB2-OB5
54	r	714	CDL	CA2-OA2-PA1-OA3
54	r	714	CDL	CA2-OA2-PA1-OA4
54	r	714	CDL	CA3-OA5-PA1-OA2
54	r	714	CDL	CA3-OA5-PA1-OA3
54	r	714	CDL	CA3-OA5-PA1-OA4
54	r	714	CDL	OA6-CA4-CA6-OA8
54	r	714	CDL	CB3-OB5-PB2-OB2
54	r	714	CDL	CB3-OB5-PB2-OB3
54	r	714	CDL	OB7-CB5-OB6-CB4
54	r	714	CDL	C51-CB5-OB6-CB4
56	s	403	UQ	C7-C8-C9-C10
56	s	403	UQ	C7-C8-C9-C11

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Mol	Chain	Res	Type	Atoms
56	s	403	UQ	C12-C13-C14-C16
56	s	403	UQ	C14-C16-C17-C18
57	w	401	ADP	C5'-O5'-PA-O1A
57	w	401	ADP	C5'-O5'-PA-O2A
57	w	401	ADP	C5'-O5'-PA-O3A
54	V	203	CDL	OA9-CA7-OA8-CA6
54	l	712	CDL	OA9-CA7-OA8-CA6
54	V	203	CDL	C31-CA7-OA8-CA6
54	l	712	CDL	C31-CA7-OA8-CA6
56	s	403	UQ	C17-C18-C19-C21
48	l	718	PEE	O4-C10-O2-C2
48	l	719	PEE	O4-C10-O2-C2
54	l	713	CDL	C59-C60-C61-C62
48	U	101	PEE	C31-C30-O3-C3
48	V	202	PEE	C17-C18-C19-C20
48	l	720	PEE	C37-C38-C39-C40
48	s	401	PEE	C37-C38-C39-C40
48	V	202	PEE	O4-C10-O2-C2
48	m	202	PEE	O4-C10-O2-C2
54	r	714	CDL	OB9-CB7-OB8-CB6
54	V	203	CDL	O1-C1-CA2-OA2
54	l	712	CDL	O1-C1-CA2-OA2
54	l	712	CDL	O1-C1-CB2-OB2
54	l	713	CDL	O1-C1-CB2-OB2
54	r	714	CDL	C71-CB7-OB8-CB6
48	U	101	PEE	O5-C30-O3-C3
48	V	202	PEE	C11-C10-O2-C2
54	N	202	CDL	C11-CA5-OA6-CA4
54	N	202	CDL	C51-CB5-OB6-CB4
49	V	205	PLX	C9-C10-C11-C12
51	J	401	NDP	C2D-C1D-N1N-C6N
49	C	312	PLX	C28-C29-C30-C31
54	l	713	CDL	C11-C12-C13-C14
49	e	201	PLX	C12-C13-C14-C15
49	j	203	PLX	C28-C29-C30-C31
54	V	203	CDL	C60-C61-C62-C63
49	i	705	PLX	C7-C8-C9-C10
54	l	712	CDL	C55-C56-C57-C58
51	J	401	NDP	O4B-C4B-C5B-O5B
54	l	713	CDL	C71-CB7-OB8-CB6
54	N	202	CDL	OA7-CA5-OA6-CA4
49	V	205	PLX	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
56	s	403	UQ	C12-C11-C9-C10
54	l	713	CDL	OB9-CB7-OB8-CB6
48	l	720	PEE	C31-C30-O3-C3
48	m	202	PEE	C33-C34-C35-C36
48	l	720	PEE	C10-C11-C12-C13
54	V	203	CDL	CB2-C1-CA2-OA2
54	i	401	CDL	CA2-C1-CB2-OB2
54	r	714	CDL	CB2-C1-CA2-OA2
48	l	720	PEE	O5-C30-O3-C3
48	l	719	PEE	C31-C30-O3-C3
48	m	202	PEE	C31-C30-O3-C3
54	V	203	CDL	C71-CB7-OB8-CB6
54	i	401	CDL	C31-CA7-OA8-CA6
54	l	713	CDL	C35-C36-C37-C38
54	i	401	CDL	O1-C1-CA2-OA2
54	i	401	CDL	OA9-CA7-OA8-CA6
56	s	403	UQ	C13-C14-C16-C17
54	N	202	CDL	OB7-CB5-OB6-CB4
48	U	101	PEE	C30-C31-C32-C33
48	l	718	PEE	C10-C11-C12-C13
54	r	714	CDL	CB5-C51-C52-C53
48	m	202	PEE	O5-C30-O3-C3
48	V	202	PEE	C10-C11-C12-C13
48	l	719	PEE	O5-C30-O3-C3
48	s	401	PEE	C30-C31-C32-C33
54	l	712	CDL	CB7-C71-C72-C73
54	l	713	CDL	CB7-C71-C72-C73
54	r	714	CDL	CB7-C71-C72-C73
54	l	713	CDL	C39-C40-C41-C42
47	A	503	NAI	O4D-C4D-C5D-O5D
49	j	203	PLX	C15-C16-C17-C18
49	e	201	PLX	C2-C1-N1-C1C
49	e	201	PLX	C2-C1-N1-C1A
54	a	201	CDL	CA7-C31-C32-C33
54	l	712	CDL	CB5-C51-C52-C53
54	r	714	CDL	C74-C75-C76-C77
56	s	403	UQ	C9-C11-C12-C13
48	l	718	PEE	C22-C23-C24-C25
54	r	714	CDL	O1-C1-CA2-OA2
54	V	203	CDL	OB9-CB7-OB8-CB6
48	U	101	PEE	C1-O3P-P-O4P
49	C	312	PLX	C3-O4-P1-O1

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Mol	Chain	Res	Type	Atoms
49	V	205	PLX	C3-O4-P1-O1
54	N	202	CDL	CA2-OA2-PA1-OA5
54	N	202	CDL	CA3-OA5-PA1-OA2
54	N	202	CDL	CB3-OB5-PB2-OB2
54	V	203	CDL	CA2-OA2-PA1-OA5
54	a	201	CDL	CA2-OA2-PA1-OA5
54	a	201	CDL	CB2-OB2-PB2-OB5
54	i	401	CDL	CA2-OA2-PA1-OA5
54	i	401	CDL	CB2-OB2-PB2-OB5
54	l	712	CDL	CA2-OA2-PA1-OA5
54	l	712	CDL	CB2-OB2-PB2-OB5
54	l	712	CDL	CB3-OB5-PB2-OB2
54	l	713	CDL	CA2-OA2-PA1-OA5
54	l	713	CDL	CA3-OA5-PA1-OA2
54	n	102	CDL	CA3-OA5-PA1-OA2
54	r	714	CDL	CA2-OA2-PA1-OA5
54	r	714	CDL	CB2-OB2-PB2-OB5
48	s	401	PEE	C31-C30-O3-C3
54	l	712	CDL	CA2-C1-CB2-OB2
49	j	203	PLX	C34-C35-C36-C37
49	e	201	PLX	O8-C24-C25-C26
49	V	205	PLX	C16-C17-C18-C19
49	i	705	PLX	C28-C29-C30-C31
54	l	713	CDL	C37-C38-C39-C40
54	l	713	CDL	C75-C76-C77-C78
48	C	311	PEE	C11-C10-O2-C2
48	l	720	PEE	C31-C32-C33-C34
49	V	205	PLX	C15-C16-C17-C18
49	V	205	PLX	C27-C28-C29-C30
49	e	201	PLX	C13-C14-C15-C16
49	i	705	PLX	C27-C28-C29-C30
50	G	201	8Q1	C11-C12-C13-C14
54	a	201	CDL	C31-C32-C33-C34
54	l	712	CDL	C62-C63-C64-C65
54	l	712	CDL	C75-C76-C77-C78
50	G	201	8Q1	O27-C28-C29-C30
50	G	201	8Q1	O27-C28-C29-C31
48	U	101	PEE	C41-C42-C43-C44
49	C	312	PLX	C17-C18-C19-C20
49	V	205	PLX	C12-C13-C14-C15
49	i	705	PLX	C33-C34-C35-C36
50	G	201	8Q1	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
54	V	203	CDL	C81-C82-C83-C84
54	l	712	CDL	C39-C40-C41-C42
54	l	712	CDL	C56-C57-C58-C59
54	r	714	CDL	C73-C74-C75-C76
54	N	202	CDL	CA6-CA4-OA6-CA5
48	C	311	PEE	O4-C10-O2-C2
48	s	401	PEE	C34-C35-C36-C37
54	V	203	CDL	C55-C56-C57-C58
49	C	312	PLX	C7-C8-C9-C10
49	e	201	PLX	C29-C30-C31-C32
49	j	203	PLX	C10-C11-C12-C13
54	r	714	CDL	C41-C42-C43-C44
54	r	714	CDL	C75-C76-C77-C78
54	N	202	CDL	O1-C1-CB2-OB2
54	V	203	CDL	O1-C1-CB2-OB2
49	i	705	PLX	C10-C11-C12-C13
54	l	712	CDL	C73-C74-C75-C76
54	r	714	CDL	C56-C57-C58-C59
48	l	719	PEE	C31-C32-C33-C34
49	e	201	PLX	C25-C26-C27-C28
49	i	705	PLX	C11-C10-C9-C8
50	G	201	8Q1	C12-C13-C14-C15
54	l	712	CDL	C81-C82-C83-C84
54	l	713	CDL	C73-C74-C75-C76
49	V	205	PLX	C28-C29-C30-C31
54	V	203	CDL	C54-C55-C56-C57
54	l	713	CDL	C40-C41-C42-C43
54	r	714	CDL	C55-C56-C57-C58
54	r	714	CDL	C71-C72-C73-C74
54	r	714	CDL	CA7-C31-C32-C33
49	e	201	PLX	C28-C29-C30-C31
49	e	201	PLX	C33-C34-C35-C36
49	i	705	PLX	C32-C33-C34-C35
49	j	203	PLX	C7-C8-C9-C10
54	V	203	CDL	C79-C80-C81-C82
54	r	714	CDL	C59-C60-C61-C62
48	U	101	PEE	C34-C35-C36-C37
49	i	705	PLX	C9-C10-C11-C12
54	V	203	CDL	C59-C60-C61-C62
54	n	102	CDL	C11-CA5-OA6-CA4
54	l	713	CDL	C54-C55-C56-C57
48	C	311	PEE	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
48	V	202	PEE	C13-C14-C15-C16
48	l	720	PEE	C33-C34-C35-C36
48	s	401	PEE	C21-C22-C23-C24
48	s	401	PEE	C33-C34-C35-C36
49	e	201	PLX	C14-C15-C16-C17
54	i	401	CDL	C36-C37-C38-C39
54	l	713	CDL	C52-C53-C54-C55
49	C	312	PLX	C11-C12-C13-C14
50	X	201	8Q1	C7-C8-C9-C10
54	V	203	CDL	C56-C57-C58-C59
54	V	203	CDL	C58-C59-C60-C61
50	G	201	8Q1	C6-C7-C8-C9
54	r	714	CDL	C14-C15-C16-C17
48	s	401	PEE	C12-C13-C14-C15
49	C	312	PLX	C33-C34-C35-C36
49	V	205	PLX	C7-C8-C9-C10
49	i	705	PLX	C14-C15-C16-C17
50	X	201	8Q1	C6-C7-C8-C9
54	i	401	CDL	C33-C34-C35-C36
49	C	312	PLX	C13-C14-C15-C16
49	C	312	PLX	C27-C28-C29-C30
49	i	705	PLX	C30-C31-C32-C33
49	e	201	PLX	C10-C11-C12-C13
54	l	712	CDL	C11-C12-C13-C14
54	r	714	CDL	C13-C14-C15-C16
49	V	205	PLX	C13-C14-C15-C16
54	l	712	CDL	C52-C53-C54-C55
54	r	714	CDL	C17-C18-C19-C20
54	n	102	CDL	OA7-CA5-OA6-CA4
48	l	720	PEE	C17-C18-C19-C20
54	l	713	CDL	C58-C59-C60-C61
54	l	712	CDL	C35-C36-C37-C38
49	e	201	PLX	C27-C28-C29-C30
54	i	401	CDL	C11-C12-C13-C14
54	l	713	CDL	C60-C61-C62-C63
54	V	203	CDL	CA7-C31-C32-C33
48	s	401	PEE	O5-C30-O3-C3
48	C	311	PEE	C42-C43-C44-C45
48	m	202	PEE	C11-C12-C13-C14
48	C	311	PEE	C13-C14-C15-C16
48	U	101	PEE	C40-C41-C42-C43
49	C	312	PLX	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
48	C	311	PEE	C11-C12-C13-C14
48	s	401	PEE	C42-C43-C44-C45
49	n	101	PLX	C10-C11-C12-C13
54	V	203	CDL	C84-C85-C86-C87
48	U	101	PEE	C21-C22-C23-C24
49	C	312	PLX	C9-C10-C11-C12
49	j	203	PLX	C27-C28-C29-C30
54	V	203	CDL	C80-C81-C82-C83
54	l	712	CDL	C14-C15-C16-C17
54	l	712	CDL	C32-C33-C34-C35
54	l	712	CDL	C71-C72-C73-C74
54	l	712	CDL	C51-CB5-OB6-CB4
48	U	101	PEE	C22-C23-C24-C25
49	j	203	PLX	C13-C14-C15-C16
49	C	312	PLX	C14-C15-C16-C17
54	V	203	CDL	C75-C76-C77-C78
54	l	712	CDL	C18-C19-C20-C21
54	l	712	CDL	C58-C59-C60-C61
48	l	718	PEE	C35-C36-C37-C38
48	s	401	PEE	C15-C16-C17-C18
48	U	101	PEE	O4-C10-O2-C2
54	l	712	CDL	C71-CB7-OB8-CB6
50	G	201	8Q1	C7-C8-C9-C10
54	r	714	CDL	C62-C63-C64-C65
50	X	201	8Q1	C11-C12-C13-C14
49	C	312	PLX	C16-C17-C18-C19
48	V	202	PEE	C12-C13-C14-C15
54	n	102	CDL	C54-C55-C56-C57
49	j	203	PLX	C9-C10-C11-C12
48	V	202	PEE	C41-C42-C43-C44
48	U	101	PEE	C11-C10-O2-C2
48	s	401	PEE	C11-C10-O2-C2
54	V	203	CDL	C51-CB5-OB6-CB4
49	C	312	PLX	O4-C3-C4-O6
50	X	201	8Q1	C10-C11-C12-C13
54	V	203	CDL	C53-C54-C55-C56
48	s	401	PEE	O4-C10-O2-C2
54	l	712	CDL	OB7-CB5-OB6-CB4
49	V	205	PLX	C14-C15-C16-C17
54	V	203	CDL	C52-C53-C54-C55
54	l	713	CDL	OA6-CA4-CA6-OA8
54	l	712	CDL	C82-C83-C84-C85

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Mol	Chain	Res	Type	Atoms
49	e	201	PLX	C2-C1-N1-C1B
50	X	201	8Q1	C12-C13-C14-C15
54	l	712	CDL	C74-C75-C76-C77
54	r	714	CDL	C12-C13-C14-C15
49	j	203	PLX	C33-C34-C35-C36
54	r	714	CDL	C43-C44-C45-C46
54	l	712	CDL	OB9-CB7-OB8-CB6
48	l	718	PEE	C14-C15-C16-C17
48	s	401	PEE	C14-C15-C16-C17
49	i	705	PLX	C25-C26-C27-C28
54	l	713	CDL	C56-C57-C58-C59
48	V	202	PEE	C36-C37-C38-C39
48	C	311	PEE	C1-O3P-P-O4P
48	l	719	PEE	C4-O4P-P-O3P
54	l	713	CDL	C77-C78-C79-C80
54	n	102	CDL	C22-C23-C24-C25
49	j	203	PLX	C14-C15-C16-C17
46	A	502	FMN	C3'-C4'-C5'-O5'
48	V	202	PEE	C11-C12-C13-C14
54	i	401	CDL	C35-C36-C37-C38
54	r	714	CDL	C78-C79-C80-C81
48	s	401	PEE	C20-C21-C22-C23
54	r	714	CDL	C36-C37-C38-C39
54	a	201	CDL	CB5-C51-C52-C53
49	j	203	PLX	C12-C13-C14-C15
54	l	712	CDL	CB2-C1-CA2-OA2
54	n	102	CDL	C75-C76-C77-C78
54	r	714	CDL	C52-C53-C54-C55
54	l	713	CDL	C14-C15-C16-C17
49	i	705	PLX	C3-C4-C5-O8
49	j	203	PLX	C3-C4-C5-O8
49	j	203	PLX	C26-C27-C28-C29
54	i	401	CDL	CB3-CB4-CB6-OB8
54	n	102	CDL	CA3-CA4-CA6-OA8
48	s	401	PEE	C17-C18-C19-C20
54	l	712	CDL	C61-C62-C63-C64
54	l	712	CDL	C21-C22-C23-C24
48	C	311	PEE	C39-C40-C41-C42
48	m	202	PEE	C19-C20-C21-C22
48	C	311	PEE	C32-C33-C34-C35
48	l	720	PEE	C11-C10-O2-C2
54	r	714	CDL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
49	e	201	PLX	C7-C8-C9-C10
54	l	713	CDL	C64-C65-C66-C67
54	r	714	CDL	C64-C65-C66-C67
54	r	714	CDL	C35-C36-C37-C38
48	m	202	PEE	C3-C2-O2-C10
54	n	102	CDL	CA6-CA4-OA6-CA5
48	V	202	PEE	C31-C32-C33-C34
50	X	201	8Q1	C13-C14-C15-C16
49	e	201	PLX	C31-C32-C33-C34
54	l	713	CDL	C62-C63-C64-C65
50	G	201	8Q1	C28-O27-P24-O3
48	l	719	PEE	C32-C33-C34-C35
49	C	312	PLX	C30-C31-C32-C33
48	V	202	PEE	C31-C30-O3-C3
54	V	203	CDL	C71-C72-C73-C74
54	i	401	CDL	C13-C14-C15-C16
54	V	203	CDL	C82-C83-C84-C85
54	r	714	CDL	C60-C61-C62-C63
48	m	202	PEE	O2-C2-C3-O3
54	r	714	CDL	OB6-CB4-CB6-OB8
54	V	203	CDL	OB7-CB5-OB6-CB4
48	U	101	PEE	C36-C37-C38-C39
54	a	201	CDL	C71-CB7-OB8-CB6
49	j	203	PLX	C25-C26-C27-C28
54	V	203	CDL	CA2-C1-CB2-OB2
54	l	713	CDL	CA2-C1-CB2-OB2
54	r	714	CDL	C81-C82-C83-C84
49	C	312	PLX	O4-C3-C4-C5
54	V	203	CDL	OB5-CB3-CB4-CB6
49	e	201	PLX	C9-C10-C11-C12
54	l	713	CDL	C32-C33-C34-C35
54	r	714	CDL	C82-C83-C84-C85
54	l	713	CDL	CB5-C51-C52-C53
54	l	713	CDL	C72-C73-C74-C75
49	j	203	PLX	C31-C32-C33-C34
49	n	101	PLX	C11-C12-C13-C14
48	U	101	PEE	C44-C45-C46-C47
48	l	719	PEE	C14-C15-C16-C17
49	V	205	PLX	C31-C32-C33-C34
49	i	705	PLX	C13-C14-C15-C16
49	V	205	PLX	C11-C12-C13-C14
48	C	311	PEE	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
48	V	202	PEE	C1-C2-C3-O3
48	l	720	PEE	C1-C2-C3-O3
49	V	205	PLX	C3-C4-C5-O8
54	N	202	CDL	CA3-CA4-CA6-OA8
54	V	203	CDL	CA3-CA4-CA6-OA8
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	O4-C10-O2-C2
48	l	719	PEE	C37-C38-C39-C40
49	e	201	PLX	C15-C16-C17-C18
49	V	205	PLX	C29-C30-C31-C32
49	e	201	PLX	C11-C12-C13-C14
48	l	720	PEE	C4-O4P-P-O3P
49	e	201	PLX	C5-C4-O6-C6
54	l	713	CDL	CB3-OB5-PB2-OB2
48	V	202	PEE	O5-C30-O3-C3
49	n	101	PLX	O7-C6-C7-C8
48	l	719	PEE	O3P-C1-C2-O2
48	s	401	PEE	O3P-C1-C2-O2
54	a	201	CDL	OA5-CA3-CA4-OA6
54	l	713	CDL	OA5-CA3-CA4-OA6
54	r	714	CDL	C31-CA7-OA8-CA6
54	a	201	CDL	C37-C38-C39-C40
48	l	719	PEE	C15-C16-C17-C18
54	n	102	CDL	C73-C74-C75-C76
50	X	201	8Q1	C42-C43-S44-C1
48	s	401	PEE	C13-C14-C15-C16
48	C	311	PEE	O2-C2-C3-O3
49	V	205	PLX	O6-C4-C5-O8
49	j	203	PLX	O6-C4-C5-O8
54	V	203	CDL	OA6-CA4-CA6-OA8
54	l	713	CDL	C55-C56-C57-C58
49	V	205	PLX	C10-C11-C12-C13
49	C	312	PLX	C31-C32-C33-C34
50	G	201	8Q1	C9-C10-C11-C12
54	l	712	CDL	C37-C38-C39-C40
54	l	713	CDL	C51-C52-C53-C54
54	r	714	CDL	CB4-CB3-OB5-PB2
54	r	714	CDL	C32-C33-C34-C35
48	U	101	PEE	C38-C39-C40-C41
54	i	401	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
54	r	714	CDL	C20-C21-C22-C23
48	l	719	PEE	C21-C22-C23-C24
49	C	312	PLX	C26-C27-C28-C29
49	e	201	PLX	C16-C17-C18-C19
50	X	201	8Q1	S44-C1-C6-C7
48	l	718	PEE	C24-C25-C26-C27
49	V	205	PLX	C33-C34-C35-C36
49	j	203	PLX	O4-C3-C4-C5
54	a	201	CDL	OA5-CA3-CA4-CA6
48	s	401	PEE	C22-C23-C24-C25
50	G	201	8Q1	C28-O27-P24-O2
54	n	102	CDL	C52-C53-C54-C55
54	r	714	CDL	C83-C84-C85-C86
54	r	714	CDL	C80-C81-C82-C83
49	e	201	PLX	C3-C4-C5-O8
54	r	714	CDL	CA3-CA4-CA6-OA8
54	a	201	CDL	OB9-CB7-OB8-CB6
54	r	714	CDL	OA9-CA7-OA8-CA6
49	i	705	PLX	O4-C3-C4-O6
54	l	713	CDL	C78-C79-C80-C81
49	e	201	PLX	C36-C37-C38-C39
54	l	712	CDL	C20-C21-C22-C23
48	s	401	PEE	C32-C33-C34-C35
48	V	202	PEE	O2-C2-C3-O3
49	i	705	PLX	O6-C4-C5-O8
54	N	202	CDL	OA6-CA4-CA6-OA8
54	l	712	CDL	C17-C18-C19-C20
47	A	503	NAI	C5B-O5B-PA-O3
48	l	718	PEE	C39-C40-C41-C42
48	V	202	PEE	C40-C41-C42-C43
54	a	201	CDL	C75-C76-C77-C78
54	r	714	CDL	C44-C45-C46-C47
48	V	202	PEE	C43-C44-C45-C46
48	l	720	PEE	C13-C14-C15-C16
54	n	102	CDL	C58-C59-C60-C61
48	l	718	PEE	C1-O3P-P-O4P
49	V	205	PLX	C2-O1-P1-O4
54	V	203	CDL	CA3-OA5-PA1-OA2
54	i	401	CDL	CB3-OB5-PB2-OB2
54	l	713	CDL	C12-C13-C14-C15
48	C	311	PEE	C1-O3P-P-O2P
48	l	718	PEE	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
48	l	719	PEE	C1-O3P-P-O2P
48	l	719	PEE	C4-O4P-P-O2P
48	l	719	PEE	C4-O4P-P-O1P
49	C	312	PLX	C2-O1-P1-O3
49	V	205	PLX	C2-O1-P1-O3
51	J	401	NDP	C5D-O5D-PN-O2N
54	a	201	CDL	CA3-OA5-PA1-OA4
54	a	201	CDL	CB2-OB2-PB2-OB4
54	i	401	CDL	CA3-OA5-PA1-OA4
54	i	401	CDL	CB2-OB2-PB2-OB3
54	l	712	CDL	CB3-OB5-PB2-OB4
54	l	713	CDL	CA2-OA2-PA1-OA3
54	l	713	CDL	CA3-OA5-PA1-OA4
54	n	102	CDL	CA3-OA5-PA1-OA3
54	r	714	CDL	CB2-OB2-PB2-OB3
54	r	714	CDL	CB2-OB2-PB2-OB4
48	m	202	PEE	O3P-C1-C2-C3
48	s	401	PEE	O3P-C1-C2-C3
49	i	705	PLX	O4-C3-C4-C5
49	i	705	PLX	C16-C17-C18-C19
49	j	203	PLX	C25-C24-O8-C5
49	j	203	PLX	C30-C31-C32-C33
48	U	101	PEE	C2-C3-O3-C30
49	n	101	PLX	C14-C15-C16-C17
49	e	201	PLX	C30-C31-C32-C33
48	m	202	PEE	O3P-C1-C2-O2
49	j	203	PLX	O4-C3-C4-O6
54	V	203	CDL	OB5-CB3-CB4-OB6
48	V	202	PEE	C38-C39-C40-C41
48	V	202	PEE	C32-C33-C34-C35
54	i	401	CDL	C14-C15-C16-C17
48	V	202	PEE	C20-C21-C22-C23
54	r	714	CDL	C31-C32-C33-C34
54	a	201	CDL	C17-C18-C19-C20
54	a	201	CDL	C39-C40-C41-C42
54	N	202	CDL	CB5-C51-C52-C53
54	l	712	CDL	CA7-C31-C32-C33
48	m	202	PEE	O3-C30-C31-C32
51	J	401	NDP	C2N-C3N-C7N-O7N
54	V	203	CDL	C78-C79-C80-C81
48	l	720	PEE	O2-C2-C3-O3
49	e	201	PLX	O6-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
54	n	102	CDL	OA6-CA4-CA6-OA8
54	n	102	CDL	C21-C22-C23-C24
54	V	203	CDL	C72-C73-C74-C75
49	C	312	PLX	O6-C6-C7-C8
49	j	203	PLX	C35-C36-C37-C38
54	l	712	CDL	C60-C61-C62-C63
49	n	101	PLX	C11-C10-C9-C8
49	n	101	PLX	C35-C36-C37-C38
48	l	720	PEE	C18-C19-C20-C21
49	i	705	PLX	O7-C6-C7-C8
54	l	712	CDL	C54-C55-C56-C57
49	i	705	PLX	C35-C36-C37-C38
49	j	203	PLX	C32-C33-C34-C35
54	V	203	CDL	C57-C58-C59-C60
54	l	712	CDL	C42-C43-C44-C45
54	r	714	CDL	C51-C52-C53-C54
54	n	102	CDL	C53-C54-C55-C56
50	X	201	8Q1	O27-C28-C29-C30
54	l	713	CDL	C76-C77-C78-C79
48	C	311	PEE	C44-C45-C46-C47
54	a	201	CDL	CA6-CA4-OA6-CA5
54	l	713	CDL	OA5-CA3-CA4-CA6
54	r	714	CDL	C33-C34-C35-C36
54	N	202	CDL	OB6-CB4-CB6-OB8
48	l	719	PEE	C20-C21-C22-C23
49	i	705	PLX	C3-O4-P1-O1
49	n	101	PLX	C2-O1-P1-O4
54	V	203	CDL	CB3-OB5-PB2-OB2
54	a	201	CDL	CB3-OB5-PB2-OB2
48	l	718	PEE	C31-C32-C33-C34
49	e	201	PLX	C19-C20-C21-C22
48	m	202	PEE	C1-C2-C3-O3
48	m	202	PEE	C16-C17-C18-C19
54	r	714	CDL	C54-C55-C56-C57
54	l	713	CDL	C74-C75-C76-C77
48	l	720	PEE	C2-C1-O3P-P
54	a	201	CDL	CB4-CB3-OB5-PB2
48	l	718	PEE	C38-C39-C40-C41
48	l	720	PEE	C16-C17-C18-C19
48	l	719	PEE	C22-C23-C24-C25
54	r	714	CDL	C57-C58-C59-C60
48	C	311	PEE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
49	C	312	PLX	C18-C19-C20-C21
48	s	401	PEE	C10-C11-C12-C13
50	X	201	8Q1	C9-C10-C11-C12
47	A	503	NAI	O4D-C1D-N1N-C2N
48	C	311	PEE	O4P-C4-C5-N
54	V	203	CDL	C63-C64-C65-C66
48	l	720	PEE	C39-C40-C41-C42
49	e	201	PLX	C24-C25-C26-C27
49	V	205	PLX	O8-C24-C25-C26
49	n	101	PLX	O6-C6-C7-C8
54	l	712	CDL	OA6-CA4-CA6-OA8
48	C	311	PEE	C38-C39-C40-C41
47	A	503	NAI	C2D-C1D-N1N-C2N
48	s	401	PEE	C39-C40-C41-C42
48	s	401	PEE	C40-C41-C42-C43
48	U	101	PEE	C12-C13-C14-C15
48	l	720	PEE	C30-C31-C32-C33
54	i	401	CDL	CA6-CA4-OA6-CA5
54	l	713	CDL	C44-C45-C46-C47
49	n	101	PLX	O4-C3-C4-O6
54	l	712	CDL	C15-C16-C17-C18
54	l	712	CDL	C41-C42-C43-C44
54	r	714	CDL	C84-C85-C86-C87
54	l	712	CDL	C79-C80-C81-C82
48	V	202	PEE	C24-C25-C26-C27
48	l	718	PEE	C32-C33-C34-C35
48	l	720	PEE	C15-C16-C17-C18
48	C	311	PEE	C37-C38-C39-C40
54	r	714	CDL	C76-C77-C78-C79
49	n	101	PLX	C34-C35-C36-C37
54	r	714	CDL	C23-C24-C25-C26
54	a	201	CDL	C18-C19-C20-C21
48	m	202	PEE	C22-C23-C24-C25
54	a	201	CDL	C38-C39-C40-C41
54	l	712	CDL	C12-C13-C14-C15
48	l	718	PEE	C17-C18-C19-C20
49	i	705	PLX	C12-C13-C14-C15
54	l	713	CDL	C33-C34-C35-C36
50	X	201	8Q1	O4-C1-C6-C7
49	C	312	PLX	O8-C24-C25-C26
49	i	705	PLX	O8-C24-C25-C26
49	j	203	PLX	O6-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
48	l	720	PEE	C12-C13-C14-C15
54	N	202	CDL	C31-C32-C33-C34
48	l	719	PEE	O3P-C1-C2-C3
54	l	713	CDL	C34-C35-C36-C37
50	X	201	8Q1	C1-C6-C7-C8
54	n	102	CDL	CB2-C1-CA2-OA2
54	V	203	CDL	OA7-CA5-OA6-CA4
54	n	102	CDL	C12-C11-CA5-OA6
50	X	201	8Q1	O33-C32-C34-N36
48	U	101	PEE	O3-C30-C31-C32
50	X	201	8Q1	O27-C28-C29-C31
54	l	713	CDL	C15-C16-C17-C18
54	n	102	CDL	C17-C18-C19-C20
48	m	202	PEE	C20-C21-C22-C23
46	A	502	FMN	O4'-C4'-C5'-O5'
48	m	202	PEE	C32-C33-C34-C35
48	l	719	PEE	C36-C37-C38-C39
48	l	718	PEE	C1-C2-C3-O3
49	j	203	PLX	C7-C6-O6-C4
54	i	401	CDL	OA5-CA3-CA4-OA6
54	l	712	CDL	C51-C52-C53-C54
48	l	720	PEE	C23-C24-C25-C26
48	l	719	PEE	C13-C14-C15-C16
48	C	311	PEE	C36-C37-C38-C39
48	U	101	PEE	O2-C10-C11-C12
54	i	401	CDL	OA5-CA3-CA4-CA6
54	N	202	CDL	C52-C51-CB5-OB6
54	a	201	CDL	C71-C72-C73-C74
48	l	718	PEE	O2-C2-C3-O3
54	V	203	CDL	OB6-CB4-CB6-OB8
54	l	712	CDL	C72-C71-CB7-OB8
49	n	101	PLX	C2-C1-N1-C1A
51	J	401	NDP	C5D-O5D-PN-O3
49	n	101	PLX	C30-C31-C32-C33
48	l	718	PEE	C2-C1-O3P-P
48	l	718	PEE	C36-C37-C38-C39
48	l	720	PEE	C38-C39-C40-C41
54	N	202	CDL	C72-C71-CB7-OB8
49	n	101	PLX	C13-C14-C15-C16
48	s	401	PEE	C44-C45-C46-C47
48	C	311	PEE	O3-C30-C31-C32
48	l	720	PEE	O2-C10-C11-C12

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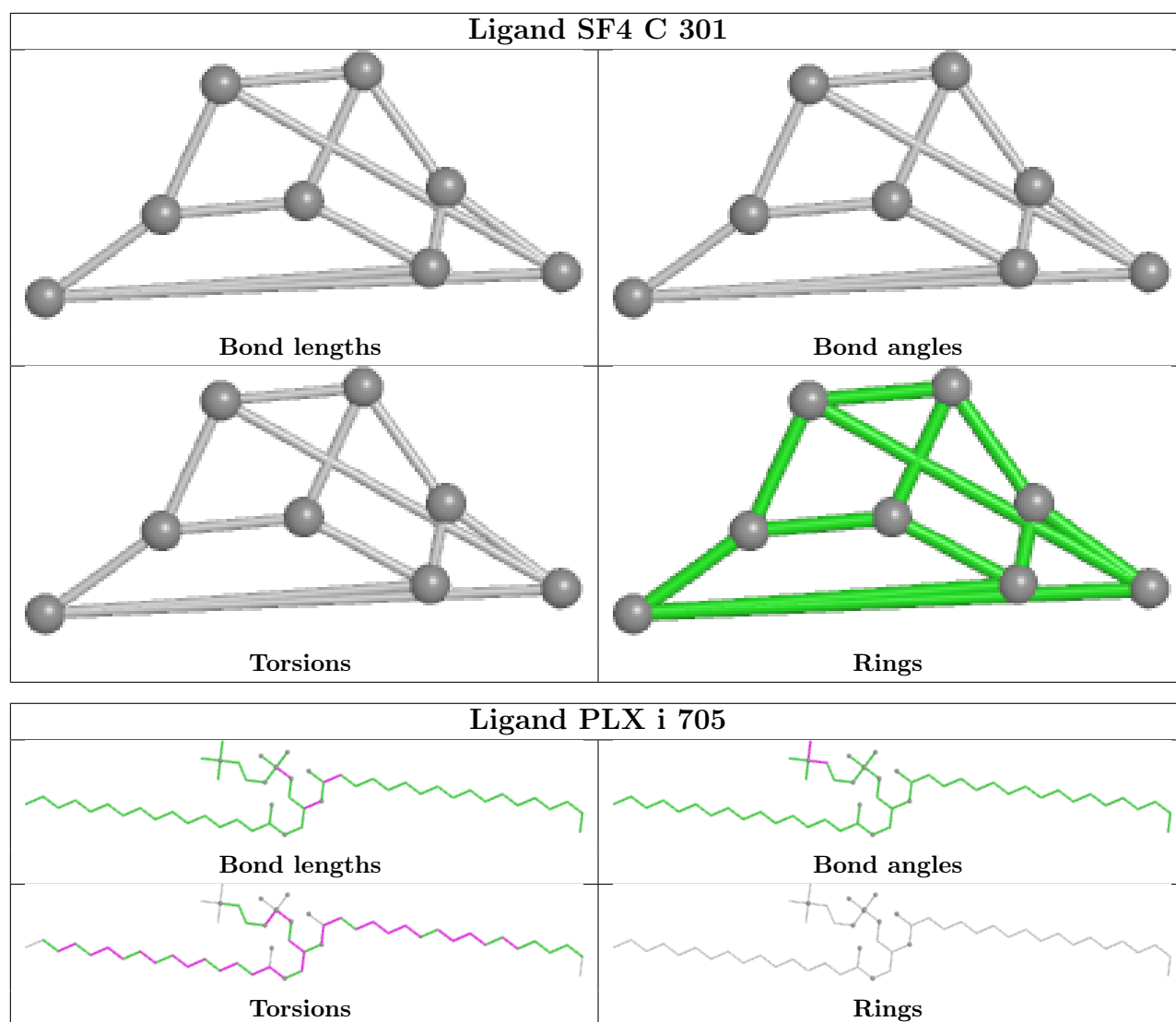
Mol	Chain	Res	Type	Atoms
49	j	203	PLX	C16-C17-C18-C19
54	V	203	CDL	C11-CA5-OA6-CA4
48	l	718	PEE	C18-C19-C20-C21
48	m	202	PEE	C18-C19-C20-C21
54	n	102	CDL	C14-C15-C16-C17
48	U	101	PEE	O5-C30-C31-C32
54	N	202	CDL	CB3-CB4-CB6-OB8
49	i	705	PLX	C2-O1-P1-O4
54	l	713	CDL	O1-C1-CA2-OA2
54	n	102	CDL	C12-C11-CA5-OA7
54	l	713	CDL	C32-C31-CA7-OA8
57	w	401	ADP	C4'-C5'-O5'-PA
48	U	101	PEE	O4-C10-C11-C12
48	V	202	PEE	C4-O4P-P-O1P
48	s	401	PEE	C1-O3P-P-O1P
49	V	205	PLX	C3-O4-P1-O3
49	i	705	PLX	C3-O4-P1-O2
49	n	101	PLX	C2-O1-P1-O2
54	V	203	CDL	CB2-OB2-PB2-OB3
54	V	203	CDL	CB3-OB5-PB2-OB3
54	l	712	CDL	CA3-OA5-PA1-OA3
54	N	202	CDL	C72-C71-CB7-OB9
54	l	712	CDL	C72-C71-CB7-OB9
50	G	201	8Q1	C13-C14-C15-C16
48	U	101	PEE	C16-C17-C18-C19
48	l	719	PEE	C18-C19-C20-C21
54	r	714	CDL	C52-C51-CB5-OB6
54	l	712	CDL	C44-C45-C46-C47
54	r	714	CDL	C11-C12-C13-C14
54	l	713	CDL	C63-C64-C65-C66
54	r	714	CDL	C15-C16-C17-C18
48	m	202	PEE	C13-C14-C15-C16
54	l	713	CDL	C12-C11-CA5-OA6
48	C	311	PEE	O5-C30-C31-C32
48	l	720	PEE	O4-C10-C11-C12
54	N	202	CDL	C52-C51-CB5-OB7
54	l	713	CDL	C32-C31-CA7-OA9
54	l	713	CDL	C71-C72-C73-C74

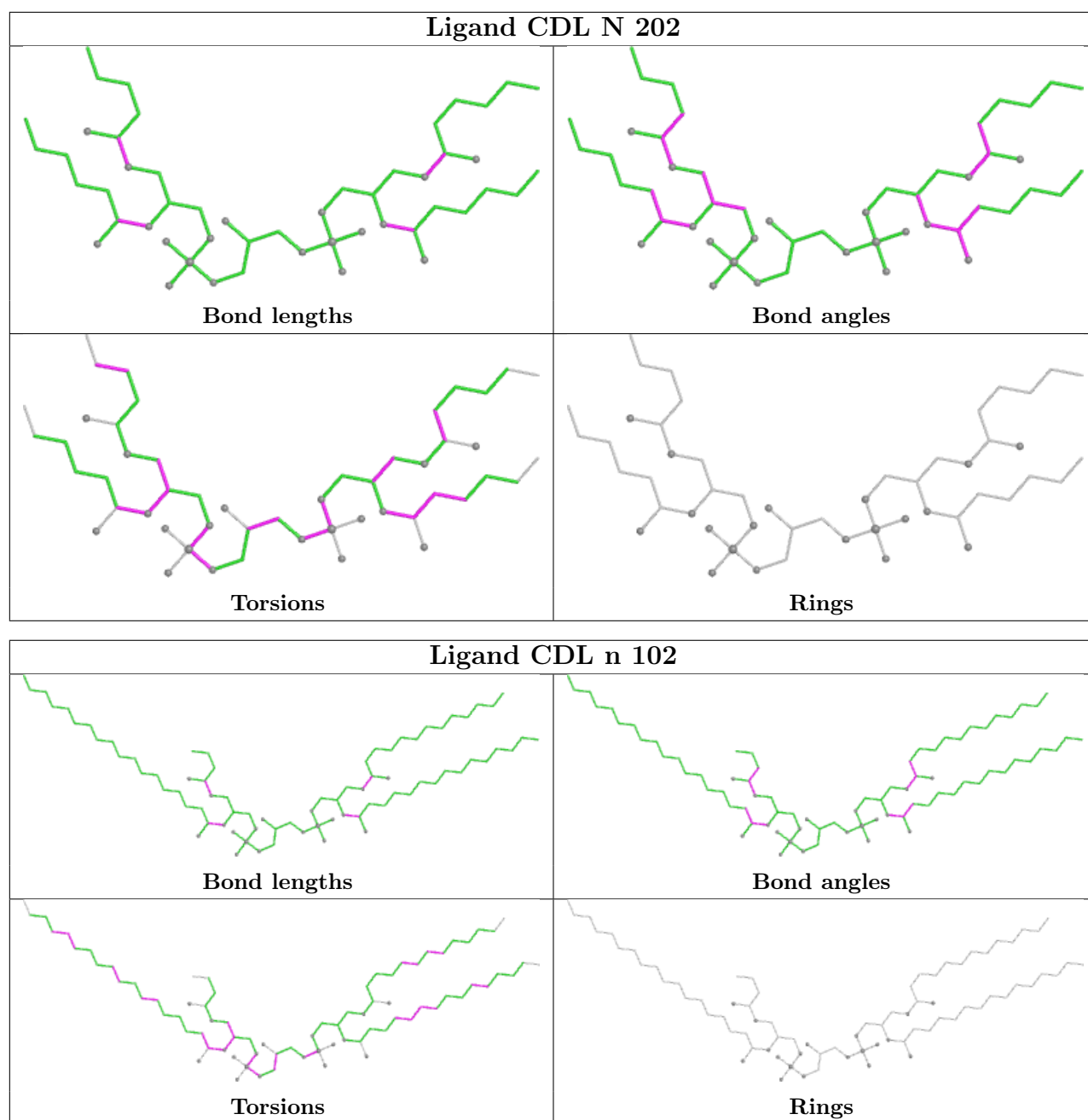
There are no ring outliers.

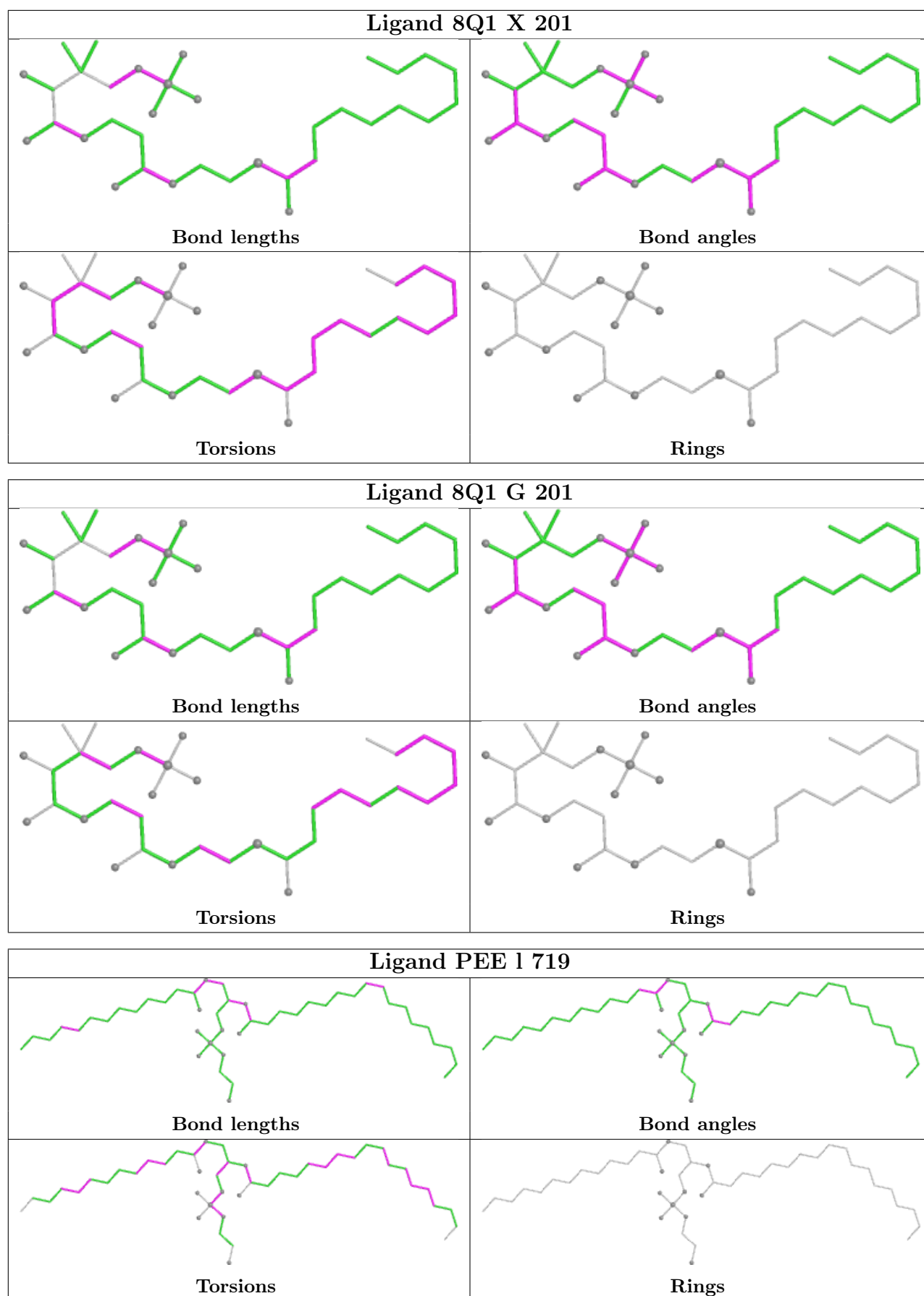
30 monomers are involved in 213 short contacts:

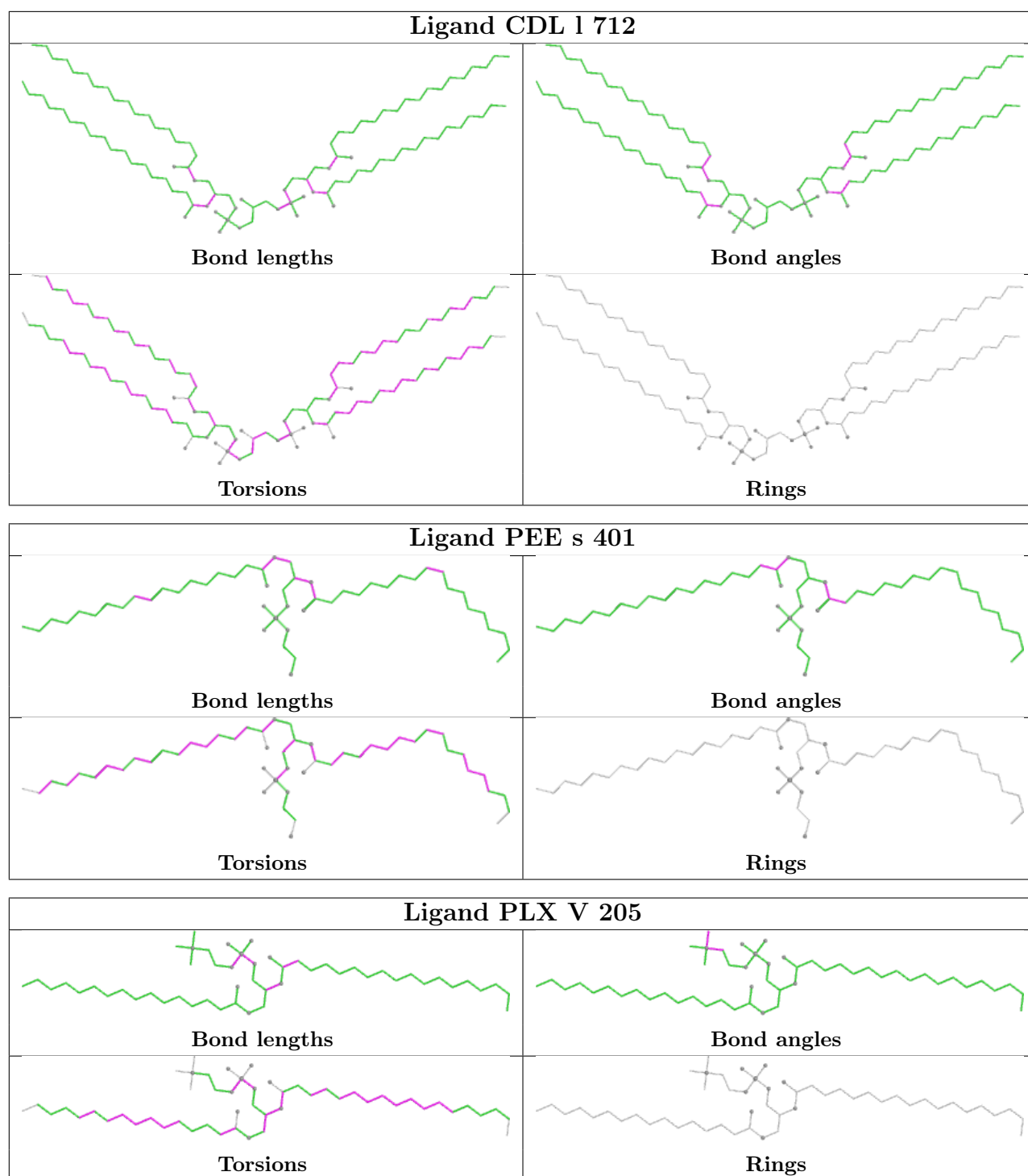
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	i	705	PLX	6	0
54	N	202	CDL	4	0
54	n	102	CDL	12	0
50	X	201	8Q1	1	0
50	G	201	8Q1	2	0
48	l	719	PEE	2	0
54	l	712	CDL	12	0
48	s	401	PEE	3	0
49	V	205	PLX	4	0
54	l	713	CDL	4	0
48	U	101	PEE	4	0
49	n	101	PLX	7	0
51	J	401	NDP	3	0
45	A	501	SF4	2	0
47	A	503	NAI	4	0
54	i	401	CDL	11	0
48	m	202	PEE	13	0
49	j	203	PLX	3	0
49	C	312	PLX	4	0
48	C	311	PEE	5	0
49	e	201	PLX	8	0
57	w	401	ADP	10	0
54	a	201	CDL	26	0
56	s	403	UQ	8	0
48	l	718	PEE	18	0
54	r	714	CDL	14	0
48	l	720	PEE	15	0
46	A	502	FMN	4	0
48	V	202	PEE	11	0
54	V	203	CDL	14	0

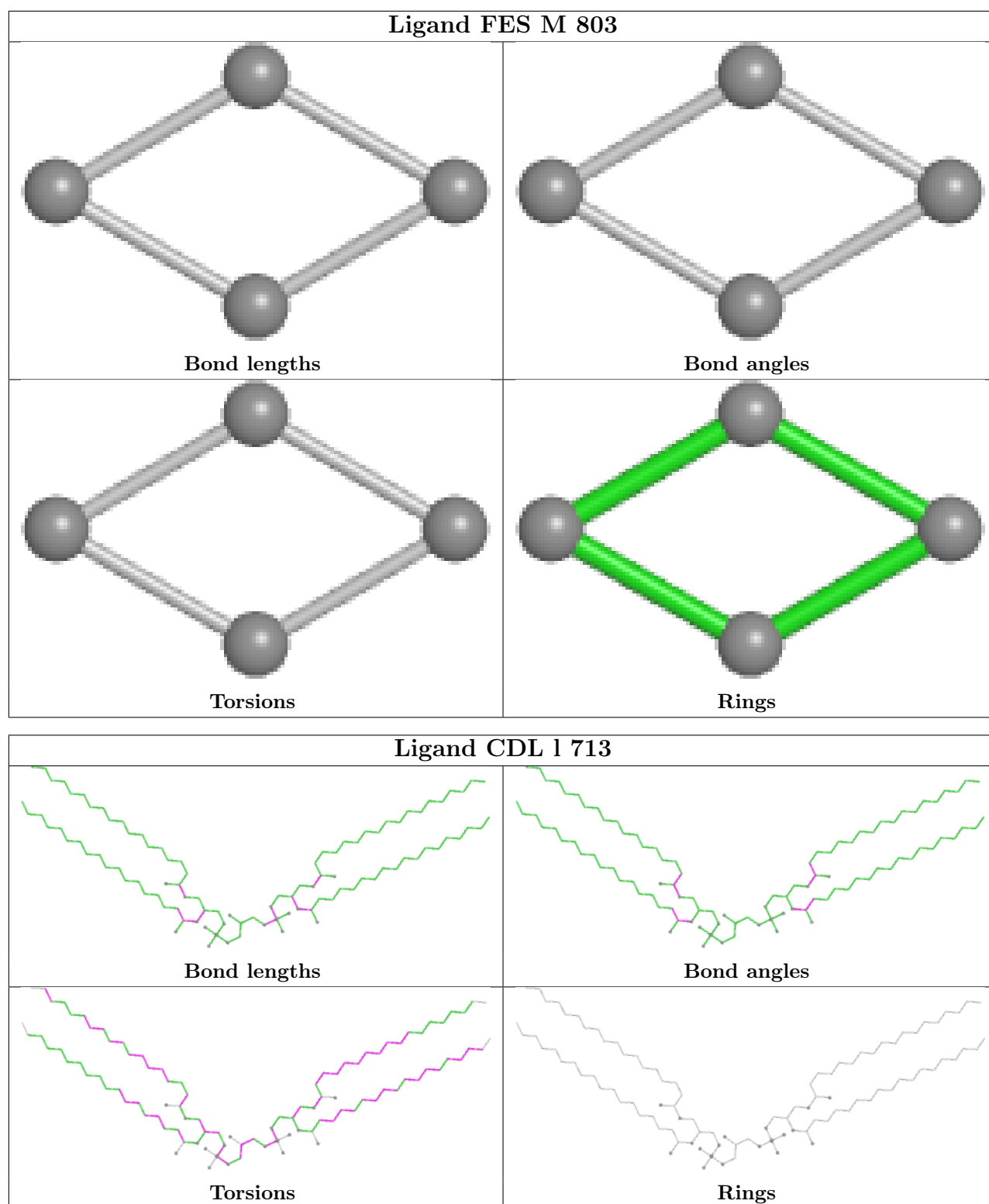
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

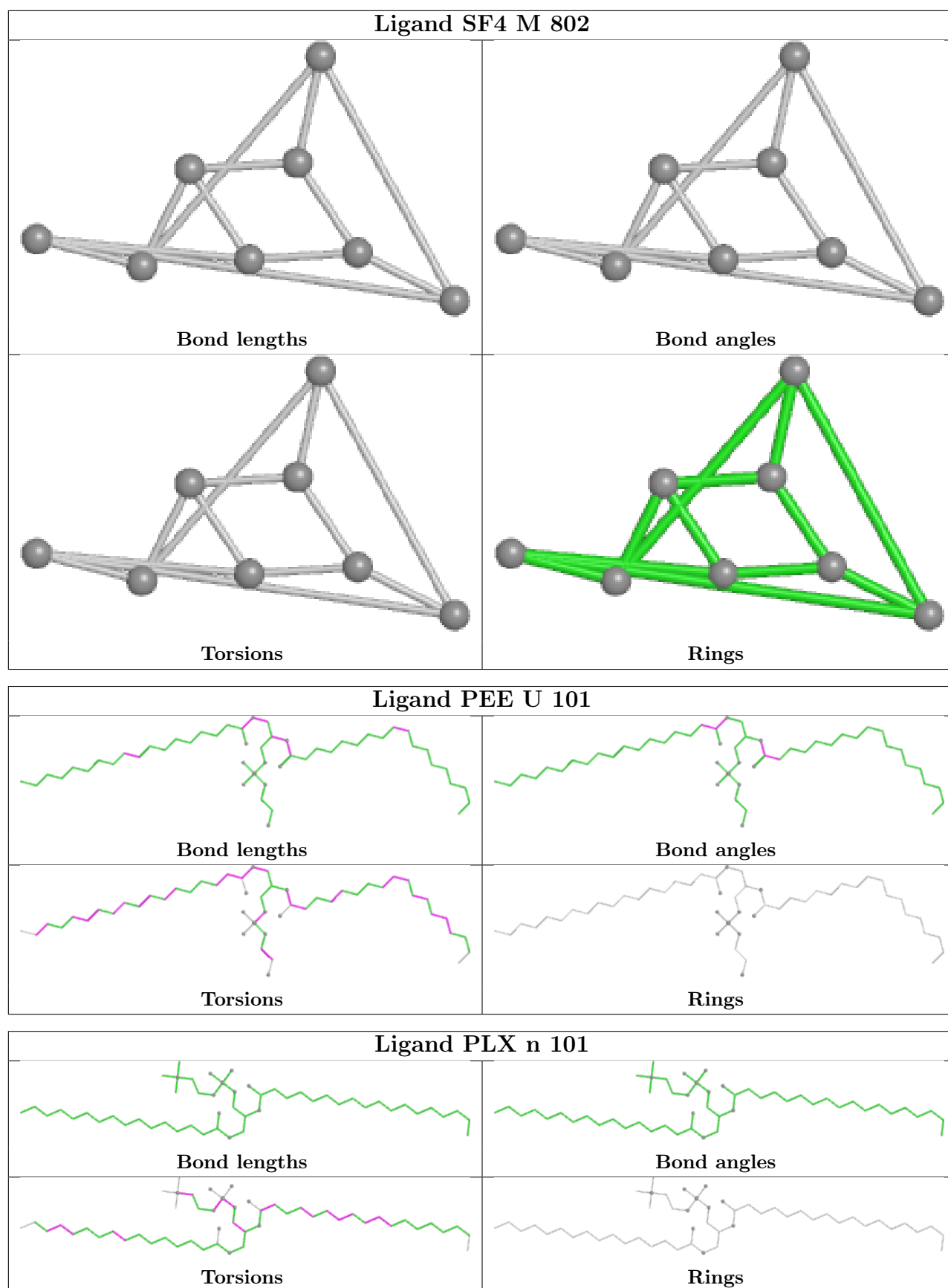


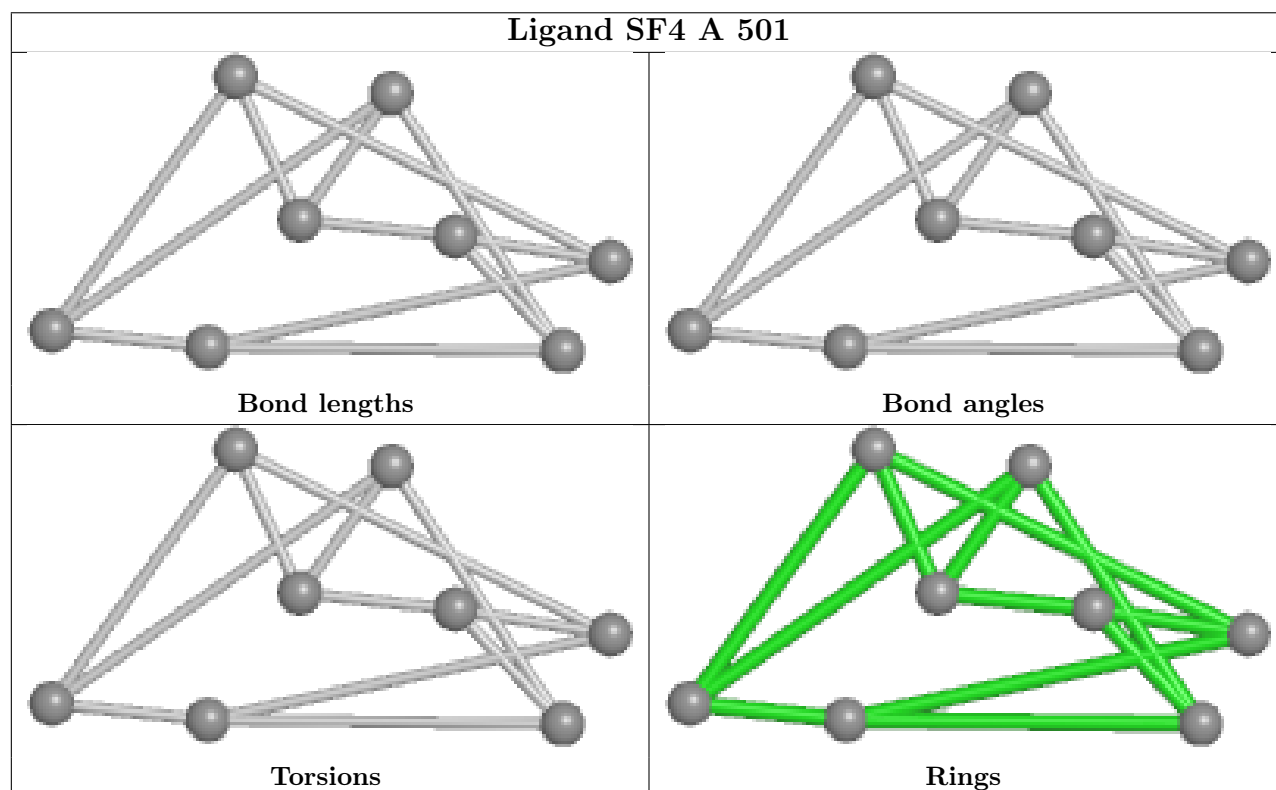
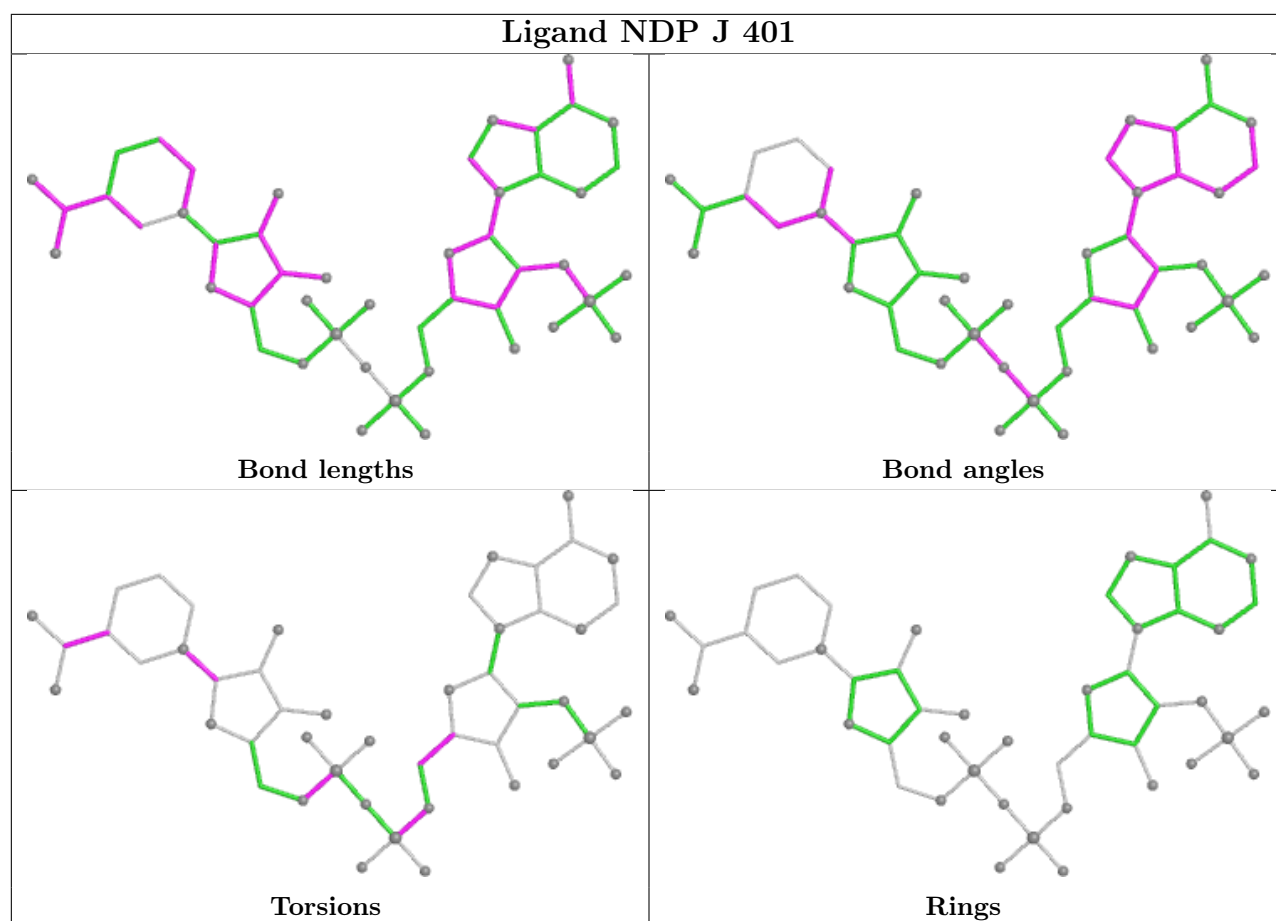


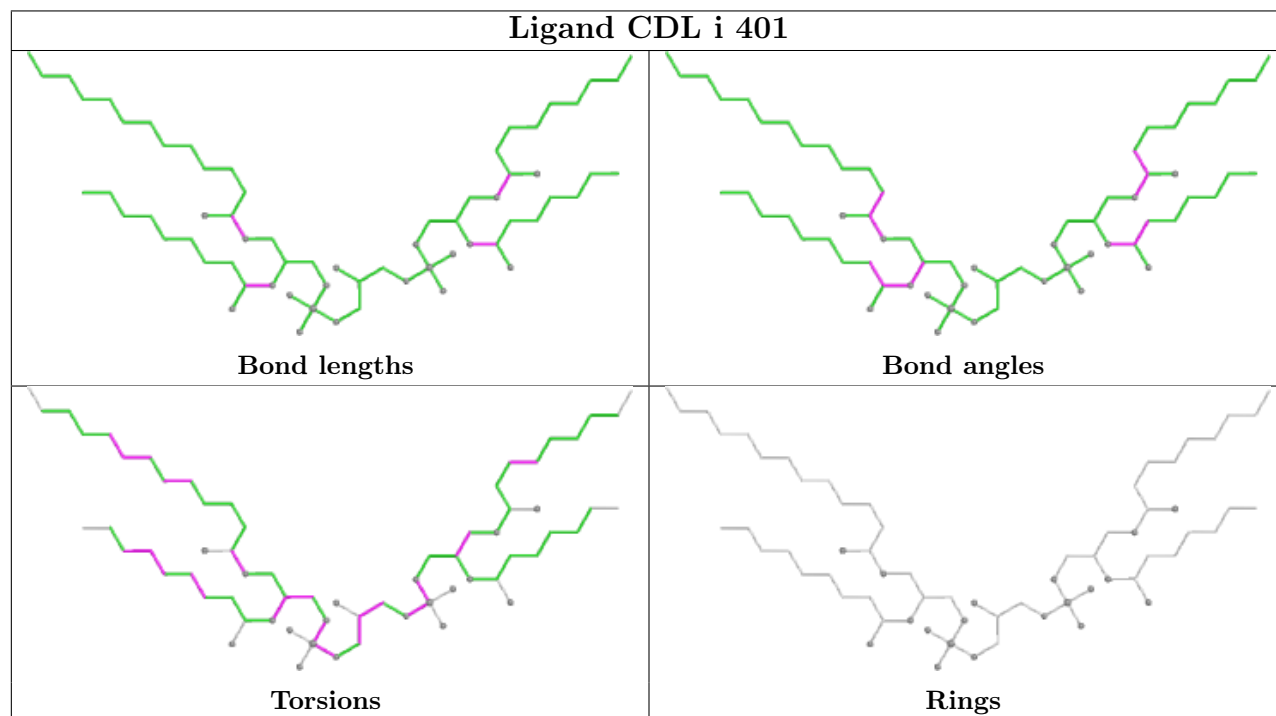
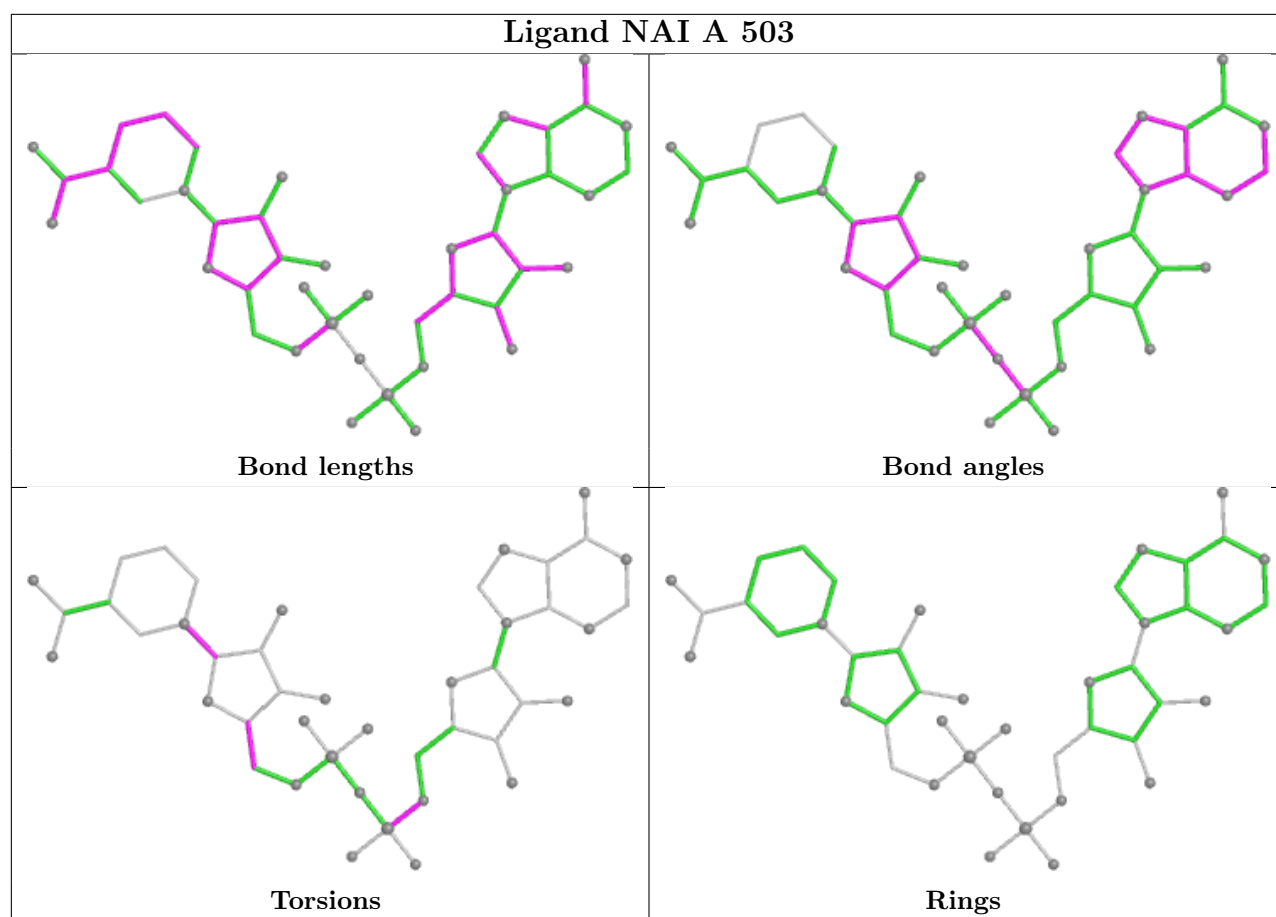


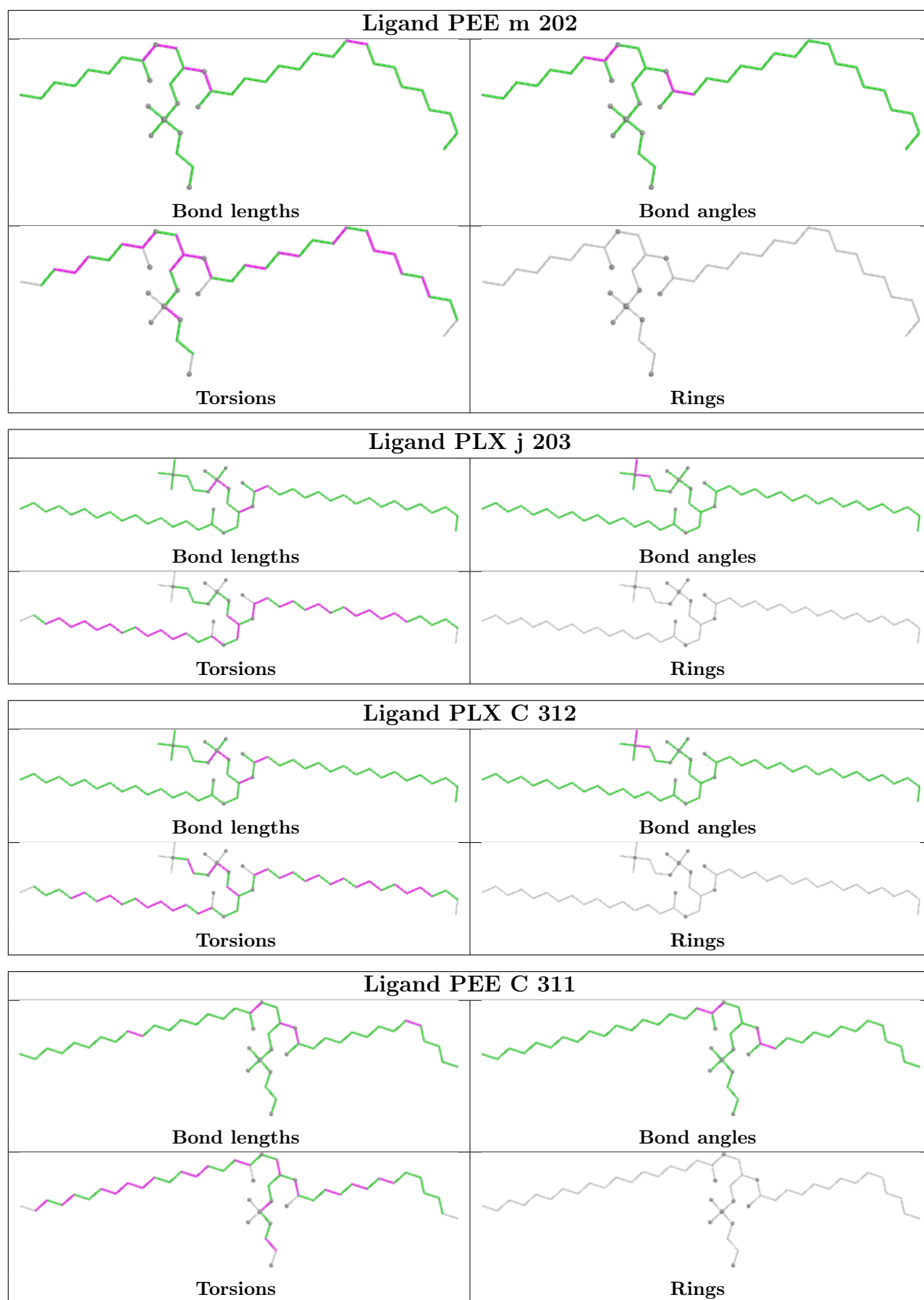


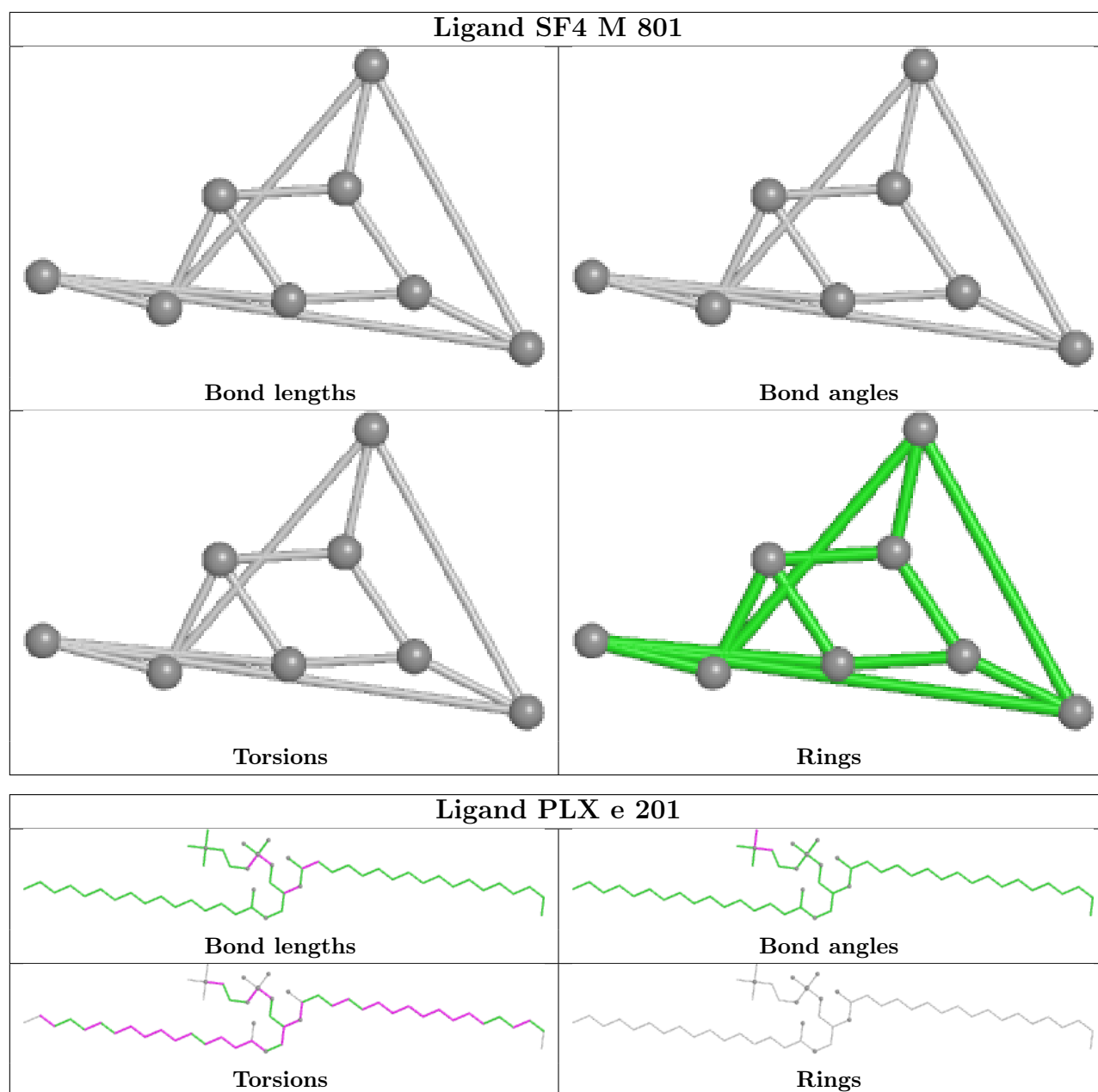


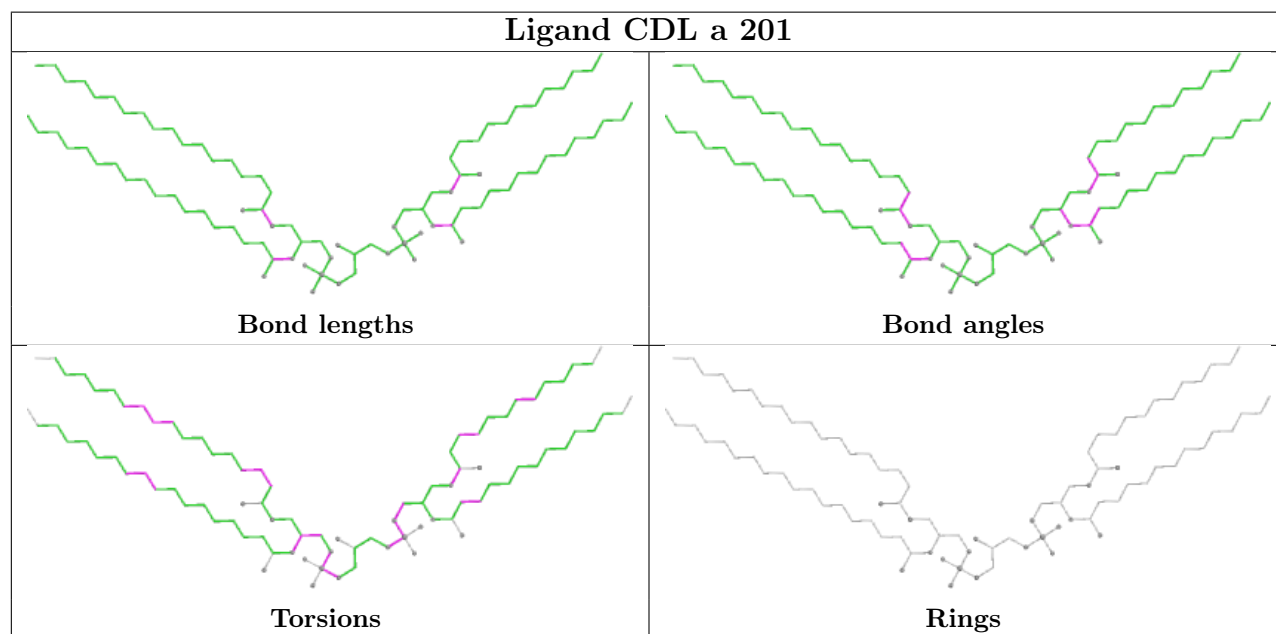
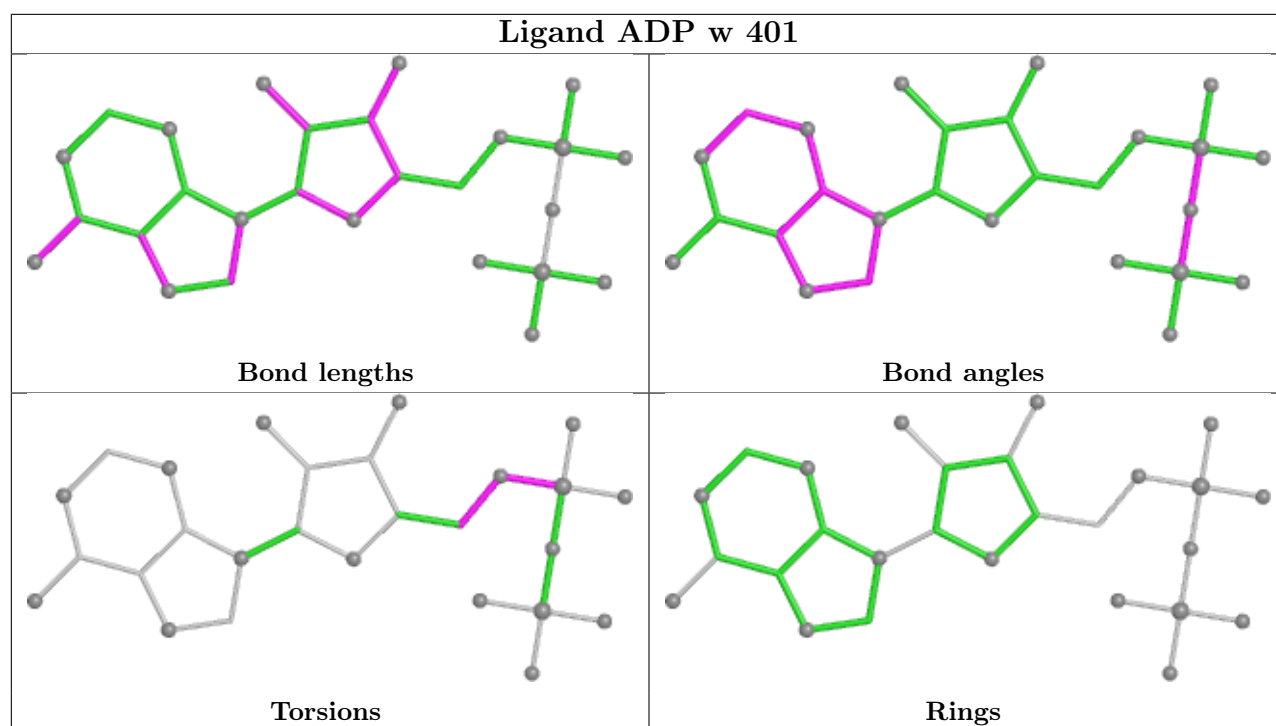


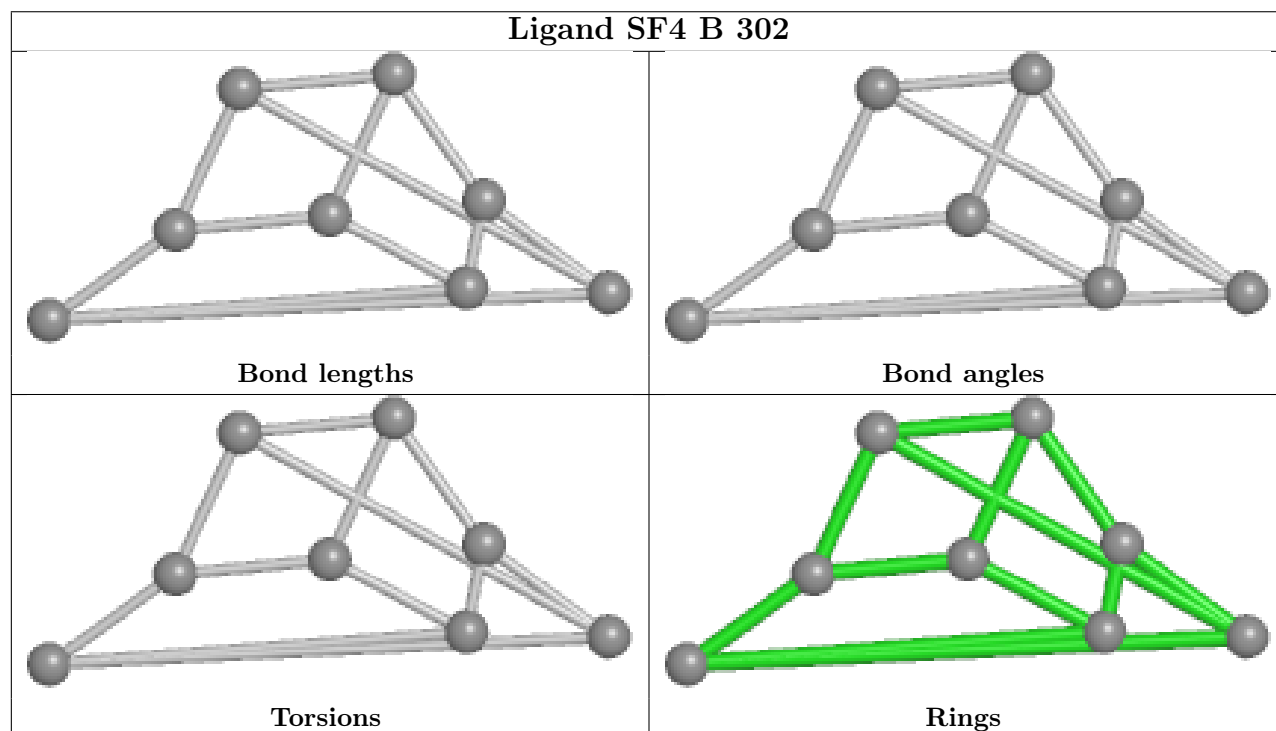
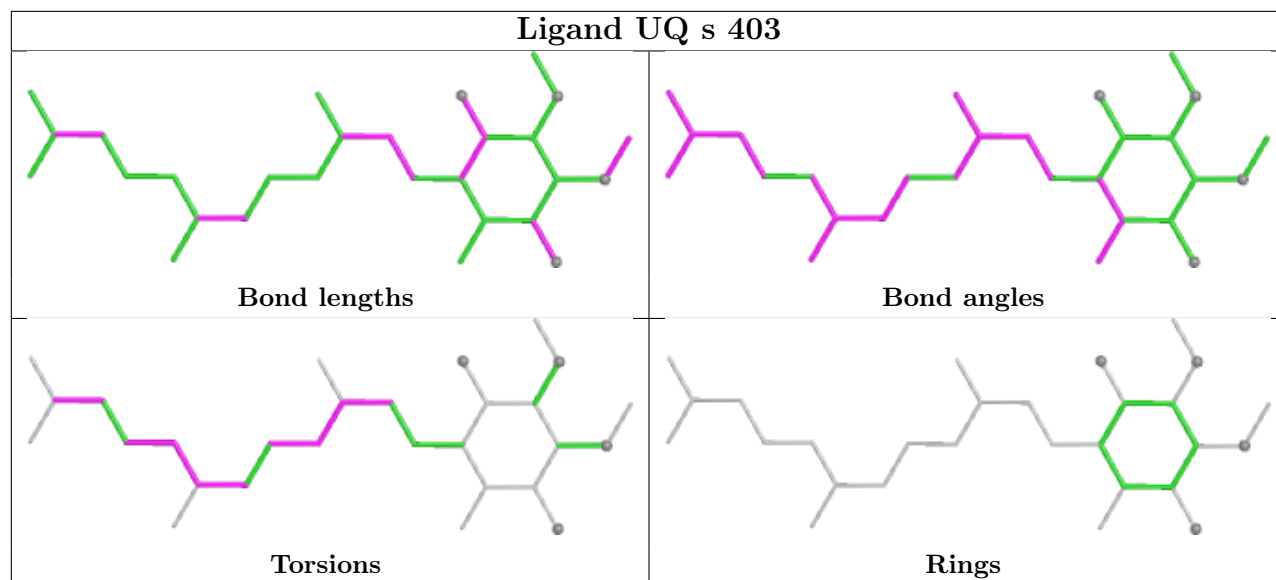


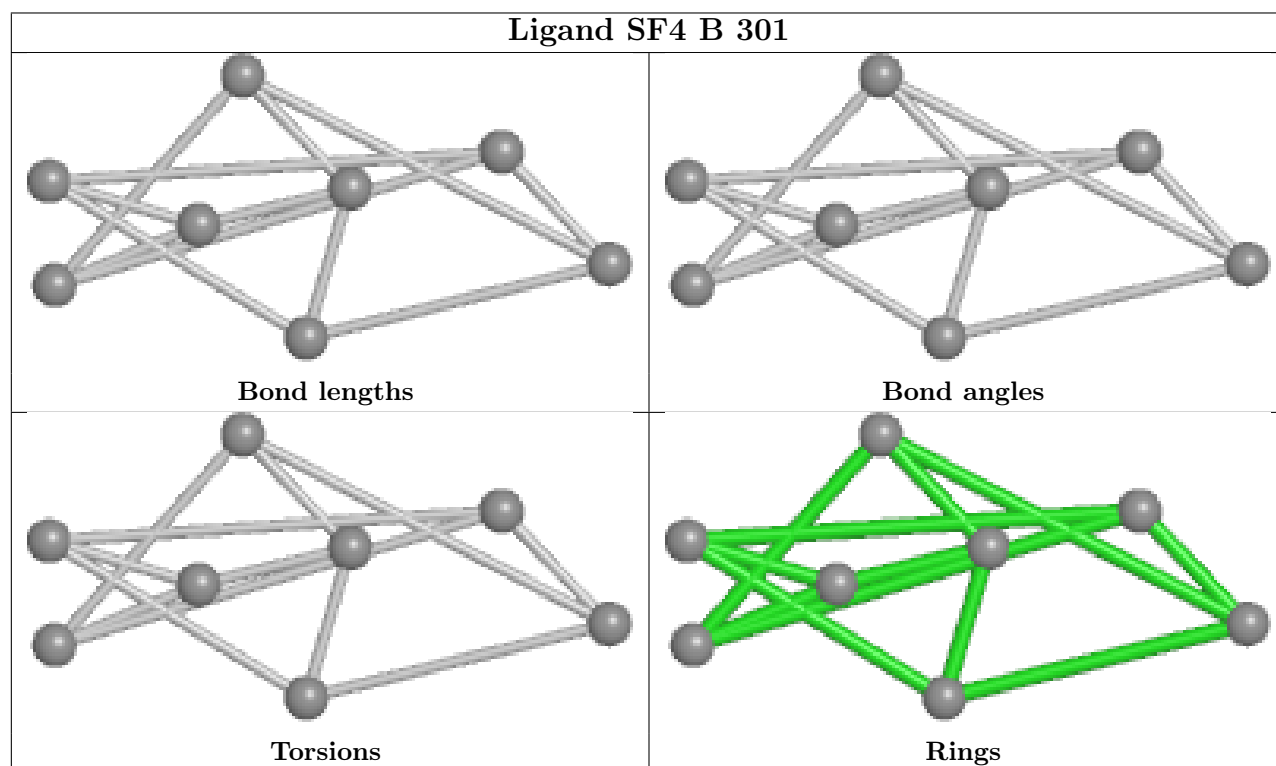
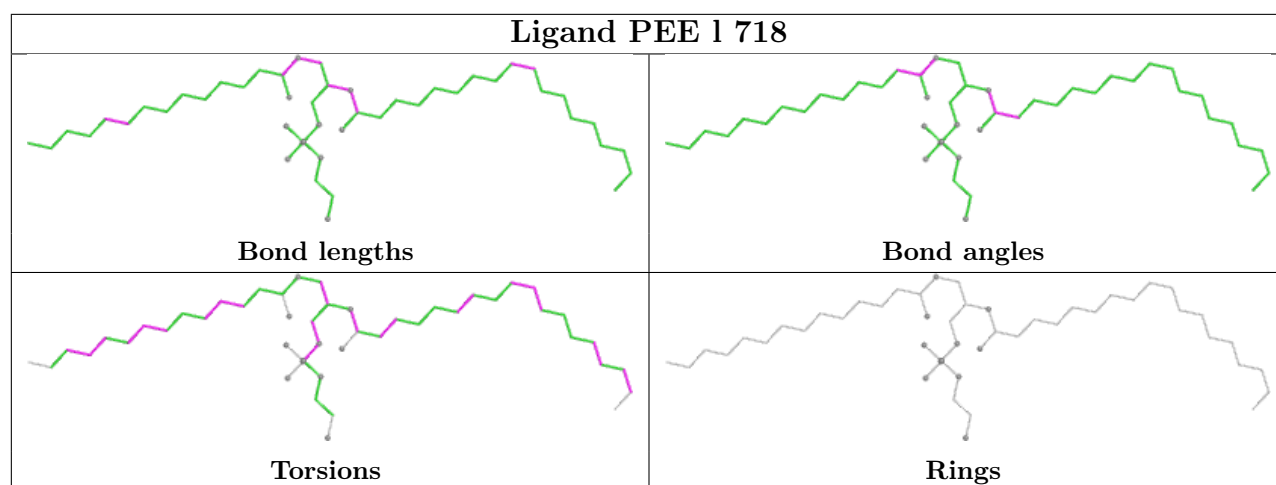


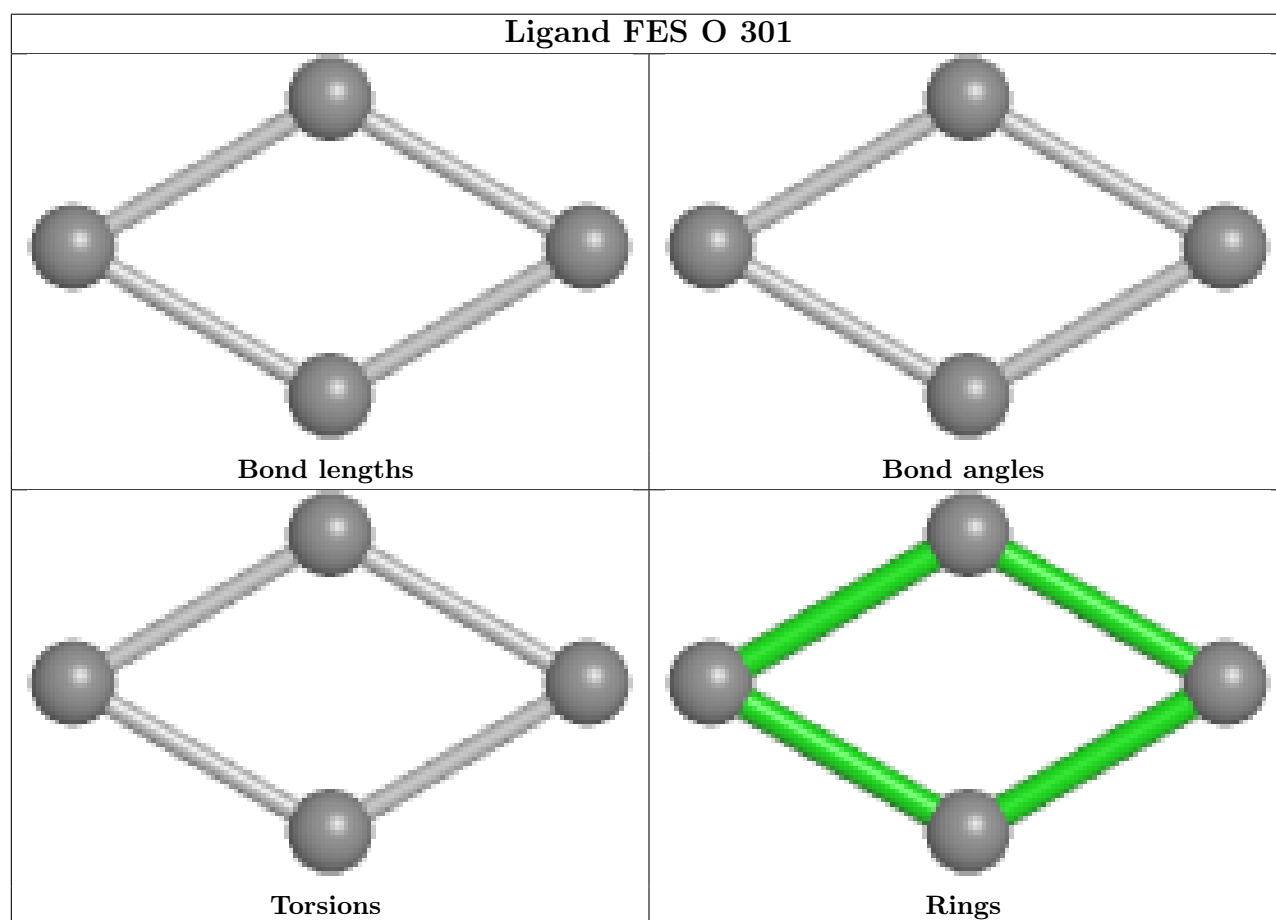
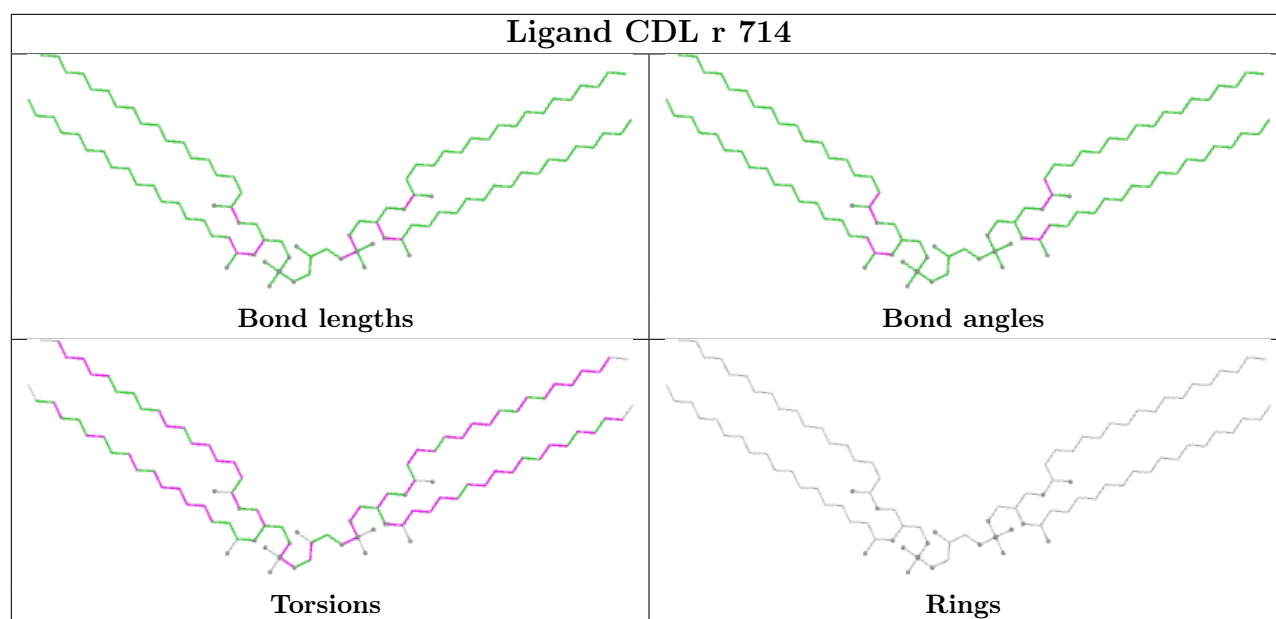


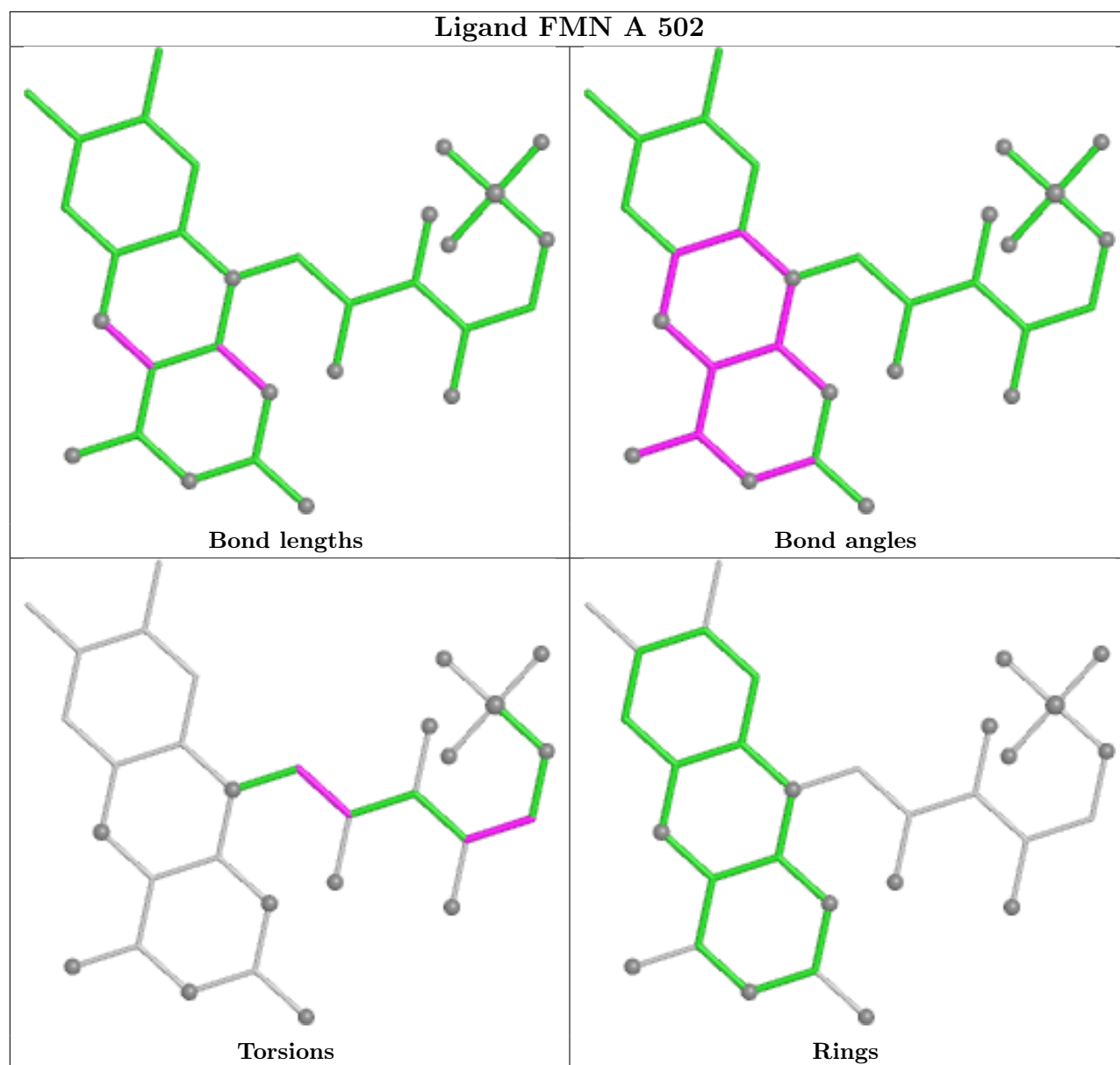
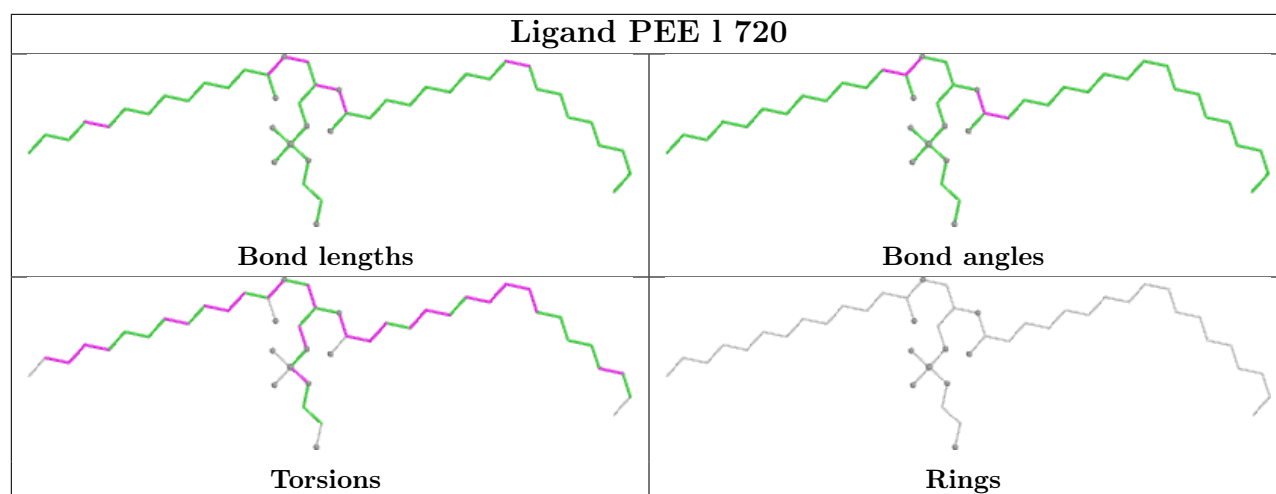


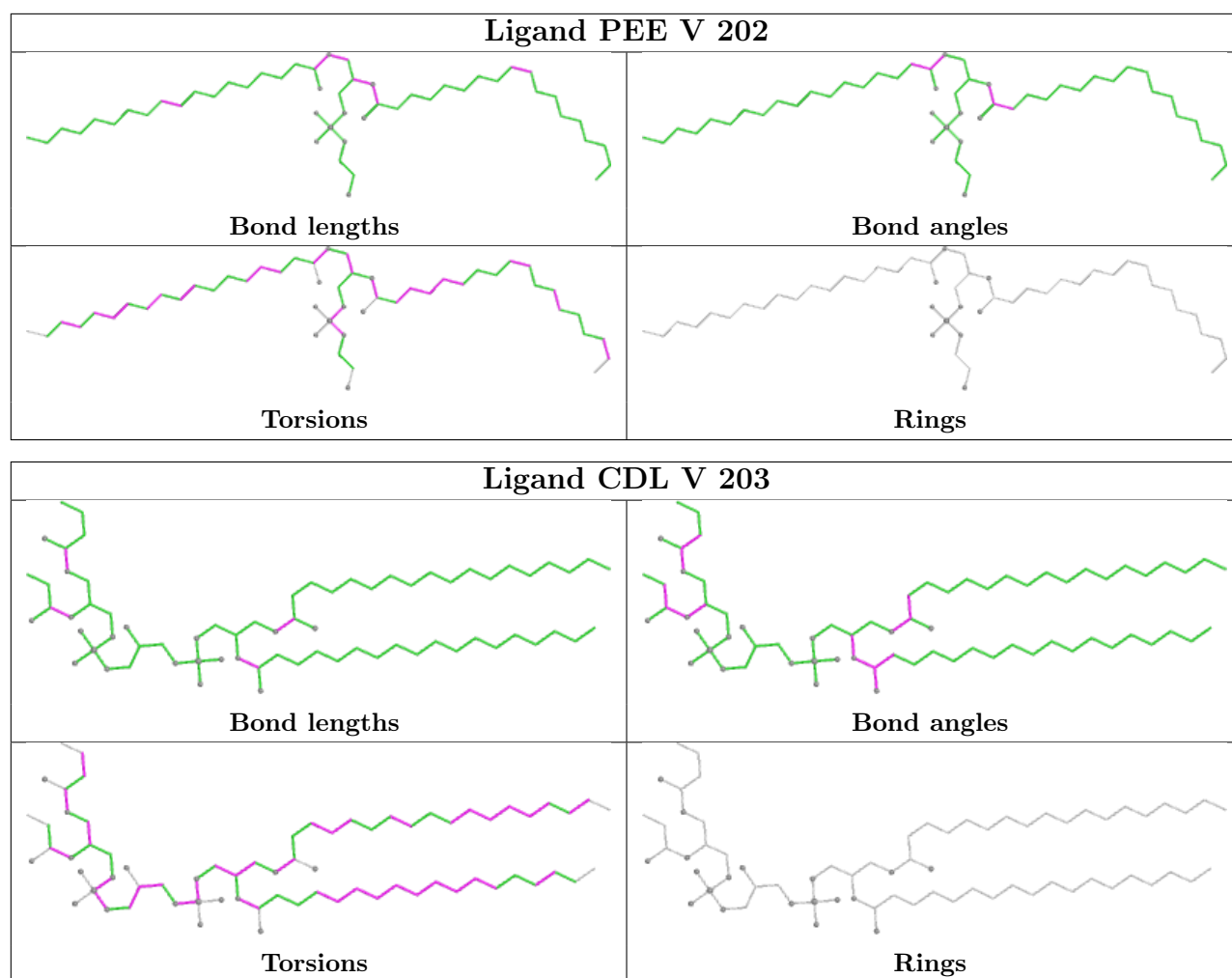












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

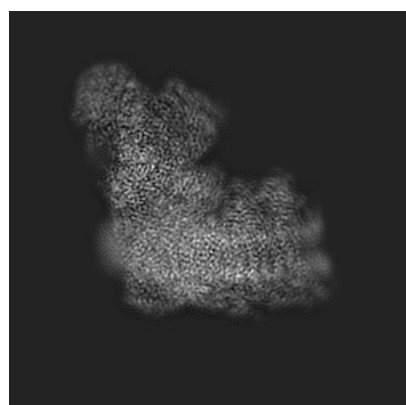
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31648. These allow visual inspection of the internal detail of the map and identification of artifacts.

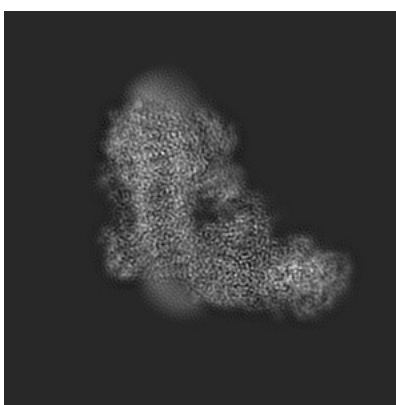
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

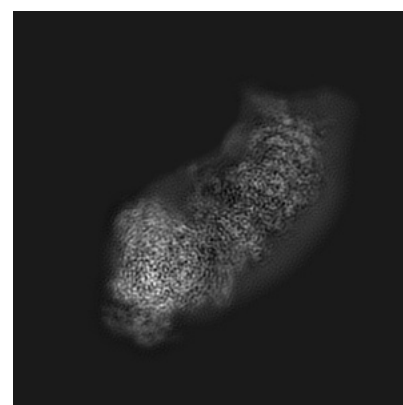
6.1.1 Primary map



X



Y

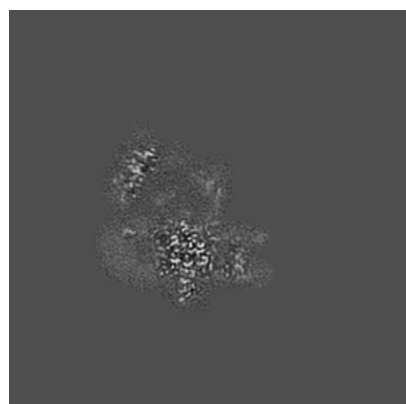


Z

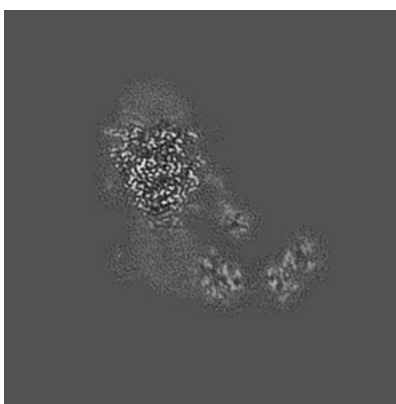
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

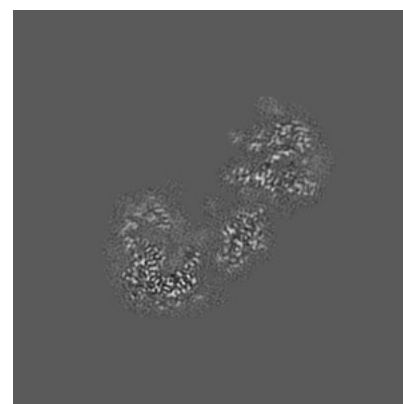
6.2.1 Primary map



X Index: 152



Y Index: 152

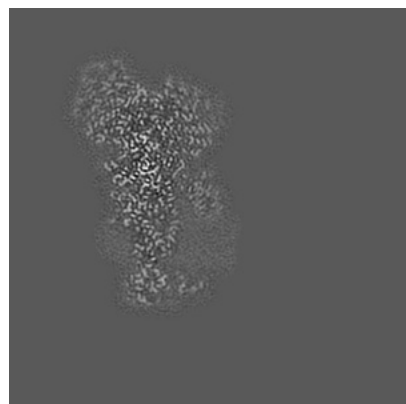


Z Index: 152

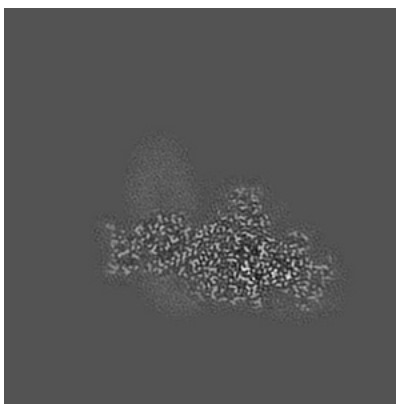
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

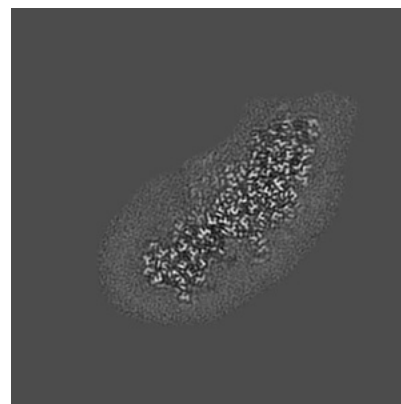
6.3.1 Primary map



X Index: 106



Y Index: 98

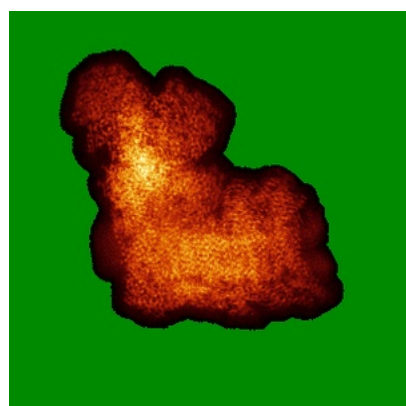


Z Index: 128

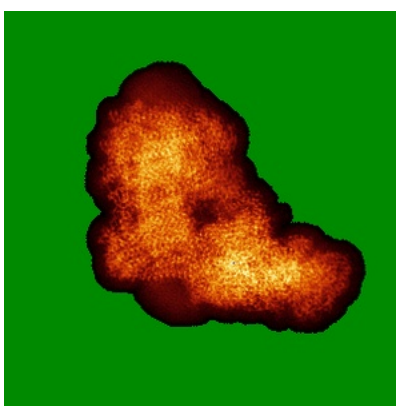
The images above show the largest variance slices of the map in three orthogonal directions.

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

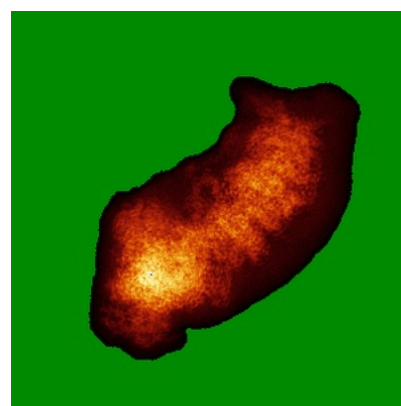
6.4.1 Primary map



X



Y

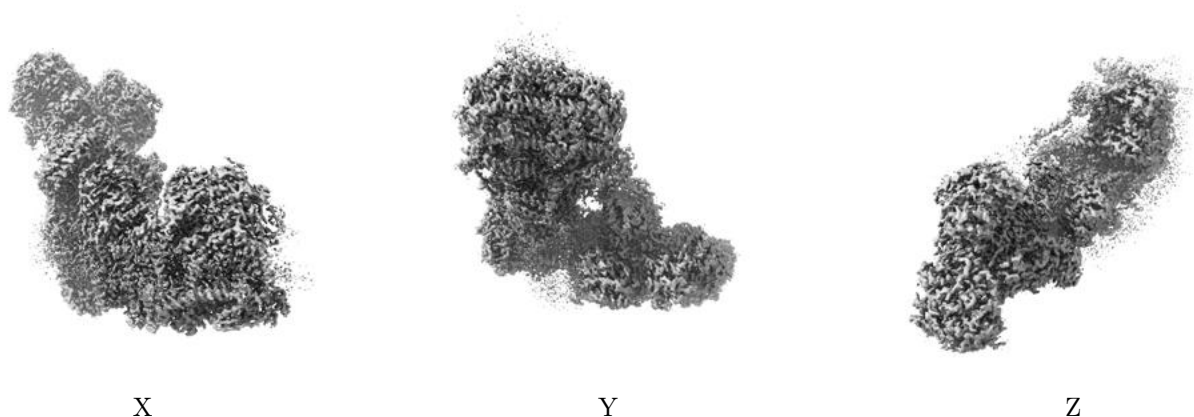


Z

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 0.0239. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

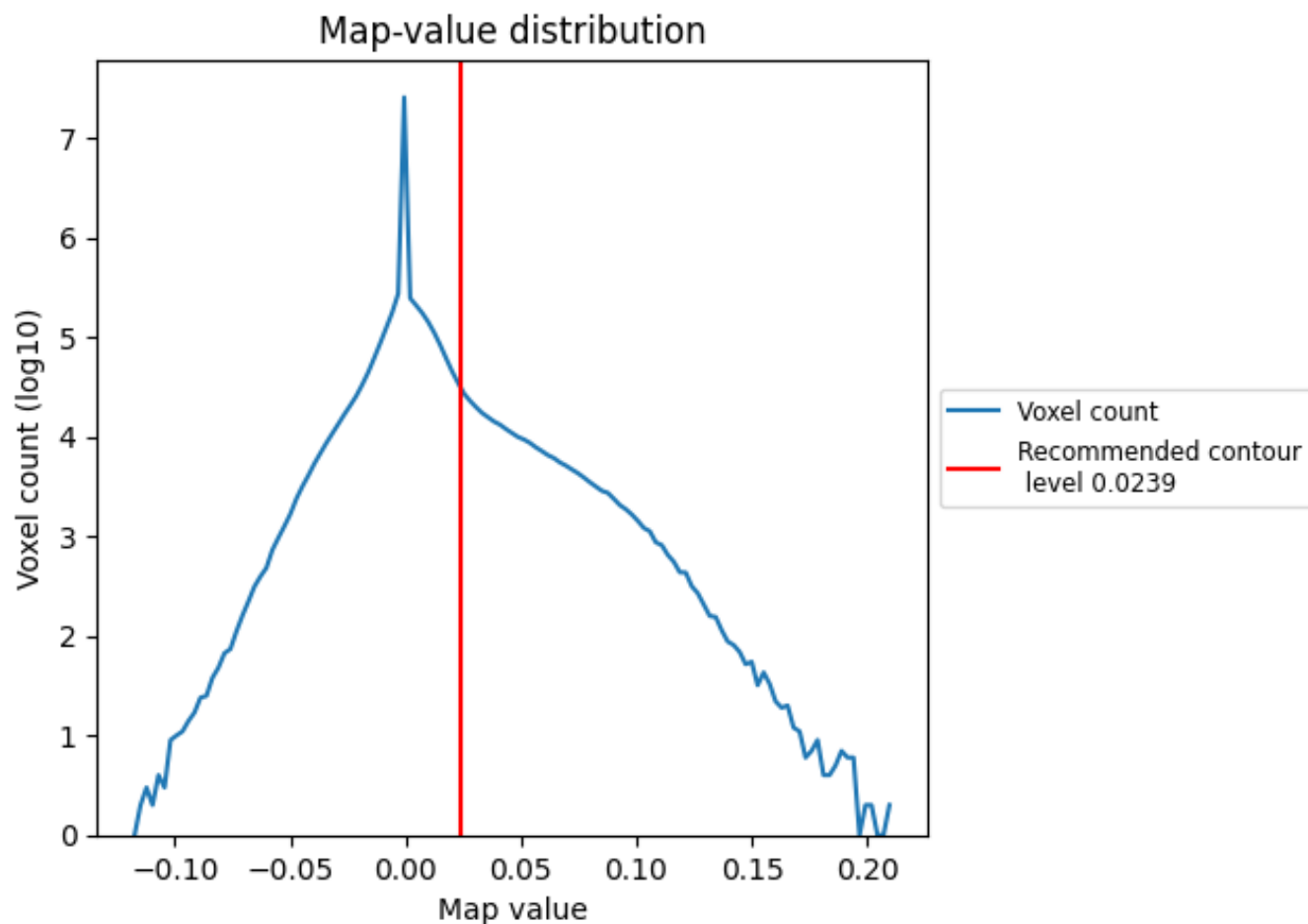
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

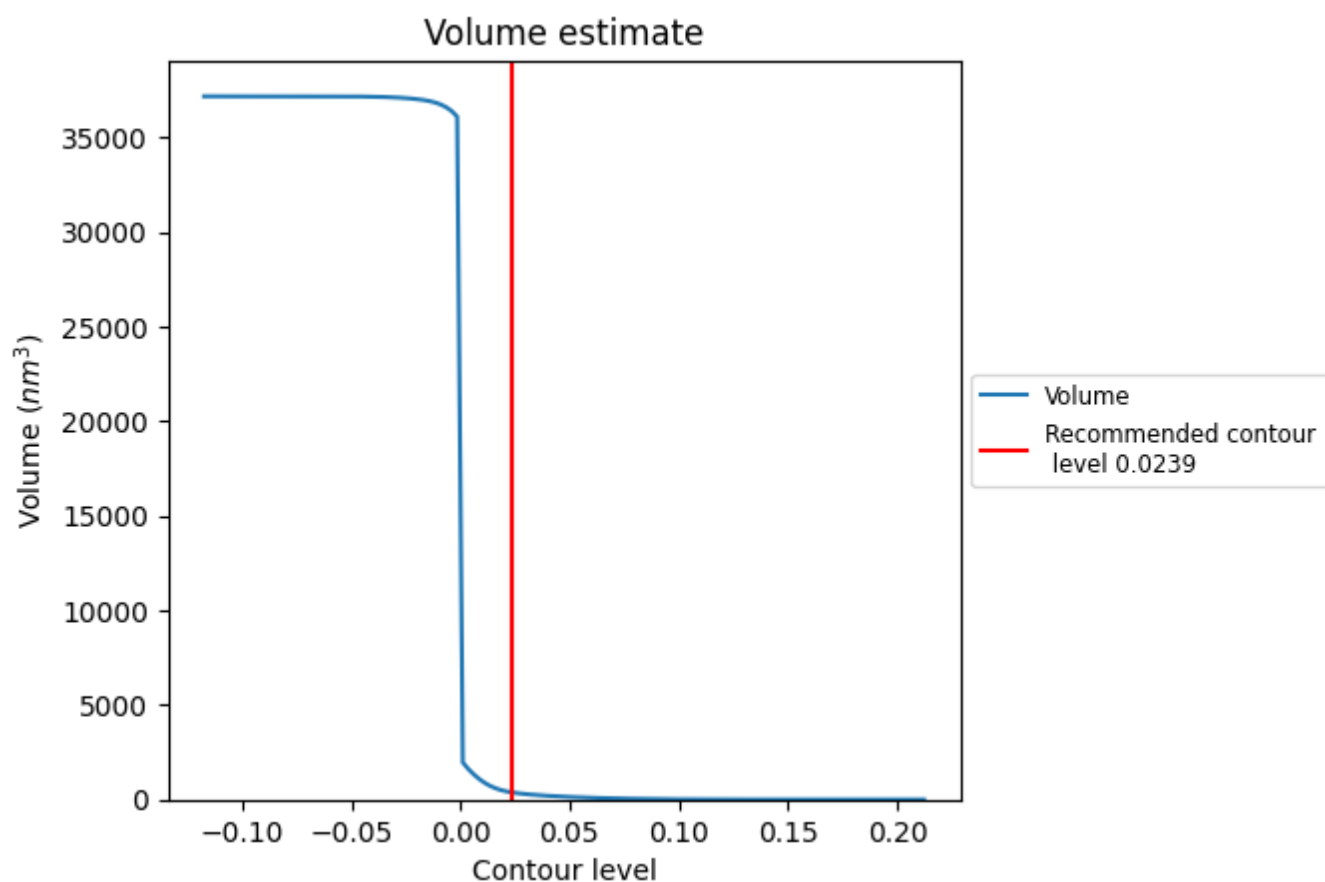
This section contains the results of statistical analysis of the map.

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.

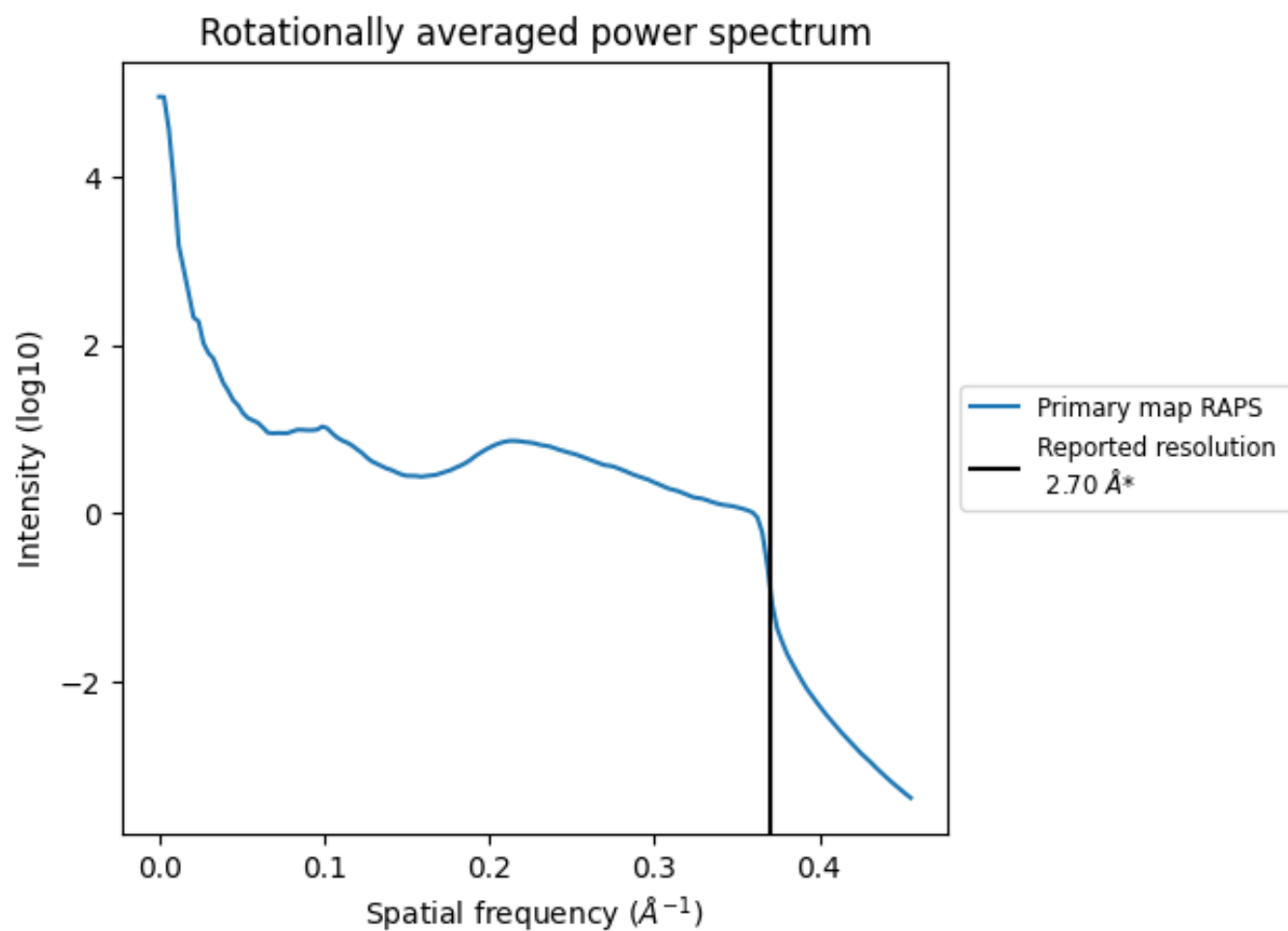
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 373 nm^3 ; this corresponds to an approximate mass of 337 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

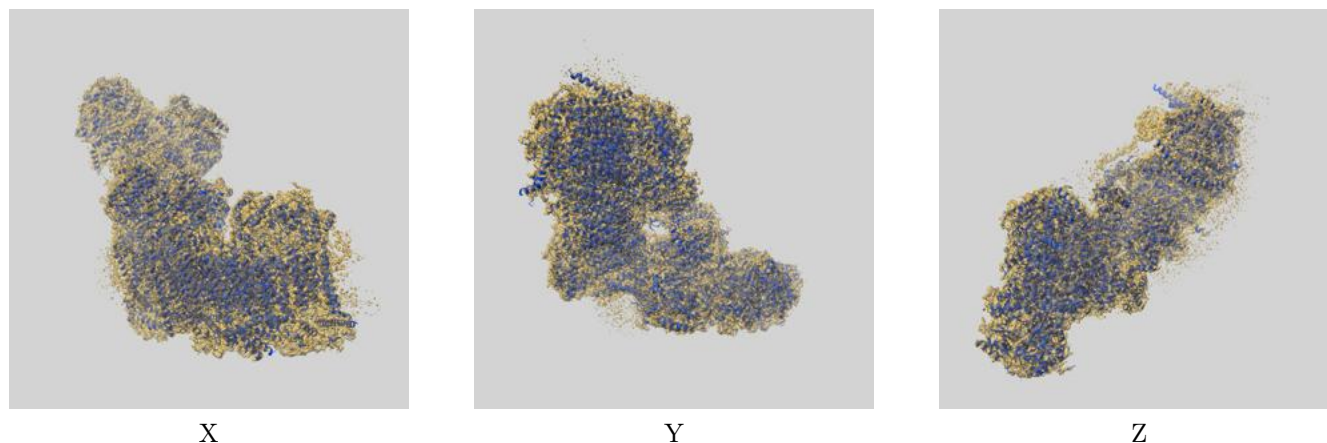
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

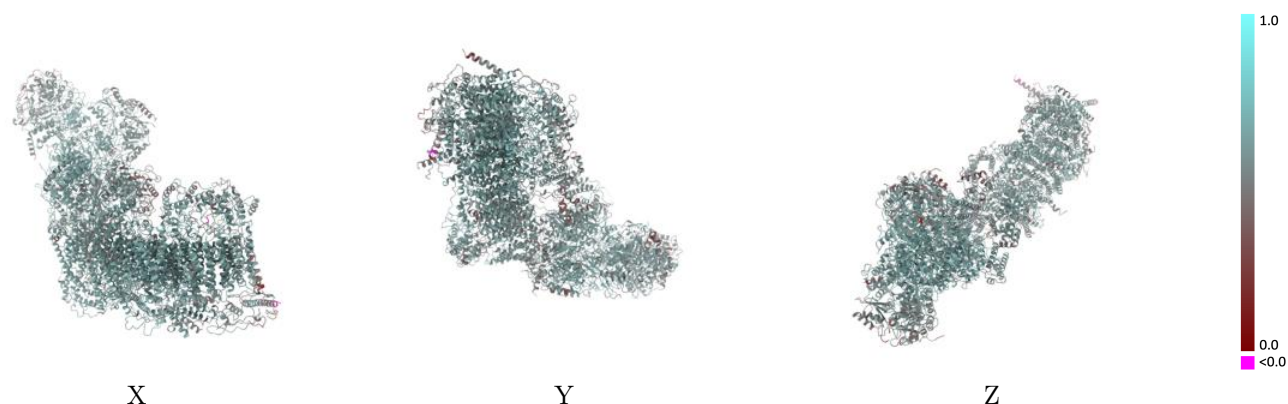
This section contains information regarding the fit between EMDB map EMD-31648 and PDB model 7V30. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



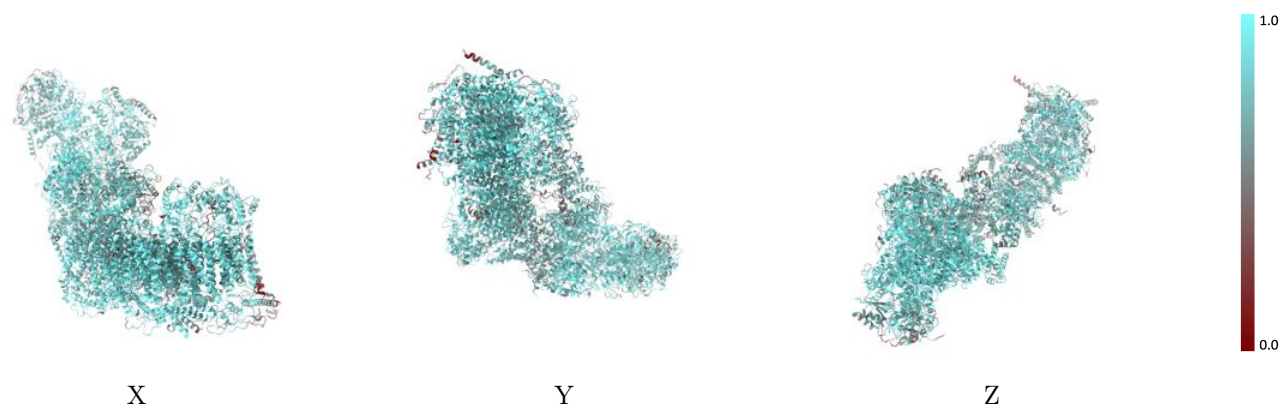
The images above show the 3D surface view of the map at the recommended contour level 0.0239 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



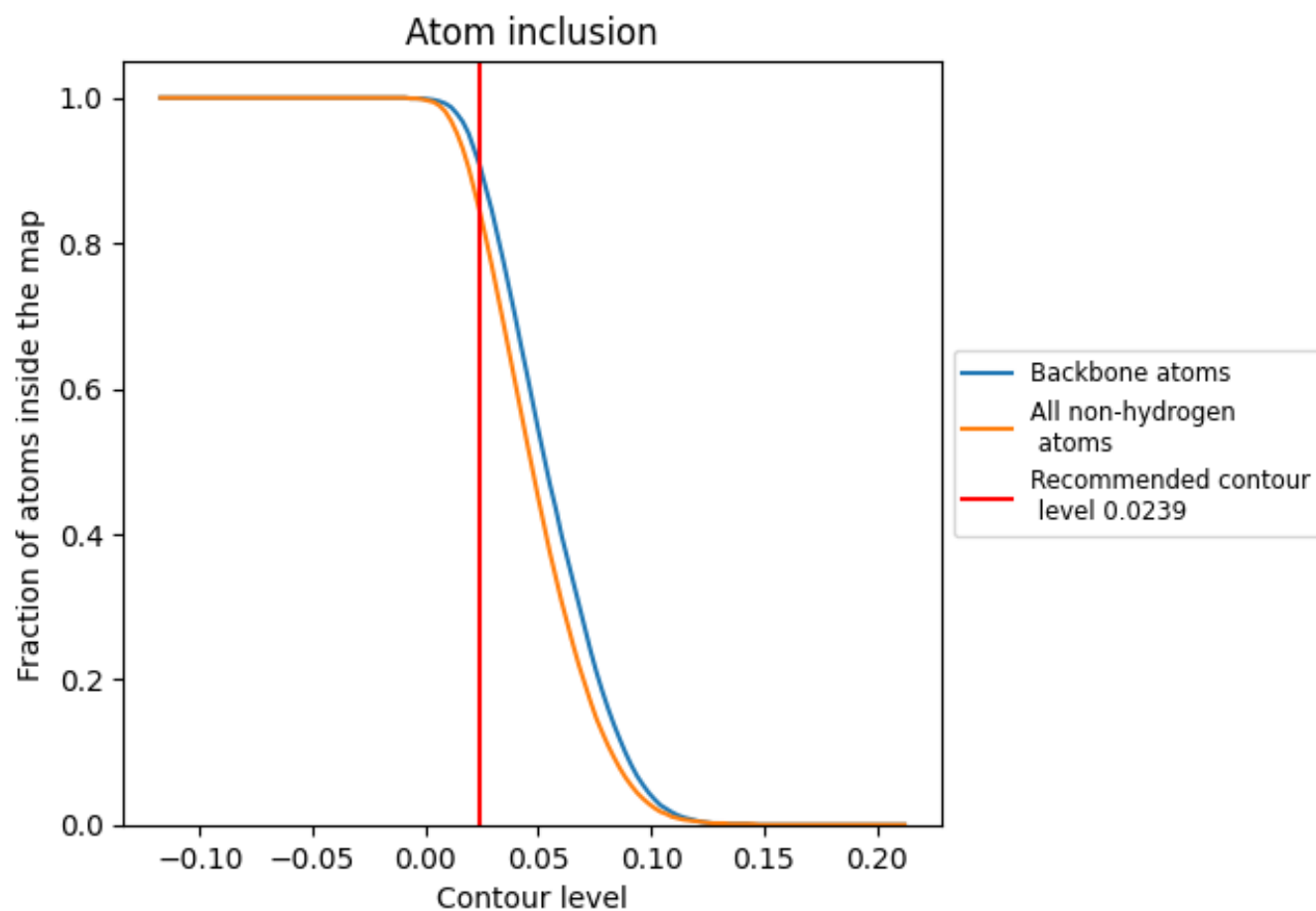
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0239).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 85% 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 (0.0239) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8460	 0.5900
A	 0.7820	 0.5530
B	 0.9630	 0.6490
C	 0.9040	 0.6250
E	 0.8270	 0.5820
F	 0.6840	 0.4920
G	 0.5430	 0.4230
H	 0.8470	 0.5700
I	 0.8470	 0.6050
J	 0.7910	 0.5600
K	 0.6830	 0.5150
L	 0.8890	 0.6180
M	 0.8810	 0.6020
N	 0.8800	 0.6180
O	 0.7300	 0.5270
P	 0.9450	 0.6450
Q	 0.9390	 0.6410
S	 0.9350	 0.6190
T	 0.8700	 0.6080
U	 0.8600	 0.5900
V	 0.6560	 0.5400
W	 0.8900	 0.6020
X	 0.7630	 0.5410
Y	 0.7130	 0.5230
Z	 0.6170	 0.4920
a	 0.8600	 0.6070
b	 0.7460	 0.5380
c	 0.8300	 0.5810
d	 0.8060	 0.5690
e	 0.7830	 0.5630
f	 0.7340	 0.5300
g	 0.9080	 0.6160
h	 0.8700	 0.6010
i	 0.9360	 0.6340
j	 0.7800	 0.5660



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Chain	Atom inclusion	Q-score
k	 0.8500	 0.5950
l	 0.8740	 0.6130
m	 0.8270	 0.5820
n	 0.7210	 0.5620
o	 0.8310	 0.5870
p	 0.8270	 0.5710
r	 0.9410	 0.6370
s	 0.9110	 0.6190
u	 0.8790	 0.6000
v	 0.6930	 0.4900
w	 0.8110	 0.5660