



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 11:05 PM JST

PDB ID : 7V2D / pdb_00007v2d
EMDB ID : EMD-31641
Title : Deactive state complex I from Q10 dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-08-08
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

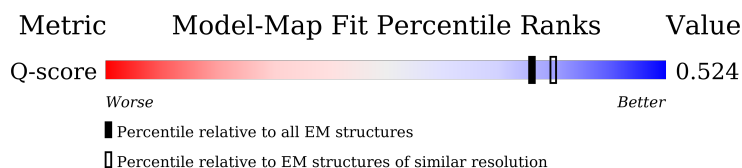
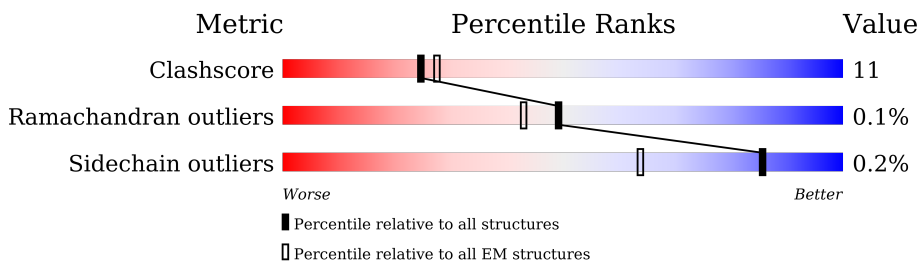
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



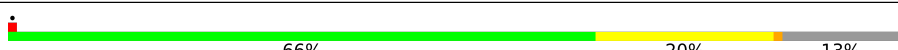
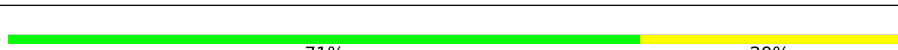
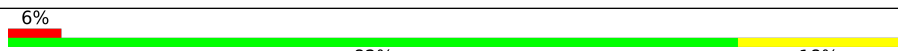
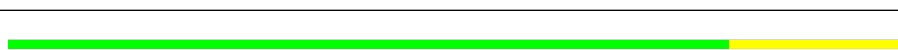
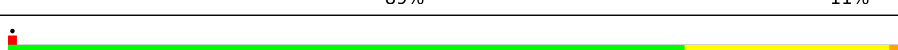
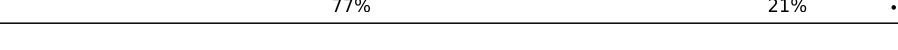
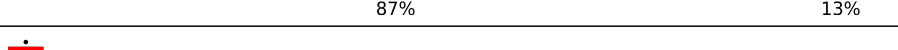
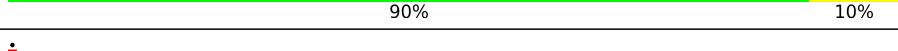
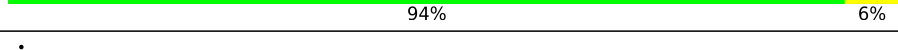
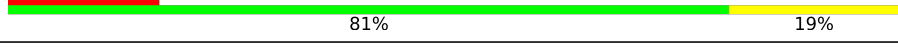
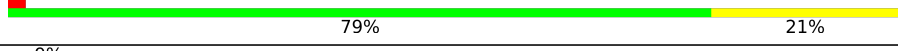
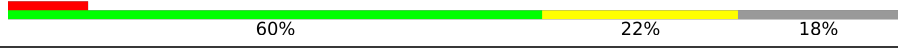
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	A	431	
2	B	176	
3	C	156	
4	E	115	

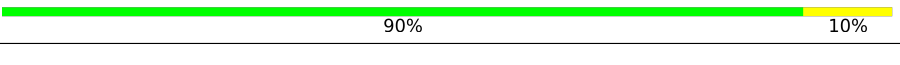
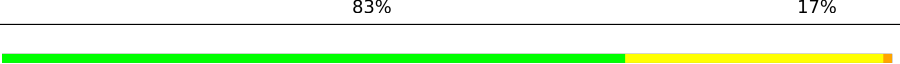
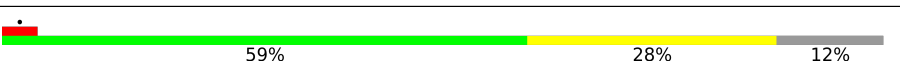
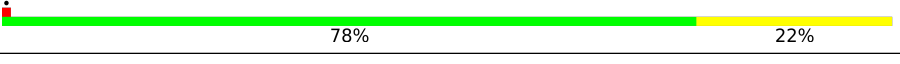
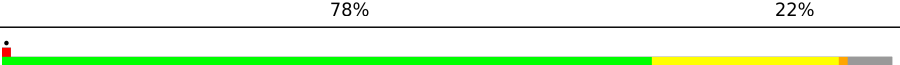
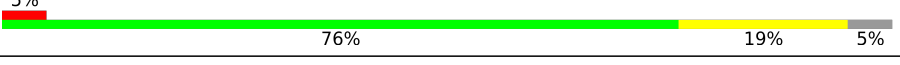
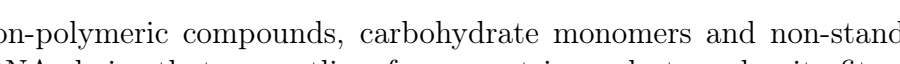
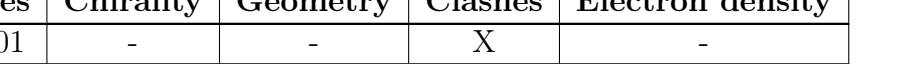
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Mol	Chain	Length	Quality of chain
5	F	86	
6	G	88	
6	X	88	
7	H	112	
8	I	112	
9	J	341	
10	K	42	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	70	
23	Z	84	
24	a	140	
25	b	126	
26	c	156	
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	-
53	CDL	a	201	-	-	X	-

2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 66899 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
			678	438	102	133	5		
6	X	88	Total	C	N	O	S	0	0
			699	450	103	141	5		

- Molecule 7 is a protein called 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
			2356	1513	421	414	8		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	70	Total	C	N	O	S	0	0
			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
			344	227	58	59		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	99	Total	C	N	O	S	0	0
			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
			4785	3173	741	820	51		

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

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

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

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

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

4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	o	128	Total	C	N	O	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		

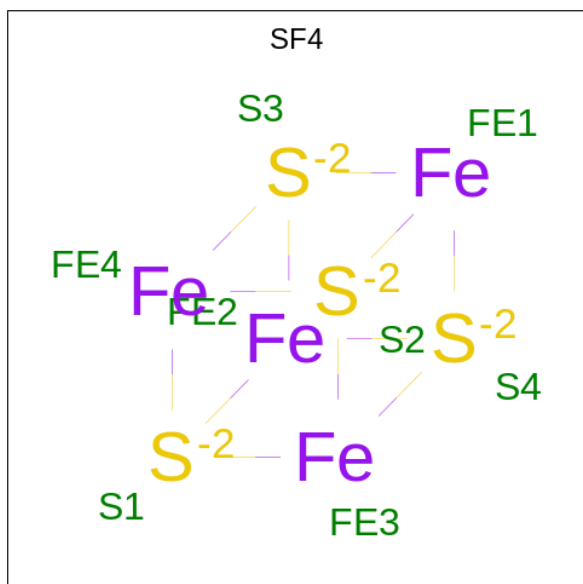
There is a discrepancy between the modelled and reference sequences:

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.

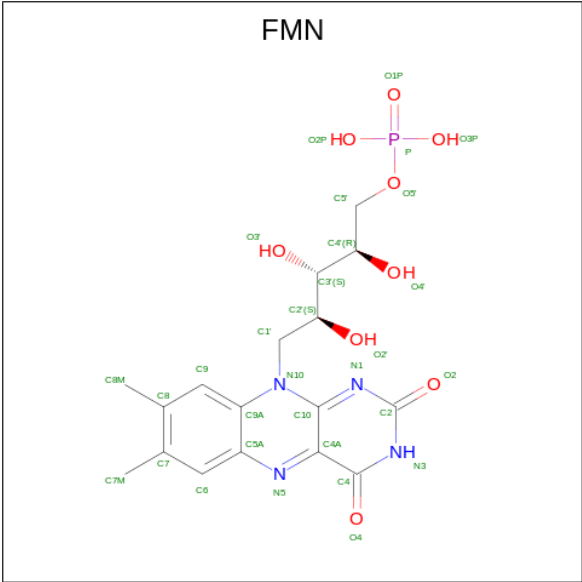
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2587	1648	440	489	10		

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



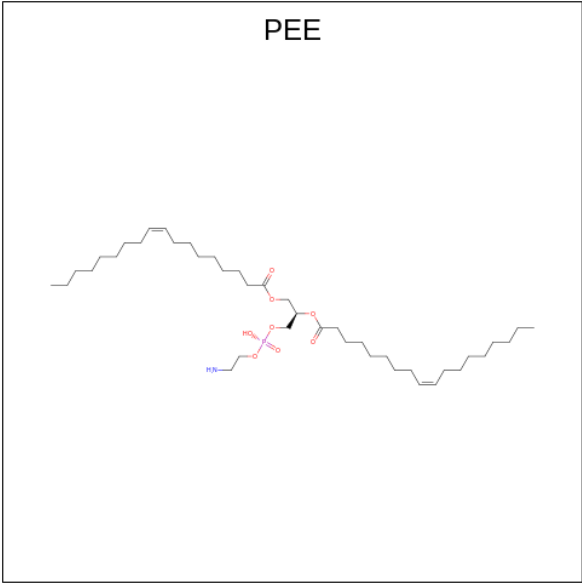
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

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



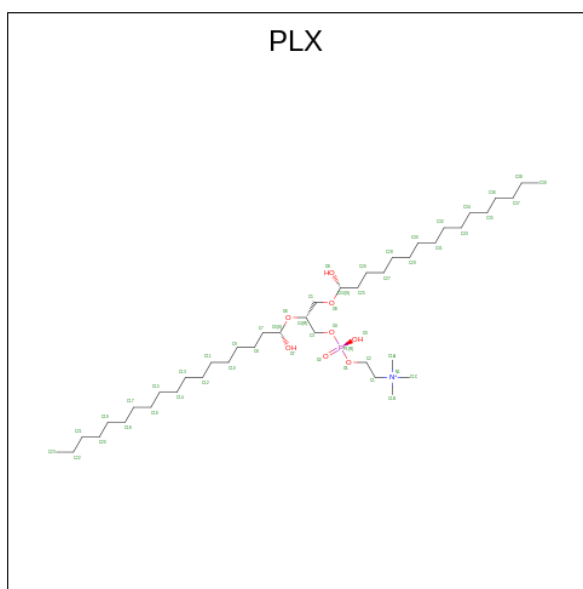
Mol	Chain	Residues	Atoms					AltConf
47	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	V	1	Total	C	N	O	P	0
			40	30	1	8	1	

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

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



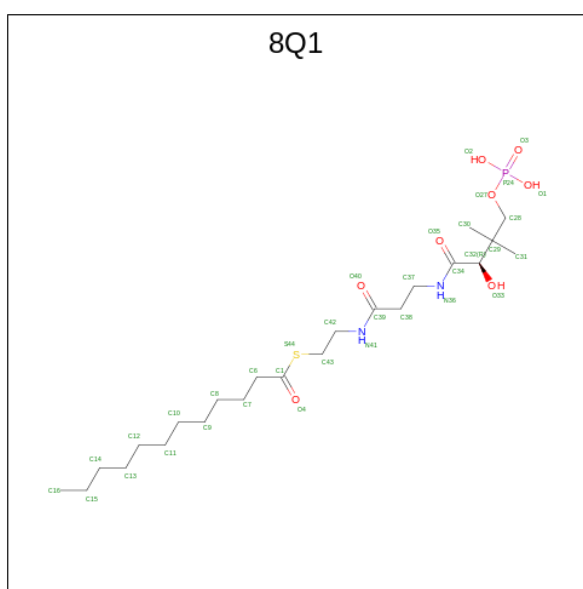
Mol	Chain	Residues	Atoms					AltConf
48	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	j	1	Total	C	N	O	P	0
			52	42	1	8	1	

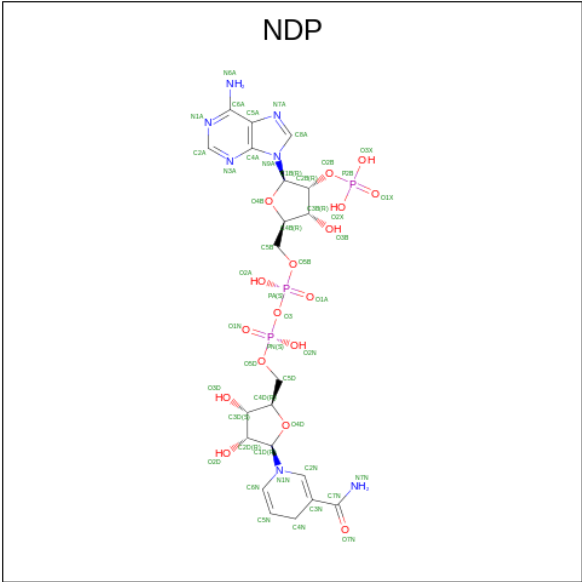
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Mol	Chain	Residues	Atoms					AltConf
48	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

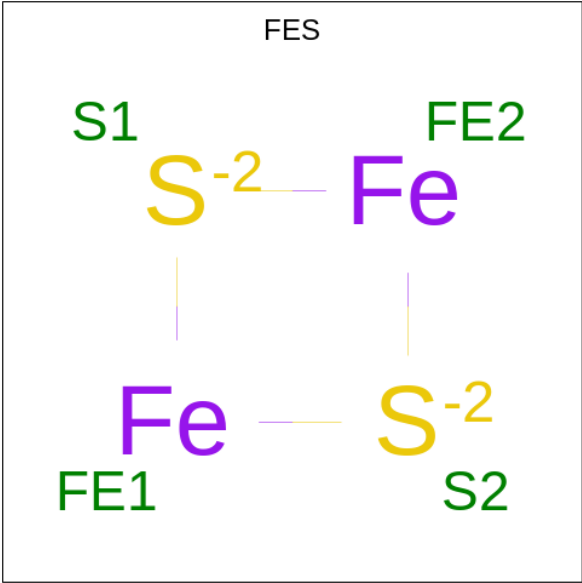
- Molecule 49 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as "Ligand of Interest" by depositor).





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

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

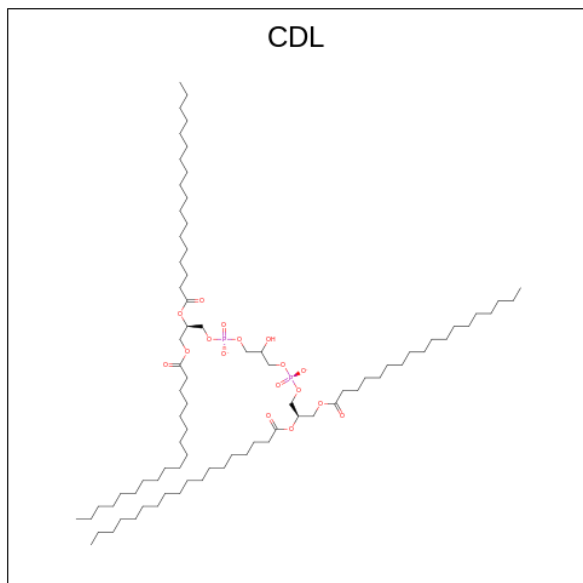


Mol	Chain	Residues	Atoms			AltConf
51	M	1	Total	Fe	S	0
			4	2	2	
51	O	1	Total	Fe	S	0
			4	2	2	

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

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

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

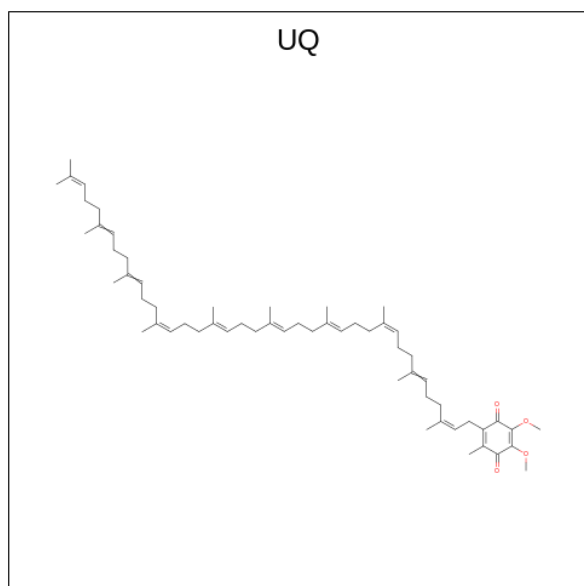


Mol	Chain	Residues	Atoms				AltConf
53	N	1	Total	C	O	P	0
			51	32	17	2	
53	V	1	Total	C	O	P	0
			94	75	17	2	
53	a	1	Total	C	O	P	0
			91	72	17	2	
53	i	1	Total	C	O	P	0
			66	47	17	2	
53	l	1	Total	C	O	P	0
			99	80	17	2	
53	l	1	Total	C	O	P	0
			100	81	17	2	
53	o	1	Total	C	O	P	0
			68	49	17	2	
53	r	1	Total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

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

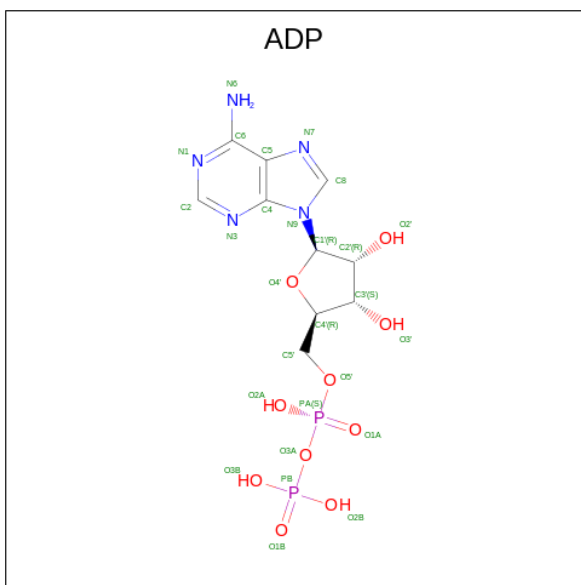
Mol	Chain	Residues	Atoms		AltConf
54	T	1	Total 1	Zn 1	0

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



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

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

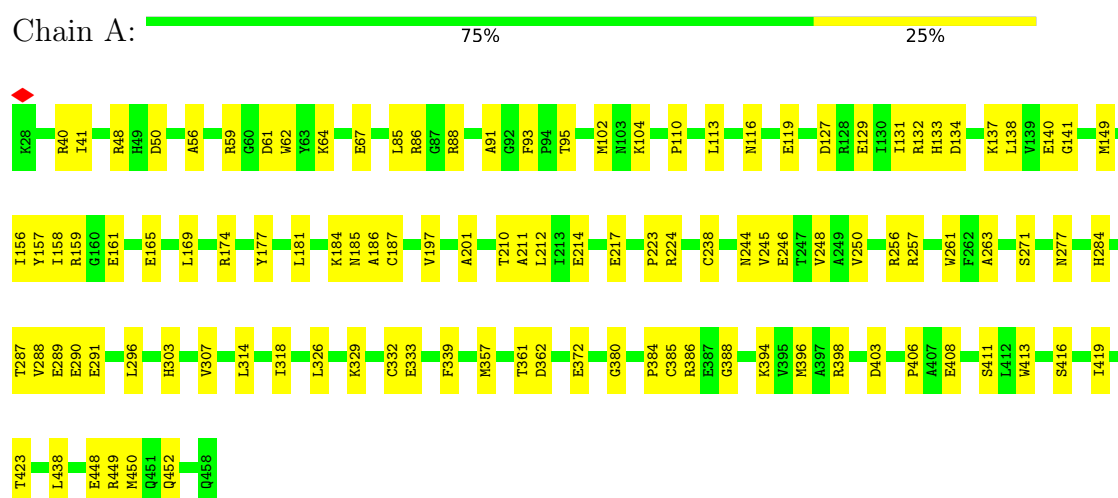


Mol	Chain	Residues	Atoms					AltConf
56	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

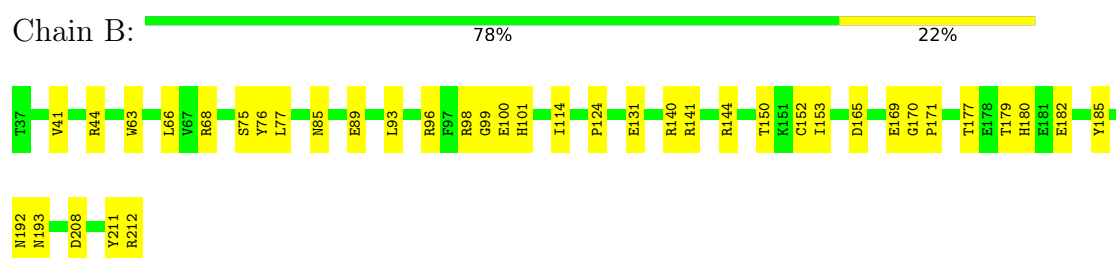
3 Residue-property plots

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

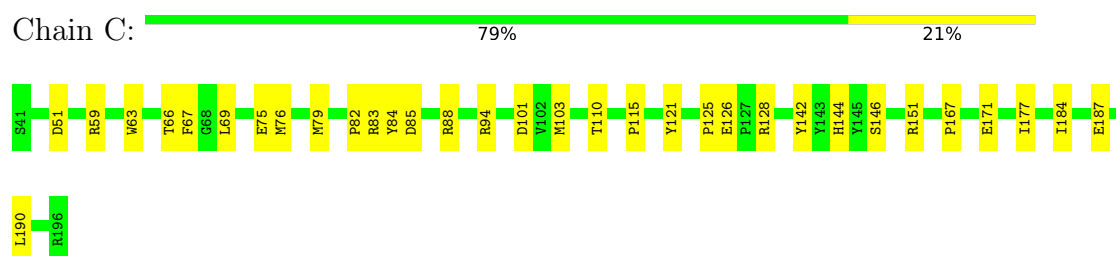
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



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

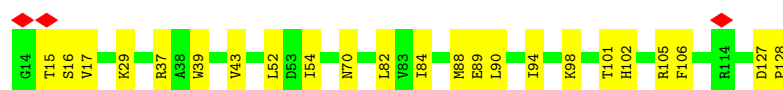


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



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

Chain E:  80% 20%



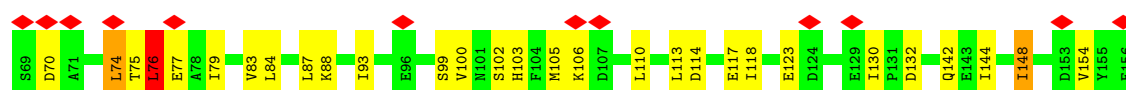
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain F:  84% 16%



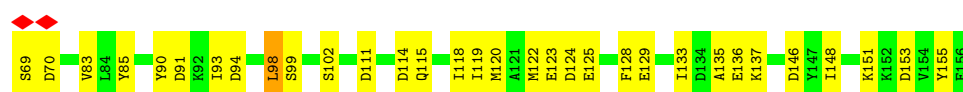
- Molecule 6: Acyl carrier protein, mitochondrial

Chain G:  14% 67% 30% ..



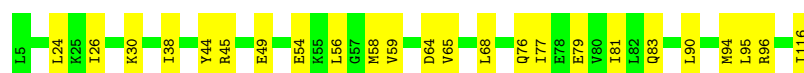
- Molecule 6: Acyl carrier protein, mitochondrial

Chain X:  64% 35% .



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

Chain H:  79% 21%



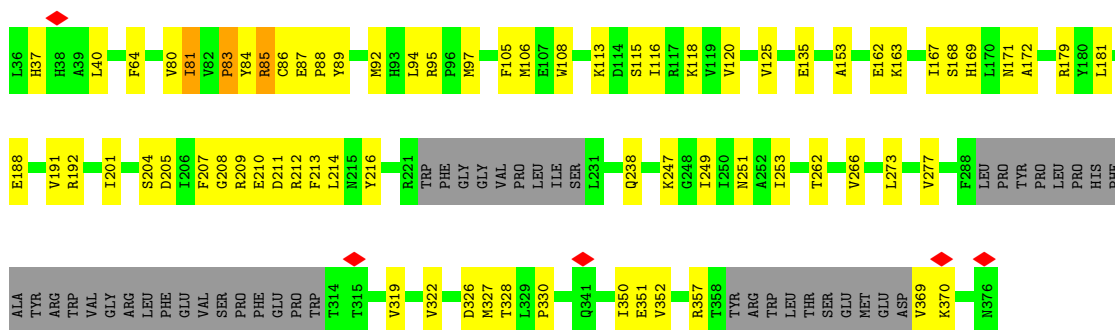
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain I:  71% 15% 13%



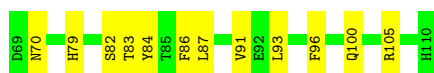
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain J:  66% 20% 13%



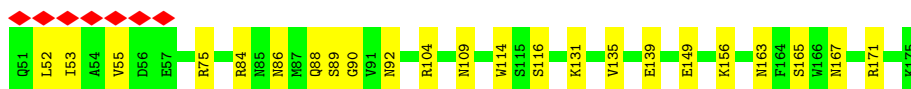
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain K: 71% 29%



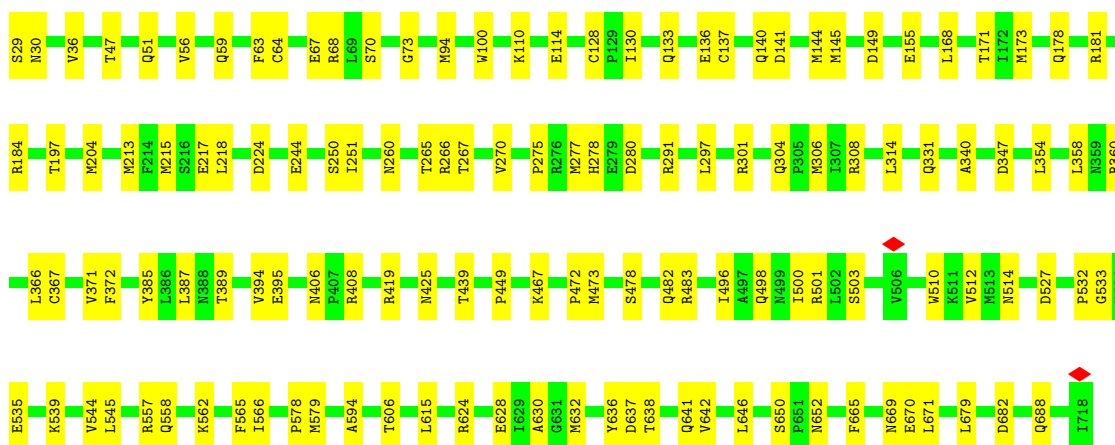
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain L: 6% 82% 18%



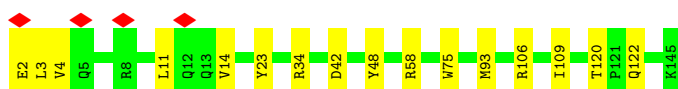
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain M: 81% 19%

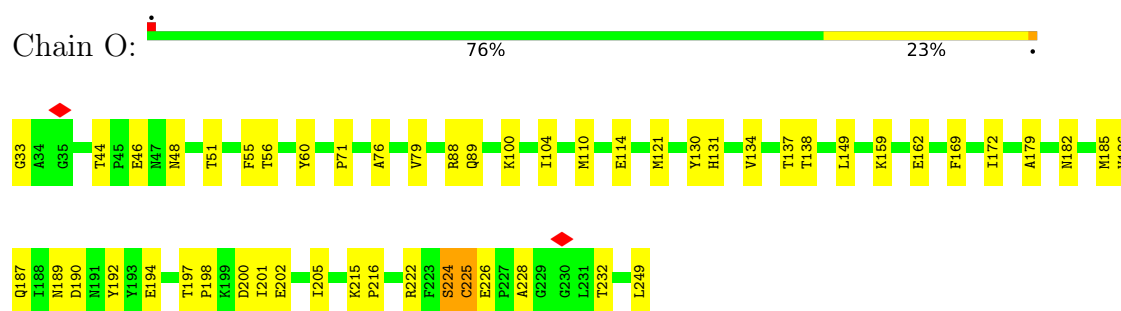


- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

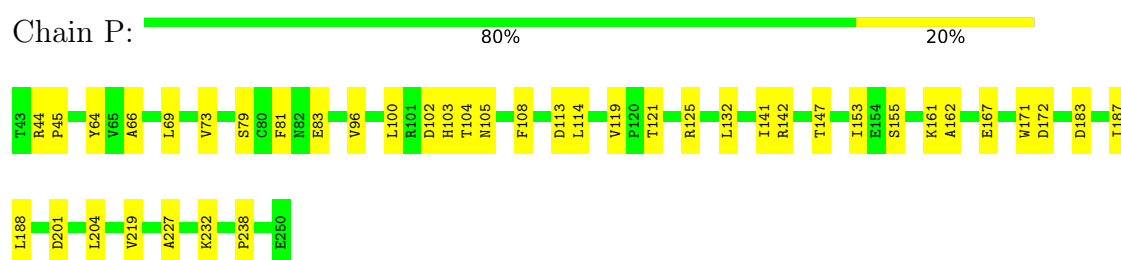
Chain N: 89% 11%



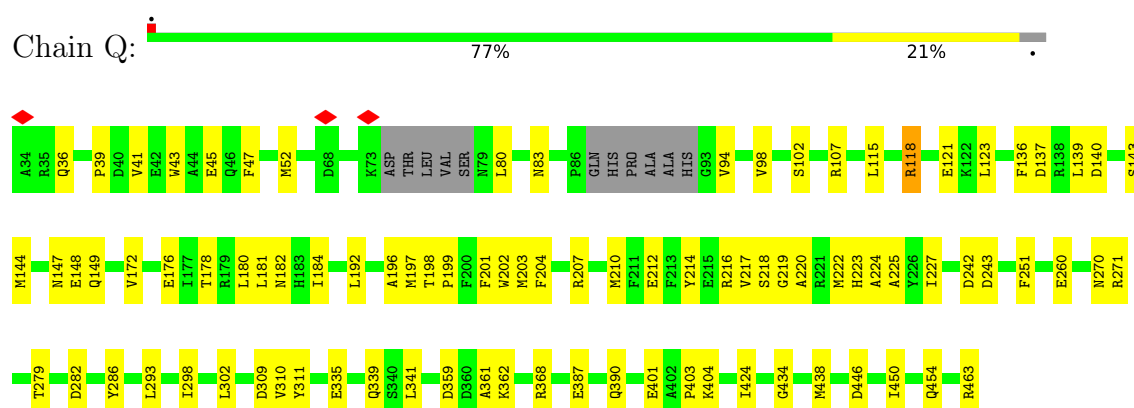
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



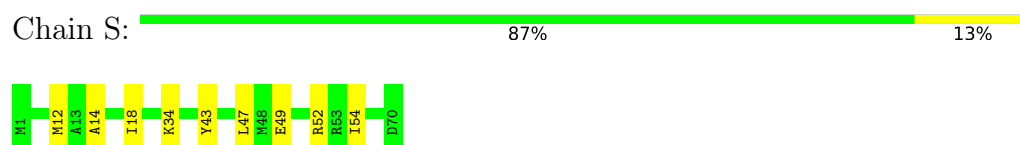
- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



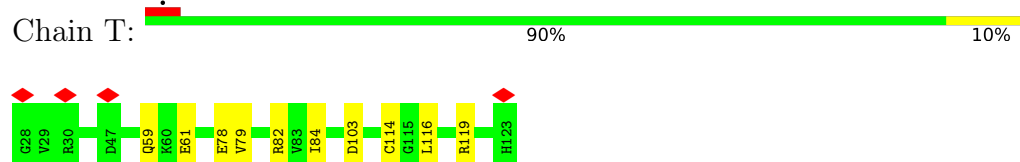
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



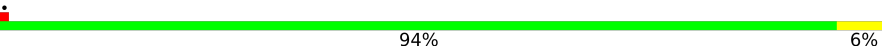
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

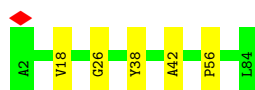


- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



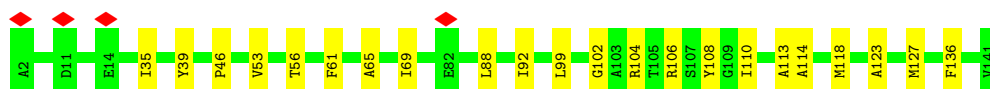
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:  94% 6%



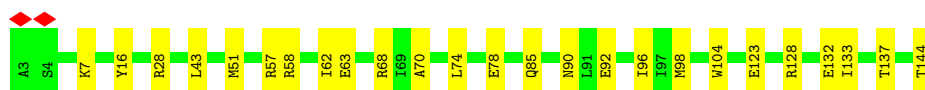
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:  84% 16%



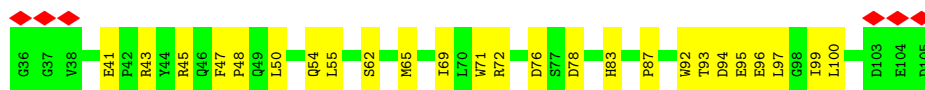
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:  82% 18%



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

Chain Y:  9% 64% 36%



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

Chain Z:  17% 81% 19%



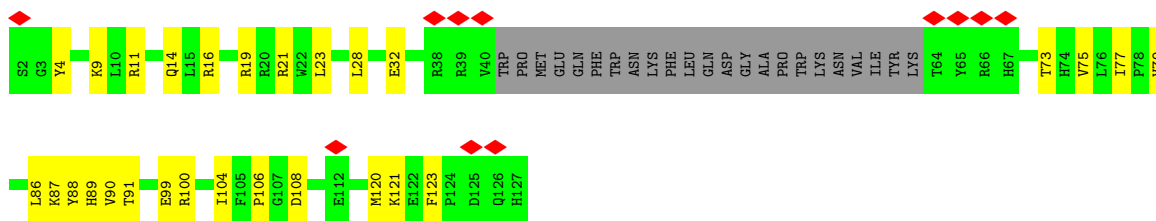
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:  79% 21%

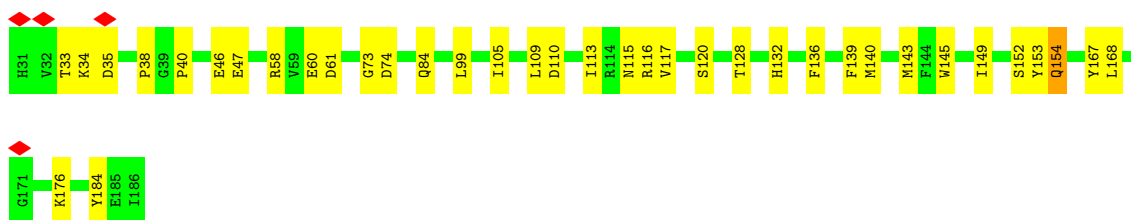
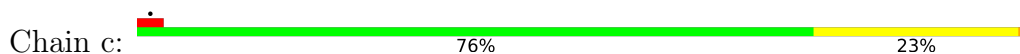


- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

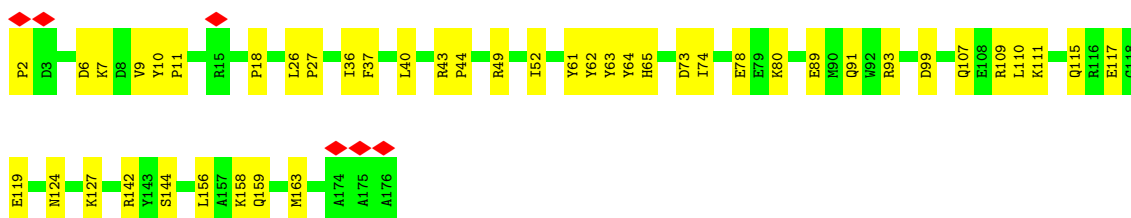
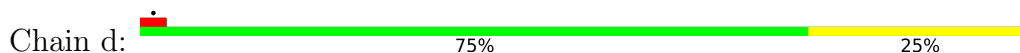
Chain b:  9% 60% 22% 18%



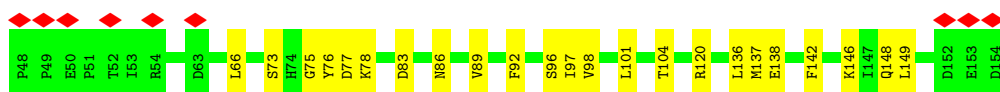
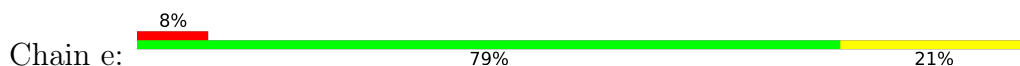
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



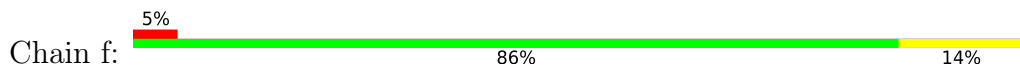
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



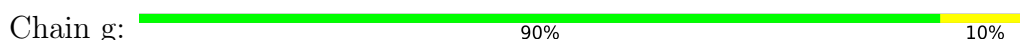
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



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

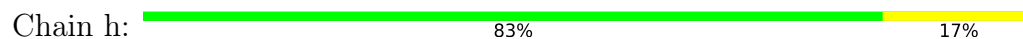


- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2





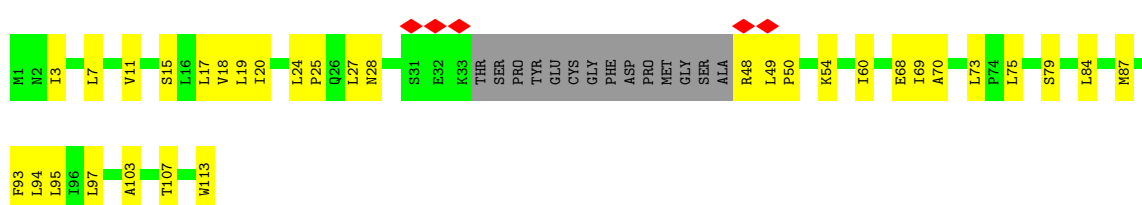
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



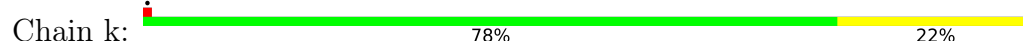
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

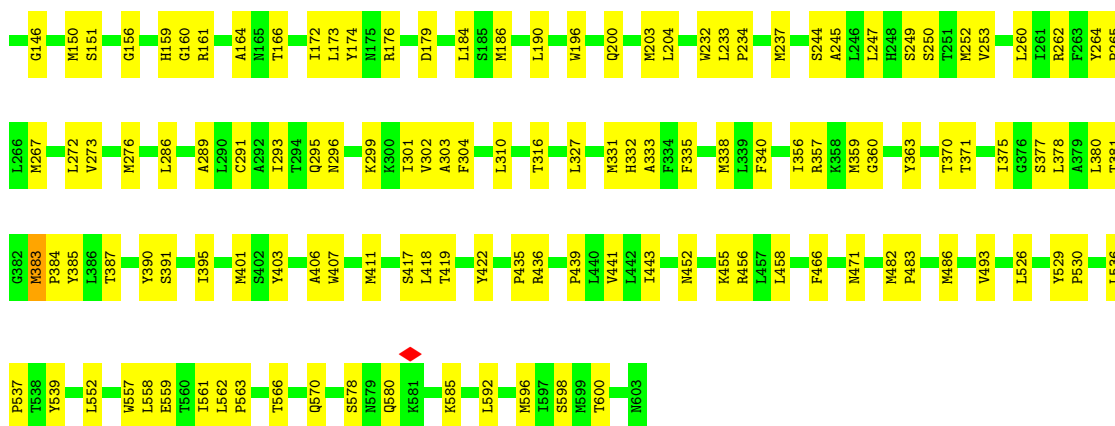


- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

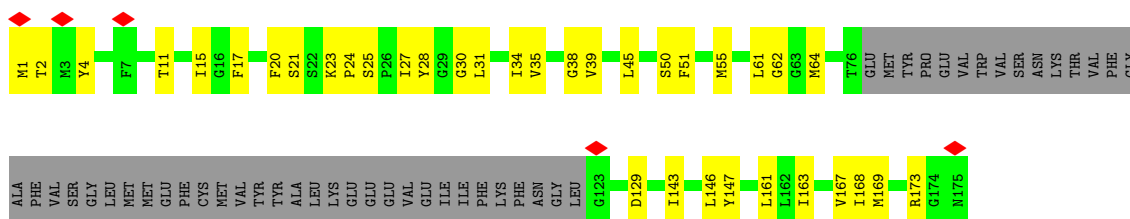


- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

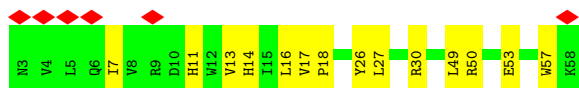
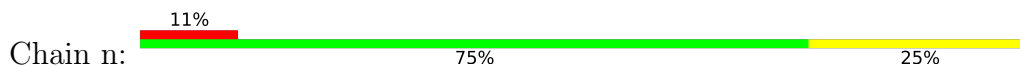




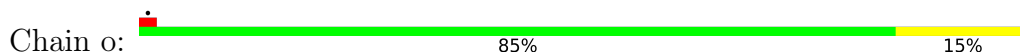
• Molecule 36: NADH-ubiquinone oxidoreductase chain 6



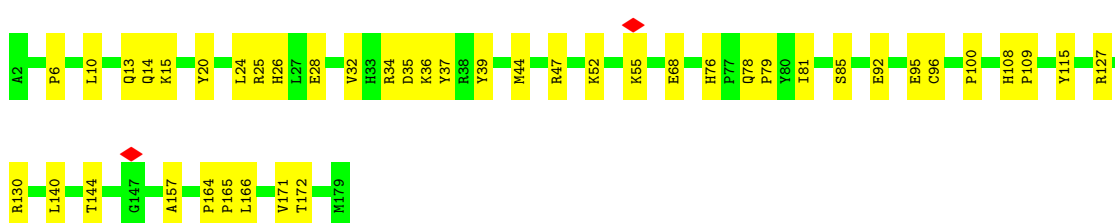
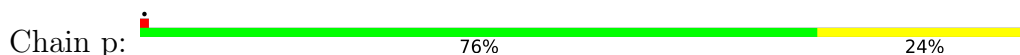
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



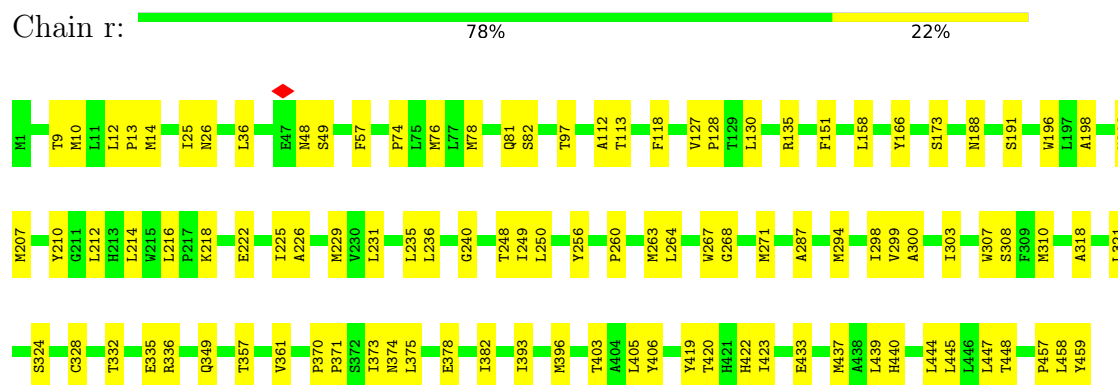
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



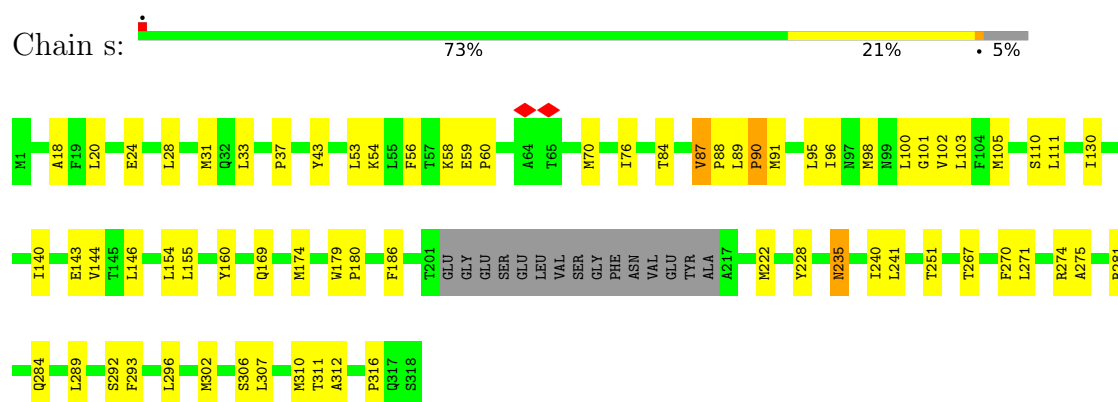
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



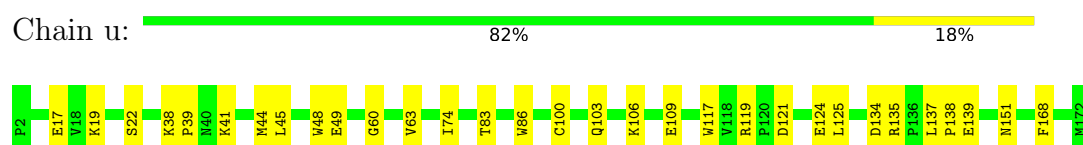
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4



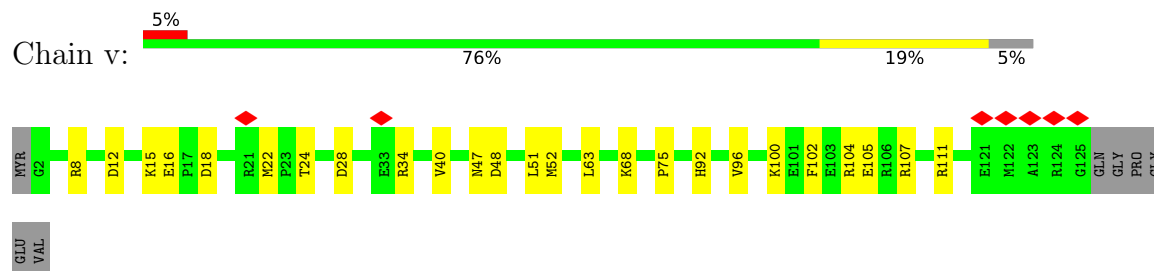
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1



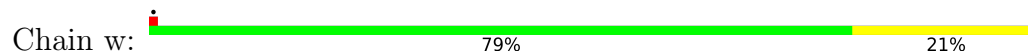
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

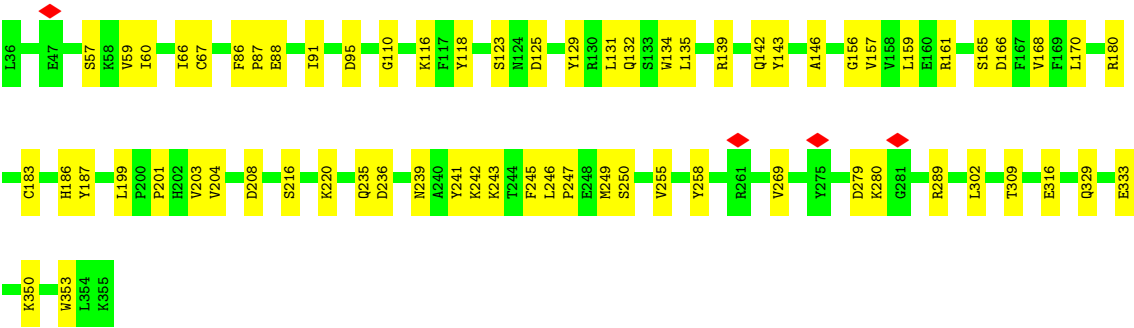


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	193234	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	0.233	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0165	Depositor
Map size ($\text{\AA}$)	354.48602, 354.48602, 354.48602	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.13	0/3393	0.33	0/4584
2	B	0.14	0/1443	0.32	0/1952
3	C	0.13	0/1279	0.31	0/1730
4	E	0.13	0/995	0.32	0/1340
5	F	0.12	0/702	0.34	0/945
6	G	0.19	0/689	0.52	0/935
6	X	0.16	0/711	0.47	0/963
7	H	0.14	0/929	0.32	0/1258
8	I	0.15	0/798	0.37	0/1079
9	J	0.14	0/2408	0.40	0/3250
10	K	0.10	0/365	0.28	0/493
11	L	0.11	0/1039	0.28	0/1403
12	M	0.12	0/5384	0.30	0/7295
13	N	0.10	0/1245	0.28	0/1694
14	O	0.15	0/1711	0.46	2/2328 (0.1%)
15	P	0.13	0/1789	0.33	0/2436
16	Q	0.16	0/3451	0.36	1/4672 (0.0%)
17	S	0.14	0/582	0.36	0/783
18	T	0.10	0/755	0.25	0/1018
19	U	0.12	0/664	0.28	0/912
20	V	0.13	0/1042	0.29	0/1411
21	W	0.12	0/1198	0.27	0/1617
22	Y	0.13	0/623	0.29	0/853
23	Z	0.14	0/695	0.34	0/939
24	a	0.14	0/1199	0.44	2/1623 (0.1%)
25	b	0.13	0/906	0.31	0/1232
26	c	0.14	0/1371	0.35	0/1875
27	d	0.11	0/1494	0.29	0/2015
28	e	0.13	0/916	0.34	0/1246
29	f	0.10	0/353	0.25	0/477
30	g	0.10	0/1031	0.26	0/1394
31	h	0.12	0/889	0.29	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.16	0/2773	0.37	1/3768 (0.0%)
33	j	0.16	0/819	0.38	0/1117
34	k	0.15	0/759	0.36	0/1029
35	l	0.16	0/4914	0.41	2/6683 (0.0%)
36	m	0.16	0/973	0.41	0/1320
37	n	0.20	0/491	0.62	1/663 (0.2%)
38	o	0.12	0/1092	0.30	0/1481
39	p	0.12	0/1590	0.30	0/2155
40	r	0.15	0/3723	0.33	0/5078
41	s	0.18	0/2464	0.44	1/3369 (0.0%)
42	u	0.13	0/1436	0.32	0/1938
43	v	0.13	0/1052	0.39	0/1411
44	w	0.13	0/2647	0.37	1/3584 (0.0%)
All	All	0.14	0/66782	0.35	11/90538 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
41	s	0	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	O	225	CYS	N-CA-C	8.98	123.78	111.39
24	a	94	GLY	N-CA-C	8.84	123.85	112.54
35	l	383	MET	CA-C-N	7.06	127.05	119.78
35	l	383	MET	C-N-CA	7.06	127.05	119.78
14	O	224	SER	N-CA-C	6.46	120.56	111.52
24	a	95	GLU	N-CA-C	6.22	119.97	111.39
37	n	16	LEU	N-CA-C	6.15	117.98	111.28
16	Q	217	VAL	N-CA-C	5.48	116.25	110.72
41	s	87	VAL	CB-CA-C	-5.45	108.57	114.35
44	w	243	LYS	N-CA-C	5.29	117.13	111.36
32	i	89	MET	N-CA-C	5.11	116.84	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
41	s	91	MET	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3318	0	3280	83	0
2	B	1412	0	1363	33	0
3	C	1248	0	1254	34	0
4	E	971	0	975	17	0
5	F	691	0	704	10	0
6	G	678	0	655	27	0
6	X	699	0	682	30	0
7	H	910	0	950	15	0
8	I	780	0	808	16	0
9	J	2356	0	2400	68	0
10	K	355	0	329	11	0
11	L	1016	0	1016	20	0
12	M	5296	0	5326	87	0
13	N	1204	0	1162	14	0
14	O	1671	0	1673	41	0
15	P	1738	0	1693	33	0
16	Q	3377	0	3320	72	0
17	S	567	0	565	7	0
18	T	741	0	702	6	0
19	U	643	0	642	5	0
20	V	1021	0	1027	27	0
21	W	1167	0	1155	22	0
22	Y	597	0	537	35	0
23	Z	674	0	643	13	0
24	a	1165	0	1174	39	0
25	b	879	0	899	29	0
26	c	1315	0	1208	28	0
27	d	1461	0	1429	49	0
28	e	890	0	837	18	0
29	f	344	0	347	3	0
30	g	1000	0	994	12	0
31	h	867	0	871	15	0
32	i	2710	0	2874	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	j	800	0	855	35	0
34	k	748	0	799	24	0
35	l	4785	0	4932	134	0
36	m	951	0	962	34	0
37	n	479	0	486	23	0
38	o	1062	0	1072	19	0
39	p	1534	0	1470	37	0
40	r	3631	0	3838	96	0
41	s	2394	0	2508	68	0
42	u	1398	0	1378	25	0
43	v	1028	0	980	25	0
44	w	2587	0	2551	57	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	3	0
47	B	51	0	82	2	0
47	V	40	0	54	11	0
47	b	46	0	69	16	0
47	i	47	0	71	15	0
47	j	98	0	153	20	0
47	l	46	0	69	3	0
47	m	41	0	59	11	0
47	r	51	0	82	15	0
48	C	52	0	88	5	0
48	g	52	0	88	4	0
48	j	52	0	88	1	0
48	r	156	0	262	11	0
49	G	35	0	0	1	0
49	X	35	0	0	1	0
50	J	48	0	26	4	0
51	M	4	0	0	1	0
51	O	4	0	0	0	0
52	M	1	0	0	0	0
53	N	51	0	46	12	0
53	V	94	0	138	11	0
53	a	91	0	132	21	0
53	i	66	0	76	19	0
53	l	199	0	307	22	0
53	o	68	0	83	17	0
53	r	100	0	156	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	u	78	0	103	14	0
54	T	1	0	0	0	0
55	s	28	0	31	3	0
56	w	27	0	11	5	0
All	All	66899	0	67618	1419	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 11.

All (1419) 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)
24:a:96:ALA:HB2	27:d:61:TYR:CE1	1.34	1.58
53:r:505:CDL:H852	53:u:201:CDL:C82	1.07	1.54
37:n:14:HIS:CE1	40:r:26:ASN:HD21	1.35	1.43
53:r:505:CDL:C85	53:u:201:CDL:C82	1.95	1.40
37:n:14:HIS:CE1	40:r:26:ASN:ND2	1.88	1.37
32:i:321:LYS:NZ	53:i:401:CDL:OA4	1.69	1.25
24:a:96:ALA:CB	27:d:61:TYR:CE1	2.19	1.24
3:C:167:PRO:HG3	16:Q:222:MET:CE	1.69	1.21
44:w:165:SER:HB3	44:w:245:PHE:CE1	1.76	1.19
24:a:96:ALA:HB2	27:d:61:TYR:CD1	1.79	1.18
22:Y:69:ILE:HD13	35:l:383:MET:HE1	1.23	1.17
24:a:96:ALA:CB	27:d:61:TYR:CD1	2.29	1.16
3:C:167:PRO:HG3	16:Q:222:MET:HE2	1.19	1.15
32:i:91:ASN:HD22	32:i:92:PRO:HD2	1.04	1.14
44:w:67:CYS:N	56:w:401:ADP:O2A	1.80	1.12
44:w:236:ASP:O	44:w:239:ASN:OD1	1.66	1.11
32:i:95:MET:HA	32:i:95:MET:HE3	1.30	1.07
47:m:201:PEE:H57	47:m:201:PEE:H25	1.08	1.06
32:i:91:ASN:ND2	32:i:92:PRO:HD2	1.69	1.05
8:I:3:SER:O	53:N:201:CDL:HA22	1.58	1.03
9:J:87:GLU:CD	9:J:88:PRO:HD2	1.86	1.01
47:m:201:PEE:H57	47:m:201:PEE:C17	1.90	1.01
53:a:201:CDL:H251	53:a:201:CDL:H211	1.42	1.00
6:G:144:ILE:O	6:G:148:ILE:HG22	1.61	1.00
33:j:27:LEU:HD13	47:j:201:PEE:H16	1.43	0.99
16:Q:148:GLU:OE1	16:Q:225:ALA:HA	1.62	0.99
24:a:96:ALA:HB2	27:d:61:TYR:HE1	1.25	0.99
22:Y:69:ILE:CD1	35:l:383:MET:HE1	1.93	0.99
37:n:13:VAL:HG12	40:r:14:MET:HG2	1.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:o:201:CDL:H781	53:o:201:CDL:H822	1.47	0.97
47:m:201:PEE:C37	47:m:201:PEE:H29	1.95	0.97
40:r:191:SER:HB3	47:r:501:PEE:H3	1.47	0.96
37:n:14:HIS:HE1	40:r:26:ASN:ND2	1.35	0.96
53:o:201:CDL:H791	53:o:201:CDL:H832	1.45	0.95
53:u:201:CDL:H161	53:u:201:CDL:HB31	1.46	0.95
53:a:201:CDL:H521	47:b:201:PEE:H13	1.46	0.94
20:V:39:TYR:CZ	53:V:201:CDL:H592	2.02	0.94
1:A:133:HIS:CE1	14:O:224:SER:OG	2.21	0.94
44:w:236:ASP:C	44:w:239:ASN:OD1	2.10	0.94
47:i:402:PEE:H37	47:i:402:PEE:H60	1.50	0.93
47:i:402:PEE:H37	47:i:402:PEE:C37	1.98	0.93
47:m:201:PEE:H25	47:m:201:PEE:C35	1.98	0.93
9:J:209:ARG:NH2	9:J:351:GLU:OE2	2.01	0.93
53:u:201:CDL:H581	53:u:201:CDL:H542	1.48	0.92
26:c:128:THR:O	26:c:132:HIS:HD2	1.53	0.92
35:l:331:MET:HB3	35:l:387:THR:HG22	1.52	0.92
47:i:402:PEE:H34	47:i:402:PEE:H42	1.51	0.91
47:V:202:PEE:H2	47:V:202:PEE:H9	1.52	0.91
1:A:133:HIS:HE1	14:O:224:SER:OG	1.54	0.90
10:K:79:HIS:CD2	14:O:216:PRO:HD2	2.08	0.89
41:s:87:VAL:HG23	41:s:88:PRO:HD3	1.52	0.88
47:b:201:PEE:H28	53:l:701:CDL:H271	1.52	0.88
22:Y:76:ASP:O	35:l:385:TYR:OH	1.90	0.88
35:l:124:PHE:CE2	35:l:247:LEU:HG	2.07	0.88
53:a:201:CDL:H532	47:b:201:PEE:H56	1.56	0.87
37:n:13:VAL:CG1	40:r:14:MET:HG2	2.04	0.86
22:Y:72:ARG:HB3	35:l:385:TYR:CD2	2.10	0.86
1:A:133:HIS:HE1	14:O:224:SER:CB	1.89	0.86
3:C:167:PRO:CG	16:Q:222:MET:HE2	2.05	0.85
24:a:96:ALA:HB1	27:d:61:TYR:CD1	2.08	0.85
24:a:97:GLU:OE2	27:d:62:TYR:CE2	2.30	0.84
53:a:201:CDL:H761	53:a:201:CDL:H201	1.59	0.84
35:l:558:LEU:HD11	53:o:201:CDL:H852	1.58	0.83
53:N:201:CDL:H532	53:N:201:CDL:CA7	2.08	0.83
6:X:98:LEU:HD12	6:X:98:LEU:O	1.78	0.83
32:i:11:MET:CE	53:i:401:CDL:C56	2.57	0.82
37:n:14:HIS:HE1	40:r:26:ASN:HD21	0.87	0.82
53:a:201:CDL:H521	47:b:201:PEE:C11	2.07	0.82
9:J:205:ASP:OD2	9:J:213:PHE:CE1	2.33	0.82
47:V:202:PEE:H9	47:V:202:PEE:C1	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:139:LEU:HD21	16:Q:424:ILE:HD13	1.62	0.81
9:J:85:ARG:HD2	50:J:401:NDP:O1X	1.80	0.81
53:r:505:CDL:C86	53:u:201:CDL:C82	2.59	0.81
6:G:74:LEU:H	6:G:74:LEU:HD23	1.46	0.80
53:a:201:CDL:H211	53:a:201:CDL:C25	2.09	0.80
37:n:14:HIS:CE1	40:r:26:ASN:HD22	1.95	0.80
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.64	0.80
32:i:91:ASN:HD22	32:i:92:PRO:CD	1.89	0.80
33:j:27:LEU:HD13	47:j:201:PEE:C12	2.12	0.80
47:j:202:PEE:C24	41:s:302:MET:HE1	2.11	0.80
35:l:380:LEU:HD23	35:l:380:LEU:O	1.82	0.79
13:N:3:LEU:HD11	53:N:201:CDL:H311	1.63	0.79
53:a:201:CDL:H201	53:a:201:CDL:C77	2.13	0.79
32:i:87:THR:HG22	32:i:88:LYS:H	1.48	0.78
53:N:201:CDL:H711	41:s:43:TYR:OH	1.82	0.78
35:l:159:HIS:CE1	40:r:349:GLN:OE1	2.37	0.78
32:i:133:TRP:HE3	53:i:401:CDL:H392	1.49	0.78
53:N:201:CDL:C55	53:N:201:CDL:H322	2.14	0.78
32:i:278:MET:HG2	32:i:282:MET:HE3	1.66	0.77
53:a:201:CDL:H201	53:a:201:CDL:C76	2.13	0.77
24:a:98:LEU:HB2	27:d:63:TYR:CE1	2.20	0.77
53:a:201:CDL:H201	53:a:201:CDL:H772	1.66	0.76
41:s:169:GLN:HE21	41:s:174:MET:HE2	1.51	0.76
34:k:58:MET:HE3	36:m:146:LEU:HA	1.67	0.76
53:a:201:CDL:H191	53:a:201:CDL:H732	1.65	0.75
22:Y:69:ILE:HD13	35:l:383:MET:CE	2.10	0.75
35:l:161:ARG:HA	39:p:92:GLU:HB2	1.68	0.75
35:l:102:GLU:OE1	35:l:456:ARG:NH2	2.18	0.75
26:c:128:THR:O	26:c:132:HIS:CD2	2.40	0.75
16:Q:144:MET:SD	16:Q:222:MET:O	2.44	0.75
2:B:99:GLY:HA3	2:B:170:GLY:O	1.87	0.74
6:X:91:ASP:HB3	23:Z:47:ARG:HH12	1.53	0.73
6:G:74:LEU:HD23	6:G:74:LEU:N	2.02	0.73
32:i:95:MET:HA	32:i:95:MET:CE	2.16	0.73
47:i:402:PEE:H36	47:i:402:PEE:H28	1.71	0.73
25:b:104:ILE:HB	43:v:48:ASP:HB3	1.70	0.72
32:i:11:MET:HE1	53:i:401:CDL:C56	2.20	0.72
53:a:201:CDL:H761	53:a:201:CDL:C20	2.18	0.72
47:i:402:PEE:H37	47:i:402:PEE:H61	1.71	0.72
12:M:498:GLN:HB2	12:M:669:ASN:HD21	1.55	0.72
47:j:202:PEE:H39	41:s:302:MET:HE1	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:h:97:HIS:HA	31:h:102:GLU:HB3	1.71	0.72
41:s:84:THR:O	41:s:87:VAL:HG22	1.90	0.72
27:d:124:ASN:HD21	43:v:47:ASN:HD21	1.38	0.71
9:J:87:GLU:OE1	9:J:88:PRO:CD	2.39	0.71
32:i:133:TRP:CE3	53:i:401:CDL:H392	2.26	0.71
3:C:126:GLU:O	9:J:89:TYR:OH	2.07	0.71
9:J:208:GLY:H	9:J:211:ASP:CB	2.03	0.71
12:M:67:GLU:HG3	12:M:68:ARG:HD2	1.71	0.71
32:i:207:ILE:HG22	32:i:211:MET:HE2	1.73	0.70
32:i:95:MET:HE3	32:i:95:MET:CA	2.15	0.70
1:A:113:LEU:HD13	1:A:149:MET:HE1	1.72	0.70
35:l:356:ILE:HA	35:l:359:MET:HE3	1.73	0.70
40:r:207:MET:HG3	40:r:294:MET:HB3	1.74	0.70
32:i:11:MET:HE3	53:i:401:CDL:C56	2.22	0.69
47:b:201:PEE:O2P	47:b:201:PEE:N	2.21	0.69
32:i:88:LYS:HD2	32:i:148:SER:OG	1.92	0.69
44:w:236:ASP:CA	44:w:239:ASN:OD1	2.39	0.69
33:j:79:SER:HA	33:j:87:MET:HE2	1.74	0.69
1:A:86:ARG:NH1	1:A:339:PHE:CD2	2.61	0.69
1:A:116:ASN:ND2	46:A:502:FMN:O3'	2.25	0.69
16:Q:446:ASP:OD1	41:s:281:ARG:NH1	2.25	0.69
33:j:27:LEU:CD1	47:j:201:PEE:H16	2.20	0.69
1:A:131:ILE:HD11	1:A:169:LEU:HD22	1.73	0.69
49:X:201:8Q1:O3	39:p:13:GLN:NE2	2.26	0.69
28:e:77:ASP:OD1	28:e:78:LYS:N	2.26	0.69
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.25	0.69
44:w:60:ILE:HG12	44:w:203:VAL:HB	1.75	0.69
13:N:3:LEU:HD12	53:N:201:CDL:OA7	1.92	0.69
24:a:96:ALA:HB1	27:d:61:TYR:HD1	1.56	0.69
25:b:11:ARG:NH2	39:p:165:PRO:O	2.25	0.69
2:B:99:GLY:CA	2:B:170:GLY:O	2.40	0.69
9:J:87:GLU:CD	9:J:88:PRO:CD	2.65	0.69
41:s:87:VAL:HG12	41:s:95:LEU:HD23	1.74	0.69
2:B:77:LEU:HD12	41:s:31:MET:HG3	1.75	0.68
9:J:247:LYS:O	9:J:251:ASN:ND2	2.26	0.68
7:H:83:GLN:HE21	15:P:104:THR:HA	1.59	0.68
24:a:96:ALA:CB	27:d:61:TYR:HE1	1.87	0.68
3:C:167:PRO:HG3	16:Q:222:MET:HE3	1.72	0.68
20:V:35:ILE:HG21	53:V:201:CDL:H781	1.76	0.68
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.27	0.68
31:h:105:ARG:NH2	42:u:17:GLU:OE2	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:383:MET:SD	35:l:384:PRO:HD2	2.34	0.68
53:l:701:CDL:H432	53:l:701:CDL:H621	1.75	0.68
44:w:236:ASP:HA	44:w:239:ASN:OD1	1.94	0.68
33:j:24:LEU:CD2	47:j:201:PEE:H67	2.23	0.68
9:J:81:ILE:HD12	9:J:81:ILE:N	2.09	0.68
53:u:201:CDL:H581	53:u:201:CDL:C54	2.21	0.67
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.27	0.67
47:b:201:PEE:H47	35:l:68:TRP:CE3	2.30	0.67
47:r:501:PEE:H77	48:r:502:PLX:H191	1.76	0.67
33:j:3:ILE:CD1	47:m:201:PEE:H50	2.25	0.67
9:J:83:PRO:HB2	9:J:108:TRP:CD1	2.30	0.67
9:J:83:PRO:HA	9:J:106:MET:O	1.95	0.67
10:K:79:HIS:HD2	14:O:216:PRO:HD2	1.60	0.67
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.24	0.67
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.78	0.66
32:i:96:THR:O	32:i:100:MET:HG2	1.95	0.66
15:P:204:LEU:HD11	16:Q:123:LEU:HD23	1.77	0.66
40:r:191:SER:CB	47:r:501:PEE:H3	2.23	0.66
2:B:76:TYR:HE2	41:s:33:LEU:HB2	1.60	0.66
47:b:201:PEE:H33	53:l:701:CDL:H241	1.76	0.66
35:l:83:ASP:OD2	35:l:262:ARG:NH1	2.28	0.66
6:X:123:GLU:HG3	6:X:129:GLU:HA	1.77	0.66
41:s:87:VAL:HG23	41:s:88:PRO:CD	2.24	0.66
6:G:148:ILE:O	6:G:148:ILE:HG13	1.92	0.66
6:X:98:LEU:HD12	6:X:98:LEU:C	2.21	0.66
38:o:101:TRP:HB2	40:r:263:MET:HE1	1.78	0.66
16:Q:136:PHE:HA	16:Q:139:LEU:HD13	1.78	0.66
53:V:201:CDL:HA62	53:V:201:CDL:OA7	1.96	0.66
47:V:202:PEE:H2	47:V:202:PEE:C4	2.24	0.66
20:V:39:TYR:CE2	53:V:201:CDL:H592	2.29	0.65
35:l:558:LEU:HB3	40:r:214:LEU:HD21	1.77	0.65
44:w:165:SER:CB	44:w:245:PHE:CE1	2.67	0.65
4:E:37:ARG:NH2	6:G:132:ASP:OD2	2.29	0.65
20:V:110:ILE:CD1	47:V:202:PEE:H48	2.26	0.65
53:a:201:CDL:H761	53:a:201:CDL:C19	2.27	0.65
16:Q:218:SER:OG	16:Q:224:ALA:HB1	1.97	0.65
21:W:85:GLN:OE1	31:h:105:ARG:NH1	2.24	0.65
37:n:30:ARG:HD3	53:u:201:CDL:OA4	1.97	0.65
44:w:88:GLU:OE2	44:w:161:ARG:NH1	2.29	0.65
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.23	0.65
4:E:127:ASP:OD1	11:L:104:ARG:NH1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:204:VAL:HG21	44:w:249:MET:HE2	1.77	0.65
14:O:134:VAL:HG21	14:O:149:LEU:HD13	1.79	0.65
15:P:69:LEU:HD23	15:P:96:VAL:HG22	1.79	0.64
20:V:114:ALA:O	20:V:118:MET:HB2	1.97	0.64
16:Q:279:THR:OG1	16:Q:282:ASP:OD1	2.15	0.64
1:A:362:ASP:OD1	1:A:449:ARG:NH2	2.31	0.64
40:r:378:GLU:O	40:r:382:ILE:HG12	1.97	0.64
24:a:95:GLU:OE2	24:a:114:LYS:HD3	1.96	0.64
12:M:472:PRO:O	12:M:510:TRP:NE1	2.29	0.64
1:A:129:GLU:OE2	14:O:224:SER:OG	2.16	0.64
9:J:87:GLU:OE1	9:J:88:PRO:HD2	1.97	0.64
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.79	0.64
14:O:182:ASN:ND2	14:O:194:GLU:OE1	2.31	0.64
6:X:124:ASP:OD1	39:p:25:ARG:NH2	2.27	0.64
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.78	0.64
32:i:236:LYS:HB2	32:i:311:MET:HE1	1.79	0.64
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.31	0.64
26:c:99:LEU:HD11	26:c:109:LEU:HD11	1.80	0.64
32:i:267:ILE:HG12	32:i:279:PRO:HB3	1.79	0.64
16:Q:178:THR:OG1	16:Q:214:TYR:OH	2.14	0.63
47:b:201:PEE:H5	47:b:201:PEE:P	2.21	0.63
36:m:30:GLY:O	36:m:34:ILE:HD12	1.98	0.63
40:r:307:TRP:HA	40:r:310:MET:HE2	1.79	0.63
2:B:177:THR:HG21	2:B:182:GLU:HB2	1.79	0.63
10:K:100:GLN:HB3	14:O:71:PRO:HA	1.80	0.63
27:d:26:LEU:HD12	27:d:27:PRO:HD2	1.79	0.63
33:j:24:LEU:HD22	47:j:201:PEE:H67	1.79	0.63
44:w:67:CYS:H	56:w:401:ADP:PA	2.18	0.63
1:A:398:ARG:HG2	1:A:403:ASP:HB3	1.79	0.63
43:v:8:ARG:NH2	43:v:18:ASP:OD1	2.31	0.63
33:j:60:ILE:HG21	36:m:168:ILE:HG21	1.80	0.63
24:a:98:LEU:HA	27:d:63:TYR:O	1.97	0.63
53:a:201:CDL:H761	53:a:201:CDL:H191	1.79	0.63
44:w:165:SER:HB3	44:w:245:PHE:CZ	2.31	0.63
1:A:41:ILE:HG21	1:A:250:VAL:HG12	1.81	0.63
6:G:99:SER:H	6:G:102:SER:HB3	1.63	0.63
8:I:102:LYS:HE3	8:I:102:LYS:HA	1.81	0.63
44:w:129:TYR:CD2	44:w:183:CYS:HB3	2.34	0.63
44:w:216:SER:O	44:w:220:LYS:HG2	1.99	0.63
9:J:205:ASP:OD2	9:J:213:PHE:CD1	2.52	0.63
24:a:97:GLU:O	27:d:62:TYR:HA	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:134:GLU:OE1	37:n:57:TRP:NE1	2.28	0.62
15:P:113:ASP:OD1	15:P:114:LEU:N	2.32	0.62
35:l:250:SER:HB2	35:l:333:ALA:HA	1.81	0.62
35:l:419:THR:HA	35:l:422:TYR:CE2	2.34	0.62
14:O:159:LYS:HB2	14:O:162:GLU:HG3	1.80	0.62
14:O:169:PHE:HE2	14:O:205:ILE:HG23	1.64	0.62
47:l:703:PEE:O5	47:l:703:PEE:H1	1.98	0.62
44:w:139:ARG:NH1	44:w:166:ASP:OD2	2.32	0.62
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.32	0.62
12:M:557:ARG:NH2	12:M:579:MET:O	2.31	0.62
27:d:2:PRO:O	27:d:7:LYS:NZ	2.31	0.62
35:l:142:ILE:HG12	40:r:370:PRO:HB2	1.81	0.62
16:Q:182:ASN:OD1	16:Q:404:LYS:NZ	2.33	0.62
35:l:558:LEU:HD12	53:o:201:CDL:H831	1.81	0.62
37:n:17:VAL:HB	37:n:18:PRO:HD3	1.82	0.62
34:k:23:ARG:HG2	36:m:23:LYS:HE2	1.81	0.62
35:l:156:GLY:HA2	35:l:164:ALA:HB1	1.82	0.62
15:P:172:ASP:OD2	15:P:187:ILE:N	2.28	0.62
16:Q:387:GLU:OE2	16:Q:390:GLN:NE2	2.33	0.62
9:J:204:SER:OG	9:J:238:GLN:O	2.16	0.62
20:V:110:ILE:HD12	47:V:202:PEE:H48	1.82	0.62
26:c:33:THR:OG1	26:c:35:ASP:OD1	2.16	0.61
6:G:144:ILE:O	6:G:148:ILE:CG2	2.44	0.61
26:c:184:TYR:OH	43:v:104:ARG:NH1	2.33	0.61
1:A:133:HIS:HE1	14:O:224:SER:HB2	1.65	0.61
9:J:171:ASN:HD22	9:J:327:MET:HG3	1.65	0.61
14:O:55:PHE:HA	14:O:89:GLN:HE22	1.66	0.61
6:X:114:ASP:O	6:X:118:ILE:HD12	2.00	0.61
9:J:210:GLU:N	9:J:210:GLU:OE1	2.34	0.61
53:o:201:CDL:H832	53:o:201:CDL:C79	2.19	0.61
2:B:85:ASN:OD1	3:C:88:ARG:NH2	2.33	0.61
35:l:380:LEU:HD23	35:l:380:LEU:C	2.25	0.61
35:l:391:SER:O	35:l:395:ILE:HG12	2.00	0.61
26:c:58:ARG:NH2	26:c:60:GLU:OE2	2.34	0.61
41:s:169:GLN:NE2	41:s:241:LEU:O	2.32	0.61
32:i:236:LYS:HE2	44:w:302:LEU:HD11	1.82	0.61
1:A:244:ASN:OD1	1:A:245:VAL:N	2.33	0.60
21:W:57:ARG:HB3	41:s:316:PRO:HG3	1.83	0.60
44:w:118:TYR:OH	56:w:401:ADP:O2'	2.16	0.60
44:w:245:PHE:HD2	44:w:246:LEU:HD22	1.65	0.60
1:A:357:MET:HB3	1:A:361:THR:HG21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:GLY:O	1:A:386:ARG:NH1	2.30	0.60
9:J:85:ARG:HH21	9:J:85:ARG:HB2	1.65	0.60
9:J:87:GLU:OE1	9:J:88:PRO:HD3	2.00	0.60
15:P:44:ARG:HB3	15:P:45:PRO:HD2	1.84	0.60
34:k:44:SER:HB2	34:k:59:MET:HE1	1.81	0.60
25:b:28:LEU:HG	25:b:32:GLU:HG2	1.83	0.60
25:b:99:GLU:OE2	35:l:2:ASN:ND2	2.32	0.60
34:k:22:TYR:O	35:l:585:LYS:NZ	2.31	0.60
44:w:246:LEU:HD12	44:w:255:VAL:HG11	1.83	0.60
12:M:389:THR:HB	12:M:473:MET:HE3	1.83	0.60
12:M:406:ASN:ND2	12:M:688:GLN:O	2.29	0.60
16:Q:220:ALA:HB3	16:Q:224:ALA:HA	1.82	0.60
27:d:144:SER:O	27:d:158:LYS:NZ	2.31	0.60
12:M:650:SER:OG	12:M:652:ASN:OD1	2.18	0.60
32:i:254:LEU:HD23	40:r:127:VAL:HG22	1.82	0.60
37:n:27:LEU:HD21	53:u:201:CDL:H112	1.84	0.60
23:Z:31:THR:HG23	23:Z:35:LYS:NZ	2.17	0.60
6:G:84:LEU:HD21	6:G:100:VAL:HG22	1.84	0.60
12:M:251:ILE:HB	12:M:606:THR:HG22	1.84	0.60
41:s:87:VAL:CG2	41:s:88:PRO:HD3	2.27	0.60
33:j:68:GLU:HG2	36:m:161:LEU:HD13	1.82	0.60
41:s:88:PRO:HG2	41:s:105:MET:SD	2.42	0.60
53:u:201:CDL:H542	53:u:201:CDL:C58	2.26	0.60
1:A:372:GLU:OE2	14:O:33:GLY:N	2.35	0.59
33:j:18:VAL:HG22	41:s:222:MET:HG3	1.83	0.59
35:l:166:THR:CG2	47:l:703:PEE:H2	2.32	0.59
43:v:12:ASP:HB3	43:v:15:LYS:HB2	1.83	0.59
47:j:202:PEE:H40	41:s:302:MET:HE1	1.82	0.59
11:L:131:LYS:NZ	11:L:149:GLU:OE2	2.34	0.59
14:O:134:VAL:HG12	14:O:186:VAL:HG12	1.84	0.59
3:C:125:PRO:HB2	41:s:58:LYS:HE3	1.85	0.59
12:M:171:THR:HG23	12:M:173:MET:HE2	1.85	0.59
1:A:50:ASP:O	1:A:59:ARG:NH2	2.33	0.59
53:a:201:CDL:OB7	47:b:201:PEE:C11	2.50	0.59
40:r:231:LEU:HD12	40:r:235:LEU:HD12	1.85	0.59
41:s:87:VAL:N	41:s:88:PRO:HD2	2.17	0.59
12:M:496:ILE:O	12:M:500:ILE:HD12	2.03	0.59
9:J:208:GLY:N	9:J:211:ASP:CB	2.66	0.59
12:M:562:LYS:HE3	12:M:562:LYS:HA	1.85	0.59
1:A:134:ASP:OD1	1:A:137:LYS:HG3	2.03	0.58
12:M:250:SER:OG	12:M:251:ILE:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:88:ARG:NH2	14:O:190:ASP:OD2	2.36	0.58
15:P:125:ARG:NH2	15:P:201:ASP:OD2	2.32	0.58
26:c:139:PHE:CZ	26:c:143:MET:HE3	2.37	0.58
32:i:276:ILE:HG21	47:r:501:PEE:C11	2.33	0.58
32:i:325:LEU:HD13	53:i:401:CDL:H132	1.85	0.58
35:l:452:ASN:HA	35:l:455:LYS:HG2	1.85	0.58
1:A:64:LYS:HG2	1:A:67:GLU:HB2	1.84	0.58
1:A:217:GLU:OE1	11:L:171:ARG:NH2	2.36	0.58
12:M:545:LEU:HB3	12:M:566:ILE:HD13	1.85	0.58
12:M:395:GLU:O	12:M:425:ASN:ND2	2.36	0.58
32:i:84:TRP:HH2	34:k:59:MET:HE2	1.68	0.58
34:k:98:CYS:HB2	35:l:580:GLN:HB2	1.84	0.58
42:u:83:THR:HA	42:u:86:TRP:CD1	2.38	0.58
9:J:249:ILE:O	9:J:253:ILE:HG12	2.02	0.58
24:a:132:ASN:ND2	40:r:49:SER:O	2.30	0.58
32:i:276:ILE:HG21	47:r:501:PEE:H14	1.85	0.58
32:i:213:LEU:HD13	53:i:401:CDL:H141	1.84	0.58
9:J:87:GLU:OE1	9:J:87:GLU:HA	2.03	0.58
3:C:59:ARG:NH1	48:C:302:PLX:O3	2.31	0.58
22:Y:100:LEU:HB2	43:v:111:ARG:HH12	1.69	0.58
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.85	0.58
38:o:31:LYS:O	38:o:35:GLU:HG3	2.03	0.58
40:r:57:PHE:CE1	40:r:113:THR:HA	2.39	0.58
40:r:207:MET:HG2	40:r:298:ILE:HG13	1.85	0.58
41:s:98:MET:HE3	41:s:101:GLY:HA2	1.84	0.58
43:v:24:THR:OG1	43:v:105:GLU:OE2	2.20	0.58
47:B:303:PEE:H16	41:s:296:LEU:CD1	2.34	0.58
22:Y:71:TRP:NE1	22:Y:72:ARG:HH21	2.02	0.58
38:o:101:TRP:CB	40:r:263:MET:HE1	2.33	0.58
1:A:211:ALA:HB2	1:A:223:PRO:HG3	1.86	0.58
30:g:32:ARG:O	30:g:36:MET:HG2	2.03	0.58
1:A:396:MET:HE1	1:A:438:LEU:HD23	1.86	0.58
12:M:449:PRO:HB2	12:M:679:LEU:HD13	1.86	0.58
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.39	0.58
53:l:701:CDL:H391	40:r:371:PRO:HD2	1.85	0.58
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.38	0.58
5:F:42:VAL:HG23	12:M:671:LEU:HG	1.86	0.57
26:c:38:PRO:HB2	38:o:75:ASN:HD22	1.67	0.57
40:r:57:PHE:HE1	40:r:113:THR:HA	1.68	0.57
1:A:159:ARG:HD3	1:A:161:GLU:HB2	1.86	0.57
6:G:100:VAL:HG12	6:G:142:GLN:NE2	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:100:LEU:HD23	41:s:103:LEU:HD12	1.85	0.57
12:M:265:THR:HG22	12:M:270:VAL:HA	1.86	0.57
32:i:46:LYS:NZ	53:i:401:CDL:HB22	2.19	0.57
36:m:45:LEU:HD23	36:m:50:SER:HA	1.86	0.57
27:d:119:GLU:HG2	43:v:52:MET:HA	1.86	0.57
47:i:402:PEE:H36	47:i:402:PEE:C18	2.34	0.57
53:o:201:CDL:H781	53:o:201:CDL:C82	2.19	0.57
2:B:96:ARG:O	16:Q:219:GLY:HA3	2.04	0.57
2:B:192:ASN:ND2	18:T:61:GLU:OE2	2.37	0.57
7:H:54:GLU:HG2	7:H:58:MET:HE2	1.86	0.57
7:H:59:VAL:HG23	7:H:68:LEU:HD21	1.86	0.57
9:J:214:LEU:HD23	9:J:352:VAL:HG11	1.86	0.57
47:j:201:PEE:H71	41:s:56:PHE:CD2	2.39	0.57
44:w:204:VAL:CG2	44:w:249:MET:HE2	2.35	0.57
53:a:201:CDL:OA7	53:a:201:CDL:HA61	2.04	0.57
32:i:79:LEU:HB2	34:k:47:ILE:HD13	1.87	0.57
6:G:75:THR:C	6:G:77:GLU:H	2.13	0.57
9:J:214:LEU:CD2	9:J:352:VAL:HG11	2.35	0.57
9:J:168:SER:OG	9:J:188:GLU:OE2	2.19	0.56
16:Q:140:ASP:OD2	16:Q:143:SER:OG	2.22	0.56
25:b:121:LYS:HD3	43:v:40:VAL:HA	1.87	0.56
35:l:592:LEU:HG	35:l:596:MET:HE2	1.86	0.56
9:J:85:ARG:NE	50:J:401:NDP:O2X	2.37	0.56
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.24	0.56
27:d:36:ILE:O	27:d:40:LEU:HD23	2.04	0.56
47:i:402:PEE:H34	47:i:402:PEE:C25	2.30	0.56
35:l:375:ILE:HD12	35:l:458:LEU:HD11	1.86	0.56
43:v:51:LEU:O	43:v:52:MET:HG3	2.05	0.56
3:C:83:ARG:NH1	16:Q:212:GLU:OE2	2.27	0.56
8:I:8:ILE:O	8:I:12:ARG:HG3	2.06	0.56
9:J:171:ASN:HD21	9:J:326:ASP:HA	1.70	0.56
11:L:84:ARG:NH1	11:L:88:GLN:O	2.37	0.56
15:P:64:TYR:OH	15:P:103:HIS:NE2	2.37	0.56
6:X:153:ASP:OD1	25:b:19:ARG:NH2	2.39	0.56
22:Y:43:ARG:NH1	22:Y:47:PHE:O	2.38	0.56
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.87	0.56
6:X:119:ILE:HG21	6:X:135:ALA:HB1	1.86	0.56
32:i:171:ASN:ND2	35:l:578:SER:OG	2.30	0.56
42:u:44:MET:HB3	42:u:48:TRP:HZ3	1.69	0.56
44:w:165:SER:HB3	44:w:245:PHE:CD1	2.37	0.56
25:b:123:PHE:HB3	43:v:40:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:85:ARG:HD2	50:J:401:NDP:P2B	2.44	0.56
22:Y:94:ASP:HB3	22:Y:99:ILE:HB	1.86	0.56
31:h:69:ARG:O	31:h:73:MET:HG2	2.06	0.56
16:Q:172:VAL:HG21	16:Q:310:VAL:HG22	1.87	0.56
32:i:125:GLN:HG2	53:i:401:CDL:OA3	2.06	0.56
1:A:290:GLU:OE1	1:A:303:HIS:NE2	2.35	0.56
20:V:39:TYR:CZ	53:V:201:CDL:C59	2.86	0.56
32:i:316:GLN:NE2	44:w:95:ASP:OD1	2.37	0.56
34:k:8:ILE:HG21	34:k:43:MET:HB2	1.86	0.56
1:A:210:THR:HB	1:A:224:ARG:HG2	1.88	0.56
2:B:75:SER:HB3	8:I:15:ALA:HB3	1.88	0.56
3:C:146:SER:OG	16:Q:118:2MR:O	2.21	0.56
33:j:3:ILE:HD11	47:m:201:PEE:H50	1.88	0.56
35:l:72:GLN:NE2	40:r:459:TYR:O	2.39	0.56
40:r:225:ILE:HG13	40:r:229:MET:HE2	1.87	0.56
3:C:187:GLU:HB2	9:J:87:GLU:OE2	2.06	0.56
33:j:3:ILE:HD13	47:m:201:PEE:H50	1.88	0.56
37:n:13:VAL:HG12	40:r:14:MET:CG	2.30	0.56
40:r:447:LEU:HD11	48:r:503:PLX:H371	1.87	0.56
9:J:84:TYR:CE2	9:J:105:PHE:HB3	2.41	0.55
39:p:44:MET:HA	39:p:47:ARG:HG2	1.88	0.55
44:w:236:ASP:HA	44:w:239:ASN:ND2	2.21	0.55
27:d:99:ASP:HB3	28:e:137:MET:HE1	1.87	0.55
1:A:201:ALA:HA	14:O:121:MET:HE2	1.88	0.55
35:l:293:ILE:HG13	35:l:418:LEU:HD22	1.89	0.55
10:K:105:ARG:NH1	11:L:167:ASN:O	2.37	0.55
44:w:236:ASP:HA	44:w:239:ASN:HD21	1.71	0.55
2:B:98:ARG:HB3	2:B:169:GLU:CD	2.32	0.55
12:M:306:MET:HB3	12:M:314:LEU:HD22	1.89	0.55
12:M:498:GLN:HB2	12:M:669:ASN:ND2	2.21	0.55
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.47	0.55
9:J:135:GLU:OE2	9:J:179:ARG:NH2	2.40	0.55
24:a:160:MET:HE3	24:a:166:GLY:HA3	1.88	0.55
40:r:324:SER:OG	40:r:440:HIS:NE2	2.37	0.55
53:V:201:CDL:H601	53:V:201:CDL:H732	1.88	0.55
32:i:133:TRP:HE3	53:i:401:CDL:C39	2.18	0.55
9:J:80:VAL:C	9:J:81:ILE:HD12	2.32	0.55
6:X:111:ASP:OD2	39:p:52:LYS:NZ	2.30	0.55
32:i:72:MET:HB2	34:k:40:LEU:HD21	1.88	0.55
33:j:73:LEU:HD13	36:m:55:MET:HE1	1.89	0.55
35:l:272:LEU:HG	35:l:276:MET:HE2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:n:7:ILE:HB	37:n:11:HIS:HD2	1.71	0.55
6:G:154:VAL:HG23	6:G:154:VAL:O	2.07	0.55
6:X:123:GLU:CD	39:p:25:ARG:HH21	2.15	0.55
24:a:96:ALA:HB1	27:d:61:TYR:O	2.06	0.55
12:M:128:CYS:SG	12:M:140:GLN:NE2	2.79	0.54
12:M:408:ARG:HD2	12:M:439:THR:HG23	1.89	0.54
13:N:2:GLU:HG3	13:N:4:VAL:HG22	1.89	0.54
40:r:12:LEU:HB2	40:r:13:PRO:HD3	1.89	0.54
9:J:125:VAL:HG11	9:J:253:ILE:HD12	1.90	0.54
12:M:624:ARG:NH1	12:M:628:GLU:OE1	2.23	0.54
16:Q:41:VAL:O	16:Q:45:GLU:HG2	2.08	0.54
16:Q:47:PHE:HD1	16:Q:52:MET:HE1	1.72	0.54
7:H:77:ILE:O	7:H:81:ILE:HD12	2.08	0.54
12:M:133:GLN:HG3	12:M:136:GLU:HG3	1.89	0.54
16:Q:121:GLU:OE2	16:Q:463:ARG:NH1	2.39	0.54
22:Y:93:THR:OG1	22:Y:96:GLU:OE2	2.25	0.54
35:l:124:PHE:CD1	35:l:124:PHE:C	2.85	0.54
6:G:93:ILE:HD11	6:G:110:LEU:HD11	1.89	0.54
35:l:359:MET:O	35:l:436:ARG:NH2	2.40	0.54
1:A:307:VAL:HG21	1:A:314:LEU:HD12	1.89	0.54
1:A:385:CYS:HB3	45:A:501:SF4:S2	2.46	0.54
47:i:402:PEE:H42	47:i:402:PEE:C21	2.27	0.54
5:F:33:VAL:O	5:F:36:PHE:HB3	2.08	0.54
20:V:39:TYR:CE1	53:V:201:CDL:H581	2.42	0.54
36:m:17:PHE:O	36:m:21:SER:OG	2.24	0.54
3:C:69:LEU:HD23	16:Q:94:VAL:HG11	1.89	0.54
6:G:103:HIS:CE1	6:G:105:MET:HB2	2.43	0.54
12:M:308:ARG:NH2	12:M:578:PRO:O	2.41	0.54
6:X:155:TYR:CE1	25:b:23:LEU:HB3	2.42	0.54
27:d:159:GLN:NE2	28:e:142:PHE:O	2.28	0.54
47:r:501:PEE:C45	48:r:502:PLX:H191	2.38	0.54
5:F:42:VAL:HG21	12:M:670:GLU:HG3	1.90	0.54
6:G:103:HIS:ND1	6:G:106:LYS:HG2	2.23	0.54
22:Y:62:SER:OG	35:l:371:THR:OG1	2.26	0.54
7:H:76:GLN:O	7:H:79:GLU:HG2	2.08	0.54
24:a:82:VAL:O	24:a:86:ILE:HG12	2.07	0.54
35:l:124:PHE:CD2	35:l:247:LEU:HG	2.42	0.54
9:J:94:LEU:HA	9:J:97:MET:SD	2.48	0.53
11:L:86:ASN:ND2	12:M:275:PRO:O	2.41	0.53
12:M:224:ASP:OD2	12:M:291:ARG:NH2	2.32	0.53
12:M:297:LEU:O	12:M:301:ARG:NH1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.89	0.53
32:i:283:ALA:HB1	40:r:158:LEU:HD13	1.90	0.53
44:w:246:LEU:N	44:w:247:PRO:HD2	2.23	0.53
1:A:64:LYS:HD2	14:O:249:LEU:HD23	1.90	0.53
53:N:201:CDL:H532	53:N:201:CDL:C31	2.37	0.53
16:Q:184:ILE:HG12	16:Q:203:MET:HE3	1.90	0.53
12:M:394:VAL:HG22	12:M:473:MET:HE1	1.90	0.53
53:N:201:CDL:C55	53:N:201:CDL:C32	2.86	0.53
21:W:51:MET:SD	41:s:311:THR:HB	2.48	0.53
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.90	0.53
32:i:230:LEU:HD11	32:i:244:MET:HE1	1.91	0.53
48:j:203:PLX:H381	48:j:203:PLX:H322	1.89	0.53
53:l:701:CDL:H541	53:l:701:CDL:HA61	1.90	0.53
44:w:236:ASP:HA	44:w:239:ASN:CG	2.33	0.53
1:A:48:ARG:NH1	10:K:70:ASN:O	2.32	0.53
1:A:394:LYS:HB3	12:M:155:GLU:HG2	1.91	0.53
6:G:84:LEU:HB3	6:G:88:LYS:HZ3	1.74	0.53
47:V:202:PEE:C1	47:V:202:PEE:C4	2.86	0.53
53:r:505:CDL:H861	53:u:201:CDL:C82	2.35	0.53
22:Y:94:ASP:OD1	43:v:107:ARG:NH1	2.42	0.53
32:i:211:MET:HG2	32:i:333:SER:HB2	1.91	0.53
39:p:10:LEU:O	39:p:15:LYS:NZ	2.41	0.53
12:M:260:ASN:HD22	12:M:278:HIS:HB2	1.74	0.53
53:a:201:CDL:OB7	47:b:201:PEE:H14	2.08	0.53
25:b:106:PRO:HG2	25:b:120:MET:HE2	1.91	0.53
35:l:200:GLN:HG3	35:l:204:LEU:HD23	1.91	0.53
41:s:140:ILE:HA	41:s:143:GLU:HG2	1.91	0.53
6:G:76:LEU:N	6:G:76:LEU:HD23	2.24	0.53
22:Y:71:TRP:HE1	22:Y:72:ARG:HH21	1.55	0.53
24:a:98:LEU:HB2	27:d:63:TYR:CZ	2.44	0.53
47:b:201:PEE:H28	53:l:701:CDL:C27	2.31	0.53
26:c:167:TYR:HD2	26:c:168:LEU:HD22	1.74	0.53
40:r:9:THR:HG21	53:u:201:CDL:H242	1.90	0.53
4:E:29:LYS:NZ	49:G:201:8Q1:O35	2.40	0.53
32:i:20:VAL:HG11	32:i:137:ALA:HB1	1.89	0.53
34:k:22:TYR:HB3	35:l:585:LYS:HG2	1.91	0.53
6:G:84:LEU:HB3	6:G:88:LYS:NZ	2.24	0.53
23:Z:76:ALA:O	23:Z:80:VAL:HG23	2.09	0.53
27:d:73:ASP:OD1	27:d:91:GLN:NE2	2.42	0.53
36:m:1:MET:HE3	36:m:2:THR:N	2.24	0.53
36:m:27:ILE:HG13	41:s:70:MET:HE1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:171:VAL:HG13	39:p:172:THR:HG23	1.91	0.53
19:U:26:GLY:HA3	47:j:202:PEE:H37	1.91	0.52
32:i:115:VAL:HG12	32:i:180:ALA:HB1	1.91	0.52
16:Q:270:ASN:HB3	41:s:284:GLN:NE2	2.24	0.52
53:i:401:CDL:H331	53:i:401:CDL:OA9	2.09	0.52
40:r:403:THR:HA	40:r:406:TYR:CE2	2.44	0.52
1:A:86:ARG:HD3	1:A:339:PHE:CE2	2.45	0.52
41:s:102:VAL:HG11	41:s:154:LEU:HD11	1.92	0.52
22:Y:69:ILE:CD1	35:l:383:MET:CE	2.77	0.52
11:L:75:ARG:HD2	11:L:104:ARG:HH21	1.73	0.52
24:a:147:ALA:HB2	40:r:173:SER:HB2	1.92	0.52
24:a:170:GLN:OE1	42:u:151:ASN:ND2	2.41	0.52
28:e:76:TYR:HB2	28:e:83:ASP:OD1	2.09	0.52
32:i:12:THR:HG21	36:m:163:ILE:HG21	1.92	0.52
35:l:327:LEU:O	35:l:331:MET:HG2	2.10	0.52
1:A:177:TYR:HB3	10:K:96:PHE:HD2	1.73	0.52
6:X:93:ILE:HG13	6:X:93:ILE:O	2.08	0.52
22:Y:65:MET:HE1	35:l:378:LEU:HD12	1.91	0.52
2:B:153:ILE:HG21	3:C:142:TYR:CD1	2.44	0.52
3:C:66:THR:OG1	3:C:76:MET:SD	2.58	0.52
32:i:170:LEU:O	32:i:295:ARG:NH2	2.36	0.52
32:i:265:MET:HE3	32:i:340:THR:HG21	1.92	0.52
33:j:24:LEU:HD21	47:j:201:PEE:H62	1.91	0.52
35:l:150:MET:HE3	35:l:150:MET:HA	1.92	0.52
35:l:159:HIS:ND1	40:r:349:GLN:OE1	2.43	0.52
53:r:505:CDL:H742	53:r:505:CDL:H271	1.92	0.52
41:s:90:PRO:HD2	41:s:240:ILE:HD13	1.92	0.52
11:L:135:VAL:O	11:L:139:GLU:HG3	2.09	0.52
26:c:116:ARG:HG2	47:l:703:PEE:H49	1.91	0.52
40:r:336:ARG:NH2	40:r:433:GLU:OE1	2.43	0.52
18:T:78:GLU:OE2	18:T:119:ARG:NH1	2.43	0.52
53:a:201:CDL:H251	53:a:201:CDL:C21	2.27	0.52
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.91	0.52
44:w:204:VAL:HG21	44:w:249:MET:CE	2.40	0.52
4:E:39:TRP:O	4:E:43:VAL:HG23	2.10	0.52
35:l:253:VAL:HB	35:l:310:LEU:HD11	1.91	0.52
36:m:17:PHE:HA	36:m:20:PHE:CE1	2.45	0.52
1:A:88:ARG:HG3	1:A:246:GLU:OE1	2.10	0.51
12:M:636:TYR:CD2	12:M:642:VAL:HG22	2.45	0.51
16:Q:242:ASP:OD1	21:W:16:TYR:OH	2.25	0.51
1:A:318:ILE:HG12	1:A:326:LEU:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.45	0.51
9:J:64:PHE:CD1	9:J:210:GLU:HB2	2.45	0.51
12:M:144:MET:O	16:Q:362:LYS:NZ	2.43	0.51
32:i:43:VAL:HG11	32:i:129:LEU:HD23	1.90	0.51
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.45	0.51
3:C:51:ASP:HB2	3:C:190:LEU:HB2	1.92	0.51
16:Q:270:ASN:HB3	41:s:284:GLN:HE21	1.75	0.51
19:U:42:ALA:HB2	41:s:312:ALA:HA	1.93	0.51
25:b:75:VAL:O	25:b:79:VAL:HG23	2.11	0.51
32:i:325:LEU:CD1	53:i:401:CDL:H132	2.39	0.51
33:j:69:ILE:HD11	41:s:144:VAL:HG13	1.92	0.51
35:l:37:LYS:HD3	35:l:98:TRP:HE1	1.76	0.51
4:E:88:MET:HE1	15:P:171:TRP:CZ2	2.45	0.51
11:L:165:SER:O	11:L:171:ARG:NH1	2.43	0.51
16:Q:182:ASN:ND2	16:Q:403:PRO:HB2	2.26	0.51
25:b:79:VAL:HG22	35:l:10:THR:HG21	1.91	0.51
32:i:155:LEU:HD12	32:i:278:MET:SD	2.50	0.51
35:l:237:MET:HB3	35:l:299:LYS:HE2	1.92	0.51
38:o:80:PHE:HE1	38:o:86:THR:HG21	1.75	0.51
40:r:78:MET:HE1	40:r:439:LEU:HD12	1.91	0.51
44:w:146:ALA:HB1	44:w:157:VAL:HG21	1.93	0.51
9:J:81:ILE:N	9:J:81:ILE:CD1	2.73	0.51
9:J:171:ASN:ND2	9:J:327:MET:H	2.09	0.51
9:J:212:ARG:O	9:J:216:TYR:HB3	2.09	0.51
20:V:113:ALA:CB	47:V:202:PEE:H53	2.40	0.51
40:r:371:PRO:O	40:r:448:THR:OG1	2.29	0.51
43:v:22:MET:HE1	43:v:102:PHE:HA	1.91	0.51
4:E:84:ILE:HG22	4:E:88:MET:HE2	1.93	0.51
23:Z:24:ILE:O	23:Z:27:THR:OG1	2.21	0.51
26:c:153:TYR:HB3	35:l:403:TYR:HD1	1.74	0.51
32:i:95:MET:HE2	32:i:95:MET:O	2.10	0.51
32:i:128:LEU:HD12	32:i:216:PHE:HB2	1.92	0.51
44:w:66:ILE:HA	56:w:401:ADP:O2A	2.10	0.51
6:X:120:MET:HE1	39:p:24:LEU:HB2	1.93	0.51
33:j:27:LEU:CD1	47:j:201:PEE:C12	2.82	0.51
8:I:6:ARG:O	8:I:10:LEU:HG	2.10	0.51
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.45	0.51
20:V:53:VAL:HA	20:V:56:THR:HG22	1.92	0.51
8:I:40:LYS:HB3	21:W:7:LYS:H	1.76	0.51
35:l:289:ALA:O	35:l:293:ILE:HG12	2.11	0.51
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:115:PRO:HG3	15:P:219:VAL:HG21	1.93	0.51
12:M:304:GLN:HG2	12:M:615:LEU:HD12	1.92	0.51
12:M:483:ARG:HH22	12:M:682:ASP:HB2	1.76	0.51
20:V:39:TYR:HB3	53:V:201:CDL:OB9	2.11	0.51
27:d:78:GLU:OE2	30:g:108:LYS:HG3	2.10	0.51
35:l:245:ALA:O	35:l:249:SER:OG	2.20	0.51
41:s:87:VAL:CG2	41:s:88:PRO:CD	2.88	0.51
1:A:157:TYR:HB3	1:A:212:LEU:HD11	1.91	0.50
11:L:156:LYS:HE2	12:M:68:ARG:HE	1.76	0.50
20:V:61:PHE:HD2	20:V:104:ARG:HH21	1.58	0.50
26:c:84:GLN:OE1	26:c:120:SER:OG	2.27	0.50
26:c:117:VAL:HG21	35:l:539:TYR:HB2	1.93	0.50
32:i:129:LEU:HD13	53:i:401:CDL:H341	1.93	0.50
35:l:237:MET:HE2	35:l:303:ALA:HB2	1.92	0.50
36:m:173:ARG:HG3	36:m:173:ARG:HH11	1.76	0.50
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.93	0.50
12:M:266:ARG:HD2	12:M:267:THR:HG23	1.94	0.50
14:O:76:ALA:O	14:O:79:VAL:HG23	2.11	0.50
14:O:130:TYR:HA	14:O:189:ASN:HD21	1.75	0.50
15:P:155:SER:OG	15:P:167:GLU:OE2	2.24	0.50
36:m:62:GLY:HA3	41:s:110:SER:HB3	1.93	0.50
38:o:23:TYR:OH	39:p:68:GLU:OE1	2.29	0.50
1:A:156:ILE:HB	1:A:197:VAL:HG22	1.92	0.50
11:L:116:SER:OG	15:P:227:ALA:O	2.23	0.50
21:W:98:MET:HG3	21:W:104:TRP:CD1	2.47	0.50
28:e:146:LYS:HE2	28:e:146:LYS:HA	1.93	0.50
32:i:177:LYS:NZ	34:k:97:GLN:O	2.31	0.50
33:j:54:LYS:HD3	33:j:113:TRP:HA	1.93	0.50
35:l:562:LEU:HB3	35:l:563:PRO:HD3	1.93	0.50
9:J:86:CYS:HB3	50:J:401:NDP:O1X	2.10	0.50
14:O:179:ALA:HB3	14:O:185:MET:SD	2.50	0.50
15:P:66:ALA:HA	15:P:73:VAL:HG11	1.94	0.50
20:V:108:TYR:HE2	53:o:201:CDL:OA6	1.95	0.50
6:X:94:ASP:OD1	6:X:94:ASP:N	2.44	0.50
40:r:299:VAL:O	40:r:303:ILE:HG12	2.12	0.50
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.93	0.50
6:X:83:VAL:HG22	6:X:122:MET:HE2	1.94	0.50
24:a:98:LEU:HD12	27:d:63:TYR:O	2.12	0.50
35:l:596:MET:O	35:l:600:THR:HG23	2.11	0.50
53:l:701:CDL:H521	48:r:503:PLX:H222	1.93	0.50
2:B:100:GLU:OE2	2:B:193:ASN:ND2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:75:THR:C	6:G:77:GLU:N	2.68	0.50
14:O:182:ASN:OD1	14:O:222:ARG:NH2	2.44	0.50
35:l:418:LEU:HD23	53:l:702:CDL:H562	1.94	0.50
39:p:100:PRO:HG3	40:r:419:TYR:CZ	2.47	0.50
1:A:406:PRO:HA	1:A:450:MET:HE1	1.94	0.50
3:C:184:ILE:O	3:C:187:GLU:HG2	2.11	0.50
53:N:201:CDL:H532	53:N:201:CDL:OA9	2.12	0.50
31:h:38:LYS:O	31:h:42:GLU:HG3	2.11	0.50
35:l:304:PHE:CZ	35:l:526:LEU:HD22	2.47	0.50
53:o:201:CDL:H791	53:o:201:CDL:C83	2.26	0.50
1:A:263:ALA:HA	1:A:271:SER:HB2	1.94	0.50
9:J:162:GLU:HG3	9:J:163:LYS:HG3	1.94	0.50
12:M:501:ARG:HH21	12:M:665:PHE:HD2	1.58	0.50
15:P:100:LEU:O	15:P:108:PHE:N	2.38	0.50
31:h:7:GLN:O	31:h:11:GLY:N	2.45	0.50
47:i:402:PEE:C20	35:l:562:LEU:HG	2.42	0.50
35:l:417:SER:HB2	35:l:493:VAL:HG22	1.93	0.50
40:r:198:ALA:HB2	47:r:501:PEE:H22	1.93	0.50
1:A:244:ASN:N	46:A:502:FMN:O1P	2.44	0.49
27:d:110:LEU:HD11	35:l:203:MET:HG2	1.93	0.49
35:l:380:LEU:C	35:l:380:LEU:CD2	2.85	0.49
37:n:30:ARG:CD	53:u:201:CDL:OA4	2.60	0.49
44:w:87:PRO:O	44:w:142:GLN:NE2	2.45	0.49
4:E:128:PRO:HD2	11:L:104:ARG:HH12	1.77	0.49
20:V:113:ALA:HB3	47:V:202:PEE:H53	1.93	0.49
22:Y:92:TRP:O	43:v:107:ARG:NH2	2.40	0.49
32:i:268:GLN:HG3	42:u:168:PHE:HZ	1.78	0.49
44:w:235:GLN:O	44:w:239:ASN:OD1	2.31	0.49
1:A:129:GLU:OE2	1:A:133:HIS:ND1	2.44	0.49
1:A:277:ASN:ND2	1:A:287:THR:OG1	2.45	0.49
3:C:101:ASP:OD2	41:s:54:LYS:HD2	2.12	0.49
9:J:169:HIS:HD2	9:J:171:ASN:H	1.61	0.49
16:Q:196:ALA:O	16:Q:197:MET:HG2	2.11	0.49
16:Q:335:GLU:OE1	16:Q:339:GLN:NE2	2.44	0.49
22:Y:71:TRP:CD1	22:Y:72:ARG:HH21	2.30	0.49
26:c:184:TYR:HA	43:v:34:ARG:HH12	1.78	0.49
27:d:115:GLN:HG2	35:l:62:ILE:HG12	1.94	0.49
40:r:82:SER:OG	40:r:335:GLU:OE1	2.28	0.49
1:A:56:ALA:HB1	1:A:61:ASP:HB2	1.95	0.49
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.45	0.49
9:J:116:ILE:O	9:J:120:VAL:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:179:ILE:HG21	31:h:38:LYS:HG3	1.93	0.49
35:l:6:SER:O	35:l:10:THR:OG1	2.15	0.49
35:l:151:SER:HB3	35:l:252:MET:HE2	1.95	0.49
4:E:16:SER:HB3	11:L:52:LEU:HD12	1.94	0.49
24:a:50:HIS:HB3	24:a:52:LYS:HZ2	1.77	0.49
32:i:125:GLN:CG	53:i:401:CDL:OA3	2.61	0.49
33:j:17:LEU:HA	33:j:20:ILE:HG12	1.93	0.49
35:l:176:ARG:HA	35:l:179:ASP:HB2	1.94	0.49
12:M:63:PHE:O	12:M:181:ARG:NH2	2.44	0.49
17:S:54:ILE:HD12	42:u:19:LYS:HA	1.94	0.49
20:V:123:ALA:O	20:V:127:MET:HG3	2.12	0.49
26:c:154:GLN:HA	26:c:154:GLN:NE2	2.27	0.49
1:A:140:GLU:OE2	1:A:256:ARG:NH2	2.46	0.49
2:B:99:GLY:N	2:B:170:GLY:O	2.46	0.49
13:N:3:LEU:CD1	53:N:201:CDL:H311	2.38	0.49
16:Q:136:PHE:HB3	16:Q:147:ASN:HB3	1.94	0.49
53:l:701:CDL:H311	53:l:701:CDL:H561	1.94	0.49
8:I:70:MET:HE2	15:P:66:ALA:HB1	1.94	0.49
9:J:207:PHE:HB2	9:J:214:LEU:HD13	1.94	0.49
41:s:307:LEU:HA	41:s:310:MET:HE3	1.94	0.49
1:A:132:ARG:HB3	1:A:165:GLU:HB3	1.94	0.49
2:B:124:PRO:HB2	3:C:142:TYR:HE1	1.77	0.49
4:E:98:LYS:HB3	4:E:102:HIS:HB2	1.93	0.49
12:M:70:SER:O	12:M:184:ARG:NH1	2.46	0.49
2:B:177:THR:HG22	2:B:179:THR:H	1.76	0.49
9:J:212:ARG:O	9:J:216:TYR:CB	2.60	0.49
21:W:128:ARG:NH1	31:h:102:GLU:OE2	2.33	0.49
6:X:115:GLN:O	6:X:119:ILE:HG12	2.13	0.49
32:i:119:THR:HG22	32:i:176:ARG:HB3	1.95	0.49
40:r:188:ASN:OD1	40:r:256:TYR:OH	2.30	0.49
41:s:24:GLU:OE1	41:s:228:TYR:OH	2.29	0.49
42:u:106:LYS:O	42:u:109:GLU:HG3	2.13	0.49
7:H:116:ILE:HG13	15:P:121:THR:HG21	1.95	0.48
25:b:87:LYS:HZ3	35:l:1:MET:HG3	1.78	0.48
38:o:60:ILE:HD12	40:r:422:HIS:HB2	1.95	0.48
41:s:235:ASN:ND2	41:s:270:PHE:CE2	2.76	0.48
44:w:91:ILE:HD11	44:w:131:LEU:HD12	1.95	0.48
44:w:170:LEU:HD22	44:w:187:TYR:CD1	2.48	0.48
12:M:94:MET:HE2	12:M:100:TRP:HH2	1.78	0.48
13:N:11:LEU:HA	13:N:14:VAL:HG12	1.95	0.48
16:Q:148:GLU:HB3	16:Q:227:ILE:HB	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:h:86:LEU:HA	31:h:89:GLU:HG2	1.94	0.48
32:i:10:ILE:HG21	53:i:401:CDL:H531	1.94	0.48
35:l:566:THR:O	35:l:570:GLN:HG2	2.13	0.48
40:r:74:PRO:O	40:r:78:MET:HG3	2.13	0.48
44:w:59:VAL:HG13	44:w:201:PRO:HA	1.95	0.48
4:E:101:THR:O	4:E:105:ARG:HG3	2.12	0.48
6:G:123:GLU:HG2	6:G:130:ILE:HG13	1.95	0.48
16:Q:102:SER:OG	16:Q:107:ARG:NH1	2.47	0.48
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.94	0.48
32:i:66:ALA:HB2	32:i:104:MET:HB3	1.94	0.48
37:n:30:ARG:HG3	37:n:30:ARG:HH11	1.78	0.48
44:w:143:TYR:OH	44:w:199:LEU:O	2.26	0.48
17:S:49:GLU:OE2	17:S:52:ARG:NH1	2.45	0.48
6:X:137:LYS:HD3	25:b:4:TYR:CE1	2.49	0.48
32:i:280:THR:O	32:i:284:MET:HG2	2.13	0.48
35:l:55:MET:HE2	35:l:471:ASN:HB3	1.95	0.48
48:r:502:PLX:H51	48:r:502:PLX:H6	1.42	0.48
12:M:197:THR:N	14:O:114:GLU:OE2	2.44	0.48
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.96	0.48
40:r:260:PRO:HG2	48:r:502:PLX:H132	1.95	0.48
4:E:101:THR:OG1	15:P:219:VAL:O	2.21	0.48
12:M:178:GLN:HG2	12:M:204:MET:HE3	1.96	0.48
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.48	0.48
32:i:234:TRP:CZ2	32:i:304:MET:HB3	2.49	0.48
53:l:701:CDL:H312	53:l:701:CDL:H761	1.95	0.48
37:n:50:ARG:HB2	37:n:53:GLU:HB2	1.96	0.48
44:w:208:ASP:OD2	44:w:242:LYS:NZ	2.30	0.48
2:B:89:GLU:HG2	13:N:58:ARG:HA	1.94	0.48
7:H:96:ARG:HG2	7:H:96:ARG:HH11	1.78	0.48
26:c:105:ILE:HG23	26:c:109:LEU:HD12	1.95	0.48
44:w:180:ARG:NH1	44:w:316:GLU:OE2	2.47	0.48
6:G:113:LEU:O	6:G:117:GLU:HG3	2.14	0.48
8:I:27:ARG:NH1	16:Q:212:GLU:OE1	2.43	0.48
10:K:87:LEU:O	10:K:91:VAL:HG23	2.13	0.48
33:j:25:PRO:HB2	41:s:60:PRO:HD3	1.96	0.48
37:n:26:TYR:HD2	37:n:27:LEU:HD12	1.79	0.48
1:A:86:ARG:HH12	1:A:339:PHE:HB2	1.77	0.48
8:I:61:ARG:NH2	12:M:145:MET:O	2.42	0.48
12:M:29:SER:OG	12:M:30:ASN:N	2.45	0.48
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	1.96	0.48
25:b:104:ILE:HD13	27:d:18:PRO:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:557:TRP:O	35:l:561:ILE:HG12	2.13	0.48
53:l:702:CDL:H781	53:l:702:CDL:H751	1.55	0.48
36:m:25:SER:O	36:m:27:ILE:N	2.46	0.48
14:O:201:ILE:O	14:O:205:ILE:HG12	2.14	0.48
16:Q:218:SER:OG	16:Q:224:ALA:CB	2.61	0.48
22:Y:72:ARG:CB	35:l:385:TYR:CD2	2.90	0.48
27:d:11:PRO:HD2	27:d:109:ARG:HD2	1.95	0.48
48:g:201:PLX:H352	32:i:342:ALA:HB3	1.95	0.48
32:i:236:LYS:HG2	32:i:237:MET:HG3	1.96	0.48
32:i:310:ASN:HB2	44:w:309:THR:HG22	1.95	0.48
35:l:186:MET:HG2	35:l:196:TRP:NE1	2.29	0.48
41:s:267:THR:O	41:s:271:LEU:HG	2.14	0.48
1:A:408:GLU:O	1:A:411:SER:HB3	2.14	0.47
20:V:136:PHE:CE1	32:i:278:MET:HE1	2.49	0.47
35:l:18:PRO:HB2	35:l:122:LEU:CD2	2.44	0.47
40:r:76:MET:HA	40:r:229:MET:HE1	1.96	0.47
1:A:288:VAL:HG11	1:A:303:HIS:HB3	1.97	0.47
4:E:52:LEU:HB3	4:E:54:ILE:HG12	1.95	0.47
5:F:45:LYS:HB3	12:M:671:LEU:HD21	1.95	0.47
9:J:84:TYR:HE2	9:J:105:PHE:HB3	1.76	0.47
9:J:153:ALA:HB2	9:J:191:VAL:HG23	1.95	0.47
14:O:198:PRO:O	14:O:202:GLU:HG3	2.13	0.47
23:Z:39:ARG:HG3	23:Z:41:LEU:HD12	1.96	0.47
28:e:98:VAL:HG22	40:r:36:LEU:HB2	1.95	0.47
32:i:154:MET:HE2	32:i:191:THR:HB	1.96	0.47
37:n:30:ARG:NE	53:u:201:CDL:OA4	2.47	0.47
39:p:81:ILE:HG22	39:p:85:SER:HB2	1.96	0.47
39:p:92:GLU:HB3	39:p:95:GLU:HG3	1.97	0.47
48:C:302:PLX:H393	48:C:302:PLX:H191	1.97	0.47
23:Z:32:VAL:HG13	39:p:39:TYR:HB2	1.96	0.47
35:l:119:LYS:HE3	53:l:701:CDL:H512	1.97	0.47
35:l:363:TYR:HD1	35:l:370:THR:HG21	1.79	0.47
35:l:552:LEU:HD21	38:o:90:GLY:HA2	1.96	0.47
1:A:102:MET:HG3	1:A:149:MET:HB3	1.95	0.47
14:O:110:MET:O	14:O:114:GLU:HG3	2.14	0.47
25:b:32:GLU:HG3	39:p:115:TYR:HA	1.95	0.47
27:d:37:PHE:CE2	35:l:3:PRO:HB3	2.49	0.47
27:d:142:ARG:NE	28:e:138:GLU:O	2.46	0.47
53:o:201:CDL:H321	53:o:201:CDL:H112	1.95	0.47
12:M:467:LYS:HE3	12:M:503:SER:HB2	1.96	0.47
12:M:638:THR:O	12:M:642:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.97	0.47
47:i:402:PEE:H31	35:l:562:LEU:CG	2.45	0.47
2:B:68:ARG:HD3	16:Q:260:GLU:OE2	2.15	0.47
36:m:38:GLY:HA3	47:m:201:PEE:H40	1.96	0.47
40:r:457:PRO:HG2	40:r:458:LEU:HD12	1.96	0.47
55:s:401:UQ:H101	55:s:401:UQ:H121	1.61	0.47
44:w:86:PHE:HB2	44:w:159:LEU:HD23	1.97	0.47
3:C:94:ARG:HH21	16:Q:192:LEU:HD21	1.80	0.47
9:J:37:HIS:HB3	9:J:40:LEU:HD12	1.97	0.47
18:T:82:ARG:NH1	18:T:103:ASP:OD1	2.48	0.47
19:U:56:PRO:HG2	42:u:45:LEU:HB2	1.97	0.47
6:X:125:GLU:HG2	35:l:439:PRO:HG2	1.97	0.47
6:X:155:TYR:HE1	25:b:23:LEU:HD22	1.79	0.47
32:i:38:LEU:HD12	34:k:73:LEU:HD22	1.96	0.47
32:i:118:VAL:O	32:i:122:ILE:HG12	2.14	0.47
53:l:701:CDL:H401	40:r:445:LEU:HD22	1.97	0.47
38:o:59:VAL:HG23	40:r:423:ILE:HG12	1.96	0.47
48:r:504:PLX:H72	48:r:504:PLX:H101	1.62	0.47
42:u:134:ASP:OD1	42:u:134:ASP:N	2.45	0.47
6:G:114:ASP:O	6:G:118:ILE:HG12	2.15	0.47
11:L:109:ASN:N	11:L:114:TRP:O	2.40	0.47
15:P:69:LEU:O	15:P:73:VAL:HG12	2.14	0.47
21:W:70:ALA:HB2	42:u:125:LEU:HD13	1.97	0.47
27:d:9:VAL:HG13	27:d:10:TYR:CD2	2.50	0.47
36:m:11:THR:O	36:m:15:ILE:HG12	2.15	0.47
39:p:10:LEU:HB2	39:p:15:LYS:HZ2	1.80	0.47
41:s:88:PRO:CG	41:s:105:MET:SD	3.02	0.47
44:w:235:GLN:O	44:w:239:ASN:CG	2.58	0.47
12:M:360:ARG:HG2	12:M:632:MET:HB3	1.96	0.47
16:Q:137:ASP:HB3	16:Q:223:HIS:ND1	2.29	0.47
20:V:110:ILE:HD13	47:V:202:PEE:H48	1.97	0.47
34:k:34:GLU:OE1	36:m:64:MET:HE1	2.15	0.47
35:l:291:CYS:O	35:l:295:GLN:HG2	2.14	0.47
35:l:407:TRP:O	35:l:411:MET:HG2	2.14	0.47
1:A:284:HIS:HD2	14:O:228:ALA:HB3	1.80	0.47
1:A:303:HIS:ND1	14:O:232:THR:OG1	2.39	0.47
7:H:26:ILE:O	7:H:30:LYS:HG3	2.13	0.47
27:d:26:LEU:HD23	43:v:75:PRO:HB2	1.96	0.47
1:A:85:LEU:HD23	1:A:95:THR:HG21	1.96	0.46
12:M:278:HIS:CE1	12:M:280:ASP:HB2	2.50	0.46
14:O:55:PHE:HB2	14:O:60:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:102:GLY:HA2	20:V:110:ILE:HG23	1.96	0.46
21:W:63:GLU:OE2	42:u:119:ARG:NH2	2.48	0.46
27:d:117:GLU:HG3	27:d:124:ASN:HB2	1.97	0.46
35:l:390:TYR:OH	35:l:466:PHE:HD1	1.98	0.46
44:w:132:GLN:NE2	44:w:166:ASP:OD1	2.48	0.46
3:C:144:HIS:O	3:C:151:ARG:NH1	2.48	0.46
6:X:98:LEU:C	6:X:98:LEU:CD1	2.88	0.46
25:b:73:THR:HA	25:b:77:ILE:HD12	1.97	0.46
27:d:107:GLN:O	27:d:111:LYS:HG3	2.15	0.46
33:j:94:LEU:HD12	36:m:147:TYR:HE1	1.80	0.46
40:r:97:THR:HG21	53:r:505:CDL:H242	1.96	0.46
44:w:258:TYR:CE2	44:w:269:VAL:HG22	2.50	0.46
12:M:47:THR:HG23	12:M:51:GLN:HB2	1.97	0.46
15:P:162:ALA:HB2	16:Q:286:TYR:C	2.41	0.46
24:a:108:GLU:N	24:a:111:GLU:OE1	2.39	0.46
32:i:72:MET:HE3	32:i:76:ILE:HG13	1.98	0.46
53:l:701:CDL:H581	53:l:701:CDL:H611	1.71	0.46
3:C:67:PHE:HB3	3:C:69:LEU:HG	1.97	0.46
5:F:64:LYS:HZ1	5:F:76:ASN:HB2	1.80	0.46
12:M:141:ASP:O	12:M:145:MET:HG2	2.15	0.46
12:M:371:VAL:HG12	12:M:533:GLY:HA2	1.98	0.46
12:M:544:VAL:HG23	12:M:565:PHE:HB3	1.96	0.46
16:Q:182:ASN:HD22	16:Q:403:PRO:HB2	1.80	0.46
16:Q:450:ILE:O	16:Q:454:GLN:HG3	2.14	0.46
22:Y:41:GLU:OE1	22:Y:41:GLU:N	2.47	0.46
22:Y:87:PRO:HG2	43:v:96:VAL:HG22	1.98	0.46
35:l:8:THR:HB	35:l:82:MET:SD	2.55	0.46
35:l:250:SER:CB	35:l:333:ALA:HA	2.45	0.46
40:r:10:MET:HE1	53:r:505:CDL:H632	1.97	0.46
7:H:24:LEU:HD11	7:H:77:ILE:HD11	1.96	0.46
9:J:369:VAL:HG12	9:J:370:LYS:HG2	1.97	0.46
17:S:12:MET:HE1	41:s:20:LEU:HD13	1.98	0.46
30:g:60:LEU:HD13	44:w:353:TRP:HB2	1.97	0.46
36:m:23:LYS:N	36:m:24:PRO:HD3	2.31	0.46
39:p:20:TYR:CZ	39:p:24:LEU:HD11	2.50	0.46
2:B:140:ARG:O	2:B:141:ARG:NH1	2.39	0.46
28:e:97:ILE:O	28:e:101:LEU:HB2	2.15	0.46
32:i:245:MET:HE1	53:r:505:CDL:H171	1.98	0.46
35:l:127:THR:HG21	35:l:146:GLY:HA3	1.98	0.46
47:m:201:PEE:H18	47:m:201:PEE:H24	1.67	0.46
17:S:47:LEU:HD22	42:u:22:SER:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:146:ASP:OD2	25:b:16:ARG:NH1	2.49	0.46
47:b:201:PEE:H38	35:l:66:TRP:HZ3	1.81	0.46
33:j:70:ALA:HA	33:j:73:LEU:HD12	1.98	0.46
35:l:559:GLU:O	35:l:563:PRO:HD2	2.15	0.46
40:r:370:PRO:HD3	40:r:375:LEU:HD22	1.96	0.46
1:A:62:TRP:CD2	1:A:181:LEU:HD13	2.51	0.46
5:F:24:CYS:O	5:F:34:ARG:NH1	2.48	0.46
11:L:92:ASN:HB3	15:P:238:PRO:HA	1.98	0.46
12:M:217:GLU:HG2	12:M:218:LEU:HG	1.98	0.46
24:a:187:PRO:HA	42:u:48:TRP:CD1	2.50	0.46
30:g:52:ARG:NH2	32:i:318:GLU:OE2	2.40	0.46
47:j:201:PEE:O5	47:j:201:PEE:H52	2.16	0.46
39:p:140:LEU:O	39:p:144:THR:HG23	2.16	0.46
3:C:126:GLU:O	3:C:128:ARG:N	2.49	0.46
4:E:89:GLU:OE1	4:E:106:PHE:HZ	1.99	0.46
8:I:46:SER:HB2	16:Q:359:ASP:OD2	2.16	0.46
9:J:92:MET:SD	9:J:95:ARG:HD2	2.56	0.46
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.98	0.46
53:a:201:CDL:H211	53:a:201:CDL:H182	1.59	0.46
26:c:38:PRO:HB2	38:o:75:ASN:ND2	2.30	0.46
32:i:95:MET:CE	32:i:95:MET:CA	2.86	0.46
53:l:701:CDL:H801	48:r:503:PLX:H212	1.98	0.46
38:o:112:LYS:O	38:o:116:ILE:HG12	2.15	0.46
10:K:82:SER:OG	10:K:83:THR:N	2.49	0.46
16:Q:180:LEU:HB3	16:Q:210:MET:HE1	1.98	0.46
20:V:35:ILE:HD13	53:V:201:CDL:H802	1.98	0.46
23:Z:22:TRP:HB3	23:Z:50:ALA:HB3	1.97	0.46
35:l:160:GLY:H	39:p:96:CYS:HB3	1.81	0.46
39:p:36:LYS:HB3	39:p:36:LYS:HE2	1.77	0.46
41:s:18:ALA:HB2	55:s:401:UQ:H152	1.97	0.46
6:G:76:LEU:N	6:G:76:LEU:CD2	2.79	0.45
12:M:340:ALA:HB1	12:M:354:LEU:HD21	1.98	0.45
12:M:637:ASP:N	12:M:641:GLN:OE1	2.39	0.45
14:O:56:THR:HG23	14:O:89:GLN:NE2	2.30	0.45
14:O:131:HIS:NE2	14:O:172:ILE:HD12	2.31	0.45
16:Q:148:GLU:OE1	16:Q:225:ALA:CA	2.50	0.45
27:d:163:MET:HE2	28:e:149:LEU:HD21	1.98	0.45
32:i:270:MET:HE3	32:i:279:PRO:HG3	1.98	0.45
53:l:701:CDL:H652	48:r:503:PLX:H122	1.97	0.45
11:L:89:SER:O	12:M:59:GLN:NE2	2.49	0.45
12:M:64:CYS:O	12:M:184:ARG:NH2	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:58:ARG:O	21:W:62:ILE:HG13	2.17	0.45
32:i:61:LEU:HD11	34:k:26:LEU:HD11	1.98	0.45
40:r:212:LEU:HD22	47:r:501:PEE:H46	1.97	0.45
2:B:171:PRO:HB2	13:N:93:MET:HE1	1.98	0.45
19:U:18:VAL:HG11	41:s:292:SER:HA	1.97	0.45
14:O:197:THR:H	14:O:200:ASP:HB2	1.81	0.45
16:Q:438:MET:HE2	16:Q:438:MET:HB3	1.86	0.45
23:Z:49:GLU:OE1	39:p:34:ARG:HB3	2.16	0.45
48:g:201:PLX:H301	32:i:347:ASN:HB3	1.98	0.45
35:l:233:LEU:HB3	35:l:234:PRO:HD3	1.98	0.45
39:p:26:HIS:CD2	39:p:79:PRO:HB3	2.51	0.45
39:p:28:GLU:HB2	39:p:37:TYR:CE1	2.51	0.45
42:u:44:MET:HE3	42:u:48:TRP:CZ3	2.52	0.45
3:C:88:ARG:HA	41:s:37:PRO:HA	1.98	0.45
21:W:128:ARG:HB3	21:W:132:GLU:OE2	2.17	0.45
23:Z:31:THR:HG23	23:Z:35:LYS:HZ1	1.82	0.45
30:g:122:ARG:NH2	38:o:113:GLU:OE2	2.49	0.45
32:i:80:TYR:CD2	32:i:91:ASN:OD1	2.70	0.45
36:m:51:PHE:CD2	36:m:143:ILE:HD13	2.52	0.45
38:o:48:LEU:HB3	39:p:166:LEU:HD13	1.97	0.45
39:p:127:ARG:HG2	39:p:130:ARG:HH21	1.80	0.45
2:B:85:ASN:HB3	2:B:89:GLU:OE1	2.17	0.45
25:b:108:ASP:OD1	43:v:68:LYS:HE3	2.17	0.45
47:j:202:PEE:H35	47:j:202:PEE:H30	1.49	0.45
40:r:231:LEU:HA	40:r:235:LEU:HB2	1.98	0.45
53:r:505:CDL:H832	53:r:505:CDL:H862	1.72	0.45
3:C:75:GLU:HG3	3:C:167:PRO:HB2	1.98	0.45
4:E:15:THR:OG1	11:L:55:VAL:O	2.30	0.45
16:Q:293:LEU:HD22	16:Q:298:ILE:HD12	1.98	0.45
24:a:82:VAL:HG11	28:e:104:THR:HG21	1.98	0.45
25:b:100:ARG:HB2	35:l:60:GLU:HB2	1.99	0.45
48:g:201:PLX:H1C3	48:g:201:PLX:H22	1.75	0.45
47:i:402:PEE:C18	47:i:402:PEE:C22	2.95	0.45
34:k:23:ARG:HD3	36:m:23:LYS:HB2	1.98	0.45
47:r:501:PEE:H74	47:r:501:PEE:H34	1.98	0.45
1:A:185:ASN:C	1:A:187:CYS:H	2.24	0.45
16:Q:184:ILE:HD11	16:Q:251:PHE:HZ	1.79	0.45
53:i:401:CDL:OA7	53:i:401:CDL:HA62	2.16	0.45
39:p:55:LYS:HE3	39:p:55:LYS:HA	1.98	0.45
53:r:505:CDL:H401	53:r:505:CDL:H211	1.97	0.45
2:B:93:LEU:O	8:I:34:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:14:VAL:HG23	13:N:23:TYR:CG	2.52	0.45
21:W:144:THR:HG21	47:m:201:PEE:H3	1.99	0.45
23:Z:90:SER:O	23:Z:90:SER:OG	2.35	0.45
24:a:139:ILE:O	24:a:143:GLU:HG2	2.17	0.45
30:g:108:LYS:HD2	30:g:108:LYS:HA	1.87	0.45
35:l:173:LEU:HD12	40:r:405:LEU:HD21	1.98	0.45
35:l:338:MET:CE	35:l:458:LEU:HA	2.47	0.45
44:w:129:TYR:CE2	44:w:183:CYS:HB3	2.52	0.45
1:A:141:GLY:HA3	1:A:248:VAL:O	2.17	0.45
12:M:260:ASN:HD21	12:M:278:HIS:HD2	1.65	0.45
53:N:201:CDL:CA7	53:N:201:CDL:C34	2.95	0.45
19:U:38:TYR:HB2	41:s:310:MET:O	2.17	0.45
6:X:99:SER:H	6:X:102:SER:HB2	1.82	0.45
32:i:26:TRP:HB3	32:i:74:ILE:HD13	1.98	0.45
47:i:402:PEE:H25	40:r:151:PHE:CB	2.47	0.45
33:j:49:LEU:N	33:j:50:PRO:HD2	2.32	0.45
38:o:91:ALA:O	38:o:95:ILE:HB	2.17	0.45
40:r:236:LEU:HD13	40:r:294:MET:HG3	1.99	0.45
9:J:84:TYR:O	9:J:84:TYR:CD1	2.70	0.44
12:M:624:ARG:NH2	12:M:637:ASP:OD1	2.37	0.44
20:V:35:ILE:HG22	53:V:201:CDL:H761	1.97	0.44
26:c:73:GLY:HA3	38:o:79:ASN:HD22	1.82	0.44
31:h:18:MET:HE3	34:k:56:ALA:HA	1.98	0.44
32:i:159:MET:HA	32:i:159:MET:HE2	1.98	0.44
35:l:401:MET:SD	35:l:482:MET:HG2	2.57	0.44
35:l:441:VAL:HG13	35:l:443:ILE:HG12	1.98	0.44
36:m:1:MET:HE2	36:m:4:TYR:HA	1.99	0.44
40:r:210:TYR:CG	40:r:268:GLY:HA3	2.52	0.44
3:C:85:ASP:O	3:C:88:ARG:HG2	2.17	0.44
9:J:207:PHE:HA	9:J:211:ASP:CB	2.47	0.44
9:J:328:THR:HG22	9:J:330:PRO:HD3	1.99	0.44
53:a:201:CDL:C25	53:a:201:CDL:C21	2.86	0.44
32:i:77:ASN:OD1	32:i:89:MET:O	2.35	0.44
47:i:402:PEE:H31	35:l:562:LEU:HG	1.99	0.44
47:r:501:PEE:H75	47:r:501:PEE:H69	1.83	0.44
6:G:83:VAL:O	6:G:87:LEU:HD23	2.16	0.44
20:V:108:TYR:CE2	53:o:201:CDL:OA6	2.71	0.44
22:Y:47:PHE:HE2	22:Y:50:LEU:HD11	1.83	0.44
32:i:268:GLN:NE2	32:i:272:LYS:HE3	2.32	0.44
35:l:377:SER:O	35:l:381:THR:HG23	2.16	0.44
53:l:702:CDL:H591	53:l:702:CDL:H622	1.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:357:THR:O	40:r:361:VAL:HG23	2.17	0.44
44:w:165:SER:CB	44:w:245:PHE:CD1	3.00	0.44
1:A:104:LYS:NZ	1:A:104:LYS:HB2	2.32	0.44
8:I:14:TRP:O	21:W:28:ARG:NH2	2.51	0.44
9:J:214:LEU:HD23	9:J:352:VAL:CG1	2.45	0.44
15:P:147:THR:HB	15:P:153:ILE:HD11	2.00	0.44
21:W:144:THR:HB	41:s:96:ILE:HG23	1.99	0.44
24:a:184:LYS:HB3	31:h:30:PRO:HB3	2.00	0.44
26:c:34:LYS:HD3	26:c:34:LYS:N	2.31	0.44
32:i:112:HIS:HB2	32:i:184:ILE:HD13	1.99	0.44
32:i:294:MET:HE2	32:i:294:MET:HB2	1.86	0.44
47:i:402:PEE:H31	35:l:562:LEU:HD21	1.99	0.44
33:j:24:LEU:CD2	47:j:201:PEE:C40	2.94	0.44
40:r:263:MET:HE3	40:r:263:MET:HB3	1.74	0.44
10:K:83:THR:HG23	10:K:84:TYR:CD2	2.52	0.44
12:M:36:VAL:HB	12:M:56:VAL:HG21	2.00	0.44
33:j:95:LEU:HD13	41:s:302:MET:HG2	1.99	0.44
35:l:184:LEU:HD13	40:r:393:ILE:HG21	2.00	0.44
48:r:503:PLX:H121	48:r:503:PLX:H152	1.53	0.44
44:w:350:LYS:HA	44:w:350:LYS:HD3	1.80	0.44
2:B:63:TRP:HB3	2:B:66:LEU:HD12	2.00	0.44
17:S:14:ALA:O	17:S:18:ILE:HG12	2.18	0.44
17:S:43:TYR:CZ	21:W:68:ARG:HG3	2.52	0.44
33:j:15:SER:O	33:j:19:LEU:HD23	2.18	0.44
40:r:216:LEU:HD23	40:r:287:ALA:HB1	1.99	0.44
12:M:277:MET:HE3	12:M:277:MET:HB3	1.91	0.44
16:Q:198:THR:HB	16:Q:199:PRO:HD3	2.00	0.44
20:V:113:ALA:CB	47:V:202:PEE:C33	2.96	0.44
21:W:74:LEU:O	21:W:78:GLU:HG3	2.18	0.44
22:Y:78:ASP:HB2	22:Y:83:HIS:HB2	1.98	0.44
26:c:46:GLU:HG2	26:c:47:GLU:N	2.32	0.44
28:e:86:ASN:ND2	40:r:81:GLN:HE22	2.15	0.44
35:l:331:MET:CB	35:l:387:THR:HG22	2.37	0.44
41:s:24:GLU:HG3	41:s:271:LEU:HD22	1.99	0.44
42:u:83:THR:HA	42:u:86:TRP:NE1	2.32	0.44
8:I:3:SER:O	53:N:201:CDL:CA2	2.48	0.44
26:c:152:SER:HB2	35:l:406:ALA:HB2	2.00	0.44
28:e:73:SER:C	28:e:75:GLY:H	2.26	0.44
30:g:84:MET:HE3	32:i:346:LEU:HD13	1.99	0.44
33:j:15:SER:HA	41:s:76:ILE:HD12	2.00	0.44
34:k:37:MET:HG3	34:k:67:ALA:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:v:92:HIS:O	43:v:96:VAL:HG23	2.18	0.44
1:A:131:ILE:HD13	1:A:158:ILE:HD13	1.99	0.44
7:H:56:LEU:HA	7:H:59:VAL:HG12	1.98	0.44
11:L:163:ASN:O	11:L:171:ARG:HA	2.18	0.44
39:p:100:PRO:HG3	40:r:419:TYR:CE1	2.52	0.44
40:r:300:ALA:O	40:r:308:SER:HB3	2.18	0.44
40:r:382:ILE:HD12	40:r:396:MET:HB3	1.99	0.44
16:Q:36:GLN:NE2	40:r:135:ARG:O	2.49	0.43
33:j:28:ASN:HB3	47:j:201:PEE:H1	2.00	0.43
40:r:267:TRP:HE1	40:r:271:MET:HE2	1.83	0.43
42:u:74:ILE:HD11	42:u:117:TRP:HZ3	1.83	0.43
16:Q:80:LEU:HD23	16:Q:80:LEU:H	1.82	0.43
16:Q:271:ARG:HD2	16:Q:271:ARG:HA	1.80	0.43
22:Y:100:LEU:HB2	43:v:111:ARG:NH1	2.31	0.43
32:i:11:MET:HE3	53:i:401:CDL:C55	2.48	0.43
35:l:125:LEU:O	35:l:129:MET:HG2	2.18	0.43
2:B:100:GLU:OE2	2:B:185:TYR:CE2	2.72	0.43
2:B:131:GLU:HB2	2:B:144:ARG:HB3	2.00	0.43
11:L:90:GLY:HA3	15:P:238:PRO:HB2	2.00	0.43
13:N:42:ASP:HB2	13:N:48:TYR:HE1	1.82	0.43
15:P:119:VAL:HG12	15:P:121:THR:HG22	2.00	0.43
16:Q:176:GLU:OE2	16:Q:311:TYR:OH	2.22	0.43
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.83	0.43
22:Y:54:GLN:HG3	22:Y:55:LEU:HD12	2.00	0.43
22:Y:83:HIS:O	22:Y:83:HIS:ND1	2.42	0.43
32:i:100:MET:HE2	35:l:598:SER:OG	2.18	0.43
47:m:201:PEE:O4	47:m:201:PEE:H7	2.18	0.43
48:r:502:PLX:H301	48:r:502:PLX:H331	1.73	0.43
3:C:110:THR:OG1	16:Q:115:LEU:O	2.29	0.43
13:N:120:THR:HG22	13:N:122:GLN:H	1.82	0.43
24:a:106:VAL:HG13	37:n:50:ARG:HH21	1.82	0.43
40:r:207:MET:HE1	40:r:240:GLY:HA2	1.99	0.43
9:J:167:ILE:HG12	9:J:201:ILE:HB	2.01	0.43
36:m:35:VAL:O	36:m:39:VAL:HG23	2.19	0.43
40:r:206:LYS:HE3	40:r:206:LYS:HB2	1.90	0.43
41:s:24:GLU:OE2	41:s:274:ARG:NH1	2.50	0.43
55:s:401:UQ:HM53	55:s:401:UQ:H72	1.74	0.43
43:v:51:LEU:HD22	43:v:63:LEU:HD22	2.01	0.43
1:A:384:PRO:HB2	1:A:423:THR:HG22	2.01	0.43
18:T:79:VAL:HG21	18:T:84:ILE:HD13	2.00	0.43
25:b:4:TYR:HB3	25:b:9:LYS:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:79:VAL:O	34:k:82:SER:OG	2.35	0.43
35:l:172:ILE:O	35:l:176:ARG:HG2	2.18	0.43
35:l:302:VAL:HG12	35:l:340:PHE:CZ	2.53	0.43
1:A:448:GLU:O	1:A:452:GLN:HG2	2.19	0.43
7:H:38:ILE:HD13	7:H:95:LEU:HD13	2.01	0.43
33:j:93:PHE:O	33:j:97:LEU:HD23	2.18	0.43
40:r:127:VAL:HB	40:r:128:PRO:HD3	1.99	0.43
40:r:207:MET:HG2	40:r:298:ILE:CG1	2.47	0.43
48:C:302:PLX:H31	13:N:75:TRP:CD2	2.54	0.43
5:F:23:LEU:O	5:F:57:GLU:HA	2.18	0.43
7:H:90:LEU:HB2	15:P:102:ASP:HB3	2.01	0.43
21:W:90:ASN:ND2	21:W:123:GLU:O	2.52	0.43
6:X:128:PHE:HZ	6:X:148:ILE:HG12	1.84	0.43
24:a:176:LYS:HD3	31:h:45:HIS:ND1	2.34	0.43
47:b:201:PEE:H60	47:b:201:PEE:H55	1.87	0.43
33:j:48:ARG:HB2	33:j:49:LEU:H	1.62	0.43
40:r:218:LYS:O	40:r:222:GLU:HG2	2.19	0.43
14:O:187:GLN:HG3	14:O:192:TYR:CE1	2.54	0.43
28:e:66:LEU:HB3	28:e:73:SER:OG	2.18	0.43
28:e:148:GLN:HB2	30:g:113:GLU:HB3	2.01	0.43
47:j:201:PEE:H20	47:j:201:PEE:H26	1.28	0.43
35:l:295:GLN:HB2	35:l:301:ILE:HG12	2.00	0.43
38:o:31:LYS:HE3	38:o:31:LYS:HB3	1.90	0.43
53:o:201:CDL:H321	53:o:201:CDL:C11	2.49	0.43
1:A:214:GLU:OE1	1:A:224:ARG:NE	2.41	0.43
9:J:85:ARG:HD3	9:J:85:ARG:C	2.44	0.43
25:b:89:HIS:CD2	47:b:201:PEE:H49	2.53	0.43
32:i:112:HIS:CE1	32:i:164:ILE:HG21	2.54	0.43
33:j:28:ASN:CB	47:j:201:PEE:H1	2.48	0.43
36:m:169:MET:HE3	36:m:169:MET:HB3	1.81	0.43
36:m:173:ARG:HD3	44:w:289:ARG:NH2	2.34	0.43
40:r:328:CYS:HB3	40:r:437:MET:HE1	2.01	0.43
44:w:123:SER:OG	44:w:125:ASP:OD1	2.23	0.43
4:E:70:ASN:HD22	4:E:82:LEU:HD13	1.84	0.42
9:J:319:VAL:HA	9:J:322:VAL:HG12	2.00	0.42
14:O:48:ASN:OD1	14:O:51:THR:OG1	2.24	0.42
14:O:137:THR:HG22	14:O:138:THR:H	1.84	0.42
21:W:98:MET:HG3	21:W:104:TRP:NE1	2.34	0.42
22:Y:97:LEU:O	43:v:104:ARG:HG3	2.19	0.42
48:g:201:PLX:H131	48:g:201:PLX:H102	1.45	0.42
32:i:334:THR:HG22	32:i:335:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:i:402:PEE:H25	40:r:151:PHE:HB2	2.02	0.42
33:j:73:LEU:O	41:s:160:TYR:OH	2.37	0.42
33:j:75:LEU:HB3	41:s:155:LEU:HD21	2.01	0.42
35:l:78:LEU:HD11	53:l:701:CDL:H251	1.99	0.42
35:l:483:PRO:HD2	35:l:486:MET:HE2	2.01	0.42
53:l:701:CDL:H792	53:l:701:CDL:H762	1.86	0.42
36:m:61:LEU:HB3	41:s:111:LEU:HD21	2.01	0.42
53:o:201:CDL:H541	53:o:201:CDL:H512	1.61	0.42
40:r:267:TRP:NE1	40:r:271:MET:HE2	2.33	0.42
1:A:296:LEU:HD23	1:A:332:CYS:HB2	2.01	0.42
3:C:79:MET:HE1	3:C:177:ILE:HG13	2.01	0.42
3:C:82:PRO:HG3	16:Q:201:PHE:HB3	2.01	0.42
16:Q:199:PRO:HA	16:Q:202:TRP:HB2	2.01	0.42
20:V:99:LEU:HD23	20:V:99:LEU:HA	1.89	0.42
28:e:92:PHE:O	28:e:96:SER:HB2	2.18	0.42
35:l:363:TYR:CD1	35:l:370:THR:HG21	2.54	0.42
37:n:13:VAL:HG13	40:r:14:MET:HA	2.01	0.42
39:p:76:HIS:O	39:p:78:GLN:N	2.51	0.42
40:r:318:ALA:HB1	40:r:374:ASN:OD1	2.18	0.42
42:u:38:LYS:HB3	42:u:39:PRO:HD3	2.01	0.42
53:u:201:CDL:H521	53:u:201:CDL:H551	1.81	0.42
44:w:57:SER:O	44:w:156:GLY:HA3	2.18	0.42
1:A:40:ARG:NH1	1:A:289:GLU:O	2.53	0.42
2:B:114:ILE:HD12	12:M:130:ILE:HG23	2.02	0.42
5:F:18:GLU:HG2	5:F:68:ARG:HB3	2.02	0.42
6:G:75:THR:O	6:G:77:GLU:N	2.52	0.42
9:J:192:ARG:HH21	9:J:262:THR:HG1	1.61	0.42
12:M:367:CYS:HB3	12:M:533:GLY:O	2.19	0.42
24:a:115:HIS:NE2	53:a:201:CDL:OB4	2.50	0.42
30:g:74:GLY:O	30:g:78:LEU:HG	2.19	0.42
36:m:25:SER:O	36:m:28:TYR:N	2.50	0.42
53:o:201:CDL:H822	53:o:201:CDL:C78	2.27	0.42
40:r:248:THR:HG23	40:r:249:ILE:HG23	2.02	0.42
41:s:251:THR:HG23	41:s:251:THR:O	2.20	0.42
43:v:28:ASP:OD1	43:v:34:ARG:HG3	2.19	0.42
14:O:56:THR:H	14:O:89:GLN:NE2	2.18	0.42
14:O:215:LYS:HA	14:O:216:PRO:HD3	1.84	0.42
35:l:190:LEU:HB2	35:l:196:TRP:NE1	2.33	0.42
47:r:501:PEE:H25	47:r:501:PEE:H32	1.84	0.42
42:u:139:GLU:H	42:u:139:GLU:CD	2.27	0.42
1:A:388:GLY:HA3	1:A:419:ILE:HD11	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:74:LEU:H	6:G:74:LEU:CD2	2.13	0.42
12:M:358:LEU:HD12	12:M:366:LEU:HD21	2.02	0.42
14:O:100:LYS:O	14:O:104:ILE:HG12	2.19	0.42
20:V:106:ARG:HA	20:V:106:ARG:NE	2.35	0.42
22:Y:92:TRP:CZ2	43:v:100:LYS:HE3	2.54	0.42
24:a:91:VAL:HG23	27:d:52:ILE:HG12	2.01	0.42
53:o:201:CDL:H872	53:o:201:CDL:H841	1.83	0.42
42:u:100:CYS:HB2	42:u:103:GLN:OE1	2.20	0.42
6:G:103:HIS:HE1	6:G:105:MET:HB2	1.84	0.42
16:Q:251:PHE:HB3	16:Q:341:LEU:HD11	2.02	0.42
21:W:28:ARG:HA	21:W:28:ARG:HD2	1.83	0.42
25:b:88:TYR:CZ	27:d:49:ARG:HG2	2.55	0.42
47:b:201:PEE:O4	47:b:201:PEE:H3	2.20	0.42
27:d:127:LYS:HB3	27:d:127:LYS:HE3	1.86	0.42
35:l:174:TYR:CD2	35:l:232:TRP:HB3	2.54	0.42
35:l:260:LEU:HD23	35:l:260:LEU:HA	1.86	0.42
36:m:51:PHE:O	36:m:55:MET:HG2	2.19	0.42
37:n:49:LEU:HD12	37:n:49:LEU:H	1.85	0.42
38:o:82:PRO:O	53:o:201:CDL:OB7	2.38	0.42
42:u:41:LYS:HA	42:u:41:LYS:HD3	1.81	0.42
44:w:110:GLY:HA2	44:w:134:TRP:CD2	2.55	0.42
1:A:86:ARG:NH1	1:A:339:PHE:HB2	2.35	0.42
15:P:183:ASP:OD1	15:P:183:ASP:N	2.51	0.42
16:Q:83:ASN:OD1	16:Q:98:VAL:HG22	2.19	0.42
47:V:202:PEE:H2	47:V:202:PEE:O4	2.20	0.42
6:X:90:TYR:CE2	6:X:118:ILE:HD11	2.55	0.42
25:b:86:LEU:HA	25:b:90:VAL:HB	2.01	0.42
31:h:65:GLU:HA	31:h:65:GLU:OE1	2.20	0.42
32:i:222:SER:O	32:i:224:ALA:N	2.53	0.42
6:X:151:LYS:HB2	6:X:151:LYS:HE2	1.71	0.42
24:a:184:LYS:O	24:a:185:THR:OG1	2.35	0.42
27:d:89:GLU:O	27:d:93:ARG:HG2	2.19	0.42
34:k:37:MET:HG3	34:k:67:ALA:HB1	2.02	0.42
40:r:373:ILE:HD11	40:r:444:LEU:HD23	2.01	0.42
43:v:8:ARG:HA	43:v:16:GLU:OE2	2.19	0.42
1:A:290:GLU:HG3	1:A:291:GLU:N	2.35	0.42
2:B:208:ASP:OD1	2:B:212:ARG:NE	2.53	0.42
3:C:167:PRO:CG	16:Q:222:MET:CE	2.64	0.42
48:C:302:PLX:H212	48:C:302:PLX:H181	1.75	0.42
12:M:133:GLN:O	12:M:137:CYS:HB2	2.20	0.42
29:f:52:VAL:O	29:f:56:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:137:ALA:HB3	32:i:138:PRO:HD3	2.01	0.42
9:J:238:GLN:HG2	9:J:266:VAL:HB	2.01	0.42
15:P:81:PHE:HD1	15:P:83:GLU:HG3	1.85	0.42
17:S:34:LYS:HE3	17:S:34:LYS:HB2	1.91	0.42
26:c:176:LYS:HD2	26:c:176:LYS:HA	1.77	0.42
28:e:136:LEU:HB3	28:e:137:MET:H	1.63	0.42
31:h:84:ASP:HA	31:h:87:ILE:HG22	2.00	0.42
6:G:79:ILE:HD13	6:G:148:ILE:HG12	2.01	0.41
9:J:92:MET:O	9:J:95:ARG:HG3	2.20	0.41
9:J:172:ALA:HA	9:J:181:LEU:HB3	2.01	0.41
12:M:73:GLY:HA2	51:M:803:FES:S2	2.60	0.41
20:V:35:ILE:CD1	53:V:201:CDL:H802	2.50	0.41
6:X:136:GLU:OE2	39:p:14:GLN:NE2	2.52	0.41
22:Y:71:TRP:HD1	22:Y:72:ARG:HE	1.68	0.41
23:Z:13:LYS:HD2	23:Z:13:LYS:HA	1.80	0.41
47:b:201:PEE:C21	53:l:701:CDL:H241	2.45	0.41
27:d:78:GLU:HG2	30:g:108:LYS:HE3	2.02	0.41
30:g:33:LEU:HD23	30:g:33:LEU:HA	1.92	0.41
32:i:106:LEU:HG	32:i:138:PRO:HB2	2.01	0.41
41:s:289:LEU:HD12	41:s:293:PHE:HB2	2.01	0.41
44:w:116:LYS:NZ	44:w:123:SER:OG	2.53	0.41
44:w:250:SER:O	44:w:280:LYS:NZ	2.42	0.41
2:B:101:HIS:HE1	2:B:152:CYS:SG	2.44	0.41
4:E:17:VAL:HG23	11:L:53:ILE:HD13	2.01	0.41
5:F:64:LYS:NZ	5:F:76:ASN:HB2	2.34	0.41
12:M:244:GLU:OE1	12:M:266:ARG:NH1	2.53	0.41
15:P:161:LYS:HB3	15:P:161:LYS:HE3	1.85	0.41
21:W:92:GLU:O	21:W:96:ILE:HG12	2.20	0.41
6:X:83:VAL:HG13	6:X:122:MET:CE	2.50	0.41
22:Y:45:ARG:HG2	35:l:439:PRO:HB3	2.02	0.41
24:a:90:ASN:HD21	53:a:201:CDL:PB2	2.43	0.41
27:d:65:HIS:ND1	28:e:120:ARG:HD2	2.35	0.41
32:i:270:MET:HE1	32:i:282:MET:SD	2.60	0.41
47:j:201:PEE:H70	41:s:53:LEU:HD23	2.01	0.41
39:p:164:PRO:HA	39:p:165:PRO:HD3	1.97	0.41
40:r:328:CYS:O	40:r:332:THR:HG23	2.19	0.41
41:s:143:GLU:HA	41:s:146:LEU:HB2	2.02	0.41
44:w:279:ASP:N	44:w:279:ASP:OD1	2.51	0.41
1:A:110:PRO:O	1:A:238:CYS:HB3	2.20	0.41
3:C:63:TRP:H	3:C:101:ASP:HB2	1.85	0.41
16:Q:434:GLY:O	16:Q:438:MET:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:133:ILE:HD11	39:p:6:PRO:HA	2.02	0.41
26:c:40:PRO:O	26:c:74:ASP:HB2	2.20	0.41
27:d:6:ASP:HB3	27:d:9:VAL:HG12	2.02	0.41
27:d:43:ARG:HB3	27:d:44:PRO:HD3	2.03	0.41
32:i:46:LYS:HZ3	53:i:401:CDL:HB22	1.85	0.41
41:s:130:ILE:O	41:s:134:ARG:HG3	2.20	0.41
42:u:44:MET:HE3	42:u:48:TRP:CH2	2.54	0.41
42:u:60:GLY:HA2	42:u:63:VAL:HG12	2.02	0.41
1:A:257:ARG:HH21	1:A:261:TRP:NE1	2.17	0.41
2:B:44:ARG:HA	2:B:44:ARG:HD2	1.73	0.41
3:C:84:TYR:CE1	3:C:171:GLU:HG2	2.55	0.41
48:C:302:PLX:H1C3	48:C:302:PLX:H21	1.87	0.41
12:M:419:ARG:NH1	12:M:439:THR:O	2.53	0.41
14:O:44:THR:HG22	14:O:46:GLU:H	1.85	0.41
22:Y:65:MET:HE3	35:l:375:ILE:HG12	2.02	0.41
26:c:145:TRP:CH2	26:c:149:ILE:HD11	2.55	0.41
29:f:44:VAL:O	29:f:48:LEU:HD23	2.20	0.41
34:k:57:ASN:HB3	36:m:143:ILE:HG13	2.01	0.41
35:l:47:SER:O	35:l:50:PRO:HD2	2.20	0.41
35:l:267:MET:HE1	35:l:273:VAL:HG12	2.02	0.41
35:l:357:ARG:HG3	39:p:32:VAL:HG13	2.01	0.41
40:r:112:ALA:HB1	40:r:118:PHE:HB2	2.02	0.41
41:s:28:LEU:HG	41:s:275:ALA:HB2	2.03	0.41
1:A:119:GLU:CG	1:A:127:ASP:HB2	2.49	0.41
1:A:138:LEU:HD13	1:A:245:VAL:HG13	2.03	0.41
1:A:413:TRP:O	1:A:416:SER:OG	2.29	0.41
3:C:126:GLU:N	41:s:59:GLU:OE2	2.52	0.41
9:J:350:ILE:HD11	9:J:357:ARG:HH22	1.85	0.41
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.51	0.41
13:N:106:ARG:HB2	13:N:109:ILE:HG13	2.03	0.41
26:c:110:ASP:OD1	26:c:110:ASP:N	2.53	0.41
32:i:62:THR:HG21	32:i:114:TRP:CD1	2.55	0.41
32:i:226:THR:HG23	32:i:229:SER:H	1.84	0.41
33:j:7:LEU:O	33:j:11:VAL:HG23	2.20	0.41
33:j:103:ALA:O	33:j:107:THR:HG23	2.20	0.41
35:l:332:HIS:HA	35:l:335:PHE:CZ	2.56	0.41
41:s:306:SER:OG	41:s:310:MET:HE2	2.20	0.41
1:A:88:ARG:HA	1:A:88:ARG:HD3	1.85	0.41
5:F:83:SER:O	5:F:87:VAL:HG12	2.21	0.41
9:J:204:SER:OG	9:J:204:SER:O	2.38	0.41
12:M:646:LEU:HD23	12:M:646:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:122:GLN:HA	18:T:59:GLN:HG2	2.02	0.41
16:Q:184:ILE:HG21	16:Q:207:ARG:HG3	2.02	0.41
18:T:114:CYS:SG	18:T:116:LEU:HG	2.61	0.41
20:V:88:LEU:O	20:V:92:ILE:HG12	2.21	0.41
22:Y:43:ARG:HG3	22:Y:48:PRO:HA	2.03	0.41
25:b:99:GLU:HG2	35:l:61:MET:SD	2.61	0.41
29:f:55:TRP:O	29:f:59:ILE:HG12	2.20	0.41
30:g:87:LEU:HD23	30:g:87:LEU:HA	1.94	0.41
33:j:84:LEU:HD23	33:j:84:LEU:HA	1.88	0.41
35:l:244:SER:O	35:l:249:SER:HB3	2.20	0.41
35:l:316:THR:OG1	35:l:395:ILE:HD12	2.20	0.41
44:w:129:TYR:OH	44:w:186:HIS:ND1	2.44	0.41
44:w:135:LEU:HD13	56:w:401:ADP:C5	2.56	0.41
1:A:88:ARG:NH1	1:A:246:GLU:OE1	2.51	0.41
1:A:149:MET:HE3	1:A:149:MET:HB2	1.97	0.41
2:B:41:VAL:HG12	8:I:113:LEU:HD12	2.02	0.41
14:O:225:CYS:O	14:O:225:CYS:SG	2.79	0.41
21:W:133:ILE:O	21:W:137:THR:HG22	2.21	0.41
22:Y:65:MET:CE	35:l:378:LEU:HD12	2.50	0.41
35:l:124:PHE:CE2	35:l:252:MET:HB2	2.56	0.41
53:l:702:CDL:H612	53:l:702:CDL:H371	2.03	0.41
38:o:102:TYR:N	40:r:263:MET:HE2	2.36	0.41
46:A:502:FMN:O4'	46:A:502:FMN:O2'	2.22	0.41
12:M:512:VAL:O	12:M:514:ASN:ND2	2.53	0.41
12:M:558:GLN:N	12:M:558:GLN:OE1	2.54	0.41
6:X:69:SER:OG	6:X:70:ASP:N	2.53	0.41
24:a:98:LEU:CB	27:d:63:TYR:CE1	2.98	0.41
26:c:58:ARG:HB2	26:c:61:ASP:HB2	2.02	0.41
32:i:185:ALA:CB	32:i:289:ASN:HD21	2.33	0.41
35:l:529:TYR:HB3	35:l:530:PRO:HD3	2.02	0.41
1:A:210:THR:O	1:A:214:GLU:HG2	2.20	0.41
1:A:329:LYS:O	1:A:333:GLU:HG2	2.21	0.41
2:B:150:THR:HG21	2:B:180:HIS:CD2	2.56	0.41
47:B:303:PEE:H70	41:s:186:PHE:CD2	2.56	0.41
3:C:103:MET:HE1	3:C:121:TYR:HB2	2.02	0.41
7:H:45:ARG:NE	7:H:49:GLU:OE2	2.41	0.41
7:H:64:ASP:OD1	7:H:65:VAL:N	2.47	0.41
10:K:86:PHE:HD2	10:K:87:LEU:HD23	1.86	0.41
12:M:213:MET:HB3	12:M:215:MET:HE2	2.02	0.41
12:M:301:ARG:HD2	12:M:301:ARG:HA	1.69	0.41
12:M:385:TYR:OH	12:M:527:ASP:OD1	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:72:ARG:HB3	35:l:385:TYR:HD2	1.77	0.41
22:Y:95:GLU:OE1	22:Y:95:GLU:N	2.51	0.41
26:c:136:PHE:O	26:c:140:MET:HG2	2.20	0.41
32:i:276:ILE:HG21	47:r:501:PEE:H7	2.03	0.41
34:k:33:LEU:HA	34:k:36:MET:CE	2.51	0.41
34:k:43:MET:O	34:k:47:ILE:HG13	2.20	0.41
37:n:7:ILE:O	37:n:11:HIS:N	2.46	0.41
38:o:82:PRO:HB2	53:o:201:CDL:HB4	2.02	0.41
39:p:35:ASP:OD1	39:p:36:LYS:N	2.52	0.41
39:p:108:HIS:CD2	39:p:109:PRO:HD2	2.56	0.41
40:r:420:THR:HG21	40:r:423:ILE:HD12	2.03	0.41
53:r:505:CDL:H792	53:r:505:CDL:H761	1.87	0.41
41:s:89:LEU:HA	41:s:90:PRO:HD3	1.89	0.41
42:u:121:ASP:N	42:u:124:GLU:OE1	2.48	0.41
44:w:165:SER:O	44:w:168:VAL:HG22	2.21	0.41
1:A:88:ARG:HG3	1:A:246:GLU:CD	2.45	0.41
1:A:184:LYS:C	1:A:186:ALA:H	2.29	0.41
8:I:66:PRO:HB3	15:P:79:SER:HA	2.03	0.41
9:J:64:PHE:HD1	9:J:210:GLU:HB2	1.86	0.41
9:J:273:LEU:O	9:J:277:VAL:HG23	2.21	0.41
12:M:372:PHE:H	12:M:532:PRO:HB2	1.86	0.41
12:M:478:SER:O	12:M:482:GLN:HG2	2.21	0.41
25:b:21:ARG:HE	25:b:21:ARG:HB3	1.73	0.41
25:b:87:LYS:O	25:b:91:THR:OG1	2.39	0.41
27:d:74:ILE:HG23	27:d:156:LEU:HD22	2.02	0.41
32:i:276:ILE:HG21	47:r:501:PEE:H13	2.02	0.41
32:i:319:HIS:HB3	32:i:322:GLN:NE2	2.36	0.41
32:i:339:MET:HE3	32:i:339:MET:HB3	1.96	0.41
35:l:286:LEU:HD12	35:l:286:LEU:HA	1.75	0.41
37:n:17:VAL:N	37:n:18:PRO:CD	2.84	0.41
41:s:179:TRP:CG	41:s:180:PRO:HD3	2.56	0.41
9:J:115:SER:HA	9:J:118:LYS:HG2	2.02	0.40
12:M:535:GLU:OE1	12:M:539:LYS:HE3	2.21	0.40
24:a:96:ALA:CB	27:d:61:TYR:HD1	2.04	0.40
47:j:202:PEE:H62	47:j:202:PEE:H69	1.89	0.40
53:o:201:CDL:H873	40:r:264:LEU:HD21	2.01	0.40
40:r:48:ASN:OD1	40:r:49:SER:N	2.50	0.40
40:r:191:SER:HB3	47:r:501:PEE:C1	2.32	0.40
40:r:226:ALA:HA	40:r:229:MET:HE3	2.03	0.40
1:A:133:HIS:CE1	14:O:224:SER:CB	2.81	0.40
9:J:192:ARG:NH2	9:J:262:THR:OG1	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:110:LYS:O	12:M:114:GLU:HG3	2.20	0.40
12:M:331:GLN:NE2	12:M:630:ALA:O	2.44	0.40
24:a:95:GLU:CD	24:a:114:LYS:HD3	2.46	0.40
32:i:321:LYS:O	32:i:321:LYS:HG3	2.21	0.40
35:l:86:SER:O	35:l:90:ILE:HG12	2.21	0.40
53:r:505:CDL:H802	53:r:505:CDL:H831	1.90	0.40
1:A:91:ALA:HB1	1:A:93:PHE:CD2	2.56	0.40
7:H:44:TYR:HE2	7:H:94:MET:HB3	1.86	0.40
9:J:113:LYS:HB3	9:J:113:LYS:HE2	1.88	0.40
12:M:260:ASN:HD21	12:M:278:HIS:CD2	2.39	0.40
15:P:103:HIS:CD2	15:P:105:ASN:HB2	2.57	0.40
22:Y:45:ARG:NH1	23:Z:48:ASN:O	2.54	0.40
24:a:99:ALA:O	27:d:64:TYR:HD1	2.04	0.40
25:b:19:ARG:HA	39:p:171:VAL:HG23	2.03	0.40
32:i:294:MET:SD	40:r:130:LEU:HD21	2.61	0.40
40:r:321:LEU:HD13	40:r:444:LEU:HG	2.04	0.40
44:w:329:GLN:O	44:w:333:GLU:HG2	2.22	0.40
15:P:232:LYS:HE2	15:P:232:LYS:HB3	1.91	0.40
20:V:65:ALA:O	20:V:69:ILE:HG12	2.22	0.40
27:d:80:LYS:HD3	27:d:80:LYS:HA	1.77	0.40
32:i:79:LEU:HB2	34:k:47:ILE:CD1	2.50	0.40
35:l:42:TYR:HA	35:l:45:THR:HG22	2.03	0.40
35:l:249:SER:HB2	35:l:340:PHE:CE2	2.57	0.40
40:r:158:LEU:HD23	40:r:158:LEU:HA	1.86	0.40
40:r:166:TYR:OH	47:r:501:PEE:O1P	2.34	0.40
4:E:90:LEU:O	4:E:94:ILE:HG12	2.21	0.40
9:J:85:ARG:HB2	9:J:85:ARG:NH2	2.35	0.40
12:M:168:LEU:HD23	12:M:168:LEU:HA	1.89	0.40
25:b:14:GLN:HE22	39:p:157:ALA:H	1.70	0.40
26:c:113:ILE:HG13	26:c:115:ASN:HB2	2.03	0.40
31:h:50:ILE:H	31:h:50:ILE:HD12	1.87	0.40
32:i:340:THR:N	32:i:341:PRO:HD2	2.36	0.40
34:k:58:MET:H	34:k:58:MET:HG3	1.74	0.40
35:l:296:ASN:HD22	35:l:357:ARG:CZ	2.35	0.40
53:l:702:CDL:H421	53:l:702:CDL:H391	1.89	0.40
36:m:31:LEU:HD12	41:s:70:MET:HE2	2.03	0.40
36:m:129:ASP:N	36:m:129:ASP:OD1	2.49	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%)	411 (96%)	18 (4%)	0	100	100
2	B	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
3	C	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
4	E	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
5	F	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
6	G	86/88 (98%)	82 (95%)	2 (2%)	2 (2%)	5	25
6	X	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
7	H	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
8	I	93/112 (83%)	83 (89%)	10 (11%)	0	100	100
9	J	289/341 (85%)	277 (96%)	11 (4%)	1 (0%)	36	65
10	K	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	668 (97%)	20 (3%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	208 (97%)	7 (3%)	0	100	100
15	P	206/208 (99%)	194 (94%)	12 (6%)	0	100	100
16	Q	412/430 (96%)	398 (97%)	14 (3%)	0	100	100
17	S	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
18	T	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
19	U	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
20	V	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	18	49
21	W	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
22	Y	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
23	Z	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
24	a	138/140 (99%)	135 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	b	99/126 (79%)	96 (97%)	3 (3%)	0	100	100
26	c	154/156 (99%)	145 (94%)	9 (6%)	0	100	100
27	d	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
28	e	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
29	f	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
30	g	119/121 (98%)	112 (94%)	7 (6%)	0	100	100
31	h	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
32	i	345/347 (99%)	336 (97%)	9 (3%)	0	100	100
33	j	95/113 (84%)	89 (94%)	6 (6%)	0	100	100
34	k	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
35	l	601/603 (100%)	577 (96%)	24 (4%)	0	100	100
36	m	125/175 (71%)	111 (89%)	14 (11%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
39	p	176/178 (99%)	168 (96%)	8 (4%)	0	100	100
40	r	457/459 (100%)	440 (96%)	17 (4%)	0	100	100
41	s	299/318 (94%)	289 (97%)	9 (3%)	1 (0%)	36	65
42	u	169/171 (99%)	162 (96%)	7 (4%)	0	100	100
43	v	122/131 (93%)	117 (96%)	5 (4%)	0	100	100
44	w	318/320 (99%)	303 (95%)	15 (5%)	0	100	100
All	All	8029/8315 (97%)	7716 (96%)	308 (4%)	5 (0%)	49	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	70	ASP
6	G	76	LEU
9	J	83	PRO
41	s	90	PRO
20	V	46	PRO

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/345 (100%)	345 (100%)	0	100	100
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	72/81 (89%)	69 (96%)	3 (4%)	26	55
6	X	78/81 (96%)	77 (99%)	1 (1%)	61	74
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	87 (100%)	0	100	100
9	J	254/295 (86%)	252 (99%)	2 (1%)	73	79
10	K	41/41 (100%)	41 (100%)	0	100	100
11	L	113/113 (100%)	113 (100%)	0	100	100
12	M	580/580 (100%)	580 (100%)	0	100	100
13	N	130/130 (100%)	130 (100%)	0	100	100
14	O	183/183 (100%)	182 (100%)	1 (0%)	81	83
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	122/123 (99%)	122 (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%)	140 (99%)	1 (1%)	76	80
27	d	155/155 (100%)	155 (100%)	0	100	100
28	e	99/99 (100%)	99 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	f	36/38 (95%)	36 (100%)	0	100	100
30	g	108/108 (100%)	108 (100%)	0	100	100
31	h	93/93 (100%)	93 (100%)	0	100	100
32	i	311/311 (100%)	308 (99%)	3 (1%)	68	76
33	j	88/99 (89%)	88 (100%)	0	100	100
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	537/537 (100%)	537 (100%)	0	100	100
36	m	99/141 (70%)	99 (100%)	0	100	100
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	113/113 (100%)	113 (100%)	0	100	100
39	p	159/159 (100%)	159 (100%)	0	100	100
40	r	410/410 (100%)	410 (100%)	0	100	100
41	s	263/275 (96%)	262 (100%)	1 (0%)	84	84
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	104/115 (90%)	104 (100%)	0	100	100
44	w	282/283 (100%)	281 (100%)	1 (0%)	84	84
All	All	7064/7238 (98%)	7051 (100%)	13 (0%)	85	88

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	G	74	LEU
6	G	76	LEU
6	G	148	ILE
9	J	81	ILE
9	J	85	ARG
14	O	226	GLU
6	X	98	LEU
26	c	154	GLN
32	i	91	ASN
32	i	93	VAL
32	i	95	MET
41	s	235	ASN
44	w	241	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	116	ASN
1	A	164	ASN
1	A	270	ASN
1	A	393	ASN
1	A	422	HIS
4	E	58	GLN
7	H	83	GLN
8	I	25	GLN
9	J	122	HIS
9	J	150	HIS
9	J	171	ASN
9	J	251	ASN
9	J	278	GLN
10	K	100	GLN
10	K	106	GLN
12	M	260	ASN
12	M	415	ASN
12	M	499	ASN
12	M	604	GLN
12	M	678	GLN
14	O	87	GLN
14	O	89	GLN
15	P	75	GLN
15	P	77	GLN
15	P	107	GLN
15	P	196	HIS
16	Q	234	GLN
16	Q	270	ASN
18	T	120	GLN
18	T	123	HIS
19	U	52	ASN
6	X	142	GLN
22	Y	54	GLN
24	a	50	HIS
24	a	90	ASN
25	b	89	HIS
25	b	126	GLN
26	c	132	HIS
27	d	124	ASN
27	d	161	GLN
29	f	73	ASN
32	i	83	GLN

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Mol	Chain	Res	Type
32	i	91	ASN
32	i	134	GLN
32	i	310	ASN
33	j	82	ASN
34	k	57	ASN
35	l	56	HIS
35	l	135	ASN
35	l	226	GLN
35	l	354	GLN
35	l	447	ASN
35	l	580	GLN
36	m	175	ASN
37	n	3	ASN
37	n	6	GLN
37	n	11	HIS
37	n	14	HIS
40	r	26	ASN
40	r	51	ASN
40	r	81	GLN
40	r	251	ASN
42	u	30	HIS
43	v	43	GLN
44	w	127	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	2MR	Q	118	16	10,12,13	1.95	1 (10%)	5,13,15	6.02	3 (60%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.60	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	130.77	119.48
16	Q	118	2MR	CD-NE-CZ	4.42	131.69	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.00	130.50	123.86

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
51	FES	M	803	12	0,4,4	-	-	-		
47	PEE	V	202	-	39,39,50	1.30	6 (15%)	41,44,55	1.05	2 (4%)
48	PLX	g	201	-	51,51,51	1.14	3 (5%)	55,59,59	0.60	1 (1%)
49	8Q1	X	201	6	31,34,34	2.16	6 (19%)	40,43,43	1.69	10 (25%)
45	SF4	C	301	3	0,12,12	-	-	-		
48	PLX	r	504	40	51,51,51	1.16	4 (7%)	55,59,59	0.60	1 (1%)
53	CDL	l	701	-	98,98,99	1.09	8 (8%)	104,110,111	0.89	4 (3%)
47	PEE	m	201	-	40,40,50	1.15	5 (12%)	43,45,55	0.98	2 (4%)
56	ADP	w	401	-	27,29,29	2.96	8 (29%)	42,45,45	2.00	10 (23%)
45	SF4	B	301	2	0,12,12	-	-	-		
53	CDL	N	201	-	50,50,99	1.28	4 (8%)	56,62,111	1.32	6 (10%)
53	CDL	l	702	-	99,99,99	1.09	8 (8%)	105,111,111	0.85	4 (3%)
48	PLX	C	302	-	51,51,51	1.15	4 (7%)	55,59,59	0.61	1 (1%)
45	SF4	M	802	12	0,12,12	-	-	-		
47	PEE	j	201	-	46,46,50	1.21	6 (13%)	49,51,55	0.95	2 (4%)
47	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	0.98	2 (3%)
53	CDL	r	505	-	99,99,99	1.09	8 (8%)	105,111,111	0.86	4 (3%)
53	CDL	o	201	-	67,67,99	1.10	4 (5%)	73,79,111	1.16	5 (6%)
50	NDP	J	401	-	49,52,52	2.23	5 (10%)	66,80,80	1.65	12 (18%)
48	PLX	r	503	-	51,51,51	1.14	4 (7%)	55,59,59	0.59	1 (1%)
45	SF4	B	302	2	0,12,12	-	-	-		
45	SF4	M	801	12	0,12,12	-	-	-		
51	FES	O	301	14	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	SF4	A	501	1	0,12,12	-	-	-		
49	8Q1	G	201	6	31,34,34	2.14	6 (19%)	40,43,43	1.67	10 (25%)
53	CDL	u	201	-	77,77,99	1.03	4 (5%)	83,89,111	1.10	4 (4%)
48	PLX	j	203	-	51,51,51	1.15	4 (7%)	55,59,59	0.60	1 (1%)
47	PEE	j	202	-	50,50,50	1.15	6 (12%)	53,55,55	0.97	2 (3%)
53	CDL	a	201	-	90,90,99	0.97	4 (4%)	96,102,111	1.04	5 (5%)
47	PEE	b	201	-	45,45,50	1.22	6 (13%)	48,50,55	1.00	2 (4%)
46	FMN	A	502	-	33,33,33	1.09	2 (6%)	48,50,50	1.21	8 (16%)
47	PEE	l	703	-	45,45,50	1.22	6 (13%)	48,50,55	0.99	2 (4%)
55	UQ	s	401	-	28,28,63	3.29	7 (25%)	34,37,79	2.72	10 (29%)
48	PLX	r	502	-	51,51,51	1.13	4 (7%)	55,59,59	0.63	1 (1%)
53	CDL	V	201	-	93,93,99	0.95	4 (4%)	99,105,111	1.08	5 (5%)
47	PEE	i	402	-	46,46,50	1.20	6 (13%)	49,51,55	0.98	2 (4%)
53	CDL	i	401	-	65,65,99	1.14	4 (6%)	71,77,111	1.19	5 (7%)
47	PEE	B	303	-	50,50,50	1.16	6 (12%)	53,55,55	0.98	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	FES	M	803	12	-	-	0/1/1/1
47	PEE	V	202	-	-	23/43/43/54	-
48	PLX	g	201	-	-	25/55/55/55	-
49	8Q1	X	201	6	-	22/41/41/41	-
45	SF4	C	301	3	-	-	0/6/5/5
48	PLX	r	504	40	-	29/55/55/55	-
53	CDL	l	701	-	-	52/109/109/110	-
47	PEE	m	201	-	-	21/44/44/54	-
56	ADP	w	401	-	-	3/16/32/32	0/3/3/3
53	CDL	l	702	-	-	56/110/110/110	-
53	CDL	N	201	-	-	20/61/61/110	-
45	SF4	B	301	2	-	-	0/6/5/5
48	PLX	C	302	-	-	29/55/55/55	-
45	SF4	M	802	12	-	-	0/6/5/5
47	PEE	j	201	-	-	21/50/50/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	PEE	r	501	-	-	24/54/54/54	-
53	CDL	r	505	-	-	65/110/110/110	-
53	CDL	o	201	-	-	32/78/78/110	-
50	NDP	J	401	-	-	9/34/77/77	0/5/5/5
48	PLX	r	503	-	-	34/55/55/55	-
45	SF4	B	302	2	-	-	0/6/5/5
45	SF4	M	801	12	-	-	0/6/5/5
51	FES	O	301	14	-	-	0/1/1/1
45	SF4	A	501	1	-	-	0/6/5/5
49	8Q1	G	201	6	-	12/41/41/41	-
53	CDL	u	201	-	-	24/88/88/110	-
48	PLX	j	203	-	-	29/55/55/55	-
47	PEE	j	202	-	-	28/54/54/54	-
53	CDL	a	201	-	-	26/101/101/110	-
47	PEE	b	201	-	-	26/49/49/54	-
46	FMN	A	502	-	-	5/18/18/18	0/3/3/3
47	PEE	l	703	-	-	22/49/49/54	-
55	UQ	s	401	-	-	8/21/45/87	0/1/1/1
48	PLX	r	502	-	-	25/55/55/55	-
53	CDL	V	201	-	-	30/104/104/110	-
47	PEE	i	402	-	-	23/50/50/54	-
53	CDL	i	401	-	-	31/76/76/110	-
47	PEE	B	303	-	-	23/54/54/54	-

All (158) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	J	401	NDP	P2B-O2B	12.67	1.83	1.59
55	s	401	UQ	C13-C14	9.35	1.55	1.33
55	s	401	UQ	C8-C9	8.97	1.54	1.33
56	w	401	ADP	C3'-C4'	-8.91	1.30	1.53
55	s	401	UQ	C18-C19	8.23	1.56	1.32
49	X	201	8Q1	P24-O27	7.85	1.85	1.60
49	G	201	8Q1	P24-O27	7.77	1.85	1.60
56	w	401	ADP	O4'-C4'	7.63	1.62	1.45
56	w	401	ADP	C6-N6	5.57	1.48	1.34
56	w	401	ADP	O4'-C1'	-4.41	1.31	1.42
53	a	201	CDL	OA8-CA7	4.29	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	u	201	CDL	OA8-CA7	4.28	1.45	1.33
53	N	201	CDL	OA8-CA7	4.28	1.45	1.33
53	i	401	CDL	OA8-CA7	4.27	1.45	1.33
53	i	401	CDL	OA6-CA5	4.26	1.46	1.34
53	V	201	CDL	OA8-CA7	4.26	1.45	1.33
53	i	401	CDL	OB8-CB7	4.25	1.45	1.33
53	o	201	CDL	OA8-CA7	4.25	1.45	1.33
53	a	201	CDL	OB8-CB7	4.24	1.45	1.33
53	N	201	CDL	OB8-CB7	4.24	1.45	1.33
53	V	201	CDL	OB8-CB7	4.22	1.45	1.33
53	u	201	CDL	OB8-CB7	4.22	1.45	1.33
53	o	201	CDL	OB8-CB7	4.21	1.45	1.33
53	a	201	CDL	OB6-CB5	4.19	1.46	1.34
53	i	401	CDL	OB6-CB5	4.17	1.46	1.34
53	V	201	CDL	OA6-CA5	4.16	1.46	1.34
53	N	201	CDL	OA6-CA5	4.13	1.45	1.34
49	G	201	8Q1	C1-S44	4.12	1.86	1.76
53	o	201	CDL	OA6-CA5	4.10	1.45	1.34
50	J	401	NDP	PN-O5D	4.08	1.75	1.59
53	u	201	CDL	OA6-CA5	4.07	1.45	1.34
53	N	201	CDL	OB6-CB5	4.06	1.45	1.34
53	a	201	CDL	OA6-CA5	4.06	1.45	1.34
53	V	201	CDL	OB6-CB5	4.06	1.45	1.34
53	o	201	CDL	OB6-CB5	4.04	1.45	1.34
49	X	201	8Q1	C1-S44	4.04	1.85	1.76
53	u	201	CDL	OB6-CB5	3.98	1.45	1.34
46	A	502	FMN	C4A-N5	3.88	1.38	1.30
47	j	201	PEE	C18-C19	3.75	1.53	1.31
47	m	201	PEE	C18-C19	3.75	1.53	1.31
47	l	703	PEE	C18-C19	3.73	1.53	1.31
47	B	303	PEE	C18-C19	3.72	1.53	1.31
47	V	202	PEE	C18-C19	3.72	1.53	1.31
47	b	201	PEE	C18-C19	3.72	1.53	1.31
47	r	501	PEE	C18-C19	3.71	1.53	1.31
47	j	202	PEE	C18-C19	3.70	1.53	1.31
47	i	402	PEE	C18-C19	3.70	1.53	1.31
47	j	201	PEE	C39-C38	3.66	1.53	1.31
49	X	201	8Q1	C34-N36	3.65	1.41	1.33
47	r	501	PEE	C39-C38	3.64	1.52	1.31
47	i	402	PEE	C39-C38	3.63	1.52	1.31
47	b	201	PEE	C39-C38	3.63	1.52	1.31
47	j	202	PEE	C39-C38	3.63	1.52	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	V	202	PEE	C39-C38	3.63	1.52	1.31
47	l	703	PEE	C39-C38	3.63	1.52	1.31
47	B	303	PEE	C39-C38	3.63	1.52	1.31
49	G	201	8Q1	C34-N36	3.60	1.41	1.33
49	X	201	8Q1	C6-C1	3.58	1.54	1.50
53	r	505	CDL	OA8-CA7	3.46	1.43	1.33
53	l	702	CDL	OA8-CA7	3.44	1.43	1.33
53	l	701	CDL	OA8-CA7	3.40	1.43	1.33
49	G	201	8Q1	C6-C1	3.39	1.54	1.50
49	G	201	8Q1	O27-C28	-3.33	1.33	1.43
49	X	201	8Q1	O27-C28	-3.29	1.33	1.43
56	w	401	ADP	O2'-C2'	-3.24	1.35	1.43
56	w	401	ADP	C8-N9	-3.17	1.31	1.37
56	w	401	ADP	O3'-C3'	3.15	1.50	1.43
49	G	201	8Q1	C39-N41	3.14	1.40	1.33
49	X	201	8Q1	C39-N41	3.10	1.40	1.33
53	l	702	CDL	OB6-CB5	3.05	1.42	1.34
53	l	701	CDL	OB6-CB5	3.03	1.42	1.34
53	r	505	CDL	OB6-CB5	3.01	1.42	1.34
53	l	702	CDL	OB8-CB7	3.00	1.42	1.33
53	r	505	CDL	OB8-CB7	2.99	1.42	1.33
50	J	401	NDP	O2B-C2B	-2.99	1.33	1.44
53	l	702	CDL	OA6-CA5	2.99	1.42	1.34
53	l	701	CDL	OB8-CB7	2.99	1.42	1.33
53	r	505	CDL	OA6-CA5	2.94	1.42	1.34
53	l	701	CDL	OA6-CA5	2.92	1.42	1.34
48	C	302	PLX	O6-C4	-2.76	1.40	1.44
48	g	201	PLX	O6-C4	-2.74	1.40	1.44
48	r	503	PLX	O6-C4	-2.66	1.41	1.44
55	s	401	UQ	C6-C1	2.65	1.54	1.46
48	r	504	PLX	O6-C4	-2.62	1.41	1.44
48	j	203	PLX	O6-C4	-2.58	1.41	1.44
47	j	201	PEE	O3-C30	2.52	1.40	1.33
47	B	303	PEE	O2-C2	-2.51	1.40	1.46
47	i	402	PEE	O3-C30	2.51	1.40	1.33
47	b	201	PEE	O3-C30	2.48	1.40	1.33
47	l	703	PEE	O2-C2	-2.47	1.40	1.46
46	A	502	FMN	C10-N1	2.46	1.38	1.33
47	r	501	PEE	O2-C2	-2.45	1.40	1.46
47	i	402	PEE	O2-C2	-2.43	1.40	1.46
47	r	501	PEE	O3-C30	2.43	1.40	1.33
47	l	703	PEE	O3-C30	2.43	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	l	701	CDL	OA6-CA4	-2.42	1.40	1.46
48	j	203	PLX	C7-C6	2.42	1.55	1.50
47	j	202	PEE	O3-C30	2.42	1.40	1.33
47	V	202	PEE	O3-C30	2.41	1.40	1.33
47	j	202	PEE	O2-C2	-2.41	1.40	1.46
47	j	201	PEE	O2-C2	-2.40	1.40	1.46
48	r	504	PLX	C7-C6	2.39	1.55	1.50
47	m	201	PEE	O2-C10	2.39	1.41	1.34
48	r	502	PLX	C7-C6	2.39	1.55	1.50
47	b	201	PEE	O2-C2	-2.38	1.40	1.46
53	r	505	CDL	OA6-CA4	-2.38	1.40	1.46
47	B	303	PEE	O3-C30	2.37	1.40	1.33
47	m	201	PEE	O3-C30	2.35	1.40	1.33
53	l	702	CDL	OA6-CA4	-2.35	1.40	1.46
50	J	401	NDP	C5A-C4A	2.34	1.43	1.39
48	r	503	PLX	C7-C6	2.34	1.55	1.50
47	V	202	PEE	O2-C10	2.33	1.40	1.34
48	g	201	PLX	C7-C6	2.32	1.55	1.50
47	V	202	PEE	O2-C2	-2.31	1.40	1.46
47	m	201	PEE	O2-C2	-2.31	1.40	1.46
55	s	401	UQ	C7-C8	2.30	1.54	1.50
48	C	302	PLX	C7-C6	2.29	1.55	1.50
56	w	401	ADP	C5-N7	-2.29	1.34	1.39
47	j	201	PEE	O2-C10	2.29	1.40	1.34
47	i	402	PEE	O2-C10	2.28	1.40	1.34
47	j	202	PEE	O2-C10	2.27	1.40	1.34
47	b	201	PEE	O2-C10	2.27	1.40	1.34
47	r	501	PEE	O2-C10	2.25	1.40	1.34
55	s	401	UQ	O4-C4	-2.25	1.18	1.23
47	B	303	PEE	O2-C10	2.22	1.40	1.34
53	l	702	CDL	PB2-OB2	2.20	1.68	1.59
53	l	701	CDL	PB2-OB2	2.20	1.68	1.59
53	r	505	CDL	PB2-OB2	2.20	1.68	1.59
53	r	505	CDL	PB2-OB5	2.20	1.68	1.59
47	m	201	PEE	O3-C3	-2.19	1.40	1.45
47	l	703	PEE	O3-C3	-2.19	1.40	1.45
47	l	703	PEE	O2-C10	2.18	1.40	1.34
48	r	502	PLX	O6-C4	-2.17	1.41	1.44
53	l	701	CDL	PB2-OB5	2.16	1.68	1.59
53	l	702	CDL	PB2-OB5	2.16	1.68	1.59
48	r	504	PLX	P1-O4	2.16	1.68	1.59
53	l	702	CDL	OB6-CB4	-2.15	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	j	203	PLX	P1-O4	2.15	1.68	1.59
53	l	701	CDL	OB6-CB4	-2.14	1.41	1.46
48	r	503	PLX	P1-O4	2.13	1.67	1.59
50	J	401	NDP	C2A-N1A	2.13	1.37	1.33
48	r	502	PLX	P1-O4	2.12	1.67	1.59
48	C	302	PLX	P1-O4	2.11	1.67	1.59
48	g	201	PLX	P1-O4	2.10	1.67	1.59
47	B	303	PEE	O3-C3	-2.10	1.40	1.45
47	j	202	PEE	O3-C3	-2.10	1.40	1.45
53	r	505	CDL	OB6-CB4	-2.10	1.41	1.46
47	V	202	PEE	O3-C3	-2.08	1.40	1.45
47	r	501	PEE	O3-C3	-2.08	1.40	1.45
47	b	201	PEE	O3-C3	-2.08	1.40	1.45
47	j	201	PEE	O3-C3	-2.06	1.40	1.45
48	C	302	PLX	P1-O1	2.05	1.67	1.59
48	r	502	PLX	P1-O1	2.04	1.67	1.59
48	r	504	PLX	P1-O1	2.04	1.67	1.59
55	s	401	UQ	O1-C1	-2.04	1.18	1.23
48	j	203	PLX	P1-O1	2.04	1.67	1.59
48	r	503	PLX	P1-O1	2.04	1.67	1.59
47	i	402	PEE	O3-C3	-2.03	1.40	1.45

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	s	401	UQ	C7-C8-C9	-9.15	111.56	126.79
50	J	401	NDP	PN-O3-PA	-7.05	108.62	132.83
55	s	401	UQ	C12-C13-C14	-5.82	113.64	127.66
56	w	401	ADP	C5-C4-N3	-5.80	119.19	126.75
49	X	201	8Q1	C6-C1-S44	4.57	118.77	113.46
55	s	401	UQ	C11-C9-C8	-4.55	111.92	121.12
55	s	401	UQ	C10-C9-C8	-4.49	112.15	123.68
49	G	201	8Q1	C6-C1-S44	4.47	118.66	113.46
56	w	401	ADP	N3-C4-N9	4.46	134.43	127.08
56	w	401	ADP	N3-C2-N1	-4.36	121.78	128.60
53	i	401	CDL	OA6-CA5-C11	4.34	120.86	111.50
53	u	201	CDL	OA6-CA5-C11	4.28	120.72	111.50
53	N	201	CDL	OB6-CB5-C51	4.20	120.55	111.50
55	s	401	UQ	C15-C14-C13	-4.14	113.05	123.68
47	B	303	PEE	O2-C10-C11	4.10	120.34	111.50
53	l	701	CDL	OB6-CB5-C51	4.09	120.32	111.50
53	a	201	CDL	OB6-CB5-C51	4.08	120.29	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	V	201	CDL	OB6-CB5-C51	4.08	120.28	111.50
53	r	505	CDL	OB6-CB5-C51	4.05	120.22	111.50
47	r	501	PEE	O2-C10-C11	4.03	120.19	111.50
55	s	401	UQ	C16-C14-C13	-4.03	112.96	121.12
53	N	201	CDL	OA6-CA5-C11	4.03	120.18	111.50
53	o	201	CDL	OB6-CB5-C51	4.02	120.16	111.50
47	m	201	PEE	O2-C10-C11	4.01	120.15	111.50
47	V	202	PEE	O2-C10-C11	4.01	120.15	111.50
47	b	201	PEE	O2-C10-C11	4.00	120.12	111.50
55	s	401	UQ	C17-C18-C19	-3.99	114.11	127.75
47	j	202	PEE	O2-C10-C11	3.98	120.09	111.50
53	l	702	CDL	OA6-CA5-C11	3.97	120.05	111.50
53	i	401	CDL	OB6-CB5-C51	3.94	119.98	111.50
53	l	701	CDL	OA6-CA5-C11	3.94	119.98	111.50
47	l	703	PEE	O2-C10-C11	3.93	119.96	111.50
47	i	402	PEE	O2-C10-C11	3.91	119.92	111.50
53	r	505	CDL	OA6-CA5-C11	3.91	119.92	111.50
53	l	702	CDL	OB6-CB5-C51	3.90	119.90	111.50
53	o	201	CDL	OA6-CA5-C11	3.88	119.86	111.50
47	j	201	PEE	O2-C10-C11	3.86	119.82	111.50
53	u	201	CDL	OB6-CB5-C51	3.77	119.62	111.50
53	V	201	CDL	OA6-CA5-C11	3.74	119.56	111.50
56	w	401	ADP	C2-N3-C4	3.68	120.45	111.75
56	w	401	ADP	N9-C8-N7	-3.62	108.97	113.91
53	a	201	CDL	OA6-CA5-C11	3.59	119.24	111.50
49	X	201	8Q1	C43-S44-C1	3.58	113.02	101.87
56	w	401	ADP	C5-N7-C8	3.49	108.46	103.51
49	G	201	8Q1	C43-S44-C1	3.43	112.56	101.87
50	J	401	NDP	O2B-P2B-O1X	-3.37	96.40	109.39
55	s	401	UQ	C21-C19-C18	-3.35	112.96	122.65
49	G	201	8Q1	O35-C34-N36	-3.21	116.11	122.99
49	X	201	8Q1	O35-C34-N36	-3.19	116.15	122.99
46	A	502	FMN	C4-N3-C2	-3.06	119.98	125.64
56	w	401	ADP	C4-N9-C8	3.05	109.03	105.73
55	s	401	UQ	C20-C19-C18	-3.03	113.88	122.65
50	J	401	NDP	PA-O5B-C5B	-3.03	103.92	121.68
53	V	201	CDL	OB8-CB7-C71	2.97	121.22	111.91
53	i	401	CDL	OA8-CA7-C31	2.92	121.08	111.91
53	a	201	CDL	OB8-CB7-C71	2.92	121.07	111.91
50	J	401	NDP	PN-O5D-C5D	-2.90	104.66	121.68
56	w	401	ADP	C4-C5-N7	-2.85	107.15	110.62
53	a	201	CDL	OA8-CA7-C31	2.84	120.81	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	G	201	8Q1	C37-C38-C39	2.83	117.07	112.36
49	X	201	8Q1	O2-P24-O27	-2.81	99.25	106.73
53	V	201	CDL	OA8-CA7-C31	2.81	120.72	111.91
47	r	501	PEE	O3-C30-C31	2.78	120.64	111.91
49	G	201	8Q1	O2-P24-O27	-2.78	99.34	106.73
53	V	201	CDL	CB4-OB6-CB5	-2.74	111.04	117.79
53	N	201	CDL	OA8-CA7-C31	2.74	120.52	111.91
53	N	201	CDL	OB8-CB7-C71	2.74	120.51	111.91
53	N	201	CDL	CB4-OB6-CB5	-2.72	111.08	117.79
47	B	303	PEE	O3-C30-C31	2.72	120.44	111.91
55	s	401	UQ	CM5-C5-C6	-2.65	120.08	124.40
46	A	502	FMN	C4A-C4-N3	2.65	119.91	113.19
56	w	401	ADP	PA-O3A-PB	-2.65	123.75	132.83
47	l	703	PEE	O3-C30-C31	2.63	120.16	111.91
53	l	701	CDL	OB8-CB7-C71	2.62	120.13	111.91
47	b	201	PEE	O3-C30-C31	2.60	120.05	111.91
53	o	201	CDL	OA8-CA7-C31	2.59	120.05	111.91
53	u	201	CDL	OA8-CA7-C31	2.58	120.01	111.91
53	u	201	CDL	OB8-CB7-C71	2.58	120.01	111.91
53	l	701	CDL	OA8-CA7-C31	2.58	120.00	111.91
47	i	402	PEE	O3-C30-C31	2.58	119.99	111.91
53	r	505	CDL	OB8-CB7-C71	2.57	119.98	111.91
47	j	202	PEE	O3-C30-C31	2.57	119.98	111.91
49	X	201	8Q1	C32-C34-N36	2.56	121.68	116.58
47	V	202	PEE	O3-C30-C31	2.56	119.95	111.91
50	J	401	NDP	O3X-P2B-O2X	2.56	117.41	107.64
53	l	702	CDL	OA8-CA7-C31	2.56	119.93	111.91
47	m	201	PEE	O3-C30-C31	2.54	119.88	111.91
47	j	201	PEE	O3-C30-C31	2.54	119.86	111.91
53	l	702	CDL	OB8-CB7-C71	2.52	119.81	111.91
53	r	505	CDL	OA8-CA7-C31	2.51	119.77	111.91
53	i	401	CDL	OB8-CB7-C71	2.49	119.73	111.91
49	G	201	8Q1	C32-C34-N36	2.49	121.54	116.58
48	r	503	PLX	C1A-N1-C1	2.48	120.08	109.92
50	J	401	NDP	O4B-C4B-C3B	2.47	110.00	105.11
46	A	502	FMN	O4-C4-C4A	-2.47	120.06	126.60
50	J	401	NDP	N3A-C4A-N9A	2.46	131.14	127.08
49	X	201	8Q1	C37-C38-C39	2.45	116.44	112.36
46	A	502	FMN	C4A-C10-N10	2.45	120.06	116.48
53	o	201	CDL	OB8-CB7-C71	2.45	119.58	111.91
49	X	201	8Q1	O1-P24-O2	2.43	116.93	107.64
48	j	203	PLX	C1A-N1-C1	2.43	119.84	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	X	201	8Q1	O40-C39-N41	-2.42	118.45	123.01
48	r	504	PLX	C1A-N1-C1	2.41	119.78	109.92
49	G	201	8Q1	O40-C39-N41	-2.41	118.47	123.01
50	J	401	NDP	O5D-PN-O1N	-2.40	99.70	109.07
48	g	201	PLX	C1A-N1-C1	2.38	119.66	109.92
49	G	201	8Q1	O1-P24-O2	2.38	116.73	107.64
48	r	502	PLX	C1A-N1-C1	2.38	119.63	109.92
50	J	401	NDP	C2A-N1A-C6A	-2.37	114.70	118.77
50	J	401	NDP	C5A-C4A-N3A	-2.36	123.68	126.75
53	o	201	CDL	CB4-OB6-CB5	-2.33	112.07	117.79
50	J	401	NDP	O2N-PN-O1N	2.31	123.65	112.24
46	A	502	FMN	C10-C4A-N5	-2.26	120.06	124.86
48	C	302	PLX	C1A-N1-C1	2.24	119.10	109.92
50	J	401	NDP	C5B-C4B-C3B	-2.24	106.78	115.18
49	X	201	8Q1	O4-C1-S44	-2.22	119.73	122.61
46	A	502	FMN	C9A-C5A-N5	-2.21	120.03	122.43
53	i	401	CDL	CA4-OA6-CA5	-2.18	112.43	117.79
56	w	401	ADP	C4'-O4'-C1'	-2.17	104.68	109.47
49	G	201	8Q1	O4-C1-S44	-2.15	119.82	122.61
46	A	502	FMN	C4A-C10-N1	-2.13	119.80	124.73
49	X	201	8Q1	O4-C1-C6	-2.11	121.49	123.99
53	a	201	CDL	CB4-OB6-CB5	-2.11	112.59	117.79
49	G	201	8Q1	O4-C1-C6	-2.09	121.52	123.99
46	A	502	FMN	C5A-C9A-N10	2.04	120.06	117.95
53	N	201	CDL	CA6-CA4-CA3	-2.02	107.01	111.79

There are no chirality outliers.

All (777) 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	V	202	PEE	C1-O3P-P-O1P
47	i	402	PEE	C11-C10-O2-C2
47	i	402	PEE	C4-O4P-P-O1P
47	j	201	PEE	C4-O4P-P-O2P
47	j	201	PEE	C4-O4P-P-O1P
47	j	201	PEE	O4P-C4-C5-N
47	j	202	PEE	C19-C20-C21-C22
47	j	202	PEE	C1-O3P-P-O2P
47	j	202	PEE	C1-O3P-P-O1P
47	j	202	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
47	j	202	PEE	C4-O4P-P-O2P
47	l	703	PEE	C11-C10-O2-C2
47	l	703	PEE	C1-O3P-P-O1P
47	l	703	PEE	C39-C40-C41-C42
47	m	201	PEE	C4-O4P-P-O1P
47	r	501	PEE	C11-C10-O2-C2
47	r	501	PEE	C4-O4P-P-O2P
47	r	501	PEE	C4-O4P-P-O1P
48	C	302	PLX	O7-C6-O6-C4
48	C	302	PLX	N1-C1-C2-O1
48	g	201	PLX	C25-C24-O8-C5
48	j	203	PLX	O7-C6-C7-C8
48	j	203	PLX	C25-C24-O8-C5
48	j	203	PLX	O9-C24-C25-C26
48	r	502	PLX	O7-C6-O6-C4
48	r	502	PLX	C5-C4-O6-C6
48	r	502	PLX	O9-C24-O8-C5
48	r	502	PLX	O9-C24-C25-C26
48	r	503	PLX	O7-C6-O6-C4
48	r	503	PLX	C3-O4-P1-O3
48	r	503	PLX	C2-O1-P1-O4
48	r	503	PLX	C2-O1-P1-O2
48	r	503	PLX	C2-O1-P1-O3
48	r	503	PLX	C25-C24-O8-C5
48	r	503	PLX	O9-C24-C25-C26
48	r	504	PLX	O7-C6-C7-C8
48	r	504	PLX	O7-C6-O6-C4
48	r	504	PLX	O4-C3-C4-O6
48	r	504	PLX	C3-O4-P1-O2
48	r	504	PLX	C3-O4-P1-O3
48	r	504	PLX	O9-C24-C25-C26
49	G	201	8Q1	O4-C1-S44-C43
49	G	201	8Q1	C6-C1-S44-C43
49	G	201	8Q1	N36-C37-C38-C39
49	G	201	8Q1	N41-C42-C43-S44
49	G	201	8Q1	C42-C43-S44-C1
49	G	201	8Q1	C28-O27-P24-O3
49	G	201	8Q1	C28-O27-P24-O2
49	G	201	8Q1	C28-O27-P24-O1
49	X	201	8Q1	C1-C6-C7-C8
49	X	201	8Q1	O4-C1-S44-C43
49	X	201	8Q1	C6-C1-S44-C43

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Mol	Chain	Res	Type	Atoms
49	X	201	8Q1	C28-C29-C32-C34
49	X	201	8Q1	C28-C29-C32-O33
49	X	201	8Q1	C30-C29-C32-C34
49	X	201	8Q1	C30-C29-C32-O33
49	X	201	8Q1	C31-C29-C32-C34
49	X	201	8Q1	C29-C32-C34-N36
49	X	201	8Q1	C29-C32-C34-O35
49	X	201	8Q1	O33-C32-C34-N36
49	X	201	8Q1	N36-C37-C38-C39
49	X	201	8Q1	C42-C43-S44-C1
49	X	201	8Q1	C28-O27-P24-O3
49	X	201	8Q1	C28-O27-P24-O2
49	X	201	8Q1	C28-O27-P24-O1
50	J	401	NDP	C5B-O5B-PA-O2A
50	J	401	NDP	C5B-O5B-PA-O3
50	J	401	NDP	C3B-C4B-C5B-O5B
50	J	401	NDP	C2B-O2B-P2B-O1X
53	N	201	CDL	CA2-OA2-PA1-OA4
53	N	201	CDL	CA3-OA5-PA1-OA2
53	N	201	CDL	CA6-CA4-OA6-CA5
53	N	201	CDL	CB2-OB2-PB2-OB4
53	V	201	CDL	CA2-OA2-PA1-OA5
53	V	201	CDL	CA3-OA5-PA1-OA2
53	V	201	CDL	CB2-OB2-PB2-OB3
53	V	201	CDL	CB2-OB2-PB2-OB4
53	V	201	CDL	CB2-OB2-PB2-OB5
53	V	201	CDL	CB3-OB5-PB2-OB3
53	V	201	CDL	CB3-OB5-PB2-OB4
53	a	201	CDL	CA2-OA2-PA1-OA3
53	a	201	CDL	CA2-OA2-PA1-OA4
53	a	201	CDL	CA2-OA2-PA1-OA5
53	a	201	CDL	CA3-OA5-PA1-OA2
53	a	201	CDL	CB2-OB2-PB2-OB3
53	a	201	CDL	CB3-OB5-PB2-OB3
53	i	401	CDL	CB2-C1-CA2-OA2
53	i	401	CDL	CA2-OA2-PA1-OA5
53	i	401	CDL	CA3-OA5-PA1-OA4
53	i	401	CDL	CB2-OB2-PB2-OB3
53	i	401	CDL	CB3-OB5-PB2-OB3
53	l	701	CDL	O1-C1-CA2-OA2
53	l	701	CDL	CA2-OA2-PA1-OA3
53	l	701	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
53	l	701	CDL	CA2-OA2-PA1-OA5
53	l	701	CDL	CA3-OA5-PA1-OA3
53	l	701	CDL	CB2-OB2-PB2-OB3
53	l	701	CDL	CB2-OB2-PB2-OB4
53	l	701	CDL	CB3-OB5-PB2-OB3
53	l	702	CDL	O1-C1-CA2-OA2
53	l	702	CDL	OA6-CA4-CA6-OA8
53	l	702	CDL	CB2-OB2-PB2-OB3
53	l	702	CDL	CB2-OB2-PB2-OB4
53	l	702	CDL	CB2-OB2-PB2-OB5
53	l	702	CDL	OB6-CB4-CB6-OB8
53	o	201	CDL	CA2-OA2-PA1-OA4
53	o	201	CDL	CA3-OA5-PA1-OA3
53	o	201	CDL	CB2-OB2-PB2-OB4
53	o	201	CDL	CB3-OB5-PB2-OB3
53	o	201	CDL	CB3-OB5-PB2-OB4
53	o	201	CDL	OB5-CB3-CB4-OB6
53	r	505	CDL	CA2-OA2-PA1-OA3
53	r	505	CDL	CA2-OA2-PA1-OA4
53	r	505	CDL	CA3-OA5-PA1-OA2
53	r	505	CDL	CA3-OA5-PA1-OA4
53	r	505	CDL	CB2-OB2-PB2-OB3
53	r	505	CDL	CB3-OB5-PB2-OB2
53	r	505	CDL	CB3-OB5-PB2-OB3
53	r	505	CDL	CB3-OB5-PB2-OB4
53	u	201	CDL	CA2-OA2-PA1-OA3
53	u	201	CDL	CA2-OA2-PA1-OA4
53	u	201	CDL	CA2-OA2-PA1-OA5
53	u	201	CDL	CA3-OA5-PA1-OA2
53	u	201	CDL	CA3-OA5-PA1-OA3
53	u	201	CDL	CA3-OA5-PA1-OA4
53	u	201	CDL	CB3-OB5-PB2-OB3
55	s	401	UQ	C7-C8-C9-C10
55	s	401	UQ	C7-C8-C9-C11
55	s	401	UQ	C12-C11-C9-C8
55	s	401	UQ	C12-C11-C9-C10
55	s	401	UQ	C9-C11-C12-C13
55	s	401	UQ	C12-C13-C14-C16
55	s	401	UQ	C17-C18-C19-C21
56	w	401	ADP	C5'-O5'-PA-O1A
56	w	401	ADP	C5'-O5'-PA-O2A
56	w	401	ADP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
53	l	701	CDL	OA9-CA7-OA8-CA6
47	i	402	PEE	O4-C10-O2-C2
47	l	703	PEE	O4-C10-O2-C2
53	N	201	CDL	OA7-CA5-OA6-CA4
53	r	505	CDL	C71-CB7-OB8-CB6
53	N	201	CDL	C11-CA5-OA6-CA4
53	l	701	CDL	C31-CA7-OA8-CA6
53	l	702	CDL	C71-CB7-OB8-CB6
47	B	303	PEE	C37-C38-C39-C40
47	b	201	PEE	C37-C38-C39-C40
47	j	202	PEE	C17-C18-C19-C20
47	r	501	PEE	O4-C10-O2-C2
53	N	201	CDL	O1-C1-CB2-OB2
53	l	701	CDL	O1-C1-CB2-OB2
53	l	702	CDL	O1-C1-CB2-OB2
47	b	201	PEE	C31-C30-O3-C3
47	m	201	PEE	C31-C30-O3-C3
53	l	702	CDL	OB9-CB7-OB8-CB6
53	r	505	CDL	OB9-CB7-OB8-CB6
48	r	502	PLX	C9-C10-C11-C12
47	j	201	PEE	C14-C15-C16-C17
47	m	201	PEE	C13-C14-C15-C16
48	j	203	PLX	C28-C29-C30-C31
47	b	201	PEE	O5-C30-O3-C3
48	r	504	PLX	C7-C8-C9-C10
53	l	702	CDL	C75-C76-C77-C78
47	j	202	PEE	C30-C31-C32-C33
48	g	201	PLX	C10-C11-C12-C13
50	J	401	NDP	O4D-C4D-C5D-O5D
47	V	202	PEE	C31-C30-O3-C3
48	r	503	PLX	C12-C13-C14-C15
53	l	702	CDL	C59-C60-C61-C62
47	V	202	PEE	C2-C3-O3-C30
53	l	702	CDL	C11-C12-C13-C14
47	V	202	PEE	O5-C30-O3-C3
47	m	201	PEE	O5-C30-O3-C3
53	l	701	CDL	C55-C56-C57-C58
47	j	202	PEE	C32-C33-C34-C35
47	l	703	PEE	C33-C34-C35-C36
53	V	201	CDL	CA2-C1-CB2-OB2
53	i	401	CDL	CA2-C1-CB2-OB2
53	l	701	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
53	l	702	CDL	CA2-C1-CB2-OB2
53	r	505	CDL	CB2-C1-CA2-OA2
53	l	702	CDL	C35-C36-C37-C38
48	r	504	PLX	C2-C1-N1-C1B
48	r	504	PLX	C2-C1-N1-C1A
47	j	202	PEE	C31-C30-O3-C3
47	l	703	PEE	C31-C30-O3-C3
53	i	401	CDL	C31-CA7-OA8-CA6
53	o	201	CDL	C31-CA7-OA8-CA6
47	b	201	PEE	C10-C11-C12-C13
48	r	502	PLX	C30-C31-C32-C33
53	V	201	CDL	O1-C1-CA2-OA2
53	i	401	CDL	O1-C1-CA2-OA2
53	i	401	CDL	OB6-CB4-CB6-OB8
53	i	401	CDL	OA9-CA7-OA8-CA6
48	g	201	PLX	C12-C13-C14-C15
47	j	202	PEE	C34-C35-C36-C37
48	j	203	PLX	C15-C16-C17-C18
53	l	701	CDL	CB7-C71-C72-C73
47	j	202	PEE	O5-C30-O3-C3
47	V	202	PEE	C30-C31-C32-C33
53	l	702	CDL	CB5-C51-C52-C53
53	r	505	CDL	CA7-C31-C32-C33
50	J	401	NDP	O4B-C4B-C5B-O5B
50	J	401	NDP	C3D-C4D-C5D-O5D
53	r	505	CDL	C74-C75-C76-C77
48	r	503	PLX	C2-C1-N1-C1A
47	l	703	PEE	O5-C30-O3-C3
53	r	505	CDL	C76-C77-C78-C79
53	l	702	CDL	C39-C40-C41-C42
53	V	201	CDL	O1-C1-CB2-OB2
53	i	401	CDL	O1-C1-CB2-OB2
53	r	505	CDL	O1-C1-CA2-OA2
47	i	402	PEE	C2-C3-O3-C30
48	g	201	PLX	C31-C32-C33-C34
53	o	201	CDL	OA9-CA7-OA8-CA6
53	l	702	CDL	CB7-C71-C72-C73
48	r	502	PLX	C11-C12-C13-C14
53	o	201	CDL	C79-C80-C81-C82
47	B	303	PEE	C11-C10-O2-C2
47	j	202	PEE	C11-C10-O2-C2
47	i	402	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
47	j	201	PEE	C4-O4P-P-O3P
47	j	202	PEE	C1-O3P-P-O4P
47	r	501	PEE	C4-O4P-P-O3P
48	C	302	PLX	C3-O4-P1-O1
48	g	201	PLX	C3-O4-P1-O1
48	r	503	PLX	C3-O4-P1-O1
48	r	504	PLX	C3-O4-P1-O1
53	N	201	CDL	CA2-OA2-PA1-OA5
53	N	201	CDL	CB2-OB2-PB2-OB5
53	V	201	CDL	CB3-OB5-PB2-OB2
53	a	201	CDL	CB2-OB2-PB2-OB5
53	i	401	CDL	CA3-OA5-PA1-OA2
53	i	401	CDL	CB3-OB5-PB2-OB2
53	l	701	CDL	CB2-OB2-PB2-OB5
53	l	701	CDL	CB3-OB5-PB2-OB2
53	o	201	CDL	CA2-OA2-PA1-OA5
53	o	201	CDL	CB2-OB2-PB2-OB5
53	o	201	CDL	CB3-OB5-PB2-OB2
53	r	505	CDL	CA2-OA2-PA1-OA5
53	u	201	CDL	CB2-OB2-PB2-OB5
53	r	505	CDL	CB5-C51-C52-C53
47	i	402	PEE	C30-C31-C32-C33
53	l	701	CDL	CA2-C1-CB2-OB2
53	l	702	CDL	CB2-C1-CA2-OA2
47	B	303	PEE	O4-C10-O2-C2
47	j	202	PEE	O4-C10-O2-C2
48	r	503	PLX	C2-C1-N1-C1C
53	l	701	CDL	C71-CB7-OB8-CB6
53	l	701	CDL	C58-C59-C60-C61
48	g	201	PLX	O8-C24-C25-C26
53	o	201	CDL	C32-C33-C34-C35
48	r	502	PLX	C27-C28-C29-C30
48	r	504	PLX	C28-C29-C30-C31
53	l	702	CDL	C37-C38-C39-C40
53	r	505	CDL	C35-C36-C37-C38
53	r	505	CDL	C51-CB5-OB6-CB4
48	r	503	PLX	C13-C14-C15-C16
48	r	504	PLX	C11-C10-C9-C8
49	X	201	8Q1	C11-C12-C13-C14
53	l	701	CDL	C52-C53-C54-C55
53	l	701	CDL	C74-C75-C76-C77
53	r	505	CDL	C56-C57-C58-C59

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Mol	Chain	Res	Type	Atoms
53	r	505	CDL	C59-C60-C61-C62
53	r	505	CDL	OB7-CB5-OB6-CB4
47	V	202	PEE	C11-C12-C13-C14
47	m	201	PEE	C33-C34-C35-C36
47	r	501	PEE	C12-C13-C14-C15
49	G	201	8Q1	C6-C7-C8-C9
47	V	202	PEE	C17-C18-C19-C20
48	r	502	PLX	C7-C8-C9-C10
53	N	201	CDL	O1-C1-CA2-OA2
48	r	504	PLX	C10-C11-C12-C13
47	l	703	PEE	C30-C31-C32-C33
53	r	505	CDL	CB7-C71-C72-C73
48	g	201	PLX	C11-C10-C9-C8
48	r	502	PLX	C14-C15-C16-C17
53	V	201	CDL	C52-C53-C54-C55
53	l	701	CDL	C35-C36-C37-C38
53	l	701	CDL	C82-C83-C84-C85
53	l	702	CDL	C55-C56-C57-C58
53	r	505	CDL	C12-C13-C14-C15
53	l	701	CDL	OB9-CB7-OB8-CB6
47	B	303	PEE	C22-C23-C24-C25
48	C	302	PLX	C25-C26-C27-C28
48	g	201	PLX	C9-C10-C11-C12
49	G	201	8Q1	C12-C13-C14-C15
53	l	701	CDL	C73-C74-C75-C76
53	l	701	CDL	C75-C76-C77-C78
53	r	505	CDL	C32-C33-C34-C35
53	r	505	CDL	C71-C72-C73-C74
53	r	505	CDL	C73-C74-C75-C76
47	B	303	PEE	C20-C21-C22-C23
47	r	501	PEE	C40-C41-C42-C43
48	C	302	PLX	C14-C15-C16-C17
48	g	201	PLX	C25-C26-C27-C28
48	j	203	PLX	C10-C11-C12-C13
48	r	503	PLX	C27-C28-C29-C30
48	r	503	PLX	C10-C11-C12-C13
53	l	701	CDL	C56-C57-C58-C59
53	V	201	CDL	C11-CA5-OA6-CA4
47	l	703	PEE	C34-C35-C36-C37
48	r	503	PLX	C14-C15-C16-C17
49	G	201	8Q1	C11-C12-C13-C14
53	l	701	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
53	l	701	CDL	C61-C62-C63-C64
53	l	702	CDL	C72-C73-C74-C75
53	u	201	CDL	C75-C76-C77-C78
47	m	201	PEE	C22-C23-C24-C25
48	C	302	PLX	C9-C10-C11-C12
48	j	203	PLX	C7-C8-C9-C10
48	j	203	PLX	C25-C26-C27-C28
48	r	502	PLX	C31-C32-C33-C34
48	r	503	PLX	C25-C26-C27-C28
53	l	701	CDL	C59-C60-C61-C62
53	l	702	CDL	C73-C74-C75-C76
47	j	201	PEE	C13-C14-C15-C16
47	B	303	PEE	C21-C22-C23-C24
47	b	201	PEE	C22-C23-C24-C25
47	b	201	PEE	C13-C14-C15-C16
48	C	302	PLX	C16-C17-C18-C19
48	r	504	PLX	C14-C15-C16-C17
48	r	503	PLX	C28-C29-C30-C31
48	r	504	PLX	C33-C34-C35-C36
53	l	701	CDL	C62-C63-C64-C65
53	r	505	CDL	C75-C76-C77-C78
53	r	505	CDL	C78-C79-C80-C81
47	j	202	PEE	C41-C42-C43-C44
48	g	201	PLX	C27-C28-C29-C30
47	b	201	PEE	C31-C32-C33-C34
47	l	703	PEE	C31-C32-C33-C34
48	j	203	PLX	C27-C28-C29-C30
48	r	502	PLX	C15-C16-C17-C18
53	r	505	CDL	C17-C18-C19-C20
48	r	502	PLX	C12-C13-C14-C15
48	r	502	PLX	C33-C34-C35-C36
48	r	504	PLX	C9-C10-C11-C12
53	l	701	CDL	C20-C21-C22-C23
47	j	201	PEE	C17-C18-C19-C20
47	l	703	PEE	C37-C38-C39-C40
48	C	302	PLX	C17-C18-C19-C20
48	r	504	PLX	C25-C26-C27-C28
53	r	505	CDL	C72-C73-C74-C75
47	V	202	PEE	C11-C10-O2-C2
47	b	201	PEE	C11-C10-O2-C2
53	o	201	CDL	C51-CB5-OB6-CB4
53	u	201	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
47	b	201	PEE	C2-C3-O3-C30
47	B	303	PEE	C33-C34-C35-C36
48	C	302	PLX	C28-C29-C30-C31
48	C	302	PLX	O9-C24-C25-C26
48	g	201	PLX	C28-C29-C30-C31
47	B	303	PEE	C15-C16-C17-C18
47	r	501	PEE	C13-C14-C15-C16
47	j	201	PEE	C41-C42-C43-C44
53	r	505	CDL	C43-C44-C45-C46
47	m	201	PEE	C32-C33-C34-C35
47	V	202	PEE	O4-C10-O2-C2
47	b	201	PEE	O4-C10-O2-C2
53	V	201	CDL	OA7-CA5-OA6-CA4
53	o	201	CDL	OB7-CB5-OB6-CB4
53	u	201	CDL	OA7-CA5-OA6-CA4
53	r	505	CDL	C41-C42-C43-C44
48	r	504	PLX	C2-C1-N1-C1C
47	B	303	PEE	C23-C24-C25-C26
48	r	503	PLX	C33-C34-C35-C36
53	r	505	CDL	C37-C38-C39-C40
48	C	302	PLX	C15-C16-C17-C18
47	b	201	PEE	C32-C33-C34-C35
48	r	503	PLX	C31-C32-C33-C34
53	a	201	CDL	C31-C32-C33-C34
53	l	701	CDL	C14-C15-C16-C17
47	j	201	PEE	C39-C40-C41-C42
53	r	505	CDL	CA5-C11-C12-C13
47	V	202	PEE	C32-C33-C34-C35
47	b	201	PEE	C14-C15-C16-C17
53	l	702	CDL	C58-C59-C60-C61
47	m	201	PEE	C23-C24-C25-C26
47	B	303	PEE	C10-C11-C12-C13
48	C	302	PLX	C31-C32-C33-C34
53	i	401	CDL	C11-C12-C13-C14
53	l	701	CDL	C32-C33-C34-C35
48	g	201	PLX	C33-C34-C35-C36
48	r	502	PLX	C13-C14-C15-C16
47	j	201	PEE	C11-C12-C13-C14
48	j	203	PLX	C14-C15-C16-C17
47	r	501	PEE	C36-C37-C38-C39
48	r	504	PLX	C26-C27-C28-C29
53	r	505	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
48	j	203	PLX	C12-C13-C14-C15
48	r	503	PLX	C29-C30-C31-C32
48	r	503	PLX	C2-C1-N1-C1B
48	r	503	PLX	C26-C27-C28-C29
47	B	303	PEE	C35-C36-C37-C38
47	B	303	PEE	C39-C40-C41-C42
47	r	501	PEE	C39-C40-C41-C42
53	a	201	CDL	CA7-C31-C32-C33
53	r	505	CDL	C57-C58-C59-C60
53	V	201	CDL	C59-C60-C61-C62
47	j	201	PEE	C33-C34-C35-C36
48	C	302	PLX	C13-C14-C15-C16
47	b	201	PEE	C33-C34-C35-C36
48	C	302	PLX	C33-C34-C35-C36
53	l	702	CDL	C74-C75-C76-C77
53	V	201	CDL	C51-CB5-OB6-CB4
48	r	503	PLX	C15-C16-C17-C18
53	l	702	CDL	C54-C55-C56-C57
53	o	201	CDL	C80-C81-C82-C83
53	l	702	CDL	CB3-OB5-PB2-OB2
53	o	201	CDL	CA3-OA5-PA1-OA2
53	r	505	CDL	CB2-OB2-PB2-OB5
53	u	201	CDL	CB3-OB5-PB2-OB2
48	j	203	PLX	C9-C10-C11-C12
53	r	505	CDL	C14-C15-C16-C17
53	r	505	CDL	CB4-CB3-OB5-PB2
47	i	402	PEE	C11-C12-C13-C14
48	g	201	PLX	C13-C14-C15-C16
53	a	201	CDL	C18-C19-C20-C21
48	r	504	PLX	O4-C3-C4-C5
53	o	201	CDL	OB5-CB3-CB4-CB6
48	C	302	PLX	C7-C8-C9-C10
48	r	502	PLX	C10-C11-C12-C13
47	j	201	PEE	C42-C43-C44-C45
47	r	501	PEE	C41-C42-C43-C44
53	o	201	CDL	C78-C79-C80-C81
53	r	505	CDL	C52-C53-C54-C55
47	r	501	PEE	C10-C11-C12-C13
53	N	201	CDL	CA2-C1-CB2-OB2
47	i	402	PEE	C18-C19-C20-C21
47	m	201	PEE	C21-C22-C23-C24
53	a	201	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
47	b	201	PEE	C1-C2-C3-O3
48	j	203	PLX	C34-C35-C36-C37
53	l	702	CDL	CB3-CB4-CB6-OB8
53	r	505	CDL	CB3-CB4-CB6-OB8
47	j	201	PEE	C32-C33-C34-C35
48	C	302	PLX	C18-C19-C20-C21
53	l	701	CDL	C60-C61-C62-C63
48	C	302	PLX	C27-C28-C29-C30
47	j	202	PEE	C36-C37-C38-C39
47	V	202	PEE	C35-C36-C37-C38
47	j	201	PEE	C15-C16-C17-C18
53	o	201	CDL	C51-C52-C53-C54
53	l	702	CDL	C56-C57-C58-C59
48	C	302	PLX	C11-C12-C13-C14
49	X	201	8Q1	C13-C14-C15-C16
48	j	203	PLX	C13-C14-C15-C16
48	j	203	PLX	C26-C27-C28-C29
53	l	701	CDL	C71-C72-C73-C74
53	l	702	CDL	C40-C41-C42-C43
53	l	702	CDL	C64-C65-C66-C67
53	V	201	CDL	CA6-CA4-OA6-CA5
53	u	201	CDL	CA6-CA4-OA6-CA5
53	V	201	CDL	OB7-CB5-OB6-CB4
48	r	504	PLX	C27-C28-C29-C30
47	B	303	PEE	C34-C35-C36-C37
47	B	303	PEE	C40-C41-C42-C43
48	g	201	PLX	C11-C12-C13-C14
47	B	303	PEE	C31-C30-O3-C3
48	C	302	PLX	O4-C3-C4-O6
47	r	501	PEE	C17-C18-C19-C20
48	r	502	PLX	C28-C29-C30-C31
53	u	201	CDL	O1-C1-CA2-OA2
47	i	402	PEE	O2-C2-C3-O3
53	i	401	CDL	OA6-CA4-CA6-OA8
53	l	701	CDL	C37-C38-C39-C40
53	l	702	CDL	C14-C15-C16-C17
49	X	201	8Q1	C31-C29-C32-O33
48	r	503	PLX	C16-C17-C18-C19
49	G	201	8Q1	C13-C14-C15-C16
48	r	503	PLX	C9-C10-C11-C12
48	r	503	PLX	C30-C31-C32-C33
53	l	702	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
53	o	201	CDL	CA7-C31-C32-C33
47	i	402	PEE	C32-C33-C34-C35
53	i	401	CDL	C37-C38-C39-C40
53	l	702	CDL	C60-C61-C62-C63
48	j	203	PLX	C33-C34-C35-C36
53	r	505	CDL	C54-C55-C56-C57
53	N	201	CDL	C51-CB5-OB6-CB4
53	o	201	CDL	C11-CA5-OA6-CA4
48	r	504	PLX	C13-C14-C15-C16
47	b	201	PEE	C23-C24-C25-C26
47	m	201	PEE	C12-C13-C14-C15
47	i	402	PEE	O3P-C1-C2-C3
53	i	401	CDL	OB5-CB3-CB4-CB6
48	r	504	PLX	C34-C35-C36-C37
53	u	201	CDL	C53-C54-C55-C56
53	r	505	CDL	C81-C82-C83-C84
47	l	703	PEE	C22-C23-C24-C25
53	l	702	CDL	C41-C42-C43-C44
53	l	701	CDL	C34-C35-C36-C37
53	l	701	CDL	C42-C43-C44-C45
47	B	303	PEE	C32-C33-C34-C35
47	i	402	PEE	C1-C2-C3-O3
47	j	201	PEE	C1-C2-C3-O3
47	m	201	PEE	C1-C2-C3-O3
47	r	501	PEE	C1-C2-C3-O3
48	r	502	PLX	C3-C4-C5-O8
48	r	503	PLX	C3-C4-C5-O8
53	r	505	CDL	CA3-CA4-CA6-OA8
53	u	201	CDL	CA3-CA4-CA6-OA8
53	l	701	CDL	C76-C77-C78-C79
47	B	303	PEE	C17-C18-C19-C20
47	b	201	PEE	C34-C35-C36-C37
53	r	505	CDL	C13-C14-C15-C16
47	l	703	PEE	C11-C12-C13-C14
48	C	302	PLX	C3-C4-O6-C6
48	j	203	PLX	C3-O4-P1-O1
48	r	503	PLX	C5-C4-O6-C6
47	B	303	PEE	O5-C30-O3-C3
53	l	702	CDL	C32-C33-C34-C35
48	g	201	PLX	O9-C24-C25-C26
47	B	303	PEE	C31-C32-C33-C34
48	r	503	PLX	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
53	r	505	CDL	C62-C63-C64-C65
53	r	505	CDL	C82-C83-C84-C85
48	g	201	PLX	O4-C3-C4-O6
53	V	201	CDL	OB5-CB3-CB4-OB6
53	i	401	CDL	OB5-CB3-CB4-OB6
47	l	703	PEE	C15-C16-C17-C18
53	r	505	CDL	C33-C34-C35-C36
47	V	202	PEE	C33-C34-C35-C36
47	i	402	PEE	C33-C34-C35-C36
48	r	504	PLX	C30-C31-C32-C33
53	l	702	CDL	C43-C44-C45-C46
47	r	501	PEE	O2-C2-C3-O3
48	r	503	PLX	O6-C4-C5-O8
53	r	505	CDL	OA6-CA4-CA6-OA8
53	r	505	CDL	C80-C81-C82-C83
53	V	201	CDL	CB2-C1-CA2-OA2
53	r	505	CDL	C60-C61-C62-C63
53	o	201	CDL	OA7-CA5-OA6-CA4
46	A	502	FMN	O2'-C2'-C3'-C4'
53	r	505	CDL	C42-C43-C44-C45
47	V	202	PEE	C15-C16-C17-C18
47	b	201	PEE	C16-C17-C18-C19
47	V	202	PEE	C18-C19-C20-C21
49	X	201	8Q1	O4-C1-C6-C7
49	X	201	8Q1	S44-C1-C6-C7
48	r	503	PLX	O8-C24-C25-C26
47	r	501	PEE	O3P-C1-C2-C3
48	C	302	PLX	O4-C3-C4-C5
48	j	203	PLX	O4-C3-C4-C5
53	i	401	CDL	OA5-CA3-CA4-CA6
48	j	203	PLX	C31-C32-C33-C34
47	j	201	PEE	C18-C19-C20-C21
47	r	501	PEE	C38-C39-C40-C41
53	u	201	CDL	C17-C18-C19-C20
48	C	302	PLX	C30-C31-C32-C33
50	J	401	NDP	O4D-C1D-N1N-C6N
53	N	201	CDL	OB7-CB5-OB6-CB4
47	r	501	PEE	C31-C30-O3-C3
53	l	702	CDL	C71-C72-C73-C74
53	o	201	CDL	CA6-CA4-OA6-CA5
53	i	401	CDL	C36-C37-C38-C39
53	a	201	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
47	j	202	PEE	C12-C13-C14-C15
53	i	401	CDL	CB3-CB4-CB6-OB8
53	l	702	CDL	CA3-CA4-CA6-OA8
47	r	501	PEE	O3P-C1-C2-O2
53	i	401	CDL	OA5-CA3-CA4-OA6
53	r	505	CDL	C55-C56-C57-C58
47	i	402	PEE	C34-C35-C36-C37
48	r	502	PLX	C16-C17-C18-C19
47	b	201	PEE	O2-C2-C3-O3
47	m	201	PEE	O2-C2-C3-O3
48	j	203	PLX	O6-C4-C5-O8
48	r	502	PLX	O6-C4-C5-O8
50	J	401	NDP	C2B-O2B-P2B-O2X
47	l	703	PEE	C13-C14-C15-C16
48	g	201	PLX	C16-C17-C18-C19
47	r	501	PEE	C30-C31-C32-C33
47	j	202	PEE	C38-C39-C40-C41
47	r	501	PEE	O5-C30-O3-C3
53	r	505	CDL	C20-C21-C22-C23
47	m	201	PEE	C11-C12-C13-C14
48	g	201	PLX	C14-C15-C16-C17
48	r	502	PLX	C18-C19-C20-C21
47	j	202	PEE	C39-C40-C41-C42
47	l	703	PEE	C1-O3P-P-O4P
47	l	703	PEE	C4-O4P-P-O3P
53	N	201	CDL	CB3-OB5-PB2-OB2
53	i	401	CDL	CB2-OB2-PB2-OB5
53	l	702	CDL	CA3-OA5-PA1-OA2
53	l	702	CDL	C12-C13-C14-C15
48	r	503	PLX	C11-C12-C13-C14
47	i	402	PEE	C4-O4P-P-O2P
47	j	202	PEE	C4-O4P-P-O1P
47	l	703	PEE	C1-O3P-P-O2P
48	C	302	PLX	C3-O4-P1-O3
48	g	201	PLX	C3-O4-P1-O3
53	N	201	CDL	CA3-OA5-PA1-OA4
53	V	201	CDL	CA2-OA2-PA1-OA4
53	V	201	CDL	CA3-OA5-PA1-OA4
53	a	201	CDL	CA3-OA5-PA1-OA4
53	a	201	CDL	CB2-OB2-PB2-OB4
53	i	401	CDL	CA2-OA2-PA1-OA4
53	i	401	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
53	l	701	CDL	CB3-OB5-PB2-OB4
53	l	702	CDL	CB3-OB5-PB2-OB3
53	l	702	CDL	CB3-OB5-PB2-OB4
53	o	201	CDL	CA3-OA5-PA1-OA4
53	o	201	CDL	CB2-OB2-PB2-OB3
53	r	505	CDL	CA3-OA5-PA1-OA3
53	u	201	CDL	CB2-OB2-PB2-OB4
53	u	201	CDL	CB3-OB5-PB2-OB4
47	l	703	PEE	C21-C22-C23-C24
48	g	201	PLX	O4-C3-C4-C5
53	l	702	CDL	OA5-CA3-CA4-CA6
53	r	505	CDL	C64-C65-C66-C67
47	i	402	PEE	C10-C11-C12-C13
47	j	201	PEE	C37-C38-C39-C40
46	A	502	FMN	C1'-C2'-C3'-O3'
47	b	201	PEE	C5-C4-O4P-P
48	r	504	PLX	C25-C24-O8-C5
48	g	201	PLX	C29-C30-C31-C32
53	N	201	CDL	C31-CA7-OA8-CA6
53	o	201	CDL	CB2-C1-CA2-OA2
47	i	402	PEE	O3P-C1-C2-O2
48	j	203	PLX	O4-C3-C4-O6
53	l	702	CDL	OA5-CA3-CA4-OA6
53	u	201	CDL	C71-C72-C73-C74
53	l	701	CDL	CA7-C31-C32-C33
47	j	201	PEE	O2-C2-C3-O3
53	u	201	CDL	OA6-CA4-CA6-OA8
47	b	201	PEE	C18-C19-C20-C21
53	N	201	CDL	OA9-CA7-OA8-CA6
48	j	203	PLX	O6-C6-C7-C8
48	r	504	PLX	O8-C24-C25-C26
53	l	701	CDL	C36-C37-C38-C39
48	C	302	PLX	O7-C6-C7-C8
53	r	505	CDL	C83-C84-C85-C86
47	i	402	PEE	C35-C36-C37-C38
53	a	201	CDL	OB9-CB7-OB8-CB6
47	i	402	PEE	C24-C25-C26-C27
47	r	501	PEE	C21-C22-C23-C24
47	m	201	PEE	C34-C35-C36-C37
47	i	402	PEE	C2-C1-O3P-P
53	o	201	CDL	CA4-CA3-OA5-PA1
53	l	702	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
47	i	402	PEE	C38-C39-C40-C41
47	j	201	PEE	C38-C39-C40-C41
53	V	201	CDL	OB6-CB4-CB6-OB8
53	o	201	CDL	OA6-CA4-CA6-OA8
53	a	201	CDL	CB3-OB5-PB2-OB2
53	l	702	CDL	CA2-OA2-PA1-OA5
48	j	203	PLX	C3-C4-C5-O8
53	i	401	CDL	CA3-CA4-CA6-OA8
48	C	302	PLX	C26-C27-C28-C29
53	i	401	CDL	C71-C72-C73-C74
48	j	203	PLX	C2-C1-N1-C1A
47	m	201	PEE	C24-C25-C26-C27
53	r	505	CDL	C39-C40-C41-C42
47	B	303	PEE	C18-C19-C20-C21
47	V	202	PEE	C38-C39-C40-C41
47	i	402	PEE	C15-C16-C17-C18
53	o	201	CDL	C84-C85-C86-C87
53	r	505	CDL	C44-C45-C46-C47
53	V	201	CDL	OB5-CB3-CB4-CB6
53	o	201	CDL	C76-C77-C78-C79
47	V	202	PEE	O4P-C4-C5-N
53	l	702	CDL	C62-C63-C64-C65
53	i	401	CDL	C33-C34-C35-C36
48	r	503	PLX	C18-C19-C20-C21
48	j	203	PLX	C19-C20-C21-C22
48	C	302	PLX	O6-C6-C7-C8
53	l	702	CDL	C63-C64-C65-C66
53	a	201	CDL	C60-C61-C62-C63
53	u	201	CDL	C54-C55-C56-C57
47	m	201	PEE	C31-C32-C33-C34
53	a	201	CDL	CA2-C1-CB2-OB2
47	b	201	PEE	C36-C37-C38-C39
53	l	701	CDL	C54-C55-C56-C57
53	r	505	CDL	C11-C12-C13-C14
53	a	201	CDL	O1-C1-CB2-OB2
47	B	303	PEE	C11-C12-C13-C14
53	i	401	CDL	CA6-CA4-OA6-CA5
47	j	201	PEE	O4-C10-O2-C2
47	j	202	PEE	C16-C17-C18-C19
53	l	702	CDL	CA7-C31-C32-C33
47	i	402	PEE	C21-C22-C23-C24
48	g	201	PLX	C5-C4-O6-C6

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Mol	Chain	Res	Type	Atoms
53	V	201	CDL	C1-CB2-OB2-PB2
53	a	201	CDL	OA5-CA3-CA4-OA6
53	l	701	CDL	C17-C18-C19-C20
46	A	502	FMN	O2'-C2'-C3'-O3'
49	X	201	8Q1	C6-C7-C8-C9
47	j	202	PEE	C22-C23-C24-C25
47	b	201	PEE	C38-C39-C40-C41
53	a	201	CDL	CB5-C51-C52-C53
48	j	203	PLX	C11-C12-C13-C14
47	V	202	PEE	C37-C38-C39-C40
47	r	501	PEE	C37-C38-C39-C40
48	g	201	PLX	C36-C37-C38-C39
53	N	201	CDL	C51-C52-C53-C54
48	g	201	PLX	C34-C35-C36-C37
53	l	701	CDL	C44-C45-C46-C47
47	m	201	PEE	C19-C20-C21-C22
53	i	401	CDL	C31-C32-C33-C34
47	l	703	PEE	C2-C3-O3-C30
53	i	401	CDL	C14-C15-C16-C17
48	C	302	PLX	O8-C24-C25-C26
48	r	502	PLX	O8-C24-C25-C26
48	r	504	PLX	O6-C6-C7-C8
53	l	701	CDL	C40-C41-C42-C43
53	l	701	CDL	C72-C73-C74-C75
47	m	201	PEE	O4P-C4-C5-N
53	V	201	CDL	C58-C59-C60-C61
47	j	202	PEE	O3-C30-C31-C32
47	V	202	PEE	C39-C40-C41-C42
53	V	201	CDL	C40-C41-C42-C43
53	N	201	CDL	C52-C51-CB5-OB6
53	a	201	CDL	O1-C1-CA2-OA2
47	b	201	PEE	O2-C10-C11-C12
47	r	501	PEE	C18-C19-C20-C21
53	l	701	CDL	C21-C22-C23-C24
47	V	202	PEE	O3-C30-C31-C32
47	l	703	PEE	C16-C17-C18-C19
47	m	201	PEE	C18-C19-C20-C21
48	j	203	PLX	C7-C6-O6-C4
47	B	303	PEE	O3P-C1-C2-O2
48	r	502	PLX	O4-C3-C4-O6
53	u	201	CDL	OA5-CA3-CA4-OA6
47	j	202	PEE	O2-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
47	m	201	PEE	O3-C30-C31-C32
48	j	203	PLX	C2-C1-N1-C1C
48	g	201	PLX	C6-C7-C8-C9
47	V	202	PEE	C16-C17-C18-C19
48	r	502	PLX	O4-C3-C4-C5
53	V	201	CDL	C38-C39-C40-C41
53	l	701	CDL	OA6-CA4-CA6-OA8
47	b	201	PEE	O3-C30-C31-C32
53	l	702	CDL	C12-C11-CA5-OA6
53	r	505	CDL	C61-C62-C63-C64
53	l	701	CDL	C23-C24-C25-C26
53	l	702	CDL	C44-C45-C46-C47
47	j	201	PEE	C11-C10-O2-C2
53	r	505	CDL	C23-C24-C25-C26
48	C	302	PLX	C24-C25-C26-C27
48	r	503	PLX	C36-C37-C38-C39
53	a	201	CDL	C54-C55-C56-C57
53	l	701	CDL	C39-C40-C41-C42
47	j	202	PEE	O4-C10-C11-C12
47	V	202	PEE	O5-C30-C31-C32
47	j	202	PEE	O5-C30-C31-C32
47	m	201	PEE	C20-C21-C22-C23
53	V	201	CDL	CB3-CB4-CB6-OB8
53	l	702	CDL	C33-C34-C35-C36
47	b	201	PEE	O4-C10-C11-C12
53	V	201	CDL	CB4-CB3-OB5-PB2
53	N	201	CDL	C52-C51-CB5-OB7
47	j	202	PEE	C40-C41-C42-C43
47	V	202	PEE	C4-O4P-P-O1P
53	l	702	CDL	C12-C11-CA5-OA7
53	l	702	CDL	C17-C18-C19-C20
55	s	401	UQ	C15-C14-C16-C17
47	B	303	PEE	C5-C4-O4P-P
48	r	502	PLX	C25-C24-O8-C5
53	a	201	CDL	CA6-CA4-OA6-CA5
48	C	302	PLX	C11-C10-C9-C8
53	l	702	CDL	C76-C77-C78-C79
53	r	505	CDL	C84-C85-C86-C87
48	j	203	PLX	C2-C1-N1-C1B
47	j	202	PEE	C20-C21-C22-C23
48	r	504	PLX	C11-C12-C13-C14
53	l	702	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
53	a	201	CDL	CB2-C1-CA2-OA2
53	a	201	CDL	CA4-CA3-OA5-PA1
47	b	201	PEE	O5-C30-C31-C32
47	l	703	PEE	C14-C15-C16-C17
48	r	504	PLX	C35-C36-C37-C38
47	V	202	PEE	C10-C11-C12-C13
53	u	201	CDL	C12-C11-CA5-OA6
53	r	505	CDL	C51-C52-C53-C54
53	o	201	CDL	C32-C31-CA7-OA8

There are no ring outliers.

32 monomers are involved in 244 short contacts:

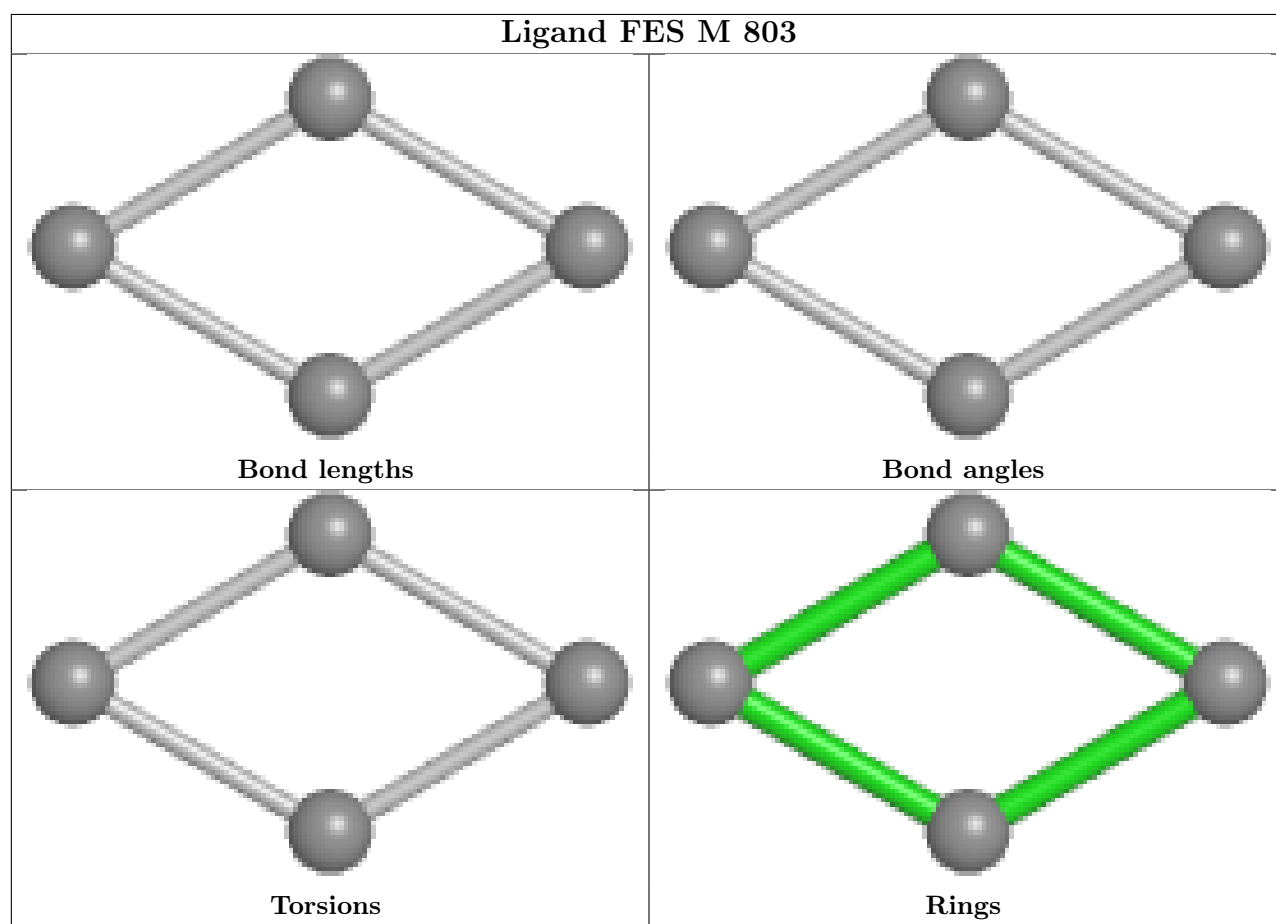
Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	M	803	FES	1	0
47	V	202	PEE	11	0
48	g	201	PLX	4	0
49	X	201	8Q1	1	0
48	r	504	PLX	1	0
53	l	701	CDL	17	0
47	m	201	PEE	11	0
56	w	401	ADP	5	0
53	N	201	CDL	12	0
53	l	702	CDL	5	0
48	C	302	PLX	5	0
47	j	201	PEE	14	0
47	r	501	PEE	15	0
53	r	505	CDL	12	0
53	o	201	CDL	17	0
50	J	401	NDP	4	0
48	r	503	PLX	5	0
45	A	501	SF4	2	0
49	G	201	8Q1	1	0
53	u	201	CDL	14	0
48	j	203	PLX	1	0
47	j	202	PEE	6	0
53	a	201	CDL	21	0
47	b	201	PEE	16	0
46	A	502	FMN	3	0
47	l	703	PEE	3	0
55	s	401	UQ	3	0
48	r	502	PLX	5	0

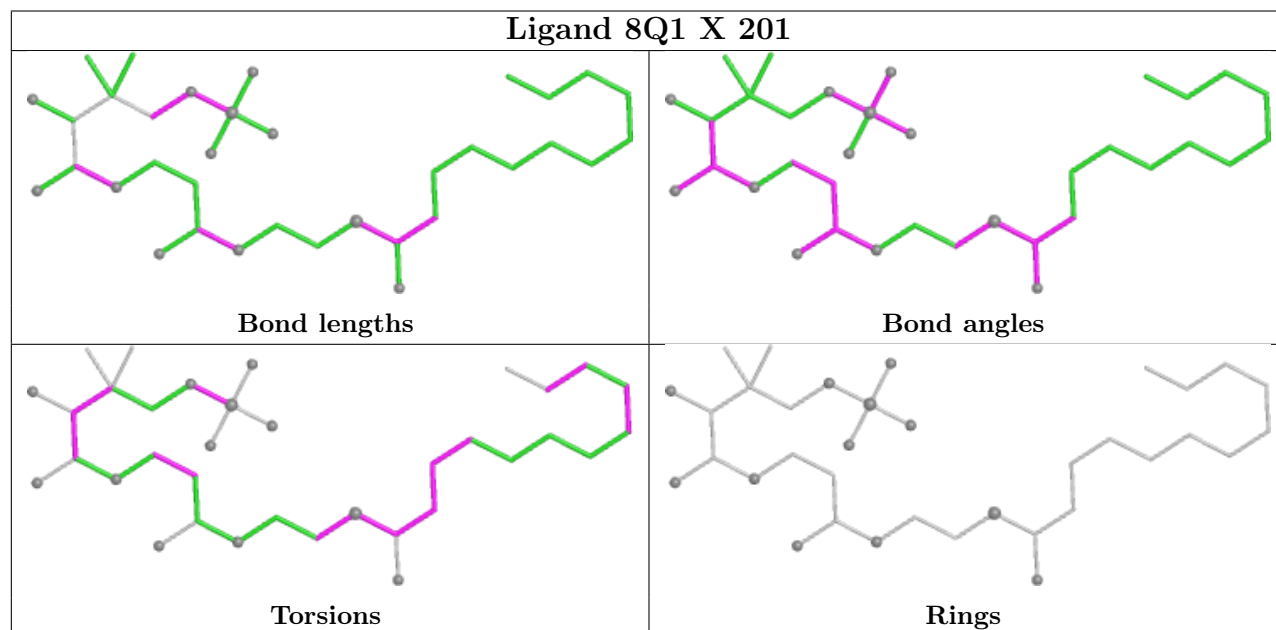
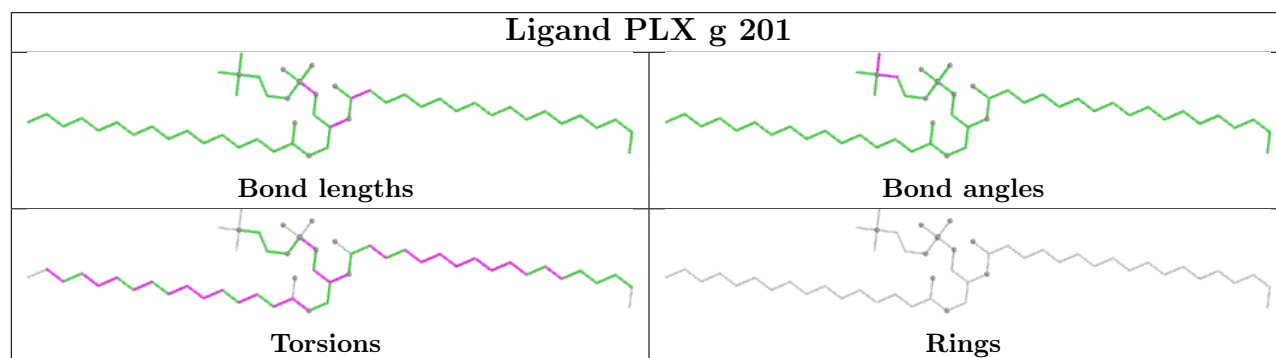
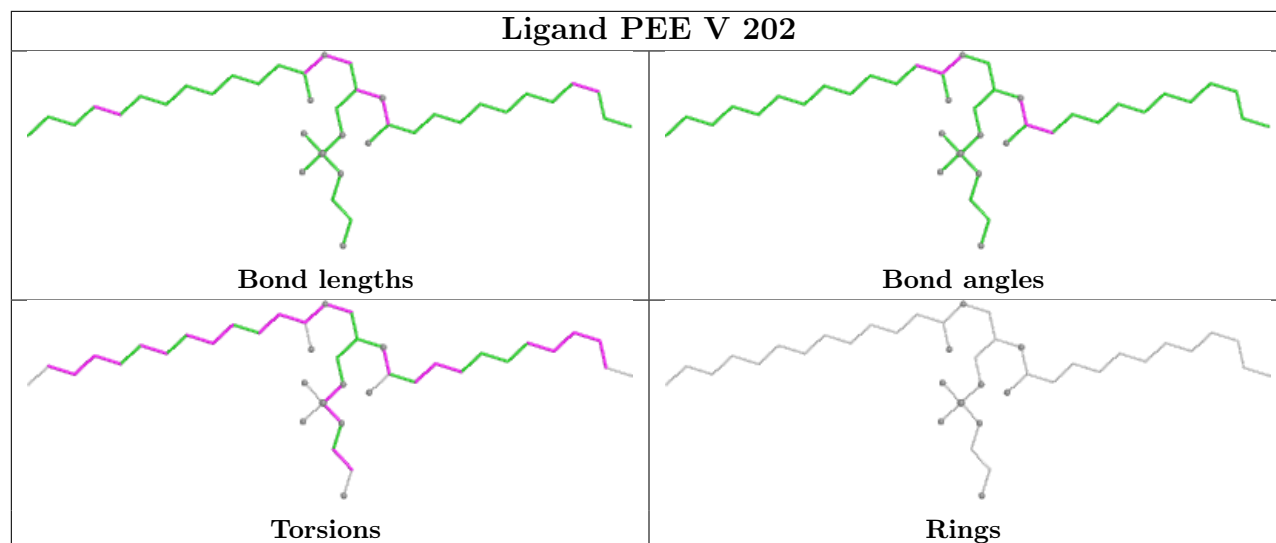
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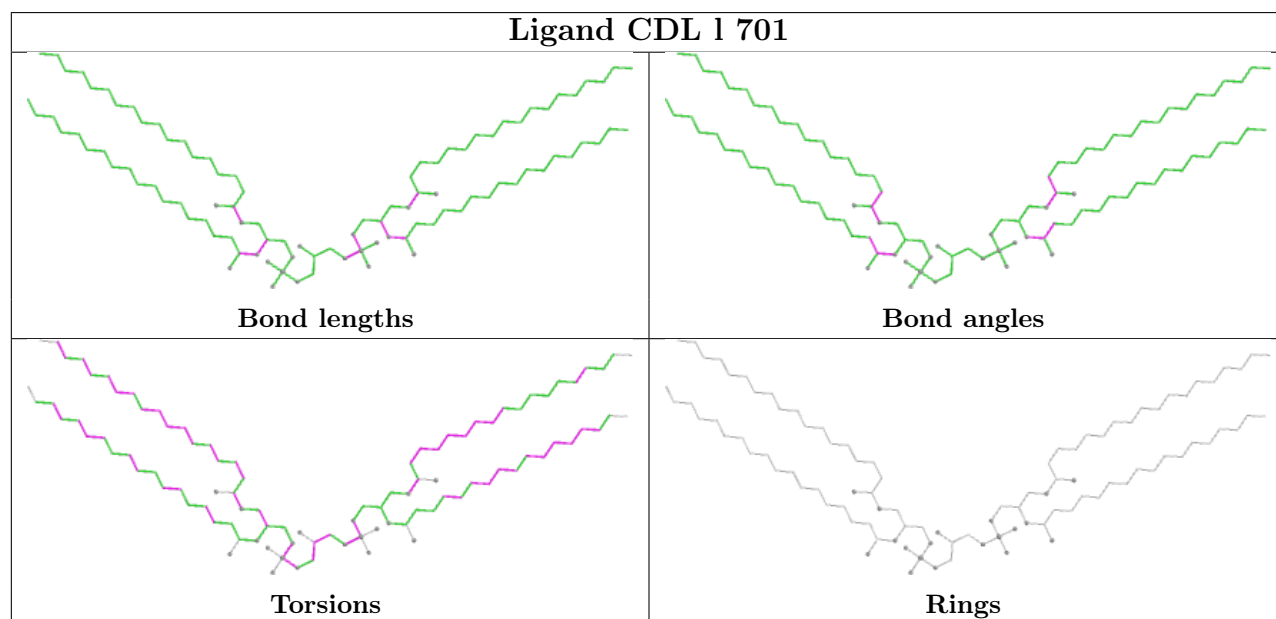
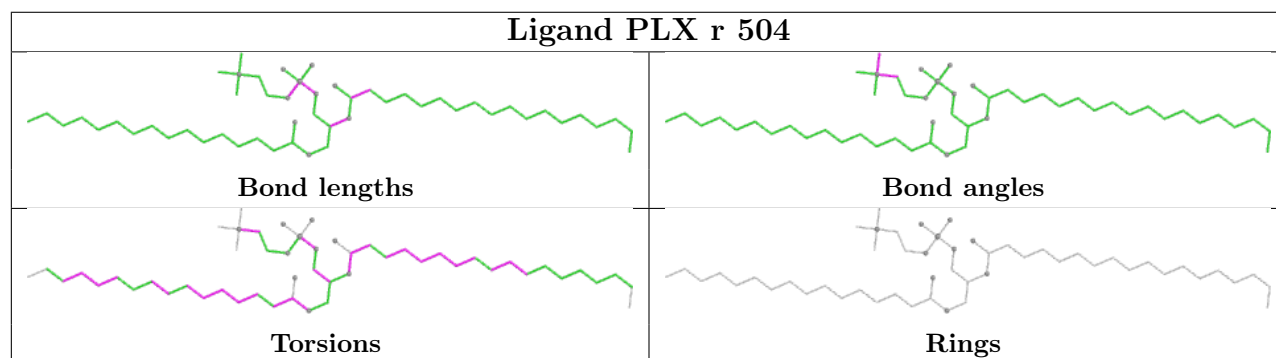
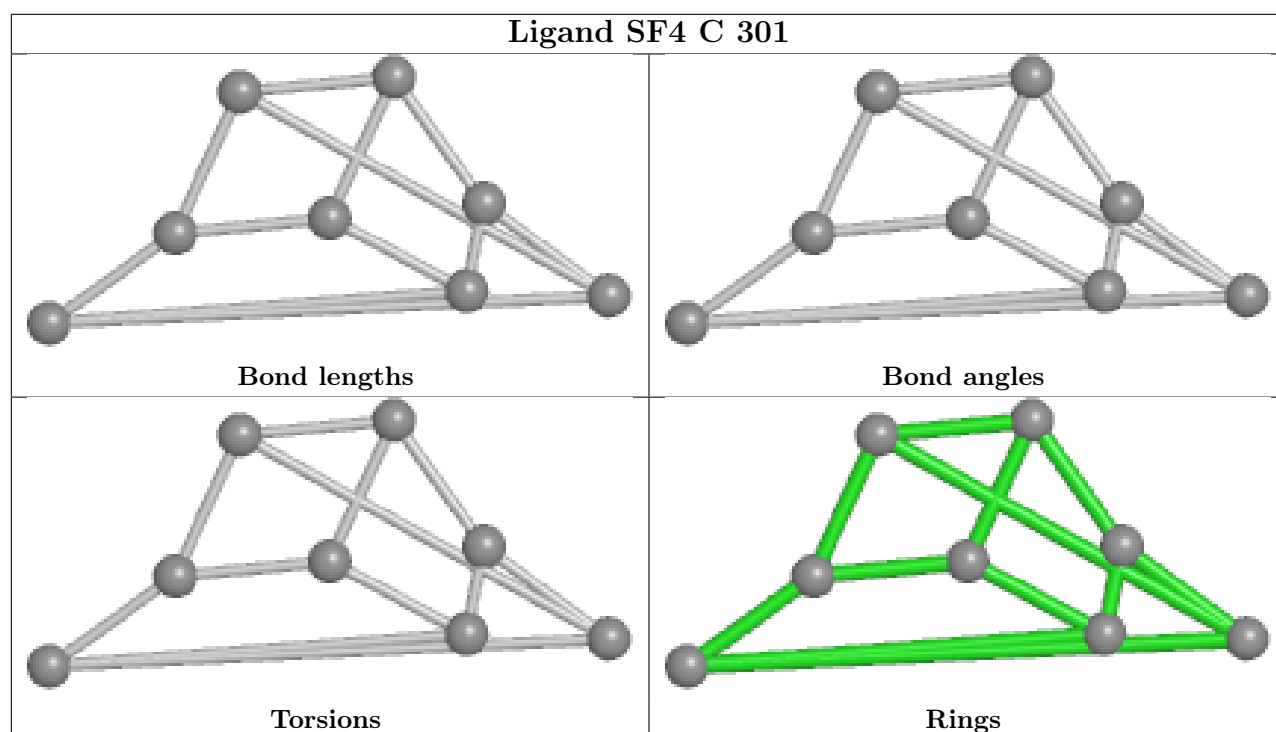
Continued from previous page...

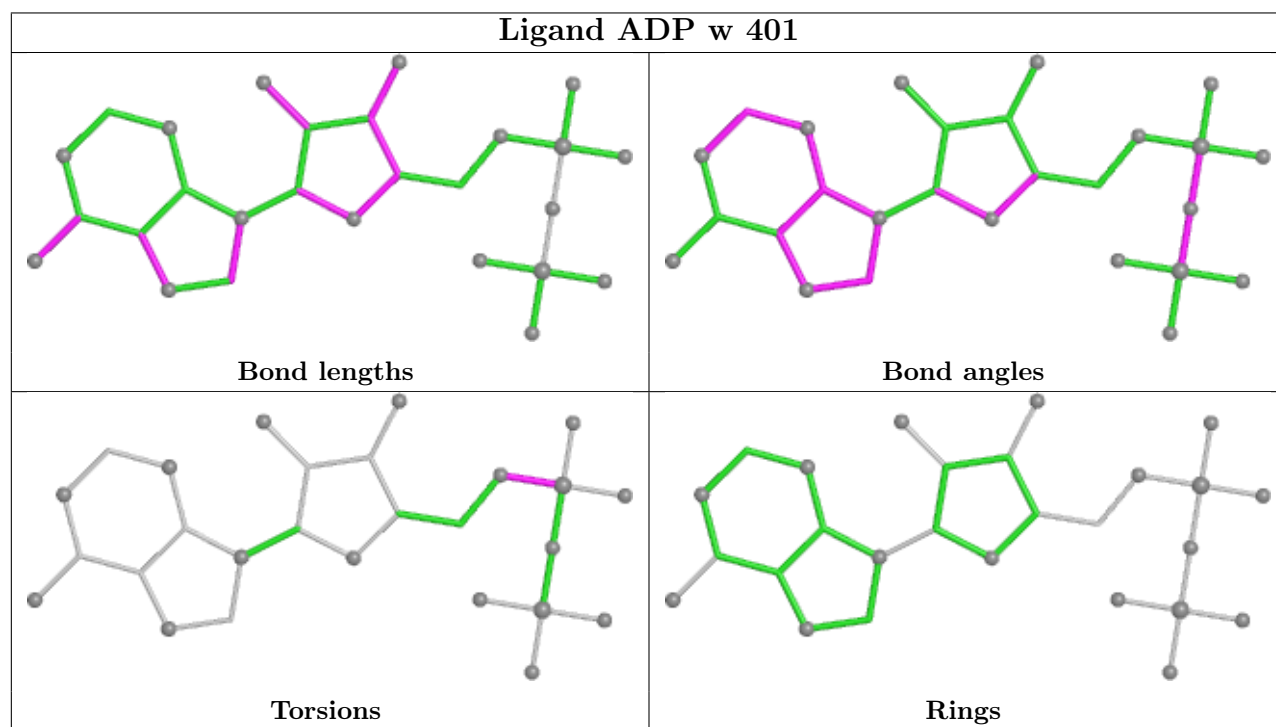
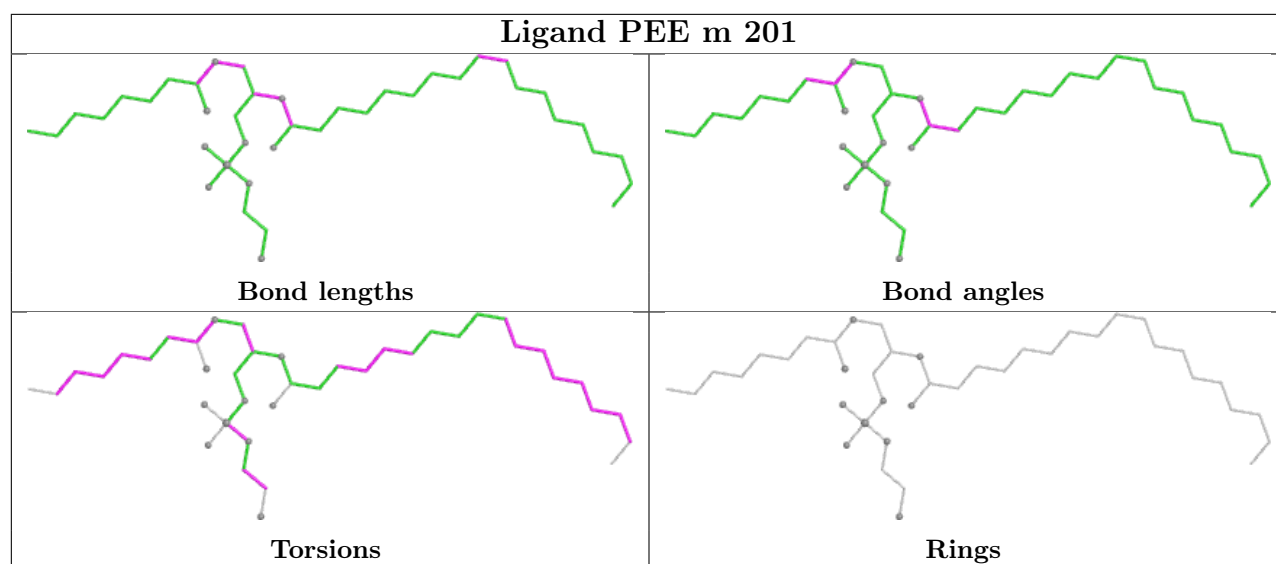
Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	V	201	CDL	11	0
47	i	402	PEE	15	0
53	i	401	CDL	19	0
47	B	303	PEE	2	0

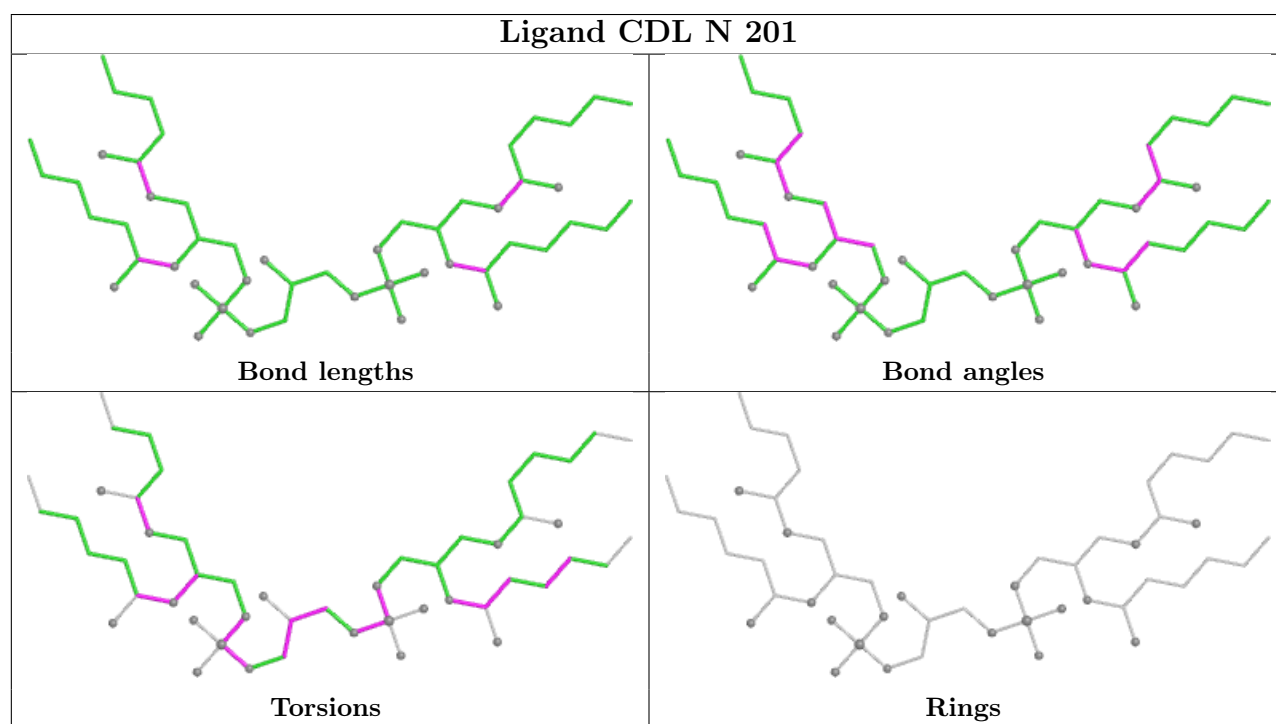
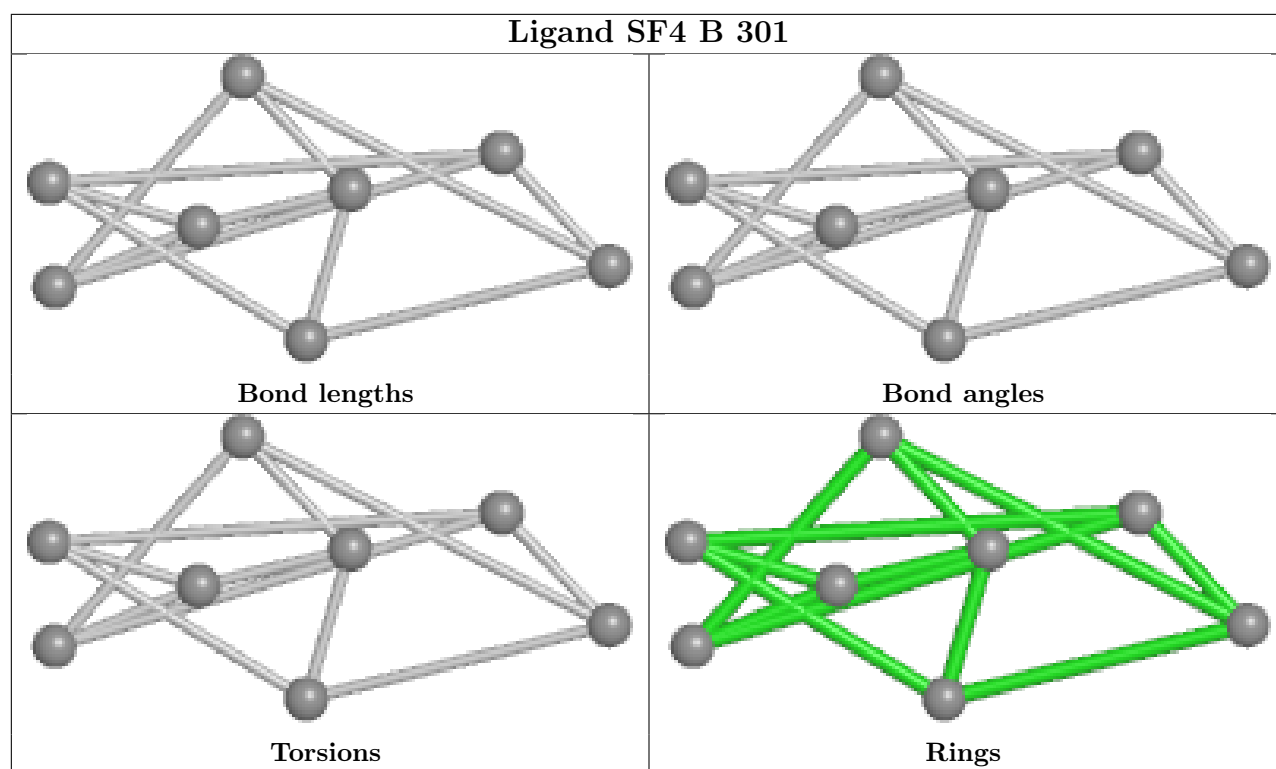
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

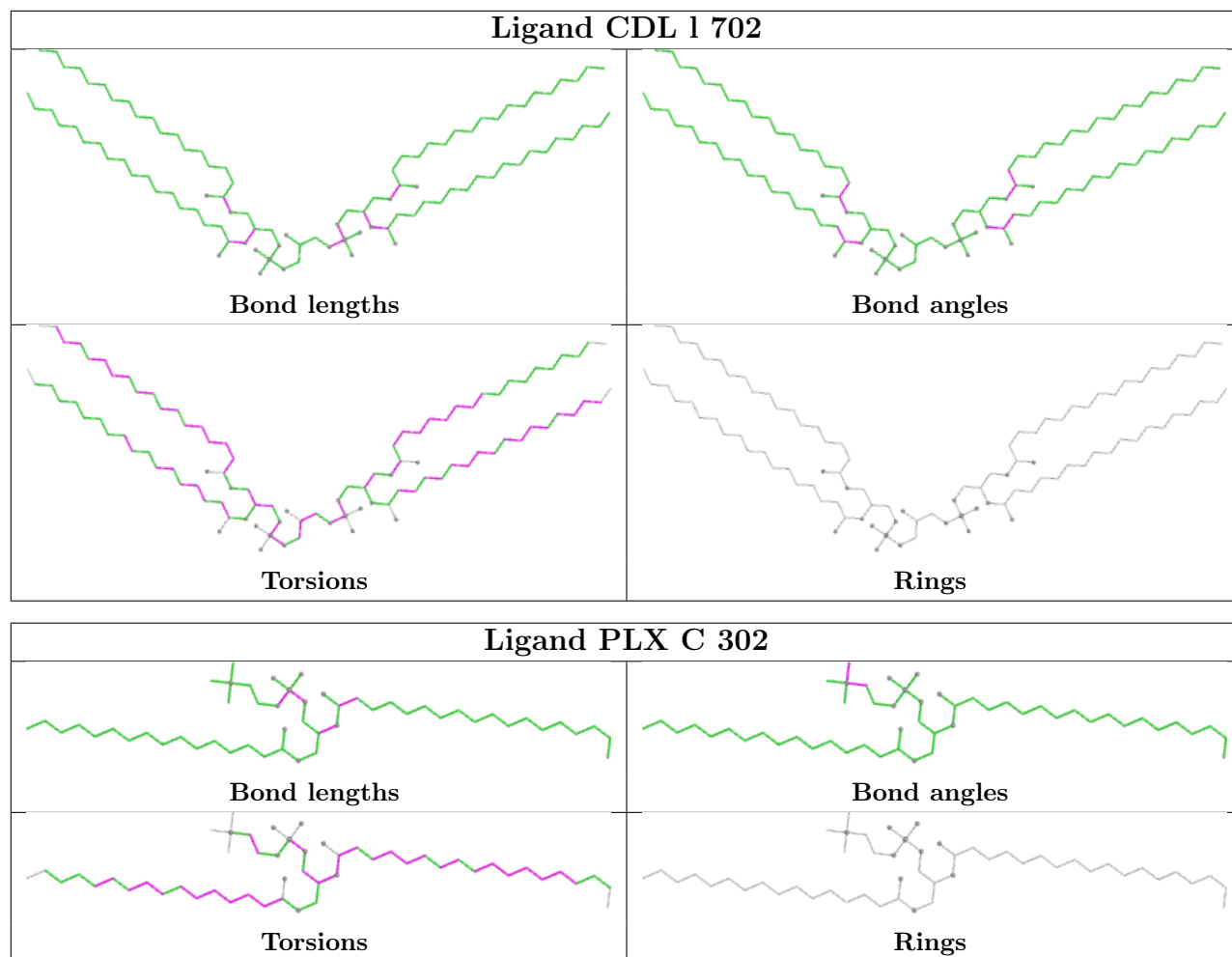


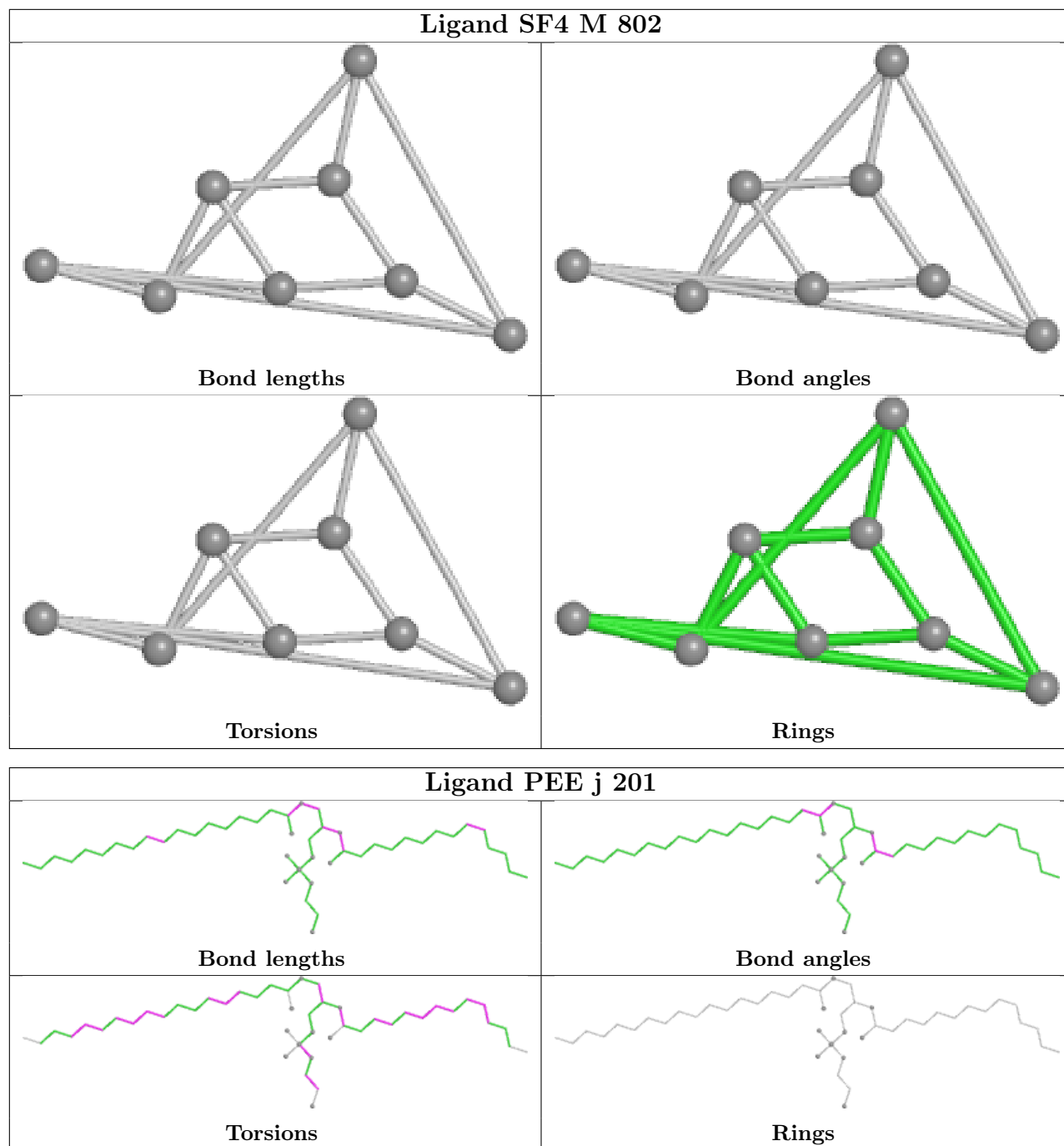


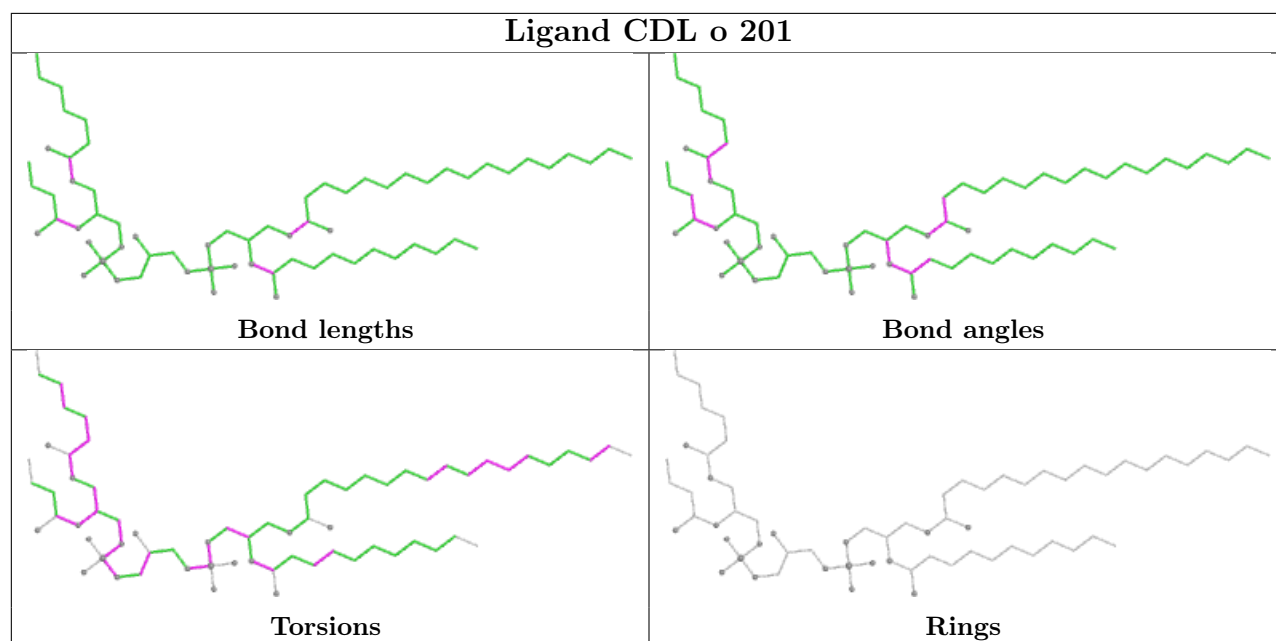
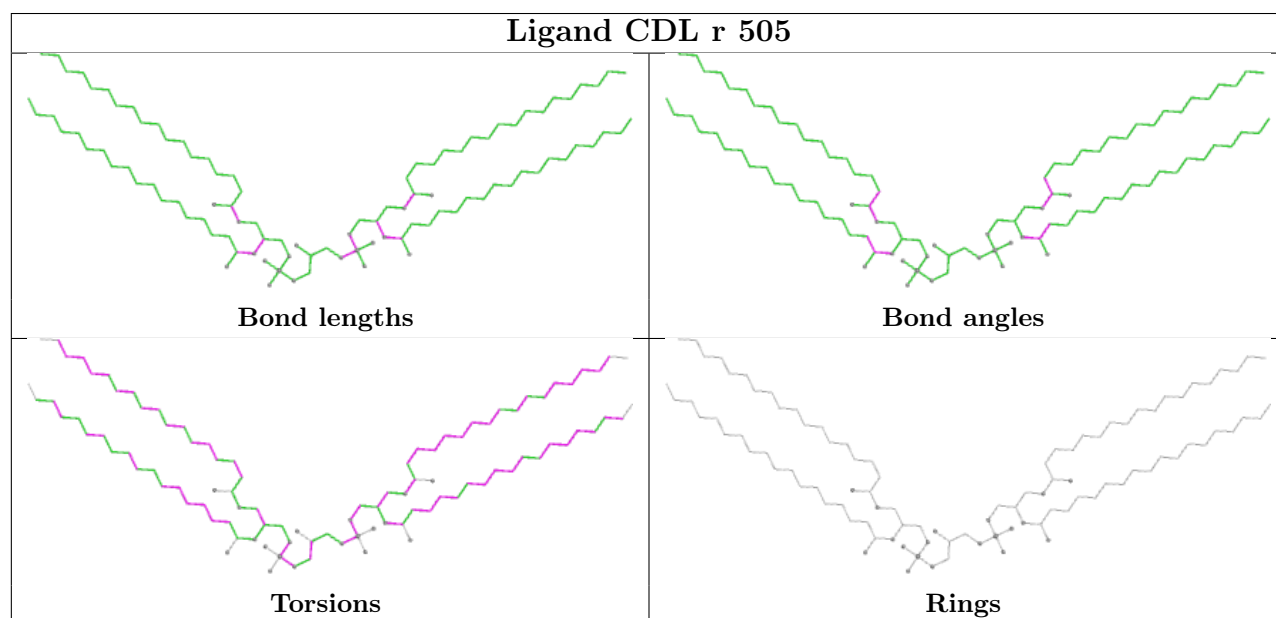
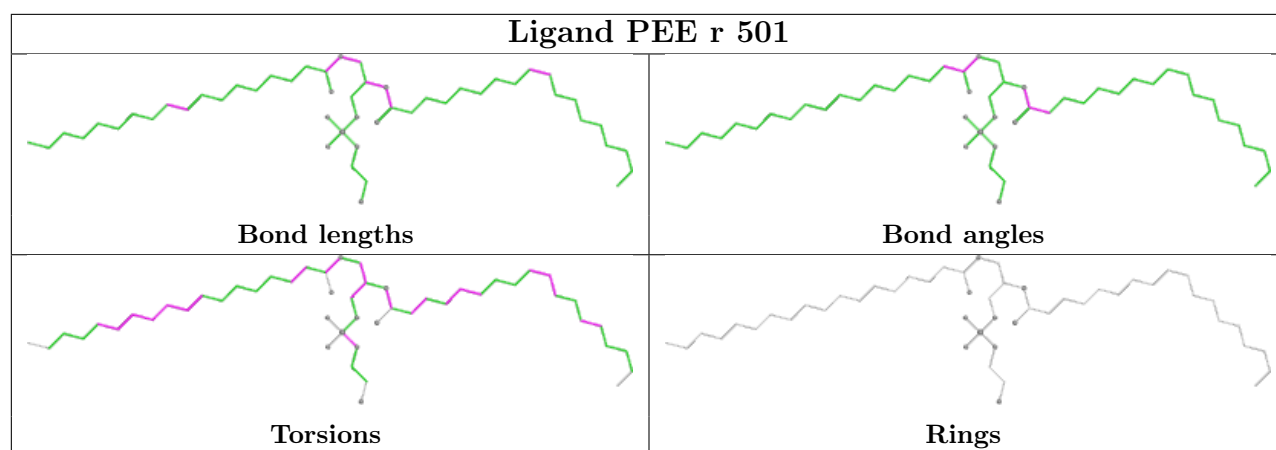


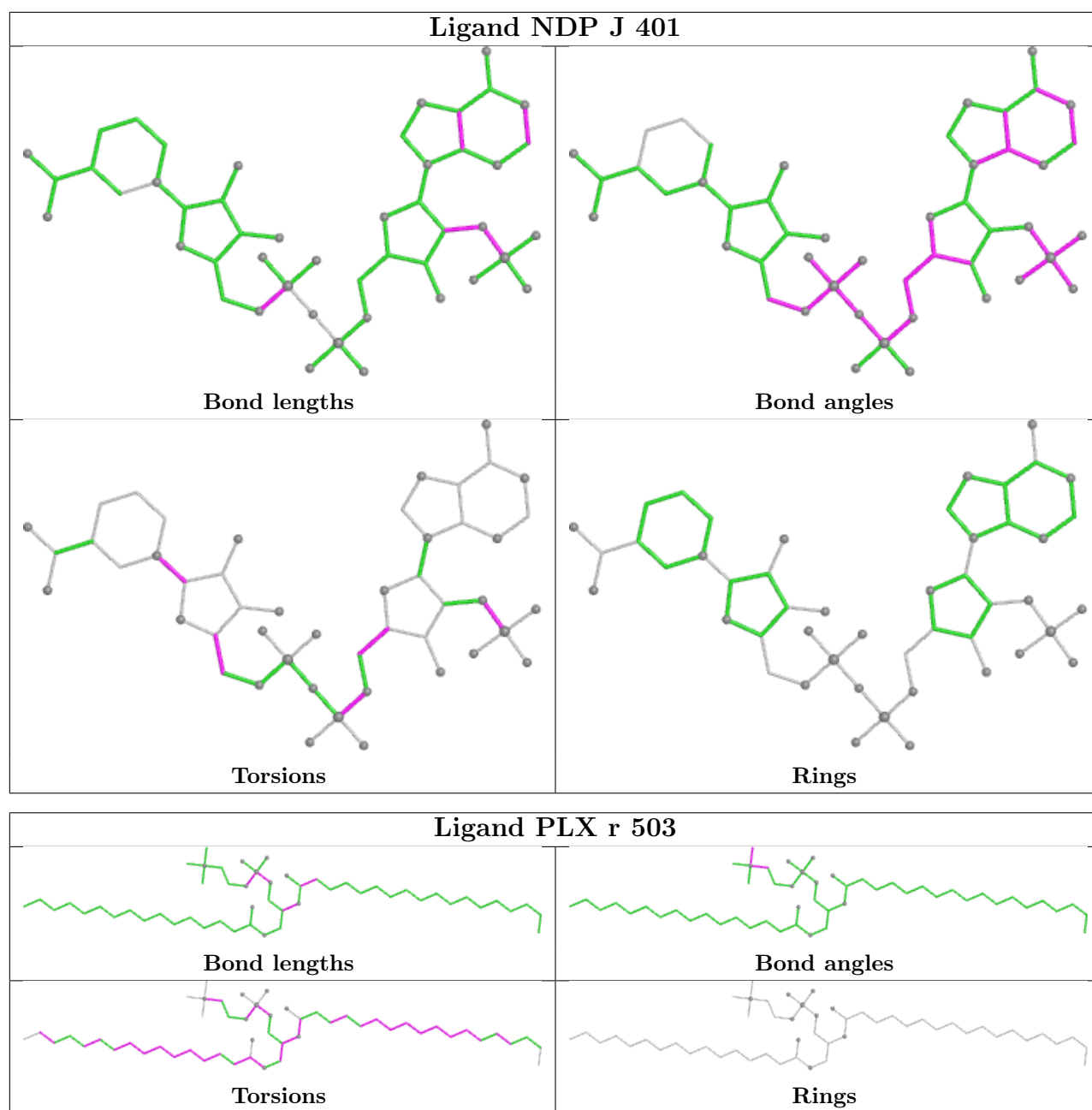




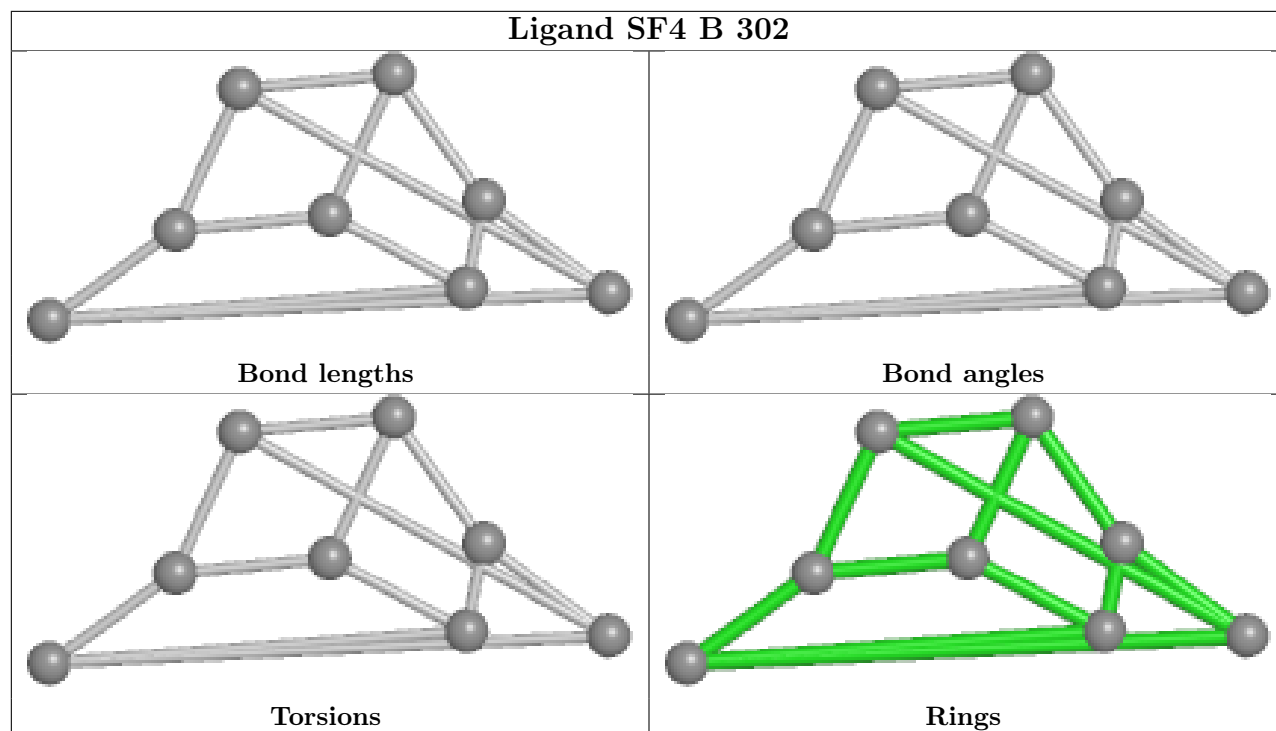




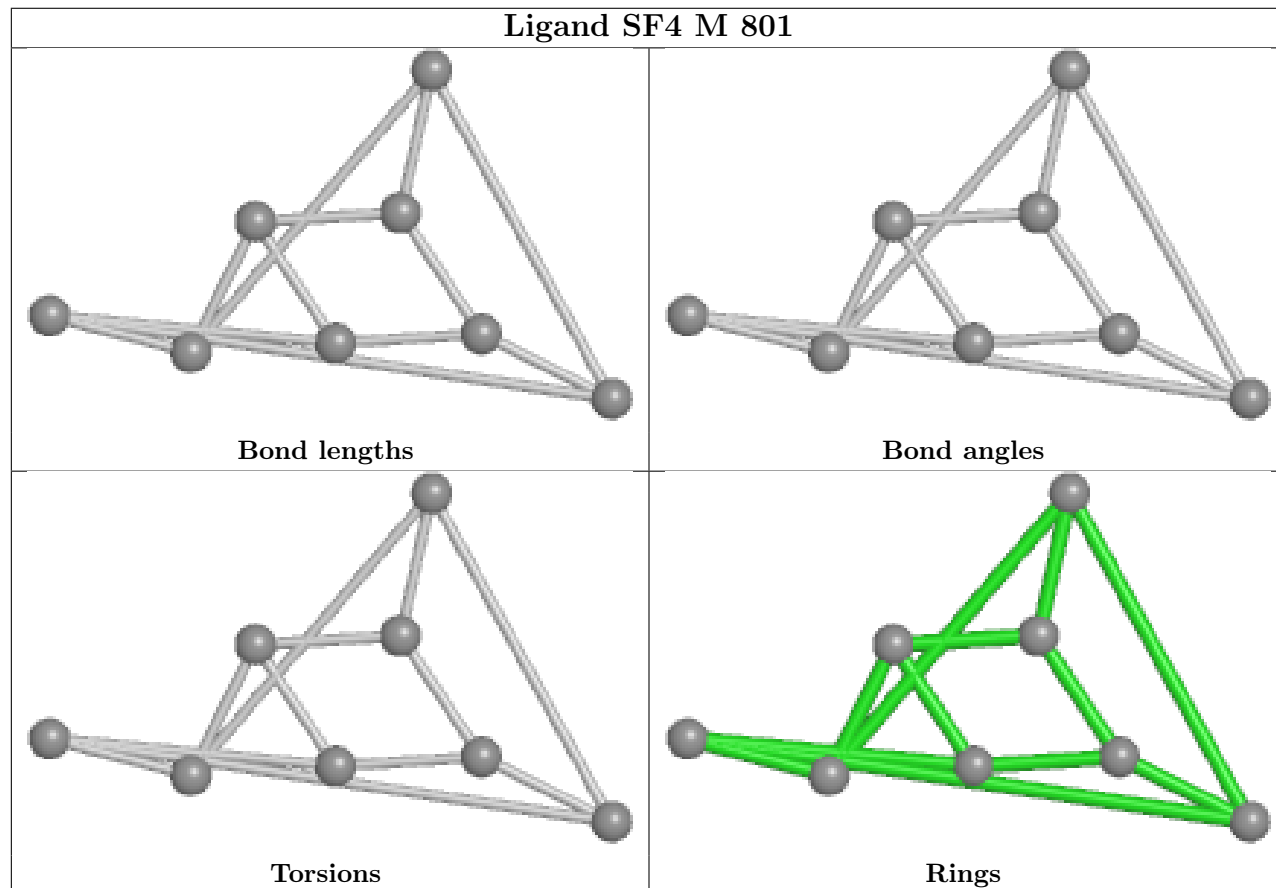


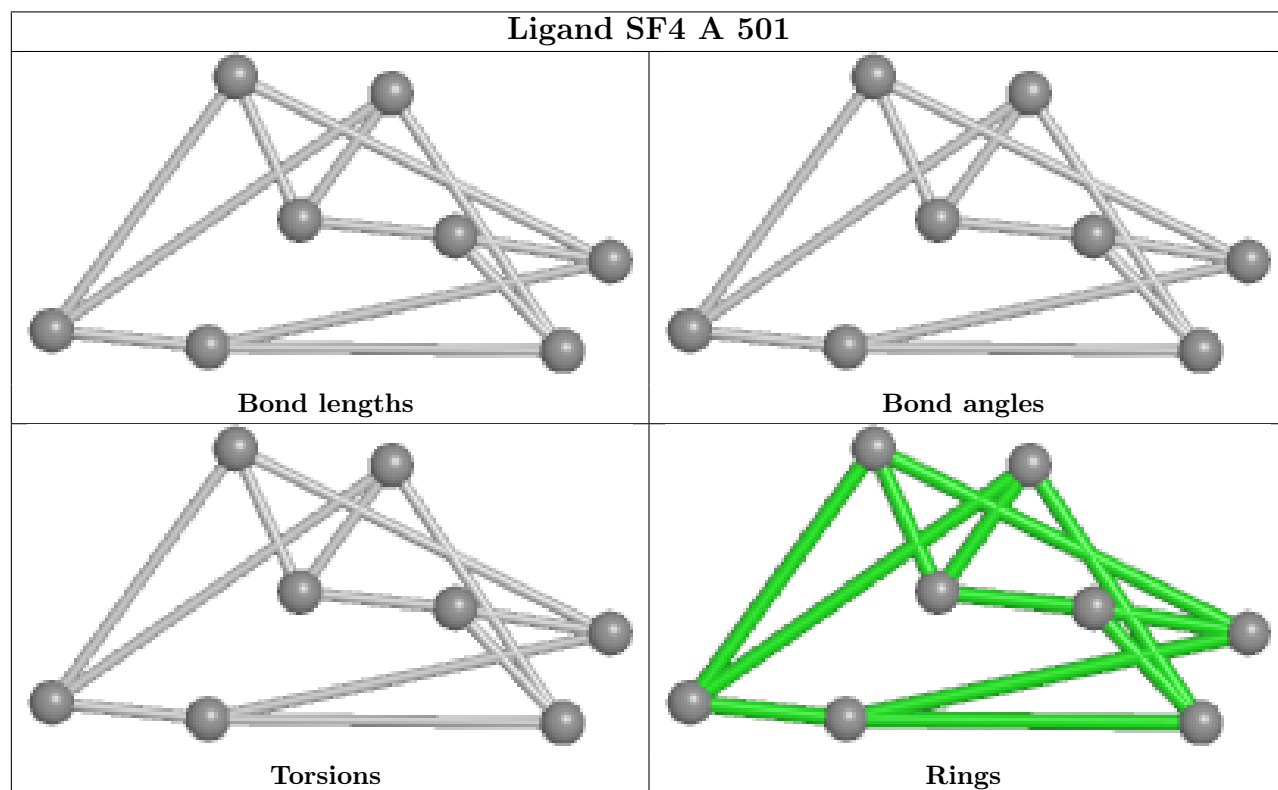
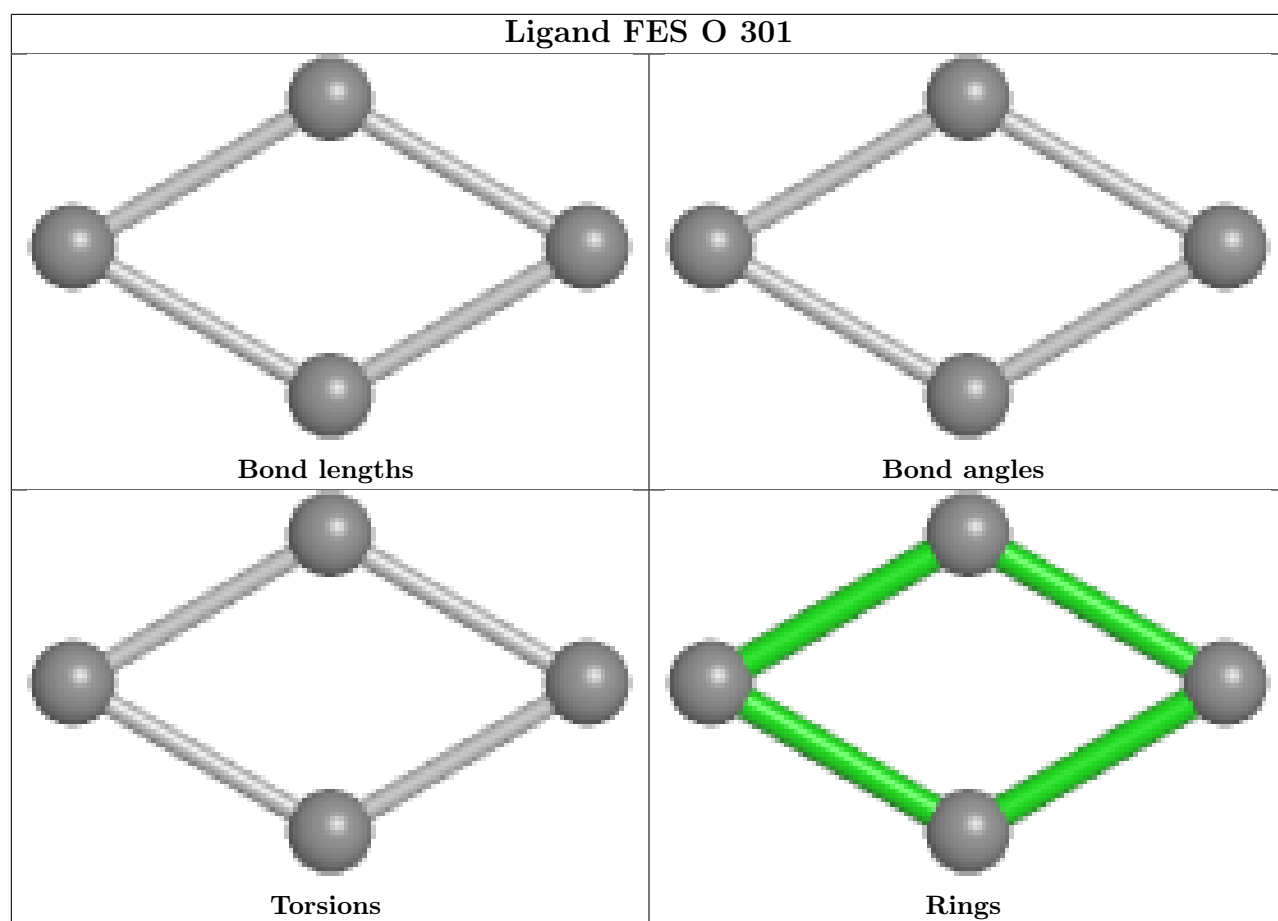


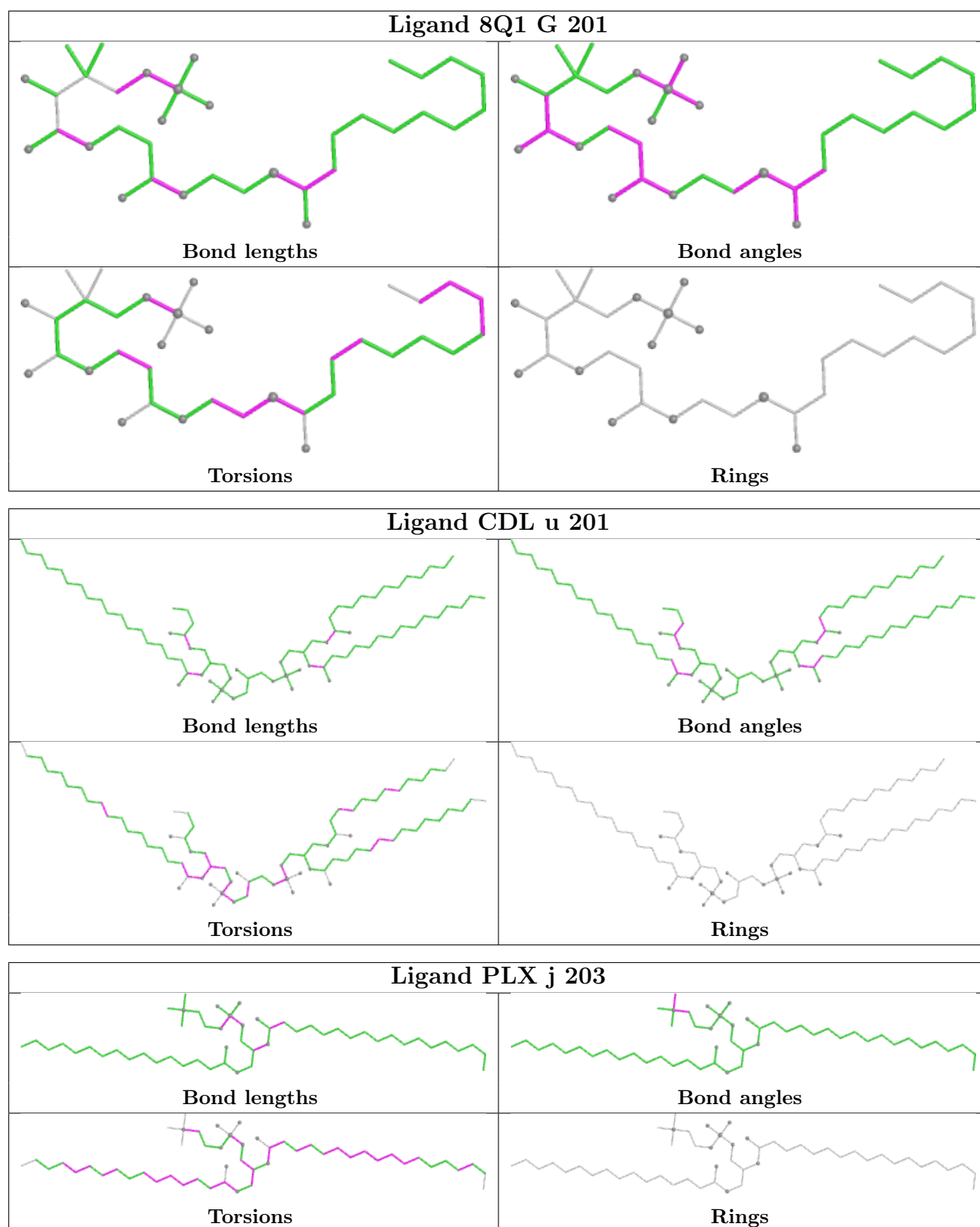
Ligand SF4 B 302

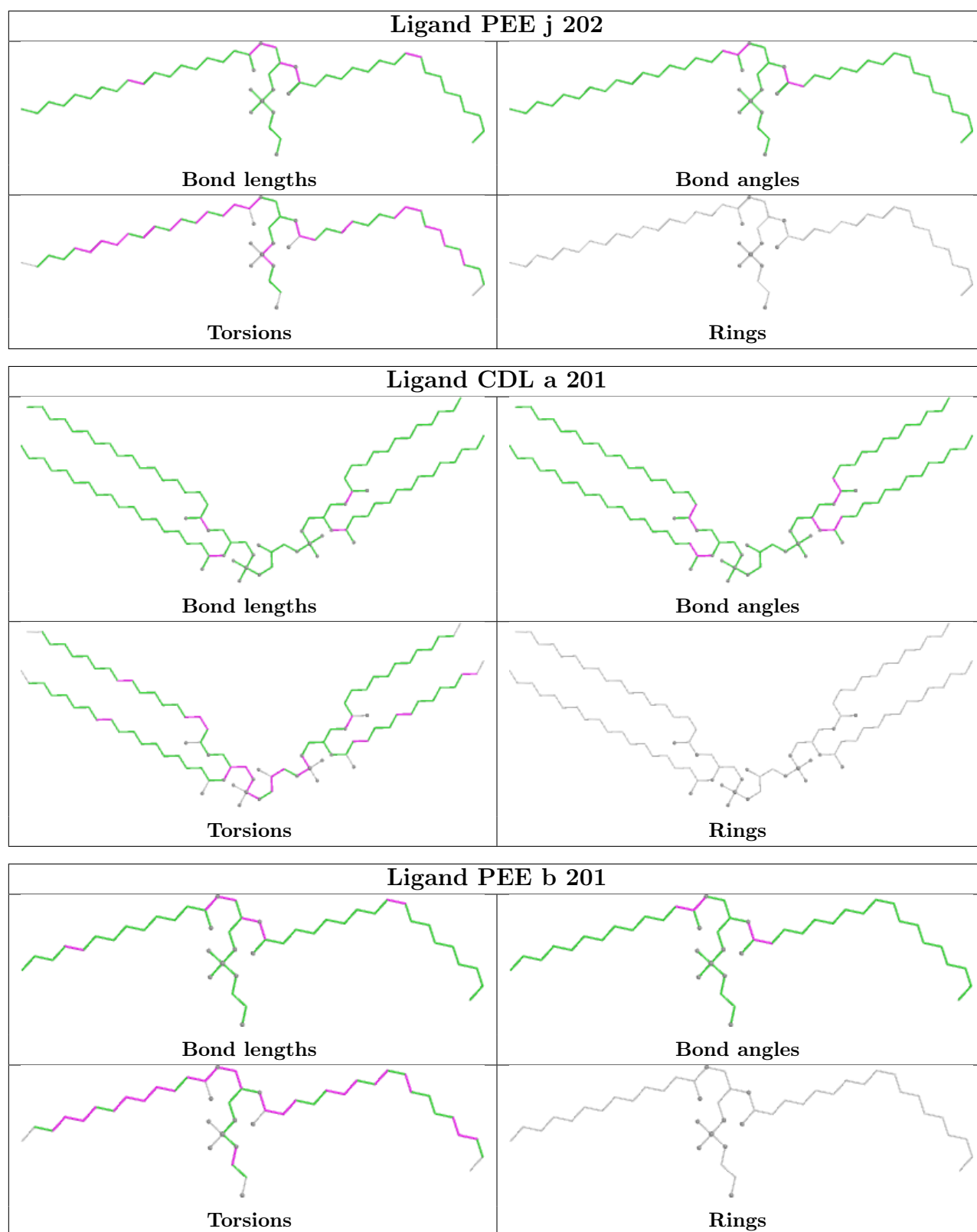


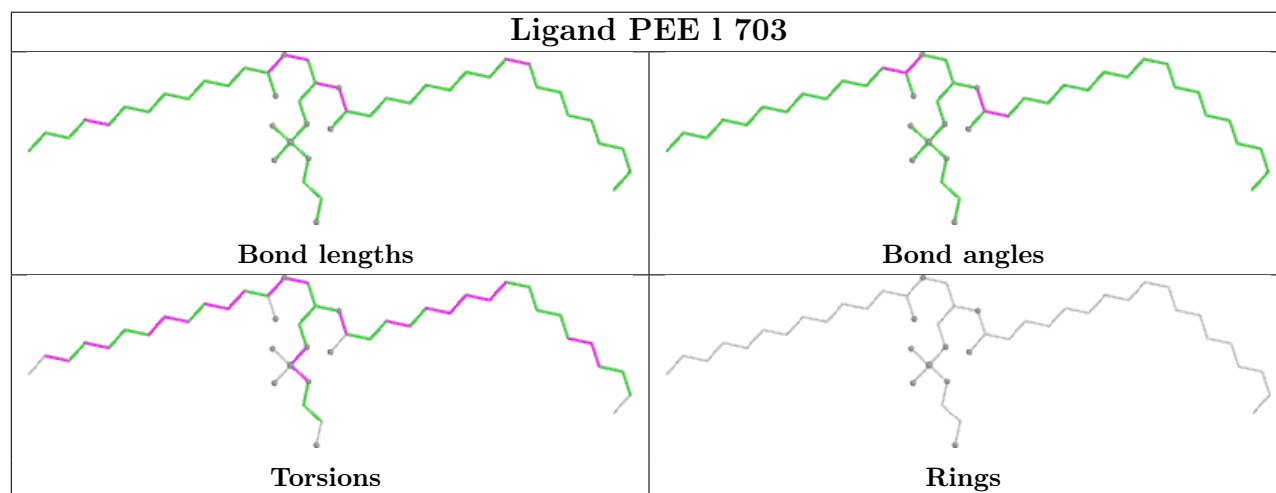
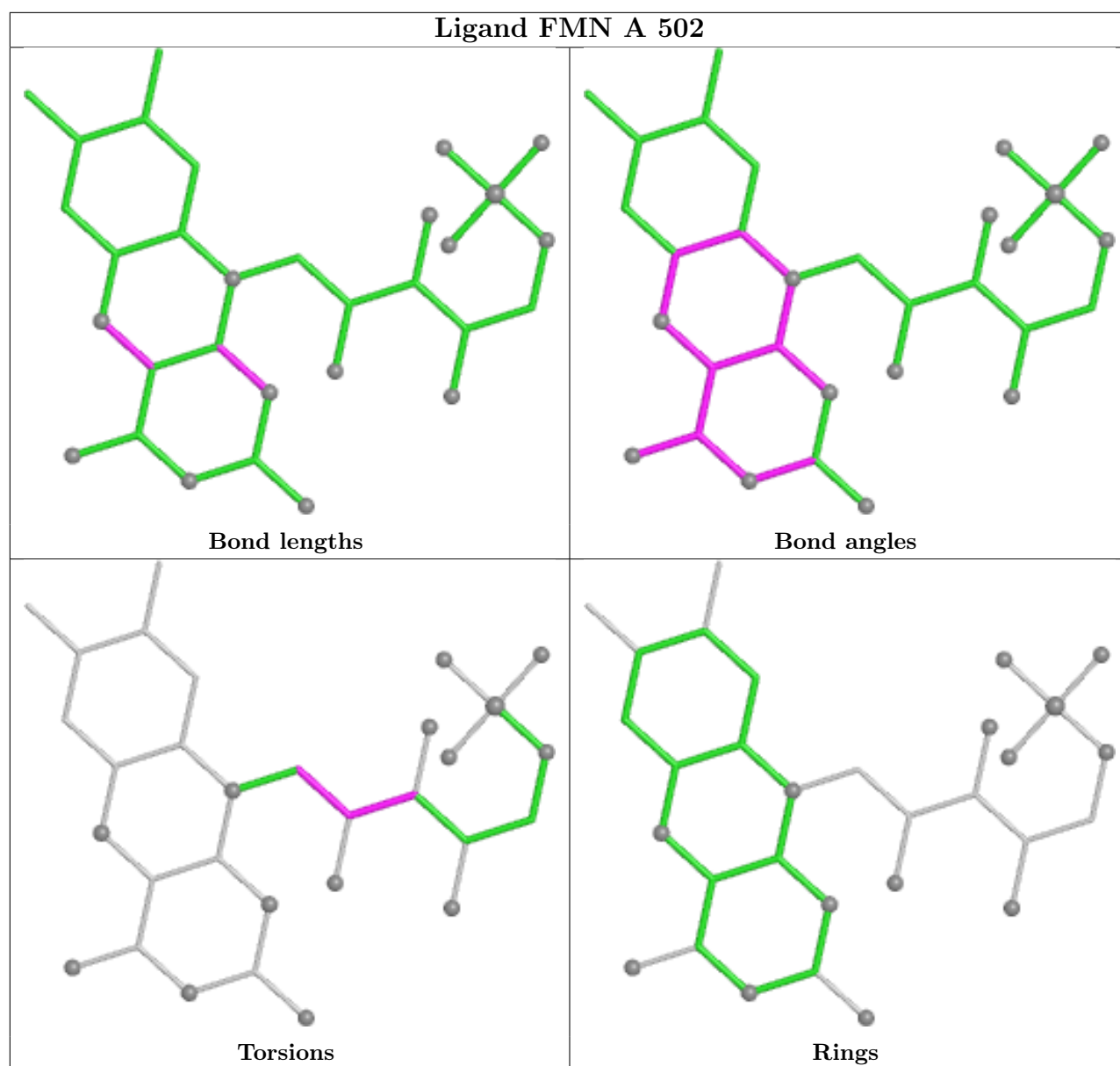
Ligand SF4 M 801

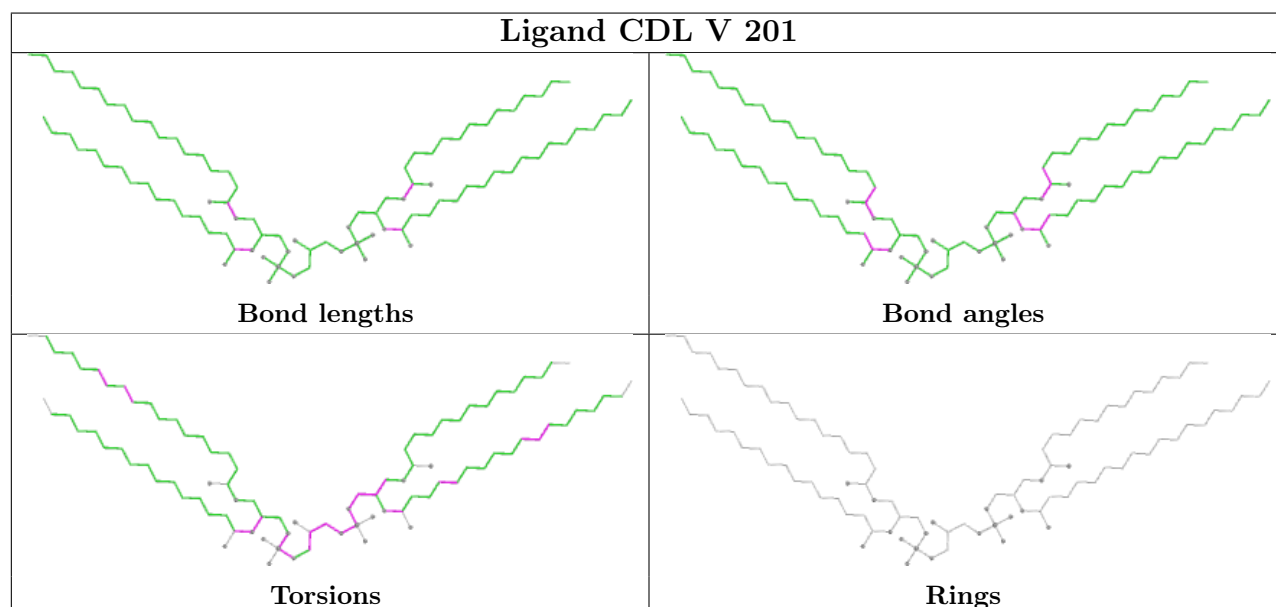
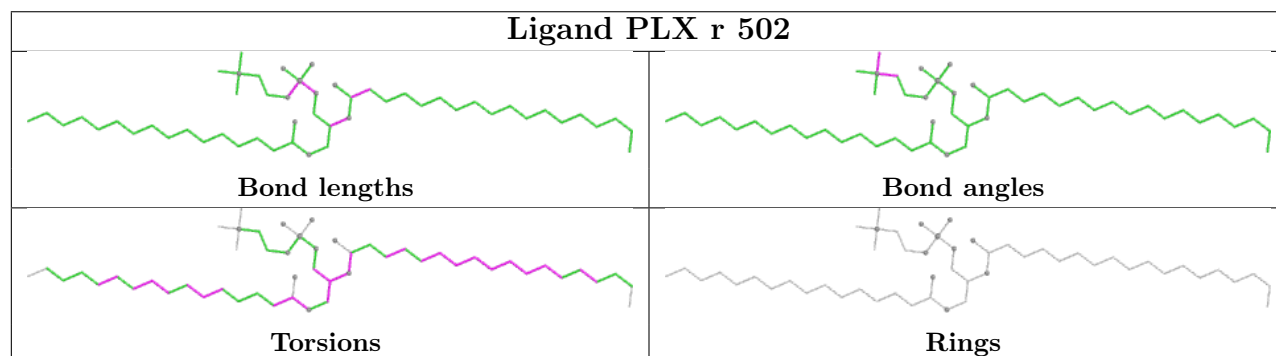
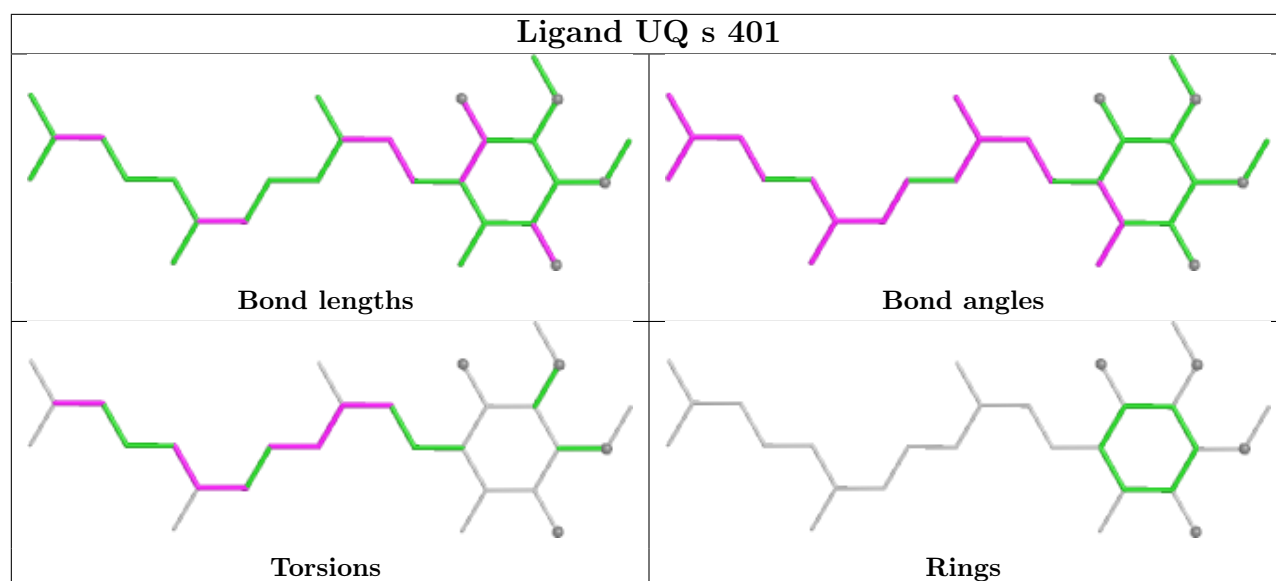


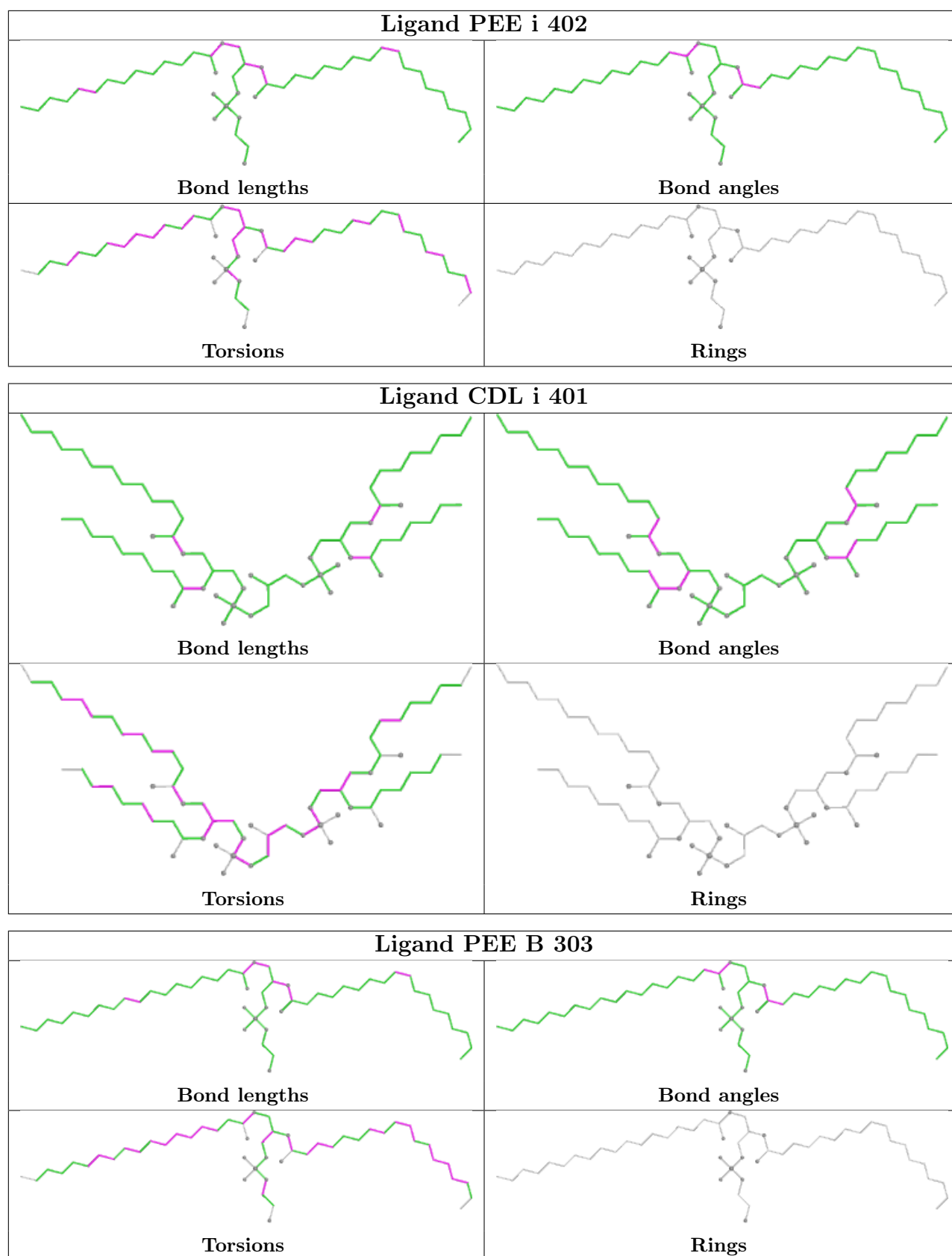












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

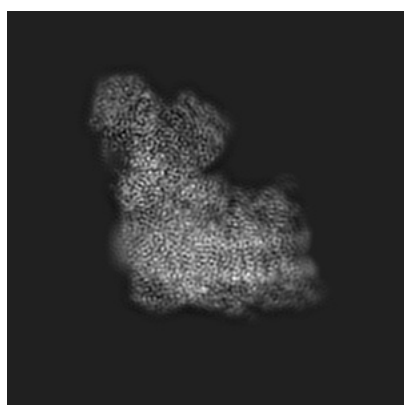
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31641. These allow visual inspection of the internal detail of the map and identification of artifacts.

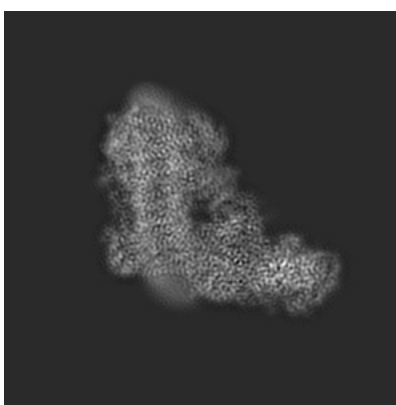
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

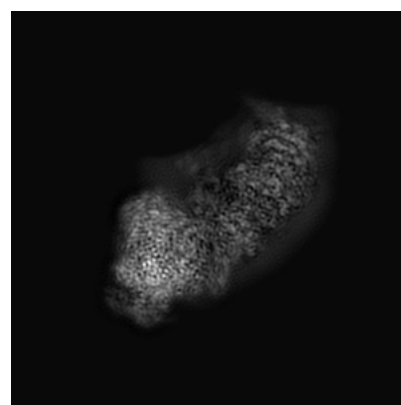
6.1.1 Primary map



X



Y

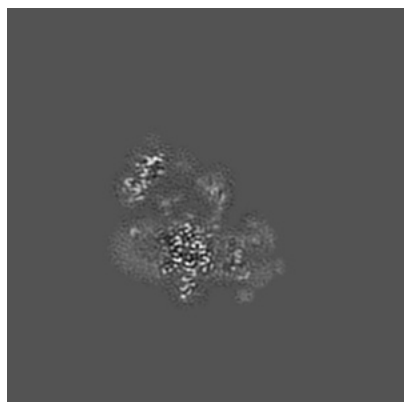


Z

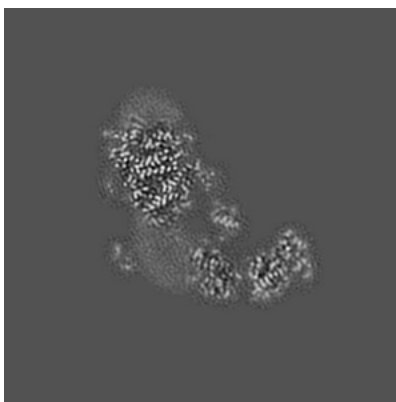
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

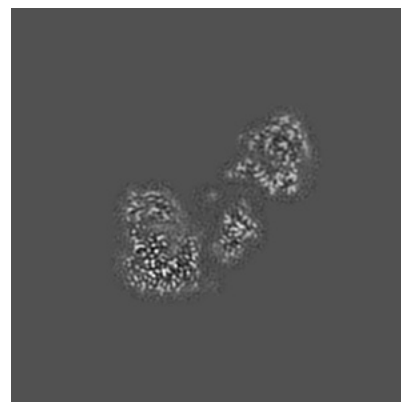
6.2.1 Primary map



X Index: 165



Y Index: 165

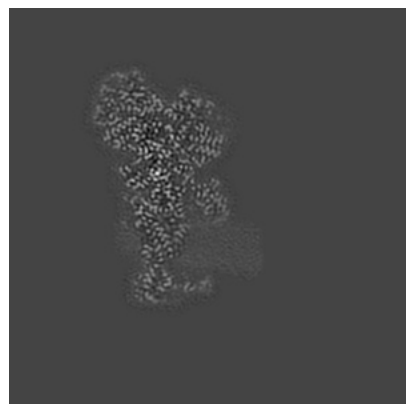


Z Index: 165

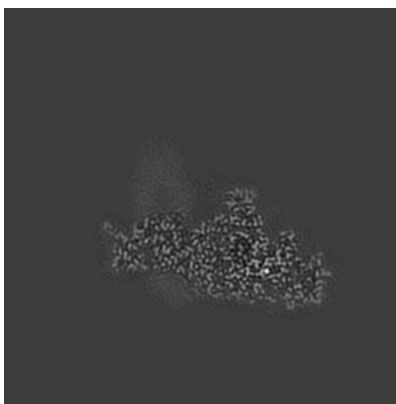
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

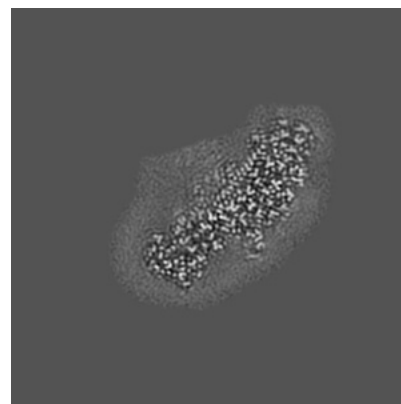
6.3.1 Primary map



X Index: 117



Y Index: 116

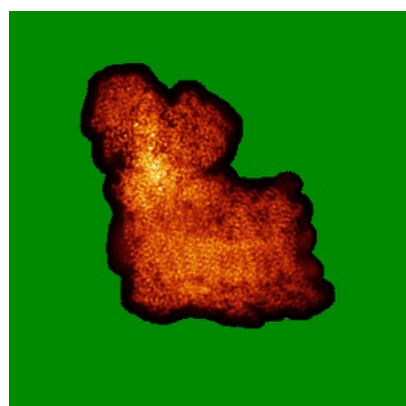


Z Index: 136

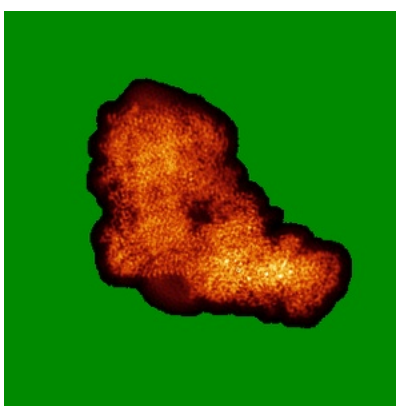
The images above show the largest variance slices of the map in three orthogonal directions.

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

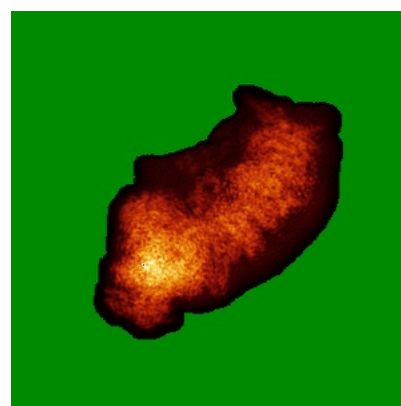
6.4.1 Primary map



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 0.0165. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

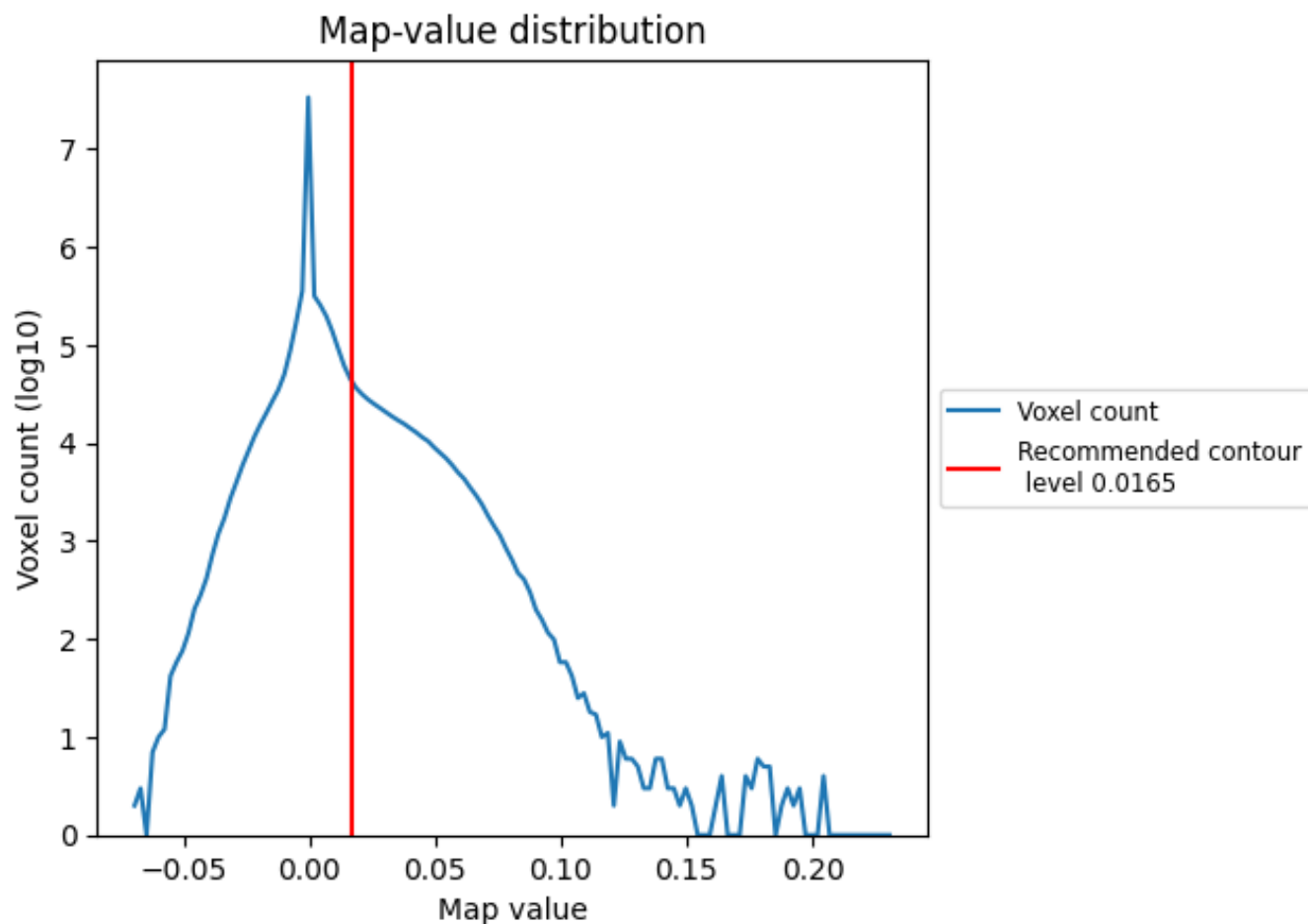
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

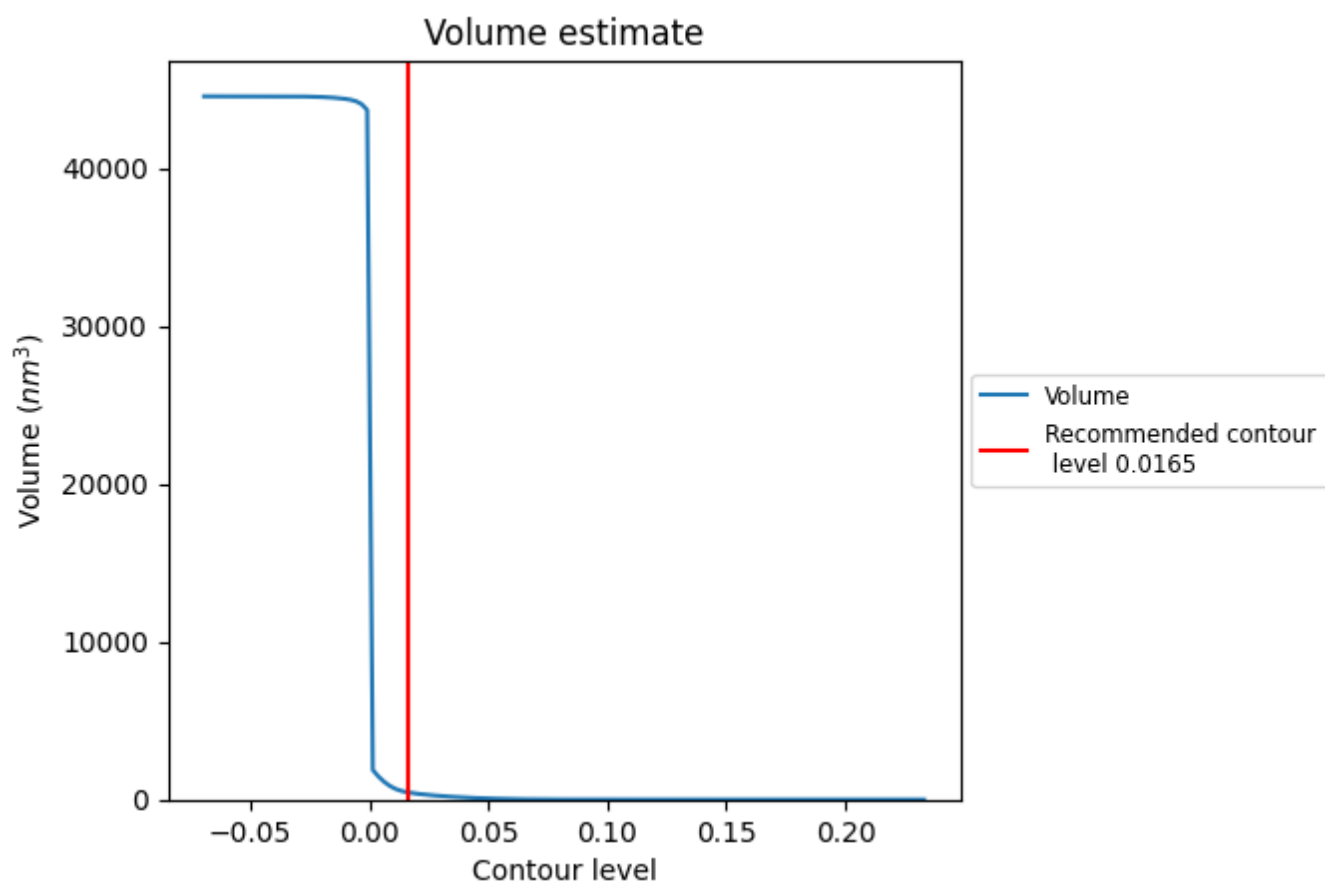
This section contains the results of statistical analysis of the map.

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.

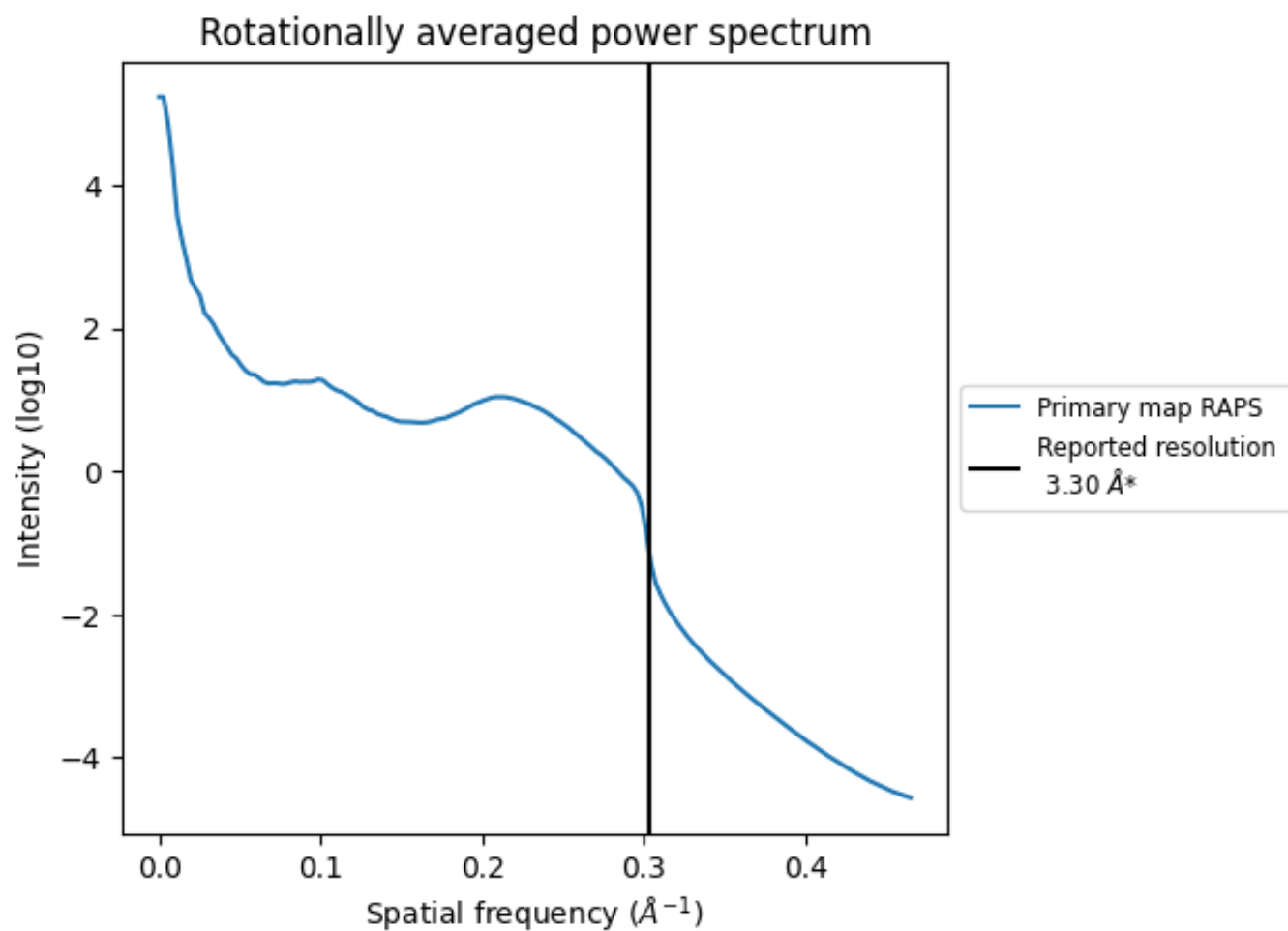
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 447 nm³; this corresponds to an approximate mass of 404 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

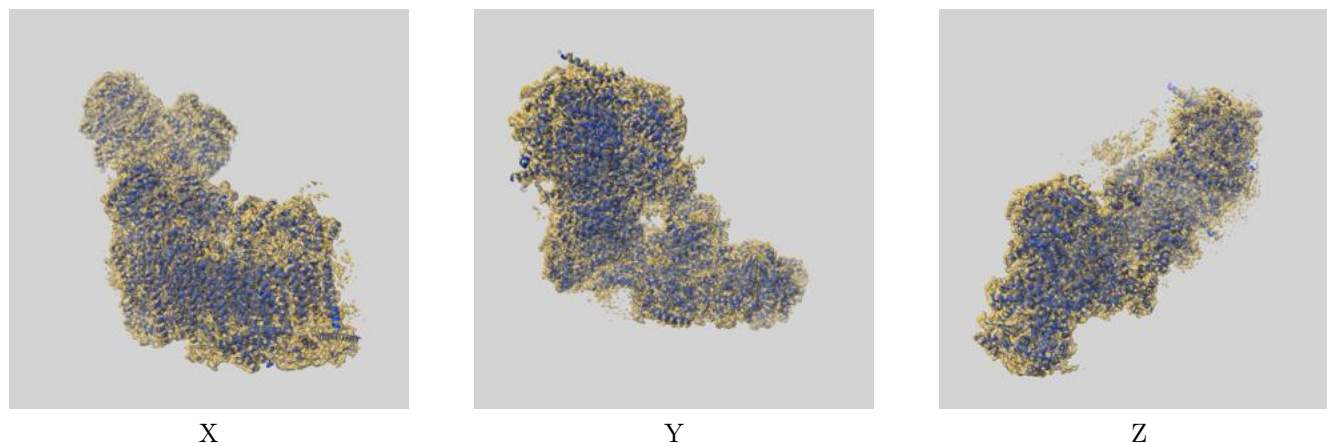
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

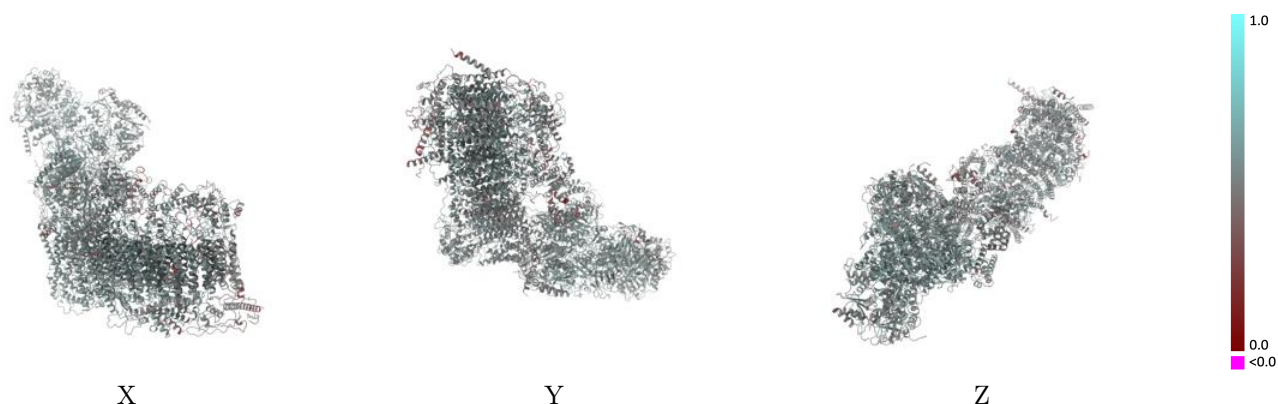
This section contains information regarding the fit between EMDB map EMD-31641 and PDB model 7V2D. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



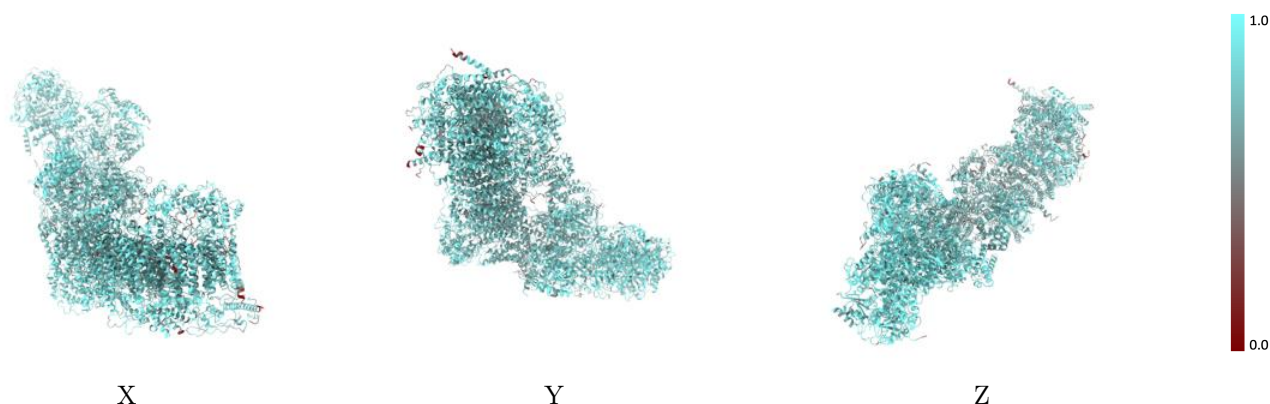
The images above show the 3D surface view of the map at the recommended contour level 0.0165 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



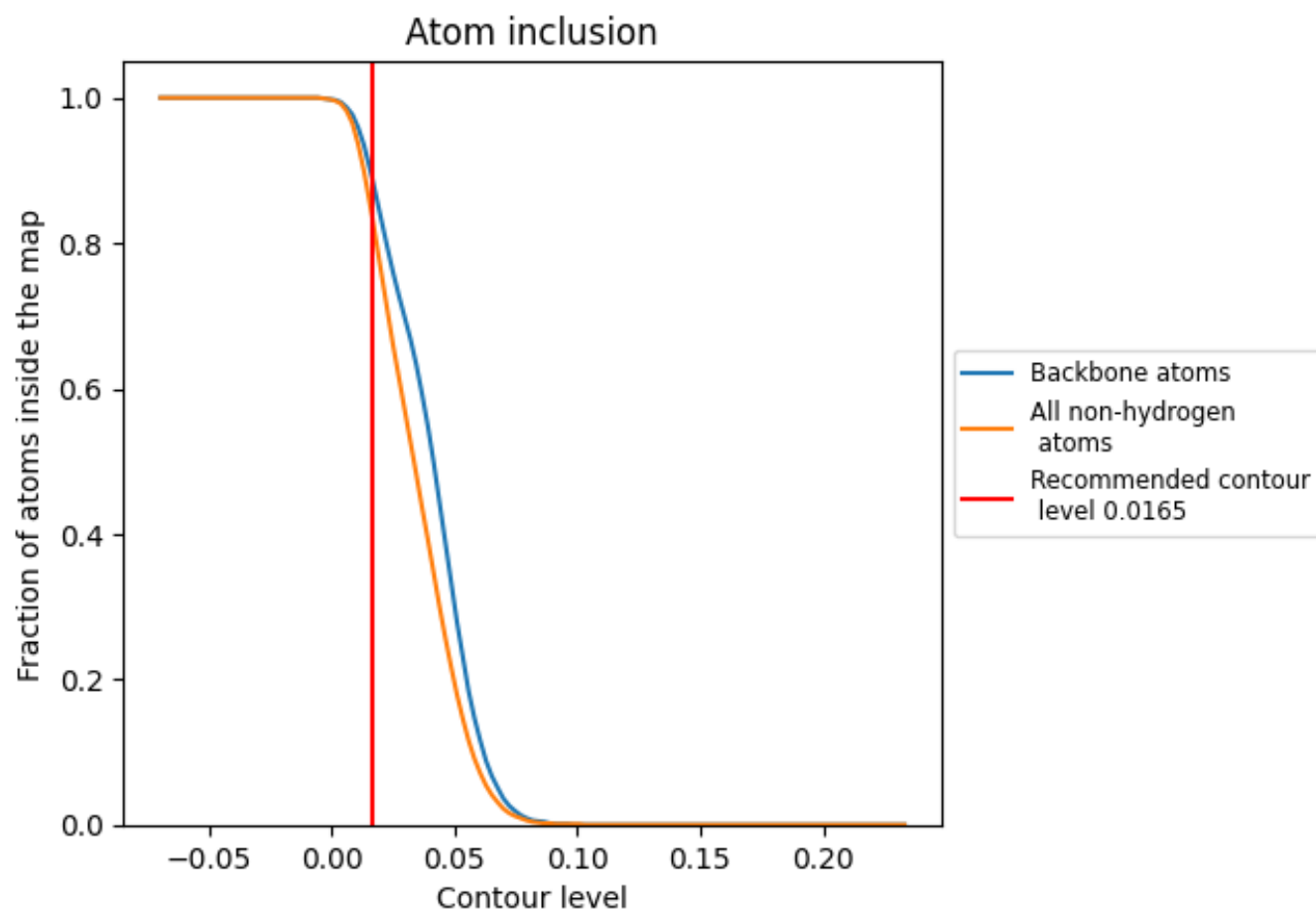
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0165).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% 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 (0.0165) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8370	 0.5240
A	 0.8720	 0.5250
B	 0.9240	 0.5640
C	 0.8830	 0.5480
E	 0.8170	 0.5230
F	 0.8230	 0.4920
G	 0.7110	 0.4220
H	 0.8490	 0.5120
I	 0.8330	 0.5360
J	 0.8400	 0.5160
K	 0.8690	 0.5200
L	 0.8550	 0.5470
M	 0.8810	 0.5420
N	 0.8250	 0.5340
O	 0.8420	 0.5120
P	 0.9100	 0.5610
Q	 0.8770	 0.5530
S	 0.8880	 0.5400
T	 0.8530	 0.5510
U	 0.8650	 0.5270
V	 0.6820	 0.4920
W	 0.8770	 0.5370
X	 0.7750	 0.4850
Y	 0.7820	 0.4720
Z	 0.7130	 0.4460
a	 0.8380	 0.5360
b	 0.7530	 0.4880
c	 0.8220	 0.5110
d	 0.8070	 0.5000
e	 0.7700	 0.5010
f	 0.8010	 0.5020
g	 0.8610	 0.5380
h	 0.8640	 0.5310
i	 0.8570	 0.5440
j	 0.7530	 0.5160



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Chain	Atom inclusion	Q-score
k	 0.8020	 0.5190
l	 0.8090	 0.5240
m	 0.8150	 0.5110
n	 0.7740	 0.4910
o	 0.7910	 0.5110
p	 0.8260	 0.5080
r	 0.8390	 0.5420
s	 0.8540	 0.5340
u	 0.8700	 0.5340
v	 0.7630	 0.4460
w	 0.8210	 0.5070