



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 11:43 PM JST

PDB ID : 7V2F / pdb_00007v2f
EMDB ID : EMD-31644
Title : Deactive state complex I from Q10-NADH dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-08-09
Resolution : 3.10 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

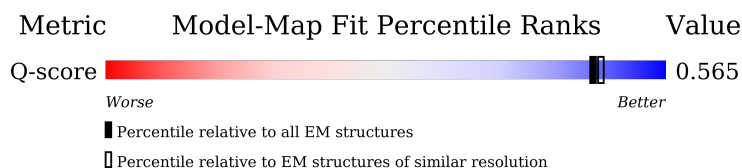
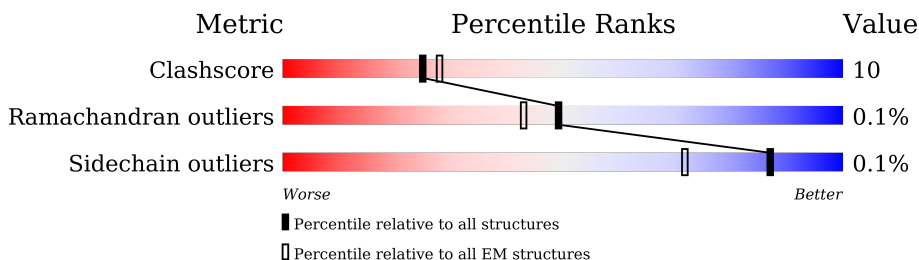
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	 73% 27%
2	B	176	 78% 22%
3	C	156	 83% 17%
4	E	115	 85% 15%

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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	125	
44	w	320	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	A	501	-	-	X	-
48	PEE	C	311	-	-	X	-
48	PEE	V	202	-	-	X	-
54	CDL	l	712	-	-	X	-

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 66939 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			693	447	102	139	5		
6	X	88	Total	C	N	O	S	0	0
			699	449	103	142	5		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	297	Total	C	N	O	S	0	0
			2359	1514	421	416	8		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	603	Total	C	N	O	S	0	0
			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
			1012	633	188	182	9		

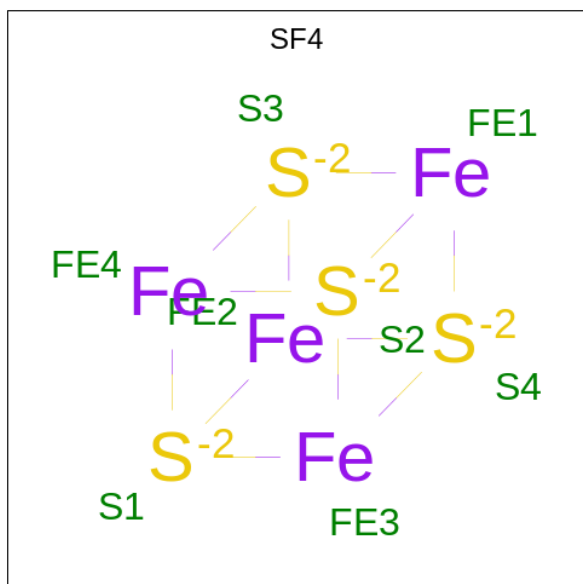
There is a discrepancy between the modelled and reference sequences:

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.

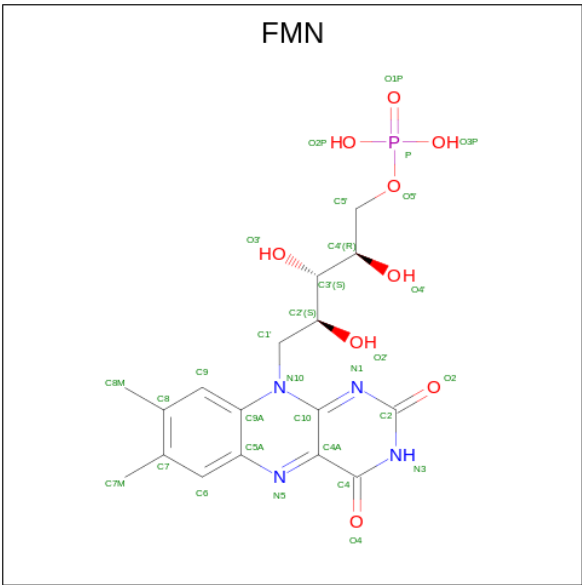
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2583	1646	437	491	9		

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



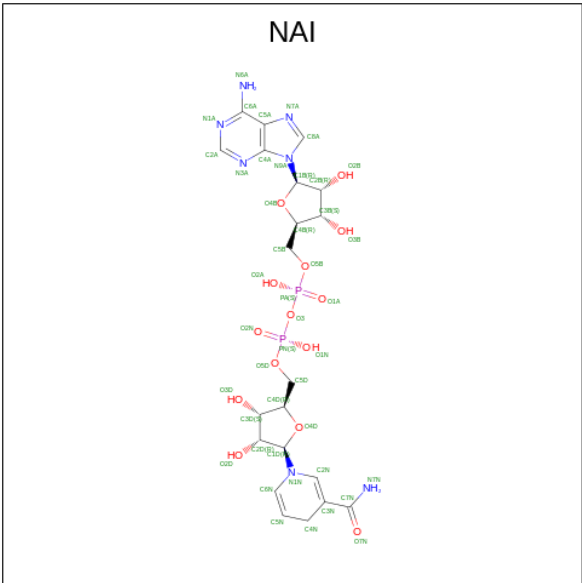
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

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



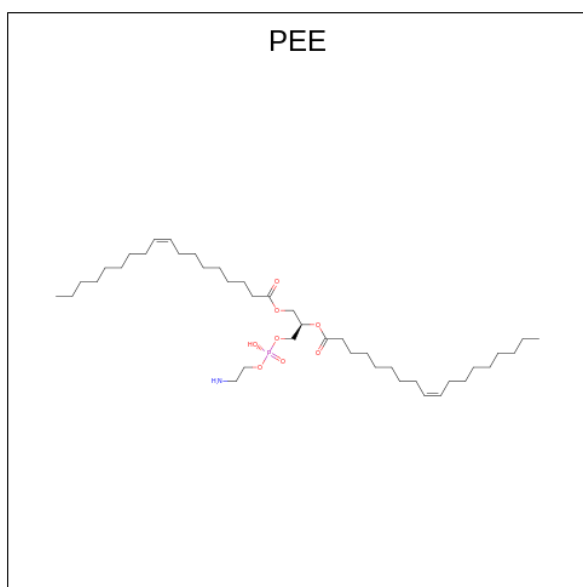
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

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



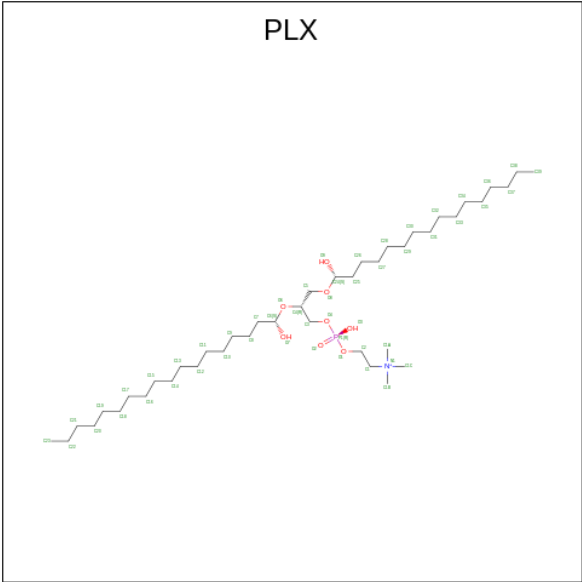
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

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



Mol	Chain	Residues	Atoms					AltConf
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	V	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	V	1	Total	C	N	O	P	0
			40	30	1	8	1	
48	l	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	s	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



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

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



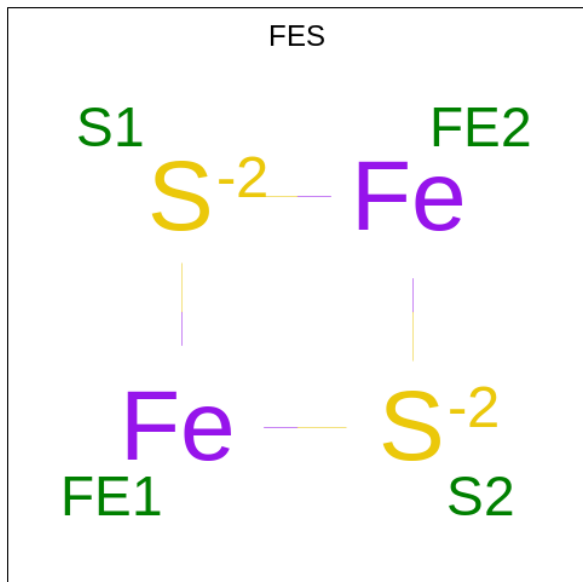
Mol	Chain	Residues	Atoms						AltCon
50	G	1	Total 35	C 23	N 2	O 8	P 1	S 1	0
50	X	1	Total 35	C 23	N 2	O 8	P 1	S 1	0

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



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

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

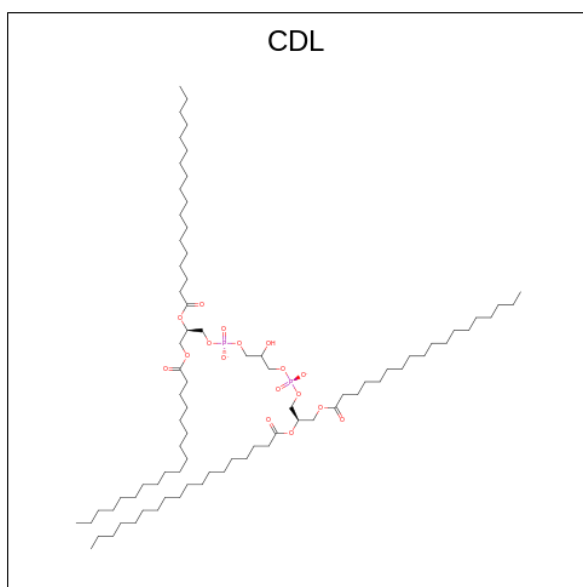


Mol	Chain	Residues	Atoms			AltConf
52	M	1	Total	Fe	S	0
			4	2	2	
52	O	1	Total	Fe	S	0
			4	2	2	

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

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

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

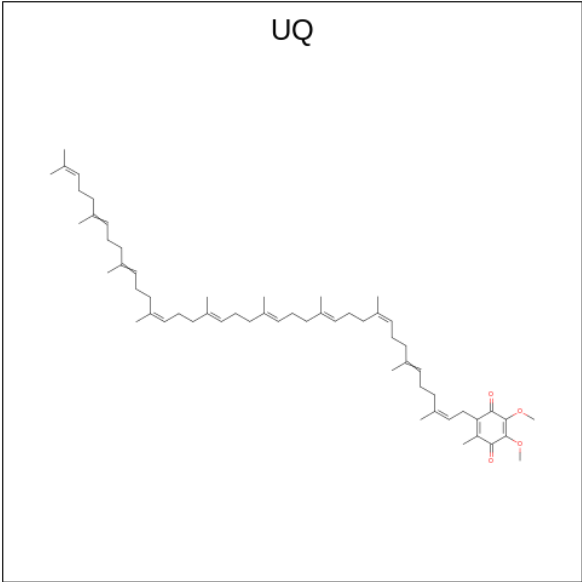


Mol	Chain	Residues	Atoms				AltConf
54	N	1	Total	C	O	P	0
			51	32	17	2	
54	V	1	Total	C	O	P	0
			94	75	17	2	
54	V	1	Total	C	O	P	0
			68	49	17	2	
54	a	1	Total	C	O	P	0
			91	72	17	2	
54	i	1	Total	C	O	P	0
			66	47	17	2	
54	l	1	Total	C	O	P	0
			99	80	17	2	
54	l	1	Total	C	O	P	0
			100	81	17	2	
54	n	1	Total	C	O	P	0
			78	59	17	2	
54	r	1	Total	C	O	P	0
			97	78	17	2	

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

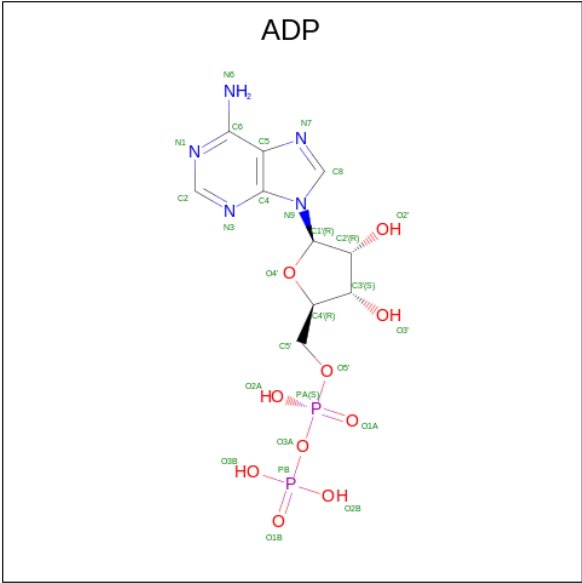
Mol	Chain	Residues	Atoms		AltConf
55	T	1	Total	Zn	0
			1	1	

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



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

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

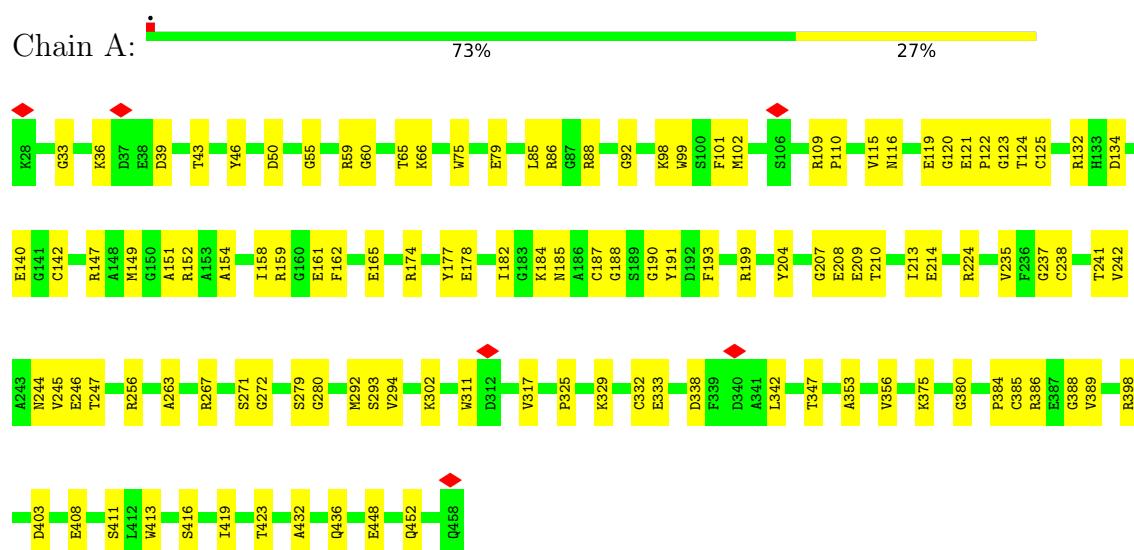


Mol	Chain	Residues	Atoms					AltConf
57	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

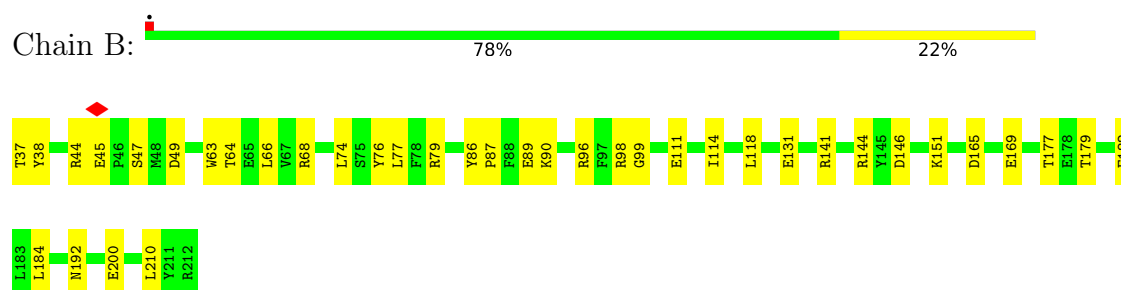
3 Residue-property plots

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

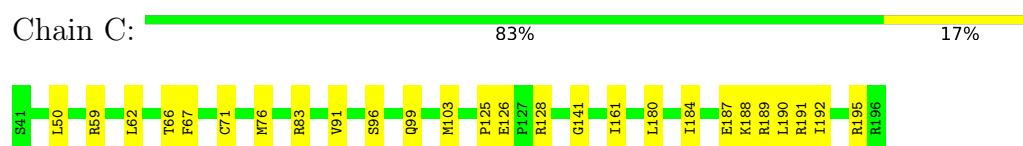
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



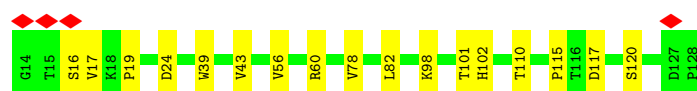
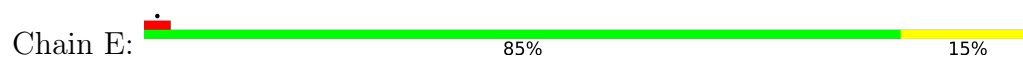
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



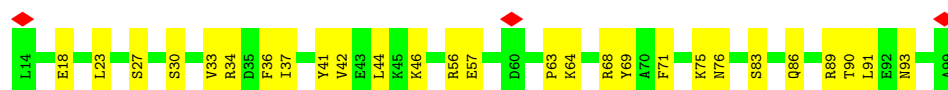
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



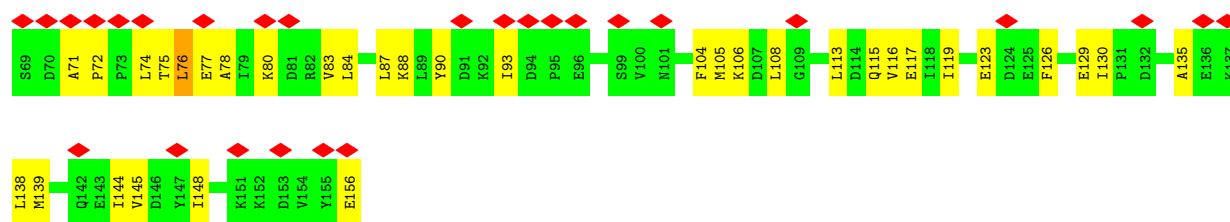
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



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



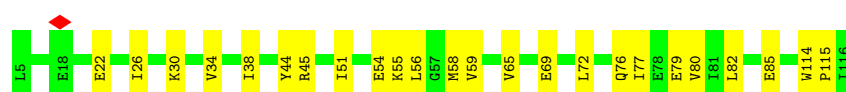
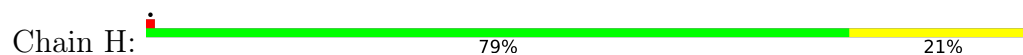
- Molecule 6: Acyl carrier protein, mitochondrial



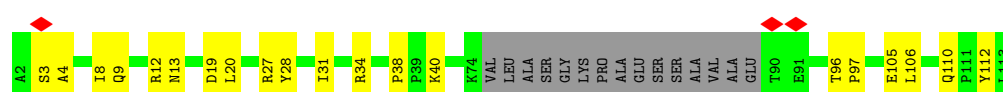
- Molecule 6: Acyl carrier protein, mitochondrial



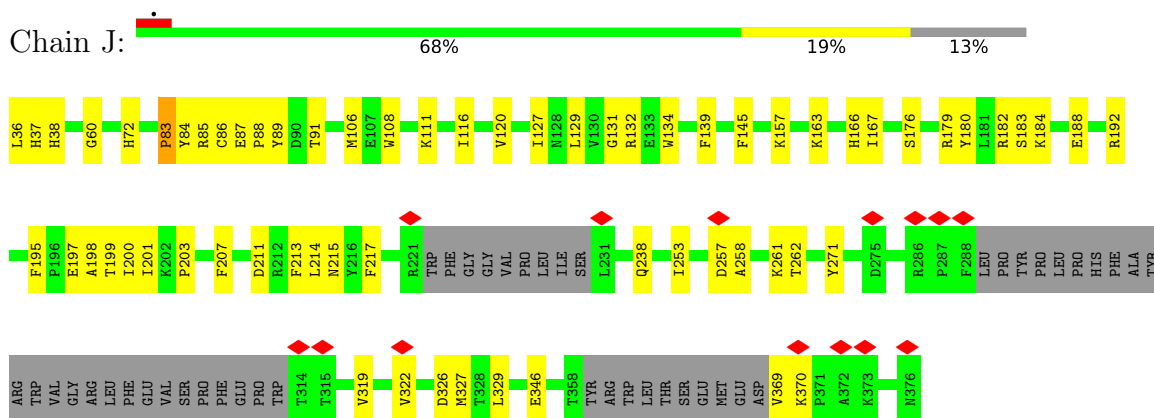
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



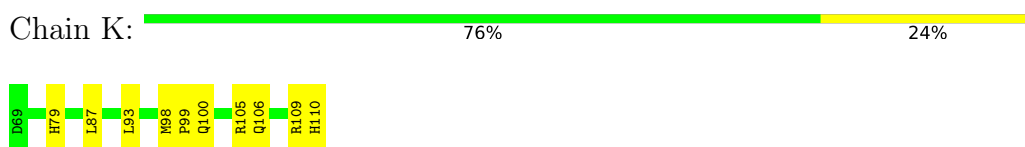
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



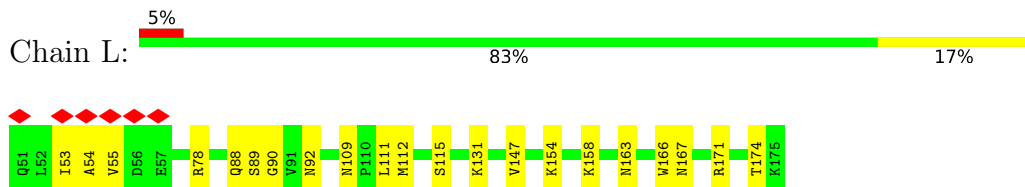
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



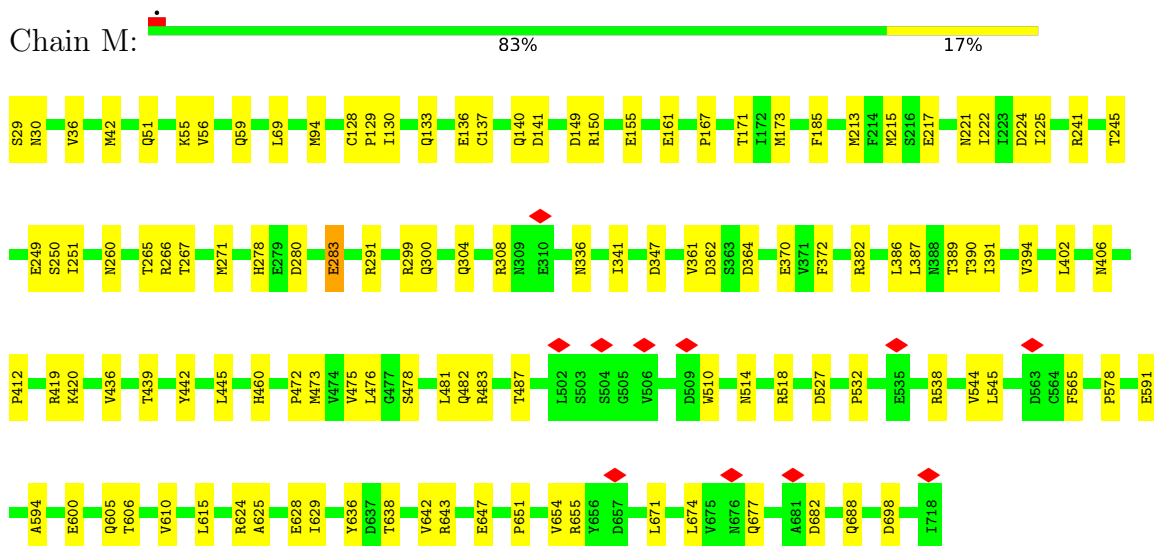
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



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



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

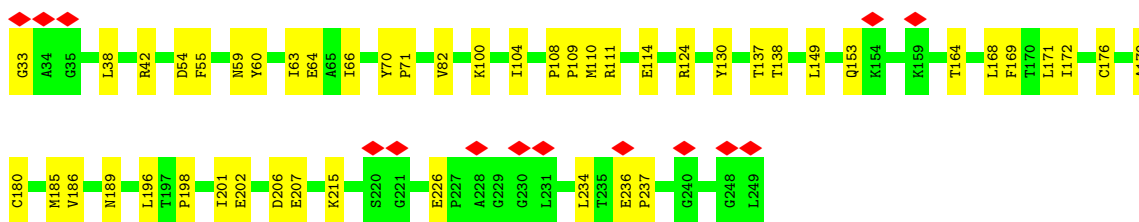
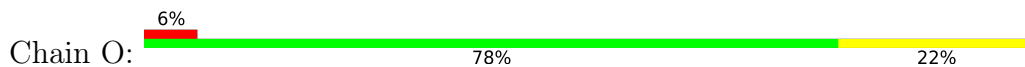


- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

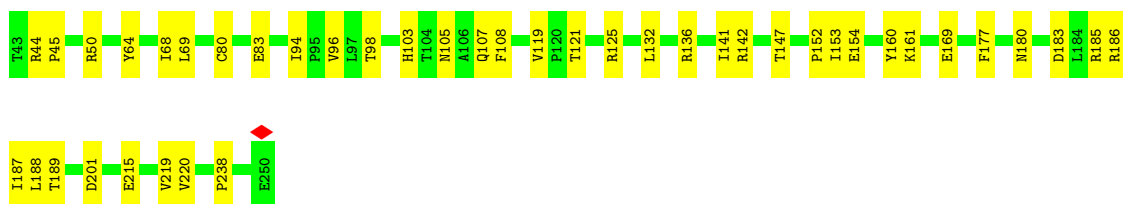
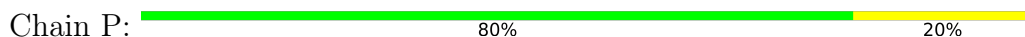




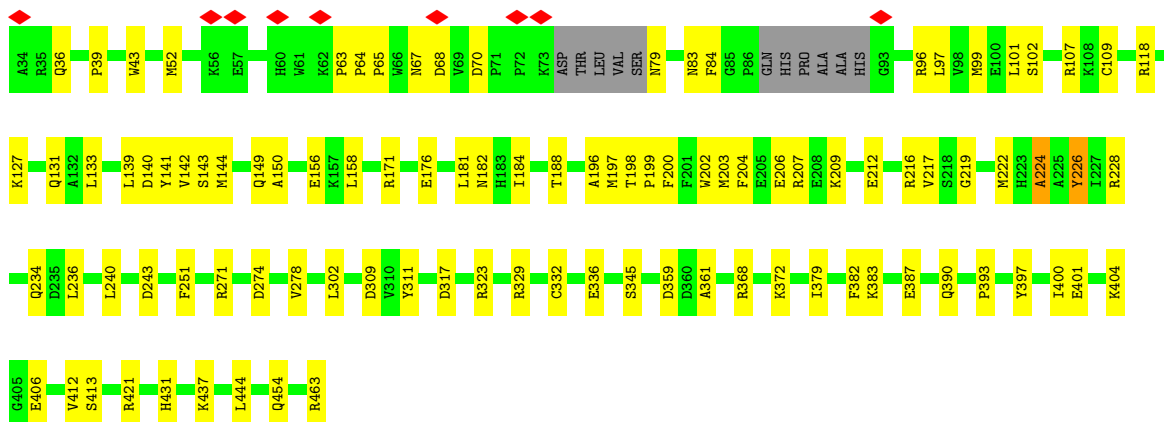
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



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



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



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

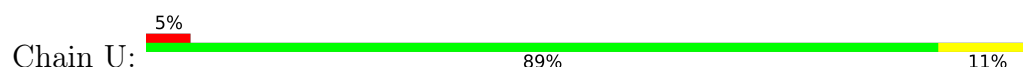




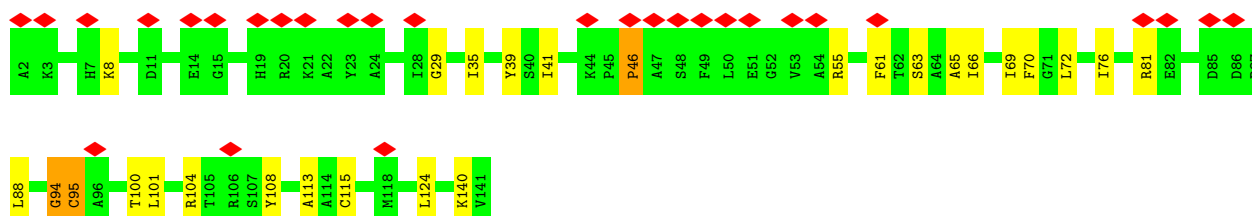
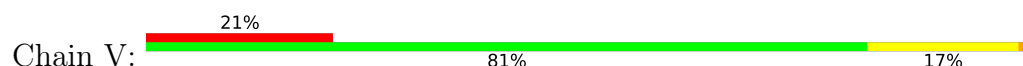
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



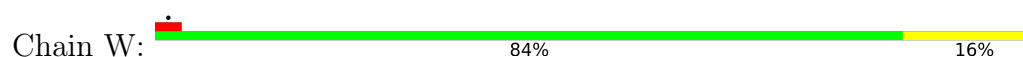
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



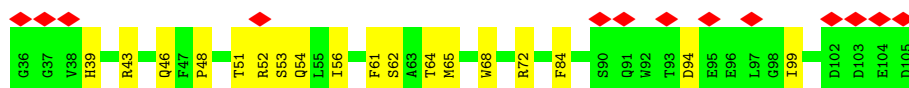
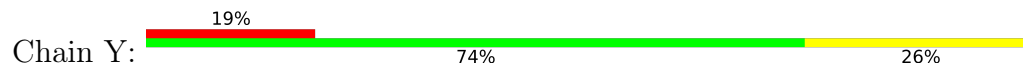
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



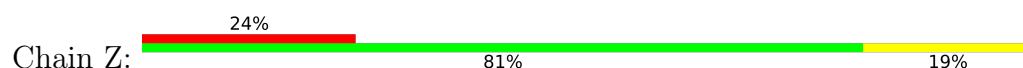
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

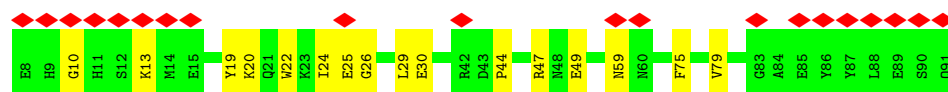


- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

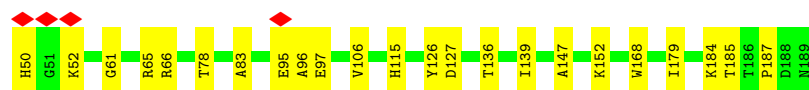
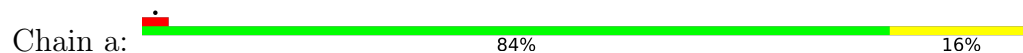


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

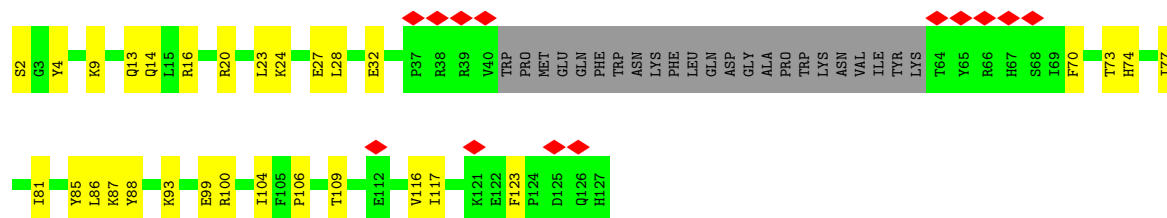




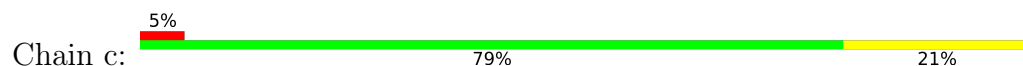
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



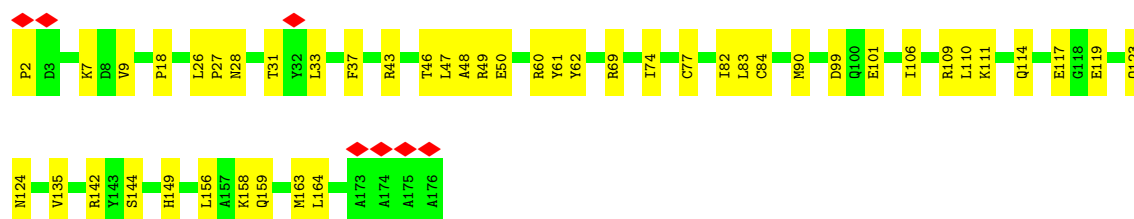
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



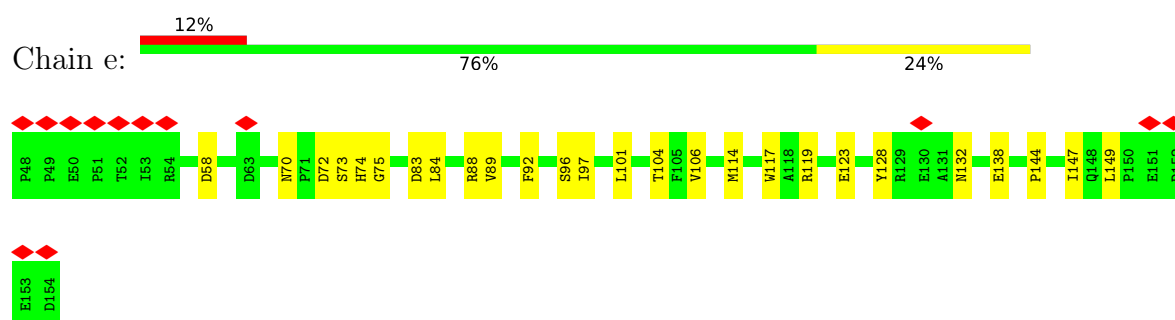
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



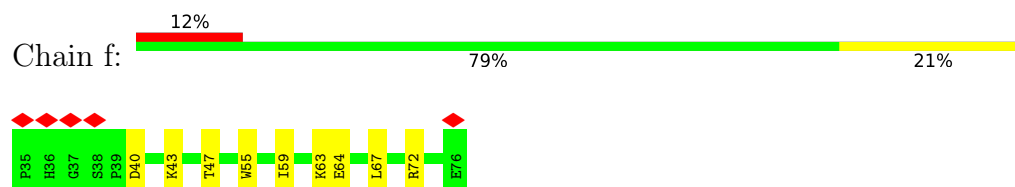
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



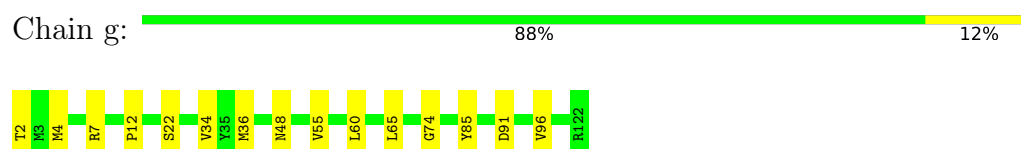
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



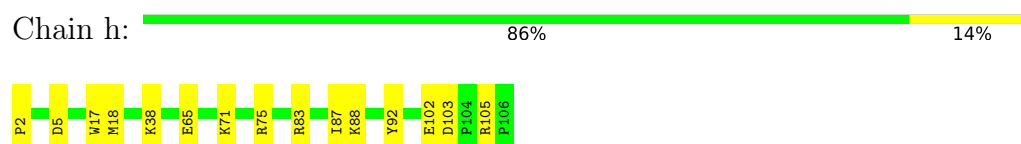
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



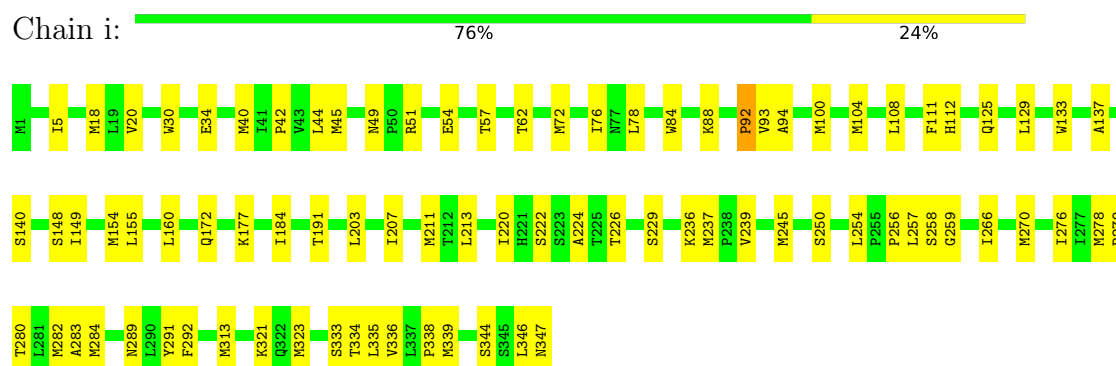
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



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

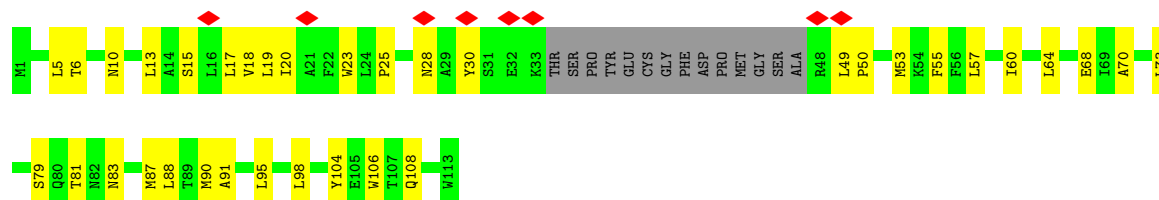


- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

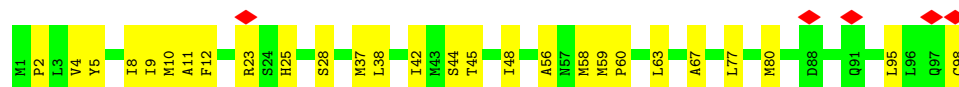


- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

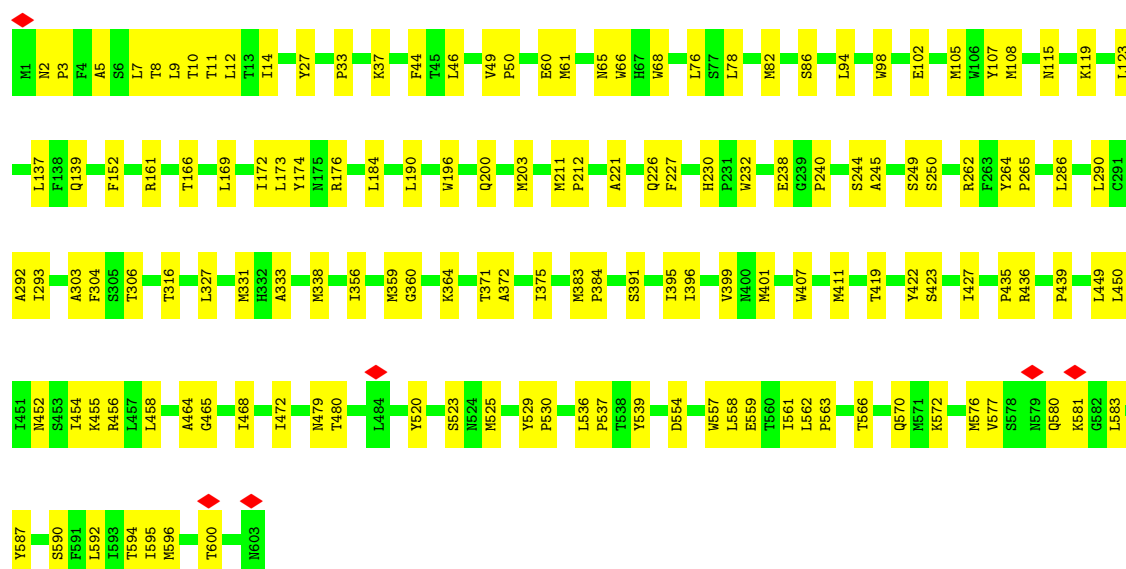
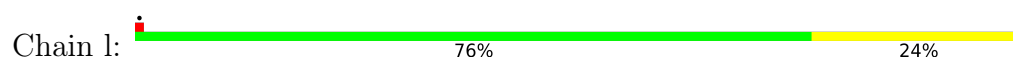




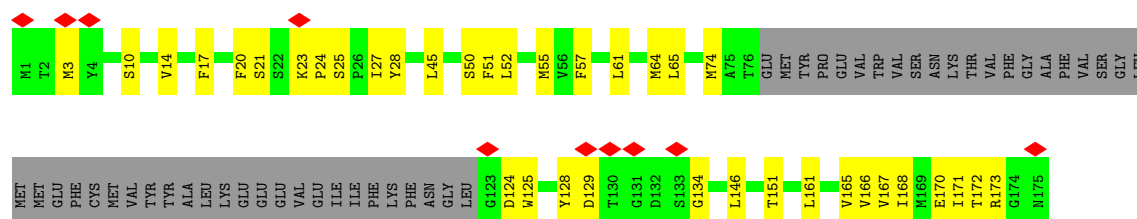
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L



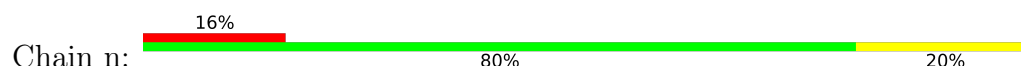
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

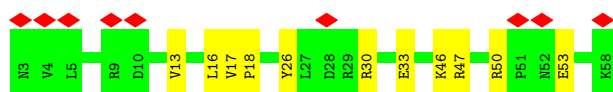


- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

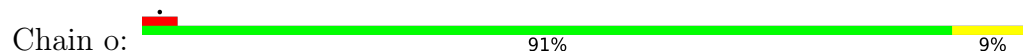


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

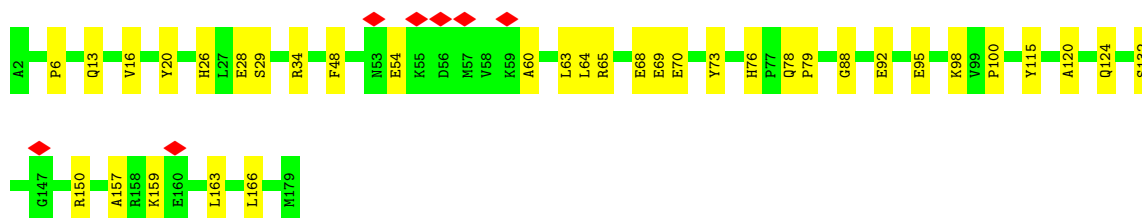
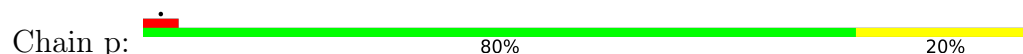




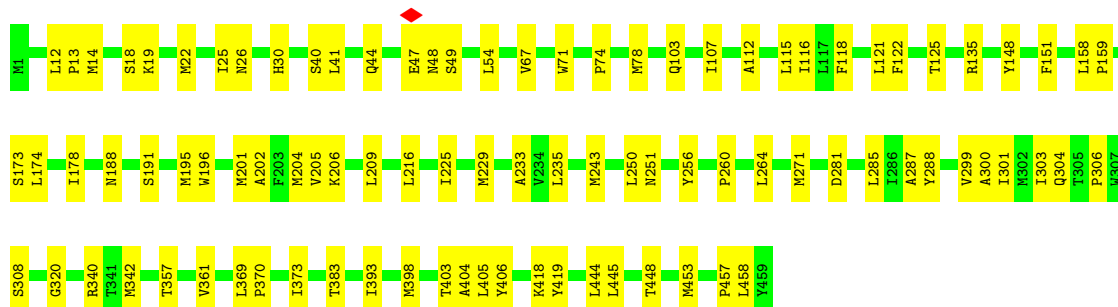
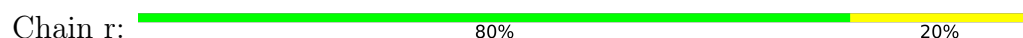
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



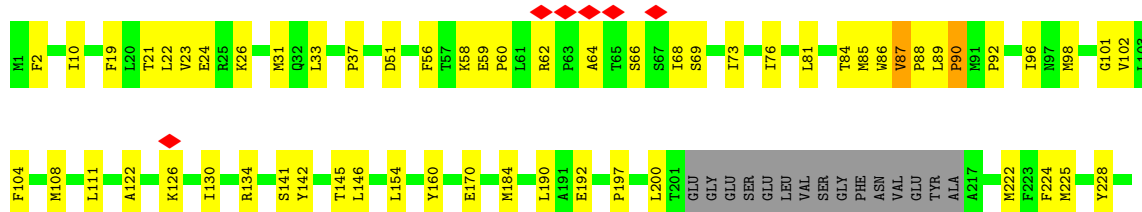
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

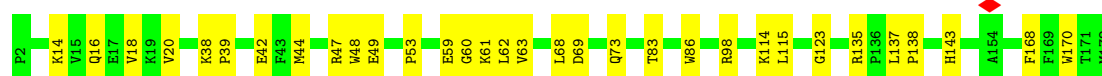
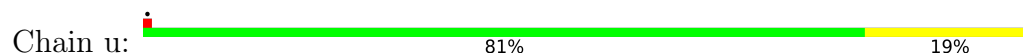


- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

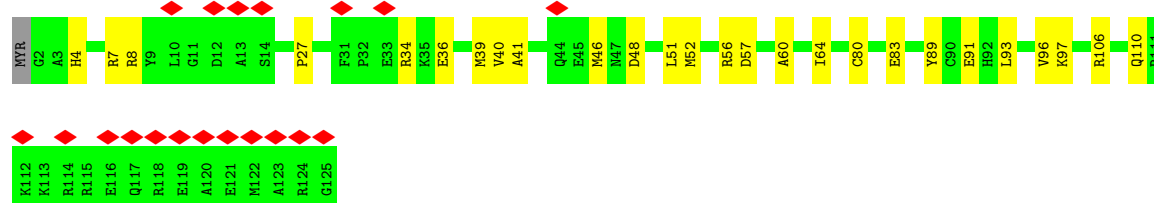
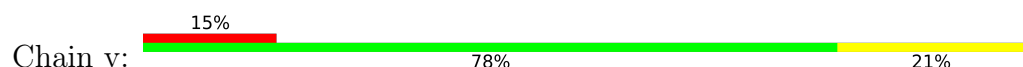




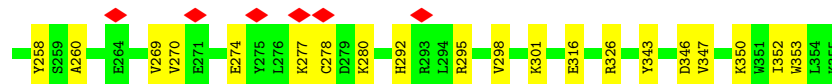
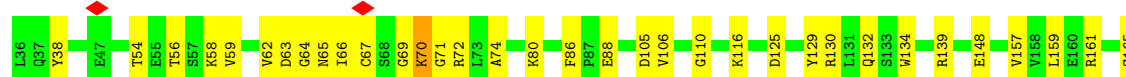
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- 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	104881	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	0.207	Depositor
Minimum map value	-0.109	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0232	Depositor
Map size ($\text{\AA}$)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	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: FES, FMN, PLX, SF4, PEE, ADP, NAI, 2MR, MG, 8Q1, CDL, ZN, UQ, NDP

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	0.19	0/3393	0.41	1/4584 (0.0%)
2	B	0.24	0/1443	0.36	0/1952
3	C	0.22	0/1279	0.35	0/1730
4	E	0.16	0/995	0.33	0/1340
5	F	0.16	0/702	0.37	0/945
6	G	0.19	0/705	0.51	0/956
6	X	0.15	0/711	0.33	0/963
7	H	0.18	0/929	0.40	0/1258
8	I	0.21	0/798	0.47	0/1079
9	J	0.18	0/2411	0.40	0/3254
10	K	0.13	0/365	0.27	0/493
11	L	0.20	0/1039	0.35	0/1403
12	M	0.19	0/5384	0.34	0/7295
13	N	0.18	0/1245	0.39	0/1694
14	O	0.17	0/1711	0.42	0/2328
15	P	0.22	0/1789	0.38	0/2436
16	Q	0.24	0/3451	0.43	4/4672 (0.1%)
17	S	0.21	0/582	0.42	0/783
18	T	0.16	0/755	0.30	0/1018
19	U	0.16	0/664	0.31	0/912
20	V	0.20	0/1042	0.42	3/1411 (0.2%)
21	W	0.19	0/1198	0.28	0/1617
22	Y	0.15	0/626	0.34	0/857
23	Z	0.16	0/695	0.35	0/939
24	a	0.19	0/1199	0.37	0/1623
25	b	0.15	0/906	0.35	0/1232
26	c	0.18	0/1371	0.35	0/1875
27	d	0.16	0/1494	0.29	0/2015
28	e	0.16	0/916	0.35	0/1246
29	f	0.15	0/350	0.30	0/473
30	g	0.18	0/1031	0.32	0/1394
31	h	0.19	0/889	0.36	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.21	0/2773	0.39	0/3768
33	j	0.23	0/819	0.42	0/1117
34	k	0.22	0/759	0.39	0/1029
35	l	0.20	0/4914	0.39	0/6683
36	m	0.21	0/973	0.41	0/1320
37	n	0.22	0/491	0.59	1/663 (0.2%)
38	o	0.17	0/1092	0.33	0/1481
39	p	0.17	0/1590	0.33	0/2155
40	r	0.22	0/3723	0.39	0/5078
41	s	0.24	0/2464	0.51	2/3369 (0.1%)
42	u	0.19	0/1436	0.40	0/1938
43	v	0.17	0/1036	0.48	0/1393
44	w	0.19	0/2643	0.45	1/3580 (0.0%)
All	All	0.20	0/66781	0.39	12/90541 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	GLY	N-CA-C	8.10	122.45	112.73
41	s	87	VAL	CA-C-N	8.07	127.65	118.85
41	s	87	VAL	C-N-CA	8.07	127.65	118.85
16	Q	217	VAL	N-CA-C	6.04	116.82	110.72
16	Q	142	VAL	N-CA-C	-6.00	107.65	113.53
20	V	95	CYS	CA-CB-SG	5.99	128.18	114.40
20	V	94	GLY	CA-C-N	-5.88	112.83	122.54
20	V	94	GLY	C-N-CA	-5.88	112.83	122.54
37	n	16	LEU	N-CA-C	5.85	117.66	111.28
44	w	245	PHE	N-CA-C	5.73	117.20	111.07
16	Q	224	ALA	N-CA-C	5.42	117.19	111.28
16	Q	226	TYR	N-CA-C	5.24	117.07	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3318	0	3280	87	0
2	B	1412	0	1363	41	0
3	C	1248	0	1254	32	0
4	E	971	0	975	13	0
5	F	691	0	704	19	0
6	G	693	0	671	24	0
6	X	699	0	674	18	0
7	H	910	0	950	16	0
8	I	780	0	808	22	0
9	J	2359	0	2402	47	0
10	K	355	0	329	14	0
11	L	1016	0	1016	22	0
12	M	5296	0	5326	89	0
13	N	1204	0	1162	33	0
14	O	1671	0	1673	36	0
15	P	1738	0	1693	28	0
16	Q	3377	0	3319	63	0
17	S	567	0	565	5	0
18	T	741	0	702	8	0
19	U	643	0	642	9	0
20	V	1021	0	1027	22	0
21	W	1167	0	1155	22	0
22	Y	600	0	539	12	0
23	Z	674	0	643	12	0
24	a	1165	0	1174	25	0
25	b	879	0	899	32	0
26	c	1315	0	1208	25	0
27	d	1461	0	1429	35	0
28	e	890	0	837	20	0
29	f	342	0	341	6	0
30	g	1000	0	994	14	0
31	h	867	0	871	13	0
32	i	2710	0	2874	78	0
33	j	800	0	855	29	0
34	k	748	0	799	23	0
35	l	4785	0	4933	114	0
36	m	951	0	962	37	0
37	n	479	0	486	14	0
38	o	1062	0	1072	9	0
39	p	1534	0	1470	29	0
40	r	3631	0	3839	88	0
41	s	2394	0	2508	83	0
42	u	1398	0	1378	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	v	1012	0	947	21	0
44	w	2583	0	2539	78	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	1	0
46	A	31	0	19	4	0
47	A	44	0	27	4	0
48	C	47	0	71	21	0
48	U	51	0	82	6	0
48	V	91	0	136	28	0
48	l	139	0	209	38	0
48	m	41	0	59	8	0
48	s	51	0	82	2	0
49	C	52	0	88	2	0
49	V	52	0	88	4	0
49	e	52	0	88	7	0
49	i	52	0	88	1	0
49	j	52	0	88	2	0
49	n	52	0	88	9	0
50	G	35	0	0	0	0
50	X	35	0	0	1	0
51	J	48	0	25	6	0
52	M	4	0	0	0	0
52	O	4	0	0	0	0
53	M	1	0	0	0	0
54	N	51	0	46	12	0
54	V	162	0	221	34	0
54	a	91	0	132	18	0
54	i	66	0	76	16	0
54	l	199	0	307	46	0
54	n	78	0	103	13	0
54	r	97	0	147	8	0
55	T	1	0	0	0	0
56	s	28	0	31	4	0
57	w	27	0	11	4	0
All	All	66939	0	67599	1406	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 10.

All (1406) 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)
3:C:50:LEU:CD2	48:C:311:PEE:H25	1.53	1.39
44:w:67:CYS:CB	44:w:218:ILE:HD11	1.65	1.27
51:J:401:NDP:O4D	51:J:401:NDP:C4D	1.68	1.21
54:V:201:CDL:H601	54:V:201:CDL:H732	1.24	1.18
3:C:50:LEU:CD2	48:C:311:PEE:C17	2.20	1.18
48:l:718:PEE:H36	48:l:718:PEE:H28	1.25	1.17
44:w:69:GLY:O	44:w:71:GLY:N	1.77	1.17
48:V:202:PEE:H78	40:r:201:MET:CE	1.75	1.15
54:V:203:CDL:H342	54:V:203:CDL:H112	1.26	1.13
54:l:712:CDL:H842	54:l:712:CDL:H631	1.14	1.13
48:V:202:PEE:H77	40:r:201:MET:HE2	1.14	1.12
3:C:50:LEU:HD21	48:C:311:PEE:C17	1.79	1.11
54:l:712:CDL:H791	54:l:712:CDL:H611	1.33	1.11
48:V:202:PEE:C45	40:r:201:MET:HE2	1.82	1.09
54:l:712:CDL:H601	54:l:712:CDL:H772	1.26	1.09
37:n:13:VAL:CG1	40:r:14:MET:HG2	1.82	1.09
41:s:87:VAL:HG23	41:s:88:PRO:HD3	1.21	1.09
48:V:207:PEE:H2	48:V:207:PEE:H9	1.25	1.07
3:C:50:LEU:HD22	48:C:311:PEE:H25	1.30	1.07
54:l:712:CDL:H541	54:l:712:CDL:HA62	1.35	1.06
54:l:712:CDL:H422	40:r:448:THR:HG21	1.36	1.06
37:n:13:VAL:HG12	40:r:14:MET:HG2	1.08	1.03
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.36	1.02
20:V:95:CYS:HB2	20:V:115:CYS:HA	1.40	1.02
24:a:95:GLU:OE2	54:a:201:CDL:O1	1.80	1.00
48:V:202:PEE:H77	40:r:201:MET:CE	1.91	0.99
44:w:67:CYS:CB	44:w:218:ILE:CD1	2.39	0.99
54:V:203:CDL:H832	54:V:203:CDL:H791	1.42	0.98
54:l:712:CDL:H312	54:l:712:CDL:H742	1.01	0.98
54:N:202:CDL:H312	54:N:202:CDL:H522	1.44	0.98
54:l:712:CDL:H742	54:l:712:CDL:C31	1.93	0.97
54:N:202:CDL:H541	54:N:202:CDL:H321	1.47	0.96
54:a:201:CDL:H521	48:l:720:PEE:H13	1.47	0.96
54:l:712:CDL:H842	54:l:712:CDL:C63	1.96	0.96
32:i:133:TRP:HE3	54:i:401:CDL:H392	1.31	0.96
48:V:202:PEE:C46	40:r:201:MET:CE	2.45	0.95
41:s:87:VAL:CG2	41:s:88:PRO:HD3	1.97	0.94
44:w:235:GLN:OE1	44:w:238:GLU:OE2	1.87	0.93
41:s:84:THR:O	41:s:87:VAL:HG22	1.69	0.92
54:a:201:CDL:H521	48:l:720:PEE:C11	1.99	0.91
32:i:133:TRP:CE3	54:i:401:CDL:H392	2.06	0.90
48:V:207:PEE:H2	48:V:207:PEE:C4	2.00	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:l:712:CDL:H791	54:l:712:CDL:C61	2.02	0.89
48:l:718:PEE:H28	48:l:718:PEE:C22	2.03	0.89
41:s:87:VAL:HG23	41:s:88:PRO:CD	2.04	0.88
48:V:202:PEE:H78	40:r:201:MET:HE3	1.55	0.88
54:l:712:CDL:H312	54:l:712:CDL:C74	1.97	0.87
48:l:719:PEE:C11	48:l:719:PEE:H7	2.04	0.87
48:V:202:PEE:C45	40:r:201:MET:CE	2.52	0.87
54:a:201:CDL:H251	54:a:201:CDL:H211	1.57	0.87
54:a:201:CDL:H532	48:l:720:PEE:H56	1.55	0.86
54:V:203:CDL:H112	54:V:203:CDL:C34	2.05	0.86
34:k:37:MET:HE1	36:m:64:MET:HE1	1.56	0.86
32:i:321:LYS:HE3	54:i:401:CDL:OA4	1.77	0.85
44:w:214:ILE:HG21	44:w:234:LEU:HD13	1.59	0.85
9:J:176:SER:O	9:J:182:ARG:NH2	2.11	0.84
54:l:712:CDL:HA62	54:l:712:CDL:C54	2.07	0.84
41:s:24:GLU:OE2	41:s:228:TYR:OH	1.95	0.83
54:N:202:CDL:H541	54:N:202:CDL:C32	2.08	0.83
54:V:203:CDL:H342	54:V:203:CDL:C11	2.07	0.83
9:J:83:PRO:HA	9:J:106:MET:O	1.79	0.82
48:m:202:PEE:H25	48:m:202:PEE:H54	1.58	0.82
37:n:13:VAL:HG12	40:r:14:MET:CG	2.02	0.82
54:V:201:CDL:H452	54:V:201:CDL:H211	1.61	0.81
54:n:102:CDL:H581	54:n:102:CDL:H542	1.61	0.81
48:C:311:PEE:H72	41:s:56:PHE:CD2	2.16	0.81
48:V:202:PEE:C46	40:r:201:MET:HE2	2.09	0.81
20:V:66:ILE:HD11	20:V:101:LEU:HD13	1.61	0.81
3:C:50:LEU:HD11	48:C:311:PEE:H59	1.62	0.81
24:a:127:ASP:OD1	49:n:101:PLX:H1C2	1.81	0.80
1:A:86:ARG:NE	1:A:92:GLY:O	2.15	0.80
6:X:91:ASP:HB3	23:Z:47:ARG:HH12	1.46	0.79
48:C:311:PEE:H72	41:s:56:PHE:HD2	1.47	0.79
33:j:68:GLU:HG2	36:m:161:LEU:HD13	1.64	0.79
32:i:133:TRP:HE3	54:i:401:CDL:C39	1.96	0.78
2:B:111:GLU:O	2:B:141:ARG:NH1	2.17	0.78
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.17	0.78
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.17	0.78
54:V:201:CDL:C74	54:V:201:CDL:H611	2.13	0.78
8:I:8:ILE:HG13	54:N:202:CDL:HA32	1.66	0.78
21:W:10:MET:HE3	21:W:11:PRO:HD2	1.64	0.78
6:G:74:LEU:H	6:G:74:LEU:HD23	1.49	0.78
1:A:204:TYR:OH	47:A:503:NAI:H5N	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.18	0.77
33:j:18:VAL:HG22	41:s:222:MET:HG3	1.66	0.77
54:l:712:CDL:H541	54:l:712:CDL:CA6	2.13	0.77
54:n:102:CDL:H542	54:n:102:CDL:C58	2.15	0.77
35:l:286:LEU:HD22	35:l:411:MET:HE3	1.68	0.76
1:A:388:GLY:HA3	1:A:419:ILE:HD11	1.67	0.76
24:a:126:TYR:O	49:n:101:PLX:H1B3	1.85	0.76
54:l:712:CDL:H772	54:l:712:CDL:C60	2.12	0.76
12:M:213:MET:HG3	12:M:215:MET:HG2	1.68	0.76
44:w:235:GLN:CD	44:w:238:GLU:OE2	2.29	0.75
41:s:87:VAL:N	41:s:88:PRO:HD2	2.02	0.75
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.69	0.74
44:w:65:ASN:ND2	44:w:238:GLU:HB3	2.03	0.74
3:C:126:GLU:O	9:J:89:TYR:OH	2.06	0.74
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.21	0.73
1:A:60:GLY:O	1:A:256:ARG:NH1	2.22	0.73
35:l:356:ILE:HA	35:l:359:MET:HE3	1.71	0.73
54:l:712:CDL:H642	54:l:712:CDL:H871	1.70	0.73
26:c:116:ARG:HG2	48:l:719:PEE:H49	1.68	0.73
24:a:179:ILE:HG21	31:h:38:LYS:HG3	1.70	0.73
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.21	0.73
9:J:83:PRO:HB2	9:J:108:TRP:CD1	2.24	0.72
44:w:69:GLY:O	44:w:70:LYS:C	2.32	0.72
11:L:112:MET:HE3	13:N:126:PRO:HB2	1.71	0.72
3:C:50:LEU:CD2	48:C:311:PEE:H26	2.15	0.72
48:V:202:PEE:O4	40:r:195:MET:HB2	1.90	0.72
48:C:311:PEE:H27	48:C:311:PEE:H58	1.71	0.72
48:V:202:PEE:H3	40:r:191:SER:HB3	1.73	0.71
54:V:201:CDL:H601	54:V:201:CDL:C73	2.14	0.71
1:A:121:GLU:HB2	47:A:503:NAI:C4N	2.20	0.71
10:K:105:ARG:NH1	11:L:167:ASN:O	2.23	0.70
32:i:129:LEU:CD1	54:i:401:CDL:H341	2.21	0.70
3:C:59:ARG:NH1	49:C:312:PLX:O3	2.23	0.70
35:l:359:MET:O	35:l:436:ARG:NH2	2.25	0.70
44:w:165:SER:HB3	44:w:245:PHE:CE1	2.26	0.70
32:i:125:GLN:HG2	54:i:401:CDL:OA3	1.90	0.70
24:a:97:GLU:OE2	27:d:60:ARG:NH1	2.24	0.70
25:b:16:ARG:HD3	25:b:20:ARG:NH1	2.07	0.70
44:w:250:SER:O	44:w:280:LYS:NZ	2.22	0.70
21:W:85:GLN:OE1	31:h:105:ARG:NH1	2.23	0.70
25:b:16:ARG:HD3	25:b:20:ARG:HH12	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:88:GLU:OE2	44:w:161:ARG:NH1	2.25	0.70
32:i:129:LEU:HD12	54:i:401:CDL:H341	1.74	0.70
48:l:719:PEE:H7	48:l:719:PEE:H14	1.74	0.70
1:A:33:GLY:O	1:A:302:LYS:NZ	2.25	0.69
12:M:472:PRO:O	12:M:510:TRP:NE1	2.22	0.69
35:l:227:PHE:O	35:l:230:HIS:ND1	2.24	0.69
40:r:188:ASN:OD1	40:r:256:TYR:OH	2.10	0.69
3:C:125:PRO:HB2	41:s:58:LYS:HE3	1.74	0.69
44:w:246:LEU:HD12	44:w:255:VAL:HG11	1.73	0.69
3:C:50:LEU:HD21	48:C:311:PEE:C18	2.23	0.69
9:J:85:ARG:NH2	51:J:401:NDP:O2X	2.23	0.69
54:n:102:CDL:H581	54:n:102:CDL:C54	2.20	0.69
48:C:311:PEE:C43	41:s:56:PHE:HD2	2.05	0.69
11:L:88:GLN:NE2	12:M:141:ASP:OD2	2.23	0.69
20:V:95:CYS:CB	20:V:115:CYS:HA	2.21	0.69
35:l:596:MET:O	35:l:600:THR:HG23	1.92	0.69
32:i:92:PRO:O	32:i:94:ALA:N	2.26	0.69
54:l:712:CDL:H622	54:l:712:CDL:H581	1.73	0.69
54:V:203:CDL:H852	35:l:558:LEU:HD21	1.74	0.69
26:c:161:TYR:HB3	26:c:166:LEU:HG	1.74	0.68
54:l:712:CDL:H631	54:l:712:CDL:C84	2.08	0.68
32:i:125:GLN:CG	54:i:401:CDL:OA3	2.42	0.68
35:l:250:SER:HB2	35:l:333:ALA:HA	1.75	0.68
54:l:712:CDL:H552	54:l:712:CDL:H792	1.75	0.68
41:s:87:VAL:CG2	41:s:88:PRO:CD	2.68	0.68
25:b:14:GLN:HE22	39:p:157:ALA:HB3	1.56	0.67
44:w:139:ARG:NH1	44:w:166:ASP:OD1	2.27	0.67
6:X:155:TYR:CE1	25:b:23:LEU:HB3	2.29	0.67
16:Q:79:ASN:HA	16:Q:101:LEU:O	1.94	0.67
54:V:201:CDL:H611	54:V:201:CDL:H741	1.75	0.67
54:V:201:CDL:HA62	54:V:201:CDL:OA7	1.92	0.67
41:s:184:MET:HE1	41:s:296:LEU:HB2	1.75	0.67
26:c:165:ASP:OD2	26:c:170:ARG:NH2	2.27	0.67
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.28	0.67
11:L:109:ASN:ND2	11:L:111:LEU:O	2.27	0.67
43:v:39:MET:HE3	43:v:41:ALA:H	1.58	0.67
29:f:40:ASP:OD2	29:f:43:LYS:NZ	2.27	0.67
22:Y:43:ARG:HB3	22:Y:46:GLN:HG2	1.77	0.67
32:i:321:LYS:CE	54:i:401:CDL:OA4	2.43	0.67
20:V:72:LEU:O	20:V:76:ILE:HG12	1.95	0.66
6:X:76:LEU:HD21	25:b:20:ARG:HH21	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:69:ARG:HH22	37:n:46:LYS:HB3	1.59	0.66
6:G:119:ILE:HG21	6:G:135:ALA:HB1	1.77	0.66
25:b:104:ILE:HB	43:v:48:ASP:HB3	1.76	0.66
33:j:25:PRO:HB2	41:s:60:PRO:HD3	1.76	0.66
35:l:401:MET:SD	35:l:479:ASN:ND2	2.66	0.66
1:A:121:GLU:HG3	1:A:122:PRO:HD2	1.77	0.66
25:b:28:LEU:HG	25:b:32:GLU:HG2	1.78	0.66
33:j:60:ILE:HG21	36:m:168:ILE:HG21	1.78	0.66
2:B:192:ASN:ND2	18:T:61:GLU:OE2	2.26	0.66
44:w:235:GLN:O	44:w:238:GLU:HG3	1.95	0.66
12:M:483:ARG:HH22	12:M:682:ASP:HB3	1.60	0.66
41:s:51:ASP:HB3	56:s:403:UQ:H8	1.77	0.66
1:A:159:ARG:NH2	14:O:176:CYS:O	2.28	0.66
1:A:185:ASN:OD1	1:A:190:GLY:N	2.21	0.66
1:A:311:TRP:NE1	1:A:333:GLU:OE2	2.28	0.66
44:w:125:ASP:O	44:w:130:ARG:NH2	2.29	0.66
1:A:152:ARG:NH2	10:K:99:PRO:O	2.29	0.65
48:V:202:PEE:H3	40:r:191:SER:CB	2.26	0.65
42:u:44:MET:HB3	42:u:48:TRP:HZ3	1.62	0.65
48:l:719:PEE:H22	48:l:719:PEE:H64	1.79	0.65
25:b:109:THR:HG22	25:b:116:VAL:HG22	1.78	0.65
32:i:100:MET:HE1	35:l:595:ILE:HG23	1.78	0.65
48:l:720:PEE:O2P	48:l:720:PEE:N	2.21	0.65
9:J:369:VAL:HG12	9:J:370:LYS:HG2	1.78	0.65
15:P:50:ARG:HH12	15:P:80:CYS:HB2	1.62	0.65
5:F:57:GLU:O	12:M:655:ARG:NH2	2.30	0.65
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.79	0.65
54:l:712:CDL:C84	54:l:712:CDL:H651	2.27	0.64
7:H:44:TYR:HB2	15:P:68:ILE:HG23	1.78	0.64
38:o:23:TYR:OH	39:p:68:GLU:OE1	2.15	0.64
41:s:235:ASN:HD21	41:s:270:PHE:HE2	1.45	0.64
3:C:83:ARG:NH1	16:Q:212:GLU:OE2	2.24	0.64
10:K:100:GLN:HB3	14:O:71:PRO:HA	1.78	0.64
54:l:712:CDL:H601	54:l:712:CDL:C77	2.16	0.64
20:V:69:ILE:HG13	20:V:100:THR:HG21	1.78	0.64
3:C:50:LEU:HD23	48:C:311:PEE:C17	2.24	0.63
6:G:105:MET:HE2	6:G:139:MET:HE1	1.79	0.63
6:G:138:LEU:HD23	6:G:144:ILE:HG12	1.80	0.63
27:d:119:GLU:HG2	43:v:52:MET:HA	1.81	0.63
49:V:205:PLX:H132	40:r:260:PRO:HG2	1.78	0.63
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:235:ASN:ND2	41:s:270:PHE:HE2	1.96	0.63
22:Y:62:SER:HG	35:l:371:THR:HG1	1.46	0.63
27:d:111:LYS:NZ	35:l:200:GLN:OE1	2.32	0.63
3:C:50:LEU:HD21	48:C:311:PEE:H26	1.73	0.63
44:w:246:LEU:N	44:w:247:PRO:HD2	2.13	0.63
9:J:213:PHE:HD1	9:J:214:LEU:HD12	1.62	0.63
54:V:201:CDL:H732	54:V:201:CDL:C60	2.16	0.63
49:e:201:PLX:O2	48:l:720:PEE:H3	1.98	0.63
44:w:233:TYR:CZ	44:w:237:ILE:HD11	2.34	0.62
35:l:391:SER:O	35:l:395:ILE:HG12	1.99	0.62
35:l:407:TRP:O	35:l:411:MET:HG2	1.99	0.62
9:J:157:LYS:NZ	9:J:197:GLU:OE2	2.33	0.62
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.81	0.62
40:r:48:ASN:OD1	40:r:49:SER:N	2.30	0.62
44:w:38:TYR:HH	44:w:292:HIS:HD1	1.48	0.62
41:s:62:ARG:HD3	41:s:64:ALA:H	1.63	0.62
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.82	0.62
9:J:132:ARG:NH2	51:J:401:NDP:O2X	2.33	0.62
9:J:327:MET:HE2	9:J:329:LEU:HD11	1.79	0.62
11:L:131:LYS:HE3	11:L:147:VAL:HG11	1.82	0.62
1:A:398:ARG:HG2	1:A:403:ASP:HB3	1.82	0.61
12:M:394:VAL:HG22	12:M:473:MET:HE1	1.82	0.61
50:X:201:8Q1:O3	39:p:13:GLN:NE2	2.33	0.61
15:P:169:GLU:OE2	16:Q:463:ARG:NH2	2.33	0.61
49:e:201:PLX:H122	54:l:712:CDL:H652	1.81	0.61
41:s:184:MET:HE2	41:s:293:PHE:HA	1.83	0.61
14:O:149:LEU:O	14:O:153:GLN:HG2	2.01	0.61
49:e:201:PLX:H102	48:l:720:PEE:H23	1.83	0.61
33:j:79:SER:HA	33:j:87:MET:HE2	1.81	0.61
2:B:177:THR:HG22	2:B:179:THR:H	1.65	0.61
9:J:145:PHE:CE1	9:J:184:LYS:HE3	2.36	0.61
16:Q:387:GLU:OE2	16:Q:390:GLN:NE2	2.34	0.61
30:g:34:VAL:HG21	54:n:102:CDL:OA7	1.99	0.61
14:O:60:TYR:O	14:O:64:GLU:HG3	2.01	0.61
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.27	0.61
27:d:2:PRO:O	27:d:7:LYS:NZ	2.33	0.61
28:e:104:THR:HG21	49:n:101:PLX:H212	1.81	0.61
11:L:78:ARG:NH2	12:M:249:GLU:OE1	2.25	0.61
12:M:636:TYR:CD1	12:M:642:VAL:HG22	2.36	0.61
25:b:73:THR:HA	25:b:77:ILE:HD12	1.83	0.61
35:l:119:LYS:NZ	54:l:712:CDL:H512	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:590:SER:O	35:l:594:THR:HG23	2.01	0.61
48:m:202:PEE:H25	48:m:202:PEE:C34	2.27	0.61
41:s:235:ASN:HD22	41:s:266:LEU:HB3	1.66	0.61
2:B:184:LEU:HD23	11:L:112:MET:HG3	1.83	0.61
28:e:92:PHE:O	28:e:96:SER:OG	2.17	0.61
54:l:712:CDL:H651	54:l:712:CDL:H841	1.83	0.61
39:p:29:SER:HB3	39:p:76:HIS:HD2	1.66	0.61
41:s:69:SER:O	41:s:73:ILE:HG12	2.00	0.61
8:I:27:ARG:NH1	16:Q:212:GLU:OE1	2.34	0.60
15:P:154:GLU:OE2	15:P:180:ASN:ND2	2.30	0.60
41:s:146:LEU:HD11	41:s:192:GLU:HG3	1.83	0.60
1:A:214:GLU:OE2	1:A:224:ARG:NE	2.29	0.60
2:B:177:THR:HG21	2:B:182:GLU:HB2	1.82	0.60
48:V:202:PEE:H14	48:V:202:PEE:H7	1.82	0.60
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.28	0.60
2:B:77:LEU:HD12	41:s:31:MET:HG3	1.83	0.60
48:V:202:PEE:H14	32:i:276:ILE:HG21	1.84	0.60
31:h:18:MET:HE3	34:k:56:ALA:HA	1.83	0.60
14:O:111:ARG:NH1	14:O:114:GLU:OE2	2.35	0.60
32:i:149:ILE:HD13	32:i:154:MET:HE3	1.84	0.60
36:m:21:SER:O	36:m:23:LYS:NZ	2.34	0.60
36:m:25:SER:O	36:m:28:TYR:N	2.34	0.60
13:N:5:GLN:OE1	13:N:9:ARG:NH1	2.34	0.60
48:V:202:PEE:C1	40:r:191:SER:HB3	2.32	0.60
26:c:62:TYR:OH	26:c:74:ASP:OD1	2.19	0.60
32:i:239:VAL:HG23	54:r:714:CDL:H311	1.83	0.60
1:A:177:TYR:HD2	10:K:93:LEU:HD22	1.66	0.60
34:k:10:MET:HE3	36:m:14:VAL:HG11	1.82	0.60
41:s:102:VAL:HG11	41:s:154:LEU:HD11	1.83	0.60
14:O:70:TYR:HB3	14:O:71:PRO:HD2	1.83	0.60
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.83	0.59
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.84	0.59
35:l:68:TRP:CE3	48:l:720:PEE:H47	2.37	0.59
44:w:176:GLN:NE2	44:w:236:ASP:OD2	2.34	0.59
6:G:115:GLN:O	6:G:119:ILE:HG12	2.01	0.59
49:e:201:PLX:O2	48:l:720:PEE:H9	2.01	0.59
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.83	0.59
54:r:714:CDL:H742	54:r:714:CDL:H271	1.83	0.59
32:i:213:LEU:HD13	54:i:401:CDL:H141	1.84	0.59
44:w:65:ASN:HD21	44:w:238:GLU:HB3	1.65	0.59
6:X:100:VAL:HG22	6:X:142:GLN:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:l:712:CDL:H422	40:r:448:THR:CG2	2.22	0.59
28:e:106:VAL:HG13	40:r:453:MET:HE2	1.84	0.59
2:B:144:ARG:NH1	2:B:146:ASP:OD2	2.34	0.59
7:H:22:GLU:O	7:H:26:ILE:HG12	2.02	0.59
54:l:712:CDL:H581	54:l:712:CDL:H872	1.85	0.59
39:p:95:GLU:OE1	39:p:98:LYS:NZ	2.29	0.59
41:s:62:ARG:HH21	41:s:68:ILE:HB	1.67	0.59
54:V:201:CDL:H611	54:V:201:CDL:H742	1.85	0.59
54:V:201:CDL:H741	54:V:201:CDL:C61	2.33	0.59
12:M:299:ARG:HG2	12:M:300:GLN:HG2	1.84	0.58
12:M:308:ARG:NH2	12:M:578:PRO:O	2.36	0.58
34:k:98:CYS:HB2	35:l:580:GLN:HB2	1.85	0.58
1:A:88:ARG:HG3	1:A:246:GLU:HG2	1.84	0.58
5:F:69:TYR:HE2	5:F:75:LYS:HG3	1.68	0.58
9:J:60:GLY:HA2	51:J:401:NDP:O3B	2.04	0.58
12:M:390:THR:HA	12:M:600:GLU:HG2	1.84	0.58
26:c:153:TYR:OH	43:v:8:ARG:NH1	2.32	0.58
43:v:93:LEU:O	43:v:97:LYS:HG3	2.02	0.58
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.86	0.58
12:M:260:ASN:HD22	12:M:278:HIS:HB2	1.67	0.58
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.85	0.58
17:S:15:CYS:HA	17:S:18:ILE:HD12	1.85	0.58
44:w:59:VAL:HG13	44:w:201:PRO:HA	1.86	0.58
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.42	0.58
3:C:71:CYS:HB3	16:Q:141:TYR:CG	2.39	0.58
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.86	0.58
32:i:278:MET:O	32:i:282:MET:HG3	2.04	0.58
48:U:101:PEE:H20	33:j:106:TRP:CE3	2.39	0.58
6:X:69:SER:OG	6:X:70:ASP:N	2.36	0.58
54:a:201:CDL:H521	48:l:720:PEE:H14	1.83	0.58
33:j:70:ALA:HA	33:j:73:LEU:HD12	1.85	0.58
35:l:66:TRP:HZ3	48:l:720:PEE:H38	1.69	0.58
12:M:336:ASN:O	12:M:336:ASN:ND2	2.37	0.58
13:N:13:GLN:NE2	13:N:33:VAL:HG23	2.19	0.58
16:Q:156:GLU:OE2	16:Q:171:ARG:NH2	2.36	0.58
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.86	0.58
11:L:90:GLY:HA3	15:P:238:PRO:HB2	1.86	0.58
12:M:304:GLN:HG2	12:M:615:LEU:HD12	1.86	0.58
12:M:647:GLU:HB2	12:M:654:VAL:HG21	1.86	0.58
23:Z:26:GLY:N	23:Z:30:GLU:OE2	2.34	0.58
12:M:283:GLU:OE2	12:M:420:LYS:NZ	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:V:202:PEE:H78	40:r:201:MET:HE1	1.77	0.57
6:X:125:GLU:HG2	35:l:439:PRO:HG2	1.84	0.57
40:r:373:ILE:HD11	40:r:444:LEU:HD23	1.86	0.57
19:U:9:LEU:HD11	48:U:101:PEE:H68	1.85	0.57
30:g:12:PRO:HB3	31:h:5:ASP:HB3	1.86	0.57
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.86	0.57
48:m:202:PEE:H52	41:s:104:PHE:HE1	1.70	0.57
44:w:132:GLN:OE1	57:w:401:ADP:N6	2.37	0.57
35:l:559:GLU:O	35:l:563:PRO:HD2	2.04	0.57
48:C:311:PEE:C43	41:s:56:PHE:CD2	2.83	0.57
34:k:5:TYR:O	34:k:9:ILE:HG12	2.04	0.57
43:v:4:HIS:HA	43:v:7:ARG:HE	1.69	0.57
12:M:370:GLU:OE2	12:M:518:ARG:NH2	2.38	0.57
54:l:712:CDL:H351	40:r:361:VAL:HG13	1.85	0.57
36:m:45:LEU:HD23	36:m:50:SER:HA	1.86	0.57
44:w:69:GLY:C	44:w:71:GLY:N	2.55	0.57
1:A:33:GLY:HA2	1:A:294:VAL:HG22	1.86	0.57
8:I:3:SER:O	54:N:202:CDL:HA22	2.05	0.57
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.38	0.57
6:X:155:TYR:HE1	25:b:23:LEU:HB3	1.70	0.57
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.40	0.57
6:G:104:PHE:HA	6:G:108:LEU:HD12	1.86	0.57
32:i:133:TRP:CE3	54:i:401:CDL:C39	2.79	0.57
16:Q:99:MET:HG2	16:Q:109:CYS:HA	1.86	0.57
35:l:290:LEU:O	35:l:523:SER:OG	2.22	0.57
15:P:94:ILE:O	15:P:98:THR:OG1	2.18	0.56
33:j:88:LEU:HD13	41:s:309:ILE:HD12	1.86	0.56
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.88	0.56
21:W:74:LEU:O	21:W:78:GLU:HG3	2.05	0.56
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.87	0.56
54:n:102:CDL:H121	54:n:102:CDL:H762	1.87	0.56
12:M:133:GLN:HG3	12:M:136:GLU:HG3	1.88	0.56
15:P:147:THR:HB	15:P:153:ILE:HD11	1.86	0.56
24:a:115:HIS:NE2	54:a:201:CDL:OB4	2.38	0.56
12:M:591:GLU:HG2	12:M:610:VAL:HG23	1.87	0.56
14:O:198:PRO:O	14:O:202:GLU:HG2	2.06	0.56
35:l:119:LYS:NZ	54:l:712:CDL:OA3	2.37	0.56
24:a:78:THR:OG1	28:e:96:SER:HB2	2.06	0.56
40:r:14:MET:SD	40:r:26:ASN:HB3	2.46	0.56
40:r:225:ILE:HG13	40:r:229:MET:HE2	1.88	0.56
44:w:62:VAL:HG21	44:w:74:ALA:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:THR:HA	14:O:234:LEU:HD11	1.87	0.56
3:C:191:ARG:O	3:C:195:ARG:HG3	2.06	0.56
13:N:7:LEU:O	13:N:11:LEU:HG	2.06	0.56
40:r:19:LYS:HD2	40:r:22:MET:HG3	1.86	0.56
41:s:277:TYR:HE2	48:s:401:PEE:H58	1.70	0.56
54:V:203:CDL:H801	54:V:203:CDL:H842	1.88	0.56
25:b:104:ILE:HD13	27:d:18:PRO:HG3	1.88	0.56
34:k:2:PRO:HD2	34:k:5:TYR:CD2	2.40	0.56
43:v:51:LEU:O	43:v:52:MET:HG3	2.05	0.56
1:A:380:GLY:O	1:A:386:ARG:NH1	2.39	0.56
32:i:62:THR:HG23	32:i:104:MET:HE2	1.88	0.56
22:Y:94:ASP:HB3	22:Y:99:ILE:HB	1.88	0.56
44:w:80:LYS:HE3	44:w:270:VAL:HG21	1.87	0.56
6:G:135:ALA:HA	6:G:138:LEU:HD13	1.87	0.56
44:w:69:GLY:O	44:w:72:ARG:N	2.39	0.56
2:B:64:THR:HG21	21:W:35:MET:HE1	1.88	0.55
48:C:311:PEE:H27	48:C:311:PEE:C36	2.36	0.55
4:E:78:VAL:O	4:E:82:LEU:HG	2.06	0.55
48:V:202:PEE:H40	48:l:718:PEE:H47	1.88	0.55
35:l:566:THR:O	35:l:570:GLN:HG2	2.05	0.55
54:l:712:CDL:H811	54:l:712:CDL:H851	1.87	0.55
1:A:375:LYS:NZ	14:O:33:GLY:O	2.40	0.55
11:L:163:ASN:O	11:L:171:ARG:HA	2.07	0.55
44:w:274:GLU:O	44:w:277:LYS:NZ	2.39	0.55
1:A:66:LYS:NZ	1:A:188:GLY:O	2.39	0.55
14:O:59:ASN:O	14:O:63:ILE:HG12	2.06	0.55
33:j:64:LEU:HD13	36:m:165:VAL:HG22	1.88	0.55
34:k:23:ARG:HD3	36:m:23:LYS:HB2	1.87	0.55
4:E:110:THR:HG21	15:P:220:VAL:HG11	1.88	0.55
12:M:51:GLN:O	12:M:55:LYS:HG2	2.06	0.55
9:J:192:ARG:NH2	9:J:262:THR:OG1	2.39	0.55
33:j:73:LEU:HD13	36:m:55:MET:HE1	1.86	0.55
35:l:464:ALA:O	35:l:468:ILE:HG12	2.07	0.55
48:l:718:PEE:C25	48:l:718:PEE:H34	2.35	0.55
48:m:202:PEE:H7	48:m:202:PEE:O4	2.05	0.55
18:T:119:ARG:HD3	18:T:122:HIS:CD2	2.42	0.55
54:a:201:CDL:OA7	54:a:201:CDL:HA61	2.06	0.55
35:l:562:LEU:HB3	35:l:563:PRO:HD3	1.89	0.55
2:B:76:TYR:HE2	41:s:33:LEU:HB2	1.72	0.55
6:G:75:THR:O	6:G:78:ALA:N	2.39	0.55
14:O:54:ASP:OD1	14:O:55:PHE:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ASN:N	46:A:502:FMN:O1P	2.38	0.55
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.88	0.55
54:V:203:CDL:H322	54:V:203:CDL:C36	2.36	0.55
35:l:11:THR:HG23	35:l:12:LEU:HD12	1.89	0.55
44:w:185:GLU:O	44:w:189:GLU:HG3	2.06	0.55
9:J:238:GLN:N	9:J:326:ASP:OD2	2.36	0.55
40:r:14:MET:O	40:r:18:SER:OG	2.22	0.55
43:v:46:MET:HE2	43:v:56:ARG:HG2	1.89	0.55
11:L:111:LEU:HD11	13:N:126:PRO:HG2	1.89	0.54
15:P:69:LEU:HD22	15:P:96:VAL:HG22	1.89	0.54
16:Q:184:ILE:HG12	16:Q:203:MET:HE3	1.89	0.54
22:Y:51:THR:HG22	22:Y:53:SER:H	1.72	0.54
37:n:50:ARG:HB2	37:n:53:GLU:HB2	1.88	0.54
40:r:398:MET:HA	40:r:398:MET:HE2	1.89	0.54
5:F:46:LYS:HE2	12:M:674:LEU:HD21	1.89	0.54
25:b:99:GLU:OE2	35:l:2:ASN:ND2	2.39	0.54
44:w:116:LYS:NZ	44:w:125:ASP:OD2	2.39	0.54
9:J:211:ASP:O	9:J:215:ASN:ND2	2.40	0.54
13:N:2:GLU:HG3	13:N:4:VAL:HG22	1.89	0.54
44:w:105:ASP:OD1	44:w:106:VAL:N	2.40	0.54
1:A:50:ASP:O	1:A:59:ARG:NH2	2.36	0.54
16:Q:127:LYS:HB3	16:Q:131:GLN:HB3	1.90	0.54
18:T:119:ARG:HD3	18:T:122:HIS:HD2	1.71	0.54
20:V:46:PRO:HB3	20:V:55:ARG:NH2	2.23	0.54
54:a:201:CDL:H211	54:a:201:CDL:C25	2.34	0.54
26:c:161:TYR:O	26:c:183:HIS:NE2	2.38	0.54
35:l:419:THR:HA	35:l:422:TYR:CE2	2.43	0.54
41:s:225:MET:HE2	56:s:403:UQ:H153	1.90	0.54
3:C:50:LEU:HD21	48:C:311:PEE:H27	1.90	0.54
13:N:6:VAL:HG12	13:N:9:ARG:NH2	2.23	0.54
15:P:152:PRO:HB3	15:P:177:PHE:HD2	1.72	0.54
35:l:7:LEU:HD22	35:l:46:LEU:HD11	1.89	0.54
48:l:720:PEE:H5	48:l:720:PEE:P	2.30	0.54
2:B:68:ARG:NH2	21:W:26:PRO:O	2.41	0.54
13:N:4:VAL:HA	13:N:7:LEU:HD12	1.88	0.54
20:V:70:PHE:HD1	20:V:94:GLY:HA2	1.73	0.54
26:c:96:ASP:OD1	26:c:97:LEU:N	2.40	0.54
44:w:132:GLN:CD	57:w:401:ADP:HN62	2.16	0.54
35:l:172:ILE:O	35:l:176:ARG:HG2	2.08	0.54
6:G:83:VAL:O	6:G:87:LEU:HD23	2.08	0.54
20:V:81:ARG:NH2	20:V:88:LEU:HD22	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:4:TYR:HB2	25:b:9:LYS:HE3	1.88	0.54
48:m:202:PEE:H25	48:m:202:PEE:C35	2.37	0.54
15:P:44:ARG:HB3	15:P:45:PRO:CD	2.38	0.54
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.40	0.54
12:M:260:ASN:HD21	12:M:278:HIS:HD2	1.56	0.53
13:N:85:GLU:HB2	13:N:98:PRO:HB3	1.89	0.53
14:O:38:LEU:O	14:O:124:ARG:NH2	2.41	0.53
27:d:28:ASN:HD21	27:d:31:THR:HG23	1.73	0.53
33:j:30:TYR:CE2	41:s:59:GLU:HB2	2.43	0.53
41:s:90:PRO:HD2	41:s:240:ILE:HD13	1.90	0.53
1:A:119:GLU:O	1:A:119:GLU:HG3	2.09	0.53
26:c:159:LYS:NZ	43:v:57:ASP:OD2	2.40	0.53
40:r:251:ASN:HD21	40:r:304:GLN:HE22	1.55	0.53
44:w:66:ILE:HD11	44:w:237:ILE:CD1	2.38	0.53
16:Q:274:ASP:OD1	16:Q:323:ARG:NH1	2.41	0.53
21:W:30:LEU:HD23	21:W:35:MET:HG2	1.90	0.53
16:Q:102:SER:OG	16:Q:107:ARG:NH1	2.42	0.53
27:d:114:GLN:HG3	35:l:203:MET:HG2	1.91	0.53
27:d:144:SER:O	27:d:158:LYS:NZ	2.40	0.53
33:j:73:LEU:O	41:s:160:TYR:OH	2.26	0.53
49:n:101:PLX:O7	49:n:101:PLX:H92	2.07	0.53
12:M:544:VAL:HG23	12:M:565:PHE:HB3	1.90	0.53
44:w:63:ASP:HB3	44:w:241:TYR:CE1	2.44	0.53
7:H:51:ILE:HG22	7:H:55:LYS:HE2	1.90	0.53
12:M:487:THR:OG1	12:M:677:GLN:OE1	2.21	0.53
30:g:36:MET:HE2	32:i:339:MET:HE2	1.90	0.53
13:N:68:MET:CG	13:N:69:ASN:H	2.22	0.53
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.44	0.53
16:Q:68:ASP:O	32:i:49:ASN:ND2	2.42	0.53
16:Q:182:ASN:OD1	16:Q:404:LYS:NZ	2.41	0.53
22:Y:43:ARG:HG3	22:Y:48:PRO:HA	1.91	0.53
54:i:401:CDL:H331	54:i:401:CDL:OA9	2.09	0.53
44:w:216:SER:O	44:w:220:LYS:HG2	2.08	0.53
2:B:99:GLY:O	2:B:169:GLU:HG3	2.09	0.53
12:M:389:THR:O	12:M:390:THR:OG1	2.24	0.53
6:X:123:GLU:HG2	6:X:129:GLU:HA	1.91	0.53
44:w:214:ILE:CG2	44:w:234:LEU:HD13	2.35	0.53
32:i:334:THR:HG21	54:r:714:CDL:H391	1.89	0.53
35:l:86:SER:OG	35:l:262:ARG:NH2	2.42	0.53
35:l:102:GLU:OE2	35:l:456:ARG:NH2	2.32	0.53
9:J:257:ASP:O	9:J:261:LYS:NZ	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:224:ASP:OD2	12:M:291:ARG:NH2	2.35	0.52
16:Q:206:GLU:OE2	16:Q:209:LYS:NZ	2.42	0.52
27:d:26:LEU:HD12	27:d:27:PRO:HD2	1.90	0.52
30:g:36:MET:HE3	30:g:74:GLY:HA2	1.90	0.52
32:i:270:MET:HE1	32:i:282:MET:SD	2.49	0.52
35:l:8:THR:HG23	35:l:82:MET:HE3	1.91	0.52
44:w:63:ASP:OD2	44:w:245:PHE:CZ	2.61	0.52
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.90	0.52
12:M:638:THR:O	12:M:642:VAL:HG23	2.10	0.52
34:k:11:ALA:HB1	36:m:17:PHE:CD2	2.44	0.52
7:H:72:LEU:HD13	7:H:80:VAL:HG11	1.91	0.52
8:I:13:ASN:HD22	8:I:19:ASP:HA	1.74	0.52
24:a:96:ALA:HB2	27:d:61:TYR:CE2	2.45	0.52
44:w:65:ASN:HB3	44:w:214:ILE:CD1	2.39	0.52
11:L:89:SER:O	12:M:59:GLN:NE2	2.41	0.52
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.45	0.52
35:l:5:ALA:HB2	35:l:61:MET:SD	2.49	0.52
35:l:66:TRP:O	35:l:78:LEU:N	2.37	0.52
37:n:30:ARG:O	37:n:33:GLU:HG2	2.10	0.52
12:M:406:ASN:ND2	12:M:688:GLN:O	2.35	0.52
24:a:152:LYS:HD3	30:g:96:VAL:HG21	1.91	0.52
33:j:87:MET:HE1	41:s:309:ILE:HD11	1.91	0.52
41:s:130:ILE:O	41:s:134:ARG:HG3	2.09	0.52
14:O:171:LEU:O	14:O:172:ILE:HD13	2.10	0.52
35:l:27:TYR:O	35:l:115:ASN:ND2	2.36	0.52
1:A:185:ASN:C	1:A:187:CYS:H	2.18	0.52
20:V:95:CYS:HB2	20:V:115:CYS:CA	2.18	0.52
54:V:203:CDL:H822	54:V:203:CDL:H781	1.91	0.52
23:Z:25:GLU:HA	23:Z:30:GLU:OE2	2.10	0.52
34:k:23:ARG:HG2	36:m:23:LYS:HE2	1.91	0.52
36:m:17:PHE:CD1	36:m:20:PHE:HE1	2.27	0.52
41:s:200:LEU:HD11	41:s:285:LEU:HD21	1.90	0.52
17:S:55:SER:O	17:S:64:LYS:NZ	2.43	0.52
32:i:40:MET:HE3	32:i:44:LEU:HD21	1.92	0.52
32:i:220:ILE:HB	32:i:323:MET:HE1	1.92	0.52
32:i:347:ASN:HB3	49:i:705:PLX:H301	1.91	0.52
1:A:102:MET:HG2	1:A:149:MET:HE2	1.91	0.52
6:G:75:THR:O	6:G:76:LEU:C	2.53	0.52
10:K:109:ARG:HH11	10:K:109:ARG:HG3	1.75	0.52
11:L:112:MET:HA	11:L:112:MET:HE2	1.92	0.52
34:k:37:MET:SD	34:k:67:ALA:HB3	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.92	0.52
4:E:39:TRP:O	4:E:43:VAL:HG23	2.10	0.51
7:H:38:ILE:O	7:H:45:ARG:NH1	2.36	0.51
40:r:403:THR:HA	40:r:406:TYR:CE2	2.45	0.51
6:G:90:TYR:OH	6:G:117:GLU:OE1	2.25	0.51
35:l:161:ARG:NH2	39:p:88:GLY:O	2.43	0.51
1:A:213:ILE:HG12	1:A:235:VAL:HG13	1.92	0.51
36:m:125:TRP:HA	36:m:128:TYR:CD2	2.46	0.51
1:A:185:ASN:O	1:A:187:CYS:N	2.43	0.51
35:l:161:ARG:NH1	35:l:238:GLU:OE2	2.40	0.51
2:B:99:GLY:H	2:B:169:GLU:HG2	1.75	0.51
32:i:236:LYS:HD3	32:i:237:MET:HE2	1.92	0.51
54:l:712:CDL:H611	54:l:712:CDL:H811	1.92	0.51
1:A:408:GLU:O	1:A:411:SER:HB3	2.11	0.51
4:E:101:THR:OG1	15:P:219:VAL:O	2.19	0.51
7:H:30:LYS:O	7:H:34:VAL:HG23	2.11	0.51
12:M:382:ARG:HG2	12:M:386:LEU:HD11	1.93	0.51
14:O:236:GLU:HG2	14:O:237:PRO:HD2	1.93	0.51
48:l:718:PEE:H34	48:l:718:PEE:H41	1.91	0.51
44:w:129:TYR:OH	44:w:186:HIS:ND1	2.27	0.51
27:d:60:ARG:NH2	27:d:62:TYR:OH	2.43	0.51
27:d:106:ILE:HG13	27:d:135:VAL:HG21	1.93	0.51
44:w:295:ARG:HA	44:w:298:VAL:HG22	1.92	0.51
44:w:343:TYR:HA	44:w:352:ILE:HD12	1.93	0.51
8:I:8:ILE:HD11	54:N:202:CDL:H142	1.93	0.51
10:K:98:MET:SD	10:K:98:MET:N	2.83	0.51
49:e:201:PLX:H131	54:l:712:CDL:H632	1.93	0.51
3:C:192:ILE:HG13	9:J:87:GLU:HG2	1.92	0.51
8:I:40:LYS:HB3	21:W:7:LYS:H	1.76	0.51
24:a:127:ASP:CG	49:n:101:PLX:H1C2	2.35	0.51
2:B:37:THR:OG1	16:Q:317:ASP:OD1	2.23	0.51
9:J:192:ARG:NH1	9:J:198:ALA:O	2.44	0.51
43:v:27:PRO:HB2	43:v:34:ARG:HE	1.76	0.51
48:C:311:PEE:C42	41:s:56:PHE:HD2	2.22	0.50
21:W:93:GLU:OE1	31:h:92:TYR:OH	2.21	0.50
54:a:201:CDL:H382	27:d:48:ALA:HB2	1.93	0.50
25:b:85:TYR:CE1	48:l:720:PEE:H48	2.45	0.50
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.46	0.50
48:m:202:PEE:O4	48:m:202:PEE:H18	2.11	0.50
39:p:92:GLU:HB3	39:p:95:GLU:HG3	1.92	0.50
13:N:39:VAL:CG2	13:N:50:GLU:HG2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:90:TYR:HE1	23:Z:44:PRO:HB2	1.76	0.50
40:r:299:VAL:O	40:r:303:ILE:HG12	2.10	0.50
12:M:347:ASP:HB3	12:M:594:ALA:HB1	1.92	0.50
12:M:538:ARG:HG2	12:M:538:ARG:HH11	1.77	0.50
35:l:76:LEU:HD21	35:l:196:TRP:HE3	1.76	0.50
54:l:712:CDL:H842	54:l:712:CDL:C64	2.40	0.50
48:l:719:PEE:H7	48:l:719:PEE:H13	1.90	0.50
36:m:61:LEU:HD23	36:m:65:LEU:HD12	1.93	0.50
43:v:39:MET:HE3	43:v:41:ALA:N	2.26	0.50
15:P:119:VAL:HG12	15:P:121:THR:HG22	1.94	0.50
32:i:88:LYS:HD2	32:i:148:SER:OG	2.12	0.50
48:l:718:PEE:C1	48:l:718:PEE:H10	2.42	0.50
36:m:125:TRP:HA	36:m:128:TYR:HD2	1.76	0.50
38:o:3:PHE:CZ	39:p:70:GLU:HG3	2.46	0.50
40:r:103:GLN:HE21	40:r:107:ILE:HD11	1.76	0.50
5:F:44:LEU:HD22	5:F:91:LEU:HD21	1.93	0.50
8:I:8:ILE:CG1	54:N:202:CDL:HA32	2.38	0.50
16:Q:36:GLN:NE2	40:r:135:ARG:O	2.43	0.50
19:U:14:ALA:O	19:U:15:LYS:HG2	2.12	0.50
24:a:66:ARG:NH1	28:e:72:ASP:OD1	2.44	0.50
54:a:201:CDL:HB21	48:l:720:PEE:H51	1.94	0.50
9:J:180:TYR:O	9:J:183:SER:OG	2.28	0.50
19:U:59:ASP:HA	19:U:63:MET:HE2	1.93	0.50
35:l:290:LEU:O	35:l:293:ILE:HG22	2.12	0.50
41:s:21:THR:CG2	41:s:224:PHE:HE1	2.25	0.50
44:w:235:GLN:NE2	44:w:238:GLU:OE2	2.45	0.50
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.93	0.50
14:O:110:MET:O	14:O:114:GLU:HG3	2.12	0.50
26:c:123:PRO:HD2	35:l:525:MET:HE1	1.93	0.50
27:d:110:LEU:HD11	35:l:203:MET:HE2	1.93	0.50
54:l:712:CDL:H331	54:l:712:CDL:OA9	2.10	0.50
40:r:300:ALA:O	40:r:308:SER:HB3	2.12	0.50
1:A:210:THR:HB	1:A:224:ARG:HG2	1.93	0.50
3:C:126:GLU:O	3:C:128:ARG:N	2.45	0.50
3:C:187:GLU:OE2	3:C:189:ARG:NH1	2.45	0.50
20:V:65:ALA:O	20:V:69:ILE:HG12	2.12	0.50
42:u:44:MET:HE3	42:u:48:TRP:CH2	2.47	0.50
42:u:83:THR:HA	42:u:86:TRP:CD1	2.46	0.50
14:O:179:ALA:HB3	14:O:185:MET:SD	2.52	0.50
34:k:4:VAL:O	34:k:8:ILE:HG12	2.11	0.50
35:l:557:TRP:O	35:l:561:ILE:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:3:SER:O	54:N:202:CDL:CA2	2.59	0.49
54:N:202:CDL:C34	54:N:202:CDL:CA7	2.89	0.49
14:O:206:ASP:OD1	14:O:207:GLU:N	2.45	0.49
15:P:125:ARG:HH22	15:P:201:ASP:CG	2.20	0.49
24:a:61:GLY:O	24:a:65:ARG:HG3	2.11	0.49
24:a:168:TRP:CD2	30:g:2:THR:HG23	2.47	0.49
26:c:81:ARG:NE	26:c:85:GLU:OE1	2.42	0.49
26:c:166:LEU:HD22	26:c:169:GLU:OE2	2.12	0.49
15:P:125:ARG:NH2	15:P:201:ASP:OD1	2.44	0.49
39:p:16:VAL:HG22	39:p:64:LEU:HD13	1.93	0.49
13:N:73:THR:HG22	13:N:73:THR:O	2.11	0.49
54:V:203:CDL:H832	54:V:203:CDL:C79	2.18	0.49
41:s:96:ILE:HG22	41:s:98:MET:HG3	1.94	0.49
44:w:69:GLY:C	44:w:71:GLY:H	2.17	0.49
2:B:44:ARG:HH21	8:I:112:TYR:HB3	1.77	0.49
54:V:203:CDL:C79	54:V:203:CDL:C83	2.86	0.49
43:v:60:ALA:O	43:v:64:ILE:HG12	2.12	0.49
16:Q:431:HIS:O	16:Q:454:GLN:NE2	2.45	0.49
40:r:204:MET:HG3	40:r:209:LEU:HB2	1.94	0.49
40:r:251:ASN:HD21	40:r:304:GLN:NE2	2.11	0.49
26:c:33:THR:OG1	26:c:35:ASP:OD1	2.26	0.49
34:k:45:THR:HG23	36:m:52:LEU:HD13	1.95	0.49
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.93	0.49
44:w:63:ASP:O	44:w:206:TYR:HD1	1.95	0.49
2:B:96:ARG:O	16:Q:219:GLY:HA3	2.13	0.49
4:E:117:ASP:OD1	4:E:120:SER:OG	2.15	0.49
12:M:149:ASP:OD2	12:M:150:ARG:NH1	2.46	0.49
15:P:64:TYR:OH	15:P:103:HIS:NE2	2.35	0.49
16:Q:176:GLU:OE2	16:Q:311:TYR:OH	2.18	0.49
32:i:84:TRP:HH2	34:k:59:MET:HE2	1.77	0.49
35:l:173:LEU:HD13	40:r:405:LEU:HD21	1.94	0.49
41:s:170:GLU:OE2	42:u:98:ARG:NH2	2.43	0.49
3:C:161:ILE:HG13	3:C:180:LEU:HB2	1.94	0.49
9:J:129:LEU:HD23	9:J:167:ILE:HG13	1.95	0.49
9:J:145:PHE:CD1	9:J:184:LYS:HE3	2.46	0.49
41:s:235:ASN:ND2	41:s:266:LEU:HB3	2.28	0.49
44:w:64:GLY:N	44:w:70:LYS:HD3	2.27	0.49
35:l:49:VAL:HB	35:l:50:PRO:HD3	1.94	0.49
38:o:48:LEU:HB3	39:p:166:LEU:HD13	1.95	0.49
40:r:271:MET:HE2	40:r:271:MET:HA	1.94	0.49
41:s:86:TRP:NE1	41:s:233:MET:HB2	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:l:718:PEE:H10	48:l:718:PEE:H2	1.94	0.49
37:n:13:VAL:HG13	40:r:14:MET:HA	1.95	0.49
44:w:213:GLU:HG2	44:w:217:ARG:HD2	1.93	0.49
7:H:69:GLU:HG2	7:H:77:ILE:HG12	1.95	0.48
39:p:100:PRO:HG3	40:r:419:TYR:CE1	2.47	0.48
1:A:182:ILE:HD11	1:A:193:PHE:HD2	1.78	0.48
5:F:37:ILE:HD12	5:F:37:ILE:H	1.78	0.48
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.95	0.48
48:V:202:PEE:H35	40:r:159:PRO:HG2	1.94	0.48
48:V:207:PEE:O4	48:V:207:PEE:H10	2.13	0.48
48:l:718:PEE:H37	48:l:718:PEE:H60	1.95	0.48
44:w:170:LEU:HD21	44:w:184:VAL:HG23	1.94	0.48
12:M:171:THR:HG23	12:M:173:MET:SD	2.52	0.48
33:j:49:LEU:N	33:j:50:PRO:HD2	2.28	0.48
35:l:105:MET:HB2	35:l:449:LEU:HD13	1.95	0.48
36:m:25:SER:O	36:m:27:ILE:N	2.46	0.48
38:o:113:GLU:O	38:o:117:GLN:HG2	2.13	0.48
44:w:110:GLY:HA2	44:w:134:TRP:CD2	2.47	0.48
14:O:100:LYS:O	14:O:104:ILE:HG12	2.13	0.48
35:l:221:ALA:HA	35:l:226:GLN:HG2	1.95	0.48
1:A:115:VAL:HG21	1:A:142:CYS:SG	2.53	0.48
3:C:67:PHE:HE2	3:C:103:MET:HE2	1.79	0.48
48:C:311:PEE:H49	33:j:28:ASN:HD22	1.78	0.48
11:L:174:THR:HG23	14:O:111:ARG:HD2	1.94	0.48
13:N:120:THR:HG22	13:N:122:GLN:H	1.78	0.48
16:Q:84:PHE:HE2	16:Q:444:LEU:HD11	1.78	0.48
20:V:108:TYR:CE2	54:V:203:CDL:OA6	2.66	0.48
31:h:88:LYS:HB3	31:h:88:LYS:HE2	1.63	0.48
2:B:47:SER:OG	2:B:49:ASP:OD1	2.24	0.48
11:L:158:LYS:NZ	12:M:69:LEU:O	2.30	0.48
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.43	0.48
27:d:159:GLN:O	27:d:163:MET:HG3	2.12	0.48
28:e:70:ASN:O	28:e:73:SER:HB2	2.14	0.48
33:j:13:LEU:HD13	41:s:10:ILE:HG21	1.96	0.48
34:k:25:HIS:O	34:k:28:SER:N	2.40	0.48
9:J:179:ARG:O	9:J:183:SER:OG	2.30	0.48
14:O:137:THR:HG22	14:O:138:THR:H	1.79	0.48
16:Q:65:PRO:HB2	16:Q:67:ASN:O	2.13	0.48
21:W:66:GLU:OE1	42:u:123:GLY:N	2.43	0.48
6:X:93:ILE:HD11	6:X:110:LEU:HD11	1.95	0.48
24:a:83:ALA:HA	54:a:201:CDL:H161	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:a:201:CDL:H772	54:a:201:CDL:H201	1.94	0.48
48:l:719:PEE:C11	48:l:719:PEE:C3	2.85	0.48
43:v:106:ARG:O	43:v:110:GLN:HG2	2.14	0.48
48:C:311:PEE:H72	41:s:56:PHE:CE2	2.48	0.48
15:P:186:ARG:NH1	15:P:189:THR:OG1	2.39	0.48
25:b:106:PRO:HA	25:b:117:ILE:HG22	1.96	0.48
33:j:15:SER:HA	41:s:76:ILE:HD12	1.95	0.48
40:r:14:MET:HE3	40:r:14:MET:HB3	1.83	0.48
44:w:148:GLU:OE1	44:w:301:LYS:NZ	2.40	0.48
6:G:75:THR:HB	6:G:156:GLU:OE1	2.14	0.48
9:J:163:LYS:NZ	9:J:253:ILE:O	2.42	0.48
13:N:73:THR:HG22	13:N:77:VAL:HG12	1.95	0.48
21:W:114:THR:OG1	42:u:143:HIS:ND1	2.35	0.48
54:a:201:CDL:H191	54:a:201:CDL:H732	1.95	0.48
32:i:222:SER:O	32:i:224:ALA:N	2.47	0.48
41:s:277:TYR:HE2	48:s:401:PEE:C36	2.27	0.48
42:u:18:VAL:HG12	42:u:20:VAL:HG22	1.96	0.48
36:m:17:PHE:O	36:m:21:SER:HB2	2.14	0.48
44:w:58:LYS:HZ3	44:w:278:CYS:HB2	1.79	0.48
9:J:127:ILE:HD11	9:J:253:ILE:HD11	1.95	0.47
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.49	0.47
32:i:321:LYS:NZ	54:i:401:CDL:OA4	2.46	0.47
42:u:114:LYS:HB2	42:u:115:LEU:HD12	1.95	0.47
1:A:109:ARG:HG2	11:L:166:TRP:CD1	2.49	0.47
5:F:71:PHE:CD1	12:M:362:ASP:HB2	2.49	0.47
7:H:38:ILE:HB	7:H:45:ARG:HD2	1.94	0.47
28:e:144:PRO:HA	28:e:147:ILE:HD12	1.96	0.47
32:i:335:LEU:HD21	54:r:714:CDL:H402	1.96	0.47
33:j:95:LEU:HD23	33:j:98:LEU:HD23	1.96	0.47
35:l:78:LEU:HD11	54:l:712:CDL:H251	1.95	0.47
35:l:152:PHE:HB2	35:l:172:ILE:HD11	1.95	0.47
2:B:98:ARG:NH2	16:Q:224:ALA:O	2.44	0.47
5:F:23:LEU:O	5:F:57:GLU:HA	2.14	0.47
16:Q:70:ASP:OD2	32:i:51:ARG:NH1	2.48	0.47
26:c:108:ASP:HB3	26:c:111:MET:HE2	1.96	0.47
31:h:103:ASP:OD1	31:h:103:ASP:O	2.32	0.47
44:w:132:GLN:HE22	57:w:401:ADP:N6	2.12	0.47
1:A:385:CYS:HB3	45:A:501:SF4:S2	2.54	0.47
3:C:50:LEU:HD23	48:C:311:PEE:H26	1.92	0.47
21:W:128:ARG:NH1	31:h:102:GLU:OE1	2.38	0.47
25:b:85:TYR:CD1	48:l:720:PEE:H48	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:20:VAL:HG11	32:i:137:ALA:HB1	1.97	0.47
35:l:166:THR:CG2	48:l:719:PEE:H2	2.44	0.47
5:F:42:VAL:HG23	12:M:671:LEU:CD1	2.44	0.47
16:Q:140:ASP:OD2	16:Q:143:SER:OG	2.25	0.47
24:a:187:PRO:HA	42:u:48:TRP:CD1	2.49	0.47
27:d:164:LEU:HD12	28:e:149:LEU:HD22	1.97	0.47
33:j:17:LEU:HA	33:j:20:ILE:HG12	1.96	0.47
33:j:53:MET:HG3	33:j:57:LEU:HD23	1.95	0.47
35:l:372:ALA:HA	35:l:458:LEU:HD21	1.97	0.47
18:T:47:ASP:O	18:T:52:ARG:NH1	2.47	0.47
29:f:47:THR:HG23	30:g:65:LEU:HD22	1.96	0.47
32:i:40:MET:HE1	32:i:129:LEU:HD23	1.97	0.47
39:p:120:ALA:O	39:p:124:GLN:HG2	2.13	0.47
41:s:85:MET:SD	41:s:108:MET:HB2	2.55	0.47
1:A:98:LYS:HA	1:A:101:PHE:HD2	1.80	0.47
3:C:126:GLU:HB2	41:s:59:GLU:OE1	2.15	0.47
4:E:98:LYS:HB3	4:E:102:HIS:HB2	1.96	0.47
4:E:98:LYS:HE2	4:E:102:HIS:HB3	1.96	0.47
9:J:37:HIS:CE1	18:T:49:ASP:HA	2.49	0.47
12:M:266:ARG:HB3	12:M:271:MET:HE3	1.96	0.47
54:N:202:CDL:C32	54:N:202:CDL:C54	2.88	0.47
20:V:81:ARG:HH22	20:V:88:LEU:HD22	1.78	0.47
54:V:201:CDL:C74	54:V:201:CDL:C61	2.88	0.47
25:b:14:GLN:NE2	39:p:157:ALA:HB3	2.26	0.47
29:f:63:LYS:O	29:f:67:LEU:HD13	2.15	0.47
34:k:58:MET:SD	36:m:146:LEU:HA	2.55	0.47
41:s:62:ARG:HH11	41:s:64:ALA:HA	1.79	0.47
41:s:66:SER:OG	41:s:122:ALA:O	2.17	0.47
44:w:161:ARG:HD3	44:w:241:TYR:OH	2.14	0.47
32:i:203:LEU:HB2	32:i:347:ASN:HD21	1.78	0.47
35:l:292:ALA:HB2	35:l:304:PHE:HB3	1.97	0.47
1:A:151:ALA:O	1:A:191:TYR:OH	2.25	0.47
2:B:98:ARG:HB3	2:B:169:GLU:CD	2.39	0.47
6:X:75:THR:OG1	6:X:156:GLU:O	2.25	0.47
54:n:102:CDL:H781	54:n:102:CDL:H752	1.62	0.47
40:r:122:PHE:CZ	40:r:206:LYS:HD3	2.49	0.47
43:v:93:LEU:HA	43:v:96:VAL:HG22	1.97	0.47
1:A:134:ASP:N	1:A:134:ASP:OD1	2.47	0.47
5:F:18:GLU:OE1	5:F:68:ARG:NH1	2.48	0.47
16:Q:196:ALA:O	16:Q:197:MET:HG2	2.14	0.47
25:b:13:GLN:HA	25:b:16:ARG:HH11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:81:ILE:HG23	48:l:720:PEE:H58	1.97	0.47
27:d:82:ILE:HG23	27:d:83:LEU:HD22	1.96	0.47
35:l:450:LEU:O	35:l:454:ILE:HG12	2.14	0.47
44:w:86:PHE:HB2	44:w:159:LEU:HD23	1.96	0.47
4:E:16:SER:HA	11:L:54:ALA:HA	1.97	0.46
54:N:202:CDL:H312	54:N:202:CDL:C52	2.31	0.46
17:S:1:MET:HB2	17:S:3:PHE:CE2	2.50	0.46
22:Y:52:ARG:O	22:Y:56:ILE:HG23	2.15	0.46
39:p:132:SER:HB2	39:p:163:LEU:HD13	1.97	0.46
40:r:281:ASP:OD1	40:r:340:ARG:HG2	2.16	0.46
44:w:65:ASN:HB3	44:w:214:ILE:HD11	1.97	0.46
1:A:177:TYR:CD2	10:K:93:LEU:HD22	2.49	0.46
8:I:12:ARG:HD3	8:I:20:LEU:HD22	1.98	0.46
9:J:213:PHE:CD1	9:J:214:LEU:HD12	2.47	0.46
12:M:251:ILE:HB	12:M:606:THR:HG22	1.96	0.46
49:V:205:PLX:H191	40:r:201:MET:HE1	1.97	0.46
6:X:143:GLU:OE1	25:b:9:LYS:HE2	2.14	0.46
25:b:24:LYS:O	25:b:27:GLU:HG3	2.15	0.46
35:l:245:ALA:O	35:l:249:SER:OG	2.24	0.46
2:B:114:ILE:HD12	12:M:130:ILE:HG23	1.97	0.46
12:M:29:SER:OG	12:M:30:ASN:N	2.48	0.46
12:M:445:LEU:HD22	12:M:460:HIS:HE1	1.80	0.46
41:s:233:MET:HE3	41:s:233:MET:HB3	1.78	0.46
19:U:9:LEU:CD1	48:U:101:PEE:H68	2.45	0.46
30:g:7:ARG:NH1	30:g:91:ASP:OD1	2.48	0.46
34:k:80:MET:HE3	36:m:172:THR:HA	1.98	0.46
54:n:102:CDL:C58	54:n:102:CDL:C54	2.86	0.46
43:v:80:CYS:HB3	43:v:83:GLU:OE1	2.16	0.46
1:A:65:THR:OG1	1:A:140:GLU:OE1	2.33	0.46
14:O:168:LEU:HB3	14:O:169:PHE:HD1	1.81	0.46
19:U:38:TYR:HB2	41:s:310:MET:O	2.16	0.46
20:V:29:GLY:O	20:V:63:SER:OG	2.33	0.46
22:Y:39:HIS:NE2	23:Z:10:GLY:HA2	2.31	0.46
41:s:87:VAL:N	41:s:88:PRO:CD	2.74	0.46
2:B:200:GLU:HG3	13:N:88:ARG:HB2	1.98	0.46
12:M:36:VAL:HB	12:M:56:VAL:HG21	1.98	0.46
54:V:201:CDL:H532	35:l:577:VAL:HA	1.96	0.46
35:l:331:MET:CE	35:l:465:GLY:HA2	2.46	0.46
35:l:529:TYR:HB3	35:l:530:PRO:HD3	1.98	0.46
35:l:581:LYS:HB3	35:l:583:LEU:HD23	1.98	0.46
39:p:63:LEU:C	39:p:65:ARG:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:74:LEU:HD23	6:G:74:LEU:N	2.24	0.46
8:I:13:ASN:ND2	8:I:20:LEU:H	2.14	0.46
25:b:86:LEU:HD11	35:l:9:LEU:HD12	1.97	0.46
25:b:93:LYS:HE2	25:b:93:LYS:HB2	1.73	0.46
28:e:104:THR:CG2	49:n:101:PLX:H212	2.45	0.46
35:l:33:PRO:HB2	35:l:105:MET:HE3	1.98	0.46
35:l:592:LEU:O	35:l:596:MET:HG3	2.15	0.46
42:u:69:ASP:O	42:u:73:GLN:HG3	2.16	0.46
44:w:248:GLU:O	44:w:251:GLU:HG2	2.16	0.46
8:I:13:ASN:ND2	8:I:19:ASP:HA	2.30	0.46
22:Y:65:MET:SD	35:l:375:ILE:HG12	2.55	0.46
24:a:168:TRP:HB3	30:g:2:THR:O	2.16	0.46
26:c:40:PRO:O	26:c:74:ASP:HB2	2.15	0.46
40:r:41:LEU:O	40:r:44:GLN:NE2	2.49	0.46
13:N:4:VAL:O	13:N:8:ARG:HG3	2.15	0.46
19:U:9:LEU:HD11	48:U:101:PEE:C41	2.46	0.46
32:i:72:MET:HE3	32:i:76:ILE:HG13	1.98	0.46
54:l:713:CDL:H421	54:l:713:CDL:H391	1.64	0.46
36:m:170:GLU:HG3	36:m:173:ARG:HH21	1.81	0.46
41:s:92:PRO:HG3	41:s:252:PRO:CB	2.46	0.46
44:w:214:ILE:CG2	44:w:215:GLN:N	2.79	0.46
44:w:258:TYR:CE2	44:w:269:VAL:HG22	2.51	0.46
5:F:68:ARG:NH2	12:M:364:ASP:OD1	2.50	0.45
5:F:90:THR:HA	5:F:93:ASN:HD22	1.80	0.45
12:M:382:ARG:HE	12:M:527:ASP:CG	2.24	0.45
12:M:445:LEU:HD22	12:M:460:HIS:CE1	2.51	0.45
20:V:8:LYS:N	20:V:8:LYS:HD2	2.31	0.45
6:X:119:ILE:HG21	6:X:135:ALA:HB1	1.98	0.45
26:c:55:TYR:OH	26:c:74:ASP:O	2.17	0.45
41:s:22:LEU:HD12	41:s:22:LEU:O	2.15	0.45
41:s:26:LYS:HE2	41:s:37:PRO:O	2.16	0.45
42:u:83:THR:HA	42:u:86:TRP:NE1	2.31	0.45
1:A:116:ASN:O	1:A:245:VAL:HG23	2.16	0.45
8:I:4:ALA:O	8:I:9:GLN:NE2	2.38	0.45
9:J:166:HIS:HB3	9:J:200:ILE:HD13	1.97	0.45
26:c:165:ASP:O	26:c:170:ARG:NH2	2.48	0.45
27:d:142:ARG:NH1	28:e:138:GLU:O	2.42	0.45
28:e:119:ARG:O	28:e:123:GLU:HG3	2.15	0.45
35:l:480:THR:HG21	43:v:91:GLU:HB2	1.97	0.45
40:r:74:PRO:O	40:r:78:MET:HG3	2.16	0.45
1:A:36:LYS:HB2	1:A:39:ASP:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:PRO:O	1:A:238:CYS:HB3	2.17	0.45
9:J:207:PHE:HB2	9:J:214:LEU:HD13	1.99	0.45
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	1.97	0.45
17:S:43:TYR:CZ	21:W:68:ARG:HG3	2.52	0.45
21:W:89:GLU:OE2	21:W:128:ARG:NH2	2.37	0.45
36:m:166:VAL:O	36:m:170:GLU:OE1	2.33	0.45
39:p:76:HIS:O	39:p:78:GLN:N	2.49	0.45
7:H:76:GLN:O	7:H:79:GLU:N	2.48	0.45
10:K:106:GLN:HB2	10:K:110:HIS:CD2	2.52	0.45
13:N:97:PRO:HG2	13:N:100:THR:HG23	1.97	0.45
32:i:313:MET:HE2	32:i:313:MET:HB3	1.79	0.45
34:k:44:SER:O	34:k:48:ILE:HG12	2.17	0.45
41:s:306:SER:O	41:s:310:MET:HG3	2.17	0.45
1:A:85:LEU:HD21	1:A:247:THR:HG23	1.98	0.45
9:J:167:ILE:HD13	9:J:201:ILE:HB	1.99	0.45
12:M:129:PRO:O	12:M:241:ARG:NH2	2.50	0.45
14:O:215:LYS:HA	14:O:215:LYS:HD2	1.83	0.45
16:Q:236:LEU:HD22	16:Q:240:LEU:HD23	1.99	0.45
18:T:60:LYS:HG2	18:T:62:VAL:HG23	1.99	0.45
27:d:99:ASP:OD2	27:d:142:ARG:NH2	2.49	0.45
28:e:128:TYR:O	28:e:132:ASN:ND2	2.41	0.45
40:r:12:LEU:HB2	40:r:13:PRO:HD3	1.97	0.45
40:r:206:LYS:HB3	40:r:206:LYS:HE2	1.70	0.45
5:F:30:SER:OG	5:F:63:PRO:HG3	2.16	0.45
25:b:123:PHE:HD2	43:v:40:VAL:HG11	1.82	0.45
34:k:38:LEU:O	34:k:42:ILE:HG12	2.17	0.45
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.49	0.45
8:I:96:THR:HB	8:I:97:PRO:HD2	1.99	0.45
12:M:478:SER:O	12:M:482:GLN:HG2	2.16	0.45
14:O:164:THR:CG2	14:O:169:PHE:H	2.29	0.45
16:Q:397:TYR:OH	16:Q:406:GLU:OE2	2.34	0.45
22:Y:68:TRP:CZ2	22:Y:72:ARG:HD2	2.52	0.45
32:i:222:SER:O	32:i:222:SER:OG	2.32	0.45
54:l:712:CDL:H311	54:l:712:CDL:H762	1.98	0.45
54:n:102:CDL:H741	54:n:102:CDL:H712	1.76	0.45
40:r:457:PRO:HG2	40:r:458:LEU:HD12	1.99	0.45
44:w:66:ILE:HD12	44:w:234:LEU:HD21	1.98	0.45
44:w:180:ARG:NH2	44:w:182:GLN:OE1	2.50	0.45
1:A:184:LYS:HD3	10:K:98:MET:HE1	1.98	0.45
9:J:84:TYR:O	9:J:84:TYR:CG	2.70	0.45
13:N:14:VAL:HA	13:N:23:TYR:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:124:LEU:HD11	48:V:202:PEE:H58	1.98	0.45
54:V:201:CDL:H512	35:l:580:GLN:HE22	1.82	0.45
21:W:68:ARG:CZ	21:W:72:MET:HE2	2.46	0.45
23:Z:13:LYS:HD2	23:Z:13:LYS:HA	1.75	0.45
40:r:112:ALA:HB1	40:r:118:PHE:HB2	1.98	0.45
1:A:380:GLY:HA2	1:A:386:ARG:HB2	1.99	0.45
3:C:188:LYS:HD3	3:C:191:ARG:HD3	1.98	0.45
12:M:341:ILE:HG13	12:M:545:LEU:HD11	1.99	0.45
14:O:198:PRO:O	14:O:201:ILE:HG22	2.17	0.45
16:Q:372:LYS:NZ	18:T:94:GLY:O	2.39	0.45
17:S:48:MET:HE1	21:W:143:TYR:CZ	2.51	0.45
23:Z:19:TYR:CZ	23:Z:20:LYS:HE2	2.51	0.45
25:b:32:GLU:HG3	39:p:115:TYR:HA	1.99	0.45
25:b:87:LYS:NZ	25:b:88:TYR:OH	2.45	0.45
32:i:250:SER:O	32:i:259:GLY:HA3	2.17	0.45
54:l:713:CDL:H622	54:l:713:CDL:H591	1.50	0.45
15:P:44:ARG:HB3	15:P:45:PRO:HD3	1.98	0.45
33:j:104:TYR:O	33:j:108:GLN:HG2	2.17	0.45
40:r:116:ILE:HG13	42:u:168:PHE:CD1	2.52	0.45
40:r:357:THR:O	40:r:361:VAL:HG23	2.16	0.45
41:s:248:ASP:OD2	41:s:251:THR:HG22	2.17	0.45
44:w:246:LEU:N	44:w:247:PRO:CD	2.79	0.45
1:A:121:GLU:HG3	1:A:122:PRO:CD	2.47	0.44
6:G:123:GLU:OE1	6:G:129:GLU:HA	2.16	0.44
9:J:195:PHE:HB3	9:J:198:ALA:HB2	1.99	0.44
12:M:278:HIS:CE1	12:M:280:ASP:HB2	2.52	0.44
6:X:134:ASP:HB3	6:X:147:TYR:CE2	2.52	0.44
28:e:58:ASP:OD2	44:w:326:ARG:NE	2.38	0.44
31:h:2:PRO:HA	32:i:140:SER:HB2	1.99	0.44
35:l:174:TYR:CD2	35:l:232:TRP:HB3	2.52	0.44
39:p:26:HIS:CD2	39:p:79:PRO:HB3	2.52	0.44
44:w:180:ARG:NH1	44:w:316:GLU:OE2	2.47	0.44
8:I:110:GLN:NE2	21:W:22:LYS:HD2	2.32	0.44
12:M:128:CYS:SG	12:M:140:GLN:NE2	2.83	0.44
22:Y:61:PHE:HA	22:Y:64:THR:HG22	1.99	0.44
30:g:85:TYR:CZ	32:i:344:SER:HB3	2.52	0.44
35:l:37:LYS:HD3	35:l:98:TRP:HE1	1.81	0.44
35:l:190:LEU:HD22	40:r:383:THR:HG21	1.99	0.44
40:r:418:LYS:HE2	40:r:419:TYR:CE2	2.52	0.44
54:r:714:CDL:H392	54:r:714:CDL:H362	1.49	0.44
1:A:116:ASN:ND2	1:A:207:GLY:O	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:LEU:HB2	41:s:272:TRP:CZ2	2.52	0.44
13:N:85:GLU:HG2	13:N:86:TRP:H	1.83	0.44
16:Q:393:PRO:HA	16:Q:413:SER:O	2.18	0.44
26:c:80:ASP:HA	26:c:106:HIS:HE2	1.81	0.44
28:e:84:LEU:HG	28:e:88:ARG:NH1	2.33	0.44
32:i:254:LEU:O	32:i:257:LEU:HB2	2.17	0.44
35:l:338:MET:HE2	35:l:338:MET:HB3	1.91	0.44
4:E:56:VAL:HG12	4:E:60:ARG:HD2	1.98	0.44
9:J:111:LYS:HE3	9:J:139:PHE:CE1	2.52	0.44
15:P:103:HIS:CD2	15:P:105:ASN:HB2	2.52	0.44
16:Q:150:ALA:HB2	16:Q:400:ILE:HG12	1.99	0.44
23:Z:49:GLU:OE2	39:p:34:ARG:HB3	2.16	0.44
25:b:81:ILE:HG23	48:l:720:PEE:C36	2.47	0.44
28:e:114:MET:HB3	28:e:117:TRP:HB3	1.98	0.44
32:i:338:PRO:HG3	54:n:102:CDL:H601	1.99	0.44
49:C:312:PLX:H311	49:C:312:PLX:H281	1.71	0.44
26:c:117:VAL:HG21	35:l:539:TYR:HB2	1.99	0.44
37:n:26:TYR:CZ	37:n:30:ARG:HD3	2.53	0.44
41:s:81:LEU:O	41:s:85:MET:HG2	2.17	0.44
4:E:24:ASP:OD1	4:E:24:ASP:N	2.51	0.44
9:J:188:GLU:C	9:J:188:GLU:CD	2.85	0.44
10:K:106:GLN:HB2	10:K:110:HIS:HD2	1.82	0.44
13:N:13:GLN:HE21	13:N:33:VAL:C	2.26	0.44
20:V:35:ILE:HG22	54:V:201:CDL:H761	1.98	0.44
1:A:154:ALA:HB2	1:A:193:PHE:CZ	2.53	0.44
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.53	0.44
10:K:79:HIS:ND1	14:O:215:LYS:HE3	2.31	0.44
13:N:26:VAL:HG13	13:N:33:VAL:HG12	1.99	0.44
26:c:32:VAL:HG13	38:o:61:GLU:OE1	2.17	0.44
26:c:122:THR:OG1	26:c:124:VAL:O	2.29	0.44
32:i:256:PRO:HB2	54:n:102:CDL:H612	2.00	0.44
35:l:65:ASN:OD1	35:l:66:TRP:N	2.48	0.44
38:o:4:PRO:HD2	39:p:73:TYR:CE2	2.53	0.44
43:v:34:ARG:NH1	43:v:36:GLU:OE1	2.51	0.44
1:A:121:GLU:HB2	47:A:503:NAI:C3N	2.48	0.44
1:A:325:PRO:HD2	1:A:347:THR:HA	2.00	0.44
2:B:179:THR:OG1	2:B:182:GLU:OE2	2.34	0.44
5:F:27:SER:O	5:F:34:ARG:NH2	2.51	0.44
16:Q:332:CYS:O	16:Q:336:GLU:HG3	2.18	0.44
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.99	0.44
19:U:26:GLY:HA3	48:U:101:PEE:H37	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:113:ALA:CB	48:V:207:PEE:H53	2.47	0.44
54:V:203:CDL:OB7	38:o:82:PRO:O	2.35	0.44
49:V:205:PLX:H1C3	49:V:205:PLX:H22	1.81	0.44
32:i:18:MET:HE2	32:i:18:MET:HA	1.99	0.44
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.99	0.44
48:m:202:PEE:H18	48:m:202:PEE:H24	1.87	0.44
37:n:17:VAL:HB	37:n:18:PRO:HD3	2.00	0.44
39:p:150:ARG:HD2	39:p:150:ARG:HA	1.85	0.44
41:s:141:SER:HB3	41:s:289:LEU:HD22	1.98	0.44
42:u:38:LYS:HB3	42:u:39:PRO:HD3	1.99	0.44
44:w:209:VAL:HG22	44:w:260:ALA:HB2	2.00	0.44
1:A:123:GLY:N	14:O:180:CYS:SG	2.85	0.44
12:M:250:SER:OG	12:M:251:ILE:N	2.44	0.44
48:V:202:PEE:C46	40:r:201:MET:HE1	2.42	0.44
54:V:203:CDL:H873	40:r:264:LEU:HD21	2.00	0.44
48:V:207:PEE:C4	48:V:207:PEE:C1	2.85	0.44
32:i:72:MET:HE3	32:i:76:ILE:CG1	2.47	0.44
32:i:270:MET:HE3	32:i:279:PRO:HG3	2.00	0.44
35:l:316:THR:OG1	35:l:395:ILE:HD12	2.17	0.44
41:s:293:PHE:O	41:s:297:THR:OG1	2.23	0.44
43:v:83:GLU:OE1	43:v:83:GLU:N	2.39	0.44
3:C:66:THR:HG21	3:C:76:MET:HE2	2.00	0.43
8:I:28:TYR:O	8:I:31:ILE:HG12	2.18	0.43
11:L:115:SER:HB2	12:M:267:THR:HB	2.00	0.43
12:M:161:GLU:OE1	14:O:42:ARG:NH2	2.51	0.43
16:Q:271:ARG:HD2	16:Q:271:ARG:HA	1.77	0.43
27:d:37:PHE:CE2	35:l:3:PRO:HB3	2.53	0.43
35:l:554:ASP:OD2	40:r:288:TYR:OH	2.32	0.43
37:n:17:VAL:HG21	40:r:30:HIS:CG	2.53	0.43
54:n:102:CDL:H601	54:n:102:CDL:H572	1.75	0.43
42:u:16:GLN:O	42:u:68:LEU:HD11	2.18	0.43
42:u:44:MET:HB3	42:u:48:TRP:CZ3	2.48	0.43
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.71	0.43
9:J:88:PRO:O	9:J:91:THR:N	2.47	0.43
9:J:217:PHE:HZ	9:J:322:VAL:HG21	1.82	0.43
9:J:271:TYR:OH	9:J:346:GLU:OE1	2.30	0.43
20:V:39:TYR:OH	35:l:594:THR:HG22	2.18	0.43
54:V:201:CDL:H322	35:l:576:MET:HE1	1.99	0.43
24:a:126:TYR:C	24:a:127:ASP:OD1	2.61	0.43
32:i:30:TRP:O	32:i:34:GLU:HG2	2.17	0.43
35:l:383:MET:SD	35:l:384:PRO:HD2	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:14:LYS:O	42:u:61:LYS:NZ	2.51	0.43
9:J:85:ARG:HD2	51:J:401:NDP:C2A	2.48	0.43
9:J:116:ILE:O	9:J:120:VAL:HG22	2.18	0.43
13:N:78:ASP:OD2	13:N:80:SER:OG	2.26	0.43
24:a:126:TYR:O	49:n:101:PLX:C1B	2.63	0.43
32:i:280:THR:O	32:i:284:MET:HG2	2.19	0.43
3:C:184:ILE:O	3:C:187:GLU:HG2	2.18	0.43
4:E:17:VAL:O	11:L:53:ILE:HD12	2.18	0.43
10:K:79:HIS:CE1	14:O:215:LYS:HB3	2.53	0.43
10:K:87:LEU:HD11	14:O:66:ILE:HD11	2.00	0.43
12:M:389:THR:HG21	12:M:473:MET:SD	2.59	0.43
16:Q:63:PRO:HA	16:Q:64:PRO:HD3	1.93	0.43
28:e:97:ILE:O	28:e:101:LEU:HB2	2.17	0.43
32:i:226:THR:HG23	32:i:229:SER:H	1.84	0.43
35:l:78:LEU:HA	35:l:139:GLN:HE21	1.82	0.43
36:m:129:ASP:OD1	36:m:129:ASP:N	2.47	0.43
54:n:102:CDL:H171	54:n:102:CDL:H201	1.84	0.43
3:C:188:LYS:HG3	3:C:188:LYS:O	2.19	0.43
6:G:75:THR:O	6:G:77:GLU:N	2.51	0.43
6:G:80:LYS:HG2	6:G:145:VAL:HG21	1.99	0.43
7:H:82:LEU:HA	7:H:85:GLU:OE2	2.18	0.43
14:O:63:ILE:HD12	14:O:82:VAL:HG22	1.99	0.43
16:Q:83:ASN:ND2	16:Q:96:ARG:HH21	2.17	0.43
25:b:88:TYR:CZ	27:d:49:ARG:HG2	2.54	0.43
35:l:244:SER:O	35:l:249:SER:HB3	2.18	0.43
54:l:713:CDL:H181	54:l:713:CDL:H212	1.76	0.43
1:A:123:GLY:O	1:A:353:ALA:HB1	2.19	0.43
1:A:149:MET:HE1	1:A:241:THR:CB	2.48	0.43
1:A:210:THR:O	1:A:214:GLU:HG2	2.18	0.43
3:C:96:SER:HB3	3:C:99:GLN:CD	2.44	0.43
9:J:36:LEU:HB3	12:M:304:GLN:OE1	2.19	0.43
12:M:347:ASP:OD1	12:M:347:ASP:N	2.43	0.43
16:Q:278:VAL:HG23	16:Q:437:LYS:NZ	2.33	0.43
48:V:202:PEE:H32	48:V:202:PEE:H25	1.70	0.43
24:a:184:LYS:O	24:a:185:THR:OG1	2.29	0.43
54:i:401:CDL:OA7	54:i:401:CDL:HA62	2.16	0.43
33:j:90:MET:SD	36:m:151:THR:HG23	2.58	0.43
35:l:102:GLU:HA	35:l:105:MET:HG3	2.00	0.43
35:l:108:MET:HE1	35:l:240:PRO:HB3	1.99	0.43
36:m:3:MET:N	36:m:3:MET:SD	2.92	0.43
36:m:10:SER:O	36:m:14:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:294:LEU:O	41:s:298:LEU:HG	2.18	0.43
42:u:38:LYS:NZ	42:u:42:GLU:OE2	2.51	0.43
1:A:174:ARG:HD2	1:A:178:GLU:OE1	2.17	0.43
15:P:161:LYS:HA	15:P:161:LYS:HD3	1.87	0.43
16:Q:431:HIS:HB3	16:Q:454:GLN:HG2	2.00	0.43
18:T:37:LYS:HE3	18:T:37:LYS:HB2	1.76	0.43
20:V:61:PHE:HD2	20:V:104:ARG:HH12	1.66	0.43
21:W:104:TRP:CH2	31:h:75:ARG:HG3	2.54	0.43
28:e:74:HIS:HB2	28:e:83:ASP:OD2	2.19	0.43
32:i:57:THR:HA	34:k:77:LEU:HD13	2.01	0.43
41:s:19:PHE:O	41:s:23:VAL:HG23	2.18	0.43
44:w:258:TYR:HE2	44:w:269:VAL:HG13	1.83	0.43
1:A:177:TYR:CD1	1:A:182:ILE:HG23	2.54	0.43
1:A:432:ALA:O	1:A:436:GLN:HG3	2.19	0.43
12:M:260:ASN:ND2	12:M:278:HIS:HB2	2.34	0.43
21:W:128:ARG:HB3	21:W:132:GLU:OE2	2.18	0.43
54:a:201:CDL:OB7	48:l:720:PEE:H14	2.19	0.43
28:e:73:SER:C	28:e:75:GLY:H	2.26	0.43
32:i:172:GLN:OE1	32:i:177:LYS:HD3	2.19	0.43
33:j:81:THR:C	33:j:83:ASN:H	2.26	0.43
39:p:65:ARG:O	39:p:69:GLU:HG3	2.19	0.43
1:A:385:CYS:O	1:A:389:VAL:HB	2.19	0.43
4:E:19:PRO:HA	11:L:53:ILE:HD11	2.01	0.43
5:F:37:ILE:HA	5:F:41:TYR:HB2	1.99	0.43
12:M:476:LEU:HD21	12:M:481:LEU:HD21	2.01	0.43
24:a:95:GLU:CD	54:a:201:CDL:O1	2.56	0.43
26:c:109:LEU:O	26:c:113:ILE:HG23	2.18	0.43
27:d:37:PHE:CD2	35:l:3:PRO:HB3	2.54	0.43
35:l:452:ASN:HA	35:l:455:LYS:HG2	2.00	0.43
54:l:712:CDL:C85	54:l:712:CDL:C81	2.97	0.43
39:p:20:TYR:HB2	39:p:48:PHE:CZ	2.54	0.43
44:w:235:GLN:HA	44:w:238:GLU:CG	2.49	0.43
3:C:190:LEU:HD23	3:C:190:LEU:HA	1.86	0.43
7:H:65:VAL:O	7:H:69:GLU:HG3	2.18	0.43
54:V:201:CDL:C51	35:l:580:GLN:HE22	2.31	0.43
49:V:205:PLX:H301	49:V:205:PLX:H331	1.65	0.43
34:k:98:CYS:SG	35:l:587:TYR:OH	2.75	0.43
41:s:21:THR:HG22	41:s:224:PHE:CE1	2.54	0.43
42:u:59:GLU:HA	42:u:62:LEU:HD12	2.00	0.43
2:B:118:LEU:HD11	16:Q:382:PHE:CE2	2.54	0.42
6:G:126:PHE:CE2	6:G:148:ILE:HG21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:105:GLU:OE1	8:I:105:GLU:HA	2.19	0.42
9:J:131:GLY:O	51:J:401:NDP:H52A	2.19	0.42
9:J:319:VAL:HA	9:J:322:VAL:HG12	2.01	0.42
36:m:57:PHE:CE1	41:s:111:LEU:HD11	2.54	0.42
37:n:47:ARG:HG2	37:n:47:ARG:HH11	1.84	0.42
40:r:71:TRP:O	40:r:74:PRO:HD2	2.19	0.42
54:r:714:CDL:H542	54:r:714:CDL:H511	1.79	0.42
42:u:44:MET:HE3	42:u:48:TRP:CZ3	2.54	0.42
9:J:132:ARG:HD2	9:J:134:TRP:CZ2	2.53	0.42
24:a:139:ILE:HG23	40:r:54:LEU:HD23	2.01	0.42
27:d:46:THR:O	27:d:50:GLU:HG3	2.20	0.42
41:s:190:LEU:HD23	41:s:270:PHE:CD1	2.53	0.42
56:s:403:UQ:H152	56:s:403:UQ:H101	2.01	0.42
2:B:210:LEU:HD23	2:B:210:LEU:HA	1.89	0.42
5:F:64:LYS:HD3	5:F:76:ASN:HB2	2.01	0.42
5:F:83:SER:OG	5:F:86:GLN:HG3	2.19	0.42
12:M:173:MET:HE1	45:M:802:SF4:S1	2.60	0.42
12:M:538:ARG:HG2	12:M:538:ARG:NH1	2.33	0.42
13:N:68:MET:SD	13:N:81:MET:HG2	2.59	0.42
16:Q:139:LEU:HD23	16:Q:139:LEU:HA	1.89	0.42
27:d:61:TYR:C	27:d:62:TYR:HD1	2.27	0.42
27:d:117:GLU:HG3	27:d:124:ASN:HB2	2.02	0.42
32:i:104:MET:HG3	32:i:111:PHE:HB3	2.01	0.42
35:l:119:LYS:HZ1	54:l:712:CDL:H512	1.81	0.42
49:n:101:PLX:H102	40:r:40:SER:HB3	2.01	0.42
40:r:306:PRO:HA	40:r:458:LEU:HD22	2.01	0.42
54:r:714:CDL:H772	54:r:714:CDL:H741	1.81	0.42
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.99	0.42
1:A:413:TRP:O	1:A:416:SER:OG	2.26	0.42
6:G:139:MET:HA	6:G:139:MET:HE3	2.00	0.42
12:M:361:VAL:HG12	12:M:361:VAL:O	2.20	0.42
25:b:70:PHE:O	25:b:74:HIS:HB2	2.18	0.42
54:l:713:CDL:H382	54:l:713:CDL:H351	1.74	0.42
40:r:178:ILE:HD12	40:r:178:ILE:H	1.84	0.42
44:w:59:VAL:HG23	44:w:157:VAL:HG23	2.01	0.42
44:w:214:ILE:CG2	44:w:234:LEU:CD1	2.97	0.42
46:A:502:FMN:HM71	46:A:502:FMN:HM83	1.84	0.42
12:M:436:VAL:O	12:M:442:TYR:OH	2.33	0.42
54:V:203:CDL:H811	38:o:94:GLY:HA3	2.00	0.42
54:a:201:CDL:H211	54:a:201:CDL:H182	1.71	0.42
29:f:64:GLU:OE1	29:f:64:GLU:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:154:MET:HE2	32:i:154:MET:HB2	1.96	0.42
32:i:211:MET:HG2	32:i:333:SER:HB2	2.01	0.42
33:j:5:LEU:HD23	41:s:2:PHE:HD2	1.85	0.42
35:l:173:LEU:HD23	48:l:719:PEE:H15	2.01	0.42
39:p:28:GLU:OE2	39:p:34:ARG:NH1	2.46	0.42
44:w:211:VAL:N	44:w:212:PRO:CD	2.83	0.42
1:A:161:GLU:N	1:A:161:GLU:OE1	2.52	0.42
11:L:92:ASN:HB3	15:P:238:PRO:HA	2.01	0.42
12:M:391:ILE:N	12:M:600:GLU:OE2	2.40	0.42
12:M:605:GLN:OE1	12:M:643:ARG:NH1	2.46	0.42
13:N:69:ASN:OD1	13:N:112:ASN:ND2	2.50	0.42
21:W:68:ARG:NH2	36:m:134:GLY:HA2	2.34	0.42
23:Z:75:PHE:O	23:Z:79:VAL:HG13	2.20	0.42
26:c:97:LEU:HB3	26:c:99:LEU:HD12	2.00	0.42
35:l:107:TYR:HD1	35:l:108:MET:HE2	1.85	0.42
40:r:115:LEU:HD12	40:r:174:LEU:HD22	2.01	0.42
41:s:126:LYS:O	41:s:130:ILE:HG12	2.18	0.42
2:B:63:TRP:HB3	2:B:66:LEU:HD12	2.00	0.42
2:B:99:GLY:N	2:B:169:GLU:HG2	2.34	0.42
3:C:62:LEU:O	3:C:91:VAL:HA	2.19	0.42
6:G:113:LEU:HA	6:G:116:VAL:HG12	2.02	0.42
12:M:140:GLN:HG2	16:Q:379:ILE:HG23	2.02	0.42
13:N:42:ASP:OD2	13:N:44:TYR:HD2	2.02	0.42
23:Z:59:ASN:HB3	35:l:364:LYS:NZ	2.34	0.42
26:c:155:PRO:HG3	43:v:4:HIS:CE1	2.54	0.42
31:h:83:ARG:O	31:h:87:ILE:HG12	2.20	0.42
37:n:47:ARG:HH22	37:n:53:GLU:CD	2.25	0.42
40:r:445:LEU:O	40:r:448:THR:HG22	2.19	0.42
1:A:263:ALA:HA	1:A:271:SER:HB3	2.01	0.42
1:A:448:GLU:O	1:A:452:GLN:HG2	2.20	0.42
2:B:200:GLU:HG3	13:N:88:ARG:HD3	2.02	0.42
7:H:56:LEU:HA	7:H:59:VAL:HG12	2.01	0.42
16:Q:97:LEU:HD11	16:Q:109:CYS:SG	2.59	0.42
54:V:201:CDL:H621	32:i:160:LEU:HD11	2.01	0.42
32:i:266:ILE:HG22	32:i:270:MET:HE2	2.01	0.42
35:l:520:TYR:CE1	54:l:713:CDL:HB22	2.54	0.42
36:m:23:LYS:N	36:m:24:PRO:HD3	2.35	0.42
39:p:54:GLU:OE1	39:p:60:ALA:HB2	2.20	0.42
44:w:214:ILE:HG22	44:w:215:GLN:N	2.34	0.42
12:M:419:ARG:NH1	12:M:439:THR:O	2.53	0.42
22:Y:84:PHE:CE2	43:v:89:TYR:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:a:201:CDL:OB7	48:l:720:PEE:C11	2.68	0.42
32:i:278:MET:HE3	32:i:278:MET:HB3	1.97	0.42
33:j:91:ALA:HB1	41:s:305:ILE:HD13	2.02	0.42
54:l:712:CDL:H842	54:l:712:CDL:H651	2.00	0.42
54:n:102:CDL:OB7	42:u:170:TRP:HA	2.20	0.42
40:r:285:LEU:HD13	40:r:342:MET:HE1	2.02	0.42
1:A:46:TYR:CD1	14:O:226:GLU:HB3	2.55	0.42
1:A:50:ASP:HB3	1:A:55:GLY:HA3	2.02	0.42
2:B:210:LEU:HD12	8:I:38:PRO:HB3	2.01	0.42
6:G:71:ALA:HB1	6:G:72:PRO:HD2	2.02	0.42
7:H:26:ILE:O	7:H:30:LYS:HG3	2.19	0.42
13:N:85:GLU:HG2	13:N:86:TRP:N	2.34	0.42
14:O:108:PRO:HA	14:O:109:PRO:HD3	1.95	0.42
16:Q:158:LEU:HD23	16:Q:158:LEU:HA	1.89	0.42
21:W:51:MET:HE2	41:s:311:THR:HB	2.02	0.42
24:a:147:ALA:HB2	40:r:173:SER:HB2	2.01	0.42
49:j:203:PLX:H372	49:j:203:PLX:H342	1.61	0.42
54:l:713:CDL:H112	54:l:713:CDL:H142	1.72	0.42
56:s:403:UQ:H72	56:s:403:UQ:H111	1.88	0.42
1:A:109:ARG:NH1	1:A:237:GLY:O	2.53	0.41
3:C:76:MET:HE3	3:C:76:MET:HB3	1.90	0.41
5:F:33:VAL:O	5:F:36:PHE:HB3	2.20	0.41
12:M:260:ASN:HD21	12:M:278:HIS:CD2	2.37	0.41
16:Q:52:MET:HE3	16:Q:52:MET:HB3	1.84	0.41
16:Q:278:VAL:HG12	16:Q:329:ARG:HH21	1.85	0.41
54:V:201:CDL:H512	35:l:580:GLN:NE2	2.34	0.41
24:a:50:HIS:HB3	24:a:52:LYS:HE2	2.02	0.41
24:a:136:THR:HG21	40:r:48:ASN:ND2	2.35	0.41
26:c:169:GLU:HA	27:d:123:GLN:HB2	2.02	0.41
27:d:149:HIS:HD2	40:r:304:GLN:NE2	2.17	0.41
30:g:48:ASN:HB3	30:g:55:VAL:HA	2.02	0.41
34:k:60:PRO:O	34:k:63:LEU:HB3	2.19	0.41
41:s:89:LEU:HA	41:s:90:PRO:HD3	1.90	0.41
41:s:197:PRO:HB3	41:s:278:PRO:O	2.20	0.41
14:O:130:TYR:HA	14:O:189:ASN:ND2	2.35	0.41
16:Q:188:THR:HB	16:Q:200:PHE:HA	2.02	0.41
48:U:101:PEE:H35	48:U:101:PEE:H30	1.50	0.41
21:W:105:LYS:HE2	21:W:105:LYS:HB2	1.90	0.41
24:a:106:VAL:HG13	37:n:50:ARG:NH2	2.35	0.41
27:d:9:VAL:O	27:d:109:ARG:NH2	2.45	0.41
49:e:201:PLX:H301	49:e:201:PLX:H331	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:207:ILE:O	32:i:211:MET:HG3	2.20	0.41
32:i:283:ALA:HB1	40:r:158:LEU:HD13	2.00	0.41
33:j:55:PHE:HB2	36:m:74:MET:HE1	2.01	0.41
35:l:303:ALA:O	35:l:306:THR:HG22	2.20	0.41
35:l:468:ILE:O	35:l:472:ILE:HG12	2.21	0.41
54:l:712:CDL:H241	48:l:720:PEE:H33	2.02	0.41
40:r:121:LEU:O	40:r:125:THR:HG23	2.20	0.41
44:w:170:LEU:HD22	44:w:187:TYR:CD1	2.54	0.41
44:w:223:ASN:O	44:w:227:MET:HG3	2.20	0.41
1:A:338:ASP:O	1:A:342:LEU:HB2	2.20	0.41
6:G:106:LYS:H	6:G:106:LYS:HG2	1.73	0.41
9:J:36:LEU:N	12:M:304:GLN:HE22	2.17	0.41
12:M:94:MET:HE2	12:M:94:MET:HB2	1.90	0.41
15:P:108:PHE:O	15:P:160:TYR:OH	2.32	0.41
16:Q:144:MET:HE3	16:Q:222:MET:HB2	2.01	0.41
54:V:201:CDL:H342	54:V:201:CDL:H371	1.92	0.41
32:i:5:ILE:HG21	36:m:170:GLU:OE2	2.20	0.41
54:l:712:CDL:H851	54:l:712:CDL:C81	2.50	0.41
41:s:98:MET:HE1	41:s:104:PHE:CG	2.56	0.41
44:w:167:PHE:O	44:w:170:LEU:HB3	2.19	0.41
1:A:329:LYS:HA	1:A:332:CYS:SG	2.61	0.41
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.55	0.41
13:N:132:LYS:NZ	13:N:136:GLU:OE1	2.53	0.41
15:P:107:GLN:NE2	15:P:136:ARG:HG2	2.36	0.41
26:c:81:ARG:HB3	26:c:85:GLU:OE1	2.20	0.41
27:d:33:LEU:HD23	27:d:33:LEU:HA	1.85	0.41
29:f:72:ARG:HE	30:g:22:SER:HB3	1.85	0.41
31:h:17:TRP:CD1	31:h:17:TRP:H	2.39	0.41
32:i:245:MET:HE3	32:i:245:MET:HB3	1.92	0.41
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.30	0.41
1:A:317:VAL:HG23	1:A:356:VAL:HG12	2.02	0.41
19:U:78:LEU:HD23	19:U:78:LEU:HA	1.94	0.41
20:V:124:LEU:CD1	48:V:202:PEE:H58	2.51	0.41
32:i:112:HIS:HB2	32:i:184:ILE:HD13	2.01	0.41
49:j:203:PLX:H312	49:j:203:PLX:H282	1.83	0.41
48:l:720:PEE:H3	48:l:720:PEE:O4	2.20	0.41
44:w:54:THR:C	44:w:56:THR:H	2.27	0.41
44:w:346:ASP:OD1	44:w:347:VAL:N	2.53	0.41
2:B:66:LEU:HB3	41:s:277:TYR:OH	2.20	0.41
2:B:151:LYS:HA	3:C:141:GLY:HA2	2.01	0.41
12:M:42:MET:HE3	12:M:42:MET:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:698:ASP:N	12:M:698:ASP:OD1	2.53	0.41
15:P:183:ASP:OD1	15:P:185:ARG:NE	2.53	0.41
16:Q:198:THR:HB	16:Q:199:PRO:HD3	2.02	0.41
22:Y:51:THR:O	22:Y:54:GLN:HG2	2.20	0.41
32:i:129:LEU:HD13	54:i:401:CDL:H341	2.01	0.41
35:l:44:PHE:HB2	35:l:94:LEU:HB3	2.02	0.41
35:l:107:TYR:CD1	35:l:108:MET:HE2	2.55	0.41
35:l:562:LEU:HG	48:l:718:PEE:H32	2.02	0.41
37:n:47:ARG:NH2	37:n:53:GLU:OE2	2.46	0.41
40:r:233:ALA:HA	40:r:320:GLY:HA2	2.03	0.41
41:s:21:THR:CG2	41:s:224:PHE:CE1	3.03	0.41
41:s:142:TYR:O	41:s:145:THR:HG22	2.21	0.41
42:u:60:GLY:O	42:u:63:VAL:HG22	2.21	0.41
8:I:8:ILE:HG13	54:N:202:CDL:CA3	2.44	0.41
12:M:185:PHE:CZ	12:M:221:ASN:HB2	2.56	0.41
12:M:625:ALA:O	12:M:629:ILE:HG12	2.21	0.41
16:Q:198:THR:HG22	16:Q:202:TRP:CE2	2.56	0.41
27:d:77:CYS:SG	27:d:84:CYS:HB3	2.60	0.41
32:i:291:TYR:HA	40:r:151:PHE:HZ	1.85	0.41
35:l:105:MET:HE2	35:l:105:MET:HB3	1.93	0.41
35:l:211:MET:N	35:l:212:PRO:HD2	2.36	0.41
35:l:423:SER:O	35:l:427:ILE:HG12	2.20	0.41
36:m:51:PHE:CZ	36:m:55:MET:HE3	2.56	0.41
36:m:124:ASP:N	36:m:124:ASP:OD1	2.48	0.41
40:r:216:LEU:HD23	40:r:287:ALA:HB1	2.01	0.41
40:r:243:MET:HB3	40:r:301:ILE:HG21	2.03	0.41
1:A:121:GLU:HA	1:A:122:PRO:HD3	1.82	0.41
2:B:76:TYR:CE2	41:s:33:LEU:HD13	2.56	0.41
2:B:99:GLY:O	2:B:169:GLU:CG	2.69	0.41
9:J:72:HIS:NE2	15:P:215:GLU:OE2	2.54	0.41
11:L:154:LYS:HE2	11:L:154:LYS:HB3	1.79	0.41
6:X:136:GLU:O	25:b:2:SER:OG	2.38	0.41
32:i:45:MET:HE1	36:m:171:ILE:HG23	2.02	0.41
32:i:344:SER:C	32:i:346:LEU:H	2.29	0.41
35:l:123:LEU:CD1	54:l:712:CDL:OA7	2.68	0.41
40:r:369:LEU:HD12	40:r:370:PRO:HD2	2.02	0.41
41:s:245:ALA:HB3	41:s:255:TYR:CE2	2.56	0.41
1:A:99:TRP:N	1:A:99:TRP:CD1	2.87	0.41
48:C:311:PEE:H20	48:C:311:PEE:H28	2.02	0.41
5:F:56:ARG:HB3	12:M:651:PRO:HD2	2.03	0.41
6:G:130:ILE:HG22	6:G:135:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:167:PRO:HD2	12:M:215:MET:HE1	2.03	0.41
12:M:372:PHE:H	12:M:532:PRO:HB2	1.86	0.41
16:Q:226:TYR:OH	16:Q:234:GLN:O	2.22	0.41
23:Z:24:ILE:HG23	23:Z:29:LEU:HB2	2.02	0.41
49:e:201:PLX:H382	40:r:67:VAL:HG12	2.02	0.41
29:f:55:TRP:O	29:f:59:ILE:HG12	2.20	0.41
30:g:2:THR:HG22	30:g:4:MET:HG3	2.03	0.41
30:g:60:LEU:HD13	44:w:353:TRP:HB2	2.03	0.41
35:l:10:THR:O	35:l:14:ILE:HG12	2.21	0.41
35:l:94:LEU:HD23	35:l:94:LEU:HA	1.92	0.41
35:l:169:LEU:HD12	35:l:169:LEU:HA	1.88	0.41
35:l:559:GLU:OE2	40:r:148:TYR:OH	2.26	0.41
49:n:101:PLX:H111	49:n:101:PLX:H81	1.60	0.41
38:o:84:PRO:O	38:o:88:LEU:HG	2.21	0.41
39:p:29:SER:HB3	39:p:76:HIS:CD2	2.52	0.41
40:r:235:LEU:HD23	40:r:235:LEU:HA	1.92	0.41
54:r:714:CDL:H812	54:r:714:CDL:H241	2.03	0.41
4:E:115:PRO:HB2	4:E:120:SER:OG	2.21	0.41
5:F:89:ARG:O	5:F:93:ASN:ND2	2.54	0.41
7:H:76:GLN:O	7:H:79:GLU:HG2	2.21	0.41
9:J:84:TYR:HD2	9:J:86:CYS:O	2.04	0.41
12:M:245:THR:HA	12:M:265:THR:O	2.21	0.41
12:M:402:LEU:HD23	12:M:475:VAL:HB	2.03	0.41
12:M:624:ARG:HH12	12:M:628:GLU:HG3	1.86	0.41
54:V:203:CDL:C36	54:V:203:CDL:C32	2.98	0.41
6:X:82:ARG:O	6:X:86:VAL:HG23	2.21	0.41
27:d:74:ILE:HG23	27:d:156:LEU:HD22	2.02	0.41
27:d:90:MET:SD	40:r:47:GLU:HB3	2.61	0.41
31:h:65:GLU:OE2	31:h:71:LYS:HB2	2.21	0.41
32:i:72:MET:HG2	34:k:12:PHE:CE2	2.56	0.41
48:m:202:PEE:H25	48:m:202:PEE:H56	2.03	0.41
42:u:47:ARG:NH2	42:u:53:PRO:HG3	2.36	0.41
1:A:75:TRP:CH2	1:A:79:GLU:HG3	2.55	0.40
1:A:122:PRO:HA	14:O:176:CYS:SG	2.60	0.40
1:A:272:GLY:O	1:A:292:MET:HB2	2.20	0.40
2:B:90:LYS:HG3	13:N:91:HIS:CE1	2.56	0.40
7:H:54:GLU:O	7:H:58:MET:HG3	2.21	0.40
25:b:32:GLU:HG3	39:p:115:TYR:CD1	2.56	0.40
35:l:137:LEU:HD23	35:l:137:LEU:HA	1.96	0.40
44:w:243:LYS:HD3	44:w:243:LYS:HA	1.88	0.40
44:w:350:LYS:HA	44:w:350:LYS:HD3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ILE:HG23	1:A:199:ARG:HG2	2.04	0.40
1:A:279:SER:OG	1:A:280:GLY:N	2.54	0.40
2:B:177:THR:CG2	2:B:182:GLU:HB2	2.50	0.40
6:G:93:ILE:HG23	6:G:108:LEU:HD22	2.01	0.40
9:J:199:THR:OG1	9:J:258:ALA:O	2.39	0.40
11:L:53:ILE:HG22	11:L:55:VAL:HB	2.02	0.40
16:Q:383:LYS:HD2	16:Q:383:LYS:HA	1.92	0.40
19:U:42:ALA:HB2	41:s:312:ALA:HA	2.03	0.40
20:V:41:ILE:HD13	20:V:55:ARG:HH11	1.86	0.40
25:b:100:ARG:HB3	35:l:60:GLU:HB2	2.03	0.40
32:i:125:GLN:HG3	54:i:401:CDL:OA3	2.20	0.40
32:i:155:LEU:HD22	32:i:278:MET:HE2	2.03	0.40
35:l:572:LYS:HA	35:l:572:LYS:HD2	1.91	0.40
39:p:159:LYS:HE3	39:p:159:LYS:HB2	1.84	0.40
6:G:84:LEU:HB3	6:G:88:LYS:HZ3	1.86	0.40
8:I:34:ARG:HB2	13:N:95:ASP:OD1	2.22	0.40
12:M:133:GLN:O	12:M:137:CYS:HB2	2.22	0.40
16:Q:345:SER:HB2	21:W:19:ILE:HD12	2.02	0.40
32:i:78:LEU:HD22	32:i:84:TRP:CZ2	2.57	0.40
33:j:6:THR:O	33:j:10:ASN:ND2	2.54	0.40
35:l:327:LEU:O	35:l:331:MET:HG2	2.21	0.40
40:r:22:MET:HE3	40:r:22:MET:HB3	1.85	0.40
44:w:132:GLN:NE2	57:w:401:ADP:HN62	2.20	0.40
1:A:147:ARG:HA	1:A:147:ARG:HD2	1.90	0.40
1:A:209:GLU:HB2	1:A:242:VAL:HG21	2.02	0.40
1:A:267:ARG:HG3	1:A:293:SER:OG	2.20	0.40
2:B:38:TYR:CZ	8:I:106:LEU:HD13	2.57	0.40
2:B:44:ARG:HD3	2:B:45:GLU:H	1.86	0.40
13:N:3:LEU:HD23	13:N:7:LEU:HD11	2.02	0.40
14:O:63:ILE:HD12	14:O:82:VAL:HG13	2.04	0.40
16:Q:133:LEU:HD22	16:Q:228:ARG:HD3	2.03	0.40
54:V:201:CDL:OA5	48:V:207:PEE:H12	2.21	0.40
27:d:101:GLU:OE1	28:e:119:ARG:NH1	2.52	0.40
32:i:49:ASN:ND2	32:i:51:ARG:HB2	2.37	0.40
32:i:258:SER:OG	32:i:336:VAL:HG22	2.22	0.40
33:j:19:LEU:O	33:j:23:TRP:HD1	2.04	0.40
35:l:396:ILE:HA	35:l:399:VAL:HG12	2.04	0.40
35:l:562:LEU:HG	48:l:718:PEE:C20	2.52	0.40
40:r:202:ALA:O	40:r:205:VAL:HG12	2.22	0.40
40:r:403:THR:O	40:r:404:ALA:C	2.65	0.40
41:s:98:MET:HE2	41:s:101:GLY:HA2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:ARG:NH2	8:I:20:LEU:HD21	2.37	0.40
9:J:201:ILE:HG22	9:J:203:PRO:HD3	2.02	0.40
14:O:186:VAL:HG22	14:O:196:LEU:HD11	2.03	0.40
20:V:140:LYS:H	20:V:140:LYS:HG2	1.75	0.40
48:V:207:PEE:H20	48:V:207:PEE:H14	1.56	0.40
6:X:133:ILE:HD11	39:p:6:PRO:HA	2.03	0.40
27:d:43:ARG:O	27:d:47:LEU:HG	2.21	0.40
32:i:54:GLU:OE2	34:k:95:LEU:HB2	2.22	0.40
35:l:184:LEU:HD13	40:r:393:ILE:HG21	2.03	0.40
54:l:713:CDL:H201	54:l:713:CDL:H232	1.96	0.40
44:w:165:SER:O	44:w:168:VAL:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	414 (96%)	15 (4%)	0	100	100
2	B	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
3	C	154/156 (99%)	146 (95%)	8 (5%)	0	100	100
4	E	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
5	F	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
6	G	86/88 (98%)	84 (98%)	1 (1%)	1 (1%)	10	37
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
8	I	93/112 (83%)	82 (88%)	11 (12%)	0	100	100
9	J	289/341 (85%)	271 (94%)	16 (6%)	2 (1%)	18	49
10	K	40/42 (95%)	40 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	662 (96%)	25 (4%)	1 (0%)	48	78
13	N	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
14	O	215/217 (99%)	205 (95%)	10 (5%)	0	100	100
15	P	206/208 (99%)	196 (95%)	10 (5%)	0	100	100
16	Q	412/430 (96%)	401 (97%)	11 (3%)	0	100	100
17	S	68/70 (97%)	63 (93%)	5 (7%)	0	100	100
18	T	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
19	U	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
20	V	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	18	49
21	W	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
22	Y	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
23	Z	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
24	a	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
25	b	99/126 (79%)	95 (96%)	4 (4%)	0	100	100
26	c	154/156 (99%)	145 (94%)	9 (6%)	0	100	100
27	d	173/175 (99%)	172 (99%)	1 (1%)	0	100	100
28	e	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
29	f	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
30	g	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
32	i	345/347 (99%)	328 (95%)	15 (4%)	2 (1%)	21	52
33	j	95/113 (84%)	89 (94%)	6 (6%)	0	100	100
34	k	96/98 (98%)	87 (91%)	9 (9%)	0	100	100
35	l	601/603 (100%)	575 (96%)	26 (4%)	0	100	100
36	m	125/175 (71%)	112 (90%)	13 (10%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
39	p	176/178 (99%)	163 (93%)	13 (7%)	0	100	100
40	r	457/459 (100%)	441 (96%)	16 (4%)	0	100	100
41	s	299/318 (94%)	285 (95%)	13 (4%)	1 (0%)	36	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	u	169/171 (99%)	162 (96%)	7 (4%)	0	100	100
43	v	122/125 (98%)	115 (94%)	7 (6%)	0	100	100
44	w	318/320 (99%)	302 (95%)	15 (5%)	1 (0%)	36	67
All	All	8029/8309 (97%)	7684 (96%)	336 (4%)	9 (0%)	49	78

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	i	93	VAL
44	w	70	LYS
9	J	38	HIS
32	i	92	PRO
6	G	76	LEU
20	V	46	PRO
12	M	283	GLU
9	J	83	PRO
41	s	90	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/345 (100%)	343 (99%)	2 (1%)	78	83
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	76/76 (100%)	76 (100%)	0	100	100
6	G	76/81 (94%)	76 (100%)	0	100	100
6	X	77/81 (95%)	77 (100%)	0	100	100
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	J	255/295 (86%)	255 (100%)	0	100	100
10	K	41/41 (100%)	41 (100%)	0	100	100
11	L	113/113 (100%)	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%)	183 (100%)	0	100	100
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	361/370 (98%)	361 (100%)	0	100	100
17	S	58/58 (100%)	58 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	101 (100%)	0	100	100
21	W	122/123 (99%)	122 (100%)	0	100	100
22	Y	63/63 (100%)	63 (100%)	0	100	100
23	Z	65/65 (100%)	65 (100%)	0	100	100
24	a	122/122 (100%)	122 (100%)	0	100	100
25	b	98/119 (82%)	98 (100%)	0	100	100
26	c	141/141 (100%)	141 (100%)	0	100	100
27	d	155/155 (100%)	155 (100%)	0	100	100
28	e	99/99 (100%)	99 (100%)	0	100	100
29	f	35/38 (92%)	35 (100%)	0	100	100
30	g	108/108 (100%)	108 (100%)	0	100	100
31	h	93/93 (100%)	93 (100%)	0	100	100
32	i	311/311 (100%)	311 (100%)	0	100	100
33	j	88/99 (89%)	88 (100%)	0	100	100
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	r	410/410 (100%)	410 (100%)	0	100	100
41	s	263/275 (96%)	263 (100%)	0	100	100
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	101/111 (91%)	101 (100%)	0	100	100
44	w	281/283 (99%)	279 (99%)	2 (1%)	76	82
All	All	7064/7234 (98%)	7060 (100%)	4 (0%)	87	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	THR
1	A	125	CYS
44	w	214	ILE
44	w	246	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	HIS
1	A	244	ASN
1	A	283	ASN
1	A	457	HIS
4	E	58	GLN
5	F	81	ASN
6	G	142	GLN
7	H	21	HIS
7	H	76	GLN
8	I	13	ASN
8	I	110	GLN
9	J	122	HIS
9	J	376	ASN
12	M	123	ASN
12	M	260	ASN
12	M	300	GLN
12	M	388	ASN
12	M	498	GLN
12	M	604	GLN
12	M	663	ASN
13	N	13	GLN

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Mol	Chain	Res	Type
13	N	135	GLN
14	O	69	ASN
14	O	133	GLN
15	P	63	GLN
15	P	107	GLN
15	P	131	ASN
15	P	181	HIS
16	Q	183	HIS
16	Q	234	GLN
16	Q	250	ASN
16	Q	306	GLN
16	Q	454	GLN
17	S	27	HIS
17	S	46	ASN
20	V	129	GLN
22	Y	83	HIS
24	a	170	GLN
24	a	181	HIS
26	c	164	ASN
30	g	119	HIS
32	i	49	ASN
32	i	63	GLN
32	i	150	ASN
32	i	174	GLN
32	i	221	HIS
33	j	82	ASN
33	j	108	GLN
34	k	57	ASN
35	l	139	GLN
35	l	192	HIS
35	l	354	GLN
35	l	580	GLN
37	n	3	ASN
37	n	11	HIS
38	o	52	ASN
38	o	75	ASN
40	r	81	GLN
40	r	103	GLN
40	r	144	ASN
40	r	175	ASN
40	r	192	ASN
40	r	251	ASN

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Mol	Chain	Res	Type
40	r	304	GLN
40	r	366	ASN
41	s	47	GLN
41	s	124	ASN
41	s	235	ASN
41	s	250	HIS
41	s	317	GLN
42	u	30	HIS
42	u	163	HIS
43	v	47	ASN
43	v	85	HIS
44	w	127	ASN
44	w	219	GLN
44	w	344	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	1.98	1 (10%)	5,13,15	6.19	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	5.54	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	12.76	131.18	119.48
16	Q	118	2MR	CD-NE-CZ	4.40	131.65	123.41
16	Q	118	2MR	CQ2-NH2-CZ	2.90	130.26	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.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 2 are monoatomic - leaving 39 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
54	CDL	n	102	-	77,77,99	1.02	4 (5%)	83,89,111	1.14	7 (8%)
48	PEE	m	202	-	40,40,50	1.14	5 (12%)	43,45,55	1.03	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
51	NDP	J	401	-	49,52,52	4.38	22 (44%)	66,80,80	2.17	14 (21%)
48	PEE	l	719	-	45,45,50	1.22	6 (13%)	48,50,55	1.01	2 (4%)
49	PLX	j	203	-	51,51,51	1.14	4 (7%)	55,59,59	0.60	1 (1%)
54	CDL	a	201	-	90,90,99	0.96	4 (4%)	96,102,111	1.06	6 (6%)
54	CDL	V	203	-	67,67,99	1.11	4 (5%)	73,79,111	1.18	6 (8%)
48	PEE	l	720	-	45,45,50	1.22	6 (13%)	48,50,55	1.00	2 (4%)
45	SF4	B	302	2	0,12,12	-	-	-	-	-
48	PEE	U	101	-	50,50,50	1.15	6 (12%)	53,55,55	0.94	2 (3%)
48	PEE	V	207	-	39,39,50	1.31	6 (15%)	41,44,55	1.04	2 (4%)
45	SF4	A	501	1	0,12,12	-	-	-	-	-
50	8Q1	G	201	6	31,34,34	2.04	6 (19%)	40,43,43	1.66	12 (30%)
49	PLX	i	705	-	51,51,51	1.12	3 (5%)	55,59,59	0.66	1 (1%)
50	8Q1	X	201	6	31,34,34	2.08	6 (19%)	40,43,43	1.70	10 (25%)
56	UQ	s	403	-	28,28,63	3.25	7 (25%)	34,37,79	2.85	10 (29%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
52	FES	M	803	12	0,4,4	-	-	-	-	-
46	FMN	A	502	-	33,33,33	1.11	2 (6%)	48,50,50	1.26	9 (18%)
48	PEE	C	311	-	46,46,50	1.21	6 (13%)	49,51,55	0.95	2 (4%)
54	CDL	N	202	-	50,50,99	1.27	4 (8%)	56,62,111	1.30	6 (10%)
54	CDL	i	401	-	65,65,99	1.14	4 (6%)	71,77,111	1.19	5 (7%)
48	PEE	V	202	-	50,50,50	1.15	6 (12%)	53,55,55	1.01	2 (3%)
49	PLX	n	101	-	51,51,51	0.62	0	55,59,59	0.69	0
48	PEE	l	718	-	46,46,50	1.20	6 (13%)	49,51,55	1.00	2 (4%)
48	PEE	s	401	-	50,50,50	1.16	6 (12%)	53,55,55	0.96	2 (3%)
47	NAI	A	503	-	45,48,48	3.91	20 (44%)	60,73,73	1.77	12 (20%)
49	PLX	C	312	-	51,51,51	1.13	3 (5%)	55,59,59	0.62	1 (1%)
49	PLX	V	205	-	51,51,51	1.14	3 (5%)	55,59,59	0.61	1 (1%)
57	ADP	w	401	-	27,29,29	2.96	8 (29%)	42,45,45	2.01	10 (23%)
45	SF4	C	301	3	0,12,12	-	-	-	-	-
45	SF4	M	802	12	0,12,12	-	-	-	-	-
52	FES	O	301	14	0,4,4	-	-	-	-	-
54	CDL	l	712	-	98,98,99	0.92	4 (4%)	104,110,111	1.16	8 (7%)
49	PLX	e	201	-	51,51,51	1.13	3 (5%)	55,59,59	0.62	1 (1%)
54	CDL	l	713	-	99,99,99	1.09	8 (8%)	105,111,111	0.83	4 (3%)
54	CDL	r	714	-	96,96,99	1.09	8 (8%)	102,108,111	0.88	4 (3%)
54	CDL	V	201	-	93,93,99	0.95	4 (4%)	99,105,111	1.07	5 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	SF4	M	801	12	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	CDL	n	102	-	-	27/88/88/110	-
48	PEE	m	202	-	-	18/44/44/54	-
51	NDP	J	401	-	-	12/34/77/77	0/4/5/5
48	PEE	l	719	-	-	20/49/49/54	-
49	PLX	j	203	-	-	25/55/55/55	-
54	CDL	a	201	-	-	27/101/101/110	-
54	CDL	V	203	-	-	34/78/78/110	-
48	PEE	l	720	-	-	26/49/49/54	-
45	SF4	B	302	2	-	-	0/6/5/5
48	PEE	U	101	-	-	25/54/54/54	-
48	PEE	V	207	-	-	20/43/43/54	-
45	SF4	A	501	1	-	-	0/6/5/5
50	8Q1	G	201	6	-	19/41/41/41	-
49	PLX	i	705	-	-	20/55/55/55	-
50	8Q1	X	201	6	-	23/41/41/41	-
56	UQ	s	403	-	-	9/21/45/87	0/1/1/1
45	SF4	B	301	2	-	-	0/6/5/5
52	FES	M	803	12	-	-	0/1/1/1
46	FMN	A	502	-	-	6/18/18/18	0/3/3/3
48	PEE	C	311	-	-	26/50/50/54	-
54	CDL	N	202	-	-	23/61/61/110	-
54	CDL	i	401	-	-	31/76/76/110	-
48	PEE	V	202	-	-	21/54/54/54	-
49	PLX	n	101	-	-	17/55/55/55	-
48	PEE	l	718	-	-	22/50/50/54	-
48	PEE	s	401	-	-	23/54/54/54	-
47	NAI	A	503	-	-	6/29/72/72	0/5/5/5
49	PLX	C	312	-	-	35/55/55/55	-
49	PLX	V	205	-	-	32/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	ADP	w	401	-	-	3/16/32/32	0/3/3/3
45	SF4	C	301	3	-	-	0/6/5/5
45	SF4	M	802	12	-	-	0/6/5/5
52	FES	O	301	14	-	-	0/1/1/1
54	CDL	l	712	-	-	40/109/109/110	-
49	PLX	e	201	-	-	36/55/55/55	-
54	CDL	l	713	-	-	66/110/110/110	-
54	CDL	r	714	-	-	65/107/107/110	-
54	CDL	V	201	-	-	38/104/104/110	-
45	SF4	M	801	12	-	-	0/6/5/5

All (184) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	J	401	NDP	C3B-C2B	-12.79	1.24	1.52
51	J	401	NDP	C6N-C5N	12.38	1.55	1.33
51	J	401	NDP	O4D-C4D	10.60	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.30	1.26	1.53
51	J	401	NDP	C3D-C4D	-9.95	1.27	1.53
56	s	403	UQ	C13-C14	9.23	1.55	1.33
47	A	503	NAI	O4B-C1B	9.04	1.63	1.42
57	w	401	ADP	C3'-C4'	-8.88	1.30	1.53
56	s	403	UQ	C8-C9	8.79	1.54	1.33
47	A	503	NAI	O4B-C4B	-8.31	1.26	1.45
56	s	403	UQ	C18-C19	8.28	1.56	1.32
51	J	401	NDP	O4B-C4B	-7.92	1.27	1.45
50	G	201	8Q1	P24-O27	7.73	1.85	1.60
57	w	401	ADP	O4'-C4'	7.61	1.62	1.45
47	A	503	NAI	C2D-C1D	-7.60	1.29	1.53
50	X	201	8Q1	P24-O27	7.52	1.84	1.60
51	J	401	NDP	C2N-C3N	7.36	1.55	1.34
47	A	503	NAI	C2B-C1B	-7.30	1.30	1.53
47	A	503	NAI	O4D-C4D	6.86	1.60	1.45
47	A	503	NAI	C2D-C3D	5.91	1.69	1.53
51	J	401	NDP	C6A-N6A	5.90	1.48	1.34
47	A	503	NAI	C7N-N7N	5.77	1.48	1.33
57	w	401	ADP	C6-N6	5.52	1.48	1.34
47	A	503	NAI	O4D-C1D	5.51	1.55	1.42
51	J	401	NDP	P2B-O2B	5.37	1.69	1.59
47	A	503	NAI	C6A-N6A	5.18	1.47	1.34
51	J	401	NDP	C3B-C4B	5.13	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	C4N-C3N	-5.07	1.40	1.49
51	J	401	NDP	O4D-C1D	-4.96	1.30	1.42
51	J	401	NDP	C6N-N1N	4.86	1.49	1.37
51	J	401	NDP	O4B-C1B	4.66	1.53	1.42
47	A	503	NAI	O2B-C2B	4.57	1.53	1.43
51	J	401	NDP	C1B-N9A	-4.52	1.33	1.46
57	w	401	ADP	O4'-C1'	-4.48	1.31	1.42
54	i	401	CDL	OA8-CA7	4.29	1.45	1.33
54	V	203	CDL	OA8-CA7	4.28	1.45	1.33
54	a	201	CDL	OA8-CA7	4.28	1.45	1.33
54	i	401	CDL	OA6-CA5	4.28	1.46	1.34
54	N	202	CDL	OB8-CB7	4.27	1.45	1.33
54	l	712	CDL	OA8-CA7	4.26	1.45	1.33
54	V	201	CDL	OA8-CA7	4.26	1.45	1.33
54	i	401	CDL	OB8-CB7	4.25	1.45	1.33
54	n	102	CDL	OB8-CB7	4.25	1.45	1.33
54	V	201	CDL	OB8-CB7	4.24	1.45	1.33
54	V	203	CDL	OB8-CB7	4.23	1.45	1.33
54	l	712	CDL	OB8-CB7	4.20	1.45	1.33
54	V	201	CDL	OA6-CA5	4.19	1.46	1.34
54	N	202	CDL	OA8-CA7	4.19	1.45	1.33
54	a	201	CDL	OB8-CB7	4.18	1.45	1.33
51	J	401	NDP	C7N-N7N	4.16	1.44	1.33
54	i	401	CDL	OB6-CB5	4.16	1.46	1.34
54	a	201	CDL	OB6-CB5	4.15	1.46	1.34
54	N	202	CDL	OA6-CA5	4.13	1.46	1.34
54	n	102	CDL	OA8-CA7	4.12	1.45	1.33
54	V	201	CDL	OB6-CB5	4.12	1.45	1.34
54	V	203	CDL	OA6-CA5	4.11	1.45	1.34
51	J	401	NDP	O2D-C2D	-4.11	1.33	1.43
54	a	201	CDL	OA6-CA5	4.07	1.45	1.34
47	A	503	NAI	C6N-C5N	4.06	1.40	1.33
54	n	102	CDL	OA6-CA5	4.00	1.45	1.34
54	l	712	CDL	OA6-CA5	3.98	1.45	1.34
54	V	203	CDL	OB6-CB5	3.98	1.45	1.34
54	l	712	CDL	OB6-CB5	3.98	1.45	1.34
54	N	202	CDL	OB6-CB5	3.96	1.45	1.34
54	n	102	CDL	OB6-CB5	3.90	1.45	1.34
50	X	201	8Q1	C1-S44	3.82	1.85	1.76
50	G	201	8Q1	C1-S44	3.76	1.85	1.76
48	m	202	PEE	C18-C19	3.75	1.53	1.31
48	C	311	PEE	C18-C19	3.74	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	V	207	PEE	C18-C19	3.73	1.53	1.31
48	s	401	PEE	C18-C19	3.73	1.53	1.31
48	V	202	PEE	C18-C19	3.72	1.53	1.31
48	l	719	PEE	C18-C19	3.71	1.53	1.31
48	l	720	PEE	C18-C19	3.71	1.53	1.31
48	l	718	PEE	C18-C19	3.70	1.53	1.31
48	U	101	PEE	C18-C19	3.66	1.53	1.31
48	C	311	PEE	C39-C38	3.66	1.53	1.31
46	A	502	FMN	C4A-N5	3.66	1.37	1.30
48	V	202	PEE	C39-C38	3.65	1.52	1.31
48	l	719	PEE	C39-C38	3.65	1.52	1.31
48	l	718	PEE	C39-C38	3.65	1.52	1.31
48	V	207	PEE	C39-C38	3.63	1.52	1.31
48	l	720	PEE	C39-C38	3.63	1.52	1.31
48	U	101	PEE	C39-C38	3.62	1.52	1.31
48	s	401	PEE	C39-C38	3.61	1.52	1.31
50	X	201	8Q1	C34-N36	3.59	1.41	1.33
50	G	201	8Q1	C34-N36	3.53	1.41	1.33
47	A	503	NAI	C7N-C3N	3.50	1.56	1.48
54	l	713	CDL	OA8-CA7	3.47	1.43	1.33
54	r	714	CDL	OA8-CA7	3.35	1.43	1.33
47	A	503	NAI	C4N-C5N	-3.35	1.40	1.48
50	X	201	8Q1	O27-C28	-3.33	1.33	1.43
50	G	201	8Q1	O27-C28	-3.27	1.33	1.43
57	w	401	ADP	O2'-C2'	-3.25	1.35	1.43
57	w	401	ADP	O3'-C3'	3.22	1.50	1.43
57	w	401	ADP	C8-N9	-3.19	1.31	1.37
50	X	201	8Q1	C39-N41	3.17	1.40	1.33
50	X	201	8Q1	C6-C1	3.13	1.54	1.50
51	J	401	NDP	C8A-N9A	-3.12	1.31	1.37
51	J	401	NDP	O3D-C3D	3.10	1.50	1.43
51	J	401	NDP	C5A-N7A	-3.06	1.33	1.39
54	r	714	CDL	OB6-CB5	3.06	1.42	1.34
54	l	713	CDL	OB6-CB5	2.99	1.42	1.34
54	l	713	CDL	OA6-CA5	2.97	1.42	1.34
54	l	713	CDL	OB8-CB7	2.97	1.42	1.33
54	r	714	CDL	OB8-CB7	2.93	1.41	1.33
51	J	401	NDP	C7N-C3N	2.87	1.54	1.48
49	C	312	PLX	O6-C4	-2.80	1.40	1.44
50	G	201	8Q1	C6-C1	2.79	1.53	1.50
54	r	714	CDL	OA6-CA5	2.79	1.42	1.34
49	e	201	PLX	O6-C4	-2.76	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	i	705	PLX	O6-C4	-2.74	1.40	1.44
50	G	201	8Q1	C39-N41	2.70	1.39	1.33
49	j	203	PLX	O6-C4	-2.61	1.41	1.44
48	s	401	PEE	O2-C2	-2.58	1.40	1.46
56	s	403	UQ	C6-C1	2.56	1.53	1.46
54	r	714	CDL	OA6-CA4	-2.56	1.40	1.46
47	A	503	NAI	C8A-N9A	-2.56	1.32	1.37
48	C	311	PEE	O3-C30	2.53	1.40	1.33
48	l	718	PEE	O3-C30	2.53	1.40	1.33
49	V	205	PLX	O6-C4	-2.52	1.41	1.44
48	V	202	PEE	O2-C2	-2.51	1.40	1.46
48	l	719	PEE	O2-C2	-2.51	1.40	1.46
51	J	401	NDP	C2D-C3D	2.50	1.60	1.53
48	l	718	PEE	O2-C2	-2.50	1.40	1.46
47	A	503	NAI	O3B-C3B	-2.49	1.37	1.43
51	J	401	NDP	O2B-C2B	2.48	1.53	1.44
48	l	720	PEE	O3-C30	2.48	1.40	1.33
48	V	207	PEE	O3-C30	2.47	1.40	1.33
48	U	101	PEE	O2-C2	-2.47	1.40	1.46
54	l	713	CDL	OA6-CA4	-2.46	1.40	1.46
48	s	401	PEE	O3-C30	2.41	1.40	1.33
48	U	101	PEE	O3-C30	2.41	1.40	1.33
49	V	205	PLX	C7-C6	2.40	1.55	1.50
48	C	311	PEE	O2-C2	-2.38	1.40	1.46
48	l	720	PEE	O2-C2	-2.38	1.40	1.46
48	l	719	PEE	O3-C30	2.38	1.40	1.33
48	V	202	PEE	O3-C30	2.38	1.40	1.33
47	A	503	NAI	PN-O5D	2.35	1.68	1.59
48	m	202	PEE	O3-C30	2.32	1.40	1.33
49	i	705	PLX	C7-C6	2.31	1.55	1.50
48	l	720	PEE	O2-C10	2.29	1.40	1.34
49	e	201	PLX	C7-C6	2.29	1.55	1.50
48	V	207	PEE	O2-C2	-2.29	1.40	1.46
57	w	401	ADP	C5-N7	-2.29	1.34	1.39
48	C	311	PEE	O2-C10	2.29	1.40	1.34
48	m	202	PEE	O2-C10	2.28	1.40	1.34
48	m	202	PEE	O2-C2	-2.28	1.40	1.46
54	l	713	CDL	OB6-CB4	-2.28	1.40	1.46
48	V	207	PEE	O2-C10	2.27	1.40	1.34
47	A	503	NAI	C5B-C4B	2.26	1.58	1.51
56	s	403	UQ	O4-C4	-2.25	1.18	1.23
46	A	502	FMN	C10-N1	2.24	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	U	101	PEE	O2-C10	2.24	1.40	1.34
48	m	202	PEE	O3-C3	-2.22	1.40	1.45
51	J	401	NDP	O7N-C7N	-2.20	1.19	1.24
49	j	203	PLX	C7-C6	2.20	1.55	1.50
48	U	101	PEE	O3-C3	-2.19	1.40	1.45
49	j	203	PLX	P1-O4	2.18	1.68	1.59
54	l	713	CDL	PB2-OB2	2.18	1.68	1.59
54	r	714	CDL	PB2-OB5	2.17	1.68	1.59
48	V	202	PEE	O3-C3	-2.17	1.40	1.45
48	l	719	PEE	O2-C10	2.17	1.40	1.34
48	l	719	PEE	O3-C3	-2.16	1.40	1.45
48	V	202	PEE	O2-C10	2.16	1.40	1.34
54	r	714	CDL	PB2-OB2	2.15	1.68	1.59
48	l	718	PEE	O2-C10	2.13	1.40	1.34
56	s	403	UQ	O1-C1	-2.13	1.18	1.23
54	l	713	CDL	PB2-OB5	2.13	1.67	1.59
48	l	720	PEE	O3-C3	-2.12	1.40	1.45
49	C	312	PLX	C7-C6	2.11	1.55	1.50
49	V	205	PLX	P1-O4	2.11	1.67	1.59
48	s	401	PEE	O2-C10	2.10	1.40	1.34
49	e	201	PLX	P1-O4	2.09	1.67	1.59
48	s	401	PEE	O3-C3	-2.09	1.40	1.45
49	j	203	PLX	P1-O1	2.06	1.67	1.59
48	V	207	PEE	O3-C3	-2.05	1.40	1.45
54	r	714	CDL	OB6-CB4	-2.05	1.41	1.46
49	C	312	PLX	P1-O4	2.05	1.67	1.59
56	s	403	UQ	O3-CM3	-2.04	1.40	1.45
48	C	311	PEE	O3-C3	-2.04	1.40	1.45
47	A	503	NAI	C5A-N7A	-2.02	1.35	1.39
48	l	718	PEE	O3-C3	-2.02	1.40	1.45
49	i	705	PLX	P1-O4	2.00	1.67	1.59

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	s	403	UQ	C7-C8-C9	-9.97	110.19	126.79
51	J	401	NDP	C3N-C2N-N1N	-7.83	111.92	123.10
51	J	401	NDP	C1D-N1N-C2N	-6.83	109.73	121.11
51	J	401	NDP	C5A-C4A-N3A	-5.92	119.03	126.75
56	s	403	UQ	C12-C13-C14	-5.90	113.45	127.66
57	w	401	ADP	C5-C4-N3	-5.78	119.21	126.75
47	A	503	NAI	C5A-C4A-N3A	-5.75	119.25	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	J	401	NDP	C1D-N1N-C6N	-5.23	109.56	120.83
54	l	712	CDL	OA6-CA5-C11	4.87	121.99	111.50
56	s	403	UQ	C10-C9-C8	-4.85	111.24	123.68
56	s	403	UQ	C11-C9-C8	-4.85	111.31	121.12
50	X	201	8Q1	C6-C1-S44	4.73	118.96	113.46
57	w	401	ADP	N3-C2-N1	-4.45	121.64	128.60
57	w	401	ADP	N3-C4-N9	4.44	134.40	127.08
50	G	201	8Q1	C6-C1-S44	4.42	118.60	113.46
54	n	102	CDL	OA6-CA5-C11	4.41	121.00	111.50
54	i	401	CDL	OA6-CA5-C11	4.36	120.89	111.50
47	A	503	NAI	N3A-C2A-N1A	-4.31	121.86	128.60
48	V	202	PEE	O2-C10-C11	4.23	120.61	111.50
48	m	202	PEE	O2-C10-C11	4.21	120.58	111.50
54	V	203	CDL	OB6-CB5-C51	4.21	120.56	111.50
51	J	401	NDP	N3A-C4A-N9A	4.15	133.92	127.08
54	r	714	CDL	OB6-CB5-C51	4.12	120.37	111.50
54	N	202	CDL	OB6-CB5-C51	4.10	120.34	111.50
56	s	403	UQ	C15-C14-C13	-4.09	113.20	123.68
48	l	719	PEE	O2-C10-C11	4.08	120.28	111.50
47	A	503	NAI	N3A-C4A-N9A	4.03	133.73	127.08
48	l	718	PEE	O2-C10-C11	4.02	120.16	111.50
51	J	401	NDP	N3A-C2A-N1A	-4.00	122.34	128.60
54	N	202	CDL	OA6-CA5-C11	4.00	120.13	111.50
56	s	403	UQ	C17-C18-C19	-4.00	114.08	127.75
48	l	720	PEE	O2-C10-C11	3.99	120.10	111.50
54	a	201	CDL	OB6-CB5-C51	3.98	120.07	111.50
54	V	201	CDL	OB6-CB5-C51	3.98	120.07	111.50
54	i	401	CDL	OB6-CB5-C51	3.92	119.96	111.50
56	s	403	UQ	C16-C14-C13	-3.89	113.25	121.12
48	V	207	PEE	O2-C10-C11	3.88	119.87	111.50
54	V	203	CDL	OA6-CA5-C11	3.87	119.84	111.50
48	C	311	PEE	O2-C10-C11	3.87	119.84	111.50
48	s	401	PEE	O2-C10-C11	3.86	119.83	111.50
54	l	713	CDL	OA6-CA5-C11	3.86	119.82	111.50
54	l	712	CDL	OB6-CB5-C51	3.85	119.81	111.50
54	r	714	CDL	OA6-CA5-C11	3.85	119.80	111.50
47	A	503	NAI	C2A-N3A-C4A	3.84	120.82	111.75
54	l	712	CDL	CA4-OA6-CA5	-3.80	108.44	117.79
54	V	201	CDL	OA6-CA5-C11	3.79	119.66	111.50
51	J	401	NDP	C2A-N3A-C4A	3.77	120.66	111.75
48	U	101	PEE	O2-C10-C11	3.77	119.62	111.50
54	l	713	CDL	OB6-CB5-C51	3.76	119.61	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	w	401	ADP	C2-N3-C4	3.72	120.55	111.75
54	a	201	CDL	OA6-CA5-C11	3.68	119.44	111.50
47	A	503	NAI	C5A-N7A-C8A	3.62	108.65	103.51
57	w	401	ADP	N9-C8-N7	-3.61	108.97	113.91
54	n	102	CDL	OB6-CB5-C51	3.57	119.20	111.50
57	w	401	ADP	C5-N7-C8	3.51	108.49	103.51
51	J	401	NDP	C5A-N7A-C8A	3.38	108.31	103.51
50	G	201	8Q1	O35-C34-N36	-3.37	115.76	122.99
46	A	502	FMN	C4-N3-C2	-3.32	119.52	125.64
50	X	201	8Q1	O35-C34-N36	-3.32	115.87	122.99
47	A	503	NAI	N9A-C8A-N7A	-3.31	109.39	113.91
50	X	201	8Q1	C43-S44-C1	3.30	112.16	101.87
56	s	403	UQ	C21-C19-C18	-3.28	113.16	122.65
51	J	401	NDP	N9A-C8A-N7A	-3.26	109.45	113.91
47	A	503	NAI	C4A-C5A-N7A	-3.17	106.76	110.62
50	G	201	8Q1	C43-S44-C1	3.16	111.71	101.87
47	A	503	NAI	C4D-O4D-C1D	-3.16	102.51	109.47
54	l	712	CDL	OB8-CB7-C71	3.06	121.50	111.91
57	w	401	ADP	C4-N9-C8	3.06	109.04	105.73
47	A	503	NAI	C3D-C2D-C1D	3.05	107.22	101.43
51	J	401	NDP	C4A-C5A-N7A	-3.03	106.93	110.62
54	a	201	CDL	OB8-CB7-C71	3.01	121.34	111.91
56	s	403	UQ	CM5-C5-C6	-2.99	119.52	124.40
54	V	201	CDL	OB8-CB7-C71	2.98	121.25	111.91
56	s	403	UQ	C20-C19-C18	-2.93	114.17	122.65
54	V	203	CDL	CB4-OB6-CB5	-2.93	110.58	117.79
48	s	401	PEE	O3-C30-C31	2.92	121.07	111.91
54	a	201	CDL	OA8-CA7-C31	2.92	121.07	111.91
54	i	401	CDL	OA8-CA7-C31	2.91	121.03	111.91
57	w	401	ADP	C4-C5-N7	-2.88	107.11	110.62
51	J	401	NDP	PN-O3-PA	-2.85	123.06	132.83
54	N	202	CDL	OA8-CA7-C31	2.84	120.82	111.91
48	V	202	PEE	O3-C30-C31	2.82	120.76	111.91
48	l	719	PEE	O3-C30-C31	2.77	120.61	111.91
54	V	203	CDL	OA8-CA7-C31	2.76	120.57	111.91
49	e	201	PLX	C1A-N1-C1	2.76	121.20	109.92
54	V	201	CDL	OA8-CA7-C31	2.72	120.43	111.91
50	X	201	8Q1	C32-C34-N36	2.71	121.98	116.58
54	V	201	CDL	CB4-OB6-CB5	-2.69	111.16	117.79
50	X	201	8Q1	O2-P24-O27	-2.69	99.57	106.73
57	w	401	ADP	PA-O3A-PB	-2.66	123.68	132.83
50	G	201	8Q1	O40-C39-N41	-2.66	118.00	123.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	V	207	PEE	O3-C30-C31	2.64	120.19	111.91
50	X	201	8Q1	C37-C38-C39	2.63	116.75	112.36
54	n	102	CDL	OA8-CA7-C31	2.63	120.17	111.91
54	N	202	CDL	OB8-CB7-C71	2.63	120.16	111.91
46	A	502	FMN	C4A-C4-N3	2.63	119.86	113.19
54	l	712	CDL	OA8-CA7-C31	2.61	120.11	111.91
47	A	503	NAI	PN-O3-PA	-2.61	123.88	132.83
48	l	720	PEE	O3-C30-C31	2.60	120.05	111.91
54	l	713	CDL	OA8-CA7-C31	2.59	120.04	111.91
54	r	714	CDL	OA8-CA7-C31	2.56	119.95	111.91
48	l	718	PEE	O3-C30-C31	2.56	119.95	111.91
48	m	202	PEE	O3-C30-C31	2.56	119.93	111.91
50	G	201	8Q1	O2-P24-O27	-2.55	99.94	106.73
47	A	503	NAI	C2D-C3D-C4D	2.54	107.58	102.64
54	r	714	CDL	OB8-CB7-C71	2.54	119.88	111.91
48	U	101	PEE	O3-C30-C31	2.54	119.87	111.91
46	A	502	FMN	C4A-C10-N10	2.53	120.19	116.48
54	l	713	CDL	OB8-CB7-C71	2.52	119.83	111.91
54	n	102	CDL	OB8-CB7-C71	2.51	119.79	111.91
48	C	311	PEE	O3-C30-C31	2.50	119.76	111.91
54	V	203	CDL	OB8-CB7-C71	2.50	119.75	111.91
54	i	401	CDL	OB8-CB7-C71	2.48	119.69	111.91
49	V	205	PLX	C1A-N1-C1	2.48	120.06	109.92
54	N	202	CDL	CB4-OB6-CB5	-2.47	111.71	117.79
50	G	201	8Q1	C37-C38-C39	2.46	116.45	112.36
46	A	502	FMN	O4-C4-C4A	-2.44	120.13	126.60
49	i	705	PLX	C1A-N1-C1	2.43	119.87	109.92
54	l	712	CDL	CB4-OB6-CB5	-2.42	111.83	117.79
49	j	203	PLX	C1A-N1-C1	2.37	119.62	109.92
50	G	201	8Q1	O1-P24-O2	2.36	116.67	107.64
46	A	502	FMN	C5A-C9A-N10	2.36	120.39	117.95
54	l	712	CDL	OA6-CA5-OA7	-2.36	118.00	123.70
50	X	201	8Q1	O1-P24-O2	2.36	116.65	107.64
50	X	201	8Q1	O4-C1-S44	-2.34	119.57	122.61
51	J	401	NDP	C4A-N9A-C8A	2.34	108.26	105.73
50	G	201	8Q1	C32-C34-N36	2.26	121.08	116.58
47	A	503	NAI	C4A-N9A-C8A	2.25	108.17	105.73
46	A	502	FMN	C4A-C10-N1	-2.25	119.50	124.73
57	w	401	ADP	C4'-O4'-C1'	-2.22	104.56	109.47
50	G	201	8Q1	O27-P24-O3	-2.19	100.32	106.47
50	G	201	8Q1	O4-C1-S44	-2.19	119.77	122.61
51	J	401	NDP	O4B-C1B-C2B	-2.17	102.76	106.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	i	401	CDL	CA4-OA6-CA5	-2.17	112.45	117.79
46	A	502	FMN	C9A-C5A-N5	-2.17	120.08	122.43
54	n	102	CDL	CA4-OA6-CA5	-2.17	112.46	117.79
49	C	312	PLX	C1A-N1-C1	2.16	118.74	109.92
54	n	102	CDL	OA6-CA5-OA7	-2.16	118.49	123.70
51	J	401	NDP	C2D-C3D-C4D	2.15	106.82	102.64
54	l	712	CDL	OB8-CB7-OB9	-2.14	118.19	123.59
50	X	201	8Q1	O4-C1-C6	-2.13	121.47	123.99
46	A	502	FMN	C10-C4A-N5	-2.12	120.37	124.86
50	X	201	8Q1	O40-C39-N41	-2.08	119.09	123.01
50	G	201	8Q1	C38-C39-N41	2.07	119.91	116.42
54	N	202	CDL	OB6-CB5-OB7	-2.05	118.76	123.70
54	a	201	CDL	OB8-CB7-OB9	-2.05	118.43	123.59
54	V	203	CDL	OB6-CB5-OB7	-2.04	118.78	123.70
46	A	502	FMN	C4-C4A-C10	2.03	120.20	116.79
54	a	201	CDL	CB4-OB6-CB5	-2.01	112.84	117.79
54	n	102	CDL	CA6-CA4-CA3	-2.01	107.04	111.79
50	G	201	8Q1	O4-C1-C6	-2.00	121.62	123.99

There are no chirality outliers.

All (795) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C1'-C2'-C3'-O3'
46	A	502	FMN	C1'-C2'-C3'-C4'
48	C	311	PEE	O4P-C4-C5-N
48	U	101	PEE	C17-C18-C19-C20
48	U	101	PEE	C4-O4P-P-O2P
48	U	101	PEE	C4-O4P-P-O1P
48	V	202	PEE	C11-C10-O2-C2
48	V	202	PEE	C4-O4P-P-O2P
48	V	202	PEE	C4-O4P-P-O1P
48	V	207	PEE	C11-C10-O2-C2
48	V	207	PEE	C1-O3P-P-O1P
48	l	718	PEE	C4-O4P-P-O3P
48	l	718	PEE	C4-O4P-P-O2P
48	l	718	PEE	C4-O4P-P-O1P
48	l	719	PEE	C11-C10-O2-C2
48	l	719	PEE	O4-C10-O2-C2
48	l	719	PEE	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
48	l	719	PEE	C4-O4P-P-O1P
48	m	202	PEE	C4-O4P-P-O1P
49	C	312	PLX	O7-C6-C7-C8
49	C	312	PLX	O4-C3-C4-O6
49	C	312	PLX	C3-O4-P1-O2
49	C	312	PLX	C3-O4-P1-O3
49	C	312	PLX	C2-O1-P1-O2
49	C	312	PLX	O9-C24-O8-C5
49	V	205	PLX	O7-C6-O6-C4
49	V	205	PLX	C3-O4-P1-O1
49	V	205	PLX	C3-O4-P1-O2
49	V	205	PLX	C3-O4-P1-O3
49	V	205	PLX	O9-C24-O8-C5
49	e	201	PLX	O7-C6-O6-C4
49	e	201	PLX	C2-O1-P1-O4
49	e	201	PLX	C2-O1-P1-O2
49	e	201	PLX	C2-O1-P1-O3
49	e	201	PLX	O9-C24-C25-C26
49	i	705	PLX	O7-C6-O6-C4
49	i	705	PLX	C3-O4-P1-O1
49	i	705	PLX	C3-O4-P1-O2
49	i	705	PLX	C25-C24-O8-C5
49	j	203	PLX	O7-C6-C7-C8
49	j	203	PLX	O7-C6-O6-C4
49	n	101	PLX	O7-C6-O6-C4
49	n	101	PLX	C3-O4-P1-O1
49	n	101	PLX	O9-C24-O8-C5
50	G	201	8Q1	O4-C1-S44-C43
50	G	201	8Q1	C6-C1-S44-C43
50	G	201	8Q1	O27-C28-C29-C32
50	G	201	8Q1	N36-C37-C38-C39
50	G	201	8Q1	N41-C42-C43-S44
50	G	201	8Q1	C42-C43-S44-C1
50	G	201	8Q1	C28-O27-P24-O2
50	G	201	8Q1	C28-O27-P24-O1
50	X	201	8Q1	O4-C1-C6-C7
50	X	201	8Q1	S44-C1-C6-C7
50	X	201	8Q1	O4-C1-S44-C43
50	X	201	8Q1	C6-C1-S44-C43
50	X	201	8Q1	C28-C29-C32-C34
50	X	201	8Q1	C28-C29-C32-O33
50	X	201	8Q1	C30-C29-C32-C34

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Mol	Chain	Res	Type	Atoms
50	X	201	8Q1	C30-C29-C32-O33
50	X	201	8Q1	C31-C29-C32-C34
50	X	201	8Q1	C29-C32-C34-N36
50	X	201	8Q1	C29-C32-C34-O35
50	X	201	8Q1	O33-C32-C34-N36
50	X	201	8Q1	N36-C37-C38-C39
50	X	201	8Q1	C28-O27-P24-O3
50	X	201	8Q1	C28-O27-P24-O2
50	X	201	8Q1	C28-O27-P24-O1
51	J	401	NDP	C5D-O5D-PN-O3
51	J	401	NDP	O4D-C4D-C5D-O5D
51	J	401	NDP	C2N-C3N-C7N-N7N
54	N	202	CDL	CA2-OA2-PA1-OA4
54	N	202	CDL	CA3-OA5-PA1-OA2
54	N	202	CDL	C11-CA5-OA6-CA4
54	N	202	CDL	CB2-OB2-PB2-OB3
54	N	202	CDL	CB2-OB2-PB2-OB4
54	N	202	CDL	CB2-OB2-PB2-OB5
54	N	202	CDL	CB3-OB5-PB2-OB2
54	V	201	CDL	CA2-OA2-PA1-OA5
54	V	201	CDL	CA3-OA5-PA1-OA4
54	V	201	CDL	CB2-OB2-PB2-OB3
54	V	201	CDL	CB2-OB2-PB2-OB4
54	V	201	CDL	CB2-OB2-PB2-OB5
54	V	201	CDL	CB3-OB5-PB2-OB3
54	V	201	CDL	CB3-OB5-PB2-OB4
54	V	203	CDL	CA2-OA2-PA1-OA4
54	V	203	CDL	CA3-OA5-PA1-OA3
54	V	203	CDL	CB2-OB2-PB2-OB3
54	V	203	CDL	CB2-OB2-PB2-OB4
54	V	203	CDL	CB2-OB2-PB2-OB5
54	V	203	CDL	CB3-OB5-PB2-OB3
54	a	201	CDL	CA2-OA2-PA1-OA3
54	a	201	CDL	CA2-OA2-PA1-OA4
54	a	201	CDL	CA2-OA2-PA1-OA5
54	a	201	CDL	CA3-OA5-PA1-OA2
54	a	201	CDL	CB2-OB2-PB2-OB3
54	i	401	CDL	CB2-C1-CA2-OA2
54	i	401	CDL	CA2-OA2-PA1-OA5
54	i	401	CDL	CB2-OB2-PB2-OB3
54	i	401	CDL	CB3-OB5-PB2-OB3
54	l	712	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
54	l	712	CDL	CB3-OB5-PB2-OB4
54	l	713	CDL	O1-C1-CA2-OA2
54	l	713	CDL	CA2-OA2-PA1-OA3
54	l	713	CDL	CA2-OA2-PA1-OA4
54	l	713	CDL	CA2-OA2-PA1-OA5
54	l	713	CDL	CA3-OA5-PA1-OA2
54	l	713	CDL	CB2-OB2-PB2-OB4
54	l	713	CDL	OB6-CB4-CB6-OB8
54	n	102	CDL	CA2-OA2-PA1-OA4
54	n	102	CDL	CA3-OA5-PA1-OA3
54	n	102	CDL	CA3-OA5-PA1-OA4
54	n	102	CDL	CB2-OB2-PB2-OB4
54	r	714	CDL	CA2-OA2-PA1-OA3
54	r	714	CDL	CA2-OA2-PA1-OA4
54	r	714	CDL	OA6-CA4-CA6-OA8
54	r	714	CDL	C51-CB5-OB6-CB4
56	s	403	UQ	C7-C8-C9-C10
56	s	403	UQ	C7-C8-C9-C11
56	s	403	UQ	C12-C11-C9-C10
56	s	403	UQ	C12-C13-C14-C16
56	s	403	UQ	C13-C14-C16-C17
56	s	403	UQ	C14-C16-C17-C18
56	s	403	UQ	C17-C18-C19-C21
57	w	401	ADP	C5'-O5'-PA-O2A
57	w	401	ADP	C5'-O5'-PA-O3A
48	V	202	PEE	O4-C10-O2-C2
48	V	207	PEE	O4-C10-O2-C2
54	N	202	CDL	OA7-CA5-OA6-CA4
54	r	714	CDL	OB7-CB5-OB6-CB4
54	l	712	CDL	C31-CA7-OA8-CA6
54	r	714	CDL	C71-CB7-OB8-CB6
48	l	720	PEE	C37-C38-C39-C40
54	l	713	CDL	C59-C60-C61-C62
54	l	712	CDL	OA9-CA7-OA8-CA6
54	r	714	CDL	OB9-CB7-OB8-CB6
54	N	202	CDL	O1-C1-CB2-OB2
54	l	712	CDL	O1-C1-CA2-OA2
54	n	102	CDL	O1-C1-CA2-OA2
48	l	720	PEE	C31-C30-O3-C3
48	m	202	PEE	C31-C30-O3-C3
54	l	713	CDL	C71-CB7-OB8-CB6
48	C	311	PEE	C11-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
48	U	101	PEE	C11-C10-O2-C2
48	l	718	PEE	C11-C10-O2-C2
54	N	202	CDL	C51-CB5-OB6-CB4
54	V	203	CDL	C51-CB5-OB6-CB4
48	U	101	PEE	C30-C31-C32-C33
49	V	205	PLX	C9-C10-C11-C12
54	l	713	CDL	C11-C12-C13-C14
54	l	713	CDL	C54-C55-C56-C57
48	l	720	PEE	O5-C30-O3-C3
49	C	312	PLX	C28-C29-C30-C31
49	V	205	PLX	C30-C31-C32-C33
48	U	101	PEE	C19-C20-C21-C22
49	e	201	PLX	C30-C31-C32-C33
51	J	401	NDP	C3D-C4D-C5D-O5D
48	l	718	PEE	O4-C10-O2-C2
49	i	705	PLX	C7-C8-C9-C10
49	n	101	PLX	C11-C10-C9-C8
54	l	713	CDL	OB9-CB7-OB8-CB6
49	j	203	PLX	C28-C29-C30-C31
54	l	713	CDL	C35-C36-C37-C38
48	m	202	PEE	O5-C30-O3-C3
54	r	714	CDL	C36-C37-C38-C39
54	V	203	CDL	C31-CA7-OA8-CA6
54	l	712	CDL	C58-C59-C60-C61
54	V	201	CDL	C11-CA5-OA6-CA4
48	U	101	PEE	C32-C33-C34-C35
54	V	201	CDL	CA2-C1-CB2-OB2
54	i	401	CDL	CA2-C1-CB2-OB2
54	r	714	CDL	CB2-C1-CA2-OA2
48	C	311	PEE	O4-C10-O2-C2
48	U	101	PEE	O4-C10-O2-C2
54	i	401	CDL	C31-CA7-OA8-CA6
54	l	713	CDL	C39-C40-C41-C42
48	l	720	PEE	C10-C11-C12-C13
54	V	203	CDL	C51-C52-C53-C54
54	a	201	CDL	C31-C32-C33-C34
54	V	203	CDL	OB5-CB3-CB4-OB6
48	V	207	PEE	C11-C12-C13-C14
54	V	201	CDL	O1-C1-CB2-OB2
54	i	401	CDL	O1-C1-CA2-OA2
54	l	713	CDL	O1-C1-CB2-OB2
54	i	401	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
54	i	401	CDL	OA9-CA7-OA8-CA6
49	e	201	PLX	C12-C13-C14-C15
54	V	201	CDL	C59-C60-C61-C62
54	r	714	CDL	C13-C14-C15-C16
48	V	207	PEE	C10-C11-C12-C13
51	J	401	NDP	C2D-C1D-N1N-C6N
54	r	714	CDL	CB5-C51-C52-C53
48	V	207	PEE	C17-C18-C19-C20
48	l	719	PEE	C37-C38-C39-C40
48	C	311	PEE	C14-C15-C16-C17
48	V	202	PEE	C30-C31-C32-C33
54	l	713	CDL	CB5-C51-C52-C53
54	r	714	CDL	CB7-C71-C72-C73
48	l	719	PEE	C31-C30-O3-C3
54	N	202	CDL	OB7-CB5-OB6-CB4
49	e	201	PLX	C2-C1-N1-C1C
49	e	201	PLX	C2-C1-N1-C1A
54	l	713	CDL	CB7-C71-C72-C73
54	r	714	CDL	CA5-C11-C12-C13
54	V	203	CDL	C32-C33-C34-C35
54	V	203	CDL	C80-C81-C82-C83
54	N	202	CDL	CB5-C51-C52-C53
54	i	401	CDL	O1-C1-CB2-OB2
54	r	714	CDL	O1-C1-CA2-OA2
54	V	201	CDL	OA7-CA5-OA6-CA4
54	V	203	CDL	OB7-CB5-OB6-CB4
48	s	401	PEE	C37-C38-C39-C40
54	V	203	CDL	OA9-CA7-OA8-CA6
48	U	101	PEE	C4-O4P-P-O3P
48	V	202	PEE	C4-O4P-P-O3P
48	V	207	PEE	C1-O3P-P-O4P
48	l	719	PEE	C4-O4P-P-O3P
48	m	202	PEE	C4-O4P-P-O3P
49	C	312	PLX	C3-O4-P1-O1
49	e	201	PLX	C3-O4-P1-O1
54	N	202	CDL	CA2-OA2-PA1-OA5
54	V	201	CDL	CA3-OA5-PA1-OA2
54	V	201	CDL	CB3-OB5-PB2-OB2
54	V	203	CDL	CA2-OA2-PA1-OA5
54	V	203	CDL	CA3-OA5-PA1-OA2
54	V	203	CDL	CB3-OB5-PB2-OB2
54	i	401	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
54	i	401	CDL	CB3-OB5-PB2-OB2
54	l	712	CDL	CA2-OA2-PA1-OA5
54	l	712	CDL	CB3-OB5-PB2-OB2
54	l	713	CDL	CB2-OB2-PB2-OB5
54	l	713	CDL	CB3-OB5-PB2-OB2
54	n	102	CDL	CA2-OA2-PA1-OA5
54	n	102	CDL	CA3-OA5-PA1-OA2
54	n	102	CDL	CB2-OB2-PB2-OB5
54	r	714	CDL	CA2-OA2-PA1-OA5
54	r	714	CDL	CB3-OB5-PB2-OB2
49	j	203	PLX	C34-C35-C36-C37
48	l	719	PEE	O5-C30-O3-C3
48	V	202	PEE	C10-C11-C12-C13
54	l	712	CDL	CB2-C1-CA2-OA2
54	l	713	CDL	CB2-C1-CA2-OA2
54	r	714	CDL	C74-C75-C76-C77
49	C	312	PLX	O6-C6-C7-C8
48	s	401	PEE	C35-C36-C37-C38
54	r	714	CDL	CA7-C31-C32-C33
49	C	312	PLX	C33-C34-C35-C36
54	l	713	CDL	C57-C58-C59-C60
54	l	712	CDL	C11-CA5-OA6-CA4
54	n	102	CDL	C11-CA5-OA6-CA4
49	C	312	PLX	C17-C18-C19-C20
49	j	203	PLX	C12-C13-C14-C15
54	r	714	CDL	C73-C74-C75-C76
50	G	201	8Q1	O27-C28-C29-C30
50	G	201	8Q1	O27-C28-C29-C31
49	V	205	PLX	C7-C8-C9-C10
49	e	201	PLX	C33-C34-C35-C36
49	j	203	PLX	C10-C11-C12-C13
54	r	714	CDL	C71-C72-C73-C74
54	N	202	CDL	CA6-CA4-OA6-CA5
54	V	201	CDL	CA6-CA4-OA6-CA5
54	n	102	CDL	OA7-CA5-OA6-CA4
46	A	502	FMN	O2'-C2'-C3'-C4'
49	i	705	PLX	C27-C28-C29-C30
54	l	713	CDL	C72-C73-C74-C75
49	V	205	PLX	C10-C11-C12-C13
48	V	202	PEE	C12-C13-C14-C15
48	l	719	PEE	C31-C32-C33-C34
48	C	311	PEE	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
50	X	201	8Q1	C12-C13-C14-C15
54	r	714	CDL	C55-C56-C57-C58
49	C	312	PLX	C16-C17-C18-C19
49	i	705	PLX	C11-C10-C9-C8
54	l	713	CDL	C53-C54-C55-C56
54	r	714	CDL	C75-C76-C77-C78
49	e	201	PLX	C31-C32-C33-C34
49	i	705	PLX	C33-C34-C35-C36
49	j	203	PLX	C13-C14-C15-C16
54	l	713	CDL	C58-C59-C60-C61
48	s	401	PEE	C33-C34-C35-C36
48	s	401	PEE	C21-C22-C23-C24
49	C	312	PLX	C11-C12-C13-C14
49	C	312	PLX	C7-C8-C9-C10
49	e	201	PLX	C15-C16-C17-C18
49	i	705	PLX	C28-C29-C30-C31
49	j	203	PLX	C27-C28-C29-C30
54	r	714	CDL	C35-C36-C37-C38
54	r	714	CDL	C43-C44-C45-C46
54	r	714	CDL	C62-C63-C64-C65
49	V	205	PLX	C15-C16-C17-C18
54	r	714	CDL	C17-C18-C19-C20
48	l	720	PEE	C13-C14-C15-C16
49	V	205	PLX	C31-C32-C33-C34
54	l	713	CDL	C33-C34-C35-C36
54	l	713	CDL	C52-C53-C54-C55
54	r	714	CDL	C41-C42-C43-C44
48	l	720	PEE	C22-C23-C24-C25
54	V	201	CDL	C52-C53-C54-C55
48	l	720	PEE	C31-C32-C33-C34
49	j	203	PLX	C25-C26-C27-C28
48	U	101	PEE	C41-C42-C43-C44
48	V	202	PEE	C20-C21-C22-C23
54	l	712	CDL	C52-C53-C54-C55
54	l	713	CDL	C56-C57-C58-C59
48	l	720	PEE	C11-C10-O2-C2
48	m	202	PEE	C11-C10-O2-C2
48	l	720	PEE	C2-C3-O3-C30
49	C	312	PLX	O9-C24-C25-C26
49	V	205	PLX	C28-C29-C30-C31
49	e	201	PLX	C11-C10-C9-C8
49	e	201	PLX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
54	l	713	CDL	C55-C56-C57-C58
54	l	713	CDL	C74-C75-C76-C77
46	A	502	FMN	O2'-C2'-C3'-O3'
48	U	101	PEE	C22-C23-C24-C25
54	n	102	CDL	C75-C76-C77-C78
54	V	201	CDL	O1-C1-CA2-OA2
47	A	503	NAI	C3D-C4D-C5D-O5D
49	C	312	PLX	C13-C14-C15-C16
54	l	713	CDL	C14-C15-C16-C17
54	l	713	CDL	C60-C61-C62-C63
49	V	205	PLX	C27-C28-C29-C30
48	l	720	PEE	O4-C10-O2-C2
48	m	202	PEE	O4-C10-O2-C2
54	l	712	CDL	OA7-CA5-OA6-CA4
50	G	201	8Q1	C10-C11-C12-C13
48	V	207	PEE	C32-C33-C34-C35
49	e	201	PLX	C32-C33-C34-C35
54	l	713	CDL	C40-C41-C42-C43
49	i	705	PLX	C25-C26-C27-C28
49	j	203	PLX	C7-C8-C9-C10
48	s	401	PEE	C31-C30-O3-C3
48	m	202	PEE	C12-C13-C14-C15
49	V	205	PLX	C16-C17-C18-C19
54	l	712	CDL	C51-C52-C53-C54
54	l	713	CDL	CA7-C31-C32-C33
48	l	718	PEE	C31-C32-C33-C34
48	l	718	PEE	C34-C35-C36-C37
49	i	705	PLX	C9-C10-C11-C12
48	l	720	PEE	C32-C33-C34-C35
49	V	205	PLX	C12-C13-C14-C15
54	l	713	CDL	C31-C32-C33-C34
48	C	311	PEE	C15-C16-C17-C18
48	U	101	PEE	C31-C30-O3-C3
49	i	705	PLX	C10-C11-C12-C13
48	l	720	PEE	C14-C15-C16-C17
54	a	201	CDL	CA7-C31-C32-C33
49	e	201	PLX	C14-C15-C16-C17
54	i	401	CDL	C11-C12-C13-C14
49	C	312	PLX	C30-C31-C32-C33
54	V	203	CDL	C11-CA5-OA6-CA4
48	V	202	PEE	C21-C22-C23-C24
49	C	312	PLX	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
50	G	201	8Q1	C11-C12-C13-C14
50	X	201	8Q1	C7-C8-C9-C10
54	a	201	CDL	CB5-C51-C52-C53
54	l	713	CDL	OA6-CA4-CA6-OA8
54	l	713	CDL	C37-C38-C39-C40
49	e	201	PLX	C2-C1-N1-C1B
48	l	719	PEE	C21-C22-C23-C24
54	l	713	CDL	C62-C63-C64-C65
48	C	311	PEE	C39-C40-C41-C42
48	m	202	PEE	C19-C20-C21-C22
49	V	205	PLX	C34-C35-C36-C37
54	r	714	CDL	C11-C12-C13-C14
48	C	311	PEE	C37-C38-C39-C40
48	l	720	PEE	C33-C34-C35-C36
48	U	101	PEE	O5-C30-O3-C3
48	s	401	PEE	O5-C30-O3-C3
48	l	718	PEE	C22-C23-C24-C25
54	r	714	CDL	C63-C64-C65-C66
48	U	101	PEE	C36-C37-C38-C39
49	C	312	PLX	C2-O1-P1-O4
54	r	714	CDL	CB2-OB2-PB2-OB5
48	V	207	PEE	C31-C30-O3-C3
49	C	312	PLX	O4-C3-C4-C5
49	e	201	PLX	C25-C26-C27-C28
49	j	203	PLX	C30-C31-C32-C33
54	V	201	CDL	C62-C63-C64-C65
49	e	201	PLX	C7-C8-C9-C10
48	V	207	PEE	C33-C34-C35-C36
48	l	719	PEE	C15-C16-C17-C18
48	s	401	PEE	C15-C16-C17-C18
48	s	401	PEE	C39-C40-C41-C42
49	V	205	PLX	C18-C19-C20-C21
54	l	712	CDL	C35-C36-C37-C38
49	V	205	PLX	C13-C14-C15-C16
49	C	312	PLX	C25-C26-C27-C28
49	j	203	PLX	C14-C15-C16-C17
48	C	311	PEE	C1-C2-C3-O3
48	l	720	PEE	C1-C2-C3-O3
48	m	202	PEE	C22-C23-C24-C25
49	V	205	PLX	C3-C4-C5-O8
49	V	205	PLX	C33-C34-C35-C36
49	e	201	PLX	C3-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
49	j	203	PLX	C3-C4-C5-O8
54	l	713	CDL	CA3-CA4-CA6-OA8
54	l	713	CDL	CB3-CB4-CB6-OB8
54	n	102	CDL	CA3-CA4-CA6-OA8
54	r	714	CDL	CB3-CB4-CB6-OB8
48	l	718	PEE	C24-C25-C26-C27
48	s	401	PEE	C14-C15-C16-C17
48	V	207	PEE	C35-C36-C37-C38
48	s	401	PEE	C20-C21-C22-C23
49	e	201	PLX	C10-C11-C12-C13
54	l	712	CDL	CB5-C51-C52-C53
48	V	202	PEE	C31-C30-O3-C3
54	r	714	CDL	C31-CA7-OA8-CA6
54	l	713	CDL	C64-C65-C66-C67
54	r	714	CDL	C33-C34-C35-C36
54	r	714	CDL	C60-C61-C62-C63
50	X	201	8Q1	C13-C14-C15-C16
54	r	714	CDL	C59-C60-C61-C62
50	G	201	8Q1	C28-O27-P24-O3
48	V	202	PEE	C17-C18-C19-C20
54	l	712	CDL	C79-C80-C81-C82
48	V	207	PEE	O5-C30-O3-C3
48	l	719	PEE	C30-C31-C32-C33
48	m	202	PEE	O2-C2-C3-O3
54	V	201	CDL	OB6-CB4-CB6-OB8
54	i	401	CDL	OA6-CA4-CA6-OA8
54	r	714	CDL	OB6-CB4-CB6-OB8
49	n	101	PLX	C7-C8-C9-C10
54	V	203	CDL	C79-C80-C81-C82
50	X	201	8Q1	C31-C29-C32-O33
54	a	201	CDL	C37-C38-C39-C40
49	n	101	PLX	C34-C35-C36-C37
54	i	401	CDL	C37-C38-C39-C40
54	l	713	CDL	C81-C82-C83-C84
54	n	102	CDL	C53-C54-C55-C56
54	l	712	CDL	C37-C38-C39-C40
54	V	203	CDL	OA7-CA5-OA6-CA4
48	l	719	PEE	C13-C14-C15-C16
49	e	201	PLX	C13-C14-C15-C16
54	r	714	CDL	C64-C65-C66-C67
48	l	720	PEE	C23-C24-C25-C26
54	r	714	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
48	C	311	PEE	C43-C44-C45-C46
49	i	705	PLX	C32-C33-C34-C35
54	r	714	CDL	C51-C52-C53-C54
48	l	718	PEE	O3P-C1-C2-C3
54	i	401	CDL	OB5-CB3-CB4-CB6
56	s	403	UQ	C9-C11-C12-C13
49	n	101	PLX	C14-C15-C16-C17
54	l	712	CDL	CB7-C71-C72-C73
49	j	203	PLX	C33-C34-C35-C36
49	i	705	PLX	C13-C14-C15-C16
48	s	401	PEE	C34-C35-C36-C37
48	m	202	PEE	C33-C34-C35-C36
54	V	201	CDL	C37-C38-C39-C40
54	r	714	CDL	C57-C58-C59-C60
48	s	401	PEE	C11-C10-O2-C2
48	l	719	PEE	C33-C34-C35-C36
54	r	714	CDL	C76-C77-C78-C79
48	V	202	PEE	O5-C30-O3-C3
48	V	202	PEE	C44-C45-C46-C47
49	n	101	PLX	C10-C11-C12-C13
54	l	713	CDL	C44-C45-C46-C47
48	l	718	PEE	C1-C2-C3-O3
49	e	201	PLX	C11-C12-C13-C14
48	m	202	PEE	C17-C18-C19-C20
48	s	401	PEE	C17-C18-C19-C20
54	r	714	CDL	OA9-CA7-OA8-CA6
48	V	202	PEE	C24-C25-C26-C27
48	l	720	PEE	C34-C35-C36-C37
54	l	713	CDL	C18-C19-C20-C21
50	G	201	8Q1	C29-C32-C34-N36
54	l	712	CDL	C14-C15-C16-C17
56	s	403	UQ	C12-C11-C9-C8
49	V	205	PLX	C5-C4-O6-C6
49	e	201	PLX	C5-C4-O6-C6
49	n	101	PLX	C5-C4-O6-C6
49	V	205	PLX	O9-C24-C25-C26
49	e	201	PLX	O7-C6-C7-C8
48	m	202	PEE	C20-C21-C22-C23
49	C	312	PLX	C36-C37-C38-C39
48	V	207	PEE	O3P-C1-C2-O2
54	V	201	CDL	OB5-CB3-CB4-OB6
54	a	201	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
54	i	401	CDL	OB5-CB3-CB4-OB6
54	l	712	CDL	OA5-CA3-CA4-OA6
54	l	713	CDL	OA5-CA3-CA4-OA6
49	C	312	PLX	O6-C4-C5-O8
48	V	202	PEE	C13-C14-C15-C16
54	r	714	CDL	C31-C32-C33-C34
54	N	202	CDL	CA2-C1-CB2-OB2
54	l	713	CDL	CA2-C1-CB2-OB2
54	n	102	CDL	CB2-C1-CA2-OA2
48	s	401	PEE	O4-C10-O2-C2
54	l	712	CDL	CA4-CA3-OA5-PA1
54	r	714	CDL	CB4-CB3-OB5-PB2
48	l	718	PEE	C11-C12-C13-C14
49	n	101	PLX	C25-C26-C27-C28
48	m	202	PEE	C13-C14-C15-C16
50	G	201	8Q1	C6-C7-C8-C9
54	r	714	CDL	C80-C81-C82-C83
48	V	202	PEE	C36-C37-C38-C39
48	l	720	PEE	C16-C17-C18-C19
49	C	312	PLX	C14-C15-C16-C17
49	e	201	PLX	C16-C17-C18-C19
54	r	714	CDL	C78-C79-C80-C81
48	C	311	PEE	C10-C11-C12-C13
47	A	503	NAI	PN-O3-PA-O5B
49	C	312	PLX	O8-C24-C25-C26
49	j	203	PLX	O4-C3-C4-C5
54	N	202	CDL	OA5-CA3-CA4-CA6
54	V	203	CDL	OB5-CB3-CB4-CB6
54	i	401	CDL	OA5-CA3-CA4-CA6
48	U	101	PEE	C38-C39-C40-C41
48	s	401	PEE	C31-C32-C33-C34
50	X	201	8Q1	C1-C6-C7-C8
54	V	203	CDL	C75-C76-C77-C78
54	r	714	CDL	C12-C13-C14-C15
48	C	311	PEE	C12-C13-C14-C15
54	l	712	CDL	C20-C21-C22-C23
48	C	311	PEE	C13-C14-C15-C16
48	l	718	PEE	C32-C33-C34-C35
54	V	201	CDL	C78-C79-C80-C81
48	V	207	PEE	C31-C32-C33-C34
48	U	101	PEE	C42-C43-C44-C45
49	C	312	PLX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
54	l	712	CDL	C76-C77-C78-C79
48	l	718	PEE	C18-C19-C20-C21
54	a	201	CDL	C54-C55-C56-C57
54	V	203	CDL	CA6-CA4-OA6-CA5
48	U	101	PEE	C44-C45-C46-C47
54	i	401	CDL	C36-C37-C38-C39
49	e	201	PLX	C26-C27-C28-C29
54	V	201	CDL	CA3-CA4-CA6-OA8
54	i	401	CDL	CB3-CB4-CB6-OB8
54	r	714	CDL	CA3-CA4-CA6-OA8
48	l	718	PEE	O3P-C1-C2-O2
54	i	401	CDL	OA5-CA3-CA4-OA6
54	V	203	CDL	C72-C73-C74-C75
54	l	713	CDL	C12-C13-C14-C15
54	V	203	CDL	C78-C79-C80-C81
48	l	718	PEE	C21-C22-C23-C24
48	C	311	PEE	O2-C2-C3-O3
48	l	720	PEE	O2-C2-C3-O3
49	e	201	PLX	O6-C4-C5-O8
54	n	102	CDL	OA6-CA4-CA6-OA8
48	C	311	PEE	C33-C34-C35-C36
48	V	202	PEE	C41-C42-C43-C44
49	j	203	PLX	C24-C25-C26-C27
54	l	713	CDL	C43-C44-C45-C46
54	l	713	CDL	C15-C16-C17-C18
54	V	201	CDL	C58-C59-C60-C61
50	X	201	8Q1	C10-C11-C12-C13
48	U	101	PEE	C1-O3P-P-O4P
49	V	205	PLX	C2-O1-P1-O4
54	i	401	CDL	CB2-OB2-PB2-OB5
48	s	401	PEE	C23-C24-C25-C26
48	s	401	PEE	C22-C23-C24-C25
48	V	207	PEE	C2-C1-O3P-P
48	C	311	PEE	C4-O4P-P-O2P
48	U	101	PEE	C1-O3P-P-O2P
48	U	101	PEE	C1-O3P-P-O1P
49	C	312	PLX	C2-O1-P1-O3
49	V	205	PLX	C2-O1-P1-O3
49	e	201	PLX	C3-O4-P1-O2
49	n	101	PLX	C3-O4-P1-O3
51	J	401	NDP	C5D-O5D-PN-O1N
51	J	401	NDP	C5D-O5D-PN-O2N

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Mol	Chain	Res	Type	Atoms
54	N	202	CDL	CA3-OA5-PA1-OA4
54	N	202	CDL	CB3-OB5-PB2-OB4
54	V	201	CDL	CA2-OA2-PA1-OA4
54	V	203	CDL	CA3-OA5-PA1-OA4
54	V	203	CDL	CB3-OB5-PB2-OB4
54	a	201	CDL	CA3-OA5-PA1-OA4
54	a	201	CDL	CB2-OB2-PB2-OB4
54	i	401	CDL	CA2-OA2-PA1-OA4
54	i	401	CDL	CA3-OA5-PA1-OA4
54	i	401	CDL	CB3-OB5-PB2-OB4
54	l	712	CDL	CA2-OA2-PA1-OA3
54	l	713	CDL	CB2-OB2-PB2-OB3
54	l	713	CDL	CB3-OB5-PB2-OB3
54	l	713	CDL	CB3-OB5-PB2-OB4
54	n	102	CDL	CB3-OB5-PB2-OB3
54	r	714	CDL	CB2-OB2-PB2-OB3
54	r	714	CDL	CB2-OB2-PB2-OB4
54	r	714	CDL	CB3-OB5-PB2-OB3
57	w	401	ADP	C5'-O5'-PA-O1A
54	a	201	CDL	OA5-CA3-CA4-CA6
54	l	712	CDL	OA5-CA3-CA4-CA6
54	r	714	CDL	OB5-CB3-CB4-CB6
48	l	719	PEE	C22-C23-C24-C25
48	l	720	PEE	C5-C4-O4P-P
49	e	201	PLX	C25-C24-O8-C5
49	j	203	PLX	C25-C24-O8-C5
54	V	201	CDL	CA5-C11-C12-C13
49	j	203	PLX	O4-C3-C4-O6
54	r	714	CDL	OB5-CB3-CB4-OB6
48	C	311	PEE	C18-C19-C20-C21
54	l	712	CDL	C51-CB5-OB6-CB4
49	j	203	PLX	C9-C10-C11-C12
48	m	202	PEE	O3-C30-C31-C32
48	m	202	PEE	C1-C2-C3-O3
49	C	312	PLX	C3-C4-C5-O8
49	C	312	PLX	N1-C1-C2-O1
49	n	101	PLX	N1-C1-C2-O1
51	J	401	NDP	C2N-C3N-C7N-O7N
54	V	201	CDL	CB3-CB4-CB6-OB8
48	l	718	PEE	O2-C2-C3-O3
49	V	205	PLX	O6-C4-C5-O8
49	j	203	PLX	O6-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
49	C	312	PLX	C35-C36-C37-C38
54	a	201	CDL	C71-C72-C73-C74
48	l	720	PEE	C18-C19-C20-C21
48	l	719	PEE	C2-C1-O3P-P
49	n	101	PLX	C15-C16-C17-C18
49	i	705	PLX	C16-C17-C18-C19
49	V	205	PLX	C14-C15-C16-C17
49	e	201	PLX	O8-C24-C25-C26
48	C	311	PEE	C16-C17-C18-C19
54	r	714	CDL	C44-C45-C46-C47
50	G	201	8Q1	C7-C8-C9-C10
54	l	712	CDL	C24-C25-C26-C27
54	N	202	CDL	O1-C1-CA2-OA2
47	A	503	NAI	O4D-C4D-C5D-O5D
49	e	201	PLX	C36-C37-C38-C39
54	n	102	CDL	CB7-C71-C72-C73
48	V	207	PEE	C38-C39-C40-C41
49	i	705	PLX	C36-C37-C38-C39
54	l	713	CDL	C73-C74-C75-C76
48	l	718	PEE	C10-C11-C12-C13
54	l	712	CDL	CA6-CA4-OA6-CA5
54	n	102	CDL	CA6-CA4-OA6-CA5
48	s	401	PEE	O3P-C1-C2-C3
54	l	713	CDL	OA5-CA3-CA4-CA6
54	l	712	CDL	C36-C37-C38-C39
54	l	712	CDL	OB7-CB5-OB6-CB4
49	e	201	PLX	C24-C25-C26-C27
48	s	401	PEE	O3P-C1-C2-O2
54	V	203	CDL	OA5-CA3-CA4-OA6
49	n	101	PLX	C2-O1-P1-O4
54	a	201	CDL	CB2-OB2-PB2-OB5
54	a	201	CDL	CB3-OB5-PB2-OB2
54	l	712	CDL	CB2-OB2-PB2-OB5
54	a	201	CDL	CA5-C11-C12-C13
54	r	714	CDL	C56-C57-C58-C59
54	l	712	CDL	C56-C57-C58-C59
54	a	201	CDL	C75-C76-C77-C78
54	i	401	CDL	CA3-CA4-CA6-OA8
54	l	713	CDL	C21-C22-C23-C24
48	l	718	PEE	C38-C39-C40-C41
54	i	401	CDL	C71-C72-C73-C74
54	V	201	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
47	A	503	NAI	O4D-C1D-N1N-C2N
51	J	401	NDP	PN-O3-PA-O2A
49	V	205	PLX	C20-C21-C22-C23
54	l	712	CDL	C83-C84-C85-C86
54	r	714	CDL	C20-C21-C22-C23
48	l	718	PEE	C2-C1-O3P-P
54	V	201	CDL	C1-CB2-OB2-PB2
54	a	201	CDL	C18-C19-C20-C21
48	l	719	PEE	C38-C39-C40-C41
54	l	713	CDL	C41-C42-C43-C44
54	V	201	CDL	OB7-CB5-OB6-CB4
49	e	201	PLX	C18-C19-C20-C21
48	C	311	PEE	C19-C20-C21-C22
49	j	203	PLX	C15-C16-C17-C18
47	A	503	NAI	C2D-C1D-N1N-C2N
54	a	201	CDL	C71-CB7-OB8-CB6
54	a	201	CDL	C39-C40-C41-C42
48	U	101	PEE	C23-C24-C25-C26
48	U	101	PEE	O4P-C4-C5-N
54	l	712	CDL	C82-C83-C84-C85
50	G	201	8Q1	C29-C32-C34-O35
54	i	401	CDL	C33-C34-C35-C36
49	i	705	PLX	O8-C24-C25-C26
54	V	203	CDL	OA6-CA4-CA6-OA8
49	i	705	PLX	C12-C13-C14-C15
49	V	205	PLX	C4-C3-O4-P1
48	l	720	PEE	C36-C37-C38-C39
54	V	203	CDL	C32-C31-CA7-OA8
54	V	203	CDL	C33-C34-C35-C36
51	J	401	NDP	O4D-C1D-N1N-C6N
50	G	201	8Q1	C12-C13-C14-C15
51	J	401	NDP	O4B-C4B-C5B-O5B
49	j	203	PLX	C35-C36-C37-C38
49	i	705	PLX	C30-C31-C32-C33
49	C	312	PLX	C27-C28-C29-C30
48	l	718	PEE	C35-C36-C37-C38
48	l	719	PEE	C3-C2-O2-C10
54	a	201	CDL	CA6-CA4-OA6-CA5
54	i	401	CDL	CA6-CA4-OA6-CA5
49	e	201	PLX	C27-C28-C29-C30
49	C	312	PLX	C5-C4-O6-C6
49	j	203	PLX	C3-O4-P1-O1

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Mol	Chain	Res	Type	Atoms
54	l	712	CDL	CA3-OA5-PA1-OA2
48	V	202	PEE	O3P-C1-C2-O2
49	n	101	PLX	C35-C36-C37-C38
54	V	201	CDL	OB5-CB3-CB4-CB6
54	V	203	CDL	OA5-CA3-CA4-CA6
50	X	201	8Q1	C42-C43-S44-C1
48	l	720	PEE	C38-C39-C40-C41
49	V	205	PLX	C26-C27-C28-C29
54	V	201	CDL	C44-C45-C46-C47
54	l	712	CDL	C54-C55-C56-C57
54	r	714	CDL	C23-C24-C25-C26
48	C	311	PEE	C38-C39-C40-C41
54	l	713	CDL	C42-C43-C44-C45
54	l	712	CDL	C39-C40-C41-C42
54	a	201	CDL	OB9-CB7-OB8-CB6
48	V	207	PEE	C37-C38-C39-C40
54	i	401	CDL	C14-C15-C16-C17
54	i	401	CDL	C31-C32-C33-C34
54	n	102	CDL	C58-C59-C60-C61
49	C	312	PLX	C26-C27-C28-C29
54	l	713	CDL	C17-C18-C19-C20
54	n	102	CDL	OA5-CA3-CA4-OA6
48	C	311	PEE	C32-C33-C34-C35
54	n	102	CDL	C77-C78-C79-C80
49	j	203	PLX	O6-C6-C7-C8
48	V	207	PEE	O3P-C1-C2-C3
48	s	401	PEE	C36-C37-C38-C39
54	l	713	CDL	C34-C35-C36-C37
54	N	202	CDL	C52-C51-CB5-OB6
54	l	712	CDL	C55-C56-C57-C58
54	l	712	CDL	C81-C82-C83-C84
54	n	102	CDL	C19-C20-C21-C22
54	l	713	CDL	C12-C11-CA5-OA6
48	l	720	PEE	O2-C10-C11-C12
48	C	311	PEE	C36-C37-C38-C39
48	l	719	PEE	C16-C17-C18-C19
48	m	202	PEE	C18-C19-C20-C21
49	C	312	PLX	C15-C16-C17-C18
54	n	102	CDL	C71-C72-C73-C74
48	U	101	PEE	C34-C35-C36-C37
48	l	718	PEE	C36-C37-C38-C39
48	m	202	PEE	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
48	l	719	PEE	O3P-C1-C2-O2
54	l	713	CDL	C32-C31-CA7-OA8
54	r	714	CDL	C42-C43-C44-C45
54	n	102	CDL	C14-C15-C16-C17
50	G	201	8Q1	C9-C10-C11-C12
48	V	202	PEE	O3P-C1-C2-C3
54	r	714	CDL	OA5-CA3-CA4-CA6
54	n	102	CDL	C55-C56-C57-C58
54	N	202	CDL	OB6-CB4-CB6-OB8
54	V	203	CDL	OB6-CB4-CB6-OB8
54	a	201	CDL	C17-C18-C19-C20
49	j	203	PLX	C18-C19-C20-C21
49	V	205	PLX	O7-C6-C7-C8
49	i	705	PLX	O9-C24-C25-C26
49	n	101	PLX	O9-C24-C25-C26
54	l	713	CDL	C31-CA7-OA8-CA6
48	s	401	PEE	C13-C14-C15-C16
48	l	720	PEE	O3-C30-C31-C32
48	V	202	PEE	C39-C40-C41-C42
54	l	713	CDL	OA9-CA7-OA8-CA6
54	V	201	CDL	CB4-CB3-OB5-PB2
48	V	207	PEE	C13-C14-C15-C16
48	V	207	PEE	C16-C17-C18-C19
51	J	401	NDP	PN-O3-PA-O1A
48	U	101	PEE	O2-C10-C11-C12
54	l	713	CDL	C51-C52-C53-C54
54	r	714	CDL	C79-C80-C81-C82
54	n	102	CDL	C54-C55-C56-C57
54	N	202	CDL	OA5-CA3-CA4-OA6
54	V	203	CDL	CB2-C1-CA2-OA2
54	l	713	CDL	C12-C11-CA5-OA7
48	s	401	PEE	C42-C43-C44-C45
49	V	205	PLX	C6-C7-C8-C9
54	V	201	CDL	C41-C42-C43-C44
54	a	201	CDL	C22-C23-C24-C25
48	l	720	PEE	O4-C10-C11-C12
48	C	311	PEE	C40-C41-C42-C43
54	N	202	CDL	C52-C51-CB5-OB7
54	r	714	CDL	C72-C73-C74-C75
48	s	401	PEE	C4-O4P-P-O1P
49	V	205	PLX	C2-O1-P1-O2
49	n	101	PLX	C2-O1-P1-O2

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Mol	Chain	Res	Type	Atoms
54	a	201	CDL	CB3-OB5-PB2-OB3
54	l	712	CDL	CA3-OA5-PA1-OA4
54	l	713	CDL	CA3-OA5-PA1-OA4
54	r	714	CDL	CA3-OA5-PA1-OA3
48	U	101	PEE	O4-C10-C11-C12
54	r	714	CDL	C32-C33-C34-C35
54	l	713	CDL	C32-C31-CA7-OA9
48	C	311	PEE	C17-C18-C19-C20
54	V	201	CDL	C35-C36-C37-C38
49	C	312	PLX	C25-C24-O8-C5
54	V	201	CDL	C39-C40-C41-C42
54	n	102	CDL	C12-C11-CA5-OA6
47	A	503	NAI	C2D-C1D-N1N-C6N
48	C	311	PEE	O3-C30-C31-C32
54	V	201	CDL	C72-C73-C74-C75
54	r	714	CDL	C12-C11-CA5-OA6
48	l	720	PEE	O5-C30-C31-C32
54	r	714	CDL	C1-CA2-OA2-PA1
48	C	311	PEE	O5-C30-C31-C32
54	V	201	CDL	CA7-C31-C32-C33

There are no ring outliers.

32 monomers are involved in 286 short contacts:

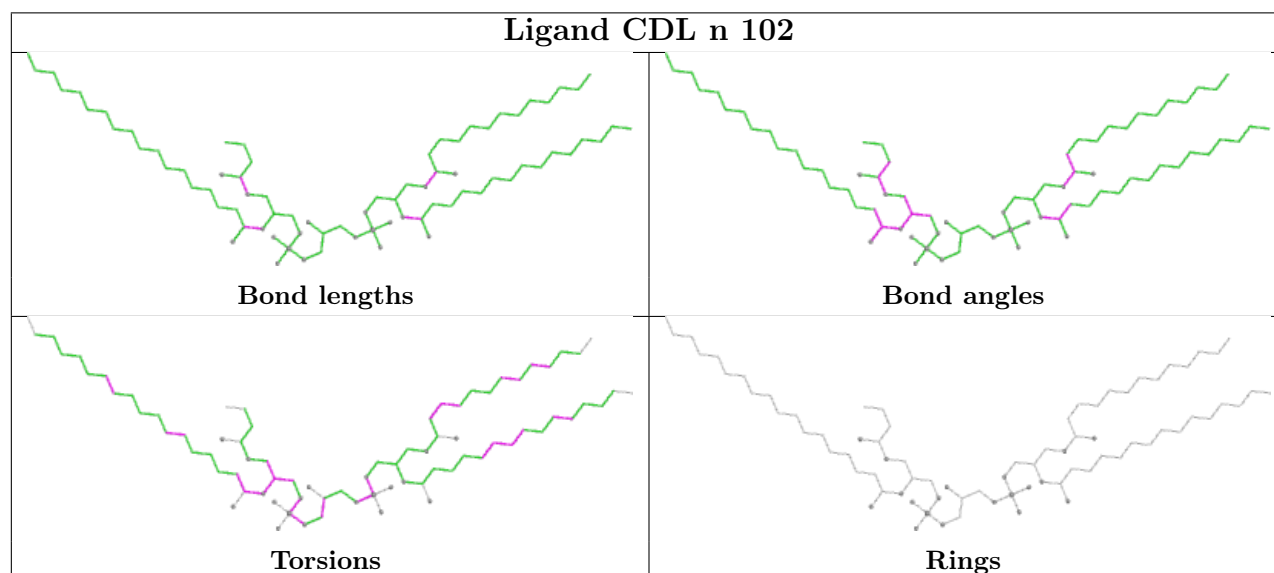
Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	n	102	CDL	13	0
48	m	202	PEE	8	0
51	J	401	NDP	6	0
48	l	719	PEE	8	0
49	j	203	PLX	2	0
54	a	201	CDL	18	0
54	V	203	CDL	15	0
48	l	720	PEE	20	0
48	U	101	PEE	6	0
48	V	207	PEE	7	0
45	A	501	SF4	2	0
49	i	705	PLX	1	0
50	X	201	8Q1	1	0
56	s	403	UQ	4	0
46	A	502	FMN	4	0
48	C	311	PEE	21	0
54	N	202	CDL	12	0

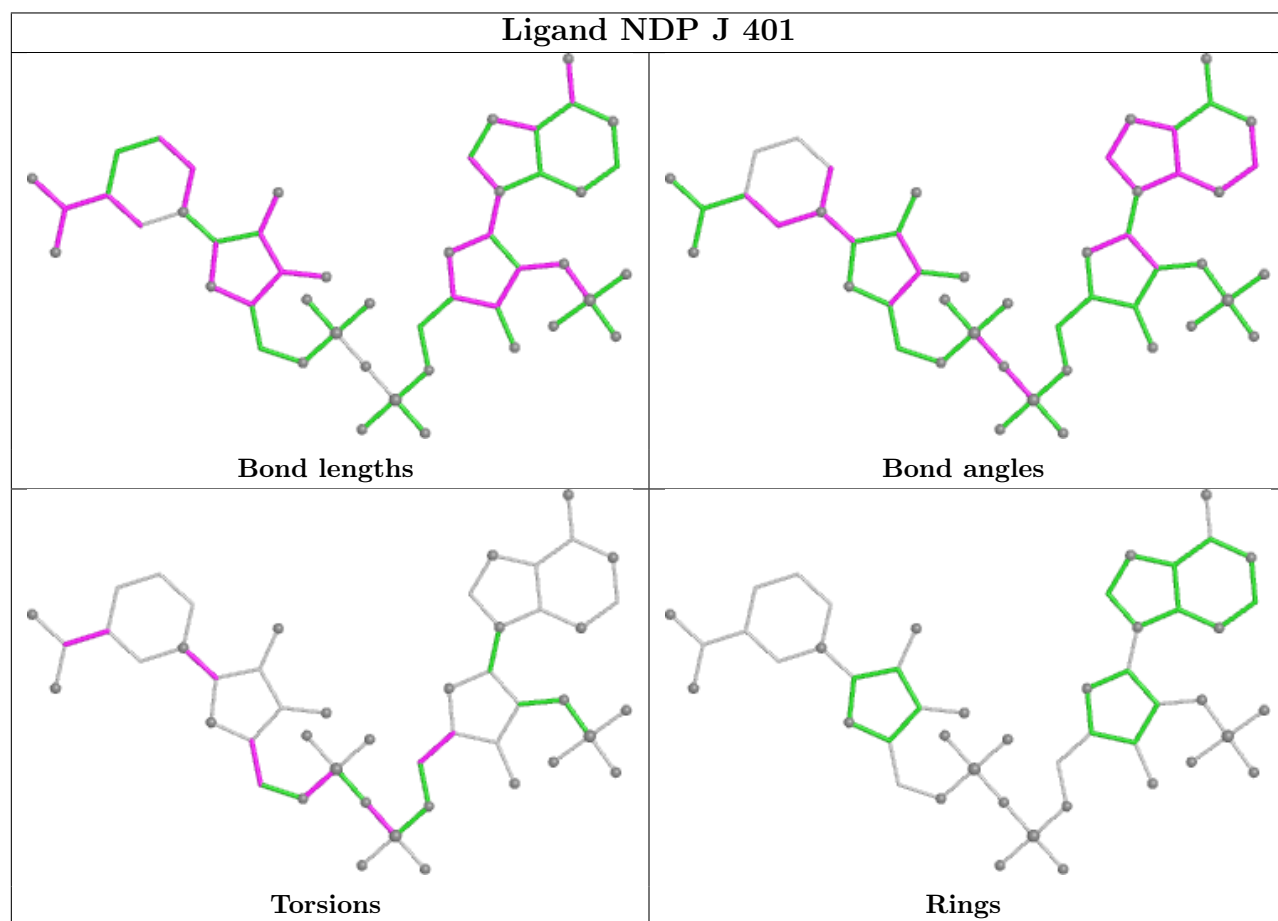
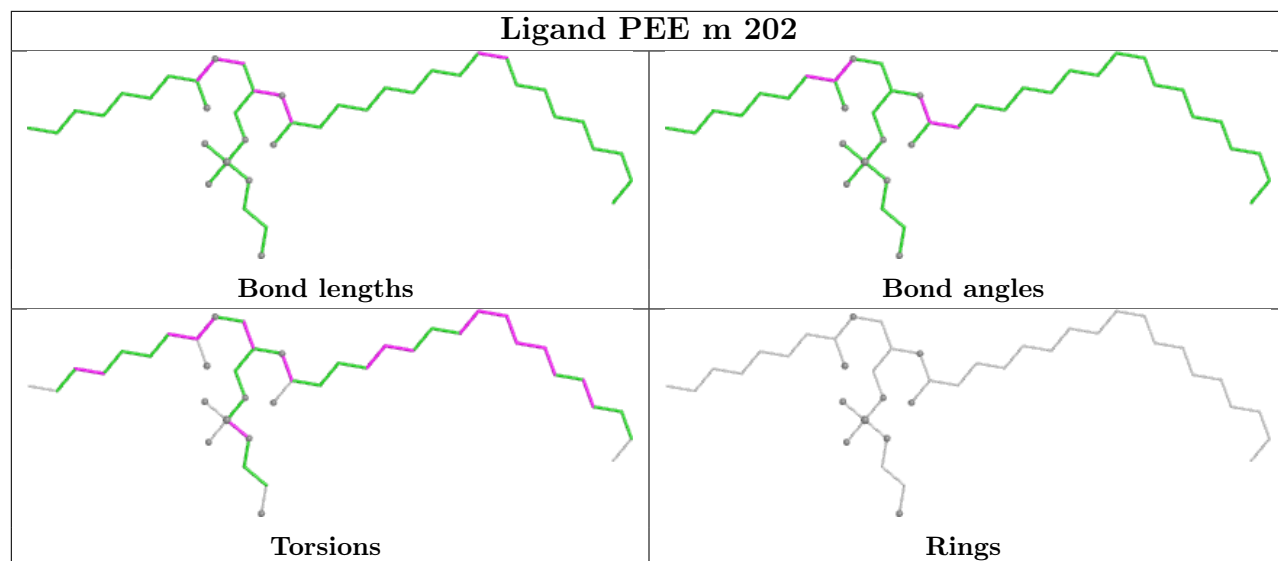
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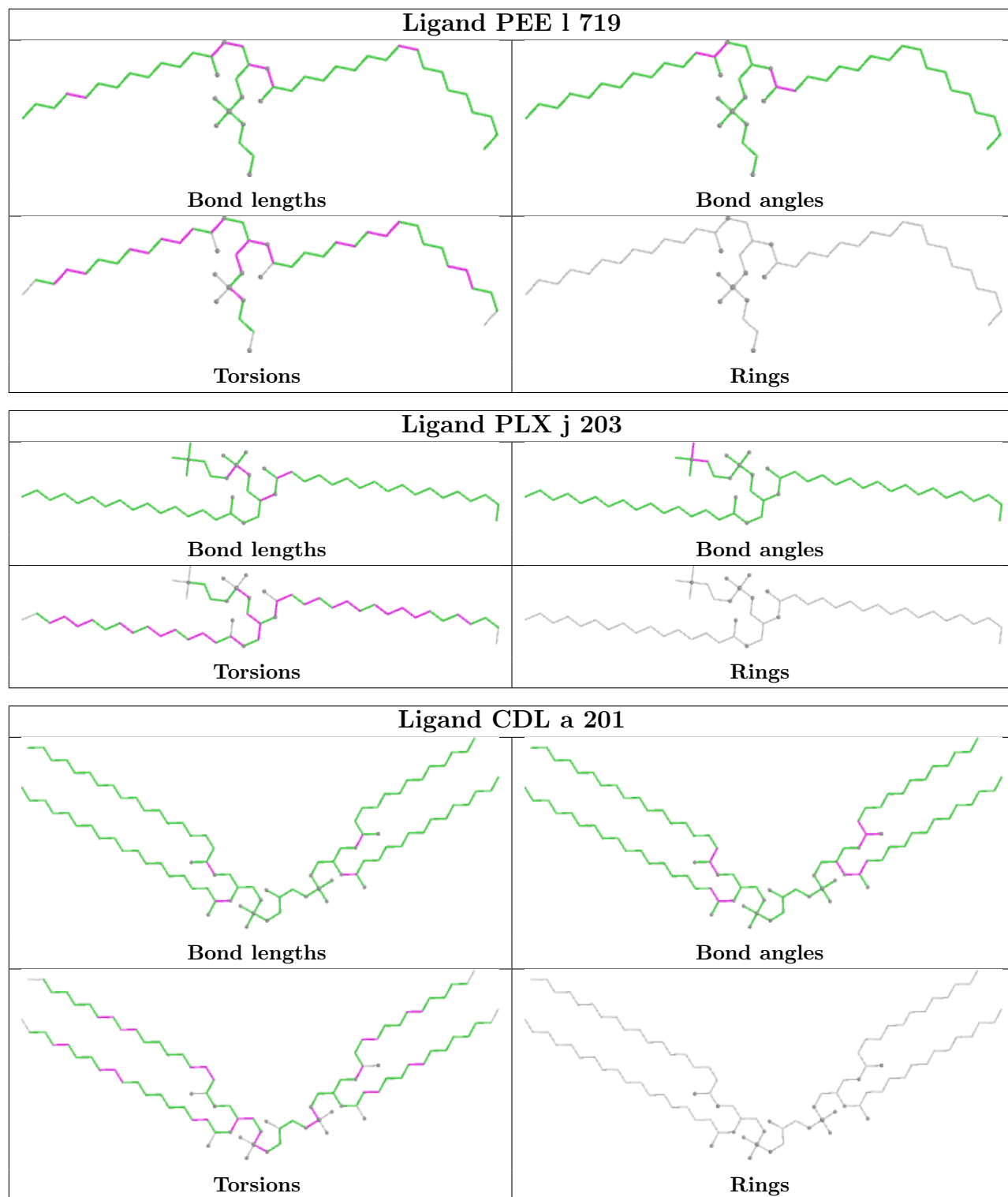
Continued from previous page...

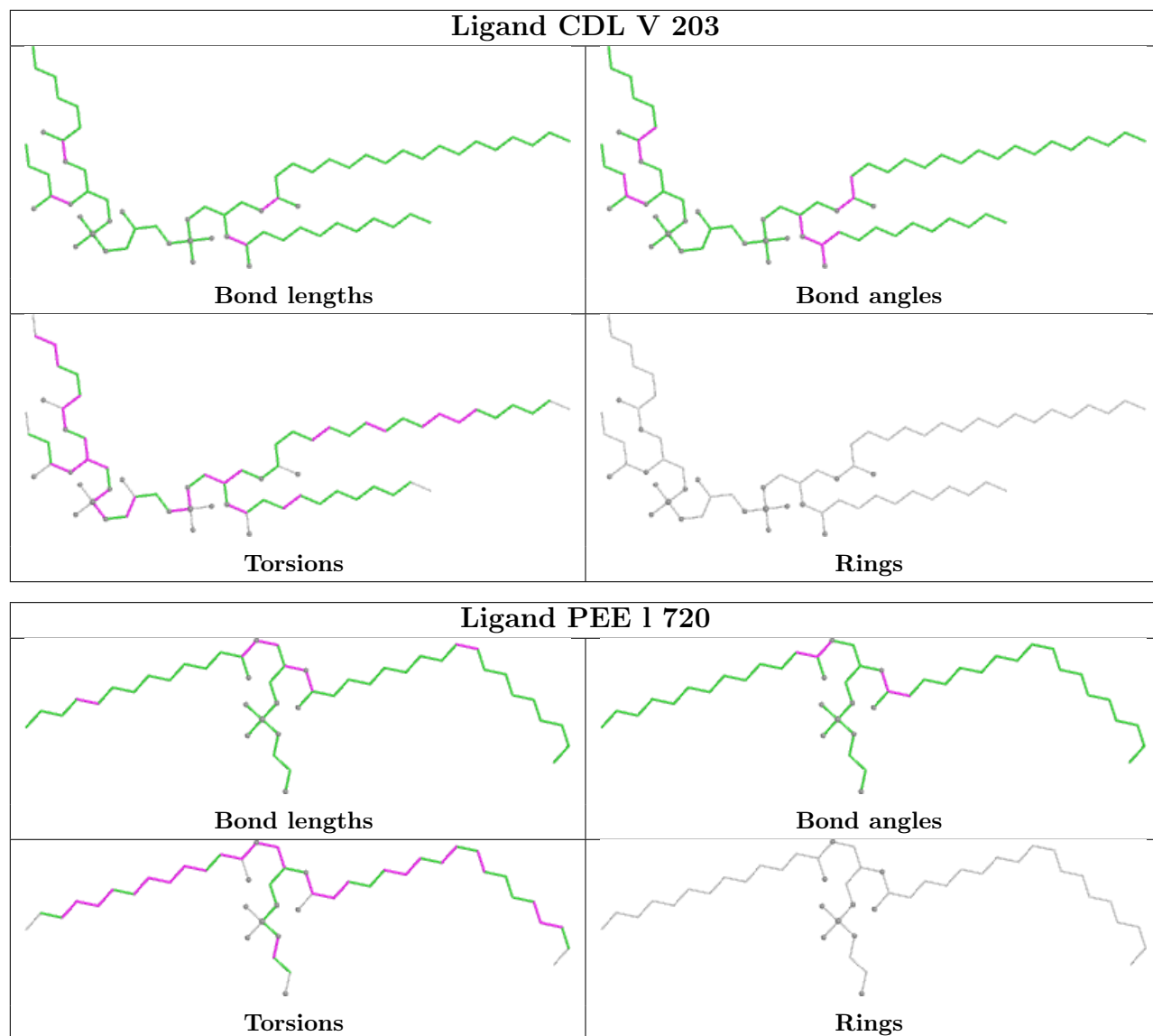
Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	i	401	CDL	16	0
48	V	202	PEE	21	0
49	n	101	PLX	9	0
48	l	718	PEE	10	0
48	s	401	PEE	2	0
47	A	503	NAI	4	0
49	C	312	PLX	2	0
49	V	205	PLX	4	0
57	w	401	ADP	4	0
45	M	802	SF4	1	0
54	l	712	CDL	39	0
49	e	201	PLX	7	0
54	l	713	CDL	7	0
54	r	714	CDL	8	0
54	V	201	CDL	19	0

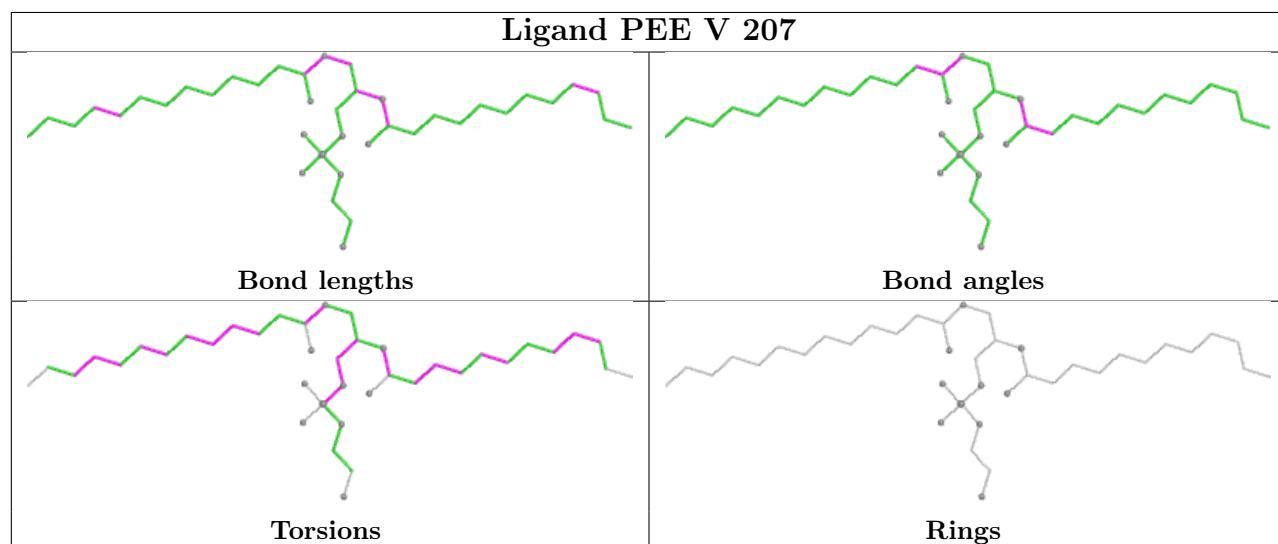
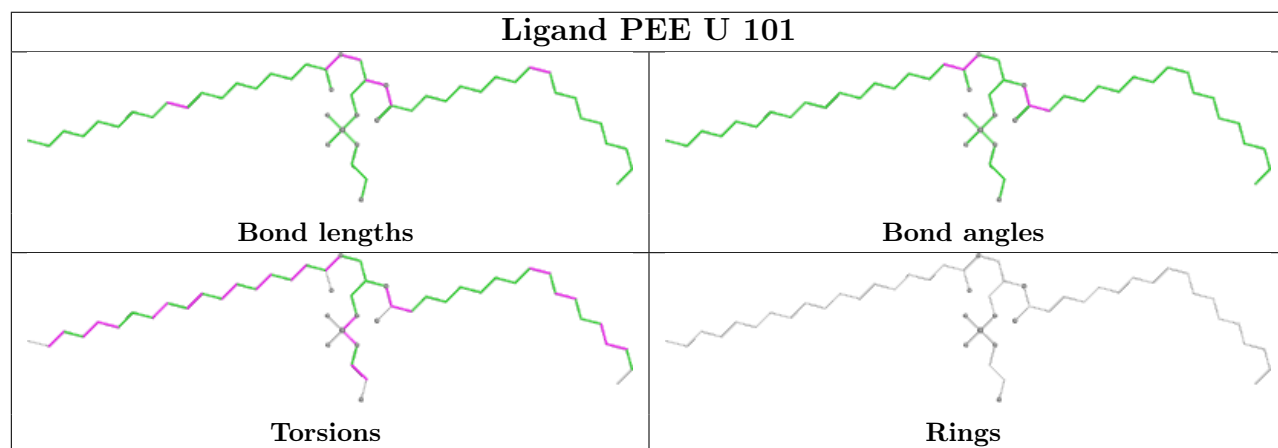
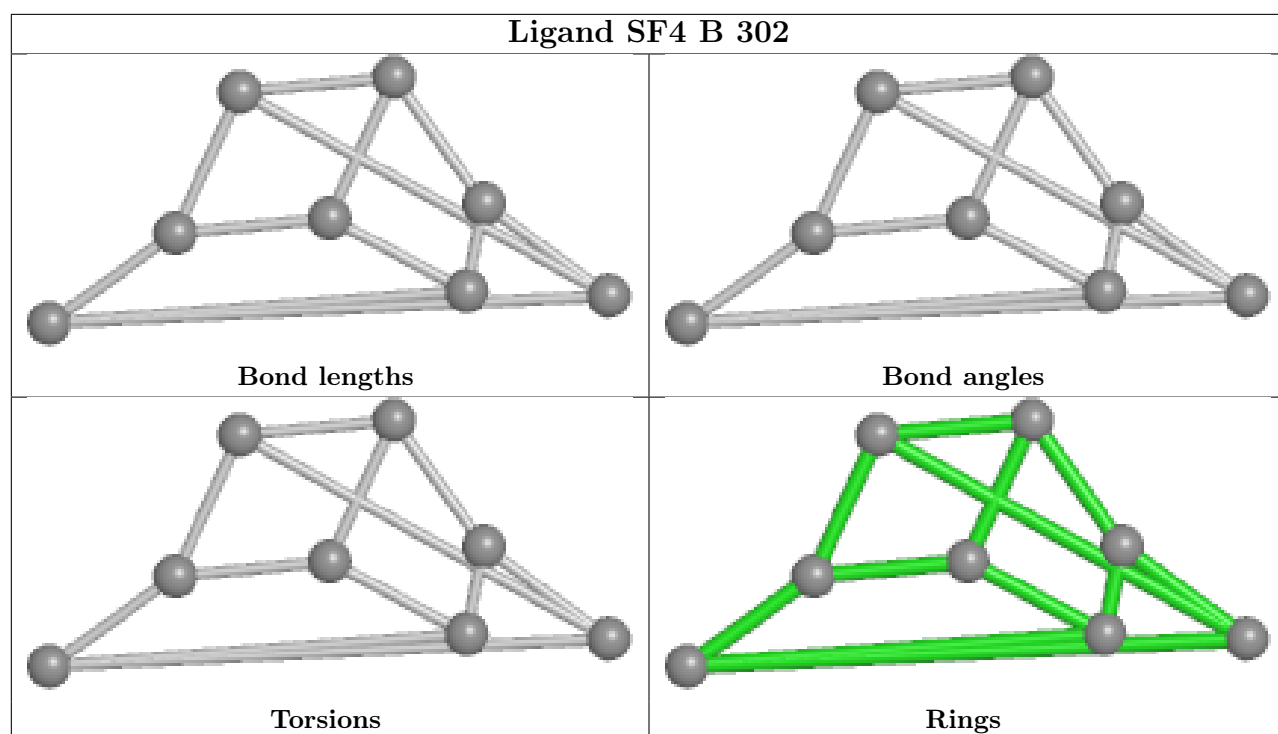
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

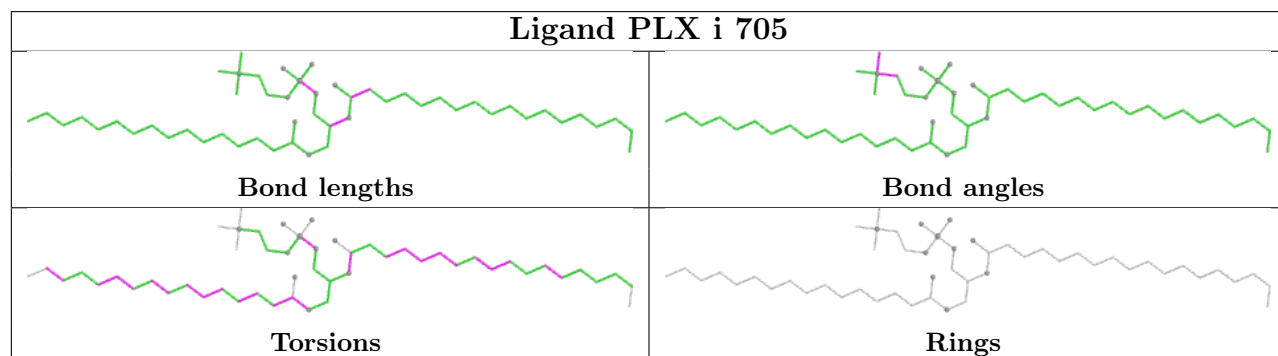
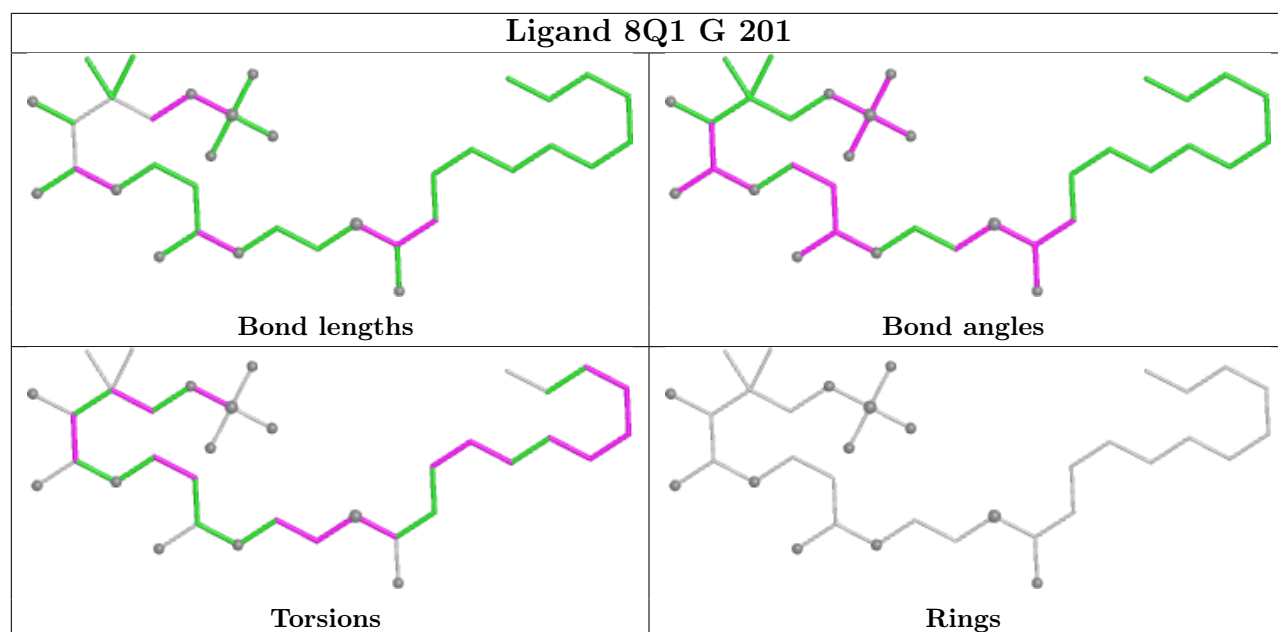
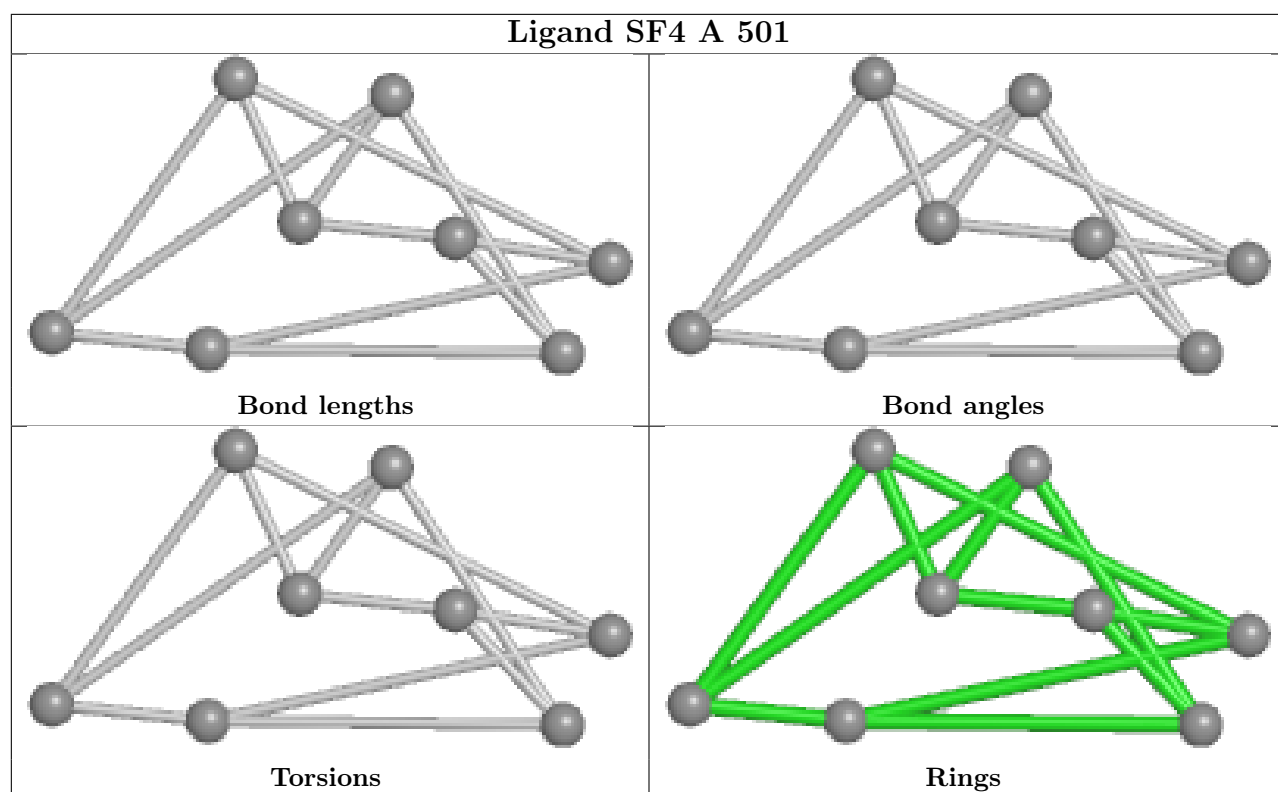


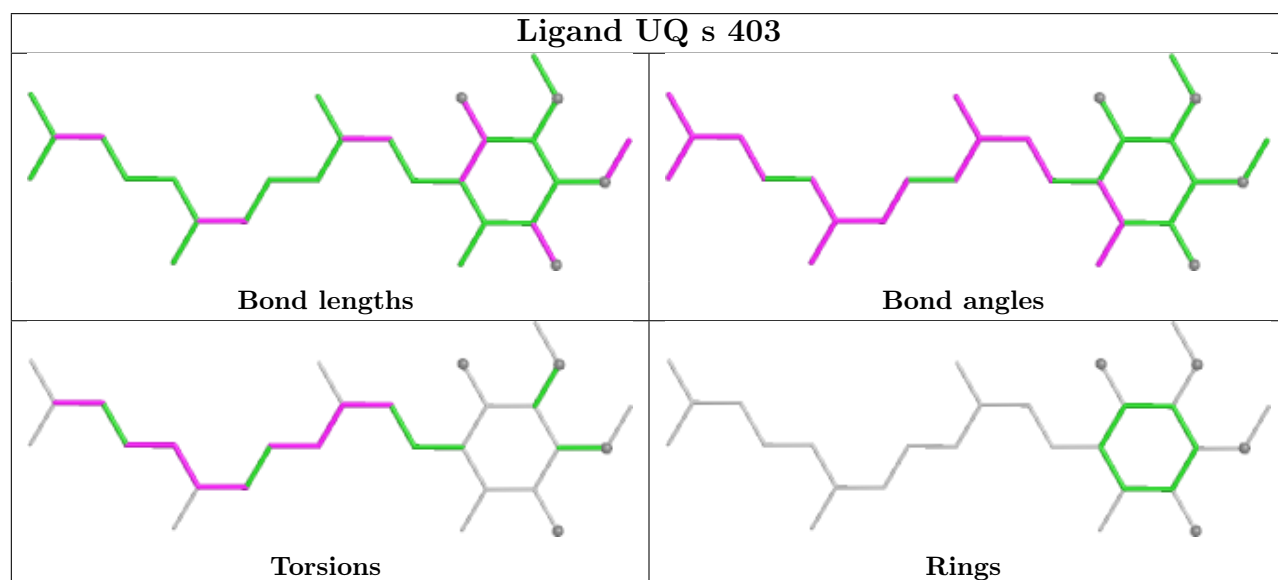
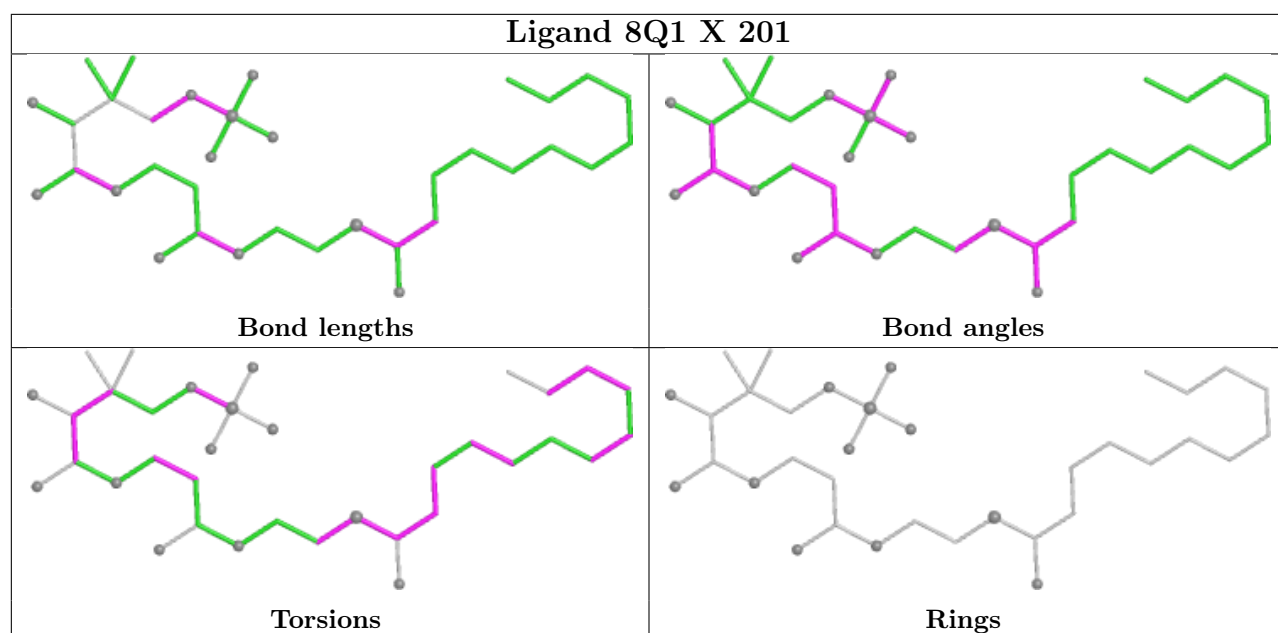


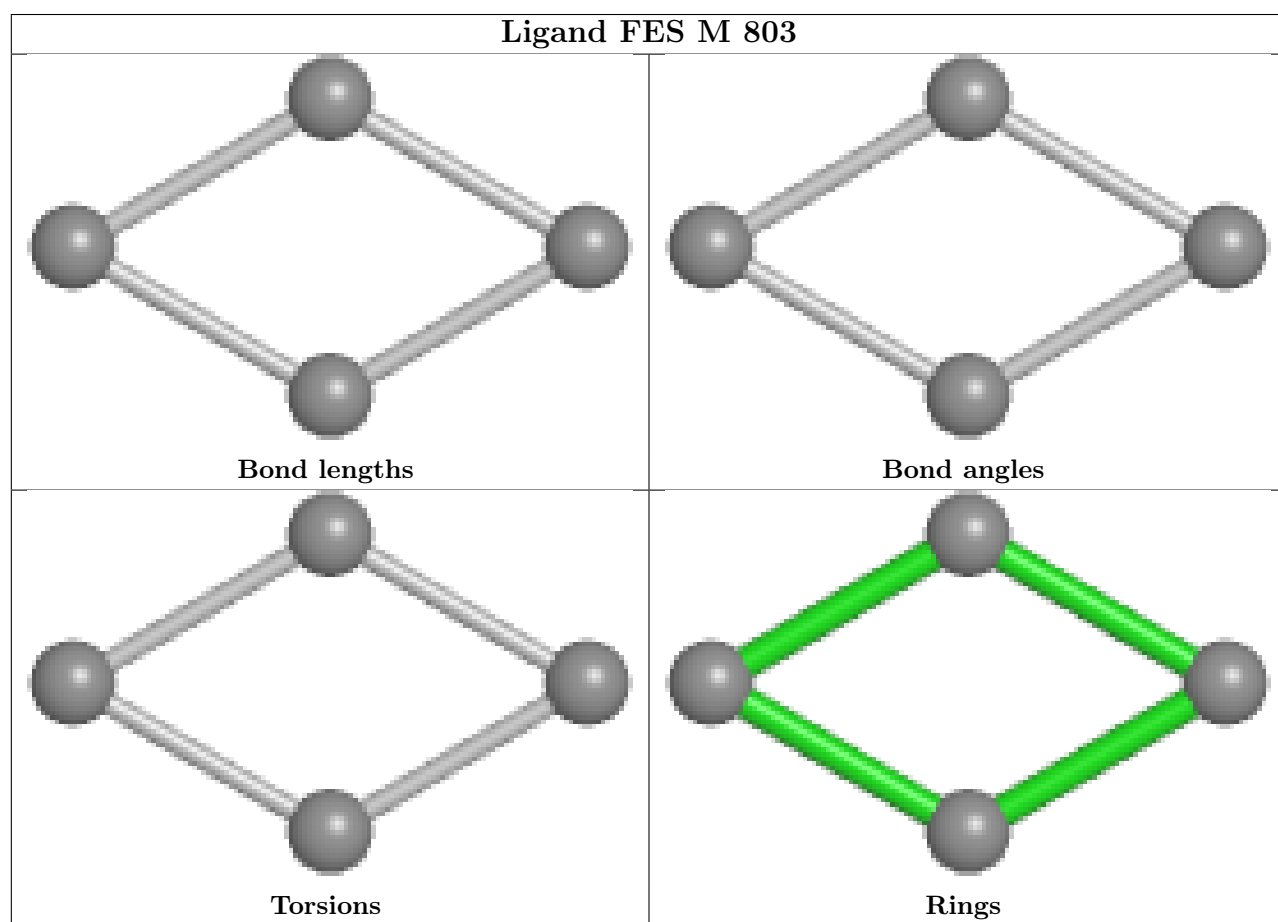
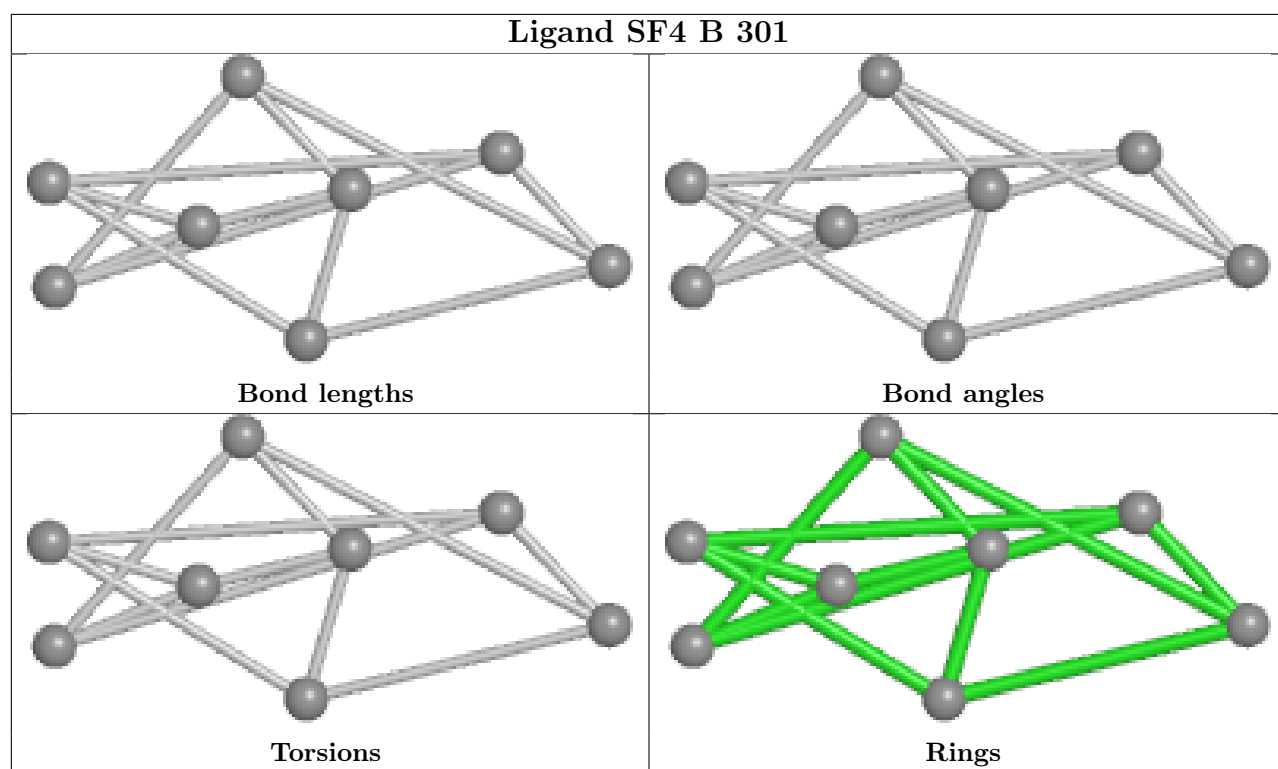


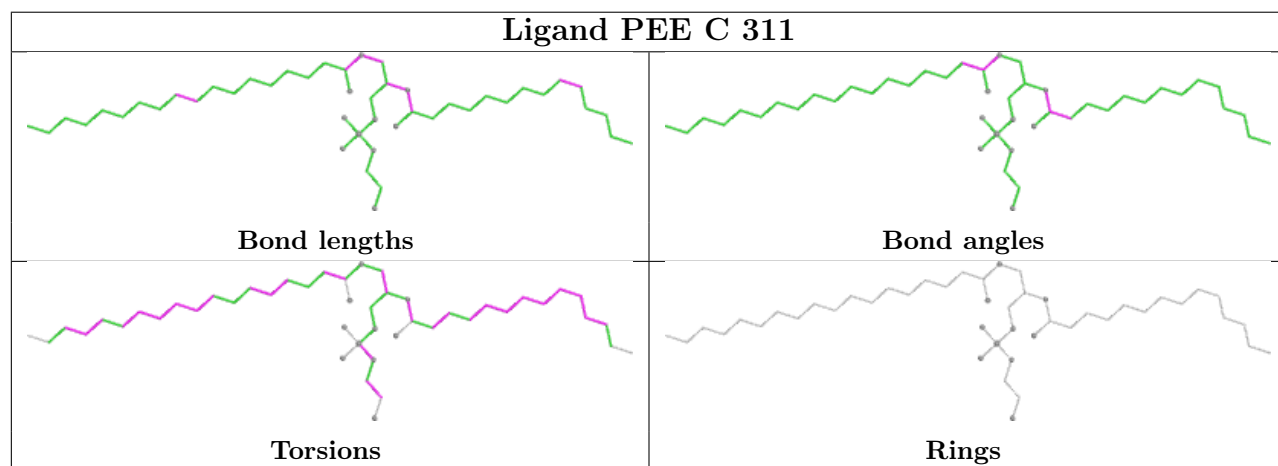
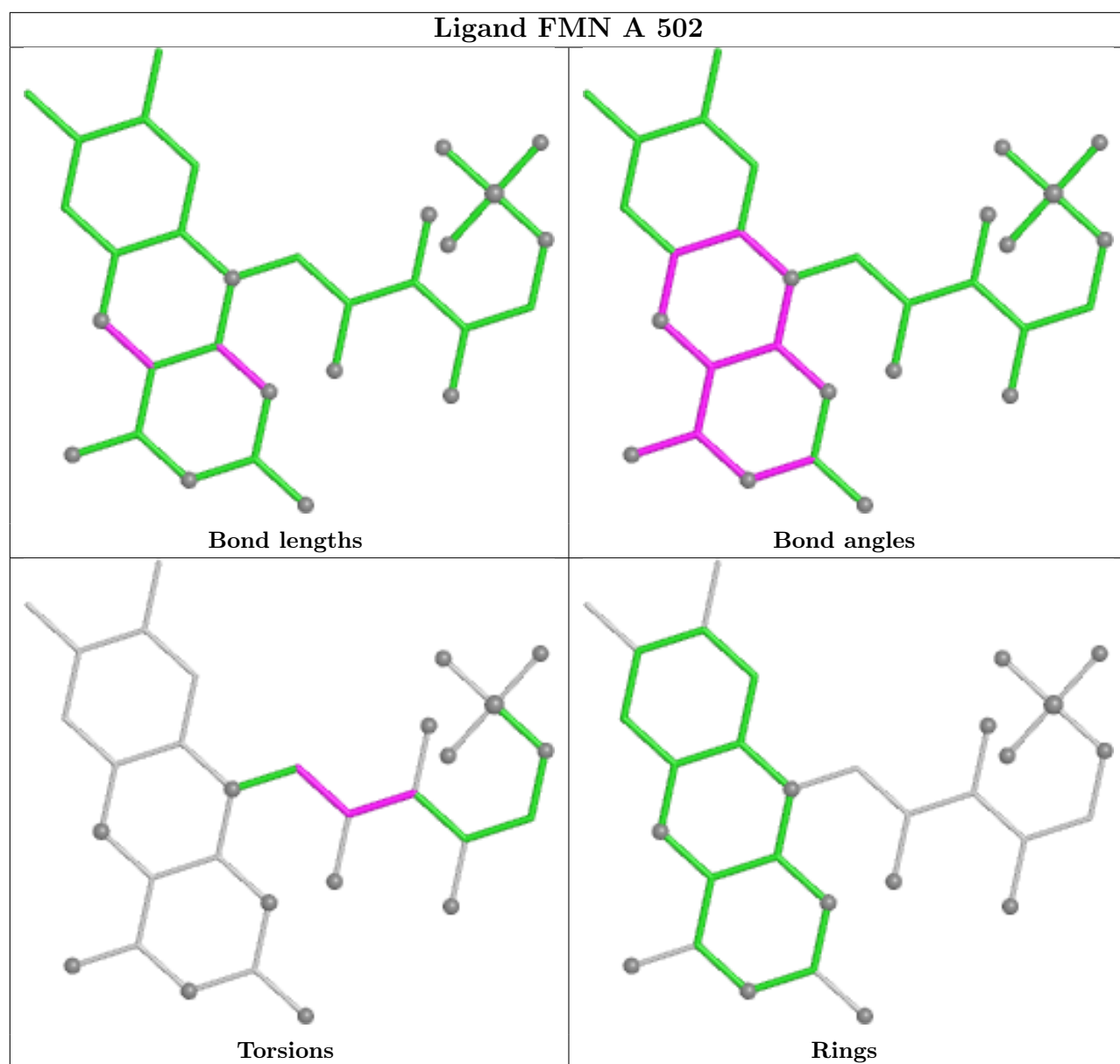


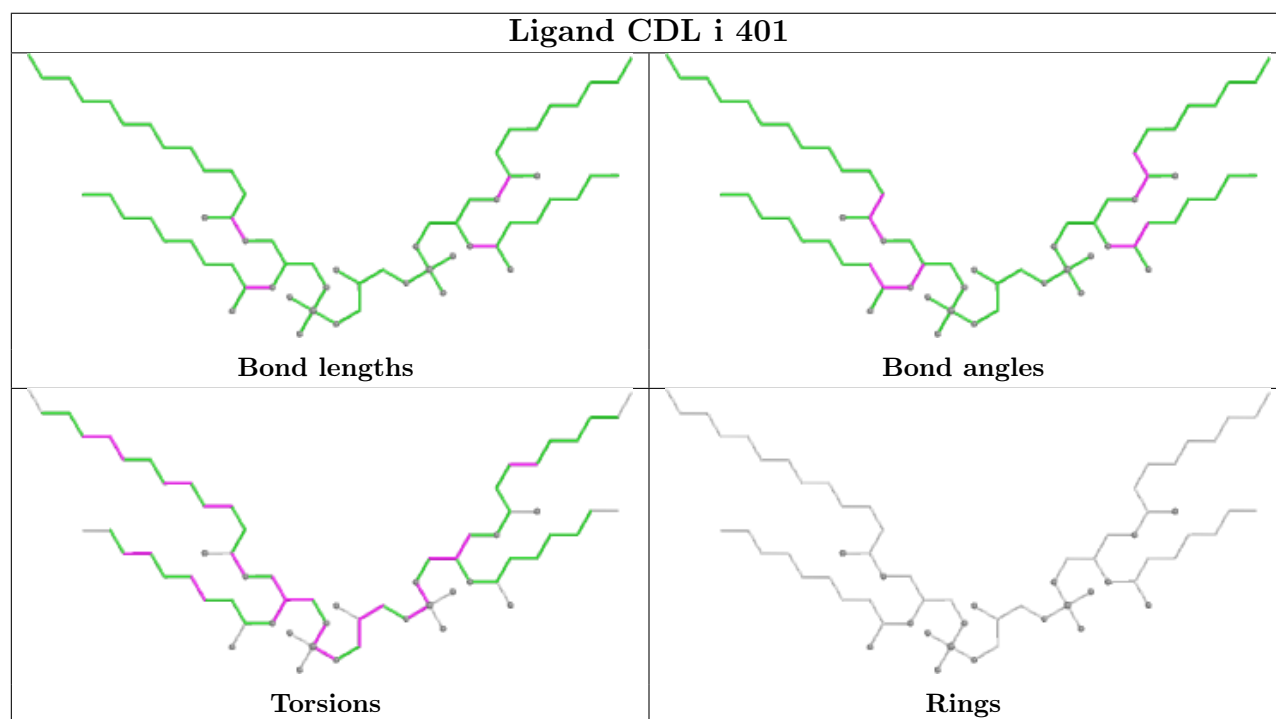
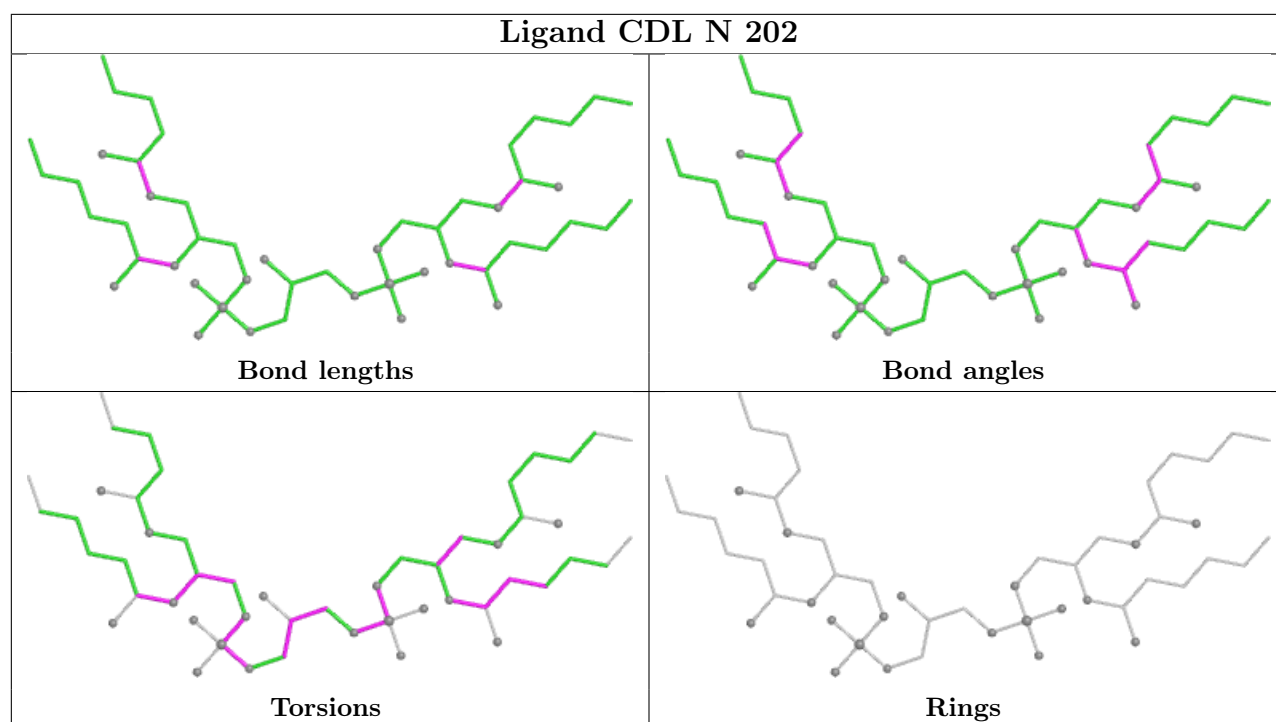


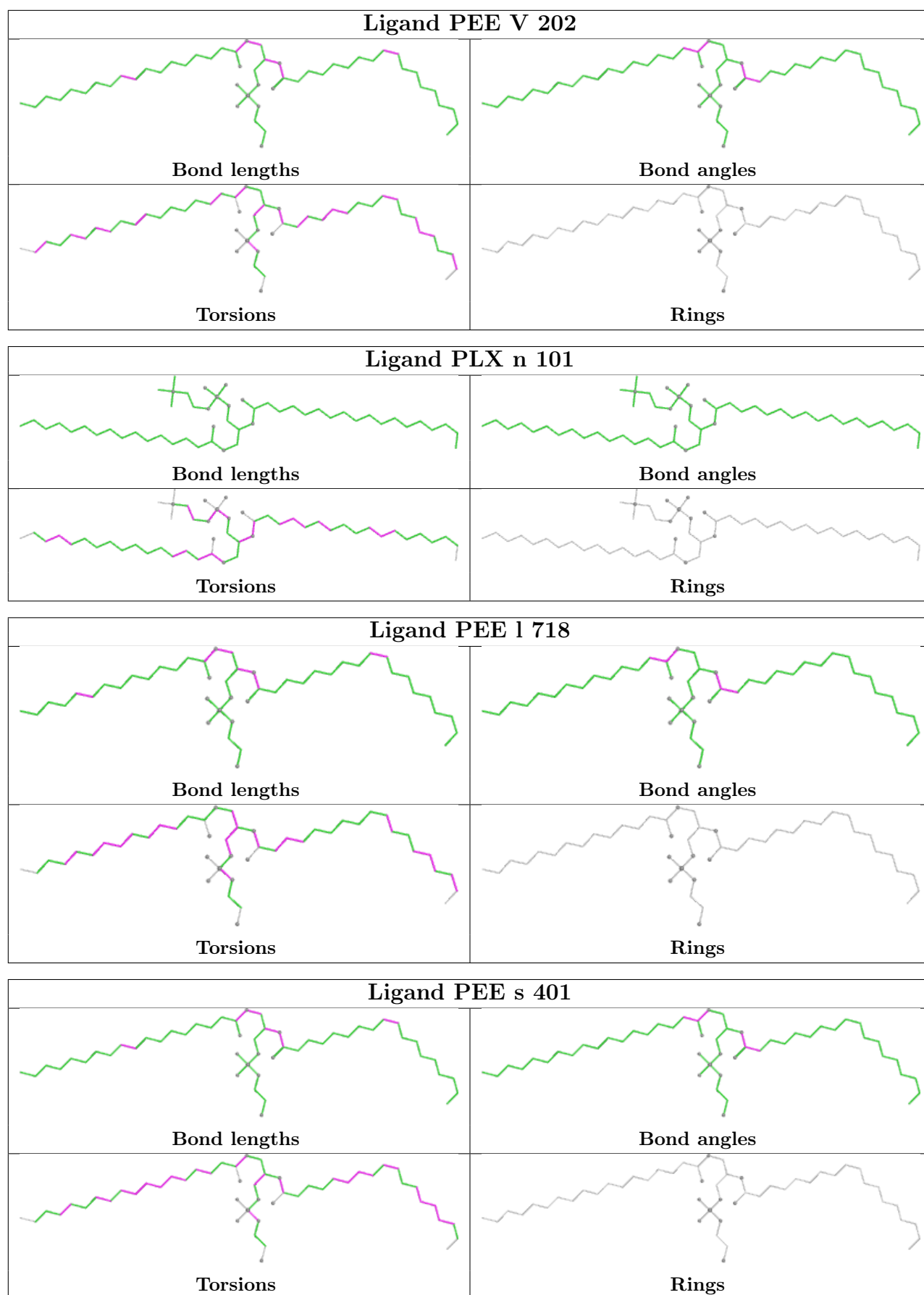


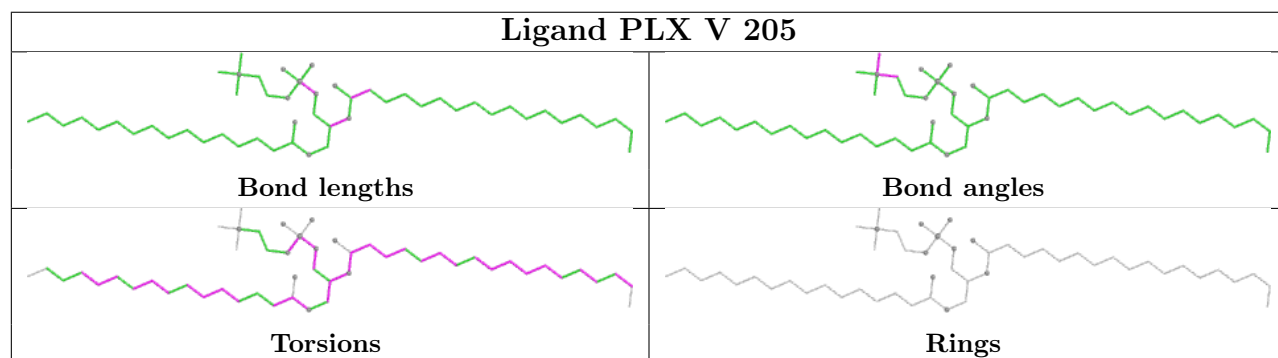
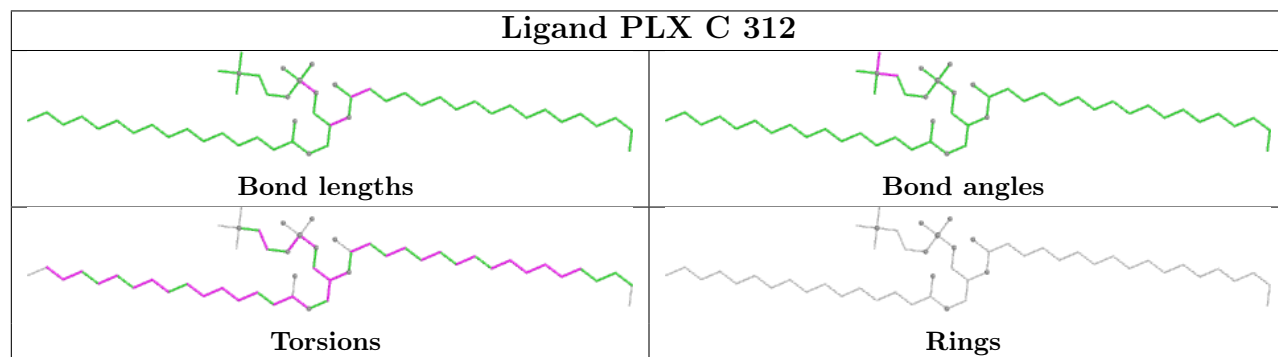
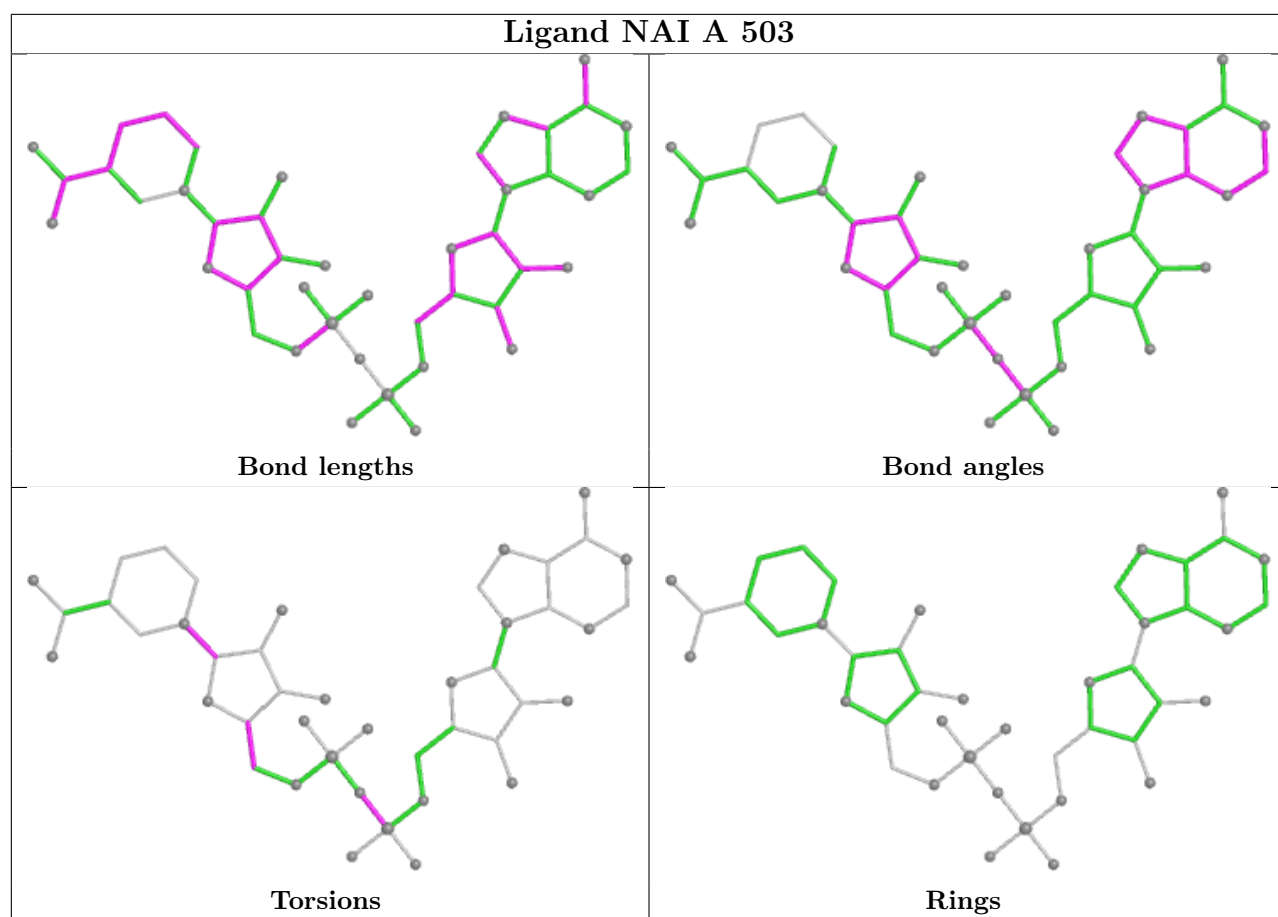


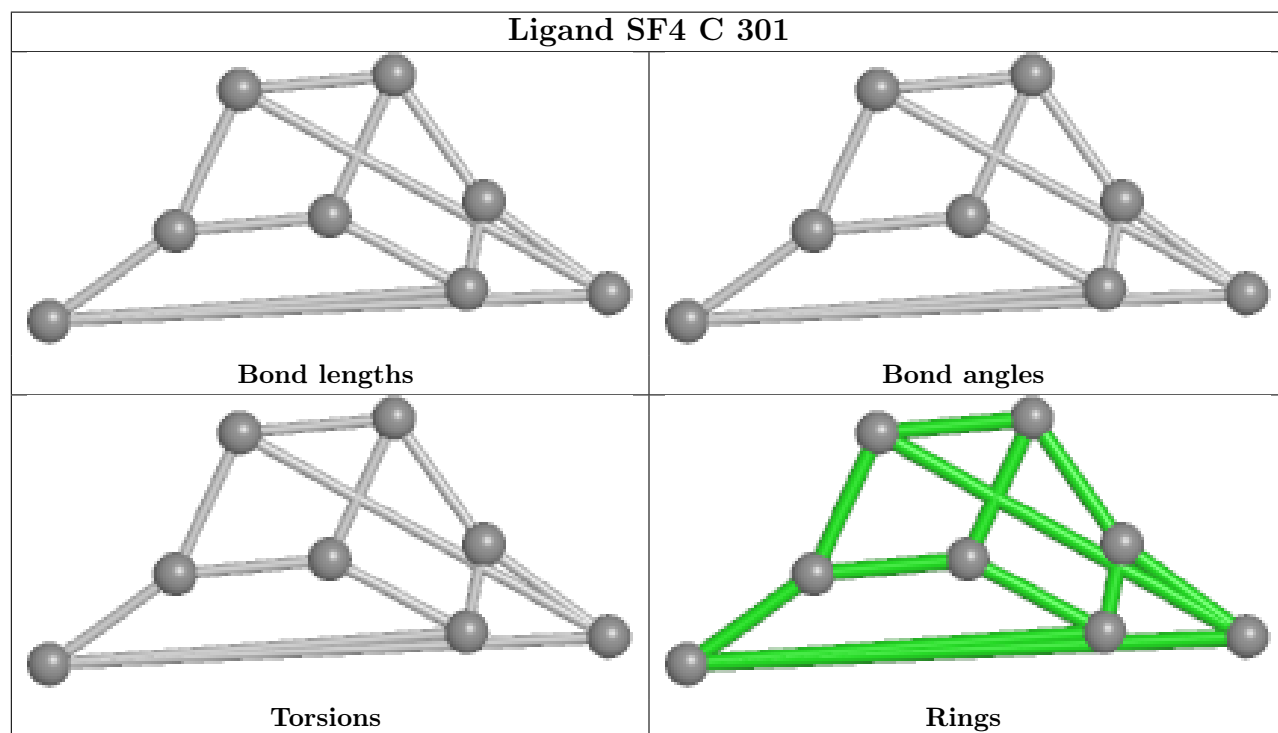
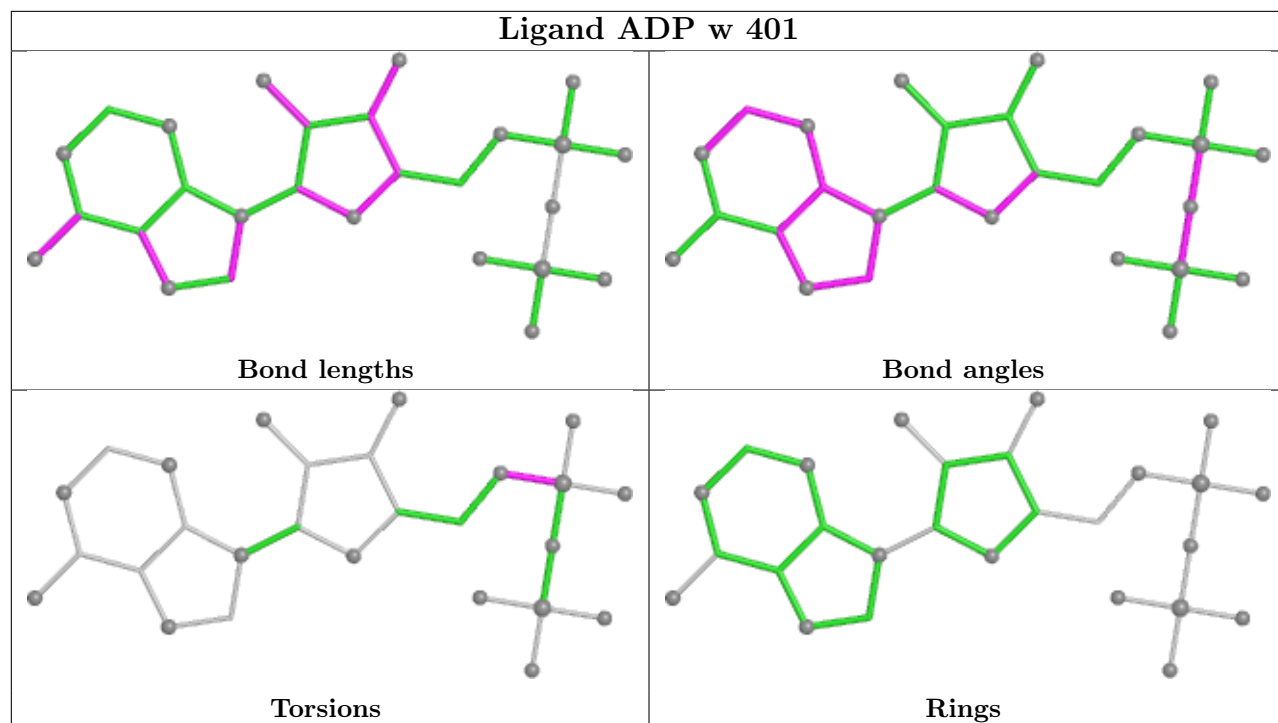


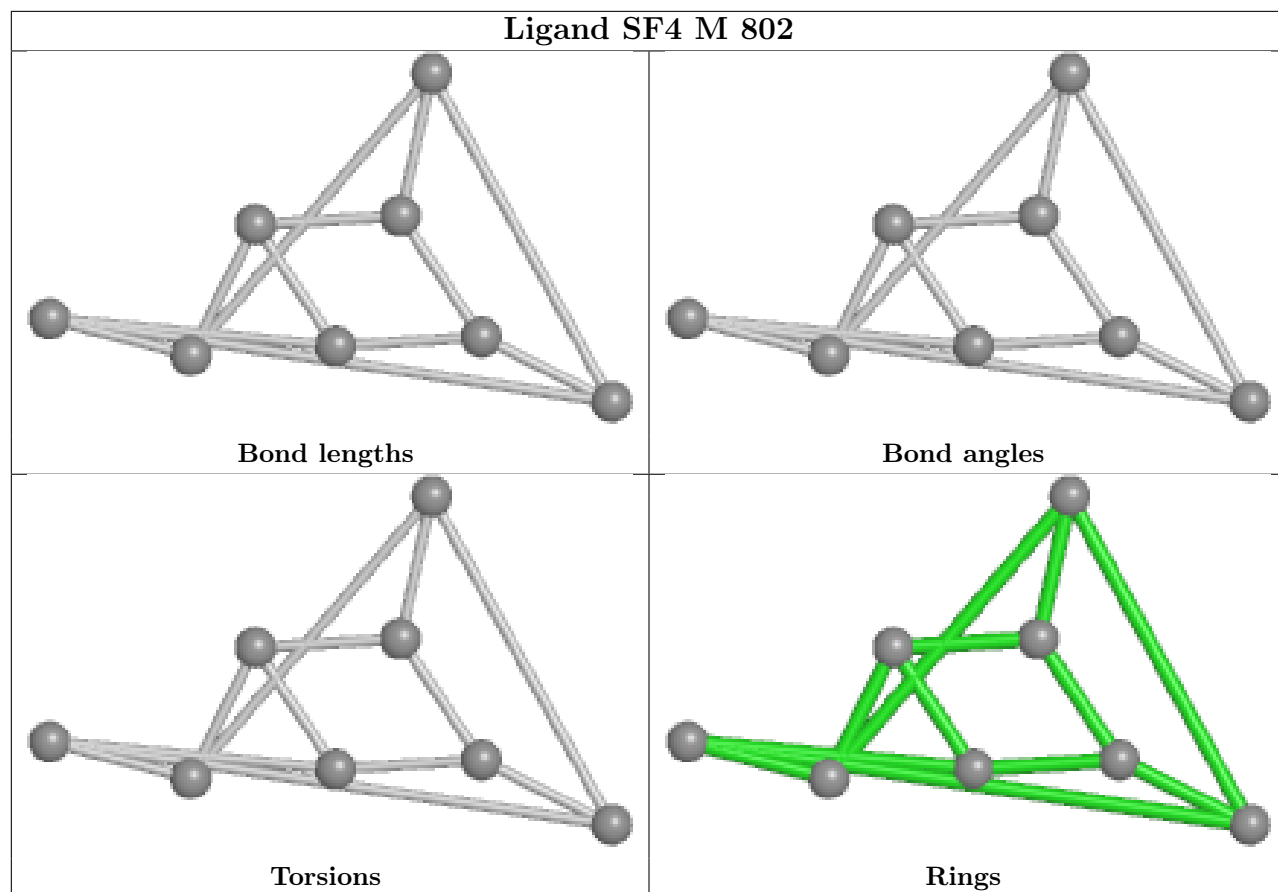


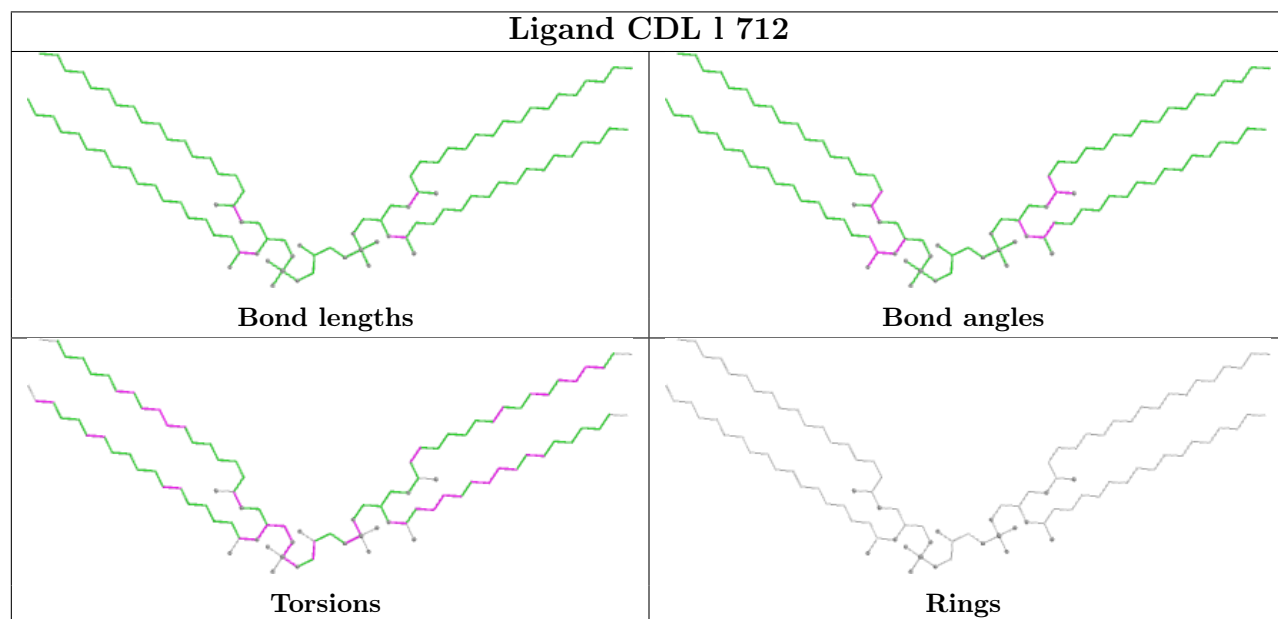
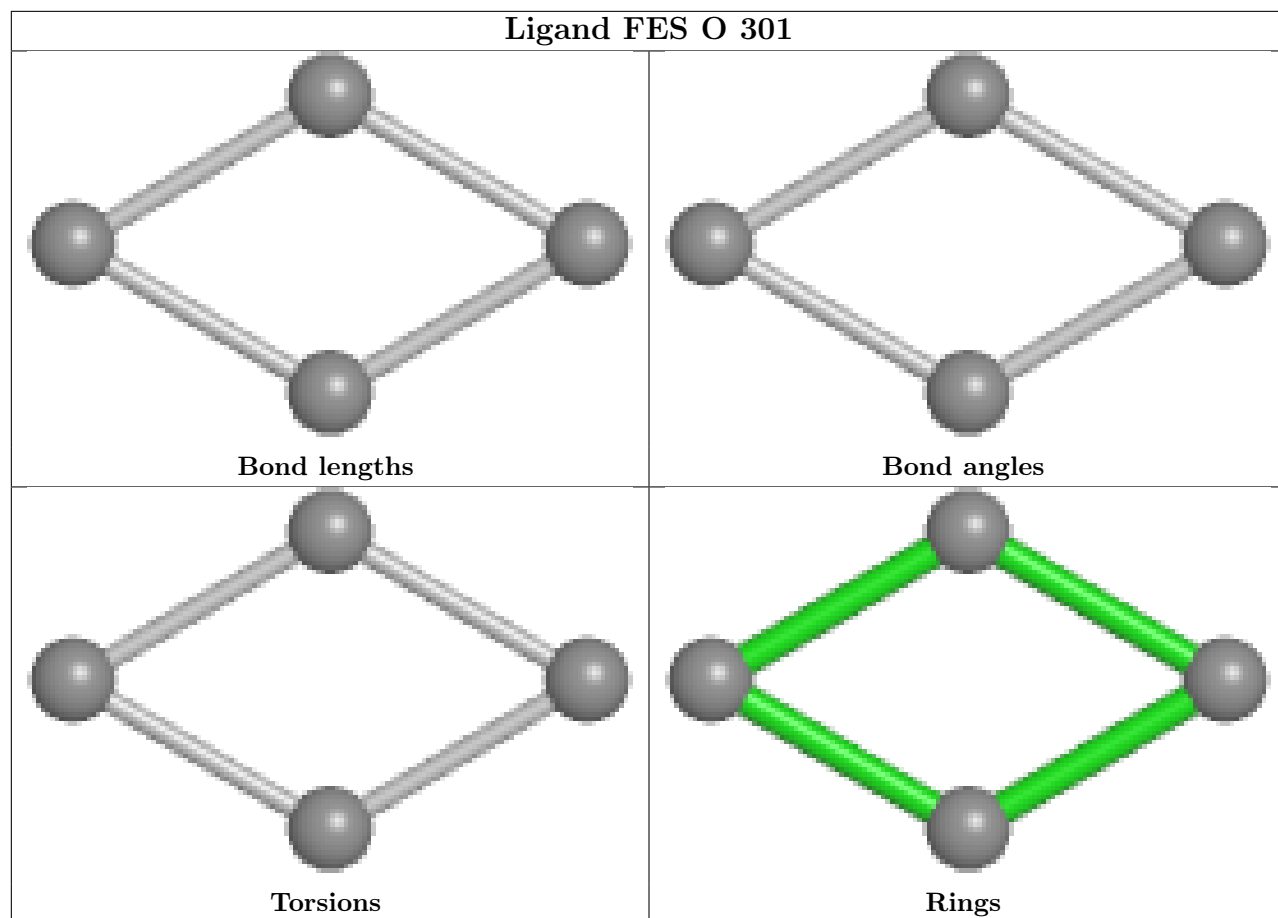


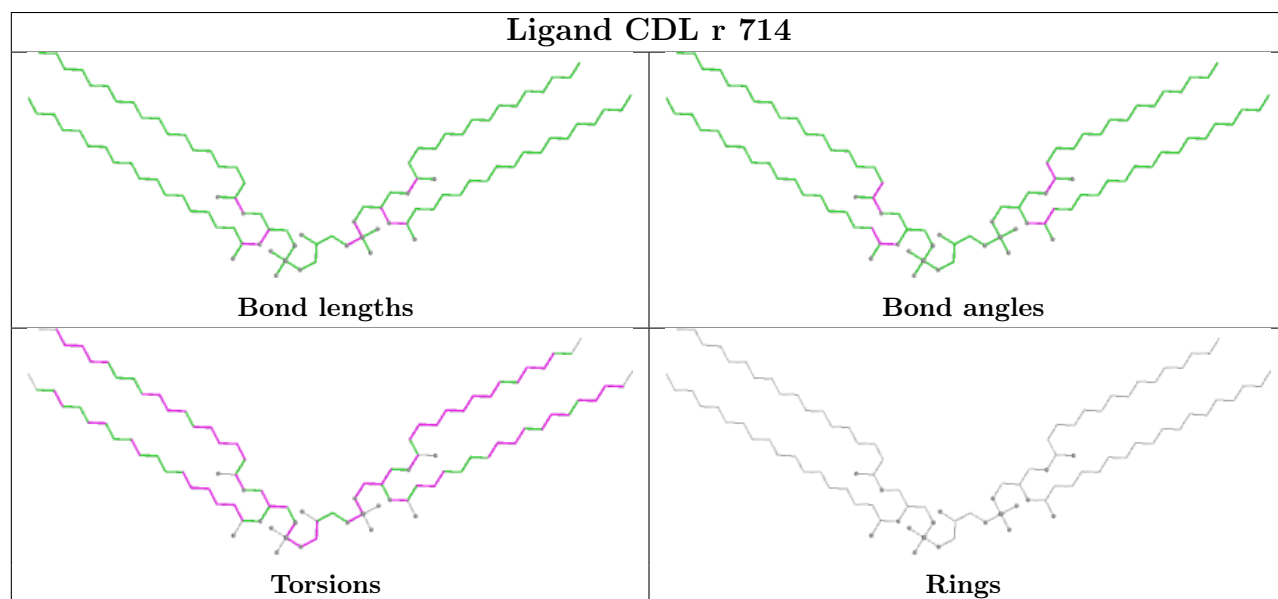
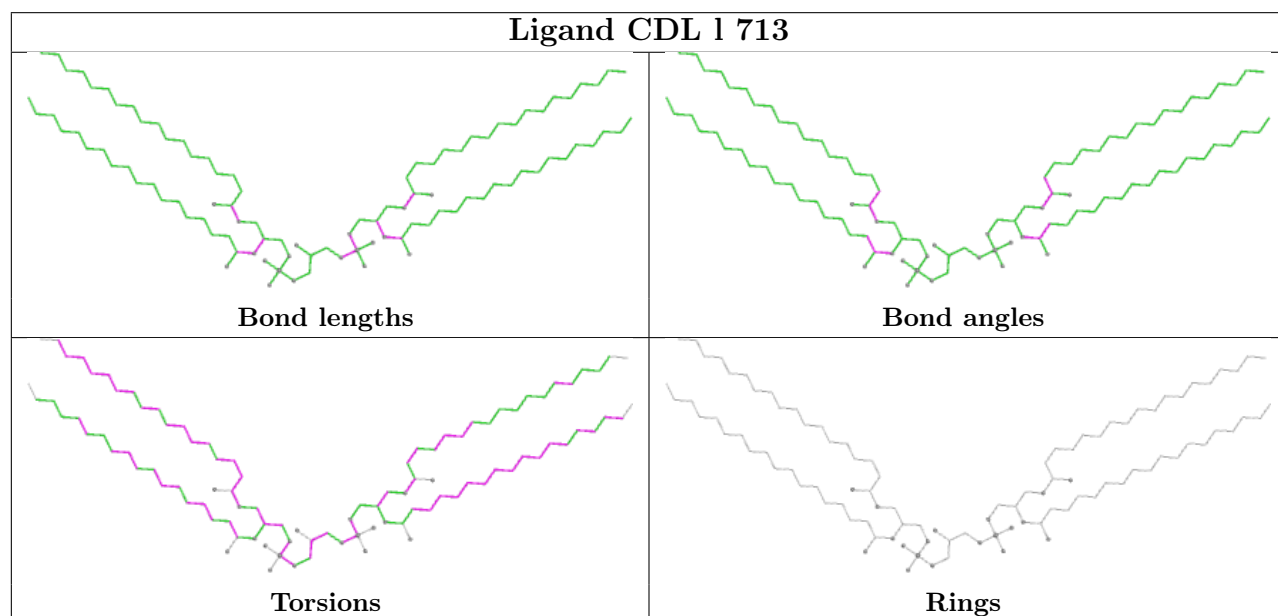
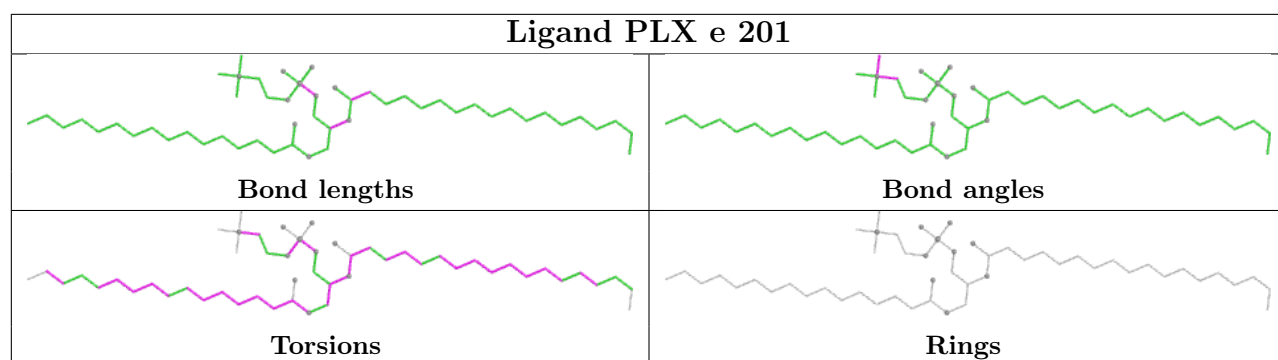


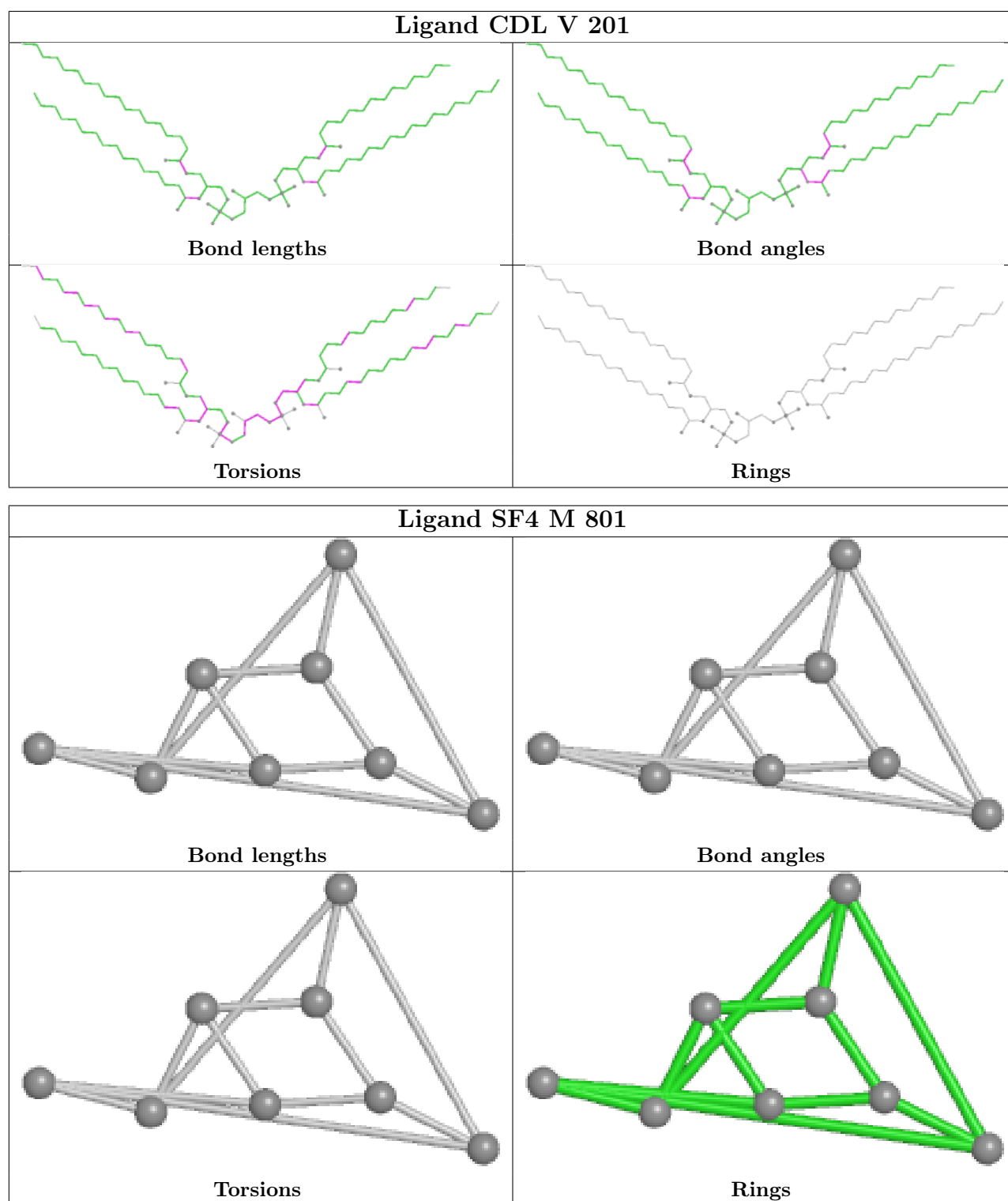












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

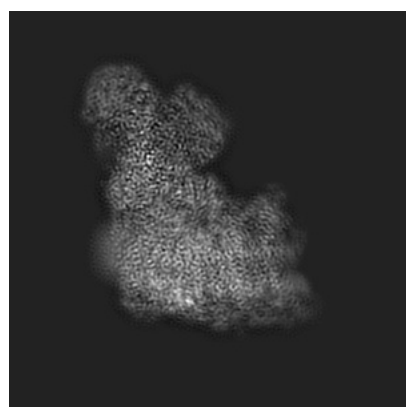
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31644. These allow visual inspection of the internal detail of the map and identification of artifacts.

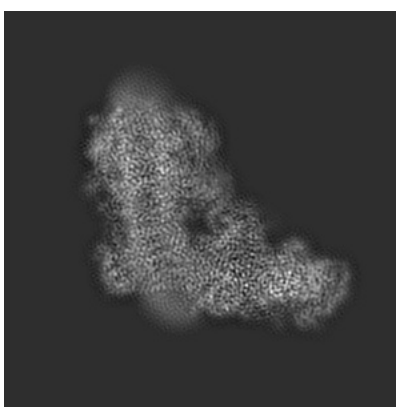
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

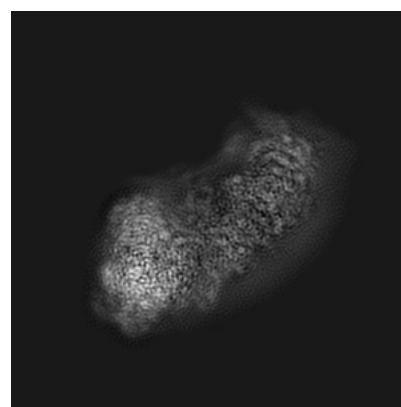
6.1.1 Primary map



X



Y

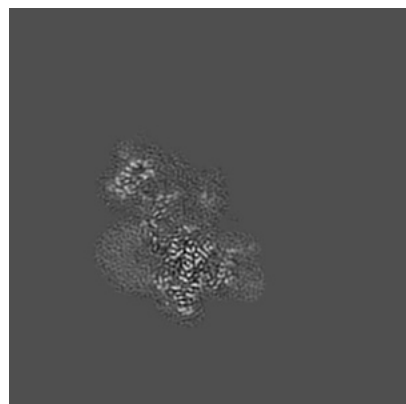


Z

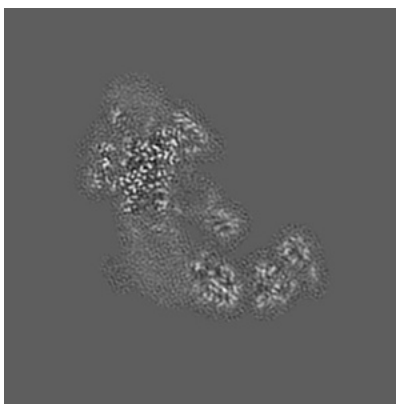
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

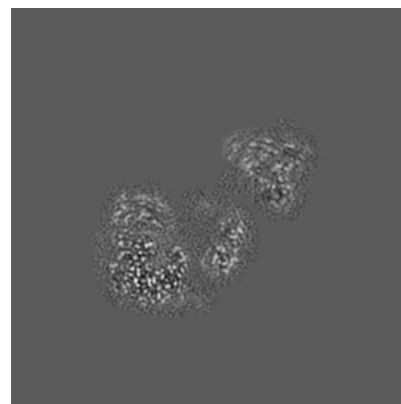
6.2.1 Primary map



X Index: 155



Y Index: 155

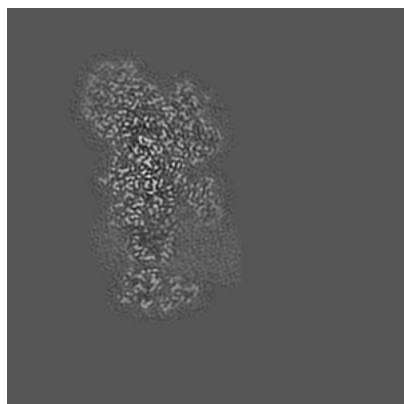


Z Index: 155

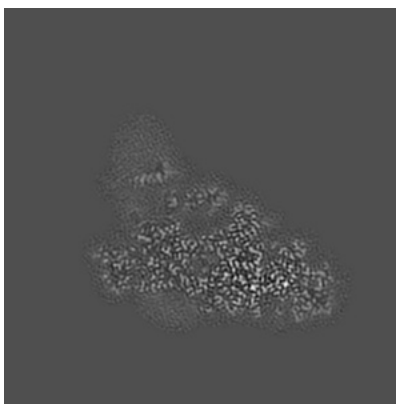
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

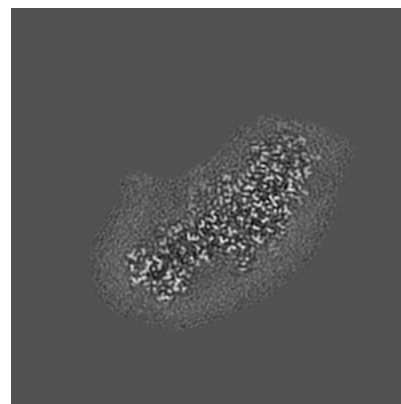
6.3.1 Primary map



X Index: 102



Y Index: 107

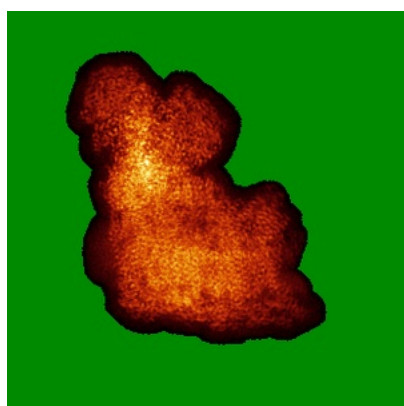


Z Index: 119

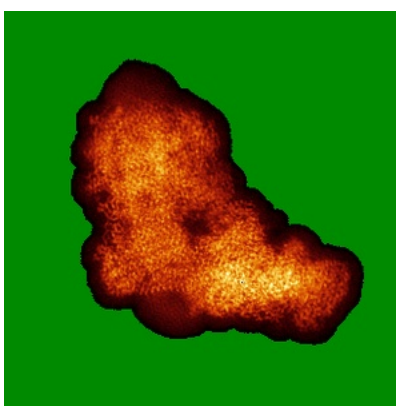
The images above show the largest variance slices of the map in three orthogonal directions.

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

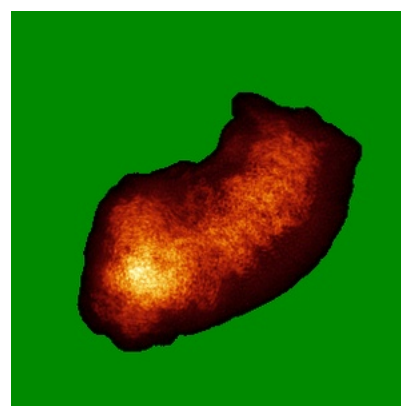
6.4.1 Primary map



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 0.0232. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

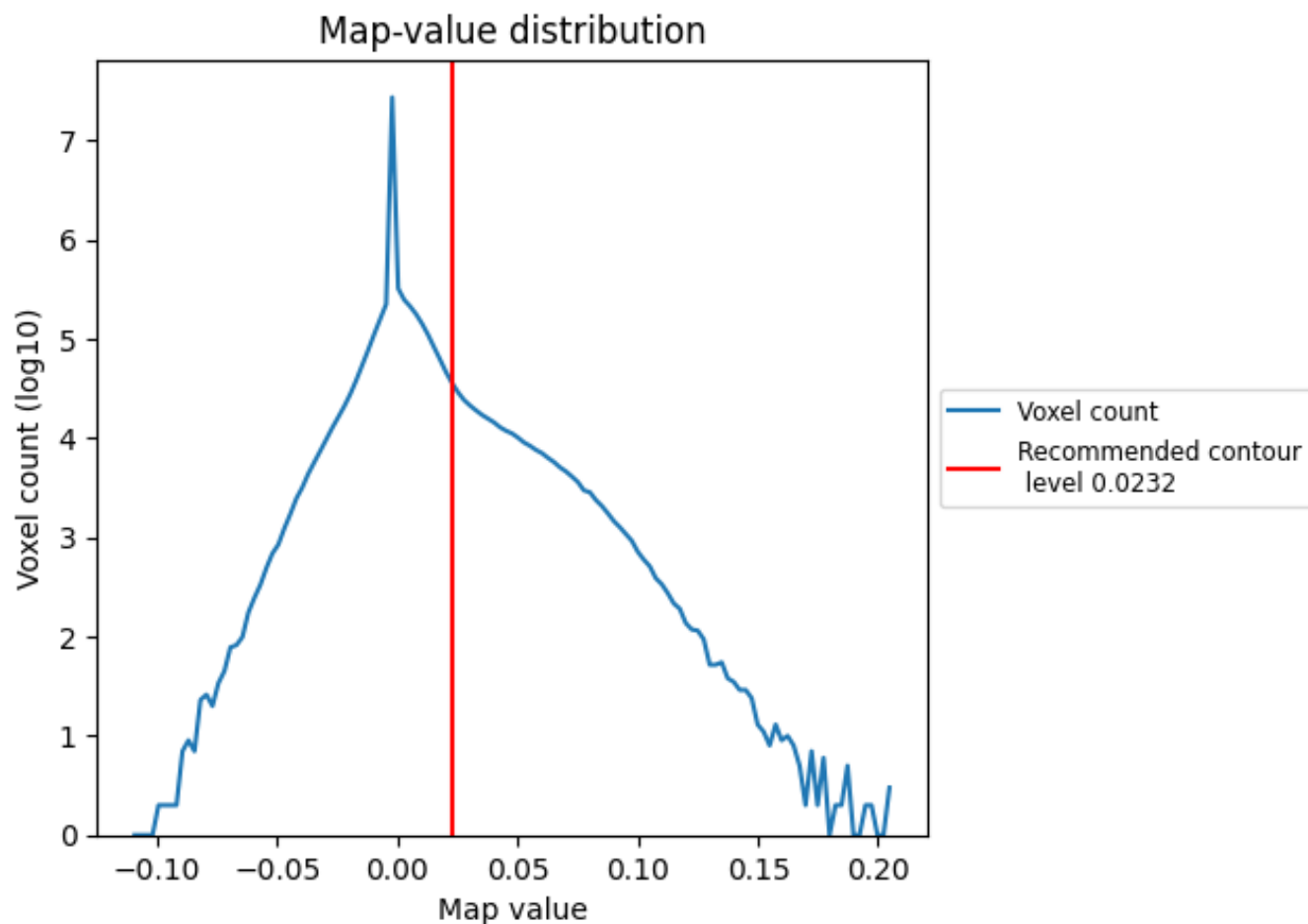
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

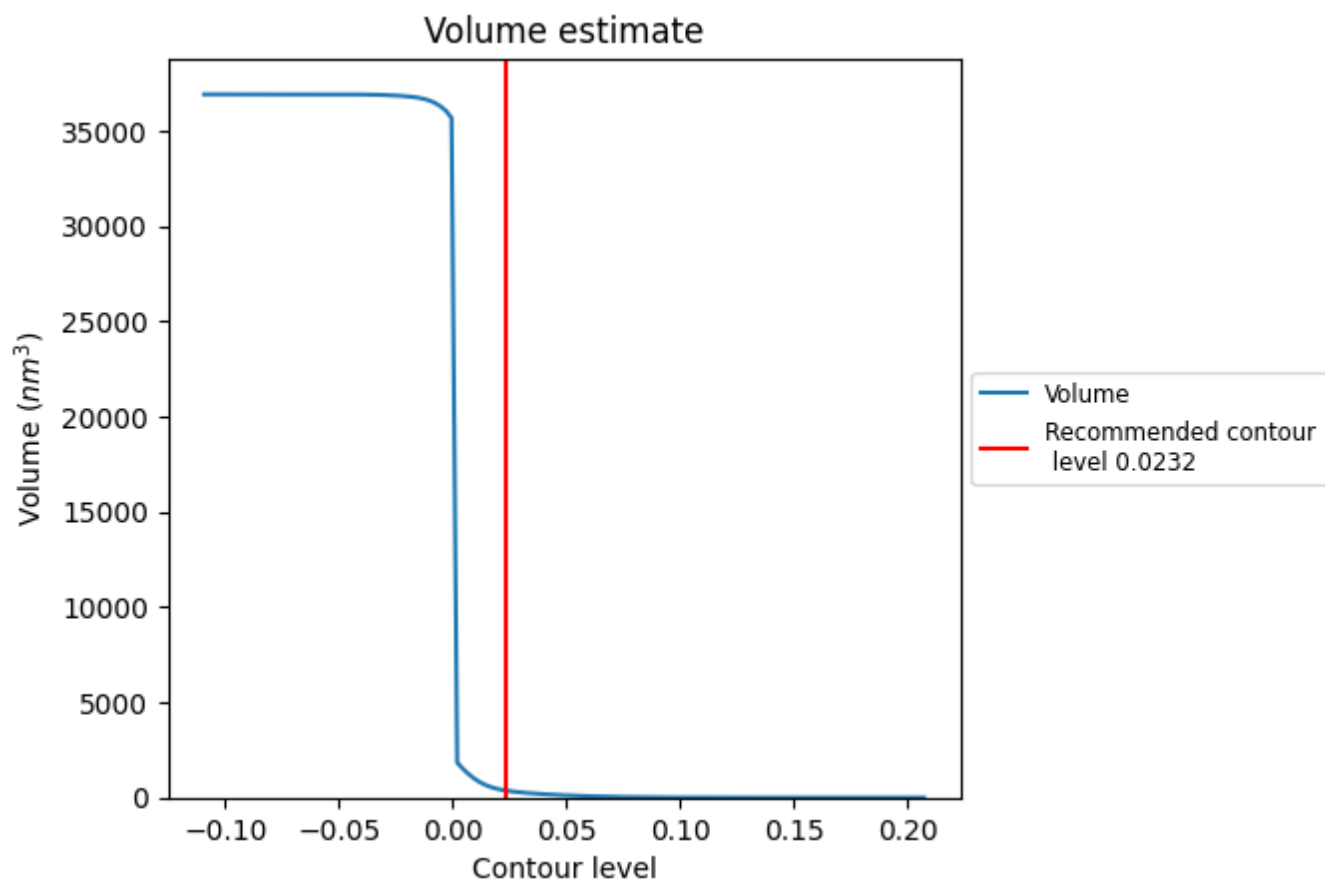
This section contains the results of statistical analysis of the map.

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.

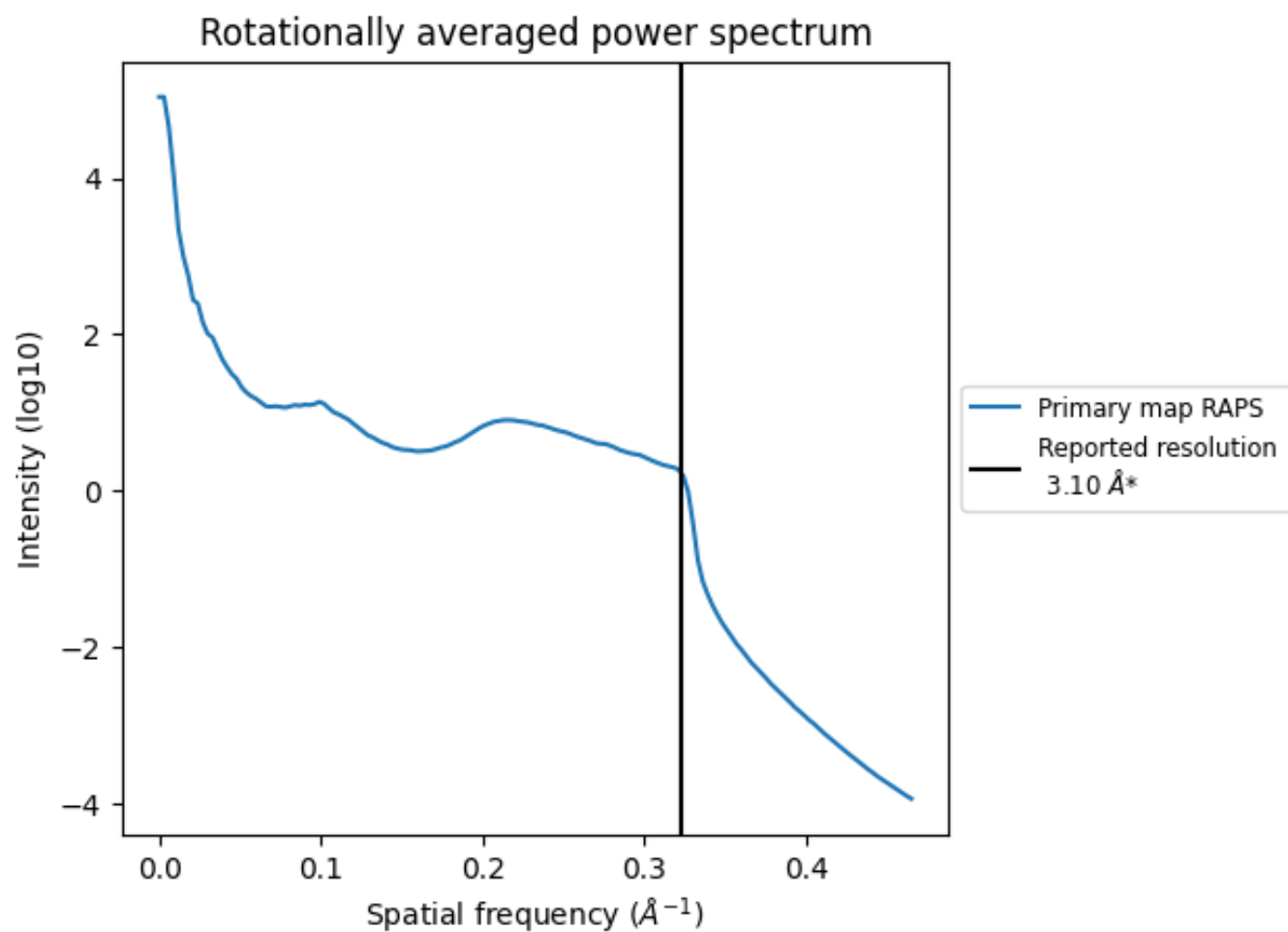
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 372 nm³; this corresponds to an approximate mass of 336 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 0.323 Å⁻¹

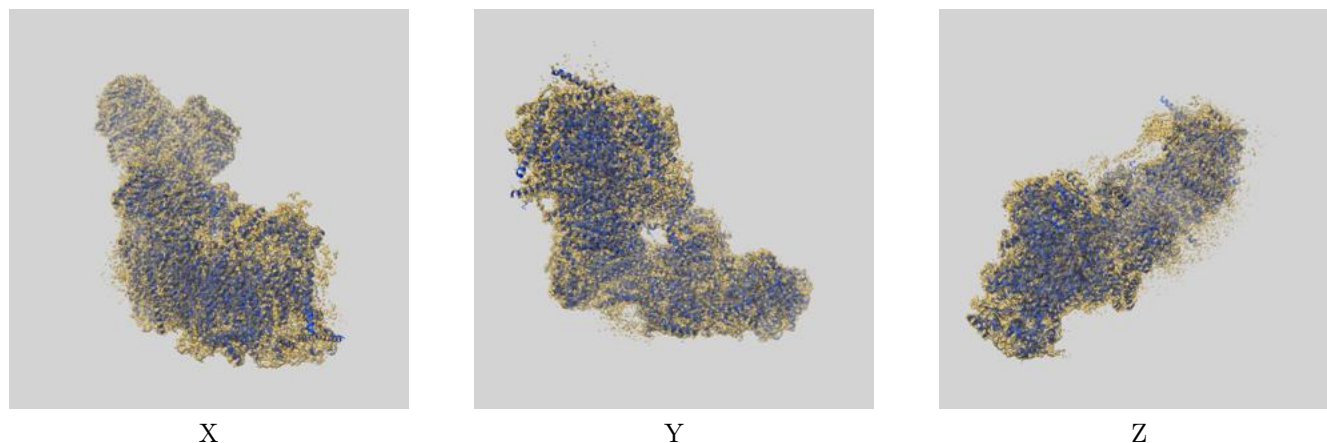
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

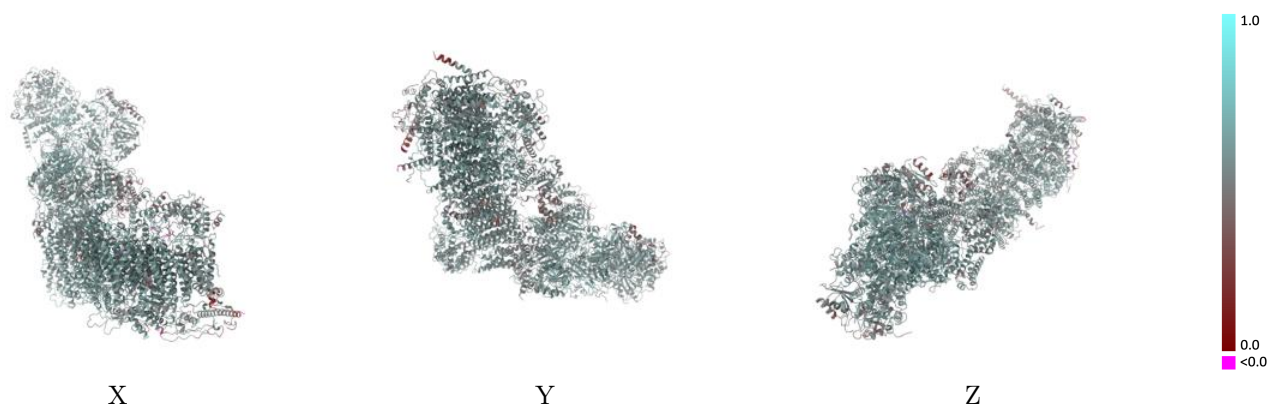
This section contains information regarding the fit between EMDB map EMD-31644 and PDB model 7V2F. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



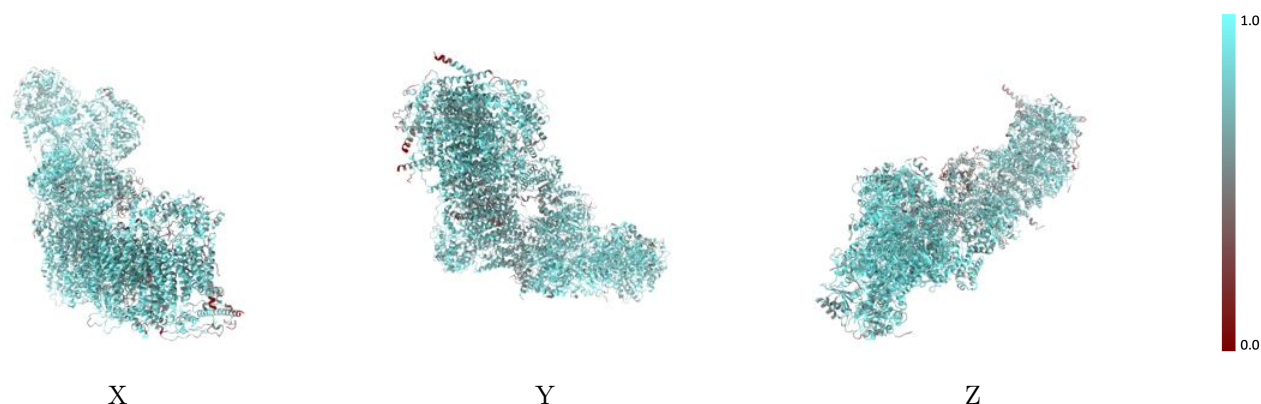
The images above show the 3D surface view of the map at the recommended contour level 0.0232 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



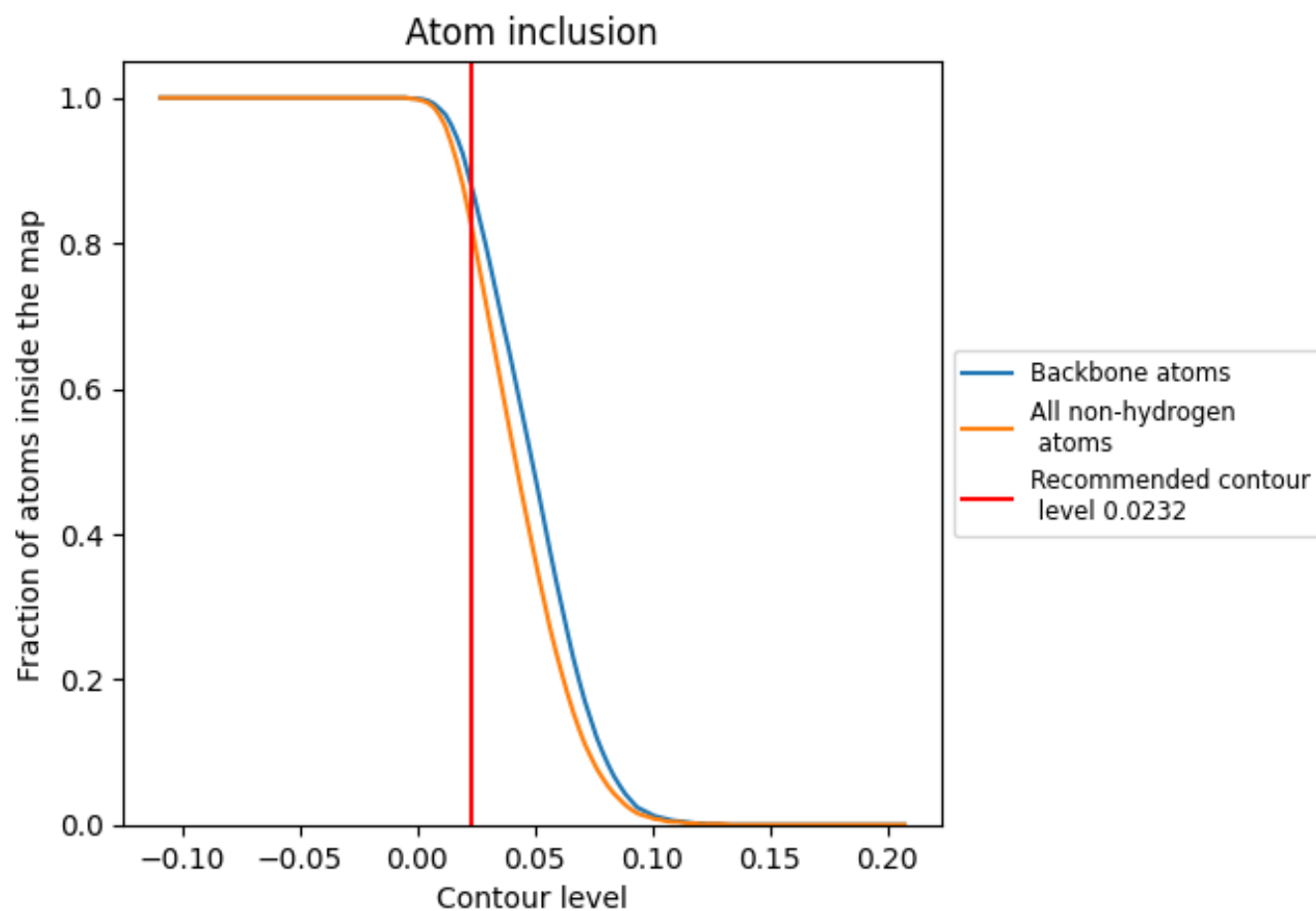
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0232).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0232) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8200	 0.5650
A	 0.8190	 0.5520
B	 0.9540	 0.6180
C	 0.8820	 0.6000
E	 0.8100	 0.5640
F	 0.7310	 0.4900
G	 0.5360	 0.4080
H	 0.8190	 0.5530
I	 0.8330	 0.5750
J	 0.7970	 0.5490
K	 0.7760	 0.5300
L	 0.8670	 0.5890
M	 0.8710	 0.5830
N	 0.8380	 0.5810
O	 0.7580	 0.5270
P	 0.9320	 0.6130
Q	 0.9000	 0.6110
S	 0.8910	 0.5840
T	 0.8770	 0.5930
U	 0.8310	 0.5590
V	 0.5440	 0.5000
W	 0.8580	 0.5780
X	 0.7350	 0.5190
Y	 0.6500	 0.4970
Z	 0.6060	 0.4530
a	 0.8230	 0.5750
b	 0.7230	 0.5090
c	 0.7890	 0.5550
d	 0.7750	 0.5420
e	 0.7530	 0.5460
f	 0.7540	 0.5390
g	 0.8720	 0.5870
h	 0.8560	 0.5750
i	 0.8850	 0.6000
j	 0.7370	 0.5440



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Chain	Atom inclusion	Q-score
k	 0.7920	 0.5650
l	 0.8090	 0.5700
m	 0.7710	 0.5510
n	 0.7090	 0.5310
o	 0.7870	 0.5530
p	 0.7980	 0.5470
r	 0.8870	 0.5990
s	 0.8580	 0.5870
u	 0.8510	 0.5750
v	 0.6940	 0.4830
w	 0.8070	 0.5520