



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 12:07 PM JST

PDB ID : 7W1T / pdb_00007w1t
EMDB ID : EMD-32255
Title : Active state CI from Rotenone dataset, Subclass 1
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-20
Resolution : 3.00 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

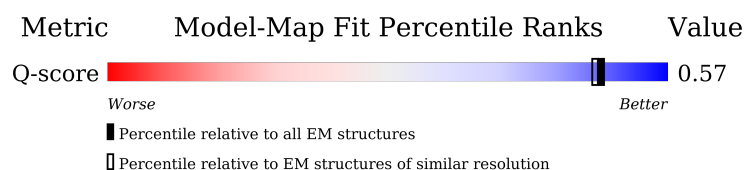
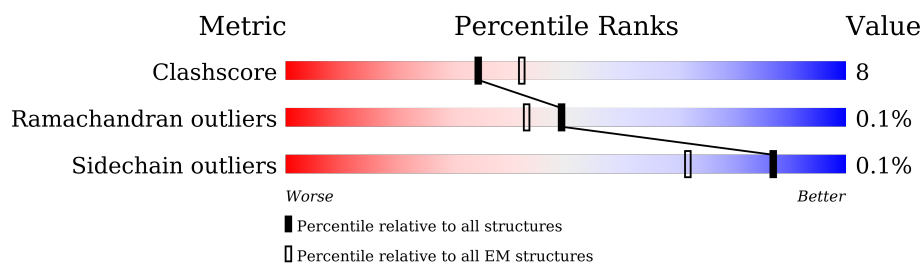
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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

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

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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	342	
10	K	43	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	67	
23	Z	80	
24	a	138	
25	b	126	
26	c	156	
27	d	175	
28	e	104	

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Mol	Chain	Length	Quality of chain
29	f	49	
30	g	121	
31	h	105	
32	i	347	
33	j	115	
34	k	98	
35	l	606	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	125	
44	w	320	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	A	501	-	-	X	-
45	SF4	C	301	-	-	X	-
46	FMN	A	502	-	-	X	-
49	UQ	C	303	-	-	X	-

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 68014 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	433	Total	C	N	O	S	0	0
			3320	2098	590	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
			1402	880	242	269	11		

- 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
			687	432	129	124	2		

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			693	447	102	139	5		
6	X	88	Total	C	N	O	S	0	0
			699	450	103	141	5		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	690	Total	C	N	O	S	0	0
			5292	3318	923	1012	39		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	430	Total	C	N	O	S	0	0
			3451	2207	593	627	24		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	83	Total	C	N	O	S	0	0
			639	414	109	115	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	142	Total	C	N	O	S	0	0
			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	67	Total	C	N	O	S	0	0
			584	385	95	103	1		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	98	Total	C	N	O	S	0	0
			819	537	144	137	1		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	49	Total	C	N	O	0	0
			377	246	65	66		

- 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	115	Total	C	N	O	S	0	0
			914	615	134	158	7		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	606	Total	C	N	O	S	0	0
			4816	3193	746	826	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	175	Total	C	N	O	S	0	0
			1284	857	188	226	13		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	318	Total	C	N	O	S	0	0
			2501	1672	385	423	21		

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

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

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

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

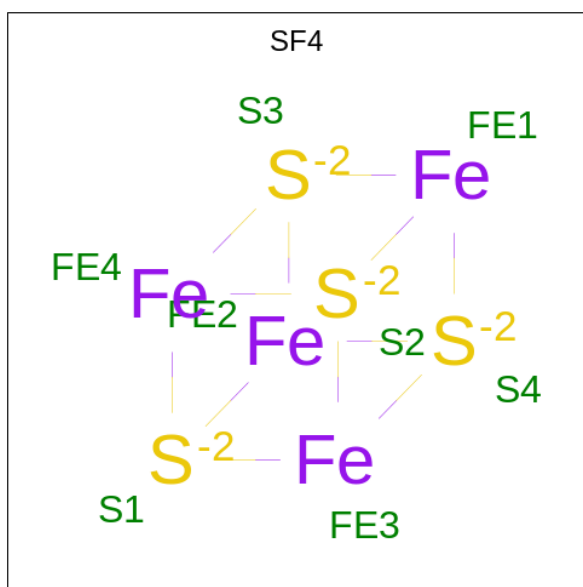
There is a discrepancy between the modelled and reference sequences:

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

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

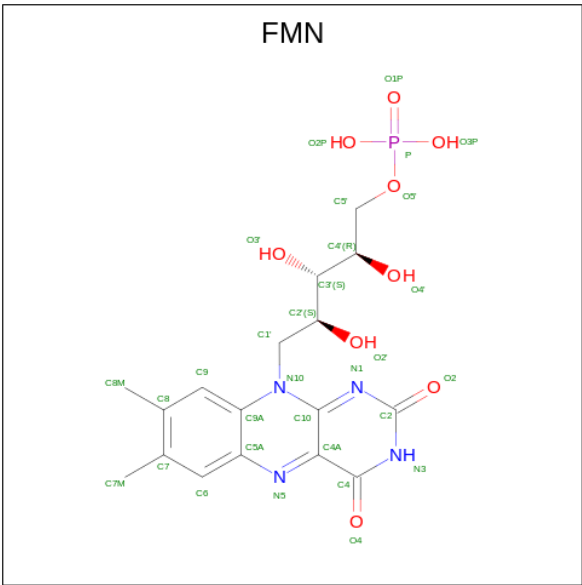
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2583	1645	439	489	10		

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



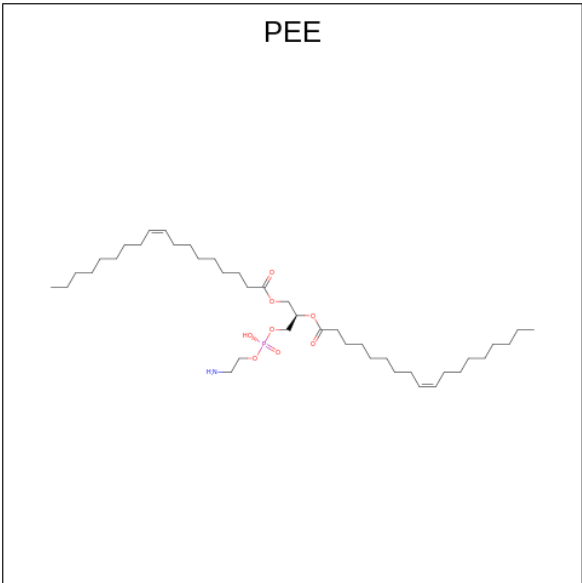
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 47 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



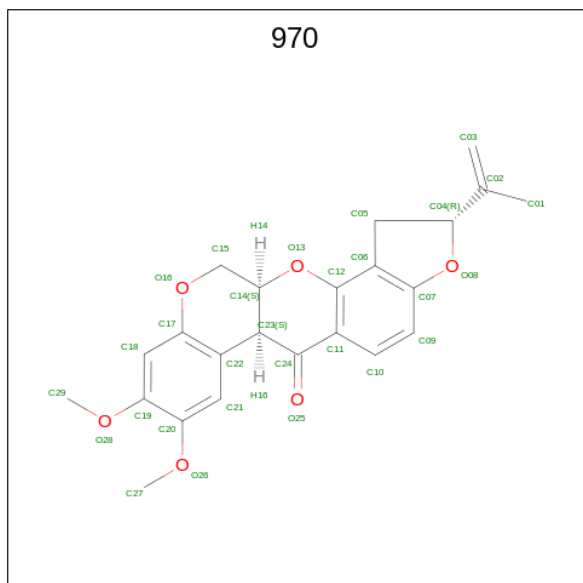
Mol	Chain	Residues	Atoms					AltConf
47	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	J	1	Total	C	N	O	P	0
			47	37	1	8	1	

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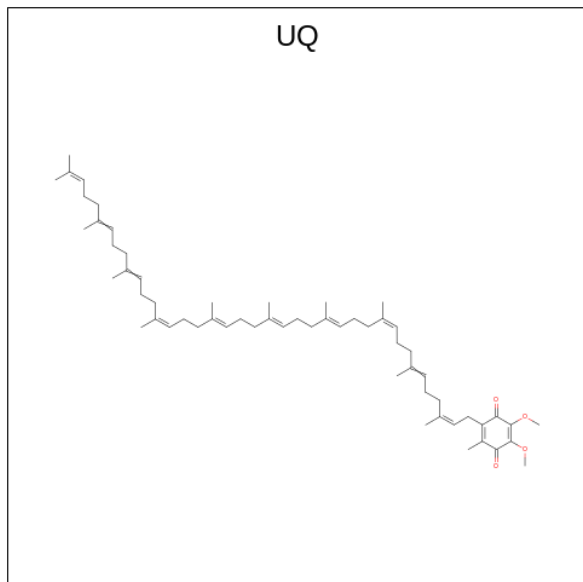
Mol	Chain	Residues	Atoms					AltConf
47	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
47	f	1	Total	N				0
			1	1				
47	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	j	1	Total	C	N	O	P	0
			41	31	1	8	1	
47	l	1	Total	C	N	O	P	0
			40	30	1	8	1	
47	l	1	Total	C	N	O	P	0
			50	40	1	8	1	
47	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
47	r	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	v	1	Total	N				0
			1	1				

- Molecule 48 is (2R,6aS,12aS)-8,9-dimethoxy-2-(prop-1-en-2-yl)-1,2,12,12a-tetrahydrofuro[2',3':7,8][1]benzopyrano[2,3-c][1]benzopyran-6(6aH)-one (CCD ID: 970) (formula: C₂₃H₂₂O₆) (labeled as "Ligand of Interest" by depositor).



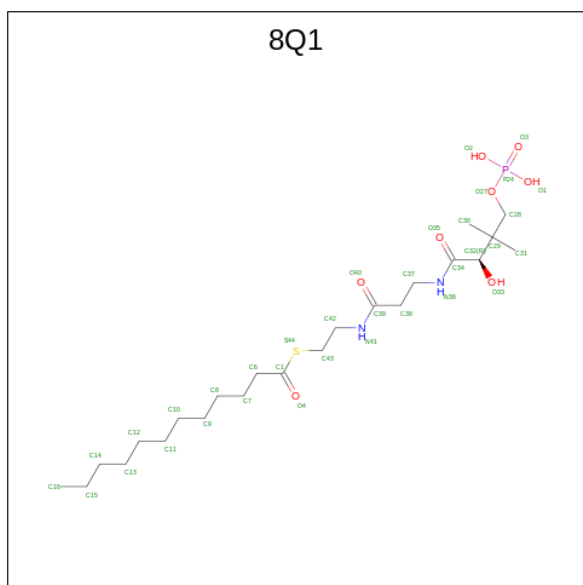
Mol	Chain	Residues	Atoms			AltConf
48	C	1	Total	C	O	0
			29	23	6	

- Molecule 49 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



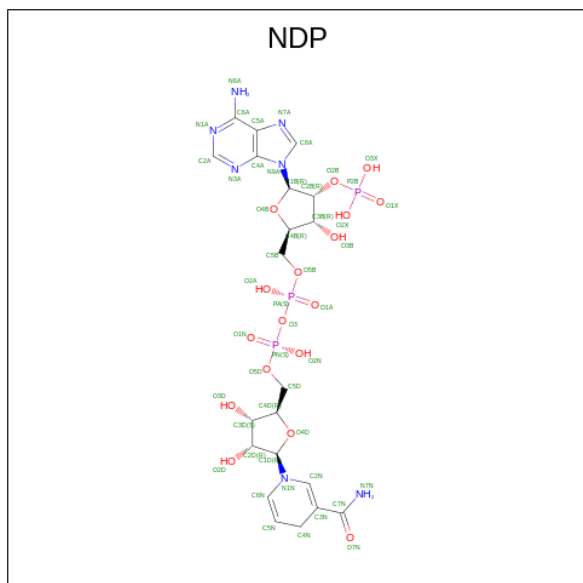
Mol	Chain	Residues	Atoms			AltConf
49	C	1	Total	C	O	0
			38	34	4	
49	J	1	Total	C	O	0
			33	29	4	

- 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).



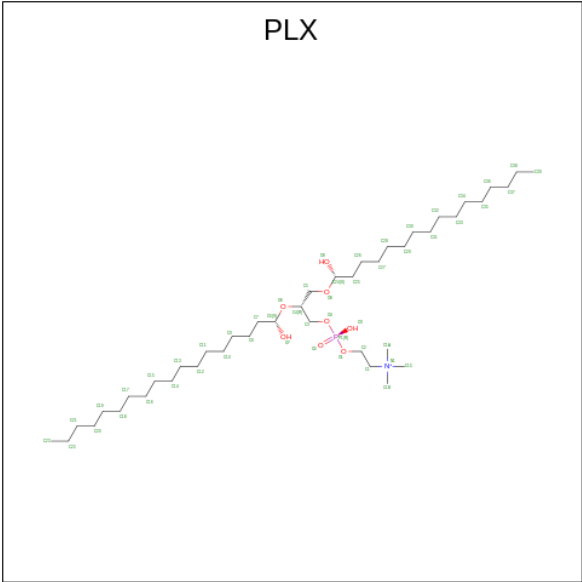
Mol	Chain	Residues	Atoms						AltConf
50	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
50	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

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



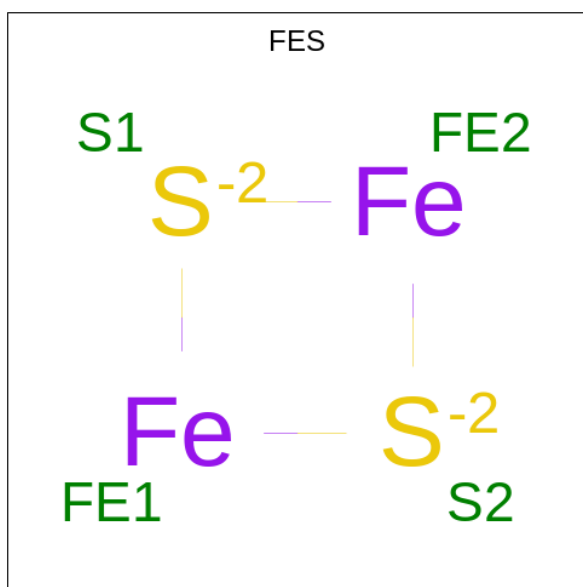
Mol	Chain	Residues	Atoms					AltConf
51	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 52 is (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: $C_{42}H_{89}NO_8P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 53 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).

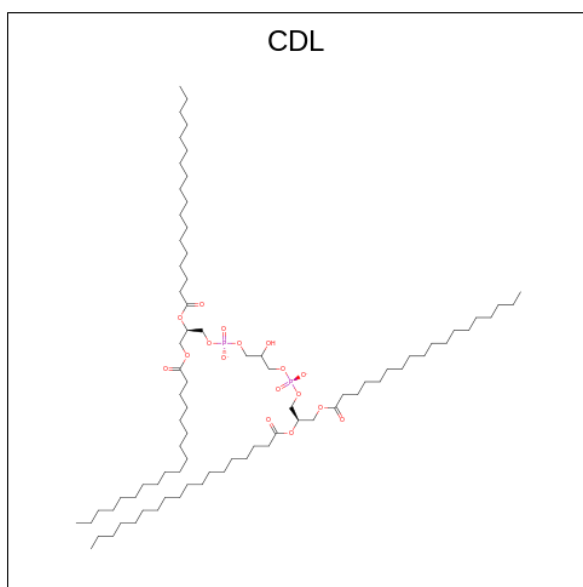


Mol	Chain	Residues	Atoms			AltConf
53	M	1	Total	Fe	S	0
			4	2	2	
53	O	1	Total	Fe	S	0
			4	2	2	

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 55 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).

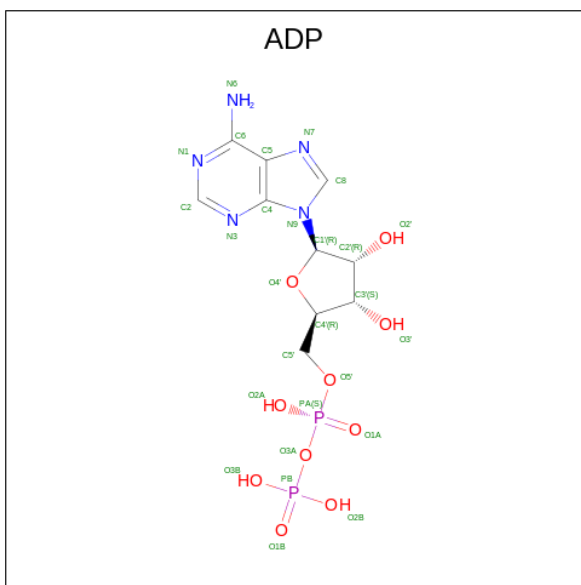


Mol	Chain	Residues	Atoms				AltConf
55	N	1	Total	C	O	P	0
			51	32	17	2	
55	V	1	Total	C	O	P	0
			94	75	17	2	
55	V	1	Total	C	O	P	0
			100	81	17	2	
55	a	1	Total	C	O	P	0
			100	81	17	2	
55	k	1	Total	C	O	P	0
			95	76	17	2	
55	l	1	Total	C	O	P	0
			99	80	17	2	
55	l	1	Total	C	O	P	0
			100	81	17	2	
55	n	1	Total	C	O	P	0
			55	36	17	2	
55	r	1	Total	C	O	P	0
			99	80	17	2	

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

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

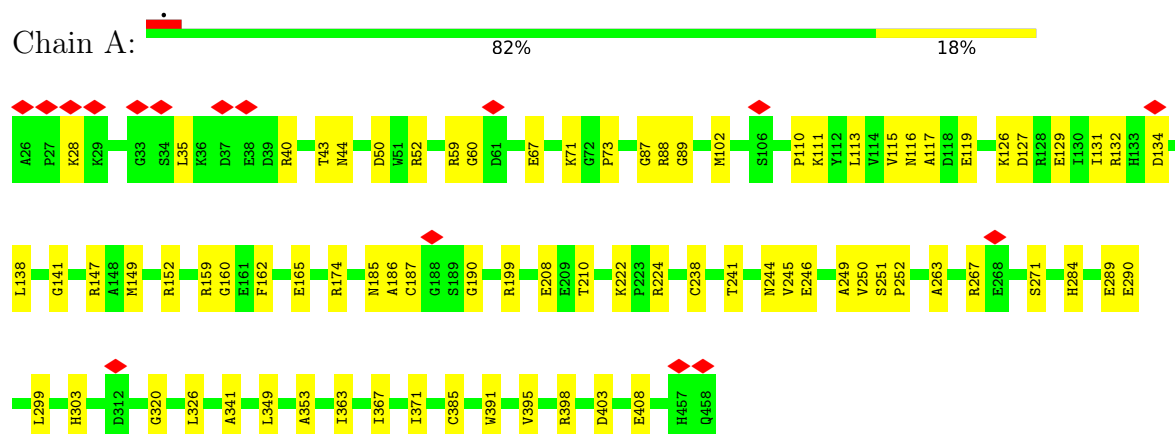


Mol	Chain	Residues	Atoms					AltConf
57	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

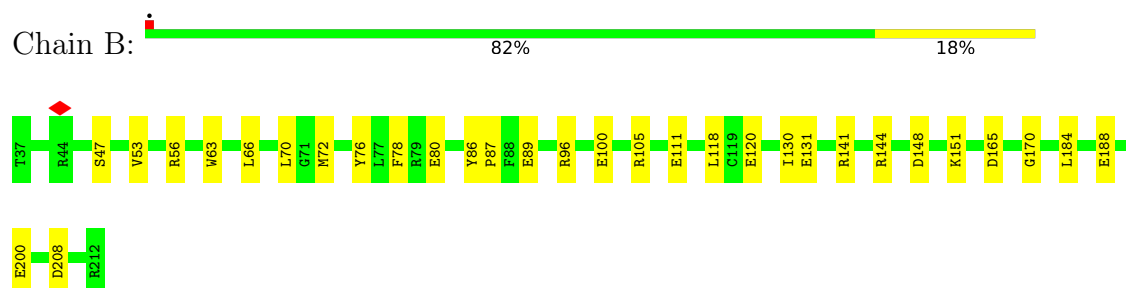
3 Residue-property plots

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.

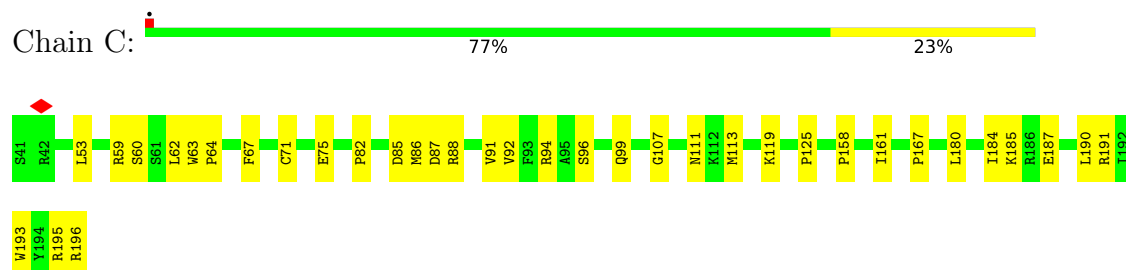
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



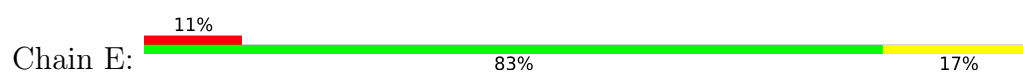
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



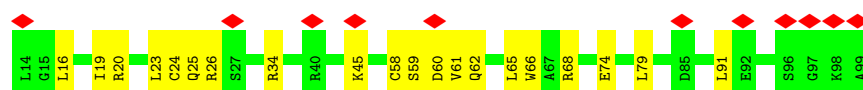
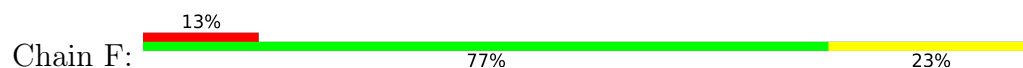
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



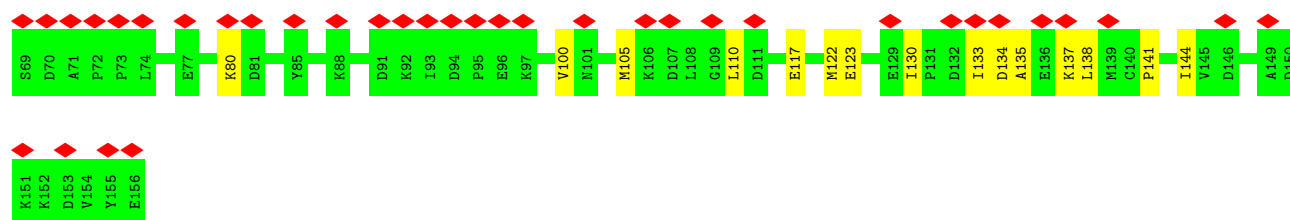
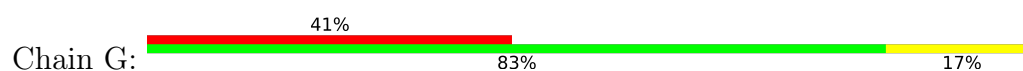
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



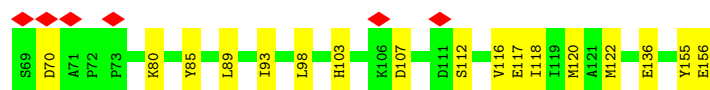
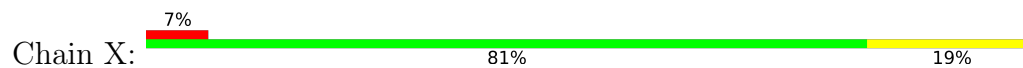
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



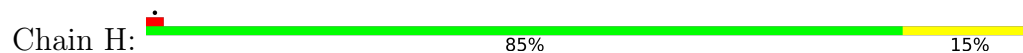
- Molecule 6: Acyl carrier protein



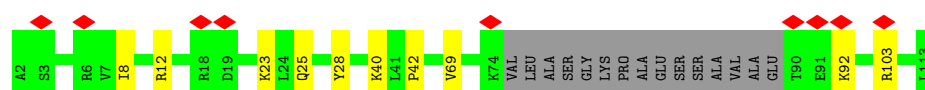
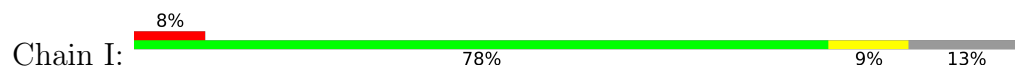
- Molecule 6: Acyl carrier protein



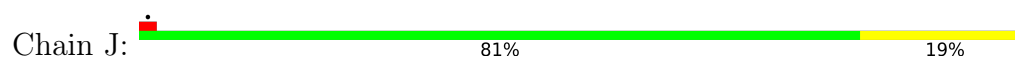
- Molecule 7: Complex I subunit B13



- Molecule 8: Complex I-B14.5a

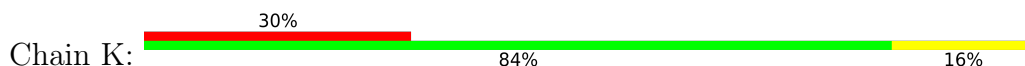


- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

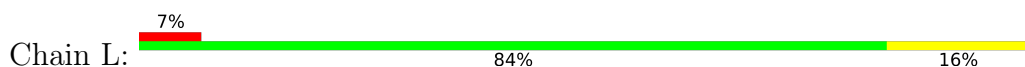




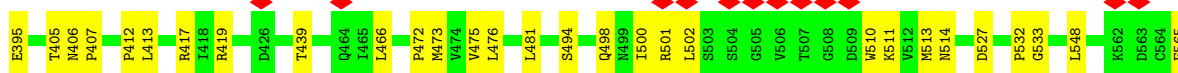
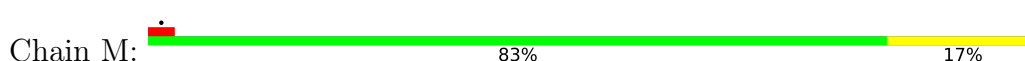
• Molecule 10: Complex I-9kD



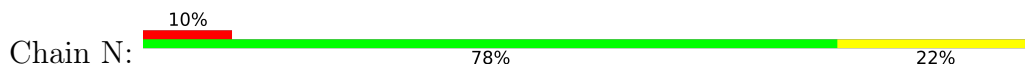
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

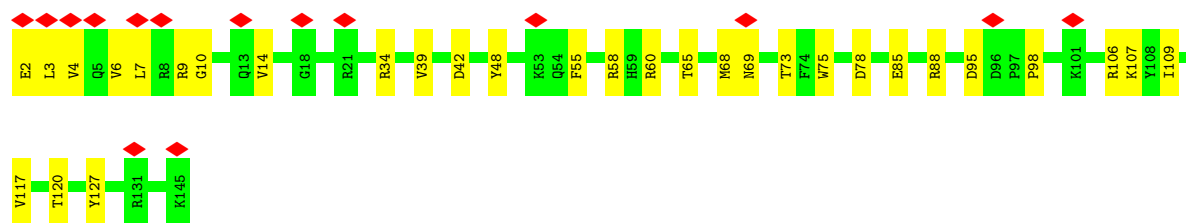


• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

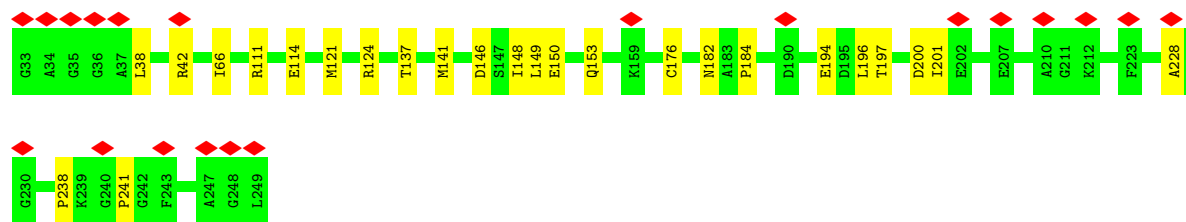
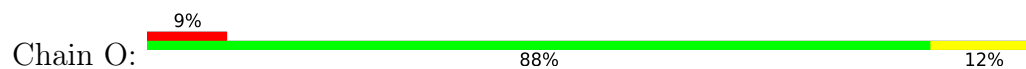


• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

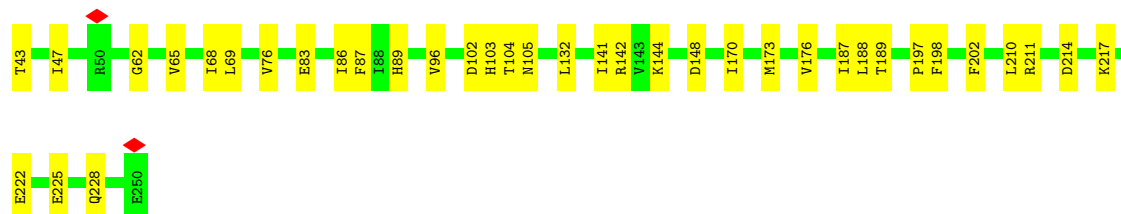
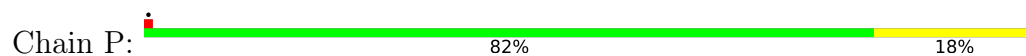




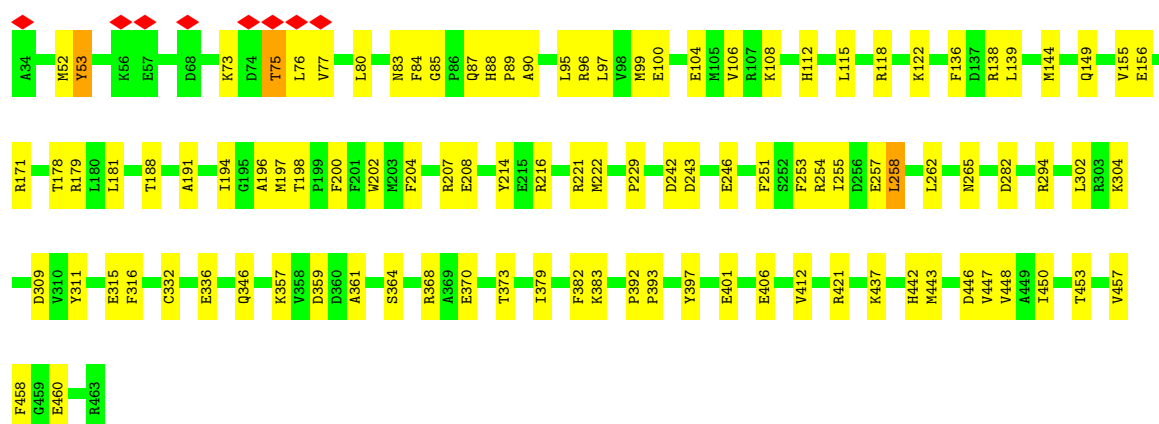
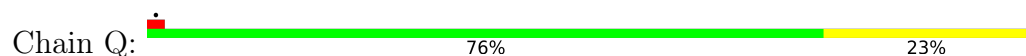
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



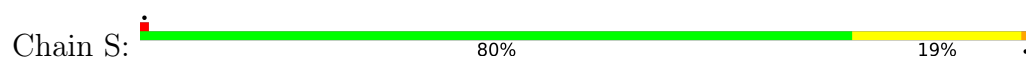
- Molecule 15: Complex I-30kD

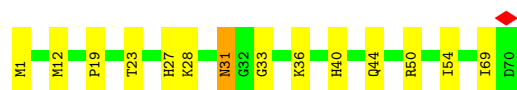


- Molecule 16: Complex I-49kD

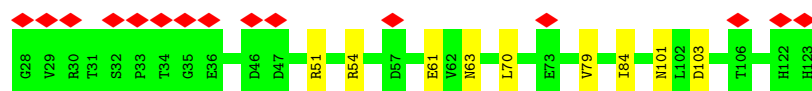
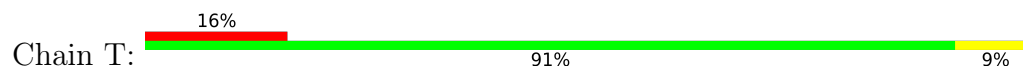


- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

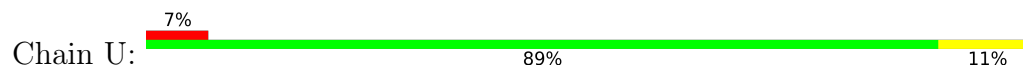




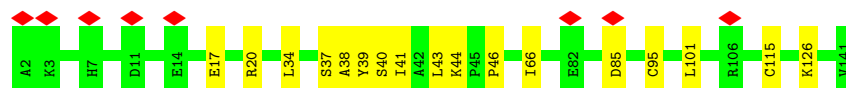
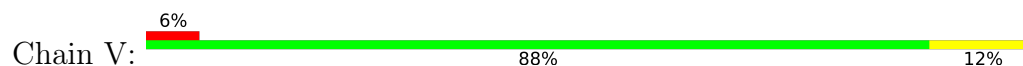
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



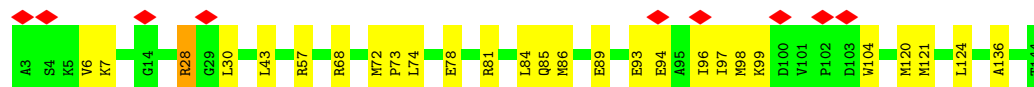
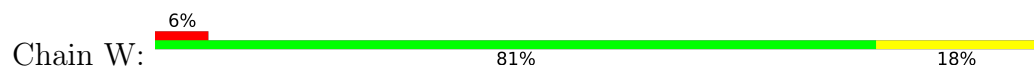
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



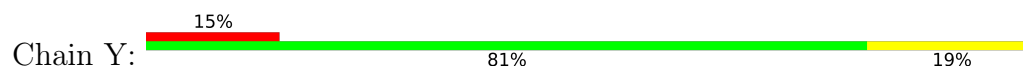
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



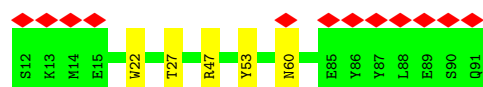
- Molecule 21: Complex I-B16.6



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



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



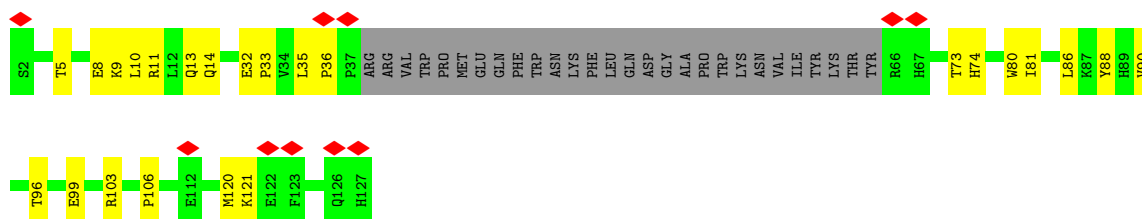
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:  91% 9%



- Molecule 25: Complex I-B17

Chain b:  8% 59% 19% 22%



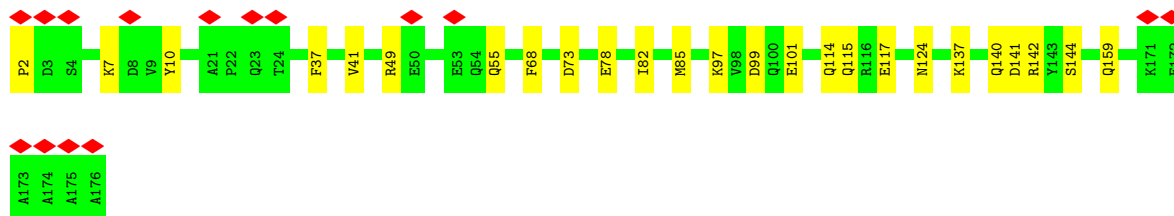
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c:  6% 85% 15%



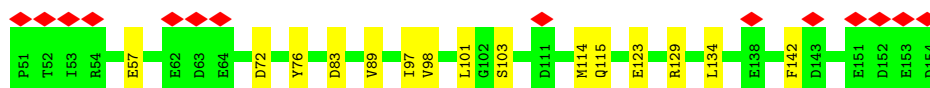
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d:  9% 86% 14%

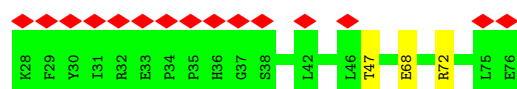


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

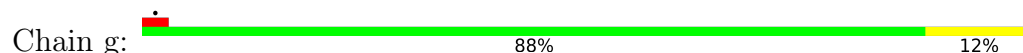
Chain e:  13% 86% 14%



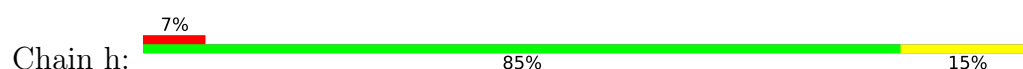
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



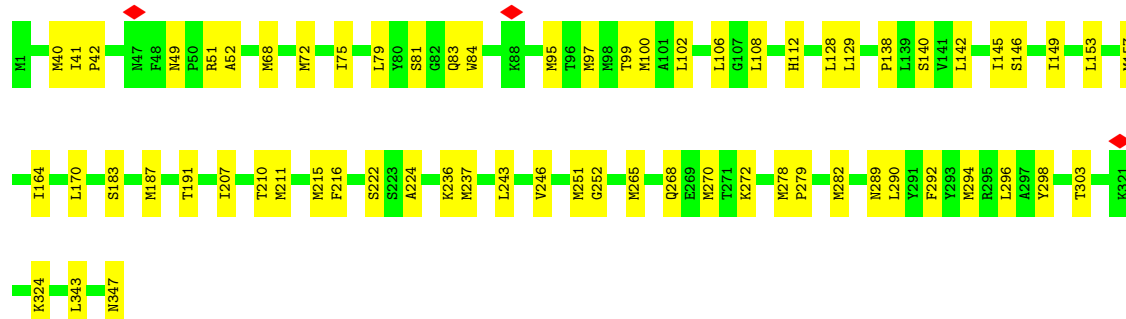
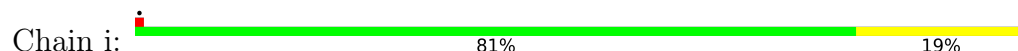
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



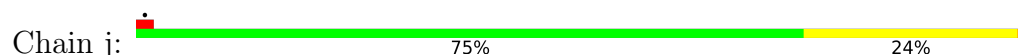
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



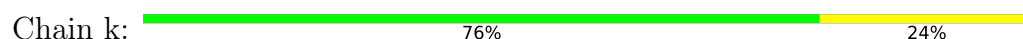
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

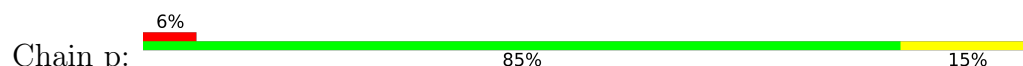


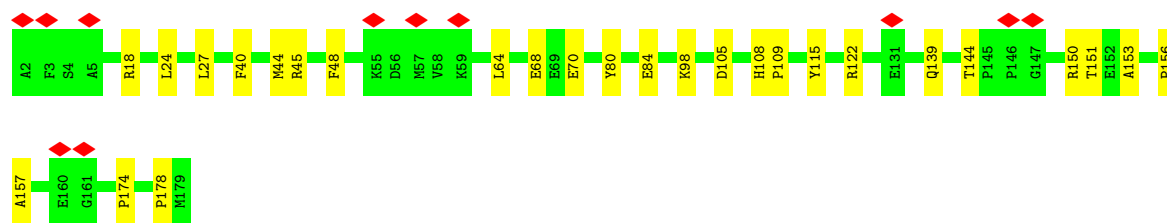
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3



- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

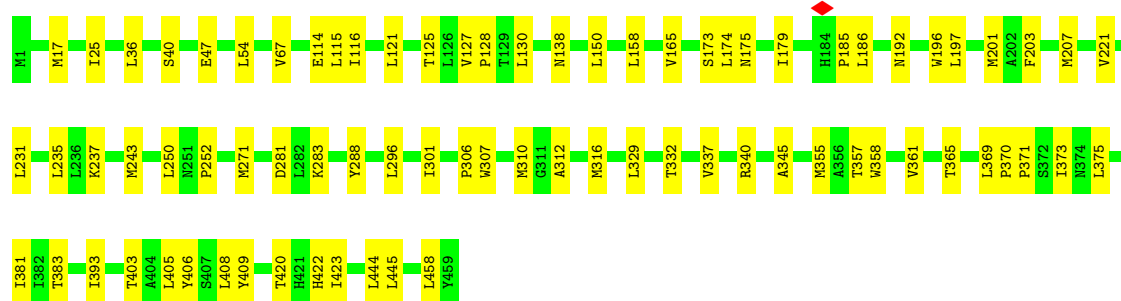






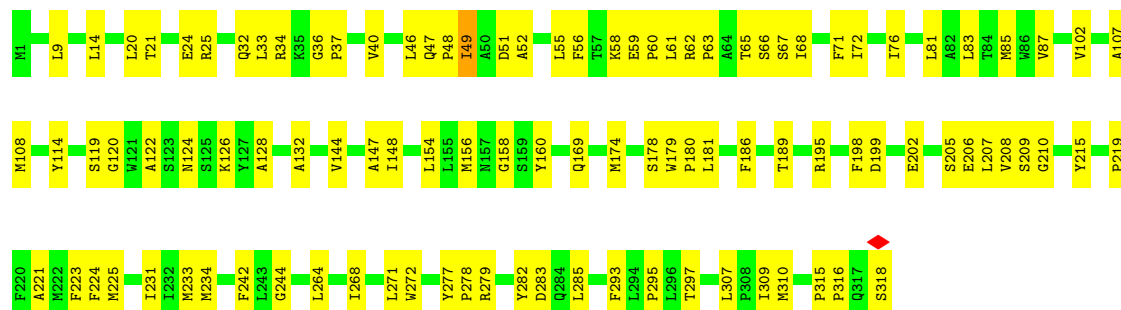
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r: 83% 17%



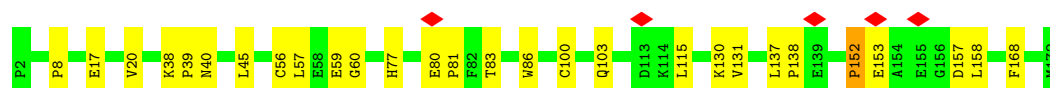
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s: 68% 32%



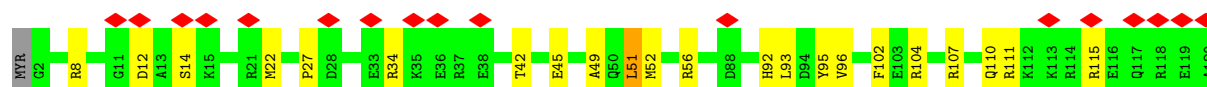
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

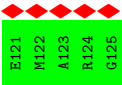
Chain u: 84% 16%



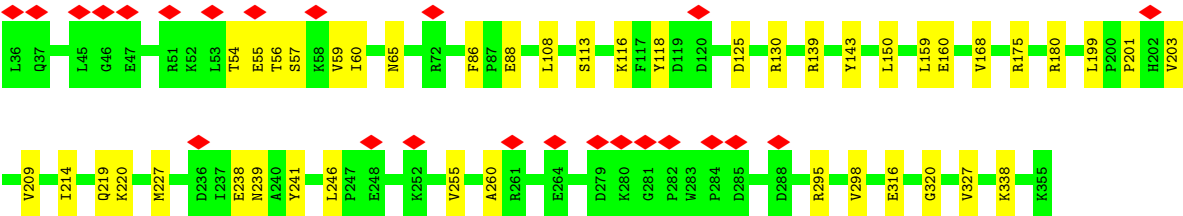
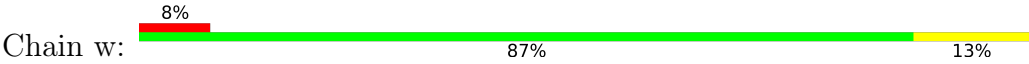
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v: 18% 82% 17%





• 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	67699	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	0.210	Depositor
Minimum map value	-0.103	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.029	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, SF4, FES, MG, 970, PLX, 8Q1, NDP, PEE, ADP, ZN, 2MR, CDL, UQ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.17	0/3396	0.34	0/4591
2	B	0.18	0/1433	0.38	0/1942
3	C	0.23	0/1279	0.40	0/1730
4	E	0.15	0/995	0.36	0/1340
5	F	0.20	0/698	0.44	0/940
6	G	0.15	0/705	0.41	0/956
6	X	0.12	0/711	0.28	0/963
7	H	0.17	0/929	0.39	0/1258
8	I	0.14	0/798	0.35	0/1079
9	J	0.16	0/2828	0.35	0/3834
10	K	0.11	0/377	0.27	0/509
11	L	0.16	0/1039	0.32	0/1403
12	M	0.16	0/5380	0.36	0/7290
13	N	0.12	0/1245	0.31	0/1694
14	O	0.15	0/1711	0.36	0/2328
15	P	0.18	0/1789	0.39	0/2436
16	Q	0.21	0/3530	0.40	1/4787 (0.0%)
17	S	0.15	0/581	0.39	0/781
18	T	0.12	0/755	0.28	0/1018
19	U	0.12	0/660	0.28	0/908
20	V	0.13	0/1042	0.26	0/1411
21	W	0.19	0/1198	0.41	0/1617
22	Y	0.13	0/610	0.31	0/836
23	Z	0.11	0/660	0.28	0/892
24	a	0.14	0/1184	0.30	0/1603
25	b	0.16	0/844	0.39	0/1149
26	c	0.13	0/1371	0.32	0/1875
27	d	0.14	0/1494	0.29	0/2015
28	e	0.13	0/891	0.29	0/1210
29	f	0.11	0/385	0.25	0/522
30	g	0.14	0/1031	0.30	0/1394
31	h	0.14	0/889	0.31	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.17	0/2773	0.35	0/3768
33	j	0.24	0/938	0.56	0/1281
34	k	0.18	0/759	0.40	0/1029
35	l	0.16	0/4947	0.34	0/6728
36	m	0.26	0/1316	0.56	1/1788 (0.1%)
37	n	0.14	0/491	0.29	0/663
38	o	0.14	0/1092	0.31	0/1481
39	p	0.15	0/1590	0.31	0/2155
40	r	0.17	0/3723	0.34	0/5078
41	s	0.21	0/2573	0.48	0/3518
42	u	0.14	0/1436	0.34	0/1938
43	v	0.12	0/1052	0.35	2/1411 (0.1%)
44	w	0.13	0/2643	0.29	0/3580
All	All	0.16	0/67771	0.36	4/91919 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	262	LEU	N-CA-C	6.30	121.86	114.04
36	m	73	ALA	N-CA-C	5.87	117.75	111.36
43	v	51	LEU	CA-C-N	5.27	133.42	122.41
43	v	51	LEU	C-N-CA	5.27	133.42	122.41

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	3320	0	3277	64	0
2	B	1402	0	1338	28	0
3	C	1248	0	1254	58	0
4	E	971	0	975	17	0
5	F	687	0	700	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	693	0	671	11	0
6	X	699	0	682	14	0
7	H	910	0	950	13	0
8	I	780	0	808	10	0
9	J	2751	0	2773	51	0
10	K	366	0	338	6	0
11	L	1016	0	1016	16	0
12	M	5292	0	5322	74	0
13	N	1204	0	1162	22	0
14	O	1671	0	1673	19	0
15	P	1738	0	1693	26	0
16	Q	3451	0	3381	88	0
17	S	566	0	561	10	0
18	T	741	0	702	7	0
19	U	639	0	631	9	0
20	V	1021	0	1025	12	0
21	W	1167	0	1155	26	0
22	Y	584	0	529	11	0
23	Z	641	0	620	6	0
24	a	1151	0	1164	11	0
25	b	819	0	835	20	0
26	c	1315	0	1208	16	0
27	d	1461	0	1429	21	0
28	e	867	0	817	12	0
29	f	377	0	353	4	0
30	g	1000	0	994	15	0
31	h	867	0	871	15	0
32	i	2710	0	2874	49	0
33	j	914	0	951	44	0
34	k	748	0	799	37	0
35	l	4816	0	4955	96	0
36	m	1284	0	1251	52	0
37	n	479	0	486	8	0
38	o	1062	0	1072	16	0
39	p	1534	0	1470	20	0
40	r	3631	0	3839	61	0
41	s	2501	0	2600	121	0
42	u	1398	0	1374	21	0
43	v	1028	0	982	16	0
44	w	2583	0	2540	27	0
45	A	8	0	0	2	0
45	B	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	C	8	0	0	3	0
45	M	16	0	0	0	0
46	A	31	0	19	9	0
47	B	51	0	82	4	0
47	J	47	0	71	6	0
47	W	41	0	59	1	0
47	f	1	0	0	0	0
47	j	92	0	141	4	0
47	l	136	0	200	11	0
47	r	51	0	82	5	0
47	v	1	0	0	0	0
48	C	29	0	0	0	0
49	C	38	0	47	21	0
49	J	33	0	39	4	0
50	G	35	0	0	0	0
50	X	35	0	0	2	0
51	J	48	0	24	3	0
52	J	52	0	88	5	0
52	N	52	0	88	10	0
52	a	52	0	88	2	0
52	e	52	0	88	6	0
52	g	52	0	88	7	0
52	j	52	0	88	2	0
52	r	52	0	88	5	0
53	M	4	0	0	0	0
53	O	4	0	0	1	0
54	M	1	0	0	0	0
55	N	51	0	46	1	0
55	V	194	0	294	15	0
55	a	100	0	156	3	0
55	k	95	0	143	15	0
55	l	199	0	307	18	0
55	n	55	0	54	1	0
55	r	99	0	151	4	0
56	T	1	0	0	0	0
57	w	27	0	11	1	0
All	All	68014	0	68642	1109	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 8.

All (1109) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:112:SER:CB	50:X:201:8Q1:O1	1.73	1.36
34:k:28:SER:HB3	36:m:23:LYS:CG	1.56	1.34
51:J:402:NDP:C4D	51:J:402:NDP:O4D	1.68	1.19
3:C:94:ARG:NH2	49:C:303:UQ:H8	1.57	1.15
16:Q:104:GLU:HB2	41:s:282:TYR:OH	1.46	1.15
3:C:125:PRO:HG2	41:s:58:LYS:CE	1.75	1.14
52:N:201:PLX:H341	52:N:201:PLX:H202	1.17	1.11
34:k:28:SER:HB3	36:m:23:LYS:HG2	1.31	1.11
3:C:125:PRO:CG	41:s:58:LYS:HE2	1.80	1.11
34:k:28:SER:HB3	36:m:23:LYS:HG3	1.21	1.10
16:Q:197:MET:HE2	41:s:32:GLN:NE2	1.67	1.09
41:s:24:GLU:HG2	41:s:271:LEU:HD22	1.17	1.09
3:C:125:PRO:HG2	41:s:58:LYS:HE2	1.07	1.03
16:Q:197:MET:HE2	41:s:32:GLN:HE22	0.81	0.98
16:Q:197:MET:CE	41:s:32:GLN:HE22	1.76	0.98
1:A:102:MET:SD	1:A:241:THR:OG1	2.22	0.97
1:A:89:GLY:HA2	1:A:244:ASN:ND2	1.79	0.97
34:k:28:SER:CB	36:m:23:LYS:HG2	1.97	0.95
36:m:64:MET:HE2	36:m:64:MET:HA	1.48	0.94
34:k:28:SER:CB	36:m:23:LYS:CG	2.47	0.93
4:E:99:GLN:HE22	33:j:42:ASP:H	1.03	0.92
33:j:73:LEU:HD12	36:m:55:MET:SD	2.08	0.92
3:C:92:VAL:HG11	49:C:303:UQ:H103	1.54	0.90
52:N:201:PLX:H202	52:N:201:PLX:C34	2.05	0.87
46:A:502:FMN:N1	46:A:502:FMN:O3'	2.08	0.87
3:C:94:ARG:HH22	49:C:303:UQ:H8	1.36	0.86
35:l:383:MET:HE3	35:l:384:PRO:HD2	1.59	0.85
16:Q:104:GLU:CB	41:s:282:TYR:OH	2.25	0.84
49:C:303:UQ:CM3	16:Q:197:MET:HE1	2.07	0.84
1:A:398:ARG:HG2	1:A:403:ASP:HB2	1.60	0.84
49:C:303:UQ:HM33	16:Q:197:MET:HE1	1.57	0.84
33:j:79:SER:O	33:j:84:LEU:HD21	1.78	0.83
1:A:89:GLY:CA	1:A:244:ASN:HD22	1.93	0.82
41:s:24:GLU:CG	41:s:271:LEU:HD22	2.05	0.81
9:J:359:TYR:HD1	41:s:65:THR:HG22	1.46	0.81
55:k:101:CDL:C17	55:k:101:CDL:H211	2.08	0.81
7:H:7:LYS:HG3	7:H:8:THR:HG23	1.63	0.80
16:Q:80:LEU:HD21	41:s:126:LYS:HD3	1.63	0.80
41:s:24:GLU:HG2	41:s:271:LEU:CD2	2.08	0.79
33:j:50:PRO:HA	36:m:76:THR:HG21	1.65	0.79
1:A:89:GLY:HA2	1:A:244:ASN:HD22	1.47	0.79
3:C:94:ARG:HH21	49:C:303:UQ:H8	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:190:LEU:HD23	40:r:383:THR:HG21	1.67	0.76
2:B:80:GLU:HG3	17:S:1:MET:SD	2.25	0.76
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.67	0.76
6:X:112:SER:CB	50:X:201:8Q1:P24	2.73	0.76
40:r:237:LYS:HD2	40:r:316:MET:HB3	1.67	0.76
1:A:244:ASN:HB2	46:A:502:FMN:O1P	1.87	0.75
9:J:359:TYR:CD1	41:s:65:THR:HG22	2.21	0.75
35:l:363:TYR:HA	35:l:370:THR:HG21	1.67	0.75
1:A:89:GLY:N	1:A:244:ASN:HD22	1.86	0.74
1:A:152:ARG:NH2	10:K:99:PRO:O	2.21	0.74
32:i:236:LYS:HG3	32:i:237:MET:HG3	1.69	0.74
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.71	0.73
47:J:401:PEE:H79	41:s:52:ALA:HB1	1.71	0.73
55:k:101:CDL:H211	55:k:101:CDL:H172	1.69	0.73
36:m:14:VAL:O	36:m:18:VAL:HG23	1.89	0.73
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.70	0.73
4:E:99:GLN:NE2	33:j:42:ASP:H	1.85	0.73
3:C:158:PRO:HB2	9:J:92:MET:HE3	1.71	0.72
32:i:207:ILE:HG22	32:i:211:MET:HE2	1.71	0.72
2:B:47:SER:O	2:B:56:ARG:NH2	2.23	0.72
35:l:295:GLN:O	35:l:425:ARG:NH1	2.22	0.72
18:T:79:VAL:HG11	18:T:84:ILE:HD13	1.72	0.72
1:A:60:GLY:HA2	14:O:241:PRO:HA	1.72	0.71
41:s:156:MET:O	41:s:315:PRO:HG3	1.90	0.71
37:n:26:TYR:HH	37:n:30:ARG:HH21	1.38	0.71
16:Q:258:LEU:C	16:Q:258:LEU:HD23	2.15	0.71
52:N:201:PLX:H341	52:N:201:PLX:C20	2.09	0.70
9:J:272:LEU:HD11	9:J:375:VAL:HG11	1.74	0.70
35:l:473:PRO:HG2	35:l:475:MET:HE2	1.73	0.70
1:A:385:CYS:HB3	45:A:501:SF4:S2	2.30	0.70
44:w:57:SER:HB3	44:w:150:LEU:HD11	1.72	0.70
11:L:123:ASN:OD1	12:M:246:ARG:NH2	2.24	0.70
3:C:125:PRO:HG2	41:s:58:LYS:NZ	2.06	0.70
3:C:125:PRO:CB	41:s:58:LYS:HE2	2.21	0.70
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.73	0.70
41:s:62:ARG:HD2	41:s:68:ILE:HD13	1.73	0.70
9:J:344:PRO:HG2	9:J:347:LEU:HD13	1.74	0.69
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.74	0.69
32:i:49:ASN:O	32:i:52:ALA:N	2.26	0.69
41:s:49:ILE:HD12	41:s:49:ILE:N	2.07	0.69
41:s:85:MET:HB3	41:s:233:MET:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:100:ARG:NH2	33:j:32:GLU:OE1	2.26	0.69
3:C:88:ARG:CB	41:s:36:GLY:O	2.42	0.68
44:w:125:ASP:O	44:w:130:ARG:NH2	2.26	0.68
13:N:75:TRP:HB3	52:N:201:PLX:O2	1.94	0.68
1:A:43:THR:HG21	14:O:238:PRO:HB3	1.75	0.68
3:C:94:ARG:HH22	49:C:303:UQ:C8	2.07	0.68
3:C:60:SER:HB3	41:s:40:VAL:HG21	1.77	0.67
9:J:192:ARG:NH1	9:J:198:ALA:O	2.27	0.67
9:J:268:PRO:HD3	9:J:342:ALA:HB1	1.75	0.67
33:j:73:LEU:N	33:j:74:PRO:HD2	2.09	0.67
1:A:249:ALA:O	1:A:252:PRO:HD2	1.93	0.67
2:B:200:GLU:HG3	13:N:88:ARG:HD3	1.76	0.67
1:A:244:ASN:N	46:A:502:FMN:O1P	2.26	0.67
3:C:119:LYS:NZ	33:j:32:GLU:OE2	2.27	0.67
49:C:303:UQ:CM3	16:Q:197:MET:CE	2.72	0.67
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.77	0.67
20:V:38:ALA:HB2	55:k:101:CDL:H251	1.75	0.67
5:F:24:CYS:HA	5:F:58:CYS:HB3	1.77	0.66
16:Q:294:ARG:NH2	16:Q:401:GLU:OE2	2.28	0.66
11:L:105:GLU:HA	12:M:611:THR:HG21	1.77	0.66
1:A:159:ARG:NH2	14:O:176:CYS:O	2.28	0.66
16:Q:104:GLU:CD	41:s:282:TYR:CE1	2.73	0.66
41:s:62:ARG:CD	41:s:68:ILE:HD13	2.25	0.66
3:C:94:ARG:NH2	49:C:303:UQ:C8	2.49	0.66
16:Q:104:GLU:OE1	41:s:282:TYR:HE1	1.78	0.66
30:g:56:VAL:HG21	40:r:17:MET:HE1	1.78	0.66
4:E:101:THR:O	4:E:105:ARG:HG3	1.95	0.66
49:C:303:UQ:HM31	16:Q:197:MET:CE	2.26	0.66
33:j:18:VAL:HG11	41:s:76:ILE:HD11	1.77	0.66
4:E:37:ARG:NH2	6:G:123:GLU:OE2	2.29	0.65
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.29	0.65
21:W:121:MET:HE2	21:W:136:ALA:HB1	1.78	0.65
36:m:26:PRO:HB2	36:m:71:THR:HG21	1.79	0.65
41:s:66:SER:HB2	41:s:122:ALA:O	1.96	0.65
12:M:161:GLU:OE2	14:O:42:ARG:NH2	2.29	0.65
24:a:152:LYS:HD3	30:g:96:VAL:HG21	1.79	0.65
12:M:308:ARG:NH2	12:M:578:PRO:O	2.30	0.65
47:l:704:PEE:H28	47:l:704:PEE:H73	1.79	0.65
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.29	0.65
44:w:54:THR:HG23	44:w:56:THR:HG22	1.79	0.65
36:m:139:GLU:O	36:m:143:ILE:HG13	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:156:MET:O	41:s:315:PRO:CG	2.45	0.65
2:B:184:LEU:HB3	11:L:112:MET:HE2	1.78	0.65
41:s:195:ARG:HD3	41:s:231:ILE:HD11	1.78	0.65
16:Q:144:MET:HE3	16:Q:222:MET:HB2	1.78	0.65
36:m:64:MET:HA	36:m:64:MET:CE	2.23	0.65
1:A:52:ARG:HH21	10:K:77:GLN:HG2	1.62	0.64
20:V:34:LEU:HD22	55:k:101:CDL:H261	1.79	0.64
33:j:67:LEU:HD21	34:k:68:ALA:HB2	1.79	0.64
55:l:703:CDL:H431	55:l:703:CDL:H642	1.80	0.64
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.78	0.64
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.31	0.64
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.78	0.64
47:l:704:PEE:H68	47:l:704:PEE:H22	1.79	0.64
9:J:188:GLU:HG3	9:J:200:ILE:HD13	1.78	0.64
12:M:94:MET:HE2	12:M:100:TRP:HH2	1.63	0.64
1:A:116:ASN:O	1:A:245:VAL:HG23	1.97	0.64
7:H:70:GLU:OE2	8:I:103:ARG:NH2	2.31	0.64
38:o:75:ASN:O	38:o:79:ASN:ND2	2.31	0.64
3:C:64:PRO:HD2	3:C:92:VAL:O	1.99	0.63
46:A:502:FMN:HO3'	46:A:502:FMN:C2	2.07	0.63
3:C:94:ARG:HH12	49:C:303:UQ:HM51	1.63	0.63
12:M:406:ASN:ND2	12:M:688:GLN:O	2.30	0.63
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.80	0.63
35:l:10:THR:HA	35:l:13:THR:HG22	1.79	0.63
38:o:118:GLU:O	38:o:120:LYS:NZ	2.29	0.63
13:N:2:GLU:HG3	13:N:4:VAL:HG12	1.80	0.63
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.79	0.63
9:J:71:ASN:HB2	9:J:97:MET:HE2	1.80	0.63
7:H:9:THR:O	7:H:76:GLN:NE2	2.31	0.62
25:b:14:GLN:HE22	39:p:157:ALA:HB3	1.62	0.62
1:A:88:ARG:C	1:A:244:ASN:HD22	2.07	0.62
3:C:88:ARG:HA	41:s:36:GLY:O	1.99	0.62
4:E:99:GLN:HE22	33:j:42:ASP:N	1.87	0.62
16:Q:448:VAL:HG21	41:s:206:GLU:HG3	1.79	0.62
3:C:82:PRO:HB3	41:s:33:LEU:O	1.99	0.62
4:E:84:ILE:HG22	4:E:88:MET:HE3	1.80	0.62
16:Q:85:GLY:HA3	16:Q:95:LEU:O	2.00	0.62
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.82	0.62
44:w:168:VAL:HG21	44:w:241:TYR:CE1	2.35	0.62
1:A:40:ARG:NH1	1:A:289:GLU:O	2.33	0.62
1:A:222:LYS:O	11:L:175:LYS:NZ	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:104:GLU:OE1	41:s:282:TYR:CE1	2.53	0.62
4:E:64:ARG:NH1	6:G:117:GLU:OE2	2.33	0.61
1:A:127:ASP:O	1:A:131:ILE:HG12	2.00	0.61
8:I:25:GLN:HG2	16:Q:254:ARG:NE	2.15	0.61
14:O:38:LEU:O	14:O:124:ARG:NH2	2.33	0.61
21:W:28:ARG:HH11	21:W:28:ARG:CG	2.13	0.61
6:X:117:GLU:OE2	39:p:45:ARG:NH1	2.33	0.61
39:p:105:ASP:OD1	39:p:122:ARG:NH1	2.32	0.61
40:r:337:VAL:HG11	40:r:345:ALA:HB2	1.81	0.61
55:k:101:CDL:H172	55:k:101:CDL:C21	2.30	0.61
40:r:231:LEU:HD23	40:r:235:LEU:HD12	1.81	0.61
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.82	0.61
16:Q:53:TYR:HB3	35:l:571:MET:HE3	1.83	0.61
3:C:88:ARG:HB2	41:s:36:GLY:O	2.00	0.61
32:i:270:MET:HE3	32:i:279:PRO:HG3	1.81	0.61
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.83	0.61
38:o:59:VAL:HG22	40:r:423:ILE:HG12	1.83	0.61
41:s:65:THR:O	41:s:124:ASN:ND2	2.31	0.61
12:M:472:PRO:O	12:M:510:TRP:NE1	2.29	0.61
27:d:101:GLU:OE2	28:e:115:GLN:NE2	2.34	0.61
31:h:18:MET:HE3	34:k:56:ALA:HA	1.81	0.61
35:l:495:ILE:HG22	35:l:499:MET:HE2	1.81	0.61
22:Y:97:LEU:HB3	43:v:104:ARG:HB2	1.82	0.60
35:l:419:THR:HA	35:l:422:TYR:CE2	2.36	0.60
2:B:111:GLU:O	2:B:141:ARG:NH1	2.35	0.60
12:M:224:ASP:OD2	12:M:291:ARG:NH1	2.35	0.60
35:l:577:VAL:O	35:l:580:GLN:NE2	2.29	0.60
44:w:116:LYS:NZ	44:w:125:ASP:OD2	2.34	0.60
20:V:44:LYS:NZ	55:V:201:CDL:OB4	2.33	0.60
30:g:4:MET:O	30:g:10:ARG:NH1	2.33	0.60
33:j:67:LEU:CD2	34:k:68:ALA:HB2	2.31	0.60
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.35	0.60
3:C:125:PRO:O	41:s:58:LYS:HE3	2.02	0.60
12:M:59:GLN:HE21	12:M:62:ARG:HH12	1.48	0.60
41:s:49:ILE:HD12	41:s:49:ILE:H	1.65	0.60
43:v:51:LEU:O	43:v:52:MET:HG3	2.01	0.60
2:B:70:LEU:O	41:s:272:TRP:HZ2	1.85	0.60
9:J:76:MET:HE1	9:J:254:LYS:HD3	1.84	0.60
7:H:9:THR:HG23	7:H:16:VAL:HG22	1.83	0.60
13:N:68:MET:HG3	13:N:69:ASN:H	1.66	0.60
16:Q:104:GLU:HB2	41:s:282:TYR:HH	1.62	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:85:MET:HE1	41:s:108:MET:HB3	1.84	0.60
42:u:152:PRO:O	42:u:153:GLU:HG2	2.02	0.60
9:J:317:ASP:OD2	9:J:321:ARG:NH1	2.34	0.59
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.28	0.59
3:C:82:PRO:HA	41:s:34:ARG:HB3	1.84	0.59
3:C:94:ARG:HH12	49:C:303:UQ:CM5	2.16	0.59
5:F:20:ARG:HB2	5:F:66:TRP:HB2	1.85	0.59
55:N:202:CDL:H722	55:N:202:CDL:H512	1.83	0.59
40:r:370:PRO:HG3	40:r:375:LEU:HD22	1.84	0.59
1:A:87:GLY:HA3	46:A:502:FMN:O2P	2.02	0.59
16:Q:77:VAL:O	16:Q:77:VAL:HG23	2.01	0.59
16:Q:73:LYS:HE2	16:Q:75:THR:HG22	1.84	0.59
25:b:80:TRP:HD1	27:d:41:VAL:HG23	1.68	0.59
17:S:12:MET:HE3	41:s:20:LEU:HB2	1.84	0.59
25:b:80:TRP:CD1	27:d:41:VAL:HG23	2.37	0.59
37:n:47:ARG:NH2	37:n:53:GLU:OE2	2.36	0.59
5:F:68:ARG:NH2	12:M:364:ASP:OD2	2.36	0.58
12:M:217:GLU:HG2	12:M:218:LEU:HG	1.85	0.58
20:V:17:GLU:OE1	20:V:20:ARG:NH1	2.31	0.58
21:W:85:GLN:O	21:W:89:GLU:HG3	2.03	0.58
41:s:221:ALA:O	41:s:225:MET:HG3	2.03	0.58
24:a:134:GLU:OE1	37:n:57:TRP:NE1	2.23	0.58
3:C:191:ARG:HB3	3:C:195:ARG:NH1	2.18	0.58
35:l:286:LEU:HD22	35:l:411:MET:SD	2.44	0.58
27:d:114:GLN:HG3	35:l:203:MET:HG2	1.84	0.58
3:C:191:ARG:HB3	3:C:195:ARG:HH12	1.69	0.58
44:w:118:TYR:OH	57:w:401:ADP:O2'	2.22	0.58
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.85	0.58
40:r:312:ALA:O	40:r:316:MET:HG3	2.04	0.58
3:C:85:ASP:CG	41:s:34:ARG:HB2	2.29	0.58
22:Y:97:LEU:HD12	43:v:107:ARG:HH21	1.69	0.58
6:G:80:LYS:HE2	6:G:100:VAL:HG21	1.86	0.57
25:b:9:LYS:HG2	25:b:13:GLN:HE22	1.69	0.57
9:J:268:PRO:HD3	9:J:342:ALA:CB	2.34	0.57
9:J:306:GLU:HG2	9:J:315:THR:HG22	1.86	0.57
52:a:202:PLX:H92	40:r:40:SER:HB3	1.85	0.57
34:k:23:ARG:NH1	36:m:81:GLU:OE1	2.36	0.57
43:v:27:PRO:O	43:v:34:ARG:NH1	2.37	0.57
21:W:98:MET:HE3	31:h:79:ILE:HD13	1.84	0.57
13:N:117:VAL:O	13:N:120:THR:OG1	2.23	0.57
30:g:13:LEU:HA	52:g:201:PLX:H32	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:151:THR:HG22	39:p:153:ALA:H	1.69	0.57
33:j:50:PRO:CA	36:m:76:THR:HG21	2.33	0.57
33:j:67:LEU:CD2	34:k:68:ALA:CB	2.82	0.57
2:B:148:ASP:HB3	2:B:151:LYS:HB2	1.86	0.57
36:m:24:PRO:O	36:m:81:GLU:HB2	2.05	0.57
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.38	0.57
35:l:128:MET:HE1	35:l:252:MET:HA	1.87	0.57
21:W:84:LEU:HD12	42:u:57:LEU:HD21	1.87	0.57
36:m:11:THR:O	36:m:15:ILE:HG13	2.05	0.57
36:m:26:PRO:HB2	36:m:71:THR:CG2	2.34	0.57
14:O:150:GLU:OE2	14:O:150:GLU:N	2.38	0.57
44:w:168:VAL:HG21	44:w:241:TYR:HE1	1.70	0.57
15:P:69:LEU:HD22	15:P:96:VAL:HG22	1.86	0.56
6:X:136:GLU:OE2	39:p:18:ARG:NH1	2.38	0.56
36:m:24:PRO:HB3	36:m:89:VAL:HG11	1.87	0.56
35:l:359:MET:O	35:l:436:ARG:NH2	2.38	0.56
40:r:307:TRP:HA	40:r:310:MET:HE2	1.87	0.56
41:s:67:SER:O	41:s:71:PHE:HB2	2.04	0.56
3:C:161:ILE:HG13	3:C:180:LEU:HB2	1.87	0.56
12:M:388:ASN:ND2	12:M:513:MET:O	2.38	0.56
12:M:389:THR:O	12:M:390:THR:OG1	2.21	0.56
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.86	0.56
30:g:52:ARG:NH2	44:w:338:LYS:O	2.38	0.56
12:M:251:ILE:HG13	12:M:604:GLN:HB3	1.86	0.56
31:h:18:MET:HE1	34:k:59:MET:HB3	1.87	0.56
9:J:310:PHE:HE1	47:J:401:PEE:H15	1.71	0.56
19:U:46:ASN:CG	33:j:80:GLN:O	2.49	0.56
1:A:50:ASP:O	1:A:59:ARG:NH2	2.37	0.56
16:Q:242:ASP:O	16:Q:246:GLU:HG2	2.06	0.56
35:l:71:LEU:HD12	40:r:310:MET:HE1	1.86	0.56
55:a:201:CDL:H751	28:e:103:SER:HB2	1.87	0.56
32:i:268:GLN:HA	40:r:165:VAL:HG11	1.87	0.56
3:C:88:ARG:HA	41:s:36:GLY:C	2.31	0.56
3:C:190:LEU:HD22	47:J:401:PEE:H13	1.88	0.56
9:J:133:GLU:OE1	9:J:321:ARG:NH2	2.39	0.56
41:s:47:GLN:HB3	41:s:48:PRO:HD3	1.87	0.56
3:C:85:ASP:OD1	41:s:34:ARG:HD2	2.06	0.55
5:F:65:LEU:HD11	5:F:91:LEU:HD21	1.87	0.55
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.87	0.55
5:F:24:CYS:CA	5:F:58:CYS:HB3	2.36	0.55
12:M:136:GLU:OE2	12:M:272:ARG:NH2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.37	0.55
6:G:135:ALA:HA	6:G:138:LEU:HD13	1.89	0.55
35:l:375:ILE:HD12	35:l:458:LEU:HD11	1.88	0.55
16:Q:457:VAL:HG13	16:Q:460:GLU:HG2	1.88	0.55
41:s:49:ILE:H	41:s:49:ILE:CD1	2.19	0.55
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.86	0.55
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.88	0.55
1:A:113:LEU:HD13	1:A:149:MET:HE1	1.87	0.55
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.88	0.55
33:j:33:LYS:HD3	41:s:61:LEU:HD21	1.89	0.55
33:j:63:LEU:HD21	36:m:63:GLY:HA2	1.88	0.55
34:k:21:MET:HE1	55:k:101:CDL:H601	1.87	0.55
40:r:403:THR:HA	40:r:406:TYR:CE2	2.41	0.55
9:J:50:SER:OG	15:P:225:GLU:OE2	2.25	0.55
21:W:89:GLU:O	21:W:93:GLU:HG2	2.07	0.55
34:k:32:CYS:SG	36:m:23:LYS:HD2	2.47	0.55
6:G:138:LEU:HD23	6:G:144:ILE:HG12	1.88	0.55
11:L:158:LYS:NZ	12:M:69:LEU:O	2.35	0.55
12:M:390:THR:HA	12:M:600:GLU:HG2	1.87	0.55
40:r:127:VAL:HG23	40:r:128:PRO:HD3	1.89	0.55
1:A:263:ALA:HA	1:A:271:SER:HB3	1.87	0.55
2:B:53:VAL:HG12	19:U:13:TRP:CD1	2.42	0.55
25:b:103:ARG:NH1	43:v:49:ALA:O	2.40	0.55
33:j:77:TRP:HD1	41:s:318:SER:O	1.89	0.55
35:l:327:LEU:O	35:l:331:MET:HG2	2.07	0.55
35:l:481:THR:HG1	43:v:92:HIS:HD1	1.52	0.54
55:l:703:CDL:H561	55:l:703:CDL:H342	1.89	0.54
38:o:45:ARG:HH12	39:p:144:THR:HG21	1.72	0.54
14:O:111:ARG:NH1	14:O:114:GLU:OE2	2.40	0.54
40:r:201:MET:HE2	47:r:501:PEE:H77	1.88	0.54
32:i:252:GLY:HA3	32:i:290:LEU:HD13	1.89	0.54
40:r:185:PRO:HB3	40:r:252:PRO:HD3	1.87	0.54
41:s:158:GLY:HA3	41:s:315:PRO:HB2	1.89	0.54
1:A:185:ASN:C	1:A:187:CYS:H	2.16	0.54
40:r:243:MET:HB3	40:r:301:ILE:HG21	1.88	0.54
9:J:199:THR:OG1	9:J:258:ALA:O	2.22	0.54
13:N:127:TYR:OH	18:T:61:GLU:O	2.22	0.54
21:W:74:LEU:O	21:W:78:GLU:HG3	2.08	0.54
4:E:119:LEU:HD11	12:M:628:GLU:HG2	1.89	0.54
30:g:15:PHE:O	30:g:16:LEU:HD22	2.07	0.54
35:l:55:MET:HE2	35:l:471:ASN:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:C:303:UQ:H161	41:s:51:ASP:HB3	1.90	0.54
40:r:420:THR:HB	40:r:423:ILE:HD12	1.90	0.54
41:s:178:SER:HB2	41:s:181:LEU:HD12	1.89	0.54
1:A:67:GLU:O	1:A:71:LYS:HG2	2.08	0.53
9:J:323:HIS:O	9:J:323:HIS:CG	2.60	0.53
32:i:84:TRP:HH2	34:k:59:MET:HE3	1.73	0.53
47:r:501:PEE:H71	47:r:501:PEE:H34	1.90	0.53
24:a:66:ARG:HA	24:a:69:LYS:HE3	1.90	0.53
12:M:285:TRP:HB2	12:M:413:LEU:HD11	1.90	0.53
16:Q:179:ARG:NH2	16:Q:401:GLU:O	2.36	0.53
55:l:702:CDL:H822	55:l:702:CDL:H631	1.91	0.53
12:M:282:ASN:O	12:M:283:GLU:HG2	2.08	0.53
1:A:89:GLY:CA	1:A:244:ASN:ND2	2.52	0.53
3:C:71:CYS:HB3	45:C:301:SF4:S4	2.46	0.53
11:L:75:ARG:NH1	11:L:119:ASP:OD1	2.35	0.53
1:A:126:LYS:NZ	1:A:246:GLU:OE2	2.33	0.53
31:h:106:PRO:HG2	42:u:17:GLU:HB3	1.91	0.53
32:i:128:LEU:HD12	32:i:216:PHE:HB3	1.91	0.53
49:C:303:UQ:HM31	16:Q:197:MET:HE3	1.90	0.53
8:I:40:LYS:HB3	21:W:7:LYS:H	1.73	0.53
12:M:367:CYS:HB2	12:M:533:GLY:O	2.09	0.53
41:s:207:LEU:O	41:s:209:SER:N	2.41	0.53
44:w:246:LEU:HD22	44:w:255:VAL:HG11	1.90	0.53
2:B:63:TRP:HZ2	47:B:303:PEE:H13	1.74	0.52
12:M:476:LEU:HD21	12:M:481:LEU:HD21	1.91	0.52
27:d:137:LYS:NZ	27:d:141:ASP:OD2	2.42	0.52
34:k:65:VAL:HG11	36:m:157:THR:HG23	1.90	0.52
35:l:227:PHE:O	35:l:230:HIS:ND1	2.42	0.52
39:p:139:GLN:NE2	39:p:156:PRO:O	2.36	0.52
41:s:21:THR:HG21	41:s:224:PHE:HE2	1.74	0.52
1:A:185:ASN:OD1	1:A:190:GLY:N	2.35	0.52
36:m:20:PHE:CD1	36:m:20:PHE:C	2.88	0.52
41:s:65:THR:O	41:s:124:ASN:CB	2.57	0.52
42:u:83:THR:HA	42:u:86:TRP:CD1	2.43	0.52
27:d:115:GLN:HG2	35:l:62:ILE:HG12	1.91	0.52
32:i:84:TRP:CH2	34:k:59:MET:HE3	2.44	0.52
3:C:60:SER:HB3	41:s:40:VAL:CG2	2.40	0.52
32:i:102:LEU:HD13	32:i:142:LEU:HG	1.92	0.52
40:r:329:LEU:O	40:r:332:THR:OG1	2.28	0.52
52:g:201:PLX:H12	31:h:2:PRO:HD2	1.92	0.52
32:i:268:GLN:NE2	32:i:272:LYS:HE3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:140:GLN:O	27:d:144:SER:HB2	2.08	0.52
40:r:306:PRO:HB3	40:r:458:LEU:HD12	1.92	0.52
41:s:49:ILE:N	41:s:49:ILE:CD1	2.73	0.52
6:G:141:PRO:HA	6:G:144:ILE:HD12	1.92	0.52
52:j:203:PLX:H152	52:j:203:PLX:H341	1.92	0.52
43:v:22:MET:HE1	43:v:102:PHE:HA	1.92	0.52
3:C:125:PRO:HB2	41:s:58:LYS:HE2	1.92	0.52
3:C:184:ILE:O	3:C:187:GLU:HG2	2.10	0.52
4:E:99:GLN:CD	33:j:41:PHE:HD1	2.18	0.52
35:l:6:SER:O	35:l:10:THR:OG1	2.24	0.52
35:l:233:LEU:HB3	35:l:234:PRO:HD3	1.92	0.52
35:l:370:THR:HG22	35:l:431:PHE:CD1	2.45	0.52
42:u:77:HIS:CE1	42:u:115:LEU:HD21	2.45	0.52
1:A:250:VAL:C	1:A:252:PRO:HD2	2.35	0.52
12:M:264:SER:HB2	12:M:272:ARG:HG2	1.92	0.52
17:S:28:LYS:O	17:S:33:GLY:N	2.42	0.52
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.92	0.51
10:K:87:LEU:O	10:K:91:VAL:HG23	2.10	0.51
24:a:139:ILE:HG23	40:r:54:LEU:HD23	1.92	0.51
27:d:10:TYR:OH	28:e:123:GLU:OE2	2.27	0.51
32:i:79:LEU:HB2	34:k:47:ILE:HD13	1.92	0.51
42:u:157:ASP:OD1	42:u:158:LEU:N	2.43	0.51
1:A:185:ASN:O	1:A:187:CYS:N	2.44	0.51
36:m:61:LEU:O	41:s:114:TYR:OH	2.21	0.51
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.45	0.51
3:C:53:LEU:HD22	52:N:201:PLX:H321	1.93	0.51
35:l:538:THR:HA	47:l:704:PEE:H59	1.91	0.51
9:J:310:PHE:CG	52:J:404:PLX:H1C2	2.45	0.51
33:j:69:ILE:HD12	41:s:147:ALA:HB1	1.93	0.51
3:C:94:ARG:NH1	49:C:303:UQ:HM51	2.24	0.51
9:J:222:TRP:HB3	49:J:403:UQ:H152	1.91	0.51
16:Q:304:LYS:NZ	16:Q:316:PHE:O	2.41	0.51
32:i:222:SER:O	32:i:224:ALA:N	2.44	0.51
5:F:61:VAL:HG23	5:F:62:GLN:H	1.76	0.51
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.32	0.51
6:X:155:TYR:CD2	6:X:156:GLU:HG3	2.46	0.51
11:L:114:TRP:HB3	15:P:228:GLN:HG3	1.93	0.51
55:V:201:CDL:H661	35:l:594:THR:HG23	1.92	0.51
1:A:87:GLY:CA	46:A:502:FMN:O2P	2.59	0.51
1:A:267:ARG:HH12	1:A:341:ALA:HB2	1.76	0.51
12:M:388:ASN:HB3	12:M:511:LYS:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:43:THR:HA	15:P:47:ILE:HD12	1.93	0.51
18:T:51:ARG:HG2	18:T:54:ARG:HH21	1.76	0.51
19:U:33:PRO:HA	41:s:310:MET:HG2	1.92	0.51
55:V:202:CDL:H712	55:V:202:CDL:H521	1.93	0.51
21:W:68:ARG:CZ	21:W:72:MET:HE2	2.41	0.51
26:c:153:TYR:OH	43:v:8:ARG:NH1	2.44	0.51
27:d:97:LYS:NZ	40:r:47:GLU:OE2	2.37	0.51
33:j:73:LEU:N	33:j:74:PRO:CD	2.73	0.51
3:C:88:ARG:CA	41:s:36:GLY:O	2.58	0.51
10:K:73:TYR:CZ	10:K:75:ASN:HB3	2.45	0.51
16:Q:282:ASP:OD2	16:Q:437:LYS:NZ	2.39	0.51
52:g:201:PLX:H233	32:i:207:ILE:HD13	1.92	0.51
33:j:77:TRP:HD1	41:s:318:SER:C	2.19	0.51
17:S:69:ILE:HD11	42:u:20:VAL:HG13	1.92	0.51
35:l:358:LYS:HG3	39:p:80:TYR:CE1	2.46	0.51
1:A:131:ILE:HD11	1:A:245:VAL:HG11	1.93	0.50
4:E:24:ASP:OD2	4:E:26:ASN:ND2	2.43	0.50
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.92	0.50
23:Z:60:ASN:HD22	35:l:433:GLY:H	1.59	0.50
32:i:100:MET:HE3	32:i:153:LEU:HD21	1.92	0.50
34:k:21:MET:CE	55:k:101:CDL:H601	2.41	0.50
40:r:130:LEU:HD22	40:r:150:LEU:HD13	1.92	0.50
40:r:373:ILE:HD11	40:r:444:LEU:HD23	1.93	0.50
6:G:122:MET:HE3	6:G:144:ILE:HG21	1.93	0.50
11:L:109:ASN:ND2	11:L:111:LEU:O	2.41	0.50
22:Y:103:ASP:OD1	22:Y:103:ASP:N	2.42	0.50
32:i:298:TYR:O	32:i:303:THR:OG1	2.29	0.50
33:j:80:GLN:O	33:j:81:THR:C	2.54	0.50
47:r:501:PEE:H81	52:r:502:PLX:H393	1.93	0.50
1:A:44:ASN:HB3	1:A:134:ASP:OD1	2.12	0.50
45:C:301:SF4:S2	16:Q:138:ARG:HG2	2.51	0.50
18:T:51:ARG:HG2	18:T:54:ARG:NH2	2.26	0.50
55:l:702:CDL:H621	55:l:702:CDL:H432	1.93	0.50
33:j:79:SER:O	33:j:84:LEU:CD2	2.55	0.50
44:w:180:ARG:NH1	44:w:316:GLU:OE2	2.44	0.50
9:J:37:HIS:CD2	9:J:40:LEU:HD12	2.46	0.50
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.47	0.50
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.47	0.50
55:l:702:CDL:H371	40:r:369:LEU:HD23	1.94	0.50
36:m:58:LEU:HD13	41:s:107:ALA:HA	1.92	0.50
44:w:219:GLN:NE2	44:w:227:MET:SD	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:GLU:HA	1:A:132:ARG:HG2	1.93	0.50
3:C:92:VAL:CG2	41:s:25:ARG:NH2	2.75	0.50
16:Q:208:GLU:OE2	16:Q:221:ARG:NH2	2.45	0.50
32:i:294:MET:HE2	40:r:130:LEU:HD21	1.94	0.50
55:k:101:CDL:C78	55:k:101:CDL:C62	2.89	0.50
37:n:26:TYR:OH	37:n:30:ARG:NH2	2.20	0.50
35:l:362:LEU:HD22	35:l:366:MET:HE2	1.93	0.50
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.94	0.49
55:a:201:CDL:H852	52:e:201:PLX:H232	1.94	0.49
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.52	0.49
5:F:58:CYS:SG	5:F:59:SER:N	2.85	0.49
7:H:116:ILE:HD12	11:L:127:THR:HG22	1.95	0.49
9:J:293:LEU:HD23	9:J:298:TYR:HB2	1.94	0.49
35:l:253:VAL:HB	35:l:310:LEU:HD11	1.94	0.49
35:l:562:LEU:HB3	35:l:563:PRO:HD3	1.92	0.49
55:r:503:CDL:H332	55:r:503:CDL:H231	1.93	0.49
5:F:25:GLN:HG2	5:F:26:ARG:HD3	1.94	0.49
16:Q:254:ARG:NH2	16:Q:257:GLU:OE2	2.45	0.49
32:i:153:LEU:HG	32:i:157:MET:HE2	1.95	0.49
34:k:76:SER:O	34:k:79:VAL:HG12	2.11	0.49
5:F:61:VAL:HG23	5:F:62:GLN:N	2.27	0.49
21:W:28:ARG:CG	21:W:28:ARG:NH1	2.73	0.49
35:l:108:MET:CE	35:l:240:PRO:HB3	2.43	0.49
41:s:85:MET:HE1	41:s:108:MET:CB	2.43	0.49
18:T:101:ASN:ND2	18:T:103:ASP:OD2	2.45	0.49
39:p:64:LEU:O	39:p:68:GLU:HG2	2.12	0.49
1:A:210:THR:HB	1:A:224:ARG:H	1.76	0.49
1:A:320:GLY:HA2	1:A:353:ALA:H	1.77	0.49
2:B:70:LEU:O	41:s:272:TRP:CZ2	2.65	0.49
2:B:120:GLU:HB2	2:B:130:ILE:HD12	1.93	0.49
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.48	0.49
6:X:120:MET:HE1	39:p:24:LEU:HB3	1.95	0.49
2:B:78:PHE:HB2	8:I:12:ARG:HG2	1.93	0.49
7:H:90:LEU:HB2	15:P:102:ASP:HB3	1.93	0.49
32:i:75:ILE:HD12	34:k:40:LEU:HD22	1.95	0.49
32:i:215:MET:HB2	32:i:251:MET:HE1	1.94	0.49
32:i:246:VAL:HG21	55:r:503:CDL:H362	1.95	0.49
35:l:515:TYR:OH	39:p:70:GLU:OE2	2.21	0.49
40:r:221:VAL:HA	40:r:283:LYS:HD3	1.95	0.49
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.25	0.49
32:i:99:THR:HG22	32:i:157:MET:HE1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:k:101:CDL:C62	55:k:101:CDL:C81	2.90	0.49
35:l:69:MET:HE2	35:l:76:LEU:HD12	1.95	0.49
36:m:34:ILE:HG13	36:m:64:MET:HG3	1.94	0.49
1:A:35:LEU:HD21	1:A:290:GLU:HA	1.95	0.49
2:B:105:ARG:NH2	18:T:63:ASN:OD1	2.46	0.49
12:M:265:THR:HG22	12:M:270:VAL:HA	1.95	0.49
15:P:214:ASP:O	15:P:217:LYS:NZ	2.44	0.49
24:a:153:GLU:HG3	30:g:92:MET:HE2	1.95	0.49
47:j:201:PEE:H26	41:s:295:PRO:HB3	1.93	0.49
34:k:38:LEU:HB2	36:m:60:TYR:CZ	2.48	0.49
35:l:27:TYR:O	35:l:115:ASN:ND2	2.44	0.49
36:m:164:GLY:O	36:m:168:ILE:HG12	2.13	0.49
9:J:222:TRP:CD1	49:J:403:UQ:H101	2.48	0.48
14:O:137:THR:O	14:O:141:MET:N	2.44	0.48
55:V:201:CDL:H512	35:l:576:MET:HG2	1.95	0.48
33:j:80:GLN:O	33:j:81:THR:O	2.31	0.48
4:E:55:SER:HB2	9:J:367:GLU:OE2	2.13	0.48
12:M:251:ILE:HG13	12:M:604:GLN:CB	2.42	0.48
13:N:42:ASP:HB2	13:N:48:TYR:HE1	1.78	0.48
20:V:40:SER:HA	55:V:201:CDL:HB61	1.95	0.48
32:i:170:LEU:HD23	32:i:292:PHE:HB3	1.93	0.48
33:j:69:ILE:HD12	41:s:147:ALA:CB	2.43	0.48
35:l:599:MET:O	35:l:603:ASN:HB3	2.13	0.48
42:u:59:GLU:N	42:u:59:GLU:OE1	2.46	0.48
3:C:88:ARG:HA	41:s:37:PRO:HA	1.94	0.48
12:M:466:LEU:HD13	12:M:500:ILE:HD11	1.94	0.48
14:O:149:LEU:O	14:O:153:GLN:HG2	2.13	0.48
32:i:68:MET:HE1	34:k:37:MET:SD	2.54	0.48
33:j:53:MET:HE3	33:j:56:PHE:HA	1.94	0.48
12:M:49:VAL:HG13	12:M:102:ILE:HD13	1.95	0.48
12:M:419:ARG:NH1	12:M:439:THR:O	2.46	0.48
13:N:3:LEU:O	13:N:7:LEU:HG	2.13	0.48
21:W:93:GLU:O	21:W:97:ILE:HD12	2.13	0.48
52:g:201:PLX:H232	32:i:210:THR:HG21	1.95	0.48
3:C:94:ARG:NH1	49:C:303:UQ:CM5	2.76	0.48
16:Q:258:LEU:HD23	16:Q:258:LEU:O	2.13	0.48
21:W:94:GLU:HG2	31:h:79:ILE:HD12	1.96	0.48
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.96	0.48
41:s:14:LEU:HD21	41:s:83:LEU:HD21	1.94	0.48
41:s:47:GLN:N	41:s:48:PRO:CD	2.77	0.48
8:I:42:PRO:HB3	21:W:6:VAL:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:69:VAL:O	15:P:76:VAL:HB	2.14	0.48
9:J:168:SER:OG	9:J:169:HIS:N	2.46	0.48
52:J:404:PLX:H32	52:J:404:PLX:H6	1.56	0.48
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.49	0.48
22:Y:76:ASP:O	35:l:385:TYR:OH	2.21	0.48
25:b:10:LEU:O	25:b:14:GLN:HG3	2.14	0.48
34:k:79:VAL:HG23	36:m:74:MET:CE	2.44	0.48
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.48	0.48
55:V:202:CDL:H732	38:o:87:SER:HB3	1.95	0.48
21:W:121:MET:HE3	36:m:130:THR:HB	1.96	0.48
52:e:201:PLX:H202	55:l:702:CDL:H812	1.95	0.48
5:F:65:LEU:HB2	5:F:79:LEU:HD11	1.95	0.48
16:Q:198:THR:HG23	41:s:32:GLN:HG2	1.95	0.48
21:W:68:ARG:O	21:W:72:MET:HG3	2.14	0.48
32:i:265:MET:HE2	32:i:343:LEU:HD21	1.96	0.48
41:s:144:VAL:O	41:s:148:ILE:HD12	2.13	0.48
44:w:54:THR:O	44:w:55:GLU:HG3	2.14	0.48
33:j:93:PHE:CZ	33:j:97:LEU:HD11	2.48	0.48
35:l:373:LEU:HD22	35:l:431:PHE:HE2	1.78	0.48
32:i:72:MET:HE2	34:k:12:PHE:CG	2.49	0.48
35:l:86:SER:OG	35:l:262:ARG:NH2	2.47	0.48
35:l:108:MET:HE3	35:l:240:PRO:HB3	1.94	0.48
2:B:63:TRP:CZ2	47:B:303:PEE:H13	2.49	0.47
12:M:340:ALA:HB3	12:M:366:LEU:HD23	1.95	0.47
15:P:65:VAL:HG11	15:P:86:ILE:HD13	1.96	0.47
15:P:173:MET:HE3	15:P:188:LEU:HB2	1.96	0.47
26:c:60:GLU:OE1	26:c:60:GLU:N	2.47	0.47
52:r:502:PLX:H122	52:r:502:PLX:H92	1.50	0.47
41:s:174:MET:HB3	41:s:242:PHE:HA	1.95	0.47
42:u:80:GLU:HB2	42:u:81:PRO:HD3	1.95	0.47
1:A:244:ASN:CB	46:A:502:FMN:O1P	2.60	0.47
1:A:391:TRP:O	1:A:395:VAL:HG23	2.13	0.47
16:Q:83:ASN:HB2	33:j:38:GLU:HG2	1.96	0.47
16:Q:397:TYR:OH	16:Q:406:GLU:OE2	2.27	0.47
35:l:190:LEU:HD21	40:r:307:TRP:CH2	2.49	0.47
37:n:50:ARG:HB2	37:n:53:GLU:HG2	1.96	0.47
9:J:167:ILE:HD13	9:J:201:ILE:HB	1.96	0.47
16:Q:443:MET:HE1	41:s:283:ASP:OD2	2.14	0.47
35:l:313:MET:HG3	35:l:328:HIS:HD2	1.79	0.47
55:l:703:CDL:H612	55:l:703:CDL:H641	1.62	0.47
44:w:86:PHE:HB2	44:w:159:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:34:ARG:HH12	13:N:58:ARG:HB3	1.80	0.47
34:k:4:VAL:O	34:k:8:ILE:HG12	2.14	0.47
35:l:78:LEU:HD11	55:l:702:CDL:H261	1.96	0.47
38:o:56:ARG:NH1	38:o:58:GLY:O	2.47	0.47
41:s:189:THR:HG22	41:s:234:MET:HE3	1.97	0.47
43:v:12:ASP:OD1	43:v:14:SER:OG	2.30	0.47
3:C:111:ASN:CG	15:P:210:LEU:HD13	2.39	0.47
9:J:132:ARG:NH2	51:J:402:NDP:O2X	2.47	0.47
12:M:64:CYS:O	12:M:184:ARG:NH2	2.28	0.47
12:M:501:ARG:HH12	12:M:666:GLN:HB3	1.79	0.47
26:c:71:GLY:HA2	38:o:79:ASN:HB2	1.95	0.47
55:k:101:CDL:H221	55:k:101:CDL:H252	1.68	0.47
1:A:102:MET:O	1:A:111:LYS:NZ	2.42	0.47
7:H:35:LEU:HD11	7:H:48:THR:HG22	1.97	0.47
22:Y:43:ARG:HB3	22:Y:46:GLN:HB2	1.97	0.47
22:Y:50:LEU:HB3	22:Y:54:GLN:HE21	1.79	0.47
29:f:47:THR:HG23	30:g:65:LEU:HD22	1.96	0.47
55:k:101:CDL:H521	36:m:88:THR:OG1	2.15	0.47
36:m:71:THR:HA	36:m:75:ALA:HB3	1.95	0.47
38:o:23:TYR:OH	39:p:68:GLU:HG3	2.15	0.47
52:r:502:PLX:H101	52:r:502:PLX:H72	1.51	0.47
55:r:503:CDL:H342	55:r:503:CDL:H181	1.97	0.47
44:w:88:GLU:HG3	44:w:139:ARG:HH12	1.79	0.47
9:J:132:ARG:HA	9:J:132:ARG:HD3	1.77	0.47
12:M:354:LEU:HD22	12:M:548:LEU:HD22	1.96	0.47
55:a:201:CDL:H541	47:l:705:PEE:H16	1.97	0.47
52:e:201:PLX:H21	47:l:705:PEE:H3	1.96	0.47
35:l:529:TYR:HB3	35:l:530:PRO:HD3	1.96	0.47
55:l:703:CDL:H351	55:l:703:CDL:H382	1.50	0.47
16:Q:99:MET:HE3	16:Q:99:MET:HB2	1.78	0.47
1:A:115:VAL:HG11	1:A:138:LEU:HD11	1.97	0.47
6:G:130:ILE:HG22	6:G:135:ALA:HB2	1.97	0.47
13:N:85:GLU:HB2	13:N:98:PRO:HB3	1.96	0.47
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.96	0.47
35:l:366:MET:O	35:l:370:THR:HG23	2.15	0.47
40:r:365:THR:HG21	40:r:444:LEU:HD13	1.97	0.47
41:s:264:LEU:O	41:s:268:ILE:HG12	2.14	0.47
44:w:60:ILE:HG12	44:w:203:VAL:HB	1.96	0.47
5:F:59:SER:OG	5:F:60:ASP:N	2.48	0.46
9:J:313:TRP:CD2	49:J:403:UQ:H72	2.50	0.46
13:N:107:LYS:HE3	18:T:70:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:95:MET:HE1	32:i:145:ILE:HD12	1.97	0.46
36:m:23:LYS:HB2	36:m:23:LYS:NZ	2.30	0.46
21:W:120:MET:O	21:W:121:MET:HB3	2.14	0.46
35:l:69:MET:HE3	35:l:71:LEU:HD21	1.95	0.46
41:s:55:LEU:HD13	41:s:221:ALA:HB2	1.97	0.46
28:e:97:ILE:O	28:e:101:LEU:HB2	2.14	0.46
34:k:18:GLY:O	36:m:23:LYS:HE3	2.16	0.46
2:B:53:VAL:HG12	19:U:13:TRP:HD1	1.80	0.46
3:C:113:MET:SD	16:Q:115:LEU:HD23	2.56	0.46
3:C:196:ARG:HB2	9:J:85:ARG:HH12	1.80	0.46
16:Q:100:GLU:OE1	16:Q:108:LYS:HB3	2.16	0.46
55:l:702:CDL:H811	55:l:702:CDL:H841	1.63	0.46
12:M:213:MET:HB3	12:M:215:MET:HG2	1.97	0.46
21:W:73:PRO:HG2	42:u:40:ASN:HB3	1.96	0.46
26:c:102:GLY:HA3	38:o:43:LEU:HD22	1.96	0.46
47:j:201:PEE:H59	47:j:201:PEE:H64	1.75	0.46
40:r:281:ASP:OD1	40:r:340:ARG:HB3	2.15	0.46
2:B:188:GLU:HG3	13:N:127:TYR:OH	2.15	0.46
3:C:107:GLY:HA2	45:C:301:SF4:S1	2.55	0.46
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.97	0.46
27:d:73:ASP:OD1	27:d:73:ASP:N	2.48	0.46
41:s:293:PHE:O	41:s:297:THR:OG1	2.24	0.46
13:N:55:PHE:CE1	13:N:58:ARG:HG3	2.51	0.46
13:N:65:THR:O	13:N:73:THR:OG1	2.32	0.46
15:P:173:MET:HE1	15:P:189:THR:HG23	1.98	0.46
16:Q:136:PHE:HA	16:Q:139:LEU:HD12	1.97	0.46
27:d:85:MET:HE2	27:d:85:MET:HB3	1.79	0.46
32:i:278:MET:O	32:i:282:MET:HG3	2.16	0.46
33:j:63:LEU:O	33:j:67:LEU:HD23	2.15	0.46
6:G:133:ILE:O	6:G:134:ASP:OD1	2.34	0.46
9:J:40:LEU:HD23	9:J:40:LEU:HA	1.79	0.46
16:Q:96:ARG:HB3	16:Q:112:HIS:HB2	1.98	0.46
16:Q:357:LYS:HD3	16:Q:364:SER:HB3	1.98	0.46
21:W:81:ARG:HH21	42:u:60:GLY:C	2.24	0.46
22:Y:43:ARG:HD3	22:Y:48:PRO:HA	1.98	0.46
34:k:31:LEU:HD21	36:m:67:VAL:HG11	1.98	0.46
55:n:101:CDL:H741	55:n:101:CDL:H711	1.70	0.46
41:s:202:GLU:HA	41:s:210:GLY:HA3	1.98	0.46
9:J:87:GLU:HG3	9:J:89:TYR:H	1.81	0.46
26:c:78:LEU:HD12	26:c:106:HIS:HA	1.98	0.46
26:c:156:VAL:HG11	43:v:95:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:41:ILE:HG13	34:k:73:LEU:HD21	1.96	0.46
32:i:146:SER:HA	32:i:149:ILE:HD12	1.98	0.46
36:m:140:ALA:O	36:m:144:ALA:HB2	2.16	0.46
5:F:20:ARG:NH2	5:F:74:GLU:OE2	2.49	0.45
12:M:395:GLU:OE2	12:M:417:ARG:NH1	2.48	0.45
16:Q:450:ILE:HA	16:Q:453:THR:HG22	1.98	0.45
55:V:201:CDL:H762	55:V:201:CDL:H401	1.97	0.45
52:j:203:PLX:H311	52:j:203:PLX:H281	1.72	0.45
36:m:82:VAL:HG22	36:m:85:SER:HB3	1.98	0.45
44:w:175:ARG:HH22	44:w:239:ASN:HD22	1.64	0.45
9:J:375:VAL:HG23	9:J:375:VAL:O	2.16	0.45
14:O:197:THR:H	14:O:200:ASP:HB2	1.81	0.45
16:Q:258:LEU:C	16:Q:258:LEU:CD2	2.85	0.45
27:d:2:PRO:O	27:d:7:LYS:NZ	2.39	0.45
38:o:38:ALA:HB2	39:p:150:ARG:HD3	1.99	0.45
43:v:111:ARG:O	43:v:115:ARG:HG2	2.16	0.45
44:w:220:LYS:HB2	44:w:220:LYS:HE3	1.67	0.45
9:J:181:LEU:CD1	9:J:324:MET:HE1	2.47	0.45
35:l:305:SER:HB2	35:l:422:TYR:CE1	2.51	0.45
35:l:530:PRO:O	35:l:534:HIS:HB2	2.16	0.45
35:l:561:ILE:HG13	35:l:562:LEU:H	1.80	0.45
3:C:67:PHE:CD1	16:Q:87:GLN:HG2	2.52	0.45
12:M:29:SER:OG	12:M:30:ASN:N	2.50	0.45
16:Q:155:VAL:HB	16:Q:229:PRO:HB3	1.99	0.45
55:l:702:CDL:H312	55:l:702:CDL:HA61	1.69	0.45
41:s:102:VAL:HG11	41:s:154:LEU:HD11	1.99	0.45
1:A:160:GLY:O	1:A:199:ARG:NH2	2.49	0.45
52:J:404:PLX:H272	52:J:404:PLX:H301	1.51	0.45
28:e:98:VAL:HG22	40:r:36:LEU:HB2	1.98	0.45
52:g:201:PLX:H112	52:g:201:PLX:H81	1.46	0.45
35:l:176:ARG:HA	35:l:176:ARG:HD3	1.76	0.45
3:C:75:GLU:OE2	16:Q:221:ARG:NH1	2.49	0.45
40:r:138:ASN:C	40:r:138:ASN:HD22	2.23	0.45
1:A:320:GLY:HA3	1:A:349:LEU:O	2.17	0.45
3:C:59:ARG:HH12	52:N:201:PLX:H32	1.81	0.45
52:J:404:PLX:H252	52:J:404:PLX:H281	1.54	0.45
12:M:494:SER:OG	12:M:669:ASN:ND2	2.47	0.45
29:f:72:ARG:NH2	30:g:18:ASN:OD1	2.50	0.45
52:g:201:PLX:H101	52:g:201:PLX:H132	1.57	0.45
36:m:141:MET:HA	36:m:144:ALA:HB3	1.98	0.45
44:w:143:TYR:OH	44:w:199:LEU:O	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:h:19:THR:HA	32:i:84:TRP:HB2	1.97	0.45
35:l:560:THR:O	35:l:565:THR:OG1	2.34	0.45
47:l:704:PEE:H58	47:l:704:PEE:H53	1.76	0.45
3:C:86:MET:HE3	3:C:91:VAL:HG12	1.99	0.45
9:J:168:SER:O	9:J:203:PRO:HD2	2.17	0.45
12:M:260:ASN:ND2	12:M:278:HIS:HD2	2.15	0.45
26:c:38:PRO:HG2	38:o:70:TYR:HD2	1.81	0.45
35:l:295:GLN:HB2	35:l:301:ILE:HG12	1.99	0.45
35:l:331:MET:HG3	35:l:391:SER:HB3	1.98	0.45
2:B:70:LEU:HB3	41:s:272:TRP:CZ2	2.52	0.45
11:L:104:ARG:HA	11:L:104:ARG:HD3	1.80	0.45
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.99	0.45
35:l:435:PRO:HB3	35:l:437:PHE:CZ	2.51	0.45
35:l:554:ASP:OD2	40:r:288:TYR:OH	2.29	0.45
40:r:115:LEU:HD12	40:r:174:LEU:HD22	1.99	0.45
41:s:198:PHE:CD1	41:s:285:LEU:HD13	2.51	0.45
8:I:23:LYS:HD2	16:Q:253:PHE:CD1	2.52	0.44
55:V:202:CDL:H742	55:V:202:CDL:H601	1.99	0.44
21:W:96:ILE:O	21:W:99:LYS:HE3	2.16	0.44
6:X:118:ILE:O	6:X:122:MET:HG2	2.17	0.44
25:b:90:VAL:O	25:b:96:THR:OG1	2.31	0.44
36:m:138:GLU:OE1	36:m:138:GLU:N	2.50	0.44
40:r:114:GLU:HG2	40:r:175:ASN:HA	1.99	0.44
47:B:303:PEE:H61	47:B:303:PEE:H55	1.66	0.44
5:F:45:LYS:HA	5:F:45:LYS:HD2	1.79	0.44
12:M:140:GLN:HG2	16:Q:379:ILE:HG23	1.98	0.44
6:X:93:ILE:HG21	6:X:98:LEU:HD13	1.99	0.44
23:Z:53:TYR:CE1	35:l:434:LYS:HG3	2.53	0.44
25:b:99:GLU:HG2	35:l:61:MET:HG2	1.99	0.44
27:d:159:GLN:NE2	28:e:142:PHE:O	2.37	0.44
28:e:76:TYR:HB2	28:e:83:ASP:OD1	2.17	0.44
38:o:60:ILE:HD12	40:r:422:HIS:HB2	1.99	0.44
39:p:98:LYS:HG2	39:p:178:PRO:HG3	1.98	0.44
40:r:203:PHE:O	40:r:207:MET:HG2	2.16	0.44
41:s:63:PRO:HB2	41:s:66:SER:HB3	1.99	0.44
1:A:299:LEU:HD12	1:A:303:HIS:HD2	1.82	0.44
13:N:6:VAL:HG12	13:N:9:ARG:NH2	2.32	0.44
13:N:78:ASP:OD1	13:N:78:ASP:N	2.50	0.44
25:b:5:THR:OG1	25:b:8:GLU:HG3	2.18	0.44
28:e:57:GLU:OE1	44:w:320:GLY:HA3	2.16	0.44
52:g:201:PLX:H361	52:g:201:PLX:H311	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:k:101:CDL:C62	55:k:101:CDL:H782	2.46	0.44
55:l:702:CDL:H452	40:r:445:LEU:HB3	2.00	0.44
36:m:163:ILE:O	36:m:167:VAL:HG23	2.17	0.44
3:C:62:LEU:O	3:C:91:VAL:HA	2.17	0.44
16:Q:370:GLU:HA	16:Q:373:THR:HG22	1.99	0.44
21:W:86:MET:SD	21:W:124:LEU:HB3	2.58	0.44
21:W:94:GLU:OE2	21:W:104:TRP:NE1	2.42	0.44
22:Y:72:ARG:HB3	35:l:385:TYR:CD1	2.52	0.44
26:c:167:TYR:CD2	26:c:178:PRO:HG3	2.52	0.44
55:l:703:CDL:H542	55:l:703:CDL:H512	1.77	0.44
36:m:24:PRO:HG3	36:m:83:TRP:NE1	2.32	0.44
16:Q:178:THR:OG1	16:Q:214:TYR:OH	2.35	0.44
19:U:16:GLU:O	19:U:20:VAL:HG23	2.18	0.44
19:U:43:ILE:HG12	33:j:84:LEU:HB2	1.99	0.44
55:V:202:CDL:H312	38:o:84:PRO:HB3	1.99	0.44
47:W:201:PEE:H42	47:W:201:PEE:H35	1.76	0.44
31:h:75:ARG:O	31:h:79:ILE:HG12	2.18	0.44
40:r:271:MET:HE2	40:r:271:MET:HA	2.00	0.44
43:v:42:THR:OG1	43:v:45:GLU:HG3	2.17	0.44
1:A:326:LEU:HD23	1:A:367:ILE:HD11	1.99	0.44
9:J:310:PHE:CD1	52:J:404:PLX:H1C2	2.53	0.44
12:M:59:GLN:NE2	12:M:62:ARG:HH12	2.15	0.44
12:M:576:GLY:HA2	12:M:579:MET:HE3	1.99	0.44
14:O:148:ILE:HD12	14:O:184:PRO:HB2	1.99	0.44
19:U:66:VAL:O	42:u:130:LYS:HE3	2.18	0.44
24:a:92:PHE:HD1	27:d:55:GLN:HE21	1.66	0.44
1:A:284:HIS:ND1	14:O:228:ALA:HB3	2.33	0.44
49:C:303:UQ:H23	41:s:52:ALA:HB2	1.99	0.44
6:G:105:MET:HG3	6:G:110:LEU:O	2.18	0.44
9:J:220:MET:HE3	9:J:226:VAL:HG13	2.00	0.44
31:h:2:PRO:HA	32:i:140:SER:HB2	2.00	0.44
32:i:40:MET:HE1	32:i:129:LEU:HD22	1.99	0.44
35:l:249:SER:HG	35:l:340:PHE:HD2	1.66	0.44
35:l:492:ILE:O	35:l:496:MET:HG2	2.18	0.44
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	1.99	0.44
24:a:147:ALA:HB2	40:r:173:SER:HB3	1.99	0.44
55:l:702:CDL:H611	55:l:702:CDL:H581	1.67	0.44
7:H:116:ILE:HG21	11:L:96:LYS:HD2	2.00	0.44
8:I:8:ILE:O	8:I:12:ARG:HG3	2.18	0.44
16:Q:90:ALA:HB2	41:s:205:SER:O	2.18	0.44
32:i:324:LYS:HA	32:i:324:LYS:HD3	1.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:76:SER:OG	36:m:168:ILE:HD12	2.18	0.44
46:A:502:FMN:O4'	46:A:502:FMN:O2'	2.31	0.43
3:C:167:PRO:HG3	16:Q:222:MET:SD	2.58	0.43
9:J:298:TYR:CE2	9:J:319:VAL:HG22	2.53	0.43
16:Q:52:MET:HE3	16:Q:52:MET:HB3	1.75	0.43
16:Q:156:GLU:OE2	16:Q:171:ARG:NH2	2.49	0.43
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	2.00	0.43
16:Q:442:HIS:HB3	16:Q:446:ASP:HB2	1.99	0.43
21:W:28:ARG:NH1	21:W:28:ARG:HG2	2.33	0.43
25:b:11:ARG:HB2	39:p:156:PRO:HB3	1.99	0.43
27:d:99:ASP:OD2	27:d:142:ARG:NH1	2.51	0.43
31:h:38:LYS:HE2	31:h:42:GLU:OE2	2.18	0.43
40:r:186:LEU:HD23	40:r:192:ASN:HB3	2.00	0.43
33:j:69:ILE:HG22	41:s:148:ILE:HD11	2.00	0.43
35:l:128:MET:HE3	35:l:251:THR:HG22	2.00	0.43
36:m:140:ALA:O	36:m:144:ALA:CB	2.67	0.43
41:s:179:TRP:CG	41:s:180:PRO:HD3	2.53	0.43
2:B:76:TYR:OH	16:Q:257:GLU:OE1	2.28	0.43
49:J:403:UQ:H171	49:J:403:UQ:H151	1.59	0.43
20:V:37:SER:O	20:V:41:ILE:HG12	2.18	0.43
32:i:49:ASN:O	32:i:51:ARG:N	2.51	0.43
33:j:22:PHE:HA	41:s:60:PRO:HG2	2.00	0.43
35:l:69:MET:HG3	35:l:71:LEU:CD2	2.47	0.43
40:r:306:PRO:O	40:r:310:MET:HG3	2.18	0.43
40:r:357:THR:O	40:r:361:VAL:HG23	2.17	0.43
44:w:295:ARG:HA	44:w:298:VAL:HG22	2.00	0.43
3:C:87:ASP:OD2	41:s:37:PRO:HD3	2.18	0.43
49:C:303:UQ:H221	49:C:303:UQ:H262	1.66	0.43
9:J:40:LEU:HD13	9:J:124:ASN:ND2	2.32	0.43
47:J:401:PEE:H82	47:J:401:PEE:H74	1.88	0.43
14:O:146:ASP:O	14:O:150:GLU:OE2	2.37	0.43
20:V:39:TYR:HB3	55:V:201:CDL:H712	2.01	0.43
25:b:121:LYS:HD3	25:b:121:LYS:O	2.19	0.43
26:c:44:THR:OG1	26:c:47:GLU:HG3	2.18	0.43
35:l:54:PHE:CZ	35:l:84:TYR:HB2	2.53	0.43
35:l:395:ILE:O	35:l:399:VAL:HG23	2.18	0.43
42:u:45:LEU:HD22	42:u:131:VAL:HB	2.00	0.43
12:M:149:ASP:OD2	12:M:150:ARG:NH1	2.51	0.43
15:P:197:PRO:HA	15:P:202:PHE:CG	2.54	0.43
31:h:17:TRP:CD1	31:h:17:TRP:H	2.36	0.43
35:l:249:SER:OG	35:l:336:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:119:VAL:HG23	9:J:120:VAL:HG13	2.01	0.43
11:L:163:ASN:O	11:L:171:ARG:HA	2.19	0.43
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.99	0.43
52:a:202:PLX:H22	52:a:202:PLX:H1C3	1.73	0.43
36:m:28:TYR:HB3	36:m:83:TRP:CH2	2.54	0.43
40:r:406:TYR:O	40:r:409:TYR:HB3	2.19	0.43
41:s:24:GLU:HA	41:s:271:LEU:HD13	2.00	0.43
42:u:100:CYS:HB2	42:u:103:GLN:OE1	2.19	0.43
1:A:141:GLY:HA2	1:A:252:PRO:HD3	2.01	0.43
47:B:303:PEE:H21	47:B:303:PEE:H15	1.76	0.43
49:C:303:UQ:H152	49:C:303:UQ:H121	1.81	0.43
47:J:401:PEE:H77	41:s:56:PHE:CD2	2.53	0.43
16:Q:265:ASN:HD21	41:s:277:TYR:HD1	1.67	0.43
16:Q:309:ASP:C	16:Q:311:TYR:H	2.26	0.43
17:S:19:PRO:HB3	41:s:9:LEU:HD12	2.01	0.43
17:S:31:ASN:CG	17:S:36:LYS:HB2	2.44	0.43
24:a:80:ILE:HB	24:a:81:PRO:HD3	2.01	0.43
26:c:85:GLU:OE1	26:c:119:THR:OG1	2.33	0.43
35:l:399:VAL:HG12	35:l:409:LEU:HD13	2.01	0.43
1:A:160:GLY:HA3	14:O:121:MET:HE1	2.00	0.43
25:b:99:GLU:HG2	35:l:61:MET:HE2	2.01	0.43
28:e:72:ASP:OD1	28:e:72:ASP:N	2.47	0.43
32:i:243:LEU:HD23	55:r:503:CDL:H361	2.00	0.43
34:k:45:THR:HG23	36:m:52:LEU:HD13	2.01	0.43
38:o:113:GLU:O	38:o:117:GLN:HG2	2.18	0.43
41:s:68:ILE:O	41:s:72:ILE:HG12	2.18	0.43
43:v:93:LEU:HA	43:v:96:VAL:HG12	1.99	0.43
1:A:117:ALA:HB2	1:A:245:VAL:HG21	2.00	0.43
7:H:47:TYR:HE1	8:I:92:LYS:O	2.01	0.43
12:M:208:THR:OG1	12:M:210:ILE:O	2.32	0.43
16:Q:315:GLU:O	16:Q:346:GLN:NE2	2.49	0.43
55:V:201:CDL:H372	55:V:201:CDL:H341	1.52	0.43
35:l:12:LEU:HD22	35:l:129:MET:HB3	2.01	0.43
35:l:332:HIS:HA	35:l:335:PHE:CZ	2.53	0.43
40:r:116:ILE:HG13	42:u:168:PHE:CD1	2.54	0.43
40:r:237:LYS:HA	40:r:237:LYS:HD3	1.94	0.43
41:s:215:TYR:HD1	41:s:219:PRO:HB2	1.83	0.43
44:w:88:GLU:N	44:w:160:GLU:HG3	2.34	0.43
3:C:53:LEU:HB2	52:N:201:PLX:H301	2.00	0.43
15:P:62:GLY:HA3	15:P:76:VAL:HG11	2.00	0.43
16:Q:194:ILE:HG22	41:s:278:PRO:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:59:ASP:OD2	42:u:130:LYS:HD3	2.18	0.43
6:X:89:LEU:HD22	23:Z:47:ARG:HB3	2.01	0.43
33:j:77:TRP:CD1	41:s:318:SER:O	2.70	0.43
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.54	0.42
3:C:92:VAL:HG23	41:s:25:ARG:NH2	2.34	0.42
9:J:37:HIS:CD2	9:J:40:LEU:HB2	2.54	0.42
20:V:43:LEU:HD13	55:V:201:CDL:H522	2.01	0.42
25:b:88:TYR:CE1	27:d:49:ARG:HG2	2.54	0.42
25:b:106:PRO:HG2	25:b:120:MET:HE2	2.01	0.42
33:j:67:LEU:HD13	33:j:67:LEU:HA	1.84	0.42
44:w:108:LEU:HD23	44:w:327:VAL:HG13	2.01	0.42
1:A:326:LEU:HD22	1:A:363:ILE:HD11	2.02	0.42
13:N:60:ARG:HH22	13:N:95:ASP:HA	1.84	0.42
16:Q:383:LYS:HB3	16:Q:383:LYS:HE3	1.92	0.42
23:Z:27:THR:HB	23:Z:53:TYR:HD2	1.83	0.42
24:a:170:GLN:HB2	30:g:6:GLY:O	2.19	0.42
32:i:296:LEU:HD12	32:i:296:LEU:HA	1.92	0.42
47:l:705:PEE:H40	47:l:705:PEE:H33	1.87	0.42
37:n:16:LEU:HD23	37:n:16:LEU:HA	1.91	0.42
40:r:174:LEU:HD23	40:r:179:ILE:HD11	2.01	0.42
40:r:296:LEU:HG	40:r:381:ILE:HG21	2.01	0.42
12:M:355:LYS:HG3	12:M:366:LEU:HD13	2.01	0.42
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	2.00	0.42
17:S:40:HIS:N	17:S:44:GLN:OE1	2.50	0.42
20:V:46:PRO:HD2	55:k:101:CDL:OA7	2.19	0.42
55:V:202:CDL:H111	55:V:202:CDL:H142	1.71	0.42
23:Z:27:THR:HB	23:Z:53:TYR:CD2	2.55	0.42
25:b:32:GLU:HB2	25:b:33:PRO:HD3	2.01	0.42
27:d:37:PHE:CD2	35:l:3:PRO:HB3	2.55	0.42
35:l:332:HIS:HA	35:l:335:PHE:CE2	2.54	0.42
47:l:701:PEE:H14	47:l:701:PEE:H20	1.69	0.42
39:p:27:LEU:HD11	39:p:40:PHE:HB3	2.01	0.42
9:J:117:ARG:O	9:J:121:GLU:HG3	2.19	0.42
16:Q:198:THR:HG22	16:Q:202:TRP:CE2	2.54	0.42
16:Q:251:PHE:CE2	16:Q:255:ILE:HD11	2.55	0.42
52:e:201:PLX:H111	55:l:702:CDL:H641	2.01	0.42
34:k:28:SER:HB2	36:m:23:LYS:HG2	1.91	0.42
44:w:59:VAL:HG12	44:w:201:PRO:HB3	2.01	0.42
1:A:73:PRO:HD3	1:A:147:ARG:NH2	2.35	0.42
1:A:119:GLU:O	1:A:159:ARG:NH1	2.52	0.42
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:131:LYS:HD2	11:L:147:VAL:HG11	2.01	0.42
12:M:689:LEU:HD23	12:M:689:LEU:HA	1.92	0.42
55:V:202:CDL:H872	35:l:558:LEU:HD21	2.01	0.42
52:e:201:PLX:H362	40:r:67:VAL:HG12	2.01	0.42
3:C:193:TRP:HA	3:C:196:ARG:HG2	2.01	0.42
7:H:105:GLU:HB3	15:P:89:HIS:CD2	2.54	0.42
9:J:108:TRP:HZ3	9:J:110:GLY:HA2	1.84	0.42
12:M:77:MET:HE2	12:M:117:MET:HE2	2.01	0.42
13:N:10:GLY:O	13:N:14:VAL:HG23	2.20	0.42
14:O:196:LEU:HD13	14:O:201:ILE:HD13	2.02	0.42
33:j:80:GLN:H	33:j:80:GLN:HG2	1.67	0.42
47:j:201:PEE:H22	47:j:201:PEE:H27	1.89	0.42
35:l:151:SER:HB2	35:l:252:MET:SD	2.60	0.42
40:r:174:LEU:HA	40:r:179:ILE:HD11	2.01	0.42
42:u:38:LYS:HB3	42:u:39:PRO:HD3	2.01	0.42
1:A:28:LYS:HD2	1:A:28:LYS:HA	1.91	0.42
12:M:329:MET:HG2	12:M:565:PHE:CG	2.54	0.42
52:N:201:PLX:H21	52:N:201:PLX:H1C3	1.56	0.42
16:Q:332:CYS:O	16:Q:336:GLU:HG3	2.20	0.42
21:W:57:ARG:HB3	41:s:316:PRO:HG3	2.00	0.42
26:c:110:ASP:HA	26:c:113:ILE:HG23	2.00	0.42
33:j:15:SER:HB3	47:j:202:PEE:H22	2.00	0.42
33:j:67:LEU:HG	34:k:68:ALA:CB	2.49	0.42
36:m:86:ASN:OD1	36:m:88:THR:HG22	2.20	0.42
41:s:199:ASP:OD1	41:s:279:ARG:NE	2.47	0.42
43:v:52:MET:O	43:v:56:ARG:HG3	2.19	0.42
27:d:68:PHE:CE1	28:e:114:MET:HE1	2.55	0.42
29:f:68:GLU:HG2	30:g:21:ARG:HE	1.85	0.42
34:k:79:VAL:HG23	36:m:74:MET:HE2	2.02	0.42
35:l:297:ASP:O	35:l:301:ILE:HG13	2.20	0.42
52:r:502:PLX:H1C3	52:r:502:PLX:H22	1.70	0.42
3:C:63:TRP:HE3	3:C:99:GLN:O	2.02	0.42
11:L:154:LYS:O	11:L:156:LYS:NZ	2.51	0.42
35:l:417:SER:OG	55:l:703:CDL:H581	2.20	0.42
40:r:355:MET:HE2	40:r:358:TRP:HD1	1.85	0.42
41:s:120:GLY:HA2	41:s:128:ALA:HB1	2.01	0.42
7:H:44:TYR:HB2	15:P:68:ILE:HG23	2.02	0.42
12:M:326:VAL:HG13	12:M:567:ILE:HD13	2.02	0.42
16:Q:188:THR:HB	16:Q:200:PHE:HA	2.02	0.42
22:Y:94:ASP:HA	22:Y:99:ILE:HD13	2.02	0.42
26:c:127:ASN:O	26:c:131:LYS:HE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:82:ILE:HD12	27:d:82:ILE:HA	1.92	0.42
28:e:129:ARG:HG2	28:e:134:LEU:HD12	2.01	0.42
30:g:10:ARG:NH2	32:i:347:ASN:O	2.47	0.42
32:i:81:SER:O	32:i:83:GLN:N	2.50	0.42
35:l:241:THR:HG21	35:l:344:GLY:HA3	2.00	0.42
9:J:272:LEU:HD11	9:J:375:VAL:CG1	2.44	0.41
12:M:386:LEU:HD23	12:M:386:LEU:HA	1.88	0.41
15:P:87:PHE:CE2	15:P:144:LYS:HE3	2.55	0.41
16:Q:85:GLY:O	33:j:39:CYS:HB3	2.20	0.41
16:Q:156:GLU:HG3	16:Q:229:PRO:O	2.20	0.41
16:Q:392:PRO:HA	16:Q:393:PRO:HD3	1.97	0.41
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.85	0.41
6:X:103:HIS:O	6:X:107:ASP:HB2	2.20	0.41
34:k:25:HIS:ND1	34:k:88:ASP:OD1	2.39	0.41
35:l:130:ILE:HD13	55:l:702:CDL:H252	2.02	0.41
47:l:705:PEE:H60	47:l:705:PEE:H55	1.87	0.41
39:p:84:GLU:OE1	39:p:84:GLU:N	2.53	0.41
44:w:113:SER:HB3	44:w:116:LYS:HB3	2.02	0.41
1:A:110:PRO:O	1:A:238:CYS:HB3	2.20	0.41
9:J:163:LYS:NZ	9:J:253:ILE:O	2.35	0.41
12:M:666:GLN:HG3	12:M:667:GLN:OE1	2.20	0.41
52:N:201:PLX:H271	52:N:201:PLX:H102	2.02	0.41
17:S:50:ARG:O	17:S:54:ILE:HG12	2.19	0.41
20:V:85:ASP:HA	20:V:126:LYS:NZ	2.35	0.41
24:a:163:ARG:NH1	30:g:102:ASP:OD2	2.44	0.41
25:b:86:LEU:HD11	35:l:9:LEU:HD12	2.01	0.41
32:i:97:MET:HE3	35:l:599:MET:HE3	2.02	0.41
32:i:268:GLN:HG3	42:u:168:PHE:CE2	2.55	0.41
55:k:101:CDL:H241	55:k:101:CDL:H351	2.01	0.41
35:l:557:TRP:O	35:l:561:ILE:HG12	2.20	0.41
41:s:307:LEU:HA	41:s:310:MET:HE3	2.02	0.41
43:v:107:ARG:HA	43:v:110:GLN:HG3	2.01	0.41
5:F:16:LEU:HD11	5:F:19:ILE:HD11	2.01	0.41
5:F:23:LEU:HD12	5:F:34:ARG:HG2	2.02	0.41
6:G:134:ASP:HA	6:G:137:LYS:NZ	2.35	0.41
9:J:279:TYR:HB2	9:J:372:ALA:HB2	2.02	0.41
17:S:1:MET:HE3	17:S:1:MET:HB3	2.00	0.41
20:V:66:ILE:HD11	20:V:101:LEU:HD13	2.02	0.41
25:b:81:ILE:HG23	47:l:705:PEE:H58	2.01	0.41
31:h:97:HIS:HB2	31:h:102:GLU:HB2	2.02	0.41
34:k:37:MET:HE2	34:k:67:ALA:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:197:LEU:HD13	47:r:501:PEE:H70	2.01	0.41
41:s:81:LEU:O	41:s:85:MET:HG2	2.20	0.41
1:A:250:VAL:O	1:A:251:SER:C	2.63	0.41
4:E:33:ARG:O	4:E:37:ARG:HG3	2.21	0.41
12:M:591:GLU:HG3	12:M:610:VAL:HG23	2.03	0.41
12:M:647:GLU:HB2	12:M:654:VAL:HG11	2.02	0.41
15:P:103:HIS:CD2	15:P:105:ASN:HB2	2.55	0.41
21:W:84:LEU:HD13	42:u:8:PRO:HG2	2.01	0.41
27:d:117:GLU:OE1	27:d:124:ASN:ND2	2.37	0.41
34:k:28:SER:CB	36:m:23:LYS:HG3	2.15	0.41
34:k:56:ALA:O	34:k:59:MET:HG3	2.20	0.41
55:k:101:CDL:OB3	35:l:585:LYS:NZ	2.43	0.41
3:C:96:SER:HB2	41:s:209:SER:HB2	2.02	0.41
8:I:28:TYR:HA	13:N:55:PHE:HA	2.03	0.41
47:J:401:PEE:C46	41:s:52:ALA:HB1	2.46	0.41
6:X:80:LYS:HE3	6:X:80:LYS:HB3	1.86	0.41
33:j:87:MET:HE1	41:s:309:ILE:HD11	2.02	0.41
37:n:49:LEU:HD22	37:n:53:GLU:HG3	2.03	0.41
39:p:44:MET:HE3	39:p:48:PHE:CE1	2.56	0.41
40:r:158:LEU:HD23	40:r:158:LEU:HA	1.91	0.41
49:C:303:UQ:H203	49:C:303:UQ:H172	1.84	0.41
4:E:14:GLY:C	4:E:16:SER:H	2.29	0.41
12:M:234:LYS:HB3	12:M:235:PRO:HD3	2.02	0.41
12:M:475:VAL:HG22	12:M:514:ASN:HB2	2.02	0.41
12:M:511:LYS:HE2	12:M:663:ASN:HB2	2.02	0.41
6:X:112:SER:O	6:X:116:VAL:HG23	2.21	0.41
25:b:73:THR:HG23	25:b:74:HIS:ND1	2.36	0.41
26:c:62:TYR:OH	26:c:74:ASP:OD1	2.36	0.41
35:l:172:ILE:HG21	40:r:408:LEU:HD12	2.03	0.41
44:w:65:ASN:HD22	44:w:238:GLU:HG3	1.86	0.41
12:M:498:GLN:HG3	12:M:502:LEU:HD23	2.03	0.41
15:P:211:ARG:NH2	15:P:222:GLU:OE2	2.49	0.41
16:Q:88:HIS:ND1	16:Q:89:PRO:HD2	2.35	0.41
55:V:202:CDL:H781	55:V:202:CDL:H812	1.78	0.41
52:e:201:PLX:H221	52:e:201:PLX:H191	1.91	0.41
32:i:183:SER:O	32:i:187:MET:HG2	2.20	0.41
36:m:163:ILE:HD13	36:m:163:ILE:HA	1.92	0.41
3:C:59:ARG:NE	3:C:185:LYS:HB2	2.35	0.41
9:J:171:ASN:OD1	9:J:327:MET:HG3	2.21	0.41
12:M:50:LEU:O	12:M:54:GLU:HG2	2.20	0.41
13:N:39:VAL:N	13:N:48:TYR:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:137:THR:HB	53:O:301:FES:S2	2.61	0.41
17:S:23:THR:HG22	17:S:27:HIS:CD2	2.56	0.41
24:a:176:LYS:HE2	24:a:176:LYS:HB3	1.70	0.41
31:h:21:GLN:HG2	31:h:37:GLU:OE1	2.21	0.41
32:i:112:HIS:CE1	32:i:164:ILE:HD13	2.55	0.41
41:s:102:VAL:HG23	41:s:160:TYR:O	2.20	0.41
44:w:209:VAL:HB	44:w:214:ILE:HD11	2.02	0.41
1:A:367:ILE:O	1:A:371:ILE:HG12	2.21	0.41
9:J:262:THR:O	9:J:333:PRO:HD2	2.21	0.41
12:M:289:LYS:HE2	12:M:694:PHE:O	2.21	0.41
12:M:338:VAL:O	12:M:363:SER:OG	2.30	0.41
52:N:201:PLX:H121	41:s:46:LEU:HD22	2.03	0.41
20:V:95:CYS:HA	20:V:115:CYS:HA	2.02	0.41
6:X:70:ASP:OD1	35:l:109:HIS:NE2	2.53	0.41
22:Y:40:ILE:HD11	35:l:444:ASN:HB2	2.03	0.41
22:Y:87:PRO:HG3	43:v:96:VAL:HG23	2.03	0.41
25:b:35:LEU:HA	25:b:36:PRO:HD3	1.98	0.41
32:i:106:LEU:HG	32:i:138:PRO:HB2	2.03	0.41
35:l:63:ILE:O	35:l:79:SER:HA	2.21	0.41
35:l:96:VAL:O	35:l:100:ILE:HG12	2.21	0.41
36:m:36:SER:HA	36:m:39:VAL:HG22	2.03	0.41
37:n:18:PRO:O	37:n:21:PHE:HB3	2.21	0.41
40:r:121:LEU:O	40:r:125:THR:HG23	2.21	0.41
41:s:120:GLY:HA3	41:s:132:ALA:HB2	2.02	0.41
41:s:186:PHE:O	41:s:189:THR:OG1	2.31	0.41
7:H:55:LYS:HE3	15:P:104:THR:HG21	2.02	0.41
15:P:170:ILE:HG22	15:P:176:VAL:HB	2.03	0.41
16:Q:80:LEU:HD13	33:j:51:PHE:CE1	2.56	0.41
29:f:68:GLU:OE2	29:f:72:ARG:HG3	2.21	0.41
30:g:92:MET:O	30:g:96:VAL:HG23	2.21	0.41
33:j:94:LEU:HD13	36:m:154:VAL:HG13	2.02	0.41
35:l:128:MET:CE	35:l:252:MET:HA	2.51	0.41
47:l:704:PEE:H55	40:r:405:LEU:HD13	2.03	0.41
38:o:61:GLU:OE2	38:o:66:ILE:HD11	2.21	0.41
9:J:131:GLY:O	51:J:402:NDP:H51A	2.22	0.40
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.51	0.40
12:M:382:ARG:HE	12:M:527:ASP:CG	2.29	0.40
16:Q:76:LEU:O	16:Q:76:LEU:HD23	2.21	0.40
26:c:126:TRP:C	26:c:128:THR:H	2.27	0.40
27:d:78:GLU:HA	30:g:110:THR:HA	2.03	0.40
35:l:298:ILE:O	35:l:302:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:561:ILE:HG13	35:l:562:LEU:N	2.36	0.40
47:r:501:PEE:H68	47:r:501:PEE:H62	1.91	0.40
2:B:144:ARG:NH1	11:L:112:MET:O	2.30	0.40
10:K:87:LEU:HD22	14:O:66:ILE:HD11	2.04	0.40
12:M:372:PHE:H	12:M:532:PRO:HB2	1.87	0.40
15:P:173:MET:HB3	15:P:198:PHE:HB2	2.02	0.40
21:W:93:GLU:HG3	31:h:98:HIS:CD2	2.56	0.40
26:c:167:TYR:CG	26:c:178:PRO:HG3	2.57	0.40
35:l:184:LEU:HD13	40:r:393:ILE:HG21	2.03	0.40
38:o:31:LYS:O	38:o:35:GLU:HG2	2.20	0.40
39:p:108:HIS:CD2	39:p:109:PRO:HD2	2.56	0.40
41:s:59:GLU:HA	41:s:60:PRO:HD3	1.88	0.40
41:s:169:GLN:HB2	41:s:244:GLY:HA3	2.03	0.40
2:B:72:MET:HE2	2:B:72:MET:HB2	1.94	0.40
2:B:118:LEU:HD11	16:Q:382:PHE:CE2	2.56	0.40
3:C:92:VAL:CG1	49:C:303:UQ:H103	2.36	0.40
4:E:17:VAL:HG21	11:L:55:VAL:HG12	2.03	0.40
4:E:104:MET:HE3	4:E:109:GLU:OE2	2.21	0.40
9:J:92:MET:HE3	9:J:92:MET:HB3	1.97	0.40
12:M:250:SER:OG	12:M:606:THR:HB	2.21	0.40
12:M:405:THR:HG23	12:M:407:PRO:HD3	2.02	0.40
15:P:197:PRO:O	16:Q:122:LYS:NZ	2.45	0.40
32:i:207:ILE:O	32:i:211:MET:HG3	2.21	0.40
33:j:37:TYR:CD1	33:j:37:TYR:C	2.99	0.40
35:l:49:VAL:HB	35:l:50:PRO:HD3	2.03	0.40
55:l:702:CDL:H411	40:r:371:PRO:HD2	2.04	0.40
40:r:370:PRO:HA	40:r:371:PRO:HA	1.85	0.40
41:s:119:SER:HG	41:s:223:PHE:HZ	1.65	0.40
42:u:56:CYS:HB2	42:u:59:GLU:OE1	2.22	0.40
2:B:96:ARG:HG2	2:B:208:ASP:OD2	2.22	0.40
12:M:394:VAL:HG22	12:M:473:MET:HE1	2.03	0.40
12:M:624:ARG:NH1	12:M:628:GLU:OE1	2.37	0.40
14:O:201:ILE:HD12	14:O:201:ILE:HA	1.97	0.40
15:P:148:ASP:OD1	15:P:148:ASP:N	2.54	0.40
26:c:83:GLN:NE2	26:c:97:LEU:O	2.54	0.40
31:h:60:PHE:O	31:h:64:VAL:HG23	2.21	0.40
52:r:502:PLX:H312	52:r:502:PLX:H342	1.91	0.40
44:w:209:VAL:HG22	44:w:260:ALA:HB2	2.02	0.40
2:B:100:GLU:O	2:B:170:GLY:N	2.43	0.40
12:M:198:THR:HG21	12:M:209:TYR:HB2	2.03	0.40
19:U:38:TYR:HB2	41:s:310:MET:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:32:GLU:HB3	39:p:115:TYR:HD1	1.86	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	431/433 (100%)	417 (97%)	13 (3%)	1 (0%)	43	76
2	B	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
3	C	154/156 (99%)	147 (96%)	7 (4%)	0	100	100
4	E	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
5	F	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
6	G	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
6	X	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
7	H	110/112 (98%)	102 (93%)	7 (6%)	1 (1%)	14	48
8	I	93/112 (83%)	80 (86%)	13 (14%)	0	100	100
9	J	340/342 (99%)	329 (97%)	11 (3%)	0	100	100
10	K	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
11	L	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
12	M	688/690 (100%)	659 (96%)	29 (4%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	201 (94%)	14 (6%)	0	100	100
15	P	206/208 (99%)	197 (96%)	9 (4%)	0	100	100
16	Q	427/430 (99%)	409 (96%)	18 (4%)	0	100	100
17	S	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
18	T	94/96 (98%)	93 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	U	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
20	V	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
21	W	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
22	Y	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
23	Z	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
24	a	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
25	b	94/126 (75%)	86 (92%)	8 (8%)	0	100	100
26	c	154/156 (99%)	142 (92%)	12 (8%)	0	100	100
27	d	173/175 (99%)	172 (99%)	1 (1%)	0	100	100
28	e	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
29	f	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
30	g	119/121 (98%)	112 (94%)	7 (6%)	0	100	100
31	h	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
32	i	345/347 (99%)	332 (96%)	13 (4%)	0	100	100
33	j	113/115 (98%)	110 (97%)	2 (2%)	1 (1%)	14	48
34	k	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
35	l	604/606 (100%)	582 (96%)	22 (4%)	0	100	100
36	m	173/175 (99%)	162 (94%)	11 (6%)	0	100	100
37	n	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
38	o	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
39	p	176/178 (99%)	170 (97%)	5 (3%)	1 (1%)	21	56
40	r	457/459 (100%)	453 (99%)	4 (1%)	0	100	100
41	s	316/318 (99%)	310 (98%)	5 (2%)	1 (0%)	36	70
42	u	169/171 (99%)	162 (96%)	6 (4%)	1 (1%)	21	56
43	v	122/125 (98%)	117 (96%)	5 (4%)	0	100	100
44	w	318/320 (99%)	307 (96%)	11 (4%)	0	100	100
All	All	8174/8313 (98%)	7861 (96%)	307 (4%)	6 (0%)	49	80

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	j	81	THR
1	A	186	ALA

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Mol	Chain	Res	Type
7	H	77	ILE
39	p	174	PRO
42	u	152	PRO
41	s	208	VAL

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	344/346 (99%)	344 (100%)	0	100	100
2	B	148/151 (98%)	148 (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	75/76 (99%)	75 (100%)	0	100	100
6	G	76/81 (94%)	76 (100%)	0	100	100
6	X	78/81 (96%)	78 (100%)	0	100	100
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	87 (100%)	0	100	100
9	J	296/296 (100%)	296 (100%)	0	100	100
10	K	42/42 (100%)	42 (100%)	0	100	100
11	L	113/113 (100%)	113 (100%)	0	100	100
12	M	579/580 (100%)	579 (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	368/370 (100%)	365 (99%)	3 (1%)	73	86
17	S	57/58 (98%)	56 (98%)	1 (2%)	51	77
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	68/69 (99%)	68 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	V	101/101 (100%)	101 (100%)	0	100	100
21	W	122/123 (99%)	120 (98%)	2 (2%)	55	79
22	Y	62/62 (100%)	62 (100%)	0	100	100
23	Z	62/62 (100%)	62 (100%)	0	100	100
24	a	121/121 (100%)	121 (100%)	0	100	100
25	b	90/119 (76%)	90 (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	96/96 (100%)	96 (100%)	0	100	100
29	f	35/45 (78%)	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	100/100 (100%)	100 (100%)	0	100	100
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	540/540 (100%)	540 (100%)	0	100	100
36	m	127/141 (90%)	124 (98%)	3 (2%)	43	73
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	113/113 (100%)	113 (100%)	0	100	100
39	p	159/159 (100%)	159 (100%)	0	100	100
40	r	410/410 (100%)	410 (100%)	0	100	100
41	s	274/275 (100%)	273 (100%)	1 (0%)	84	90
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	104/111 (94%)	104 (100%)	0	100	100
44	w	281/283 (99%)	281 (100%)	0	100	100
All	All	7147/7240 (99%)	7137 (100%)	10 (0%)	87	93

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	Q	53	TYR
16	Q	75	THR
16	Q	258	LEU

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Mol	Chain	Res	Type
17	S	31	ASN
21	W	28	ARG
21	W	30	LEU
36	m	23	LYS
36	m	65	LEU
36	m	146	LEU
41	s	49	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	ASN
3	C	179	GLN
4	E	58	GLN
4	E	70	ASN
4	E	99	GLN
4	E	126	HIS
5	F	80	ASN
7	H	83	GLN
8	I	47	HIS
9	J	37	HIS
9	J	122	HIS
9	J	128	ASN
11	L	71	HIS
12	M	123	ASN
12	M	205	GLN
12	M	278	HIS
12	M	304	GLN
12	M	453	GLN
12	M	604	GLN
13	N	91	HIS
14	O	41	HIS
14	O	48	ASN
14	O	69	ASN
14	O	187	GLN
15	P	55	HIS
15	P	75	GLN
15	P	124	ASN
15	P	164	ASN
16	Q	92	HIS
17	S	31	ASN
17	S	68	ASN

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Mol	Chain	Res	Type
18	T	120	GLN
20	V	134	GLN
21	W	90	ASN
22	Y	39	HIS
23	Z	21	GLN
23	Z	60	ASN
24	a	170	GLN
25	b	67	HIS
27	d	55	GLN
28	e	86	ASN
28	e	145	ASN
29	f	61	GLN
31	h	70	GLN
31	h	97	HIS
32	i	47	ASN
32	i	112	HIS
32	i	134	GLN
32	i	172	GLN
32	i	174	GLN
33	j	83	ASN
34	k	57	ASN
34	k	91	GLN
35	l	59	GLN
35	l	135	ASN
35	l	199	GLN
35	l	470	ASN
35	l	479	ASN
36	m	175	ASN
39	p	13	GLN
40	r	175	ASN
40	r	180	HIS
40	r	338	HIS
41	s	250	HIS
42	u	30	HIS
43	v	44	GLN
43	v	82	HIS
43	v	84	GLN
44	w	188	ASN
44	w	323	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	2MR	Q	118	16	10,12,13	2.01	1 (10%)	5,13,15	6.06	3 (60%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.67	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	12.46	130.90	119.48
16	Q	118	2MR	CD-NE-CZ	4.18	131.24	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.00	130.50	123.86

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 2 are modelled with single atom and 2 are monoatomic - leaving 41 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
47	PEE	B	303	-	50,50,50	1.16	6 (12%)	53,55,55	0.99	2 (3%)
49	UQ	J	403	-	33,33,63	3.46	8 (24%)	40,43,79	2.81	14 (35%)
49	UQ	C	303	-	38,38,63	3.54	11 (28%)	46,49,79	2.80	16 (34%)
57	ADP	w	401	-	27,29,29	2.96	8 (29%)	42,45,45	2.02	10 (23%)
52	PLX	r	502	-	51,51,51	1.14	4 (7%)	55,59,59	0.60	1 (1%)
48	970	C	302	-	33,33,33	4.79	15 (45%)	48,50,50	2.86	22 (45%)
52	PLX	g	201	-	51,51,51	1.14	3 (5%)	55,59,59	0.64	1 (1%)
50	8Q1	G	201	-	31,34,34	1.69	6 (19%)	40,43,43	1.65	5 (12%)
47	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	0.97	2 (3%)
52	PLX	J	404	-	51,51,51	1.14	3 (5%)	55,59,59	0.60	1 (1%)
53	FES	M	803	12	0,4,4	-	-	-	-	-
52	PLX	e	201	-	51,51,51	1.14	3 (5%)	55,59,59	0.54	1 (1%)
55	CDL	l	702	-	98,98,99	1.08	8 (8%)	104,110,111	0.89	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	CDL	l	703	-	99,99,99	1.09	8 (8%)	105,111,111	0.87	4 (3%)
52	PLX	a	202	-	51,51,51	1.15	3 (5%)	55,59,59	0.59	1 (1%)
47	PEE	J	401	-	46,46,50	1.20	6 (13%)	49,51,55	0.99	2 (4%)
53	FES	O	301	14	0,4,4	-	-	-		
45	SF4	B	301	2	0,12,12	-	-	-		
47	PEE	W	201	-	40,40,50	1.14	5 (12%)	43,45,55	1.02	2 (4%)
47	PEE	j	202	-	40,40,50	1.15	5 (12%)	43,45,55	1.00	2 (4%)
45	SF4	M	801	12	0,12,12	-	-	-		
55	CDL	N	202	-	50,50,99	1.40	9 (18%)	56,62,111	1.18	4 (7%)
55	CDL	k	101	-	94,94,99	0.93	4 (4%)	100,106,111	1.03	4 (4%)
50	8Q1	X	201	-	31,34,34	1.69	6 (19%)	40,43,43	1.57	6 (15%)
47	PEE	l	705	-	45,45,50	1.22	6 (13%)	48,50,55	0.95	2 (4%)
45	SF4	B	302	2	0,12,12	-	-	-		
55	CDL	V	202	-	99,99,99	1.08	8 (8%)	105,111,111	0.87	4 (3%)
46	FMN	A	502	-	33,33,33	1.41	5 (15%)	48,50,50	1.32	8 (16%)
47	PEE	l	701	-	39,39,50	1.31	6 (15%)	41,44,55	1.05	2 (4%)
47	PEE	l	704	-	49,49,50	1.17	6 (12%)	52,54,55	0.94	2 (3%)
55	CDL	a	201	-	99,99,99	1.09	8 (8%)	105,111,111	0.85	4 (3%)
55	CDL	n	101	-	54,54,99	1.36	9 (16%)	60,66,111	1.11	4 (6%)
52	PLX	N	201	-	51,51,51	0.65	0	55,59,59	0.74	0
45	SF4	A	501	1	0,12,12	-	-	-		
51	NDP	J	402	-	49,52,52	4.38	23 (46%)	66,80,80	2.19	14 (21%)
55	CDL	r	503	-	98,98,99	1.08	8 (8%)	104,110,111	0.86	4 (3%)
45	SF4	C	301	3	0,12,12	-	-	-		
45	SF4	M	802	12	0,12,12	-	-	-		
52	PLX	j	203	-	51,51,51	1.14	4 (7%)	55,59,59	0.61	1 (1%)
55	CDL	V	201	-	93,93,99	1.11	9 (9%)	99,105,111	0.87	4 (4%)
47	PEE	j	201	-	50,50,50	1.16	6 (12%)	53,55,55	0.95	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	PEE	B	303	-	-	22/54/54/54	-
49	UQ	J	403	-	-	12/27/51/87	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	UQ	C	303	-	-	13/33/57/87	0/1/1/1
57	ADP	w	401	-	-	6/16/32/32	0/3/3/3
52	PLX	r	502	-	-	21/55/55/55	-
48	970	C	302	-	-	4/8/41/41	0/5/5/5
52	PLX	g	201	-	-	36/55/55/55	-
50	8Q1	G	201	-	-	16/41/41/41	-
47	PEE	r	501	-	-	25/54/54/54	-
52	PLX	J	404	-	-	26/55/55/55	-
53	FES	M	803	12	-	-	0/1/1/1
52	PLX	e	201	-	-	30/55/55/55	-
55	CDL	l	702	-	-	55/109/109/110	-
55	CDL	l	703	-	-	49/110/110/110	-
52	PLX	a	202	-	-	31/55/55/55	-
47	PEE	J	401	-	-	24/50/50/54	-
53	FES	O	301	14	-	-	0/1/1/1
45	SF4	B	301	2	-	-	0/6/5/5
47	PEE	W	201	-	-	25/44/44/54	-
47	PEE	j	202	-	-	25/44/44/54	-
45	SF4	M	801	12	-	-	0/6/5/5
55	CDL	N	202	-	-	34/61/61/110	-
55	CDL	k	101	-	-	35/105/105/110	-
50	8Q1	X	201	-	-	21/41/41/41	-
47	PEE	l	705	-	-	27/49/49/54	-
45	SF4	B	302	2	-	-	0/6/5/5
55	CDL	V	202	-	-	59/110/110/110	-
46	FMN	A	502	-	-	6/18/18/18	0/3/3/3
47	PEE	l	701	-	-	25/43/43/54	-
47	PEE	l	704	-	-	28/53/53/54	-
55	CDL	a	201	-	-	58/110/110/110	-
55	CDL	n	101	-	-	31/65/65/110	-
52	PLX	N	201	-	-	13/55/55/55	-
45	SF4	A	501	1	-	-	0/6/5/5
51	NDP	J	402	-	-	10/34/77/77	0/4/5/5
55	CDL	r	503	-	-	55/109/109/110	-
45	SF4	C	301	3	-	-	0/6/5/5
45	SF4	M	802	12	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	PLX	j	203	-	-	32/55/55/55	-
55	CDL	V	201	-	-	62/104/104/110	-
47	PEE	j	201	-	-	24/54/54/54	-

All (225) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	C	302	970	O16-C17	17.92	1.57	1.37
51	J	402	NDP	C3B-C2B	-12.93	1.24	1.52
51	J	402	NDP	C6N-C5N	12.29	1.55	1.33
48	C	302	970	O25-C24	10.73	1.37	1.22
51	J	402	NDP	O4D-C4D	10.68	1.68	1.45
51	J	402	NDP	C3D-C4D	-9.90	1.27	1.53
49	C	303	UQ	C18-C19	9.68	1.56	1.33
49	J	403	UQ	C18-C19	9.64	1.56	1.33
49	J	403	UQ	C13-C14	9.32	1.55	1.33
49	C	303	UQ	C13-C14	9.26	1.55	1.33
49	C	303	UQ	C23-C24	9.05	1.54	1.33
49	C	303	UQ	C8-C9	8.94	1.54	1.33
57	w	401	ADP	C3'-C4'	-8.91	1.30	1.53
49	J	403	UQ	C8-C9	8.79	1.54	1.33
48	C	302	970	C23-C24	8.68	1.61	1.52
51	J	402	NDP	O4B-C4B	-7.92	1.27	1.45
49	J	403	UQ	C23-C24	7.87	1.55	1.32
49	C	303	UQ	C28-C29	7.65	1.54	1.32
57	w	401	ADP	O4'-C4'	7.65	1.62	1.45
48	C	302	970	C14-C23	-7.36	1.45	1.52
51	J	402	NDP	C2N-C3N	7.35	1.55	1.34
48	C	302	970	O08-C07	6.41	1.47	1.37
51	J	402	NDP	C6A-N6A	5.84	1.48	1.34
51	J	402	NDP	P2B-O2B	5.49	1.69	1.59
57	w	401	ADP	C6-N6	5.49	1.47	1.34
50	X	201	8Q1	C34-N36	5.45	1.45	1.33
51	J	402	NDP	C3B-C4B	5.33	1.66	1.53
50	G	201	8Q1	C34-N36	5.30	1.45	1.33
50	G	201	8Q1	C39-N41	5.28	1.45	1.33
50	X	201	8Q1	C39-N41	5.27	1.45	1.33
48	C	302	970	C05-C04	-5.16	1.46	1.54
51	J	402	NDP	O4D-C1D	-4.95	1.30	1.42
48	C	302	970	O13-C12	4.93	1.45	1.37
51	J	402	NDP	C6N-N1N	4.93	1.49	1.37
48	C	302	970	C03-C02	4.73	1.53	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	A	502	FMN	C9A-C5A	4.64	1.49	1.41
51	J	402	NDP	O4B-C1B	4.50	1.52	1.42
51	J	402	NDP	C1B-N9A	-4.49	1.33	1.46
57	w	401	ADP	O4'-C1'	-4.40	1.31	1.42
51	J	402	NDP	O2D-C2D	-4.28	1.32	1.43
55	k	101	CDL	OA8-CA7	4.18	1.45	1.33
51	J	402	NDP	C7N-N7N	4.16	1.44	1.33
55	k	101	CDL	OA6-CA5	4.11	1.45	1.34
55	k	101	CDL	OB8-CB7	4.09	1.45	1.33
55	k	101	CDL	OB6-CB5	4.08	1.45	1.34
47	J	401	PEE	C18-C19	3.75	1.53	1.31
47	B	303	PEE	C18-C19	3.73	1.53	1.31
47	l	701	PEE	C18-C19	3.73	1.53	1.31
47	l	705	PEE	C18-C19	3.73	1.53	1.31
47	j	201	PEE	C18-C19	3.72	1.53	1.31
47	l	704	PEE	C18-C19	3.71	1.53	1.31
47	j	202	PEE	C18-C19	3.71	1.53	1.31
47	r	501	PEE	C18-C19	3.69	1.53	1.31
47	W	201	PEE	C18-C19	3.69	1.53	1.31
47	r	501	PEE	C39-C38	3.65	1.53	1.31
47	l	705	PEE	C39-C38	3.65	1.52	1.31
47	J	401	PEE	C39-C38	3.65	1.52	1.31
47	B	303	PEE	C39-C38	3.64	1.52	1.31
47	l	701	PEE	C39-C38	3.64	1.52	1.31
47	j	201	PEE	C39-C38	3.61	1.52	1.31
47	l	704	PEE	C39-C38	3.60	1.52	1.31
55	n	101	CDL	OA8-CA7	3.49	1.43	1.33
48	C	302	970	C15-C14	3.46	1.57	1.51
55	V	201	CDL	OA8-CA7	3.46	1.43	1.33
55	l	703	CDL	OA8-CA7	3.45	1.43	1.33
57	w	401	ADP	O2'-C2'	-3.41	1.34	1.43
55	V	202	CDL	OA8-CA7	3.41	1.43	1.33
55	l	702	CDL	OA8-CA7	3.41	1.43	1.33
55	N	202	CDL	OA8-CA7	3.39	1.43	1.33
55	a	201	CDL	OA8-CA7	3.38	1.43	1.33
55	r	503	CDL	OA8-CA7	3.36	1.43	1.33
46	A	502	FMN	C8-C7	3.26	1.49	1.40
48	C	302	970	C11-C24	3.23	1.54	1.48
57	w	401	ADP	C8-N9	-3.19	1.31	1.37
48	C	302	970	O16-C15	3.15	1.52	1.44
55	N	202	CDL	OA6-CA5	3.14	1.43	1.34
51	J	402	NDP	C8A-N9A	-3.12	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	w	401	ADP	O3'-C3'	3.09	1.50	1.43
55	a	201	CDL	OB6-CB5	3.08	1.43	1.34
55	V	201	CDL	OA6-CA5	3.06	1.42	1.34
55	N	202	CDL	OB8-CB7	3.06	1.42	1.33
55	r	503	CDL	OB6-CB5	3.04	1.42	1.34
55	a	201	CDL	OB8-CB7	3.03	1.42	1.33
55	r	503	CDL	OB8-CB7	3.01	1.42	1.33
51	J	402	NDP	O3D-C3D	3.01	1.50	1.43
55	l	702	CDL	OB8-CB7	3.00	1.42	1.33
55	l	703	CDL	OB8-CB7	2.99	1.42	1.33
55	V	201	CDL	OB6-CB5	2.98	1.42	1.34
55	n	101	CDL	OB6-CB5	2.98	1.42	1.34
55	l	703	CDL	OB6-CB5	2.97	1.42	1.34
55	a	201	CDL	OA6-CA5	2.97	1.42	1.34
51	J	402	NDP	C5A-N7A	-2.96	1.33	1.39
55	V	202	CDL	OB6-CB5	2.96	1.42	1.34
55	N	202	CDL	OB6-CB5	2.96	1.42	1.34
55	V	201	CDL	OB8-CB7	2.95	1.41	1.33
55	l	702	CDL	OB6-CB5	2.94	1.42	1.34
55	n	101	CDL	OB8-CB7	2.94	1.41	1.33
55	l	703	CDL	OA6-CA5	2.94	1.42	1.34
55	V	202	CDL	OB8-CB7	2.94	1.41	1.33
49	J	403	UQ	C6-C1	2.92	1.54	1.46
55	V	202	CDL	OA6-CA5	2.91	1.42	1.34
55	n	101	CDL	OA6-CA5	2.89	1.42	1.34
55	l	702	CDL	OA6-CA5	2.89	1.42	1.34
55	r	503	CDL	OA6-CA5	2.86	1.42	1.34
51	J	402	NDP	C7N-C3N	2.85	1.54	1.48
52	g	201	PLX	O6-C4	-2.85	1.40	1.44
46	A	502	FMN	C4-N3	-2.77	1.33	1.38
49	C	303	UQ	C6-C1	2.68	1.54	1.46
52	r	502	PLX	O6-C4	-2.67	1.41	1.44
52	a	202	PLX	O6-C4	-2.66	1.41	1.44
52	e	201	PLX	O6-C4	-2.64	1.41	1.44
48	C	302	970	C12-C06	2.64	1.43	1.39
48	C	302	970	C09-C07	2.60	1.45	1.39
47	l	705	PEE	O3-C30	2.53	1.40	1.33
47	l	705	PEE	O2-C2	-2.52	1.40	1.46
55	r	503	CDL	OA6-CA4	-2.50	1.40	1.46
47	B	303	PEE	O2-C2	-2.49	1.40	1.46
47	j	202	PEE	O3-C30	2.48	1.40	1.33
55	l	702	CDL	OA6-CA4	-2.48	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	J	401	PEE	O3-C30	2.47	1.40	1.33
47	j	201	PEE	O3-C30	2.46	1.40	1.33
47	l	701	PEE	O3-C30	2.46	1.40	1.33
47	j	201	PEE	O2-C2	-2.46	1.40	1.46
47	r	501	PEE	O2-C2	-2.46	1.40	1.46
49	J	403	UQ	C7-C8	2.45	1.54	1.50
52	j	203	PLX	O6-C4	-2.44	1.41	1.44
49	C	303	UQ	C7-C8	2.44	1.54	1.50
47	B	303	PEE	O3-C30	2.44	1.40	1.33
47	W	201	PEE	O2-C2	-2.43	1.40	1.46
55	a	201	CDL	OA6-CA4	-2.42	1.40	1.46
47	J	401	PEE	O2-C2	-2.42	1.40	1.46
52	J	404	PLX	C7-C6	2.42	1.55	1.50
47	j	202	PEE	O2-C2	-2.42	1.40	1.46
55	n	101	CDL	OA6-CA4	-2.42	1.40	1.46
52	e	201	PLX	C7-C6	2.42	1.55	1.50
47	l	704	PEE	O3-C30	2.42	1.40	1.33
52	j	203	PLX	C7-C6	2.40	1.55	1.50
55	V	202	CDL	OA6-CA4	-2.40	1.40	1.46
50	X	201	8Q1	C1-S44	2.39	1.81	1.76
55	l	703	CDL	OA6-CA4	-2.38	1.40	1.46
47	W	201	PEE	O3-C30	2.38	1.40	1.33
47	l	704	PEE	O2-C2	-2.37	1.40	1.46
50	G	201	8Q1	C1-S44	2.37	1.81	1.76
47	r	501	PEE	O3-C30	2.36	1.40	1.33
51	J	402	NDP	O2B-C2B	2.35	1.52	1.44
52	g	201	PLX	C7-C6	2.33	1.55	1.50
50	G	201	8Q1	O40-C39	-2.33	1.18	1.23
52	r	502	PLX	C7-C6	2.33	1.55	1.50
47	l	701	PEE	O2-C10	2.32	1.40	1.34
50	G	201	8Q1	O35-C34	-2.32	1.18	1.23
46	A	502	FMN	C4A-N5	2.32	1.35	1.30
52	a	202	PLX	C7-C6	2.31	1.55	1.50
47	l	701	PEE	O2-C2	-2.30	1.40	1.46
52	J	404	PLX	O6-C4	-2.29	1.41	1.44
55	l	703	CDL	OB6-CB4	-2.28	1.40	1.46
57	w	401	ADP	C5-N7	-2.27	1.34	1.39
50	G	201	8Q1	C6-C1	2.26	1.53	1.50
50	X	201	8Q1	C6-C1	2.26	1.53	1.50
47	l	704	PEE	O2-C10	2.26	1.40	1.34
47	j	201	PEE	O2-C10	2.26	1.40	1.34
55	l	702	CDL	OB6-CB4	-2.25	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	J	402	NDP	O7N-C7N	-2.25	1.19	1.24
50	X	201	8Q1	O35-C34	-2.25	1.18	1.23
55	V	202	CDL	PB2-OB2	2.24	1.68	1.59
47	l	704	PEE	O3-C3	-2.24	1.40	1.45
47	j	202	PEE	O2-C10	2.23	1.40	1.34
55	V	202	CDL	OB6-CB4	-2.23	1.41	1.46
50	X	201	8Q1	O40-C39	-2.23	1.18	1.23
55	V	201	CDL	PB2-OB2	2.23	1.68	1.59
55	n	101	CDL	OB6-CB4	-2.22	1.41	1.46
51	J	402	NDP	C2D-C3D	2.22	1.59	1.53
49	J	403	UQ	O4-C4	-2.21	1.18	1.23
55	V	201	CDL	PB2-OB5	2.21	1.68	1.59
55	r	503	CDL	PB2-OB2	2.21	1.68	1.59
47	J	401	PEE	O2-C10	2.21	1.40	1.34
55	N	202	CDL	OB6-CB4	-2.20	1.41	1.46
55	n	101	CDL	PB2-OB2	2.20	1.68	1.59
55	l	703	CDL	PB2-OB2	2.20	1.68	1.59
47	B	303	PEE	O2-C10	2.20	1.40	1.34
47	r	501	PEE	O3-C3	-2.20	1.40	1.45
47	l	705	PEE	O2-C10	2.19	1.40	1.34
55	N	202	CDL	PB2-OB5	2.19	1.68	1.59
55	V	201	CDL	OB6-CB4	-2.19	1.41	1.46
49	C	303	UQ	O4-C4	-2.18	1.18	1.23
47	r	501	PEE	O2-C10	2.18	1.40	1.34
47	W	201	PEE	O2-C10	2.18	1.40	1.34
55	r	503	CDL	PB2-OB5	2.18	1.68	1.59
52	j	203	PLX	P1-O4	2.18	1.68	1.59
55	a	201	CDL	OB6-CB4	-2.17	1.41	1.46
55	a	201	CDL	PB2-OB2	2.16	1.68	1.59
55	l	703	CDL	PB2-OB5	2.15	1.68	1.59
55	a	201	CDL	PB2-OB5	2.15	1.68	1.59
52	a	202	PLX	P1-O4	2.15	1.68	1.59
47	W	201	PEE	O3-C3	-2.15	1.40	1.45
55	V	202	CDL	PB2-OB5	2.14	1.68	1.59
55	n	101	CDL	PB2-OB5	2.14	1.68	1.59
55	V	201	CDL	OA6-CA4	-2.13	1.41	1.46
46	A	502	FMN	C5A-N5	-2.13	1.35	1.39
55	N	202	CDL	PB2-OB2	2.13	1.67	1.59
55	l	702	CDL	PB2-OB2	2.12	1.67	1.59
55	l	702	CDL	PB2-OB5	2.12	1.67	1.59
55	N	202	CDL	OA6-CA4	-2.12	1.41	1.46
55	r	503	CDL	OB6-CB4	-2.11	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	j	201	PEE	O3-C3	-2.11	1.40	1.45
51	J	402	NDP	PA-O5B	2.11	1.67	1.59
52	e	201	PLX	P1-O4	2.10	1.67	1.59
52	r	502	PLX	P1-O4	2.10	1.67	1.59
47	J	401	PEE	O3-C3	-2.10	1.40	1.45
47	l	701	PEE	O3-C3	-2.10	1.40	1.45
52	g	201	PLX	P1-O4	2.08	1.67	1.59
52	j	203	PLX	P1-O1	2.08	1.67	1.59
52	J	404	PLX	P1-O4	2.07	1.67	1.59
52	r	502	PLX	P1-O1	2.07	1.67	1.59
49	C	303	UQ	O1-C1	-2.06	1.18	1.23
55	N	202	CDL	C11-CA5	2.06	1.56	1.50
47	B	303	PEE	O3-C3	-2.04	1.40	1.45
48	C	302	970	O26-C20	2.04	1.40	1.37
49	C	303	UQ	C21-C19	2.03	1.55	1.51
55	V	201	CDL	C11-CA5	2.02	1.56	1.50
47	l	705	PEE	O3-C3	-2.02	1.40	1.45
55	n	101	CDL	C11-CA5	2.01	1.56	1.50
48	C	302	970	O28-C19	2.01	1.40	1.37
49	C	303	UQ	O3-CM3	-2.01	1.40	1.45
47	j	202	PEE	O3-C3	-2.01	1.40	1.45
49	J	403	UQ	O3-CM3	-2.01	1.40	1.45

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	C	302	970	O25-C24-C23	-8.62	108.61	121.00
49	C	303	UQ	C7-C8-C9	-8.26	113.05	126.79
48	C	302	970	O25-C24-C11	-8.20	108.83	121.98
49	J	403	UQ	C7-C8-C9	-8.15	113.23	126.79
51	J	402	NDP	C3N-C2N-N1N	-7.96	111.74	123.10
51	J	402	NDP	C1D-N1N-C2N	-7.20	109.13	121.11
48	C	302	970	O08-C07-C06	-7.08	108.68	113.00
50	G	201	8Q1	C6-C1-S44	6.65	121.20	113.46
49	C	303	UQ	C22-C23-C24	-5.99	113.24	127.66
49	C	303	UQ	C12-C13-C14	-5.97	113.28	127.66
50	X	201	8Q1	C6-C1-S44	5.97	120.41	113.46
49	J	403	UQ	C12-C13-C14	-5.89	113.48	127.66
57	w	401	ADP	C5-C4-N3	-5.87	119.09	126.75
49	J	403	UQ	C17-C18-C19	-5.84	113.59	127.66
51	J	402	NDP	C5A-C4A-N3A	-5.83	119.15	126.75
49	C	303	UQ	C17-C18-C19	-5.67	114.01	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	J	402	NDP	C1D-N1N-C6N	-5.49	109.00	120.83
48	C	302	970	C06-C05-C04	5.49	106.37	101.45
49	J	403	UQ	C10-C9-C8	-4.71	111.58	123.68
57	w	401	ADP	N3-C4-N9	4.56	134.60	127.08
57	w	401	ADP	N3-C2-N1	-4.48	121.59	128.60
49	C	303	UQ	C27-C28-C29	-4.40	112.72	127.75
49	J	403	UQ	C22-C23-C24	-4.35	112.87	127.75
49	C	303	UQ	C10-C9-C8	-4.34	112.55	123.68
49	C	303	UQ	C25-C24-C23	-4.31	112.63	123.68
55	N	202	CDL	OA6-CA5-C11	4.28	120.73	111.50
55	N	202	CDL	OB6-CB5-C51	4.16	120.46	111.50
55	k	101	CDL	OA6-CA5-C11	4.13	120.40	111.50
49	J	403	UQ	C11-C9-C8	-4.12	112.79	121.12
55	k	101	CDL	OB6-CB5-C51	4.10	120.34	111.50
47	l	701	PEE	O2-C10-C11	4.08	120.29	111.50
47	r	501	PEE	O2-C10-C11	4.08	120.29	111.50
55	a	201	CDL	OB6-CB5-C51	4.07	120.28	111.50
51	J	402	NDP	N3A-C4A-N9A	4.07	133.78	127.08
48	C	302	970	C01-C02-C03	-4.03	111.68	121.38
55	V	202	CDL	OA6-CA5-C11	4.02	120.17	111.50
49	J	403	UQ	C16-C14-C13	-4.02	112.98	121.12
49	J	403	UQ	C21-C19-C18	-4.02	112.98	121.12
55	V	201	CDL	OA6-CA5-C11	4.02	120.16	111.50
47	W	201	PEE	O2-C10-C11	4.01	120.14	111.50
55	l	702	CDL	OB6-CB5-C51	4.01	120.14	111.50
49	C	303	UQ	C20-C19-C18	-4.00	113.42	123.68
55	l	703	CDL	OB6-CB5-C51	3.99	120.11	111.50
49	C	303	UQ	C26-C24-C23	-3.99	113.04	121.12
55	l	702	CDL	OA6-CA5-C11	3.98	120.08	111.50
55	V	201	CDL	OB6-CB5-C51	3.97	120.05	111.50
55	n	101	CDL	OA6-CA5-C11	3.96	120.03	111.50
55	l	703	CDL	OA6-CA5-C11	3.95	120.02	111.50
51	J	402	NDP	N3A-C2A-N1A	-3.94	122.44	128.60
47	B	303	PEE	O2-C10-C11	3.94	119.98	111.50
47	j	202	PEE	O2-C10-C11	3.94	119.98	111.50
49	J	403	UQ	C15-C14-C13	-3.93	113.59	123.68
55	V	202	CDL	OB6-CB5-C51	3.93	119.97	111.50
47	J	401	PEE	O2-C10-C11	3.91	119.92	111.50
49	C	303	UQ	C21-C19-C18	-3.89	113.24	121.12
55	r	503	CDL	OA6-CA5-C11	3.88	119.86	111.50
47	j	201	PEE	O2-C10-C11	3.86	119.83	111.50
48	C	302	970	O08-C07-C09	3.84	131.68	123.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	r	503	CDL	OB6-CB5-C51	3.83	119.76	111.50
55	n	101	CDL	OB6-CB5-C51	3.83	119.75	111.50
47	l	704	PEE	O2-C10-C11	3.82	119.72	111.50
49	J	403	UQ	C20-C19-C18	-3.79	113.95	123.68
57	w	401	ADP	C2-N3-C4	3.74	120.59	111.75
50	G	201	8Q1	O4-C1-C6	-3.72	119.59	123.99
57	w	401	ADP	N9-C8-N7	-3.71	108.84	113.91
51	J	402	NDP	C2A-N3A-C4A	3.70	120.50	111.75
55	a	201	CDL	OA6-CA5-C11	3.70	119.47	111.50
49	C	303	UQ	C15-C14-C13	-3.67	114.26	123.68
49	C	303	UQ	C11-C9-C8	-3.66	113.71	121.12
47	l	705	PEE	O2-C10-C11	3.66	119.38	111.50
50	X	201	8Q1	O4-C1-C6	-3.60	119.74	123.99
48	C	302	970	C04-C02-C03	-3.56	112.28	120.31
57	w	401	ADP	C5-N7-C8	3.54	108.53	103.51
49	C	303	UQ	C30-C29-C28	-3.41	112.79	122.65
48	C	302	970	C22-C23-C14	3.35	114.25	109.56
49	J	403	UQ	C25-C24-C23	-3.33	113.02	122.65
48	C	302	970	C09-C07-C06	-3.33	119.64	123.20
49	J	403	UQ	C7-C6-C1	3.28	122.43	118.48
55	n	101	CDL	OA8-CA7-C31	3.27	119.95	111.38
48	C	302	970	C05-C04-C02	-3.26	110.84	115.62
49	C	303	UQ	C31-C29-C28	-3.26	113.22	122.65
51	J	402	NDP	C5A-N7A-C8A	3.26	108.14	103.51
57	w	401	ADP	C4-N9-C8	3.20	109.19	105.73
49	J	403	UQ	C26-C24-C23	-3.19	113.43	122.65
51	J	402	NDP	N9A-C8A-N7A	-3.12	109.65	113.91
49	C	303	UQ	C16-C14-C13	-3.05	114.94	121.12
51	J	402	NDP	C4A-C5A-N7A	-3.02	106.94	110.62
47	B	303	PEE	O3-C30-C31	3.01	121.35	111.91
50	X	201	8Q1	C37-C38-C39	3.00	117.36	112.36
48	C	302	970	O28-C19-C20	2.98	119.57	115.41
48	C	302	970	O26-C20-C19	2.97	119.55	115.41
48	C	302	970	O13-C14-C23	2.89	115.32	112.40
57	w	401	ADP	C4-C5-N7	-2.87	107.13	110.62
46	A	502	FMN	C4A-C10-N1	-2.80	118.24	124.73
49	J	403	UQ	CM5-C5-C6	-2.76	119.91	124.40
55	V	202	CDL	OB8-CB7-C71	2.74	120.51	111.91
55	N	202	CDL	OA8-CA7-C31	2.72	120.43	111.91
55	l	702	CDL	OA8-CA7-C31	2.71	120.43	111.91
55	n	101	CDL	OB8-CB7-C71	2.69	120.34	111.91
47	j	202	PEE	O3-C30-C31	2.68	120.33	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	l	704	PEE	O3-C30-C31	2.68	120.33	111.91
47	r	501	PEE	O3-C30-C31	2.68	120.32	111.91
47	J	401	PEE	O3-C30-C31	2.68	120.31	111.91
55	l	703	CDL	OB8-CB7-C71	2.67	120.30	111.91
55	V	201	CDL	OB8-CB7-C71	2.67	120.30	111.91
55	a	201	CDL	OB8-CB7-C71	2.66	120.26	111.91
47	W	201	PEE	O3-C30-C31	2.64	120.19	111.91
55	k	101	CDL	OB8-CB7-C71	2.64	120.18	111.91
47	j	201	PEE	O3-C30-C31	2.63	120.18	111.91
47	l	705	PEE	O3-C30-C31	2.63	120.17	111.91
55	l	702	CDL	OB8-CB7-C71	2.63	120.17	111.91
55	N	202	CDL	OB8-CB7-C71	2.63	120.15	111.91
50	G	201	8Q1	O4-C1-S44	-2.62	119.21	122.61
55	r	503	CDL	OB8-CB7-C71	2.62	120.12	111.91
55	l	703	CDL	OA8-CA7-C31	2.60	120.07	111.91
55	r	503	CDL	OA8-CA7-C31	2.57	119.96	111.91
47	l	701	PEE	O3-C30-C31	2.56	119.95	111.91
50	G	201	8Q1	C38-C39-N41	2.56	120.73	116.42
55	k	101	CDL	OA8-CA7-C31	2.53	119.85	111.91
55	V	202	CDL	OA8-CA7-C31	2.53	119.85	111.91
52	g	201	PLX	C1A-N1-C1	2.50	120.16	109.92
55	a	201	CDL	OA8-CA7-C31	2.49	119.72	111.91
49	C	303	UQ	CM5-C5-C6	-2.45	120.40	124.40
51	J	402	NDP	C2B-C3B-C4B	2.45	107.31	101.99
55	V	201	CDL	OA8-CA7-C31	2.44	119.56	111.91
46	A	502	FMN	C4-C4A-N5	2.44	121.70	118.23
52	r	502	PLX	C1A-N1-C1	2.39	119.69	109.92
52	a	202	PLX	C1A-N1-C1	2.39	119.68	109.92
48	C	302	970	C21-C22-C17	2.35	120.39	117.06
57	w	401	ADP	PA-O3A-PB	-2.34	124.78	132.83
52	j	203	PLX	C1A-N1-C1	2.34	119.50	109.92
51	J	402	NDP	PN-O3-PA	-2.33	124.83	132.83
48	C	302	970	O28-C19-C18	-2.33	120.11	124.12
50	X	201	8Q1	C43-S44-C1	2.30	109.02	101.87
50	G	201	8Q1	C37-C38-C39	2.29	116.17	112.36
46	A	502	FMN	O4-C4-C4A	-2.28	120.55	126.60
51	J	402	NDP	C4A-N9A-C8A	2.27	108.19	105.73
52	J	404	PLX	C1A-N1-C1	2.26	119.17	109.92
46	A	502	FMN	C10-N1-C2	2.26	121.41	116.90
48	C	302	970	C11-C12-C06	-2.23	119.56	123.16
46	A	502	FMN	C4A-C4-N3	2.19	118.74	113.19
48	C	302	970	O16-C17-C22	-2.18	120.39	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	502	FMN	O2-C2-N1	-2.15	118.27	121.83
51	J	402	NDP	C2B-C1B-N9A	-2.14	109.92	113.53
48	C	302	970	C01-C02-C04	-2.14	111.51	116.47
50	X	201	8Q1	O4-C1-S44	-2.12	119.86	122.61
52	e	201	PLX	C1A-N1-C1	2.11	118.55	109.92
48	C	302	970	C21-C22-C23	-2.11	117.16	121.17
46	A	502	FMN	C4-N3-C2	-2.10	121.76	125.64
48	C	302	970	C07-C06-C12	2.03	120.73	118.74
48	C	302	970	C29-O28-C19	-2.02	114.47	117.53
57	w	401	ADP	C2'-C3'-C4'	2.02	106.57	102.64
50	X	201	8Q1	C38-C39-N41	2.01	119.81	116.42
48	C	302	970	O26-C20-C21	-2.01	120.67	124.12
46	A	502	FMN	C5A-C9A-N10	2.01	120.03	117.95

There are no chirality outliers.

All (940) 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'
47	B	303	PEE	C11-C10-O2-C2
47	W	201	PEE	C1-O3P-P-O2P
47	W	201	PEE	C1-O3P-P-O1P
47	W	201	PEE	C4-O4P-P-O2P
47	W	201	PEE	O4P-C4-C5-N
47	j	201	PEE	C17-C18-C19-C20
47	j	201	PEE	C1-O3P-P-O1P
47	j	202	PEE	C4-O4P-P-O2P
47	j	202	PEE	C4-O4P-P-O1P
47	l	701	PEE	C1-O3P-P-O1P
47	l	704	PEE	C4-O4P-P-O3P
47	l	705	PEE	C1-O3P-P-O1P
47	r	501	PEE	C1-O3P-P-O2P
47	r	501	PEE	C1-O3P-P-O1P
48	C	302	970	C03-C02-C04-C05
48	C	302	970	C03-C02-C04-O08
49	C	303	UQ	C7-C8-C9-C11
49	C	303	UQ	C17-C18-C19-C21
49	C	303	UQ	C18-C19-C21-C22
49	C	303	UQ	C22-C23-C24-C26
49	J	403	UQ	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
49	J	403	UQ	C5-C6-C7-C8
49	J	403	UQ	C7-C8-C9-C10
49	J	403	UQ	C12-C13-C14-C16
49	J	403	UQ	C14-C16-C17-C18
50	G	201	8Q1	C28-C29-C32-C34
50	G	201	8Q1	C30-C29-C32-C34
50	G	201	8Q1	C30-C29-C32-O33
50	G	201	8Q1	C31-C29-C32-C34
50	G	201	8Q1	O33-C32-C34-N36
50	G	201	8Q1	C42-C43-S44-C1
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	C31-C29-C32-C34
50	X	201	8Q1	O33-C32-C34-N36
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	402	NDP	C5B-O5B-PA-O1A
51	J	402	NDP	O4B-C4B-C5B-O5B
51	J	402	NDP	C2N-C3N-C7N-N7N
52	J	404	PLX	O7-C6-C7-C8
52	J	404	PLX	O7-C6-O6-C4
52	J	404	PLX	C3-C4-O6-C6
52	N	201	PLX	C2-O1-P1-O4
52	N	201	PLX	N1-C1-C2-O1
52	a	202	PLX	O7-C6-O6-C4
52	a	202	PLX	C3-O4-P1-O2
52	a	202	PLX	C3-O4-P1-O3
52	a	202	PLX	C2-O1-P1-O4
52	a	202	PLX	C2-O1-P1-O2
52	a	202	PLX	C2-O1-P1-O3
52	e	201	PLX	O7-C6-O6-C4
52	e	201	PLX	O9-C24-O8-C5
52	g	201	PLX	O7-C6-O6-C4
52	g	201	PLX	C3-O4-P1-O2
52	g	201	PLX	C2-O1-P1-O4
52	g	201	PLX	C2-O1-P1-O2
52	g	201	PLX	C2-O1-P1-O3
52	j	203	PLX	O7-C6-C7-C8
52	j	203	PLX	C2-O1-P1-O2
52	j	203	PLX	O9-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
52	r	502	PLX	O6-C6-C7-C8
52	r	502	PLX	O9-C24-C25-C26
55	N	202	CDL	O1-C1-CB2-OB2
55	N	202	CDL	C11-CA5-OA6-CA4
55	N	202	CDL	CB2-OB2-PB2-OB3
55	N	202	CDL	CB3-OB5-PB2-OB3
55	V	201	CDL	O1-C1-CA2-OA2
55	V	201	CDL	CA2-OA2-PA1-OA3
55	V	201	CDL	CA2-OA2-PA1-OA4
55	V	201	CDL	CA2-OA2-PA1-OA5
55	V	201	CDL	OA7-CA5-OA6-CA4
55	V	201	CDL	CB2-OB2-PB2-OB3
55	V	201	CDL	CB2-OB2-PB2-OB4
55	V	201	CDL	CB3-OB5-PB2-OB4
55	V	202	CDL	CA2-C1-CB2-OB2
55	V	202	CDL	OA6-CA4-CA6-OA8
55	V	202	CDL	CB2-OB2-PB2-OB3
55	V	202	CDL	CB3-OB5-PB2-OB3
55	V	202	CDL	CB3-OB5-PB2-OB4
55	V	202	CDL	OB6-CB4-CB6-OB8
55	a	201	CDL	CB2-OB2-PB2-OB3
55	a	201	CDL	CB2-OB2-PB2-OB4
55	a	201	CDL	CB3-OB5-PB2-OB3
55	a	201	CDL	CB3-OB5-PB2-OB4
55	a	201	CDL	C51-CB5-OB6-CB4
55	k	101	CDL	CA2-OA2-PA1-OA3
55	k	101	CDL	CA3-OA5-PA1-OA2
55	k	101	CDL	CA3-OA5-PA1-OA3
55	k	101	CDL	CA3-OA5-PA1-OA4
55	k	101	CDL	CB2-OB2-PB2-OB3
55	k	101	CDL	CB2-OB2-PB2-OB4
55	k	101	CDL	CB3-OB5-PB2-OB2
55	k	101	CDL	CB3-OB5-PB2-OB3
55	k	101	CDL	CB3-OB5-PB2-OB4
55	l	702	CDL	O1-C1-CA2-OA2
55	l	702	CDL	OA6-CA4-CA6-OA8
55	l	702	CDL	OA9-CA7-OA8-CA6
55	l	702	CDL	C31-CA7-OA8-CA6
55	l	702	CDL	CB2-OB2-PB2-OB4
55	l	702	CDL	CB3-OB5-PB2-OB3
55	l	703	CDL	O1-C1-CB2-OB2
55	l	703	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
55	l	703	CDL	CB2-OB2-PB2-OB4
55	l	703	CDL	CB3-OB5-PB2-OB3
55	l	703	CDL	CB3-OB5-PB2-OB4
55	n	101	CDL	CB2-C1-CA2-OA2
55	n	101	CDL	CA2-OA2-PA1-OA4
55	n	101	CDL	OA5-CA3-CA4-OA6
55	n	101	CDL	CB2-OB2-PB2-OB3
55	n	101	CDL	CB2-OB2-PB2-OB4
55	n	101	CDL	CB2-OB2-PB2-OB5
55	n	101	CDL	CB3-OB5-PB2-OB2
55	n	101	CDL	CB3-OB5-PB2-OB4
55	r	503	CDL	CB2-C1-CA2-OA2
55	r	503	CDL	CA2-OA2-PA1-OA3
55	r	503	CDL	CA3-OA5-PA1-OA3
55	r	503	CDL	CB3-OB5-PB2-OB3
55	r	503	CDL	C51-CB5-OB6-CB4
57	w	401	ADP	C5'-O5'-PA-O1A
57	w	401	ADP	C5'-O5'-PA-O2A
57	w	401	ADP	C5'-O5'-PA-O3A
47	B	303	PEE	O4-C10-O2-C2
47	J	401	PEE	O4-C10-O2-C2
47	j	201	PEE	O4-C10-O2-C2
47	l	704	PEE	O4-C10-O2-C2
55	N	202	CDL	OA7-CA5-OA6-CA4
55	r	503	CDL	OB7-CB5-OB6-CB4
47	J	401	PEE	C11-C10-O2-C2
47	j	201	PEE	C11-C10-O2-C2
55	V	201	CDL	C11-CA5-OA6-CA4
47	l	704	PEE	C31-C30-O3-C3
47	l	705	PEE	C31-C30-O3-C3
55	V	201	CDL	C31-CA7-OA8-CA6
55	l	703	CDL	C71-CB7-OB8-CB6
47	l	705	PEE	C37-C38-C39-C40
47	r	501	PEE	C17-C18-C19-C20
49	C	303	UQ	C7-C8-C9-C10
55	a	201	CDL	OB7-CB5-OB6-CB4
47	l	705	PEE	O5-C30-O3-C3
55	N	202	CDL	O1-C1-CA2-OA2
55	l	702	CDL	O1-C1-CB2-OB2
55	n	101	CDL	O1-C1-CA2-OA2
55	n	101	CDL	O1-C1-CB2-OB2
55	r	503	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
47	l	704	PEE	O5-C30-O3-C3
47	j	202	PEE	C11-C10-O2-C2
47	l	701	PEE	C11-C10-O2-C2
47	l	704	PEE	C11-C10-O2-C2
52	J	404	PLX	C27-C28-C29-C30
55	V	202	CDL	C37-C38-C39-C40
52	r	502	PLX	C7-C8-C9-C10
55	n	101	CDL	C71-C72-C73-C74
52	J	404	PLX	C25-C26-C27-C28
52	g	201	PLX	C11-C10-C9-C8
52	r	502	PLX	C9-C10-C11-C12
55	V	201	CDL	C62-C63-C64-C65
55	V	201	CDL	OA9-CA7-OA8-CA6
55	l	703	CDL	OB9-CB7-OB8-CB6
49	J	403	UQ	C22-C23-C24-C26
49	J	403	UQ	C13-C14-C16-C17
52	g	201	PLX	C10-C11-C12-C13
49	C	303	UQ	C14-C16-C17-C18
52	N	201	PLX	C25-C26-C27-C28
49	C	303	UQ	C27-C28-C29-C31
47	l	701	PEE	C11-C12-C13-C14
52	j	203	PLX	C28-C29-C30-C31
55	N	202	CDL	CA2-C1-CB2-OB2
55	a	201	CDL	CA2-C1-CB2-OB2
55	k	101	CDL	CB2-C1-CA2-OA2
55	l	702	CDL	CA2-C1-CB2-OB2
55	l	703	CDL	CA2-C1-CB2-OB2
55	n	101	CDL	CA2-C1-CB2-OB2
47	j	202	PEE	O4-C10-O2-C2
47	j	201	PEE	C31-C30-O3-C3
47	l	701	PEE	C31-C30-O3-C3
55	r	503	CDL	C71-CB7-OB8-CB6
52	j	203	PLX	C13-C14-C15-C16
55	V	202	CDL	C11-C12-C13-C14
55	l	702	CDL	C81-C82-C83-C84
55	l	703	CDL	C17-C18-C19-C20
55	V	202	CDL	CB7-C71-C72-C73
55	l	703	CDL	CA7-C31-C32-C33
55	l	703	CDL	CB5-C51-C52-C53
52	j	203	PLX	C32-C33-C34-C35
55	l	703	CDL	C39-C40-C41-C42
55	l	703	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
55	V	202	CDL	O1-C1-CB2-OB2
55	k	101	CDL	O1-C1-CA2-OA2
55	N	202	CDL	CB7-C71-C72-C73
52	g	201	PLX	O6-C4-C5-O8
55	l	703	CDL	C12-C13-C14-C15
55	l	703	CDL	C35-C36-C37-C38
47	l	701	PEE	O5-C30-O3-C3
47	l	701	PEE	O4-C10-O2-C2
47	r	501	PEE	C12-C13-C14-C15
55	N	202	CDL	CA7-C31-C32-C33
55	V	201	CDL	CA7-C31-C32-C33
55	a	201	CDL	CA5-C11-C12-C13
55	r	503	CDL	OB9-CB7-OB8-CB6
55	V	201	CDL	C34-C35-C36-C37
55	a	201	CDL	C71-CB7-OB8-CB6
52	r	502	PLX	C31-C32-C33-C34
47	W	201	PEE	C10-C11-C12-C13
55	V	201	CDL	CB7-C71-C72-C73
47	B	303	PEE	C34-C35-C36-C37
47	l	701	PEE	C10-C11-C12-C13
55	l	702	CDL	CA7-C31-C32-C33
55	l	702	CDL	CB7-C71-C72-C73
55	n	101	CDL	CB7-C71-C72-C73
55	r	503	CDL	CB7-C71-C72-C73
47	J	401	PEE	C30-C31-C32-C33
55	n	101	CDL	CB5-C51-C52-C53
47	r	501	PEE	C41-C42-C43-C44
55	a	201	CDL	C34-C35-C36-C37
52	g	201	PLX	C17-C18-C19-C20
55	l	702	CDL	C34-C35-C36-C37
55	a	201	CDL	O1-C1-CB2-OB2
55	l	702	CDL	C71-CB7-OB8-CB6
47	j	201	PEE	O5-C30-O3-C3
55	l	703	CDL	C41-C42-C43-C44
47	l	701	PEE	C17-C18-C19-C20
55	V	202	CDL	C57-C58-C59-C60
47	W	201	PEE	C1-O3P-P-O4P
47	W	201	PEE	C4-O4P-P-O3P
47	j	202	PEE	C4-O4P-P-O3P
47	l	701	PEE	C1-O3P-P-O4P
47	l	701	PEE	C4-O4P-P-O3P
47	r	501	PEE	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
52	a	202	PLX	C3-O4-P1-O1
52	j	203	PLX	C3-O4-P1-O1
55	N	202	CDL	CA2-OA2-PA1-OA5
55	V	201	CDL	CB2-OB2-PB2-OB5
55	V	202	CDL	CB2-OB2-PB2-OB5
55	V	202	CDL	CB3-OB5-PB2-OB2
55	a	201	CDL	CB2-OB2-PB2-OB5
55	a	201	CDL	CB3-OB5-PB2-OB2
55	k	101	CDL	CB2-OB2-PB2-OB5
55	l	702	CDL	CB2-OB2-PB2-OB5
55	l	702	CDL	CB3-OB5-PB2-OB2
55	l	703	CDL	CB2-OB2-PB2-OB5
55	l	703	CDL	CB3-OB5-PB2-OB2
55	n	101	CDL	CA2-OA2-PA1-OA5
55	r	503	CDL	CA3-OA5-PA1-OA2
55	r	503	CDL	CB2-OB2-PB2-OB5
51	J	402	NDP	C2D-C1D-N1N-C6N
55	V	201	CDL	C71-CB7-OB8-CB6
55	l	703	CDL	CA5-C11-C12-C13
55	N	202	CDL	CB2-C1-CA2-OA2
55	V	201	CDL	CB2-C1-CA2-OA2
55	l	702	CDL	CB2-C1-CA2-OA2
55	r	503	CDL	C51-C52-C53-C54
47	W	201	PEE	C31-C30-O3-C3
55	l	703	CDL	C61-C62-C63-C64
52	j	203	PLX	O6-C6-C7-C8
47	W	201	PEE	C11-C12-C13-C14
52	j	203	PLX	C7-C8-C9-C10
55	V	201	CDL	C51-CB5-OB6-CB4
47	J	401	PEE	C42-C43-C44-C45
52	g	201	PLX	C14-C15-C16-C17
52	g	201	PLX	C25-C26-C27-C28
55	V	201	CDL	C17-C18-C19-C20
55	V	202	CDL	C55-C56-C57-C58
52	a	202	PLX	C28-C29-C30-C31
52	e	201	PLX	C13-C14-C15-C16
52	e	201	PLX	C10-C11-C12-C13
52	j	203	PLX	C11-C12-C13-C14
55	V	201	CDL	C56-C57-C58-C59
55	V	202	CDL	C14-C15-C16-C17
55	V	202	CDL	C52-C53-C54-C55
55	l	702	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
55	n	101	CDL	C55-C56-C57-C58
55	V	201	CDL	OB7-CB5-OB6-CB4
47	l	704	PEE	C30-C31-C32-C33
47	l	705	PEE	C22-C23-C24-C25
52	J	404	PLX	C26-C27-C28-C29
55	l	703	CDL	C32-C33-C34-C35
55	r	503	CDL	C31-C32-C33-C34
55	a	201	CDL	OB9-CB7-OB8-CB6
55	l	702	CDL	OA5-CA3-CA4-OA6
47	B	303	PEE	C17-C18-C19-C20
52	J	404	PLX	C9-C10-C11-C12
52	J	404	PLX	C31-C32-C33-C34
52	J	404	PLX	C34-C35-C36-C37
52	a	202	PLX	C9-C10-C11-C12
52	j	203	PLX	C25-C26-C27-C28
55	V	202	CDL	C17-C18-C19-C20
55	a	201	CDL	C35-C36-C37-C38
55	l	702	CDL	C59-C60-C61-C62
55	l	703	CDL	C74-C75-C76-C77
55	r	503	CDL	C32-C33-C34-C35
55	r	503	CDL	C80-C81-C82-C83
55	V	202	CDL	O1-C1-CA2-OA2
55	N	202	CDL	C71-C72-C73-C74
55	a	201	CDL	C17-C18-C19-C20
55	l	702	CDL	C71-C72-C73-C74
55	n	101	CDL	C52-C53-C54-C55
55	n	101	CDL	C73-C74-C75-C76
47	l	705	PEE	C14-C15-C16-C17
52	g	201	PLX	C9-C10-C11-C12
55	V	201	CDL	C35-C36-C37-C38
55	V	201	CDL	C37-C38-C39-C40
55	V	202	CDL	C12-C13-C14-C15
55	a	201	CDL	C62-C63-C64-C65
55	l	702	CDL	C35-C36-C37-C38
55	l	702	CDL	C52-C53-C54-C55
55	l	702	CDL	C62-C63-C64-C65
55	r	503	CDL	C73-C74-C75-C76
47	l	701	PEE	C32-C33-C34-C35
52	g	201	PLX	C7-C8-C9-C10
55	V	201	CDL	C55-C56-C57-C58
55	V	202	CDL	C41-C42-C43-C44
55	V	202	CDL	C82-C83-C84-C85

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Mol	Chain	Res	Type	Atoms
47	J	401	PEE	C32-C33-C34-C35
52	a	202	PLX	C33-C34-C35-C36
52	e	201	PLX	C14-C15-C16-C17
52	e	201	PLX	C28-C29-C30-C31
52	j	203	PLX	C18-C19-C20-C21
55	a	201	CDL	C22-C23-C24-C25
55	l	703	CDL	C75-C76-C77-C78
55	l	702	CDL	OB9-CB7-OB8-CB6
47	j	202	PEE	C12-C13-C14-C15
52	N	201	PLX	C10-C11-C12-C13
52	a	202	PLX	C13-C14-C15-C16
52	r	502	PLX	C14-C15-C16-C17
47	J	401	PEE	C33-C34-C35-C36
52	J	404	PLX	C13-C14-C15-C16
52	g	201	PLX	C32-C33-C34-C35
52	j	203	PLX	C16-C17-C18-C19
52	r	502	PLX	C11-C10-C9-C8
55	a	201	CDL	C32-C33-C34-C35
47	j	202	PEE	C30-C31-C32-C33
55	V	202	CDL	CA7-C31-C32-C33
47	W	201	PEE	C12-C13-C14-C15
47	j	201	PEE	C21-C22-C23-C24
47	j	202	PEE	C14-C15-C16-C17
47	l	705	PEE	C33-C34-C35-C36
52	J	404	PLX	C28-C29-C30-C31
52	e	201	PLX	C25-C26-C27-C28
52	j	203	PLX	C14-C15-C16-C17
52	j	203	PLX	C33-C34-C35-C36
55	V	201	CDL	C38-C39-C40-C41
55	V	202	CDL	C36-C37-C38-C39
55	V	202	CDL	C61-C62-C63-C64
55	l	702	CDL	C11-C12-C13-C14
55	l	702	CDL	C56-C57-C58-C59
55	r	503	CDL	C52-C53-C54-C55
55	N	202	CDL	C11-C12-C13-C14
55	a	201	CDL	C23-C24-C25-C26
55	l	702	CDL	C37-C38-C39-C40
55	r	503	CDL	C14-C15-C16-C17
47	J	401	PEE	C34-C35-C36-C37
47	j	202	PEE	C23-C24-C25-C26
52	J	404	PLX	C16-C17-C18-C19
52	g	201	PLX	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	C82-C83-C84-C85
55	l	702	CDL	C75-C76-C77-C78
55	l	702	CDL	C82-C83-C84-C85
55	V	201	CDL	OB9-CB7-OB8-CB6
47	r	501	PEE	C32-C33-C34-C35
52	J	404	PLX	C11-C12-C13-C14
52	j	203	PLX	C10-C11-C12-C13
55	V	201	CDL	C11-C12-C13-C14
55	V	201	CDL	C52-C53-C54-C55
55	V	201	CDL	C74-C75-C76-C77
47	j	202	PEE	C11-C12-C13-C14
47	l	704	PEE	C21-C22-C23-C24
55	V	202	CDL	C59-C60-C61-C62
47	B	303	PEE	C23-C24-C25-C26
47	B	303	PEE	C14-C15-C16-C17
47	B	303	PEE	C11-C12-C13-C14
47	l	704	PEE	C31-C32-C33-C34
52	g	201	PLX	C30-C31-C32-C33
55	r	503	CDL	C55-C56-C57-C58
47	l	705	PEE	C31-C32-C33-C34
52	r	502	PLX	C27-C28-C29-C30
55	r	503	CDL	C41-C42-C43-C44
55	V	201	CDL	CB3-CB4-CB6-OB8
50	X	201	8Q1	C6-C7-C8-C9
55	V	201	CDL	C75-C76-C77-C78
55	r	503	CDL	C43-C44-C45-C46
52	a	202	PLX	C25-C26-C27-C28
52	g	201	PLX	O9-C24-C25-C26
52	r	502	PLX	O7-C6-C7-C8
47	l	701	PEE	C13-C14-C15-C16
52	a	202	PLX	C27-C28-C29-C30
55	V	201	CDL	C78-C79-C80-C81
55	n	101	CDL	C56-C57-C58-C59
47	J	401	PEE	C19-C20-C21-C22
47	l	701	PEE	C35-C36-C37-C38
47	l	704	PEE	C39-C40-C41-C42
52	J	404	PLX	C30-C31-C32-C33
52	r	502	PLX	C12-C13-C14-C15
55	N	202	CDL	C51-C52-C53-C54
55	l	702	CDL	C73-C74-C75-C76
47	B	303	PEE	C20-C21-C22-C23
47	l	704	PEE	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
55	V	201	CDL	C51-C52-C53-C54
55	k	101	CDL	C13-C14-C15-C16
55	r	503	CDL	C11-C12-C13-C14
47	W	201	PEE	O5-C30-O3-C3
52	e	201	PLX	C11-C12-C13-C14
55	a	201	CDL	C75-C76-C77-C78
55	l	703	CDL	C11-C12-C13-C14
52	g	201	PLX	C2-C1-N1-C1A
47	B	303	PEE	C21-C22-C23-C24
55	V	201	CDL	C33-C34-C35-C36
47	r	501	PEE	C11-C10-O2-C2
52	a	202	PLX	C11-C12-C13-C14
52	a	202	PLX	C10-C11-C12-C13
55	V	202	CDL	C15-C16-C17-C18
55	n	101	CDL	C54-C55-C56-C57
52	g	201	PLX	C28-C29-C30-C31
55	l	703	CDL	C64-C65-C66-C67
55	k	101	CDL	CA5-C11-C12-C13
52	J	404	PLX	C7-C8-C9-C10
52	a	202	PLX	C7-C8-C9-C10
47	J	401	PEE	C13-C14-C15-C16
55	a	201	CDL	C18-C19-C20-C21
55	k	101	CDL	C16-C17-C18-C19
52	e	201	PLX	C27-C28-C29-C30
47	l	704	PEE	C10-C11-C12-C13
47	l	705	PEE	C30-C31-C32-C33
52	a	202	PLX	C30-C31-C32-C33
55	V	201	CDL	C44-C45-C46-C47
55	V	202	CDL	C35-C36-C37-C38
55	l	703	CDL	C56-C57-C58-C59
55	l	703	CDL	C73-C74-C75-C76
52	J	404	PLX	C33-C34-C35-C36
55	a	201	CDL	C60-C61-C62-C63
47	W	201	PEE	C21-C22-C23-C24
55	a	201	CDL	C71-C72-C73-C74
55	r	503	CDL	C62-C63-C64-C65
47	j	202	PEE	C10-C11-C12-C13
55	V	202	CDL	C51-CB5-OB6-CB4
55	l	702	CDL	C11-CA5-OA6-CA4
47	l	704	PEE	O3P-C1-C2-O2
55	k	101	CDL	OA5-CA3-CA4-OA6
55	V	201	CDL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
49	C	303	UQ	C27-C28-C29-C30
47	r	501	PEE	O4-C10-O2-C2
55	V	202	CDL	OB7-CB5-OB6-CB4
55	V	201	CDL	C59-C60-C61-C62
55	V	201	CDL	OB6-CB4-CB6-OB8
52	e	201	PLX	C11-C10-C9-C8
52	j	203	PLX	C27-C28-C29-C30
52	j	203	PLX	C30-C31-C32-C33
55	l	702	CDL	C74-C75-C76-C77
55	r	503	CDL	C37-C38-C39-C40
47	B	303	PEE	C35-C36-C37-C38
47	r	501	PEE	C15-C16-C17-C18
47	r	501	PEE	C39-C40-C41-C42
49	C	303	UQ	C13-C14-C16-C17
55	V	201	CDL	C53-C54-C55-C56
55	n	101	CDL	C51-C52-C53-C54
51	J	402	NDP	O4D-C4D-C5D-O5D
52	a	202	PLX	C34-C35-C36-C37
55	V	202	CDL	C75-C76-C77-C78
52	r	502	PLX	C16-C17-C18-C19
47	l	701	PEE	C33-C34-C35-C36
52	e	201	PLX	C9-C10-C11-C12
52	g	201	PLX	C18-C19-C20-C21
52	j	203	PLX	C31-C32-C33-C34
46	A	502	FMN	O2'-C2'-C3'-C4'
47	j	201	PEE	C4-O4P-P-O3P
52	j	203	PLX	C2-O1-P1-O4
55	N	202	CDL	CB3-OB5-PB2-OB2
55	r	503	CDL	CA2-OA2-PA1-OA5
55	r	503	CDL	CB3-OB5-PB2-OB2
52	g	201	PLX	C27-C28-C29-C30
52	r	502	PLX	C10-C11-C12-C13
55	V	201	CDL	C14-C15-C16-C17
55	V	201	CDL	C73-C74-C75-C76
47	j	202	PEE	O3P-C1-C2-C3
52	J	404	PLX	O4-C3-C4-C5
55	N	202	CDL	OA5-CA3-CA4-CA6
55	k	101	CDL	OA5-CA3-CA4-CA6
55	l	702	CDL	OA5-CA3-CA4-CA6
55	n	101	CDL	OA5-CA3-CA4-CA6
52	e	201	PLX	C32-C33-C34-C35
55	V	202	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
55	l	702	CDL	C24-C25-C26-C27
52	g	201	PLX	C13-C14-C15-C16
47	l	704	PEE	C42-C43-C44-C45
47	B	303	PEE	C15-C16-C17-C18
47	l	704	PEE	C15-C16-C17-C18
55	l	702	CDL	OA7-CA5-OA6-CA4
55	V	202	CDL	C74-C75-C76-C77
52	e	201	PLX	C30-C31-C32-C33
55	l	703	CDL	C59-C60-C61-C62
47	J	401	PEE	C1-C2-C3-O3
47	W	201	PEE	C1-C2-C3-O3
47	l	705	PEE	C1-C2-C3-O3
52	g	201	PLX	C3-C4-C5-O8
55	V	201	CDL	CA3-CA4-CA6-OA8
55	V	202	CDL	CB3-CB4-CB6-OB8
55	k	101	CDL	C79-C80-C81-C82
55	l	702	CDL	CA3-CA4-CA6-OA8
55	V	202	CDL	CB5-C51-C52-C53
55	r	503	CDL	C17-C18-C19-C20
52	r	502	PLX	O8-C24-C25-C26
50	G	201	8Q1	O33-C32-C34-O35
50	X	201	8Q1	O33-C32-C34-O35
47	W	201	PEE	C24-C25-C26-C27
47	l	705	PEE	C13-C14-C15-C16
55	r	503	CDL	C15-C16-C17-C18
47	J	401	PEE	C11-C12-C13-C14
47	j	201	PEE	C32-C33-C34-C35
52	e	201	PLX	C18-C19-C20-C21
55	a	201	CDL	C52-C53-C54-C55
47	W	201	PEE	C15-C16-C17-C18
47	j	202	PEE	C19-C20-C21-C22
47	j	202	PEE	C15-C16-C17-C18
55	V	201	CDL	C32-C33-C34-C35
50	G	201	8Q1	O27-C28-C29-C30
50	G	201	8Q1	O27-C28-C29-C31
55	a	201	CDL	C84-C85-C86-C87
52	g	201	PLX	C16-C17-C18-C19
55	k	101	CDL	C14-C15-C16-C17
55	r	503	CDL	C59-C60-C61-C62
55	N	202	CDL	CA6-CA4-OA6-CA5
47	B	303	PEE	O3P-C1-C2-O2
55	k	101	CDL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
55	l	702	CDL	C55-C56-C57-C58
52	J	404	PLX	O6-C4-C5-O8
52	r	502	PLX	O6-C4-C5-O8
55	n	101	CDL	C75-C76-C77-C78
50	G	201	8Q1	C31-C29-C32-O33
50	X	201	8Q1	C30-C29-C32-O33
50	X	201	8Q1	C31-C29-C32-O33
47	r	501	PEE	C24-C25-C26-C27
52	e	201	PLX	C31-C32-C33-C34
52	r	502	PLX	C30-C31-C32-C33
47	j	201	PEE	C36-C37-C38-C39
47	r	501	PEE	C36-C37-C38-C39
47	l	704	PEE	C32-C33-C34-C35
55	l	702	CDL	C53-C54-C55-C56
55	a	201	CDL	C31-C32-C33-C34
55	V	202	CDL	CB2-C1-CA2-OA2
47	r	501	PEE	C40-C41-C42-C43
52	e	201	PLX	C35-C36-C37-C38
55	V	202	CDL	C60-C61-C62-C63
55	l	703	CDL	C44-C45-C46-C47
55	a	201	CDL	C42-C43-C44-C45
52	g	201	PLX	C12-C13-C14-C15
52	g	201	PLX	C2-C1-N1-C1B
47	l	704	PEE	O3P-C1-C2-C3
55	a	201	CDL	OA5-CA3-CA4-CA6
55	l	703	CDL	OB5-CB3-CB4-CB6
55	r	503	CDL	OB5-CB3-CB4-CB6
47	j	202	PEE	O4P-C4-C5-N
50	G	201	8Q1	C29-C32-C34-O35
55	r	503	CDL	C36-C37-C38-C39
55	V	201	CDL	C40-C41-C42-C43
55	a	201	CDL	C15-C16-C17-C18
47	j	201	PEE	C23-C24-C25-C26
55	n	101	CDL	C71-CB7-OB8-CB6
55	l	702	CDL	CB5-C51-C52-C53
55	r	503	CDL	CA5-C11-C12-C13
55	a	201	CDL	C61-C62-C63-C64
55	r	503	CDL	C82-C83-C84-C85
55	r	503	CDL	C1-CB2-OB2-PB2
47	B	303	PEE	C38-C39-C40-C41
47	j	201	PEE	C38-C39-C40-C41
55	a	201	CDL	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
46	A	502	FMN	C2'-C1'-N10-C10
55	V	201	CDL	C54-C55-C56-C57
55	N	202	CDL	C31-CA7-OA8-CA6
47	r	501	PEE	C1-C2-C3-O3
52	a	202	PLX	C3-C4-C5-O8
52	e	201	PLX	C3-C4-C5-O8
52	j	203	PLX	C3-C4-C5-O8
55	r	503	CDL	C12-C13-C14-C15
55	l	702	CDL	C33-C34-C35-C36
47	W	201	PEE	C13-C14-C15-C16
55	a	201	CDL	C14-C15-C16-C17
47	j	201	PEE	C1-O3P-P-O4P
47	l	705	PEE	C1-O3P-P-O4P
52	e	201	PLX	C5-C4-O6-C6
52	g	201	PLX	C5-C4-O6-C6
52	r	502	PLX	C3-C4-O6-C6
55	V	201	CDL	CB3-OB5-PB2-OB2
55	a	201	CDL	CB5-C51-C52-C53
52	a	202	PLX	O9-C24-C25-C26
52	g	201	PLX	O7-C6-C7-C8
47	j	202	PEE	O3P-C1-C2-O2
55	a	201	CDL	OB5-CB3-CB4-OB6
55	l	703	CDL	OB5-CB3-CB4-OB6
46	A	502	FMN	O2'-C2'-C3'-O3'
47	j	201	PEE	C11-C12-C13-C14
52	r	502	PLX	C25-C26-C27-C28
47	W	201	PEE	O2-C2-C3-O3
47	l	701	PEE	O2-C2-C3-O3
52	j	203	PLX	O6-C4-C5-O8
55	N	202	CDL	OB6-CB4-CB6-OB8
55	V	202	CDL	C78-C79-C80-C81
47	W	201	PEE	C11-C10-O2-C2
55	V	201	CDL	C64-C65-C66-C67
55	k	101	CDL	C40-C41-C42-C43
47	l	704	PEE	C13-C14-C15-C16
47	j	201	PEE	C44-C45-C46-C47
55	N	202	CDL	C31-C32-C33-C34
55	a	201	CDL	C54-C55-C56-C57
47	W	201	PEE	O4-C10-O2-C2
55	l	703	CDL	C40-C41-C42-C43
52	e	201	PLX	C16-C17-C18-C19
52	e	201	PLX	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
47	l	701	PEE	C18-C19-C20-C21
47	B	303	PEE	O3P-C1-C2-C3
47	l	701	PEE	O3P-C1-C2-C3
47	r	501	PEE	O3P-C1-C2-C3
55	N	202	CDL	OB5-CB3-CB4-CB6
55	a	201	CDL	OB5-CB3-CB4-CB6
55	l	703	CDL	OA5-CA3-CA4-CA6
47	B	303	PEE	C36-C37-C38-C39
47	r	501	PEE	C38-C39-C40-C41
55	a	201	CDL	C37-C38-C39-C40
52	J	404	PLX	C11-C10-C9-C8
55	a	201	CDL	C40-C41-C42-C43
55	l	702	CDL	C38-C39-C40-C41
55	l	702	CDL	C17-C18-C19-C20
57	w	401	ADP	PA-O3A-PB-O1B
52	g	201	PLX	C2-C1-N1-C1C
55	V	201	CDL	CA6-CA4-OA6-CA5
52	a	202	PLX	C35-C36-C37-C38
47	l	704	PEE	C19-C20-C21-C22
52	j	203	PLX	C7-C6-O6-C4
55	V	202	CDL	CA3-CA4-CA6-OA8
47	l	705	PEE	O3P-C1-C2-O2
47	r	501	PEE	O3P-C1-C2-O2
52	j	203	PLX	O4-C3-C4-O6
55	V	201	CDL	OA5-CA3-CA4-OA6
55	V	202	CDL	OA5-CA3-CA4-OA6
55	a	201	CDL	OA5-CA3-CA4-OA6
55	l	703	CDL	OA5-CA3-CA4-OA6
55	r	503	CDL	OB5-CB3-CB4-OB6
55	V	201	CDL	C32-C31-CA7-OA8
50	G	201	8Q1	C6-C7-C8-C9
52	a	202	PLX	C32-C33-C34-C35
52	r	502	PLX	C11-C12-C13-C14
50	X	201	8Q1	C30-C29-C32-C34
51	J	402	NDP	O4D-C1D-N1N-C6N
55	n	101	CDL	OB9-CB7-OB8-CB6
55	V	202	CDL	C54-C55-C56-C57
47	J	401	PEE	O2-C2-C3-O3
47	l	705	PEE	O2-C2-C3-O3
47	r	501	PEE	O2-C2-C3-O3
52	N	201	PLX	O6-C4-C5-O8
55	V	201	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
55	V	202	CDL	C39-C40-C41-C42
47	j	201	PEE	C42-C43-C44-C45
55	a	201	CDL	C11-C12-C13-C14
55	l	702	CDL	C31-C32-C33-C34
47	l	705	PEE	C11-C10-O2-C2
47	J	401	PEE	C15-C16-C17-C18
55	V	202	CDL	C62-C63-C64-C65
55	N	202	CDL	OA9-CA7-OA8-CA6
47	l	705	PEE	O4-C10-O2-C2
55	V	202	CDL	C64-C65-C66-C67
55	a	201	CDL	C73-C74-C75-C76
55	V	201	CDL	C71-C72-C73-C74
55	l	703	CDL	C62-C63-C64-C65
47	W	201	PEE	C23-C24-C25-C26
50	G	201	8Q1	C13-C14-C15-C16
55	r	503	CDL	C39-C40-C41-C42
55	V	201	CDL	C43-C44-C45-C46
55	l	703	CDL	C36-C37-C38-C39
52	g	201	PLX	C3-O4-P1-O1
55	N	202	CDL	CB2-OB2-PB2-OB5
55	l	702	CDL	CA2-OA2-PA1-OA5
52	a	202	PLX	C11-C10-C9-C8
47	B	303	PEE	C4-O4P-P-O1P
47	J	401	PEE	C1-O3P-P-O2P
47	W	201	PEE	C4-O4P-P-O1P
47	j	201	PEE	C1-O3P-P-O2P
47	j	201	PEE	C4-O4P-P-O2P
47	j	202	PEE	C1-O3P-P-O1P
47	l	701	PEE	C1-O3P-P-O2P
47	l	701	PEE	C4-O4P-P-O2P
47	l	704	PEE	C4-O4P-P-O2P
52	N	201	PLX	C2-O1-P1-O3
52	g	201	PLX	C3-O4-P1-O3
52	j	203	PLX	C3-O4-P1-O2
52	j	203	PLX	C2-O1-P1-O3
55	N	202	CDL	CA2-OA2-PA1-OA4
55	N	202	CDL	CB2-OB2-PB2-OB4
55	N	202	CDL	CB3-OB5-PB2-OB4
55	V	201	CDL	CB3-OB5-PB2-OB3
55	V	202	CDL	CB2-OB2-PB2-OB4
55	l	702	CDL	CB3-OB5-PB2-OB4
55	n	101	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
55	r	503	CDL	CA2-OA2-PA1-OA4
55	r	503	CDL	CB2-OB2-PB2-OB3
55	r	503	CDL	CB2-OB2-PB2-OB4
55	r	503	CDL	CB3-OB5-PB2-OB4
55	l	703	CDL	C15-C16-C17-C18
47	l	705	PEE	O3P-C1-C2-C3
52	e	201	PLX	O4-C3-C4-C5
52	j	203	PLX	O4-C3-C4-C5
55	V	201	CDL	OA5-CA3-CA4-CA6
55	V	202	CDL	OA5-CA3-CA4-CA6
55	V	202	CDL	OB5-CB3-CB4-CB6
55	n	101	CDL	C72-C71-CB7-OB8
55	k	101	CDL	C73-C74-C75-C76
52	g	201	PLX	C33-C34-C35-C36
47	B	303	PEE	C13-C14-C15-C16
52	J	404	PLX	C1-C2-O1-P1
52	J	404	PLX	C25-C24-O8-C5
52	N	201	PLX	C25-C24-O8-C5
52	a	202	PLX	C25-C24-O8-C5
52	g	201	PLX	C25-C24-O8-C5
55	l	703	CDL	C43-C44-C45-C46
55	a	201	CDL	C51-C52-C53-C54
47	J	401	PEE	C12-C13-C14-C15
52	a	202	PLX	C14-C15-C16-C17
47	l	701	PEE	O3P-C1-C2-O2
51	J	402	NDP	C3D-C4D-C5D-O5D
52	J	404	PLX	O4-C3-C4-O6
52	e	201	PLX	O4-C3-C4-O6
55	N	202	CDL	OA5-CA3-CA4-OA6
55	l	702	CDL	C51-CB5-OB6-CB4
47	J	401	PEE	C43-C44-C45-C46
47	j	202	PEE	C1-C2-C3-O3
50	G	201	8Q1	C28-C29-C32-O33
50	X	201	8Q1	O27-C28-C29-C32
50	X	201	8Q1	C28-C29-C32-O33
51	J	402	NDP	C2N-C3N-C7N-O7N
52	J	404	PLX	C3-C4-C5-O8
52	J	404	PLX	N1-C1-C2-O1
52	r	502	PLX	C3-C4-C5-O8
55	l	702	CDL	OB7-CB5-OB6-CB4
47	j	202	PEE	O2-C2-C3-O3
52	e	201	PLX	O6-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
47	j	202	PEE	C24-C25-C26-C27
55	r	503	CDL	C74-C75-C76-C77
47	l	705	PEE	C18-C19-C20-C21
52	J	404	PLX	C10-C11-C12-C13
47	W	201	PEE	C22-C23-C24-C25
47	l	705	PEE	C32-C33-C34-C35
47	r	501	PEE	C18-C19-C20-C21
50	X	201	8Q1	C12-C13-C14-C15
55	k	101	CDL	C17-C18-C19-C20
52	a	202	PLX	C26-C27-C28-C29
47	B	303	PEE	C44-C45-C46-C47
50	X	201	8Q1	O27-C28-C29-C31
47	r	501	PEE	C13-C14-C15-C16
55	V	202	CDL	C22-C23-C24-C25
47	l	704	PEE	C3-C2-O2-C10
47	j	201	PEE	C30-C31-C32-C33
55	V	201	CDL	CA4-CA3-OA5-PA1
55	n	101	CDL	C1-CB2-OB2-PB2
47	B	303	PEE	C42-C43-C44-C45
55	n	101	CDL	C74-C75-C76-C77
55	r	503	CDL	C76-C77-C78-C79
49	J	403	UQ	C15-C14-C16-C17
55	a	201	CDL	C33-C34-C35-C36
55	l	702	CDL	C54-C55-C56-C57
47	l	705	PEE	C34-C35-C36-C37
52	a	202	PLX	O6-C4-C5-O8
47	l	704	PEE	C40-C41-C42-C43
52	N	201	PLX	C3-O4-P1-O1
52	e	201	PLX	C2-O1-P1-O4
55	N	202	CDL	CA3-OA5-PA1-OA2
55	l	703	CDL	CA2-OA2-PA1-OA5
55	l	703	CDL	CA3-OA5-PA1-OA2
55	n	101	CDL	CA3-OA5-PA1-OA2
55	l	703	CDL	C53-C54-C55-C56
55	V	202	CDL	C31-C32-C33-C34
55	N	202	CDL	CB3-CB4-CB6-OB8
52	J	404	PLX	C14-C15-C16-C17
47	l	704	PEE	C41-C42-C43-C44
47	W	201	PEE	C20-C21-C22-C23
55	l	702	CDL	CB4-CB3-OB5-PB2
47	j	201	PEE	C34-C35-C36-C37
55	V	202	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
47	l	704	PEE	C38-C39-C40-C41
47	l	705	PEE	C16-C17-C18-C19
49	C	303	UQ	C23-C24-C26-C27
47	J	401	PEE	C31-C30-O3-C3
47	l	705	PEE	C15-C16-C17-C18
47	B	303	PEE	C12-C13-C14-C15
55	a	201	CDL	C16-C17-C18-C19
48	C	302	970	C20-C19-O28-C29
47	l	701	PEE	O4P-C4-C5-N
55	V	201	CDL	C31-C32-C33-C34
55	l	703	CDL	C82-C83-C84-C85
55	r	503	CDL	C42-C43-C44-C45
55	k	101	CDL	OB5-CB3-CB4-OB6
55	l	703	CDL	C72-C73-C74-C75
49	C	303	UQ	C12-C11-C9-C10
55	N	202	CDL	C52-C53-C54-C55
55	k	101	CDL	C35-C36-C37-C38
55	k	101	CDL	C71-C72-C73-C74
55	r	503	CDL	C21-C22-C23-C24
47	j	201	PEE	C37-C38-C39-C40
47	r	501	PEE	C21-C22-C23-C24
55	r	503	CDL	OA6-CA4-CA6-OA8
52	N	201	PLX	C27-C28-C29-C30
52	j	203	PLX	C17-C18-C19-C20
47	l	705	PEE	C38-C39-C40-C41
47	j	202	PEE	C33-C34-C35-C36
55	l	703	CDL	OB7-CB5-OB6-CB4
55	l	702	CDL	C84-C85-C86-C87
55	r	503	CDL	C13-C14-C15-C16
52	j	203	PLX	C9-C10-C11-C12
47	J	401	PEE	O5-C30-O3-C3
47	l	701	PEE	C1-C2-C3-O3
55	l	703	CDL	C34-C35-C36-C37
50	X	201	8Q1	O27-C28-C29-C30
49	C	303	UQ	C22-C23-C24-C25
55	a	201	CDL	C31-CA7-OA8-CA6
50	G	201	8Q1	C29-C32-C34-N36
52	g	201	PLX	C6-C7-C8-C9
55	k	101	CDL	CA3-CA4-OA6-CA5
47	l	704	PEE	C36-C37-C38-C39
47	r	501	PEE	C16-C17-C18-C19
52	a	202	PLX	C5-C4-O6-C6

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Mol	Chain	Res	Type	Atoms
50	X	201	8Q1	C9-C10-C11-C12
55	r	503	CDL	C61-C62-C63-C64
55	a	201	CDL	CA7-C31-C32-C33
55	N	202	CDL	OB5-CB3-CB4-OB6
55	V	201	CDL	OB5-CB3-CB4-OB6
55	l	702	CDL	OB5-CB3-CB4-OB6
49	C	303	UQ	C6-C7-C8-C9
55	V	202	CDL	C24-C25-C26-C27
47	l	704	PEE	C34-C35-C36-C37
55	N	202	CDL	C12-C13-C14-C15
47	j	202	PEE	C31-C30-O3-C3
55	a	201	CDL	OA9-CA7-OA8-CA6
55	l	703	CDL	C14-C15-C16-C17
50	X	201	8Q1	C42-C43-S44-C1
47	J	401	PEE	C37-C38-C39-C40
47	j	202	PEE	O5-C30-O3-C3
55	V	202	CDL	C81-C82-C83-C84
55	V	201	CDL	C57-C58-C59-C60
47	j	201	PEE	C40-C41-C42-C43
55	r	503	CDL	C20-C21-C22-C23
52	j	203	PLX	C26-C27-C28-C29
55	V	201	CDL	C72-C73-C74-C75
52	a	202	PLX	C6-C7-C8-C9
52	e	201	PLX	C24-C25-C26-C27
55	a	201	CDL	C76-C77-C78-C79
52	N	201	PLX	C19-C20-C21-C22
52	g	201	PLX	C31-C32-C33-C34
52	a	202	PLX	C12-C13-C14-C15
55	k	101	CDL	C19-C20-C21-C22
47	J	401	PEE	C38-C39-C40-C41
47	l	701	PEE	C16-C17-C18-C19
55	V	202	CDL	OB5-CB3-CB4-OB6
52	e	201	PLX	C12-C13-C14-C15
55	a	201	CDL	C64-C65-C66-C67
52	a	202	PLX	O6-C6-C7-C8
52	e	201	PLX	O8-C24-C25-C26
47	l	705	PEE	O4P-C4-C5-N
47	J	401	PEE	C36-C37-C38-C39
55	V	202	CDL	C71-C72-C73-C74
47	r	501	PEE	C14-C15-C16-C17
47	l	704	PEE	C33-C34-C35-C36
55	V	202	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
47	W	201	PEE	C34-C35-C36-C37
55	a	201	CDL	C58-C59-C60-C61
49	J	403	UQ	C12-C11-C9-C10
47	l	705	PEE	C23-C24-C25-C26
47	l	705	PEE	C21-C22-C23-C24
55	k	101	CDL	CA2-OA2-PA1-OA5
55	l	702	CDL	C72-C71-CB7-OB8
47	B	303	PEE	C18-C19-C20-C21
47	j	202	PEE	C18-C19-C20-C21
47	J	401	PEE	O3-C30-C31-C32
55	N	202	CDL	C72-C71-CB7-OB8
50	G	201	8Q1	N36-C37-C38-C39
55	l	703	CDL	C57-C58-C59-C60
55	V	202	CDL	C58-C59-C60-C61
55	a	201	CDL	C12-C11-CA5-OA6
55	k	101	CDL	C12-C11-CA5-OA6
47	W	201	PEE	C16-C17-C18-C19
47	l	701	PEE	C38-C39-C40-C41
55	k	101	CDL	C41-C42-C43-C44
52	g	201	PLX	O4-C3-C4-O6
47	B	303	PEE	C16-C17-C18-C19
57	w	401	ADP	PA-O3A-PB-O2B
57	w	401	ADP	PA-O3A-PB-O3B
55	k	101	CDL	C34-C35-C36-C37
55	r	503	CDL	C56-C57-C58-C59
52	N	201	PLX	C30-C31-C32-C33
55	V	202	CDL	C34-C35-C36-C37
55	r	503	CDL	C72-C71-CB7-OB8
47	l	704	PEE	C22-C23-C24-C25
51	J	402	NDP	C5B-O5B-PA-O3
52	N	201	PLX	O7-C6-C7-C8
52	N	201	PLX	O9-C24-C25-C26
47	j	201	PEE	O3-C30-C31-C32
47	j	202	PEE	C16-C17-C18-C19
55	a	201	CDL	C32-C31-CA7-OA8
55	V	202	CDL	C76-C77-C78-C79
47	r	501	PEE	C44-C45-C46-C47
55	l	703	CDL	C51-CB5-OB6-CB4
55	k	101	CDL	C12-C11-CA5-OA7
47	l	704	PEE	C18-C19-C20-C21
55	l	702	CDL	C72-C71-CB7-OB9
55	r	503	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
55	r	503	CDL	C72-C73-C74-C75
52	r	502	PLX	C35-C36-C37-C38
47	J	401	PEE	O5-C30-C31-C32
55	a	201	CDL	C12-C11-CA5-OA7
47	J	401	PEE	C44-C45-C46-C47
55	k	101	CDL	C23-C24-C25-C26
52	j	203	PLX	C3-O4-P1-O3
55	a	201	CDL	CA2-OA2-PA1-OA3
55	l	702	CDL	CA2-OA2-PA1-OA3
55	l	703	CDL	CA3-OA5-PA1-OA3
51	J	402	NDP	C3B-C4B-C5B-O5B
55	N	202	CDL	C72-C71-CB7-OB9
49	J	403	UQ	C22-C23-C24-C25
47	l	705	PEE	C10-C11-C12-C13
55	r	503	CDL	C72-C71-CB7-OB9
55	V	202	CDL	C77-C78-C79-C80
52	j	203	PLX	C25-C24-O8-C5
47	j	201	PEE	O5-C30-C31-C32
55	a	201	CDL	C32-C31-CA7-OA9
50	X	201	8Q1	C11-C10-C9-C8
55	k	101	CDL	C36-C37-C38-C39
52	e	201	PLX	C2-C1-N1-C1C
52	e	201	PLX	C2-C1-N1-C1A
55	V	201	CDL	C12-C11-CA5-OA6
55	l	702	CDL	C12-C11-CA5-OA6
49	J	403	UQ	C7-C8-C9-C11
52	r	502	PLX	O4-C3-C4-O6
55	n	101	CDL	C52-C51-CB5-OB6
47	l	701	PEE	O3-C30-C31-C32
48	C	302	970	C18-C19-O28-C29
49	J	403	UQ	C11-C12-C13-C14
55	V	202	CDL	C52-C51-CB5-OB6
52	e	201	PLX	C2-C1-N1-C1B
55	a	201	CDL	C36-C37-C38-C39

There are no ring outliers.

34 monomers are involved in 165 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	B	303	PEE	4	0
49	J	403	UQ	4	0
49	C	303	UQ	21	0

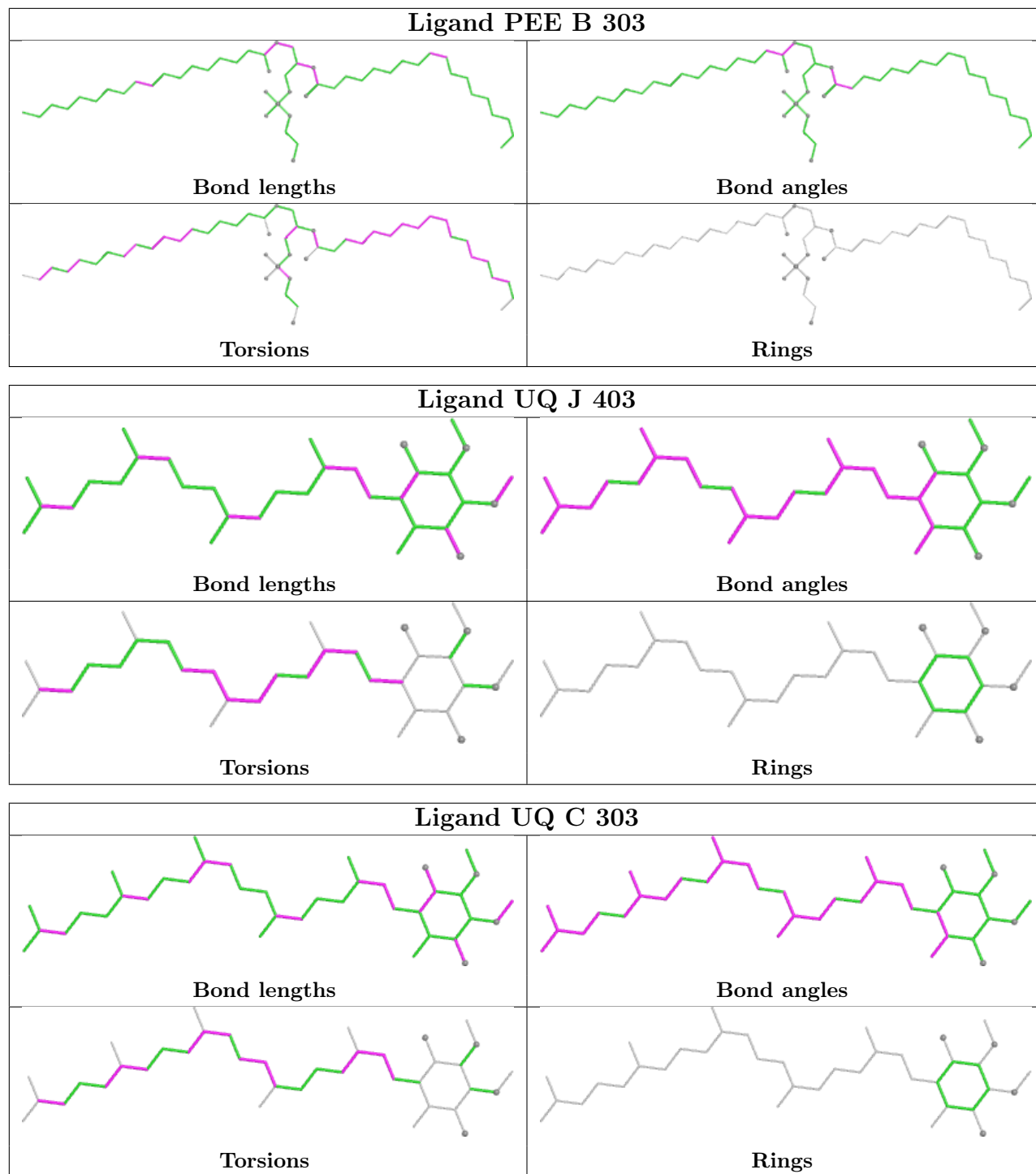
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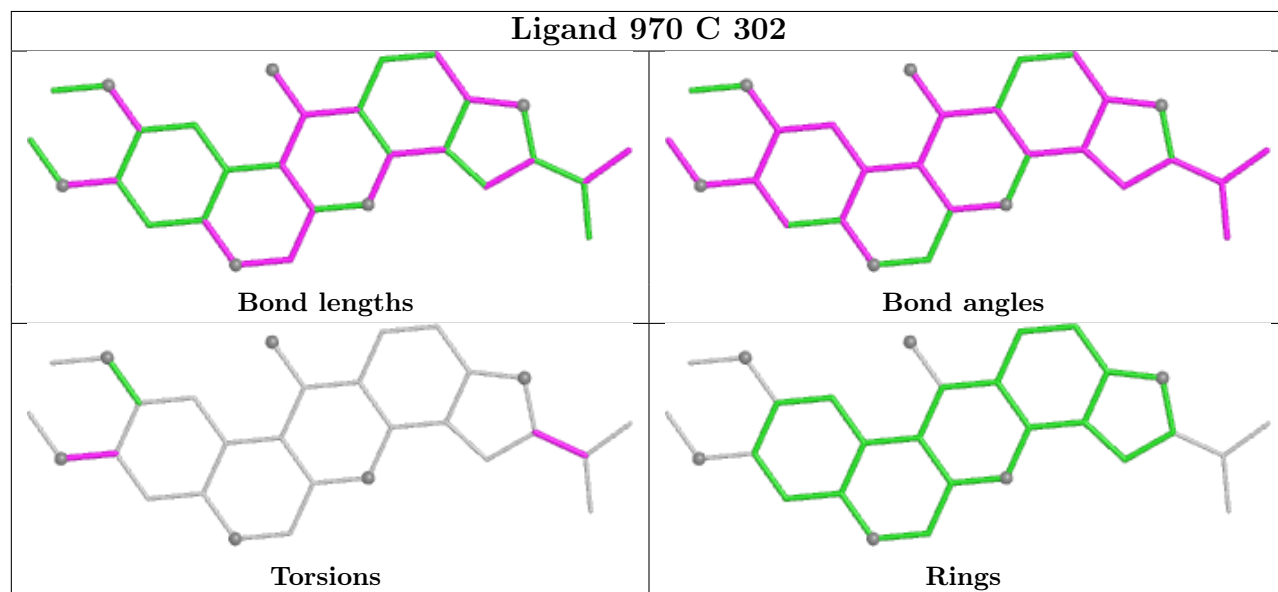
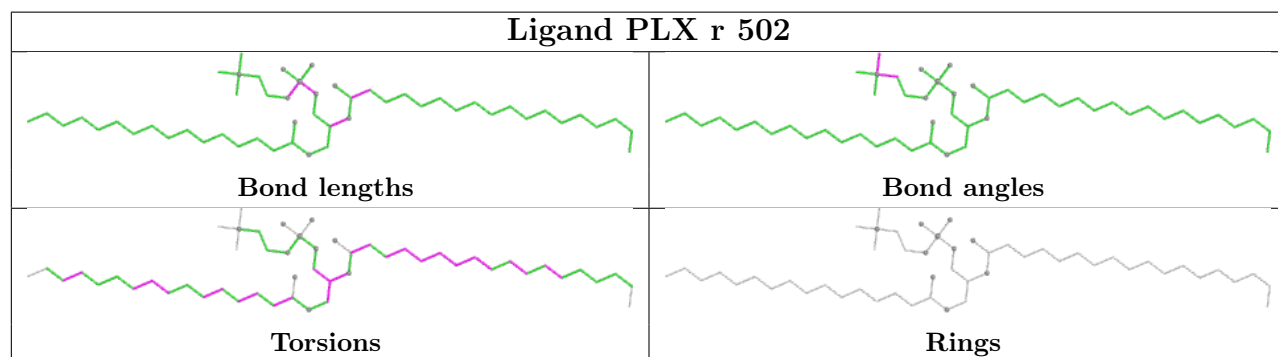
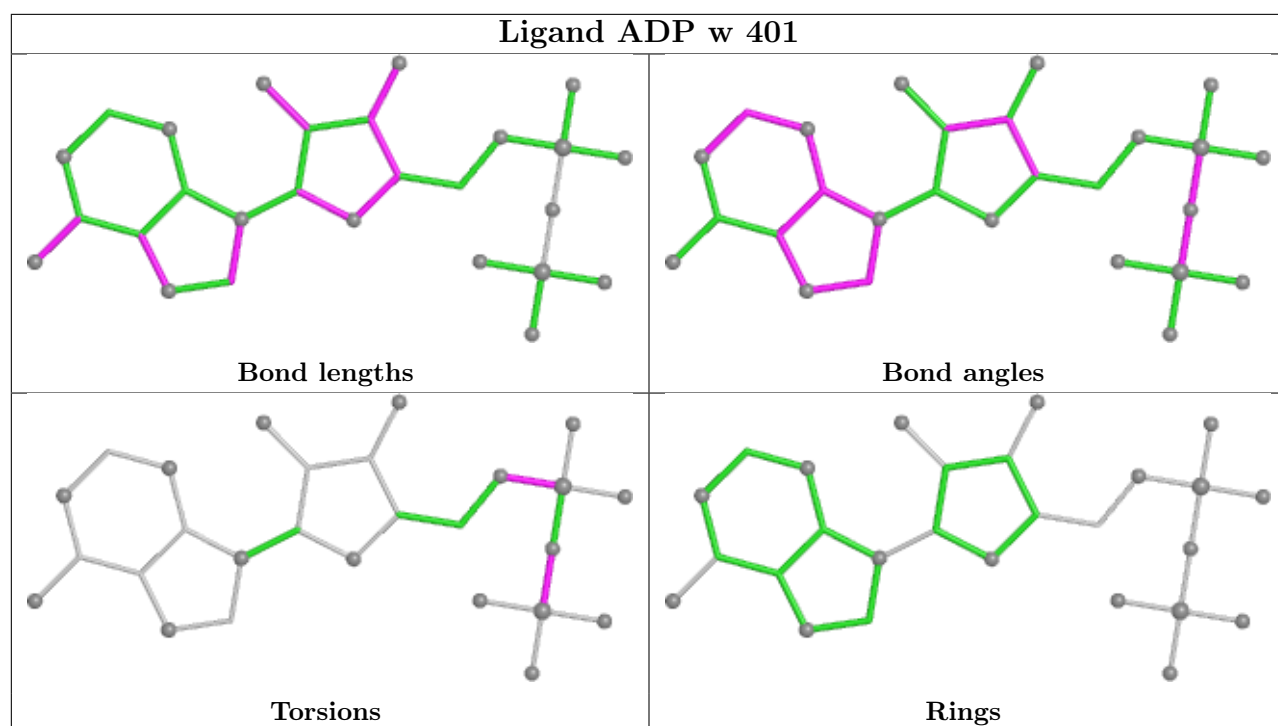
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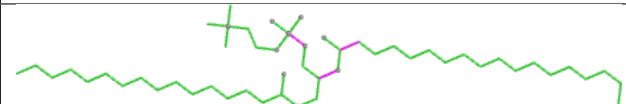
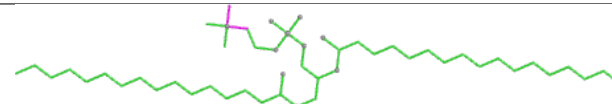
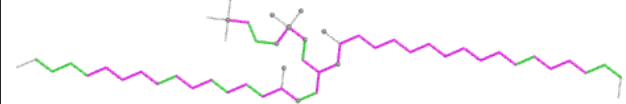
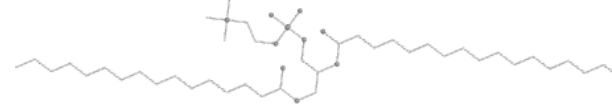
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	w	401	ADP	1	0
52	r	502	PLX	5	0
52	g	201	PLX	7	0
47	r	501	PEE	5	0
52	J	404	PLX	5	0
52	e	201	PLX	6	0
55	l	702	CDL	12	0
55	l	703	CDL	6	0
52	a	202	PLX	2	0
47	J	401	PEE	6	0
53	O	301	FES	1	0
47	W	201	PEE	1	0
47	j	202	PEE	1	0
55	N	202	CDL	1	0
55	k	101	CDL	15	0
50	X	201	8Q1	2	0
47	l	705	PEE	5	0
55	V	202	CDL	7	0
46	A	502	FMN	9	0
47	l	701	PEE	1	0
47	l	704	PEE	5	0
55	a	201	CDL	3	0
55	n	101	CDL	1	0
52	N	201	PLX	10	0
45	A	501	SF4	2	0
51	J	402	NDP	3	0
55	r	503	CDL	4	0
45	C	301	SF4	3	0
52	j	203	PLX	2	0
55	V	201	CDL	8	0
47	j	201	PEE	3	0

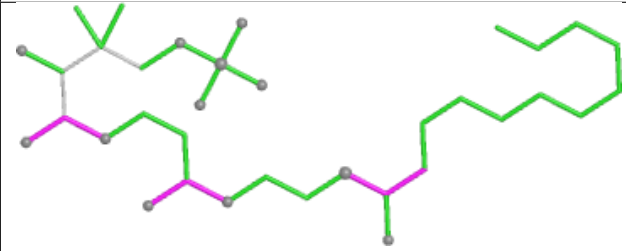
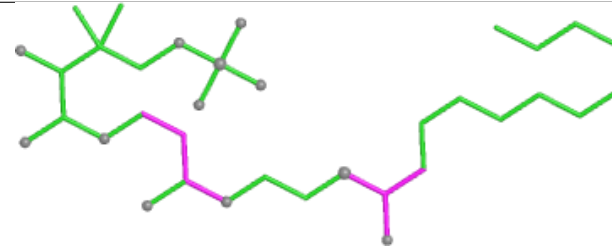
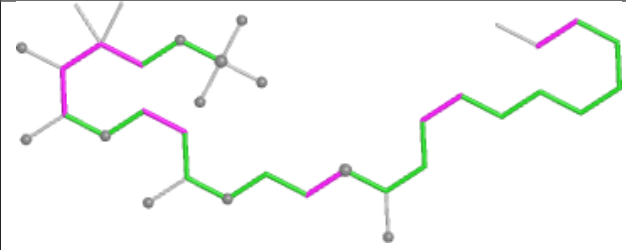
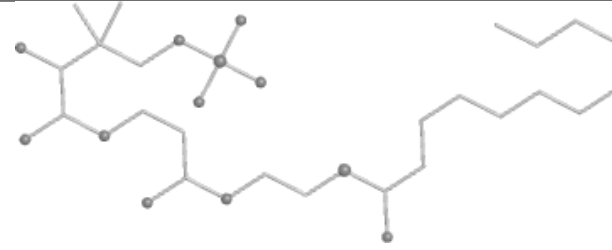
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

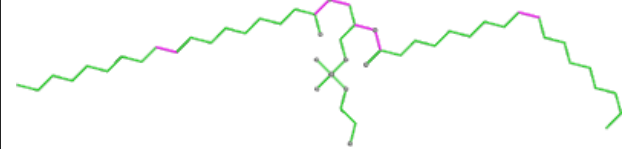
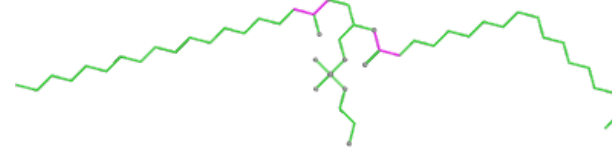
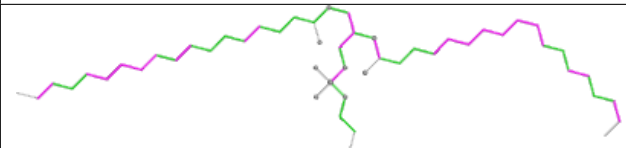
equivalents in the CSD to analyse the geometry.

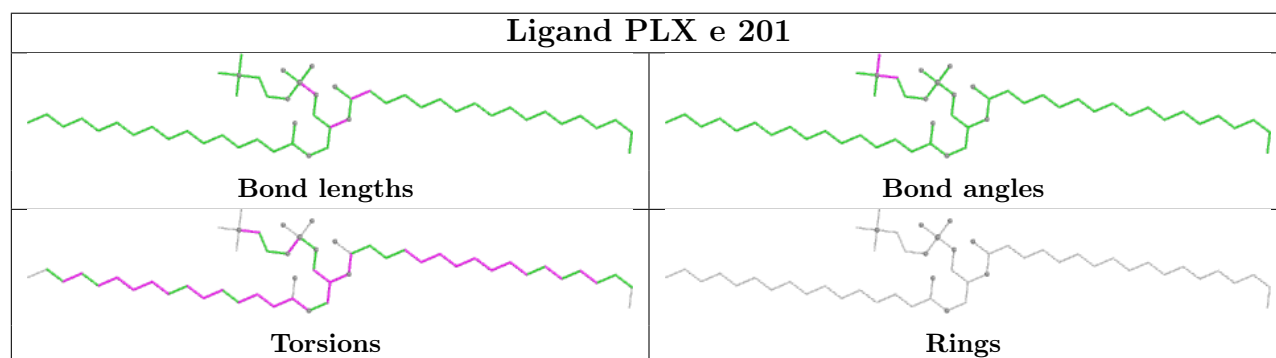
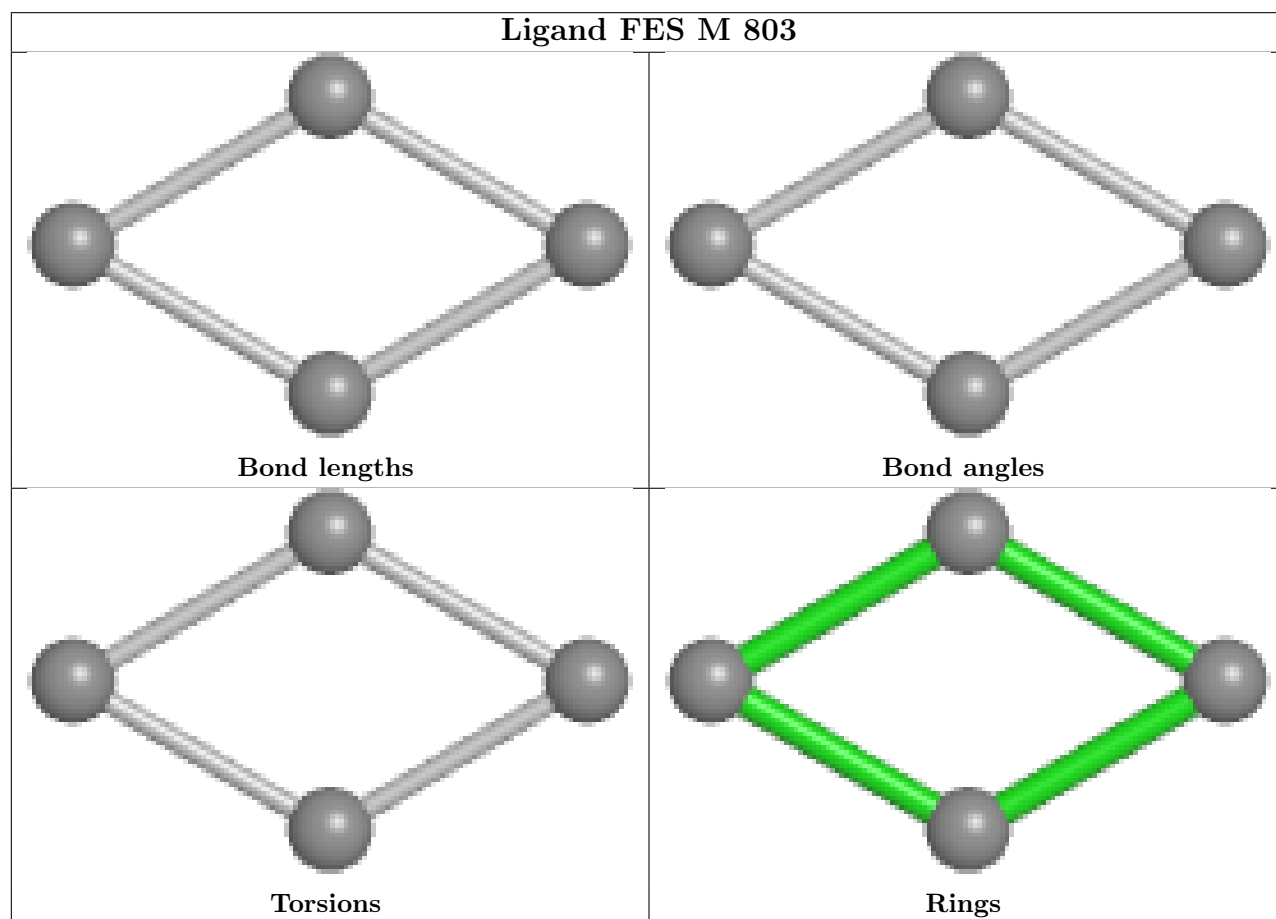
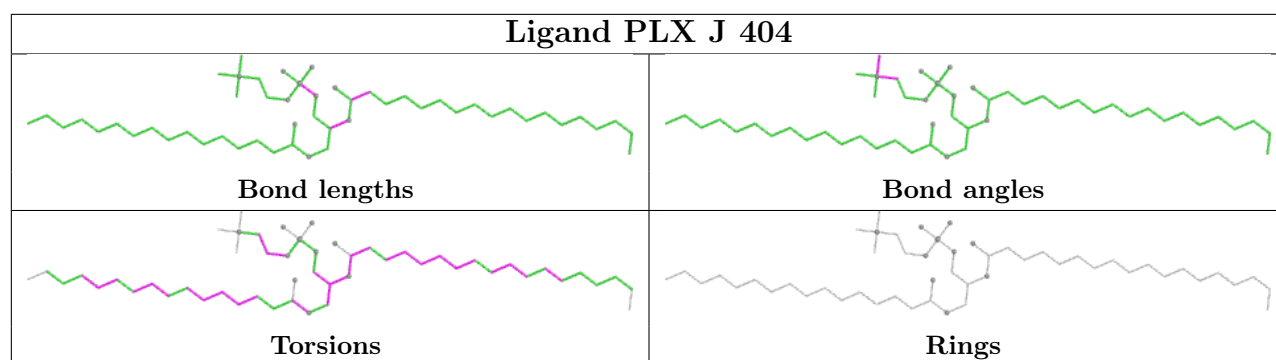


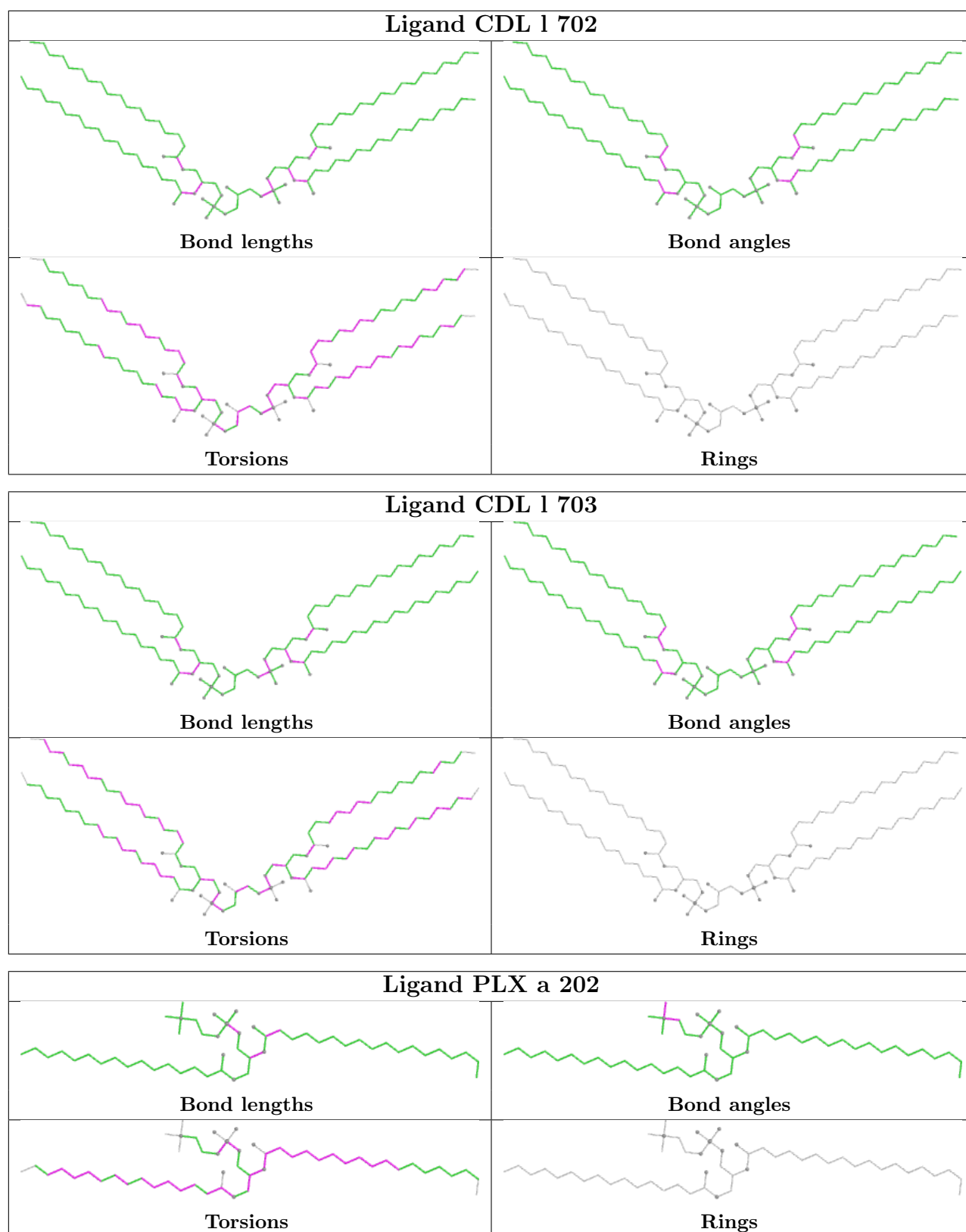


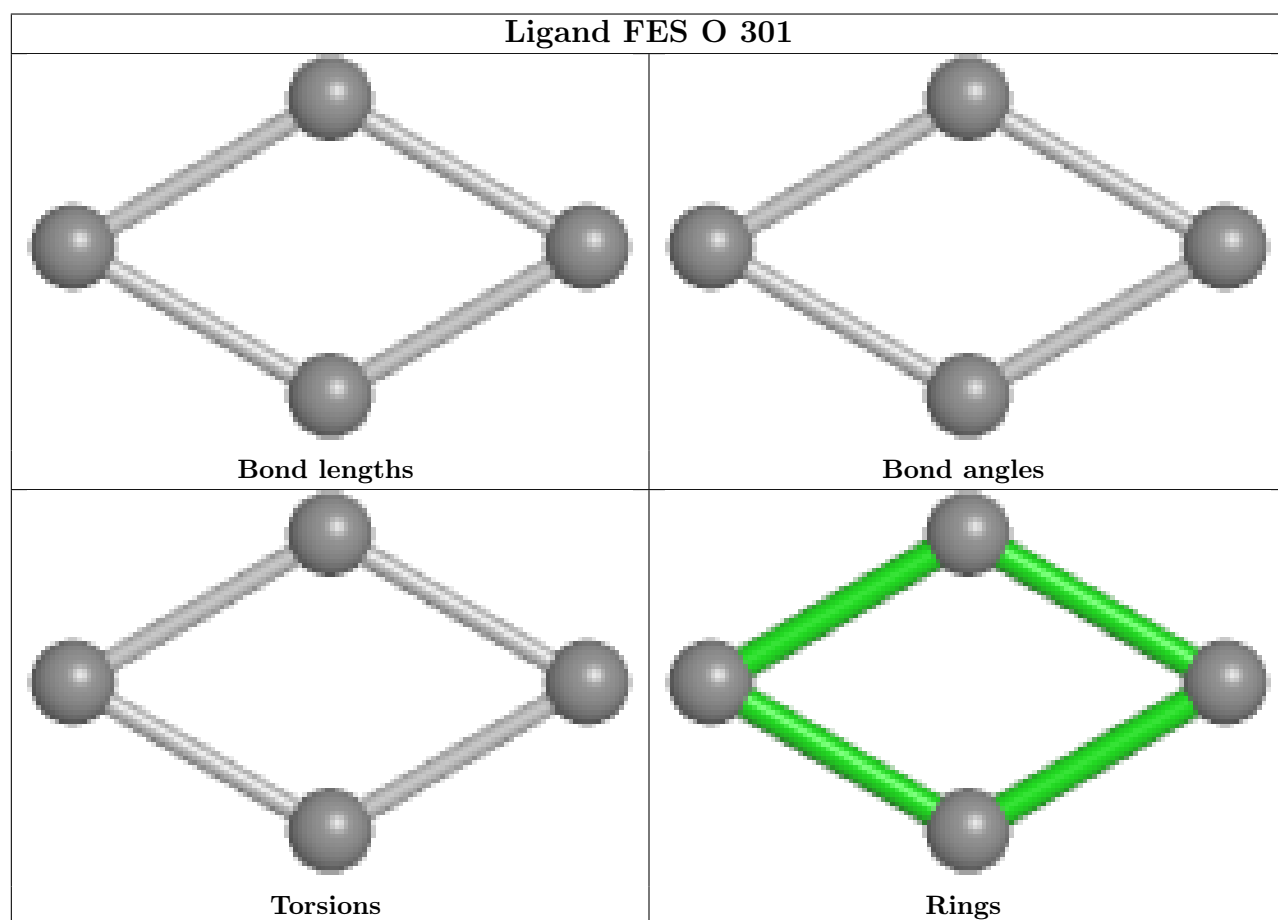
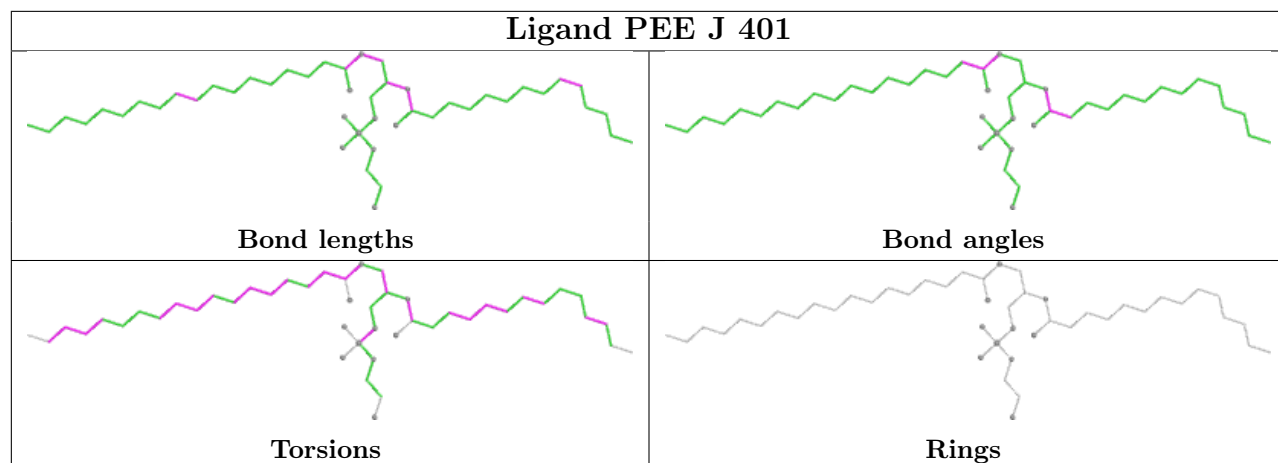
Ligand PLX g 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

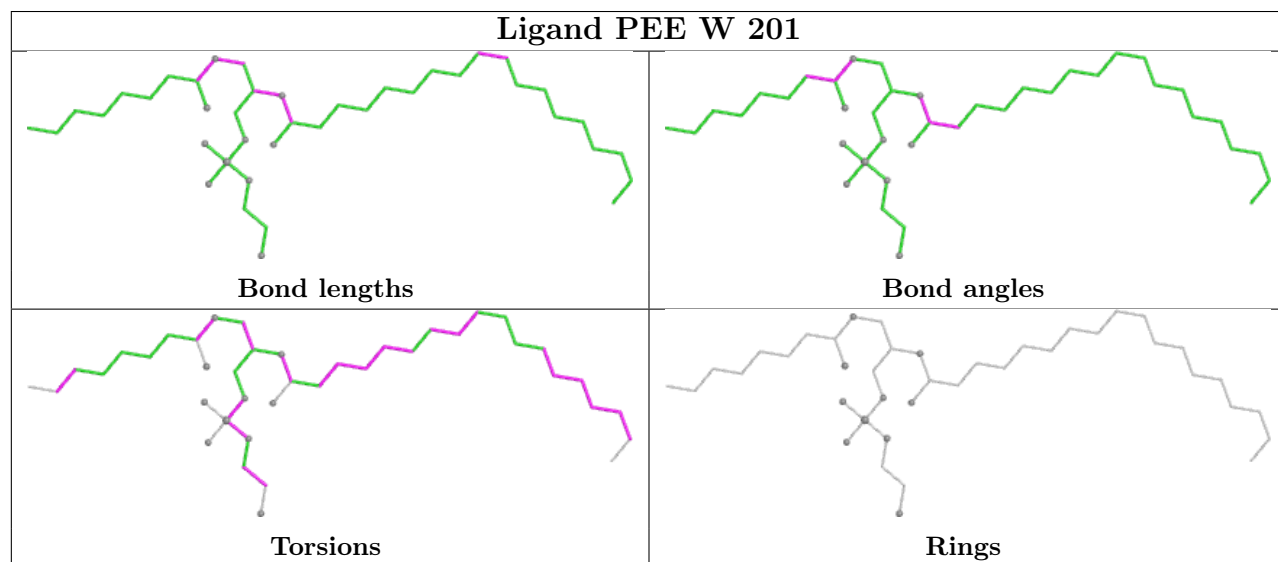
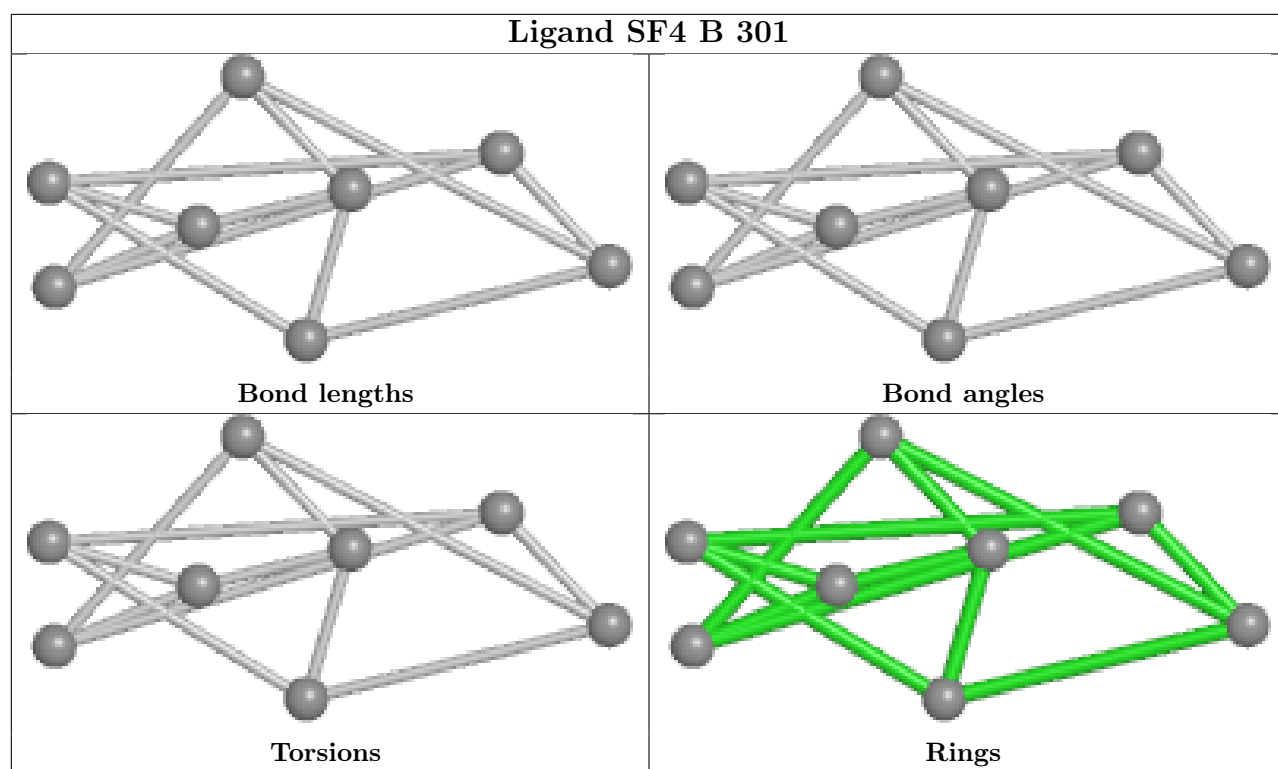
Ligand 8Q1 G 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

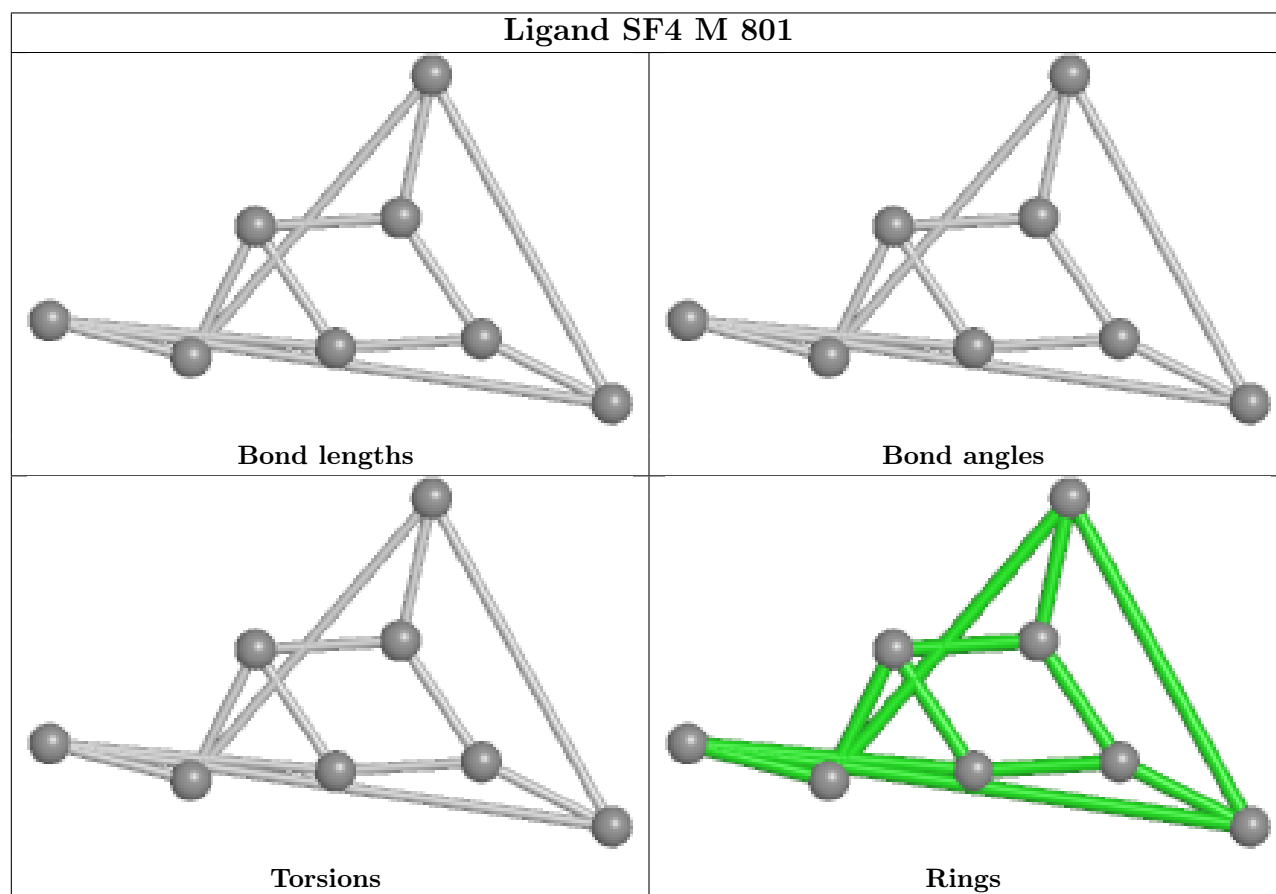
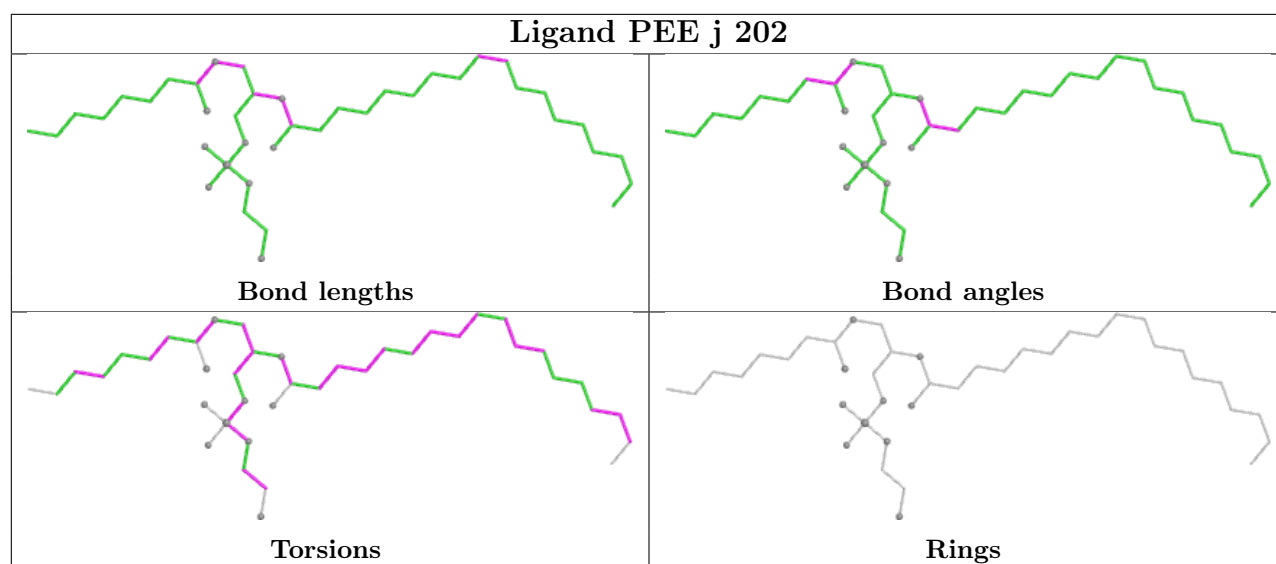
Ligand PEE r 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

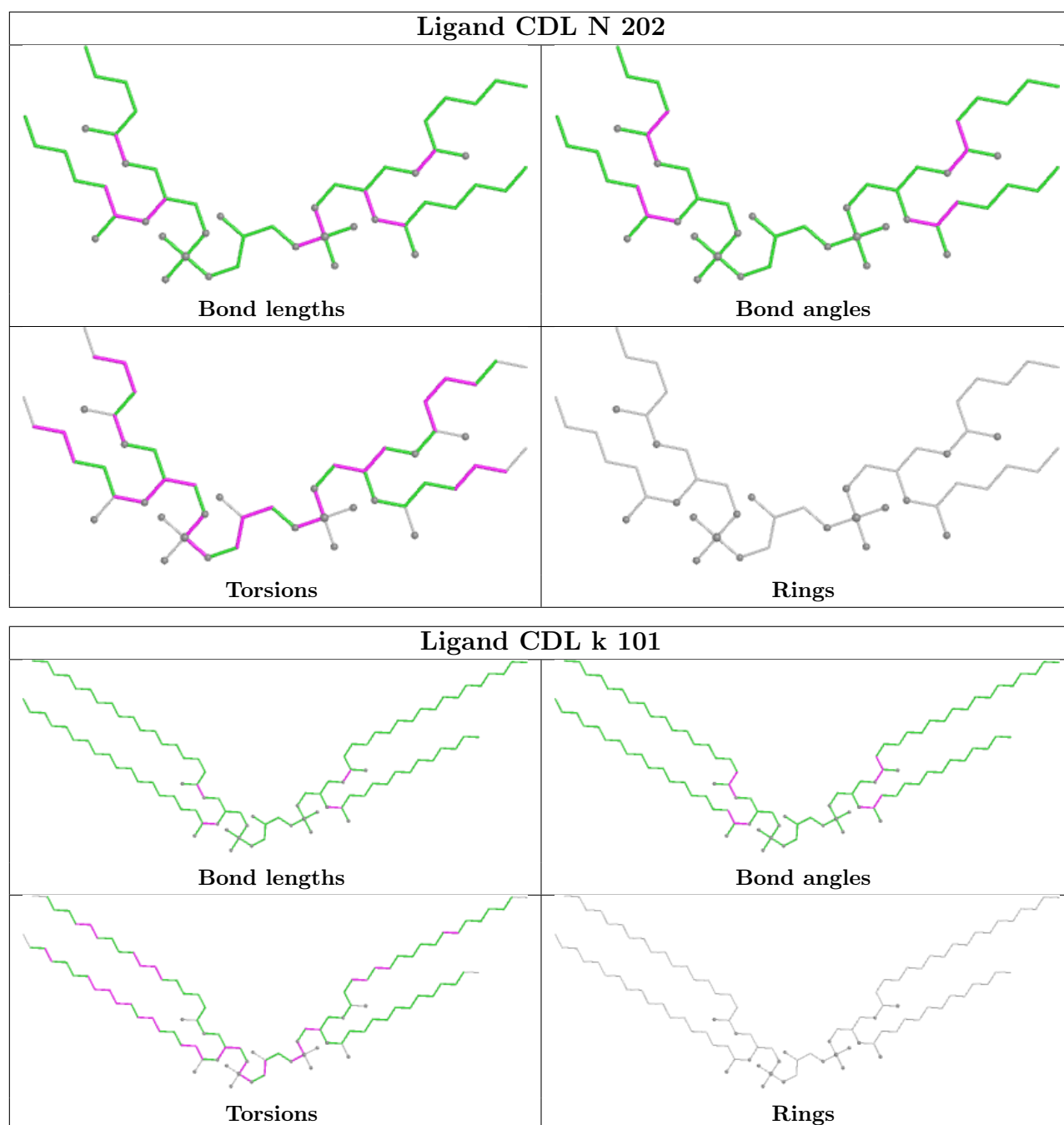


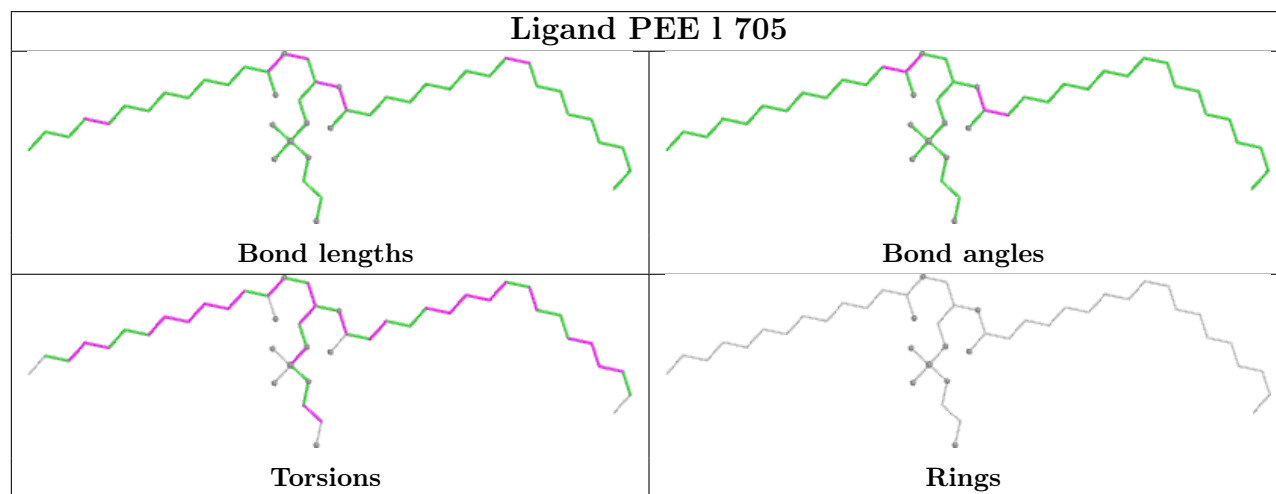
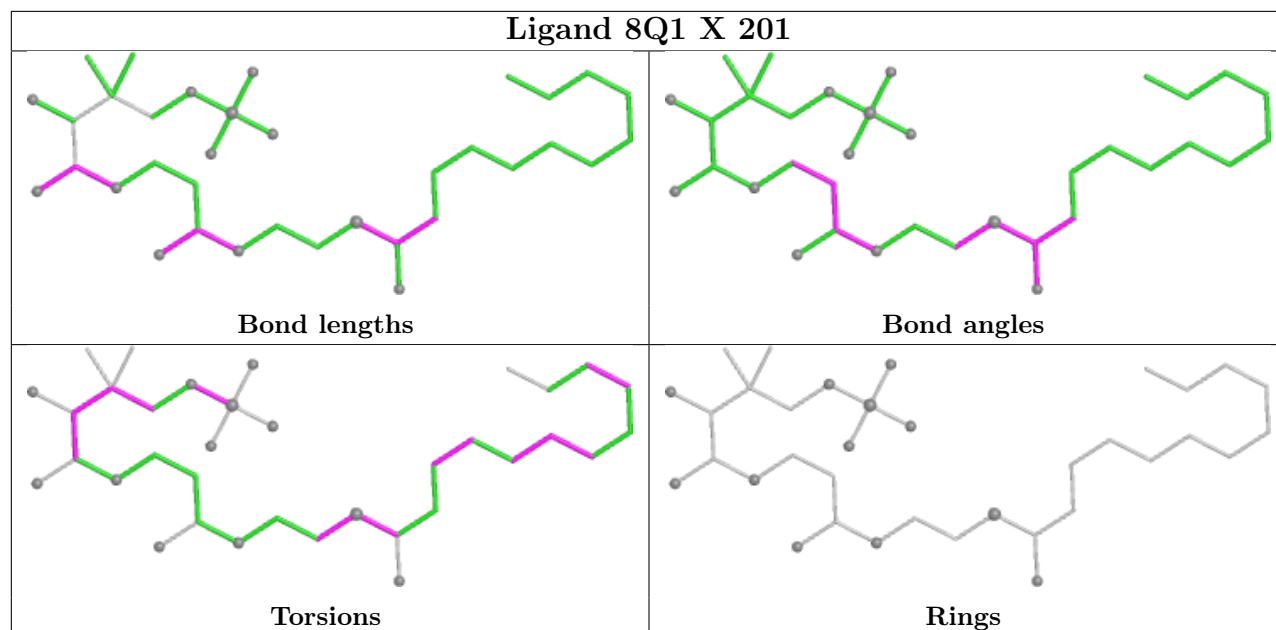


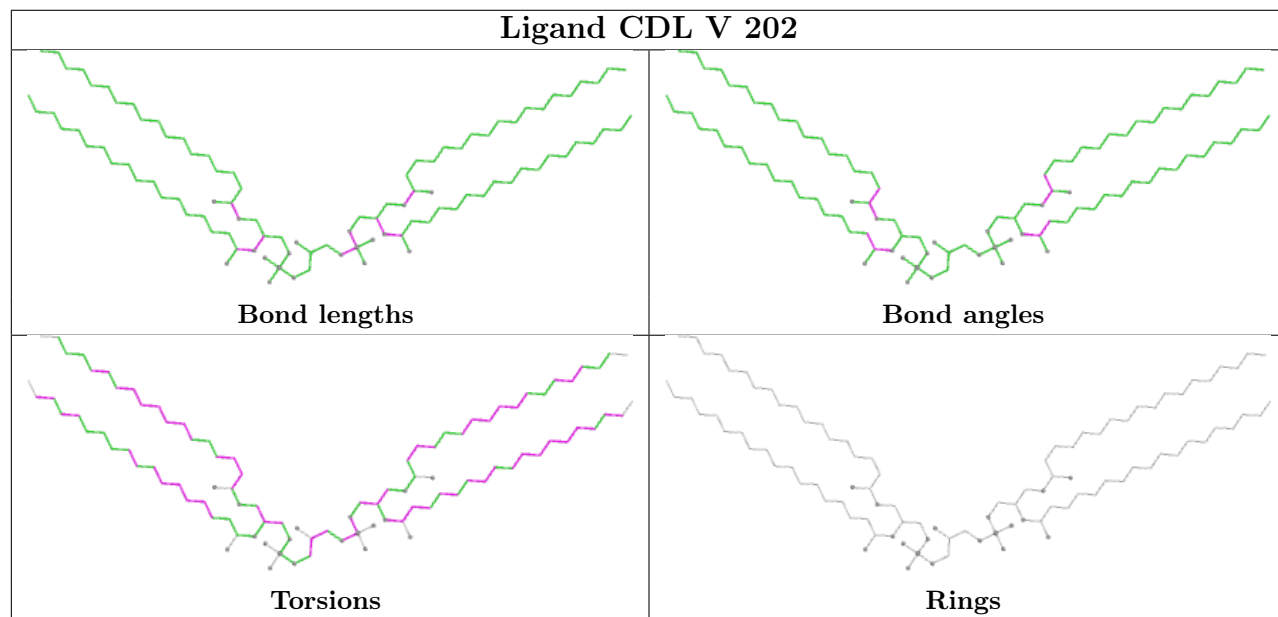
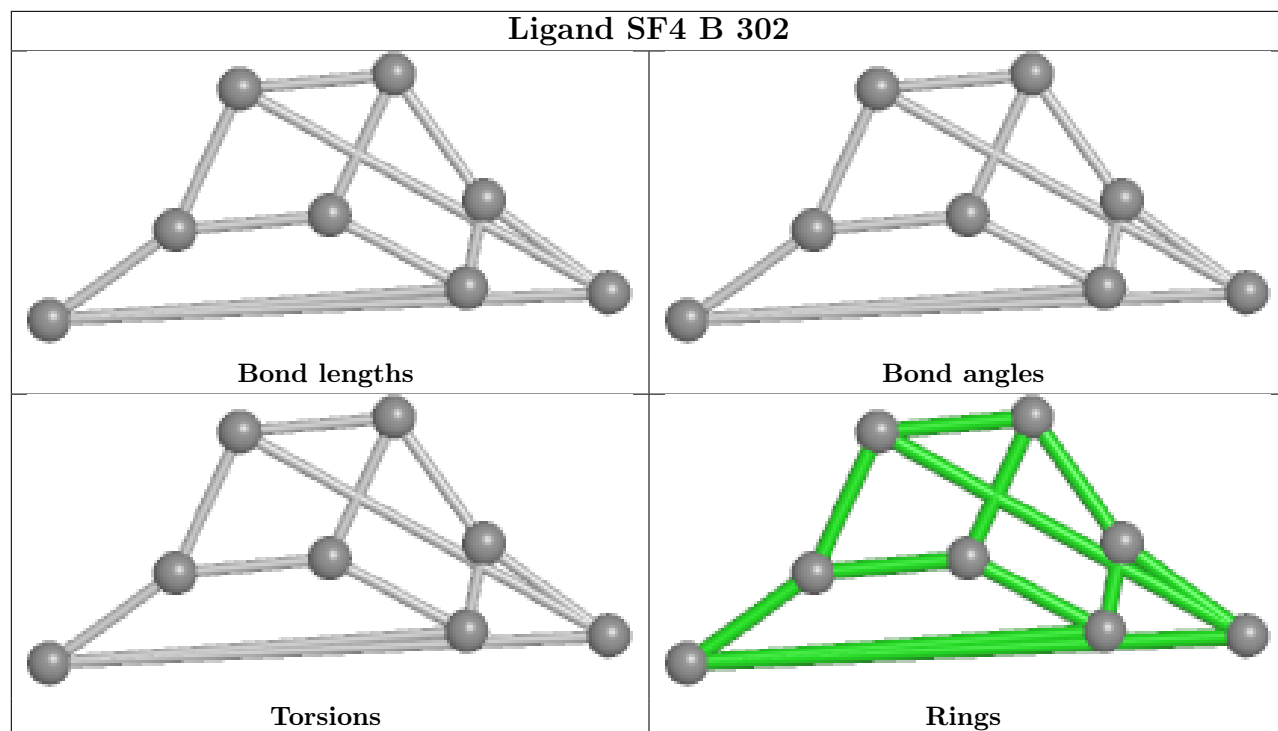


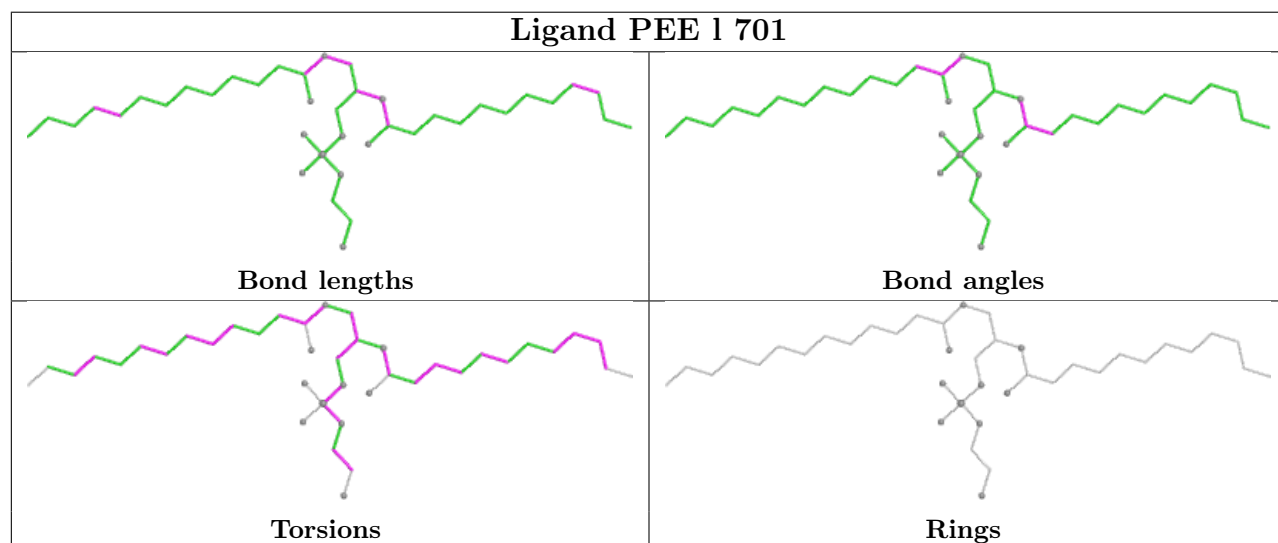
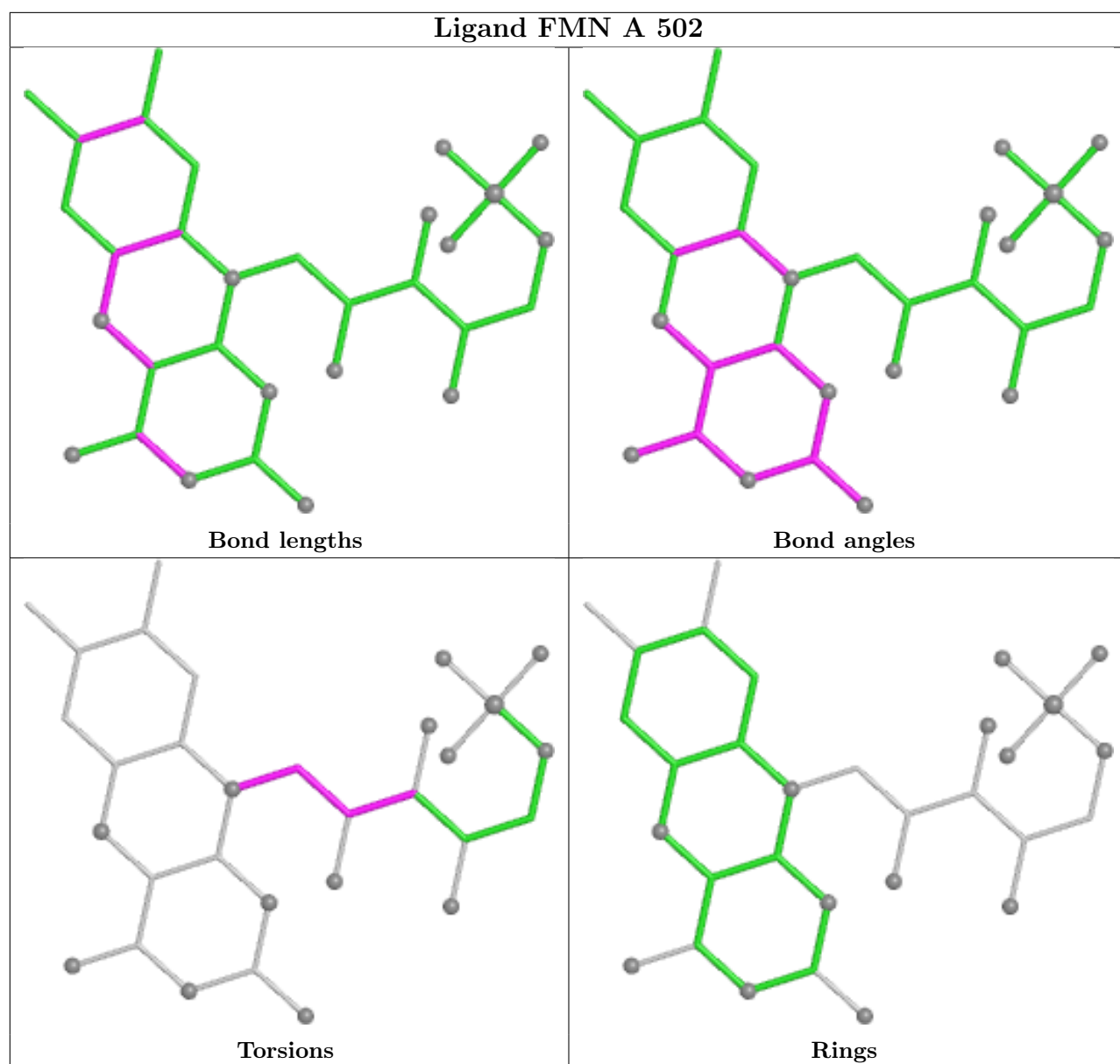


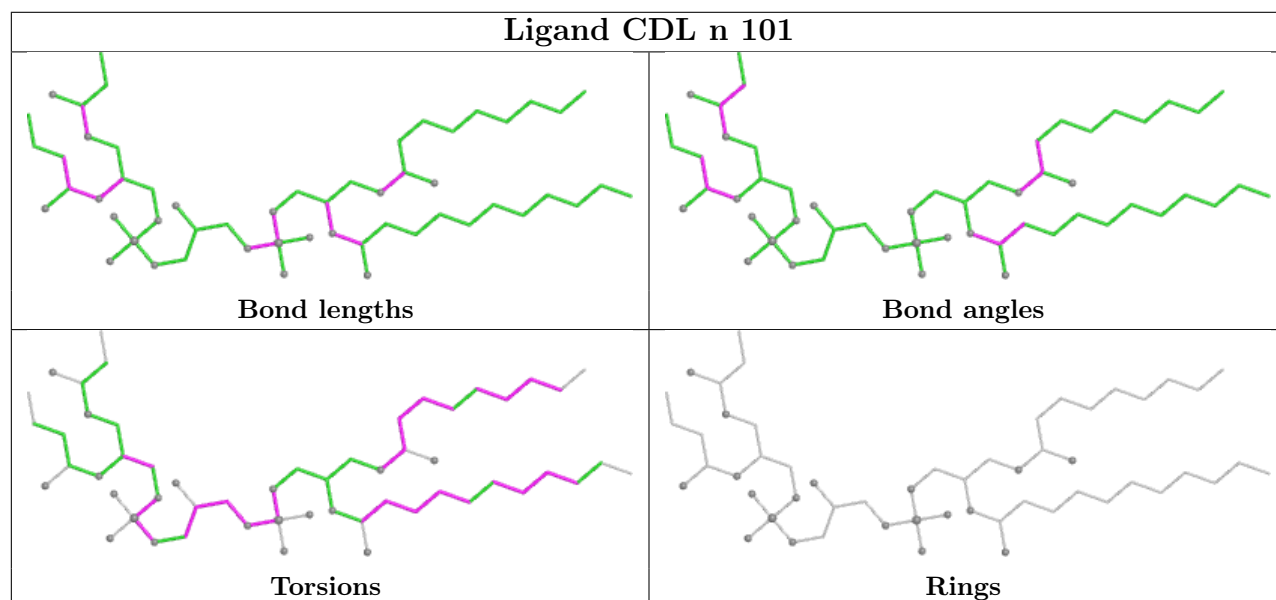
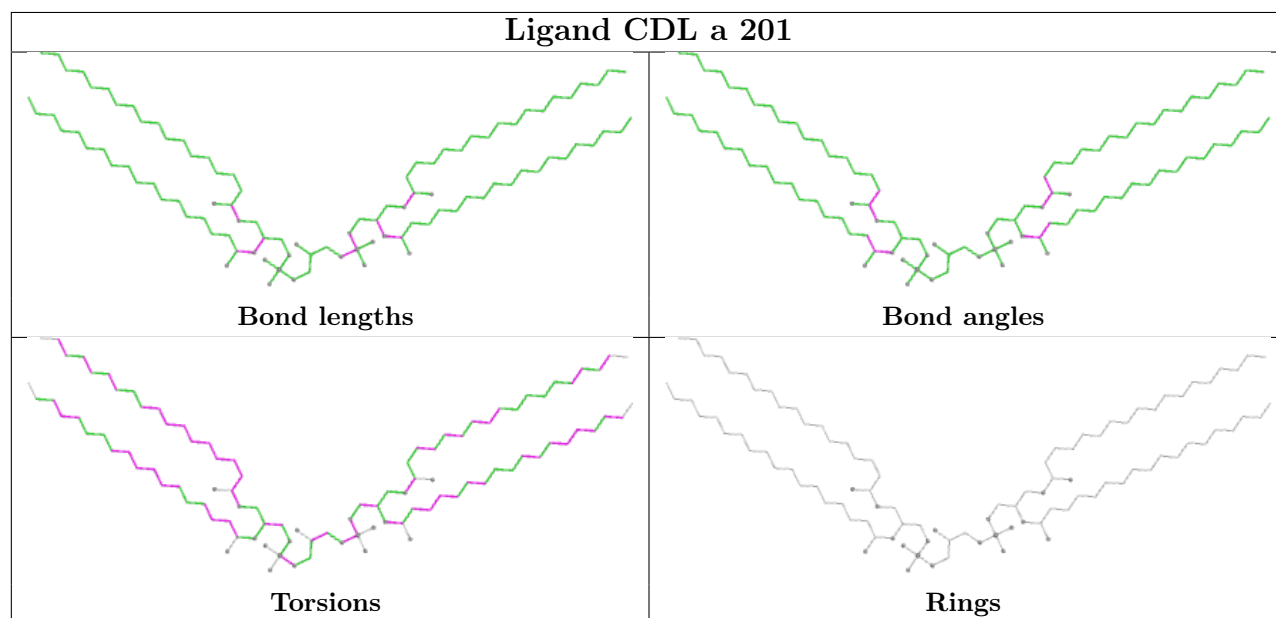
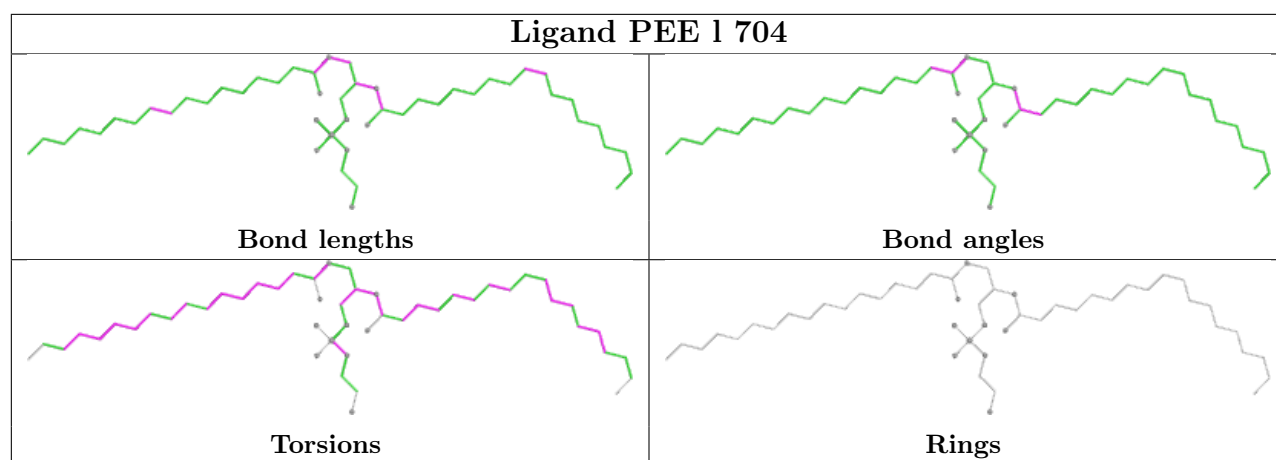


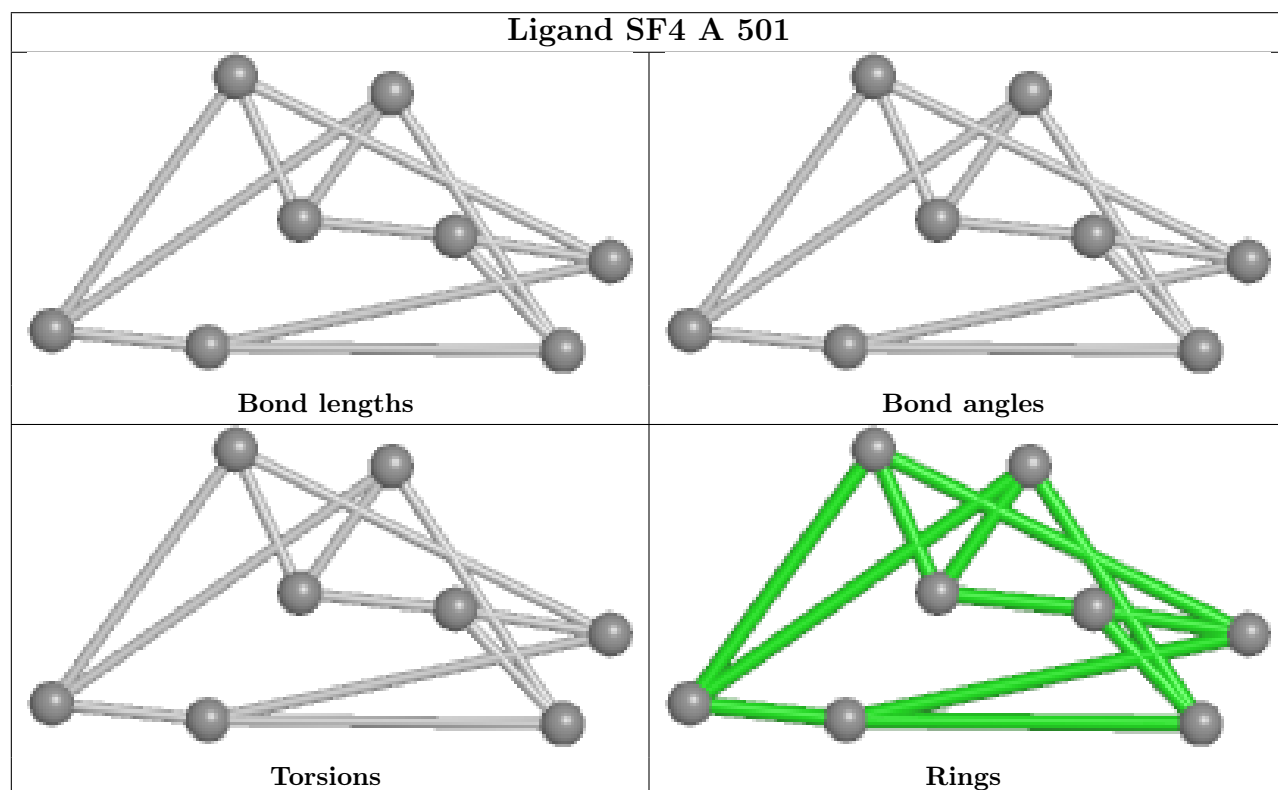
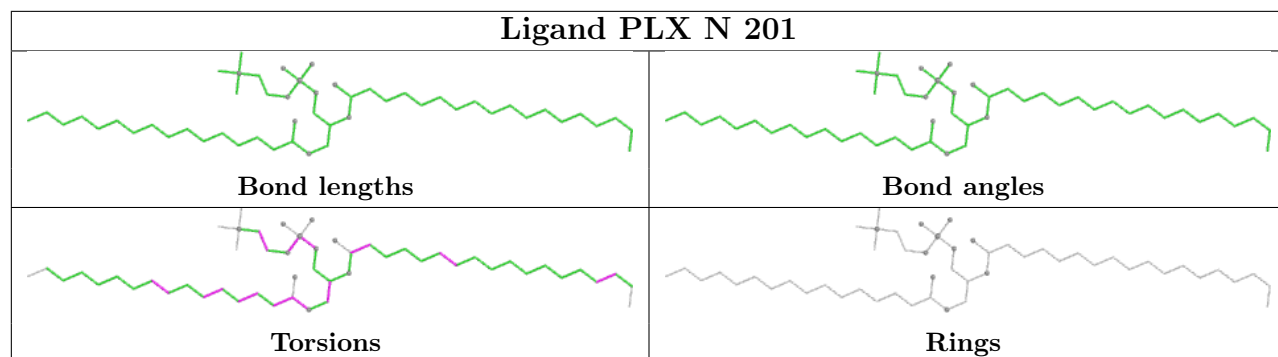


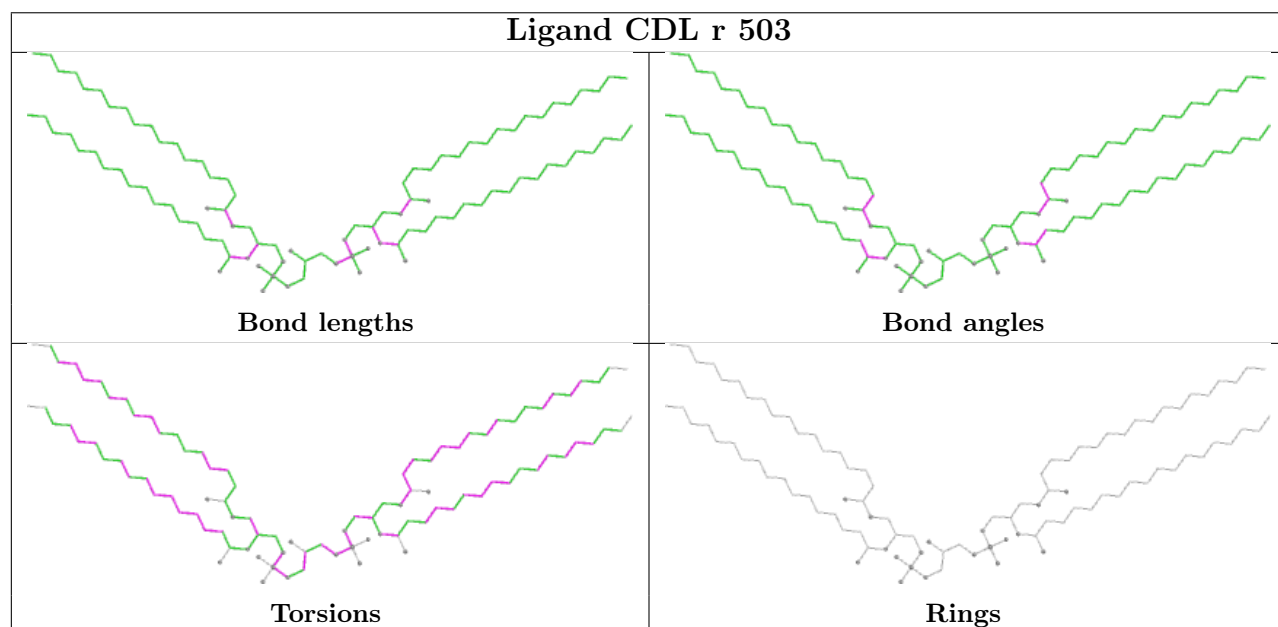
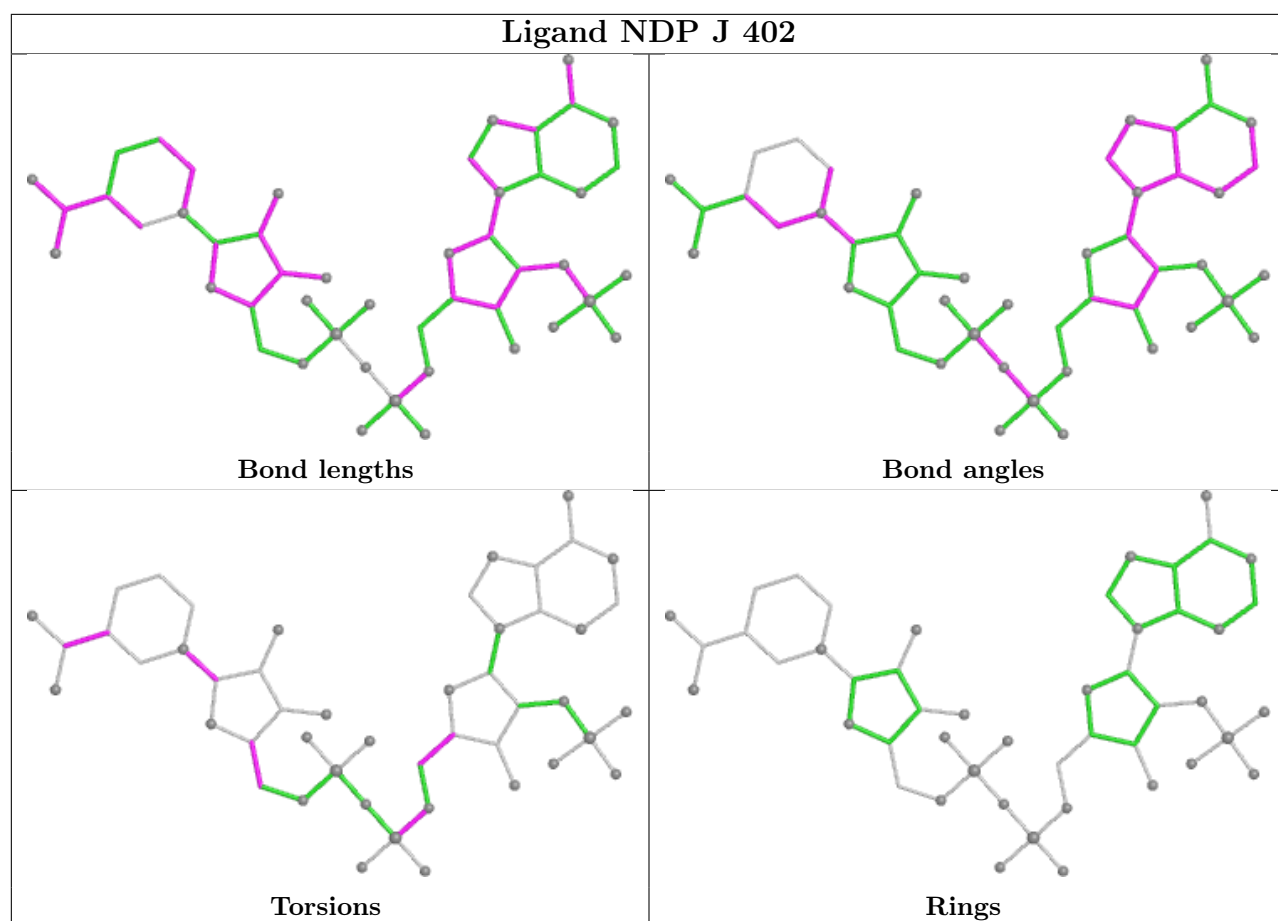


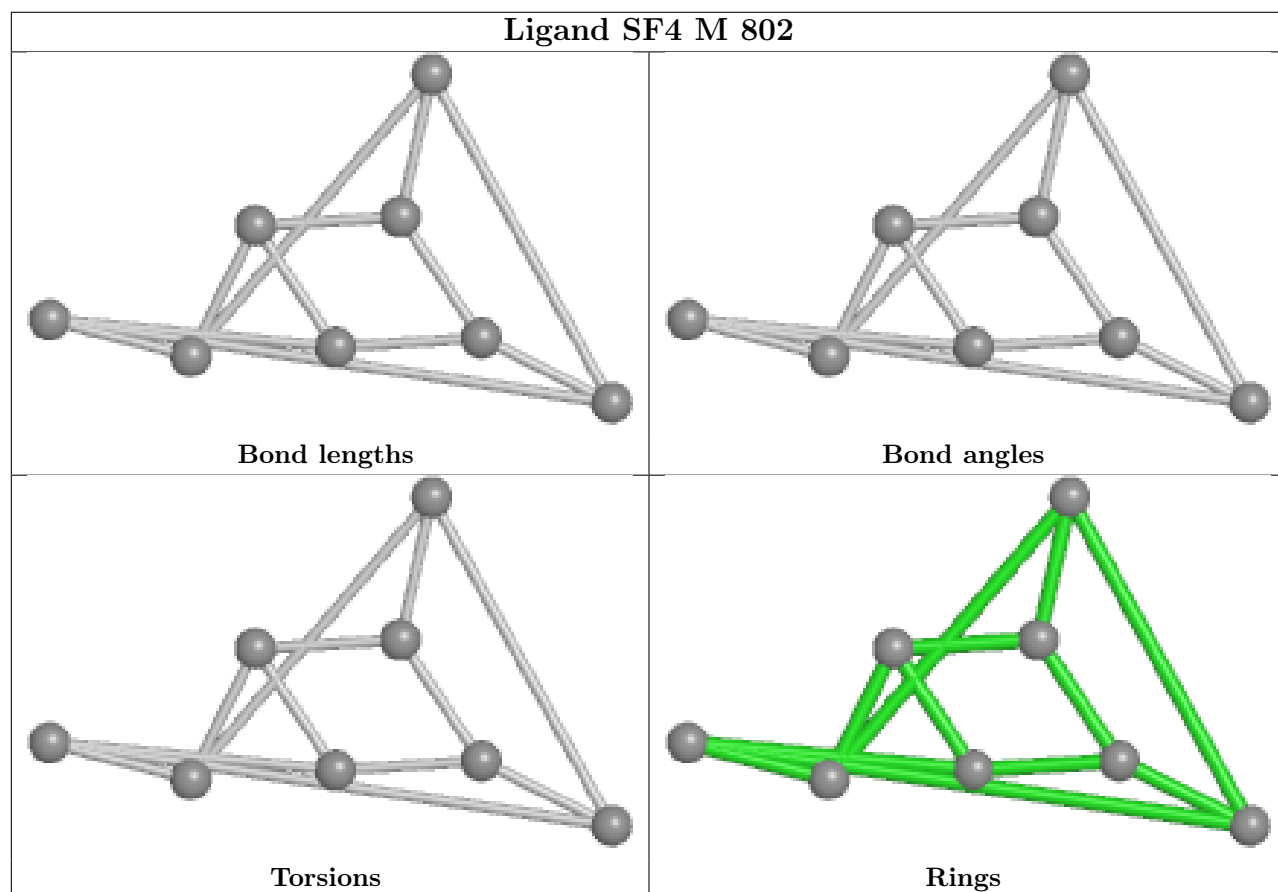
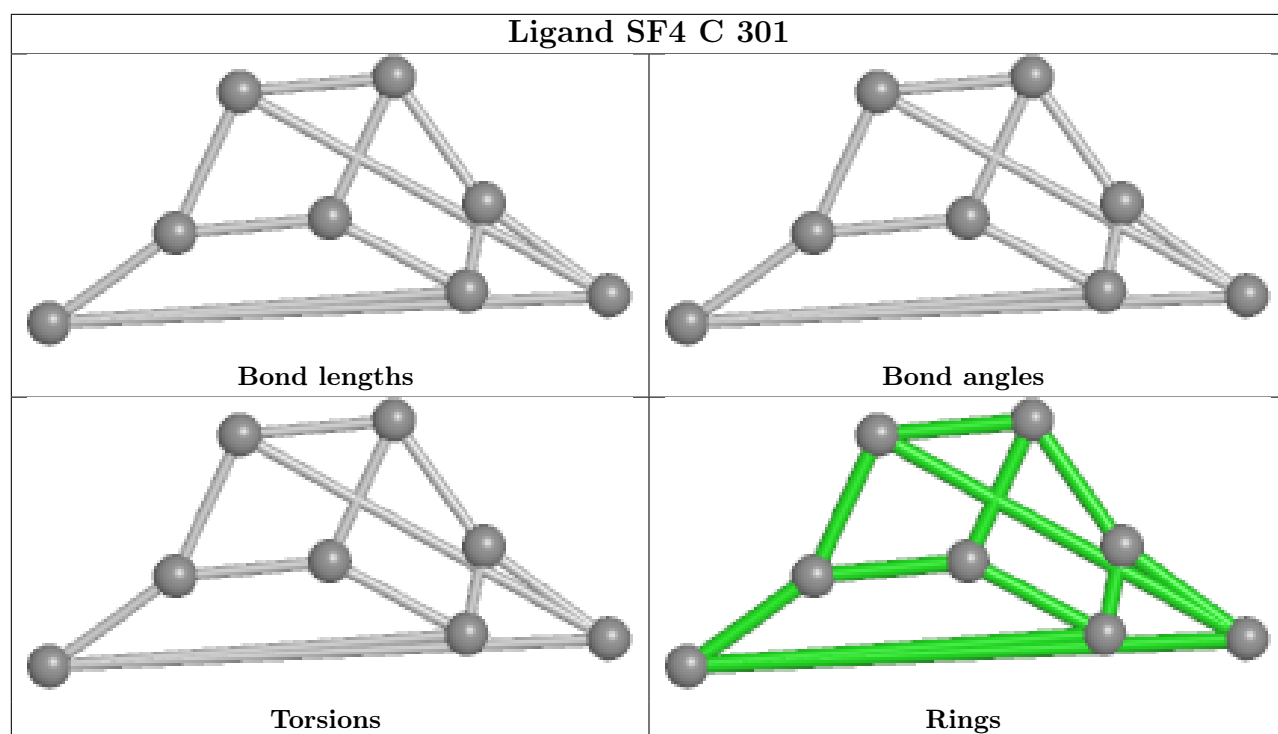


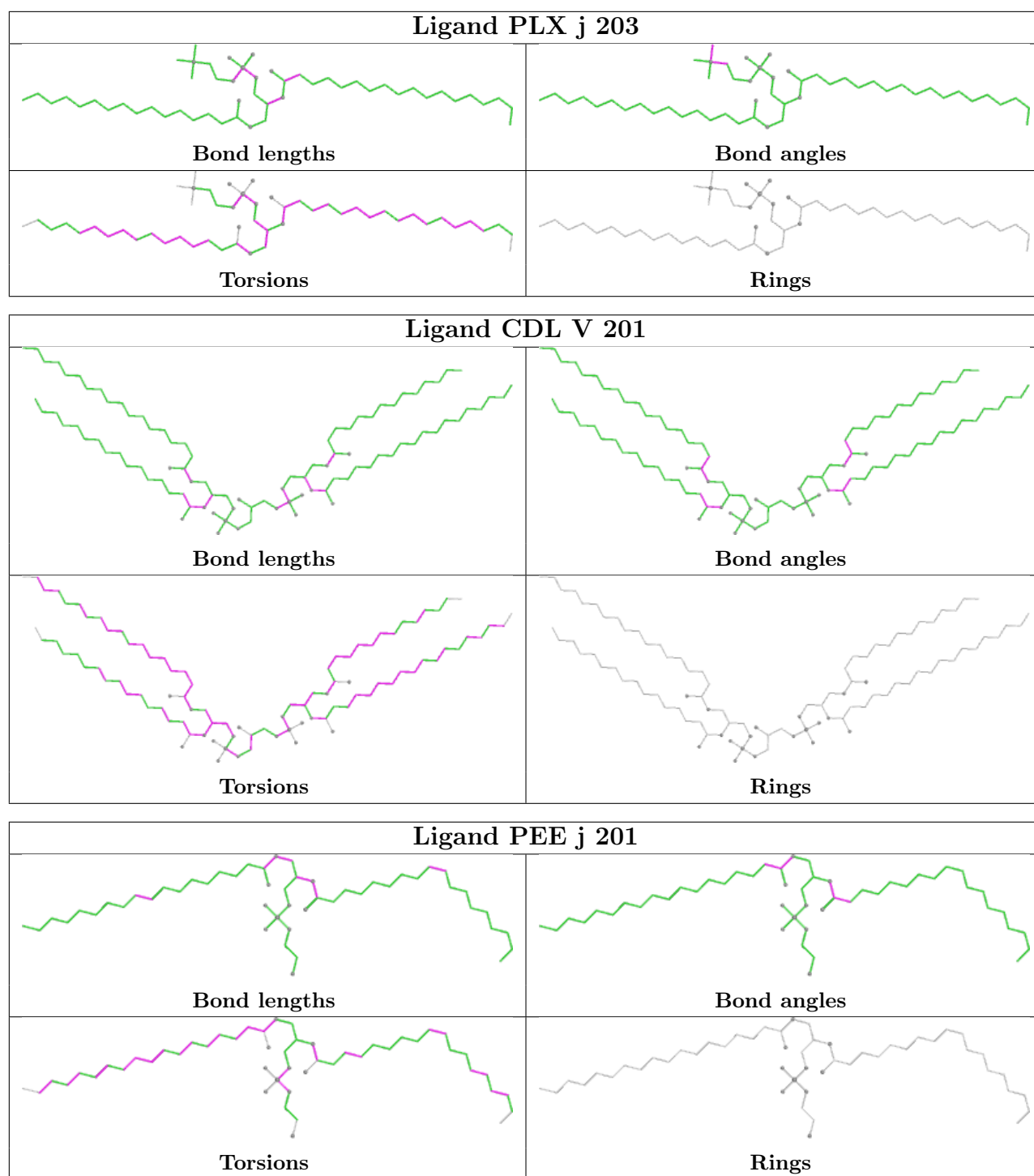












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

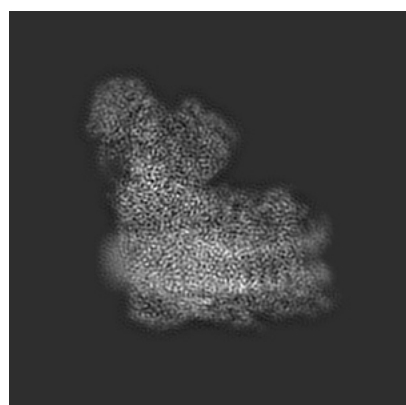
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32255. These allow visual inspection of the internal detail of the map and identification of artifacts.

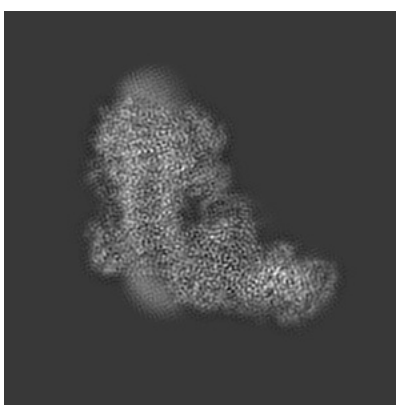
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

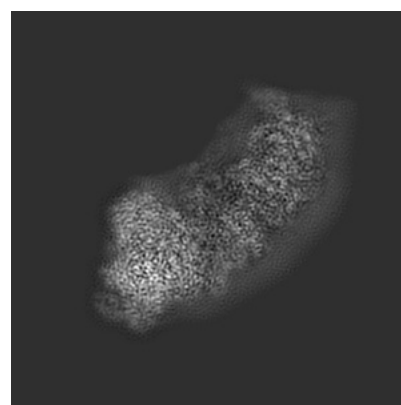
6.1.1 Primary map



X



Y

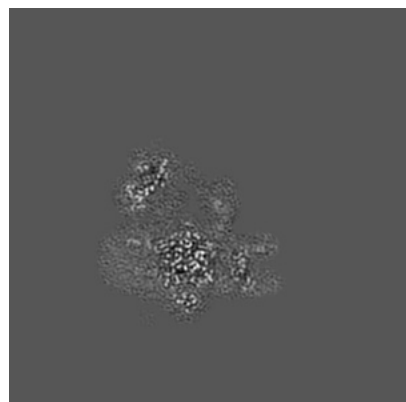


Z

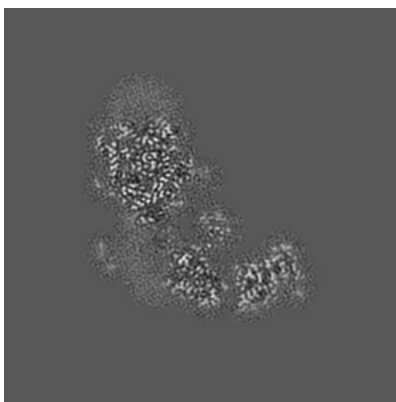
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

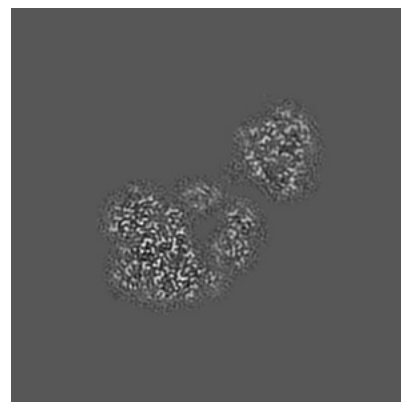
6.2.1 Primary map



X Index: 155



Y Index: 155

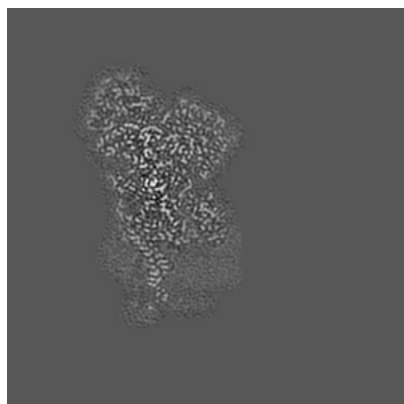


Z Index: 155

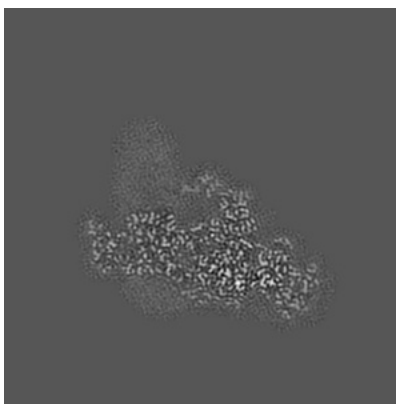
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

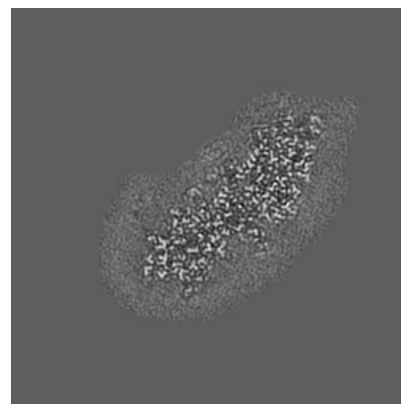
6.3.1 Primary map



X Index: 105



Y Index: 111

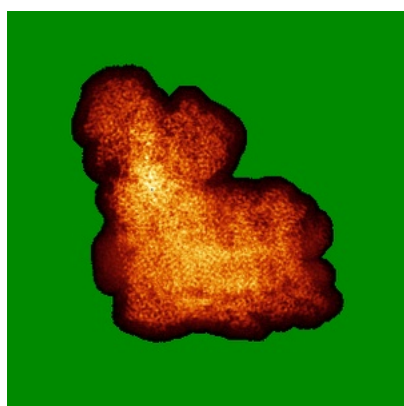


Z Index: 123

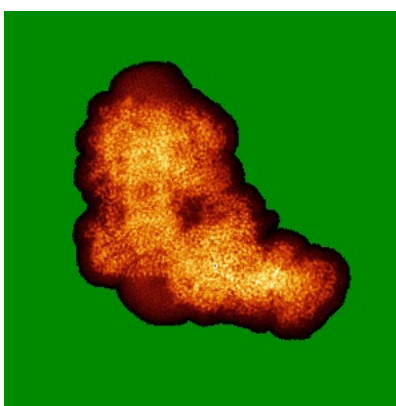
The images above show the largest variance slices of the map in three orthogonal directions.

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

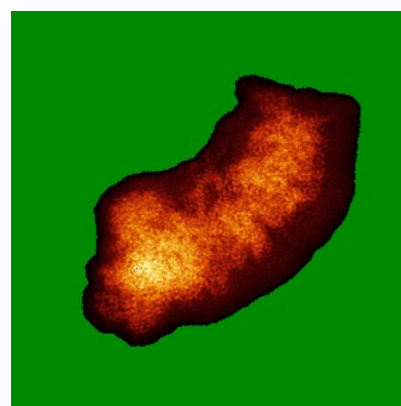
6.4.1 Primary map



X



Y

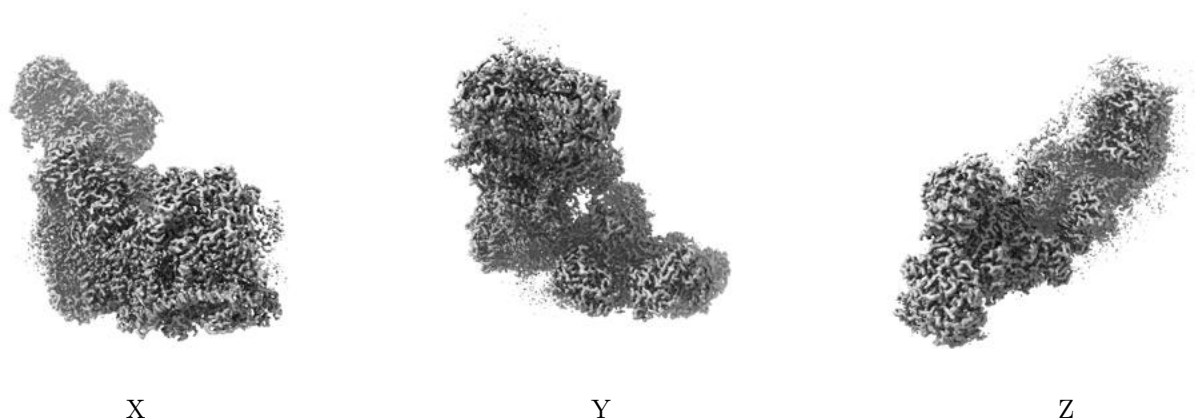


Z

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

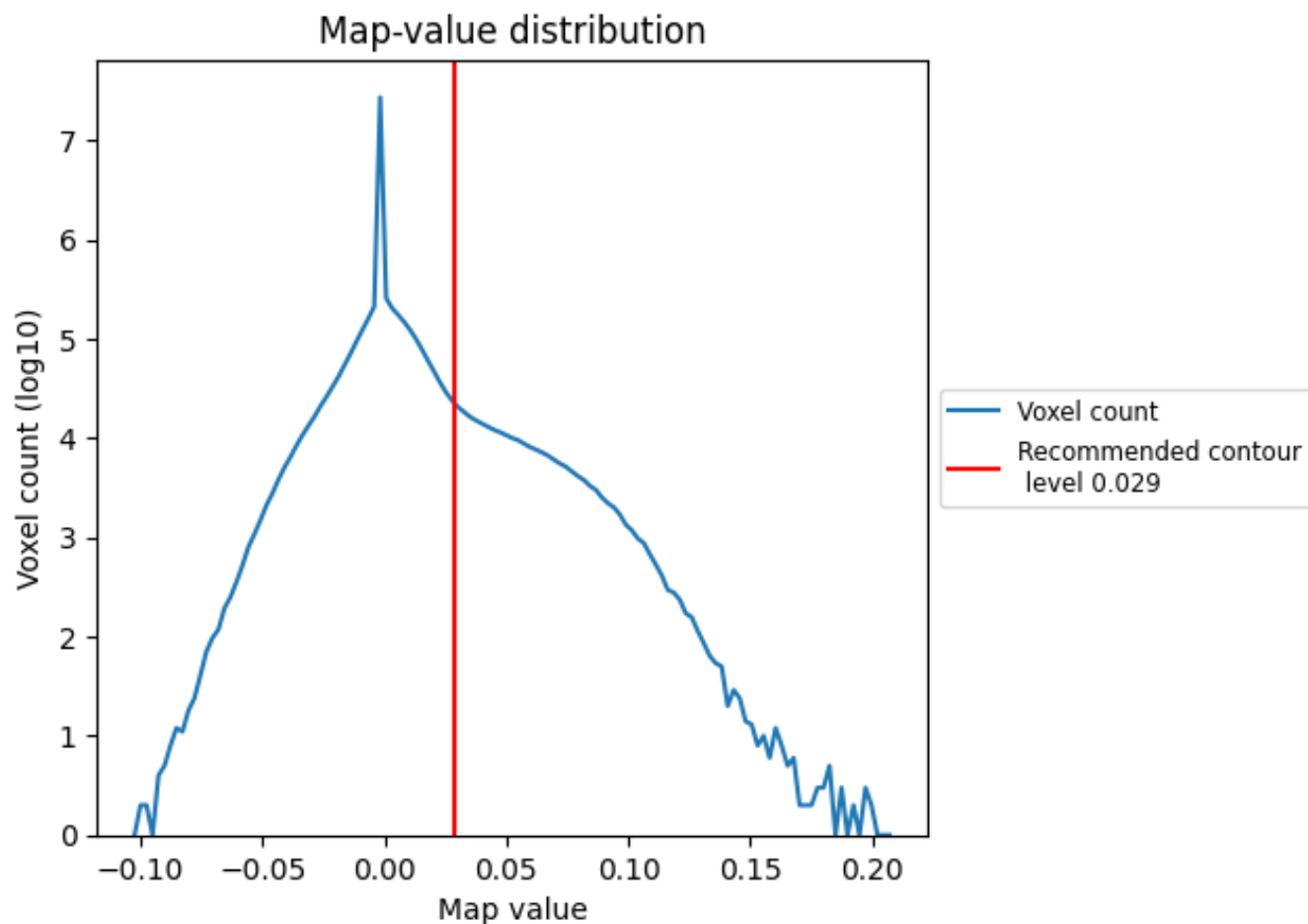
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

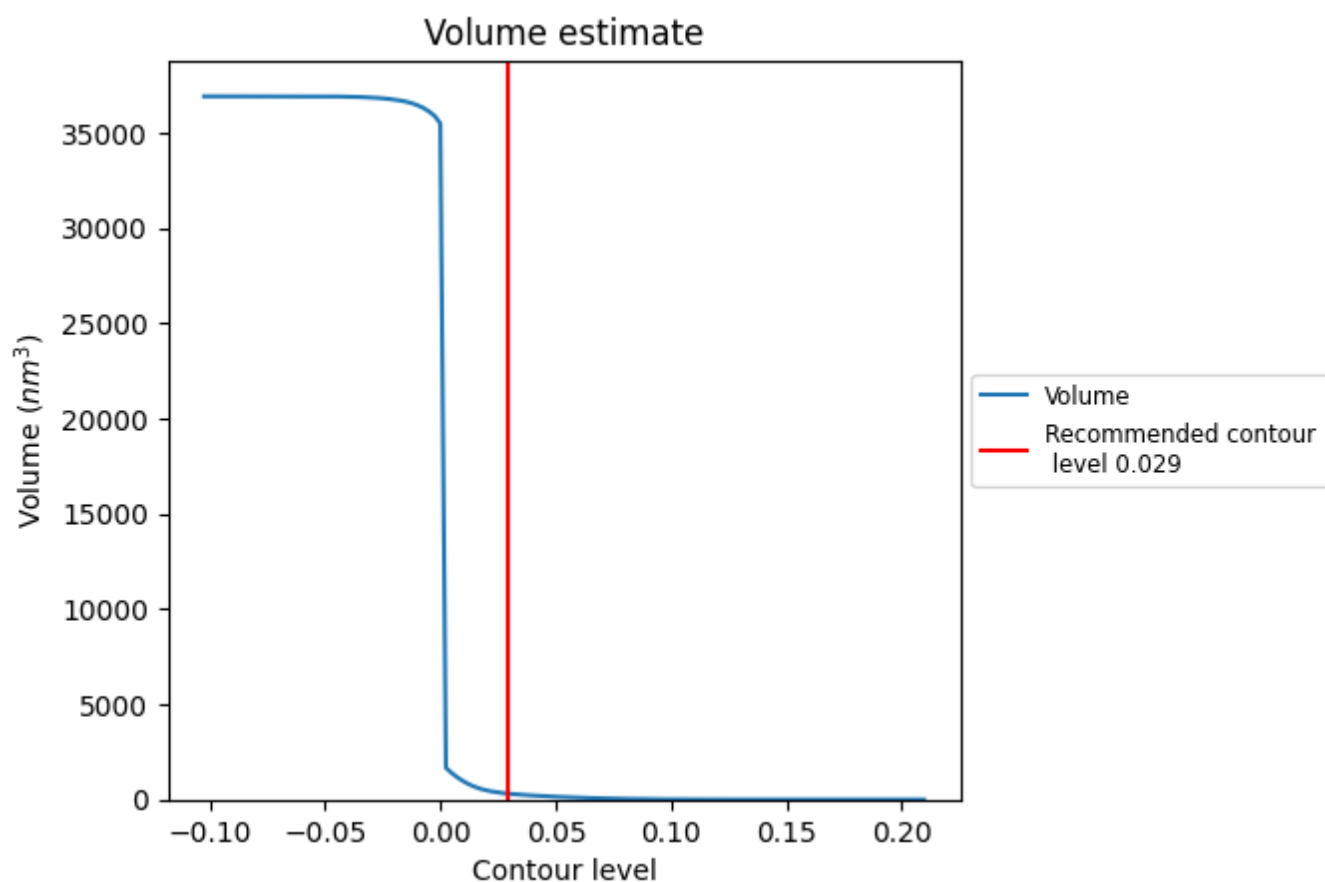
This section contains the results of statistical analysis of the map.

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.

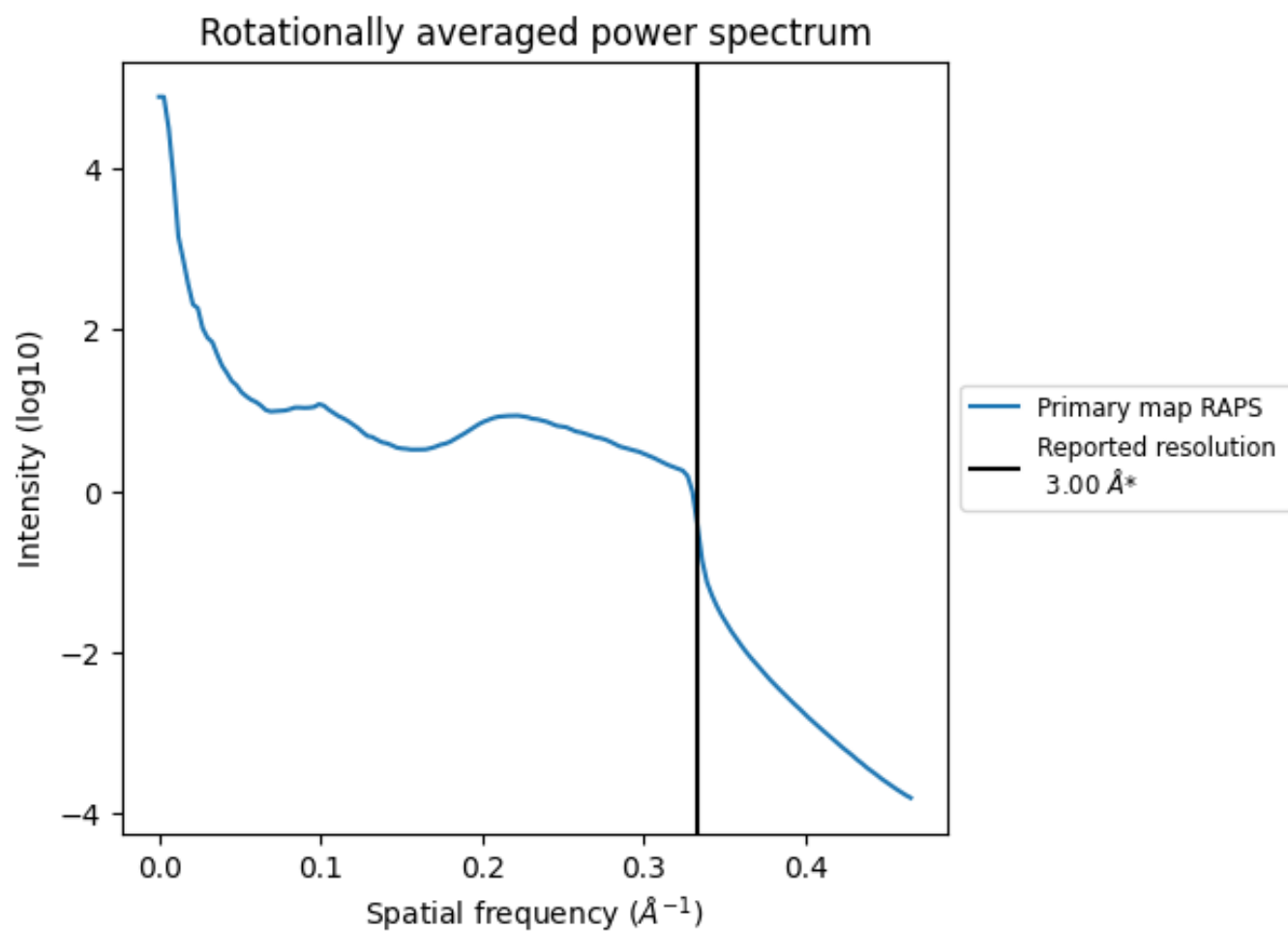
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 314 nm³; this corresponds to an approximate mass of 284 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 0.333 Å⁻¹

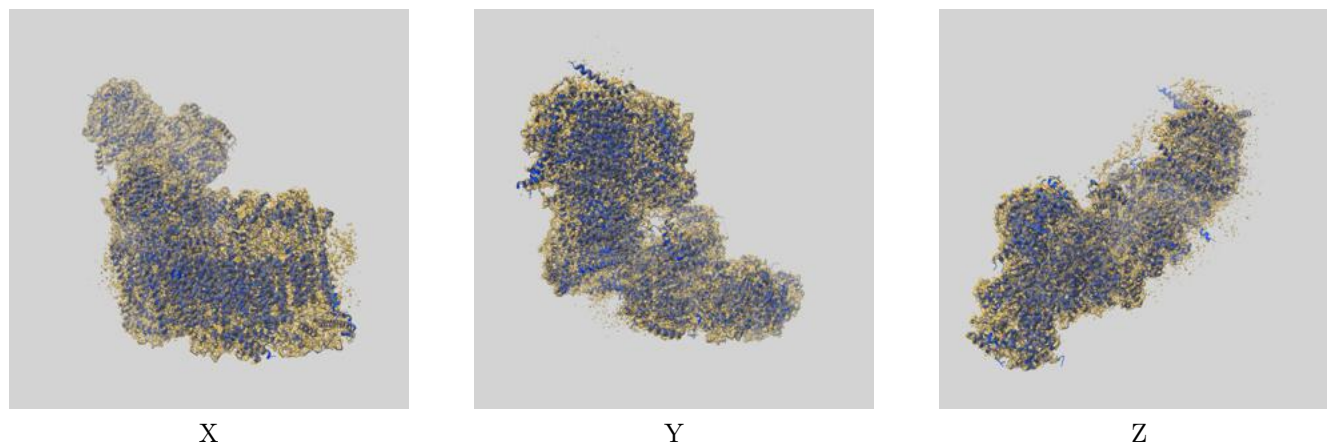
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

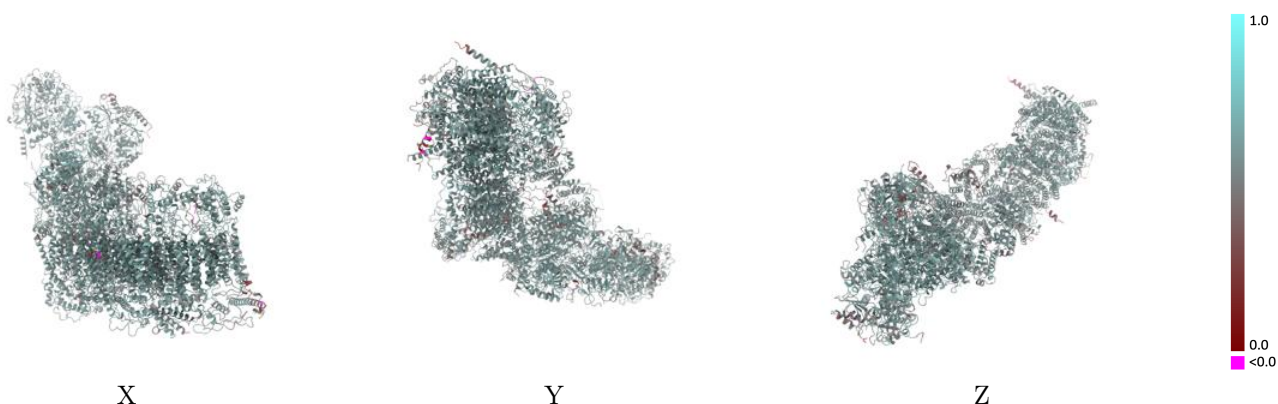
This section contains information regarding the fit between EMDB map EMD-32255 and PDB model 7W1T. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



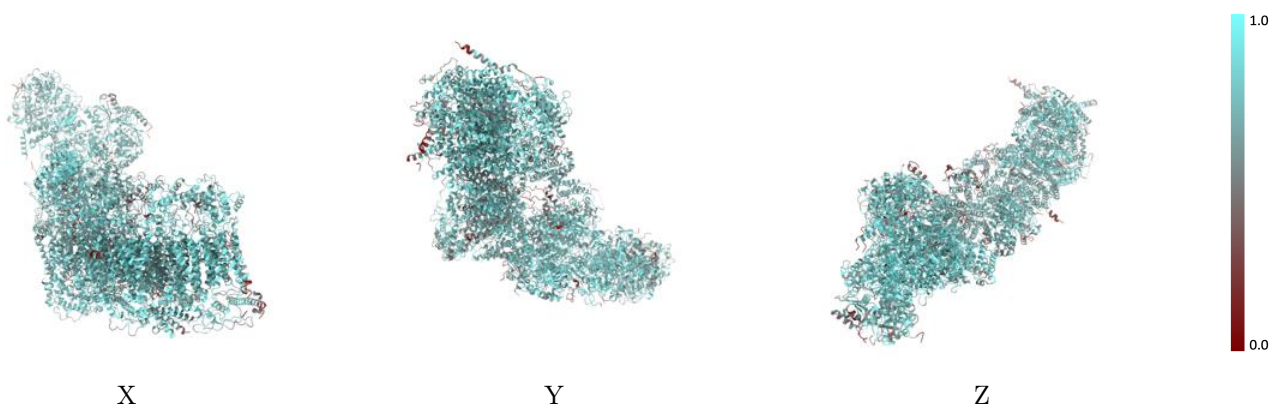
The images above show the 3D surface view of the map at the recommended contour level 0.029 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



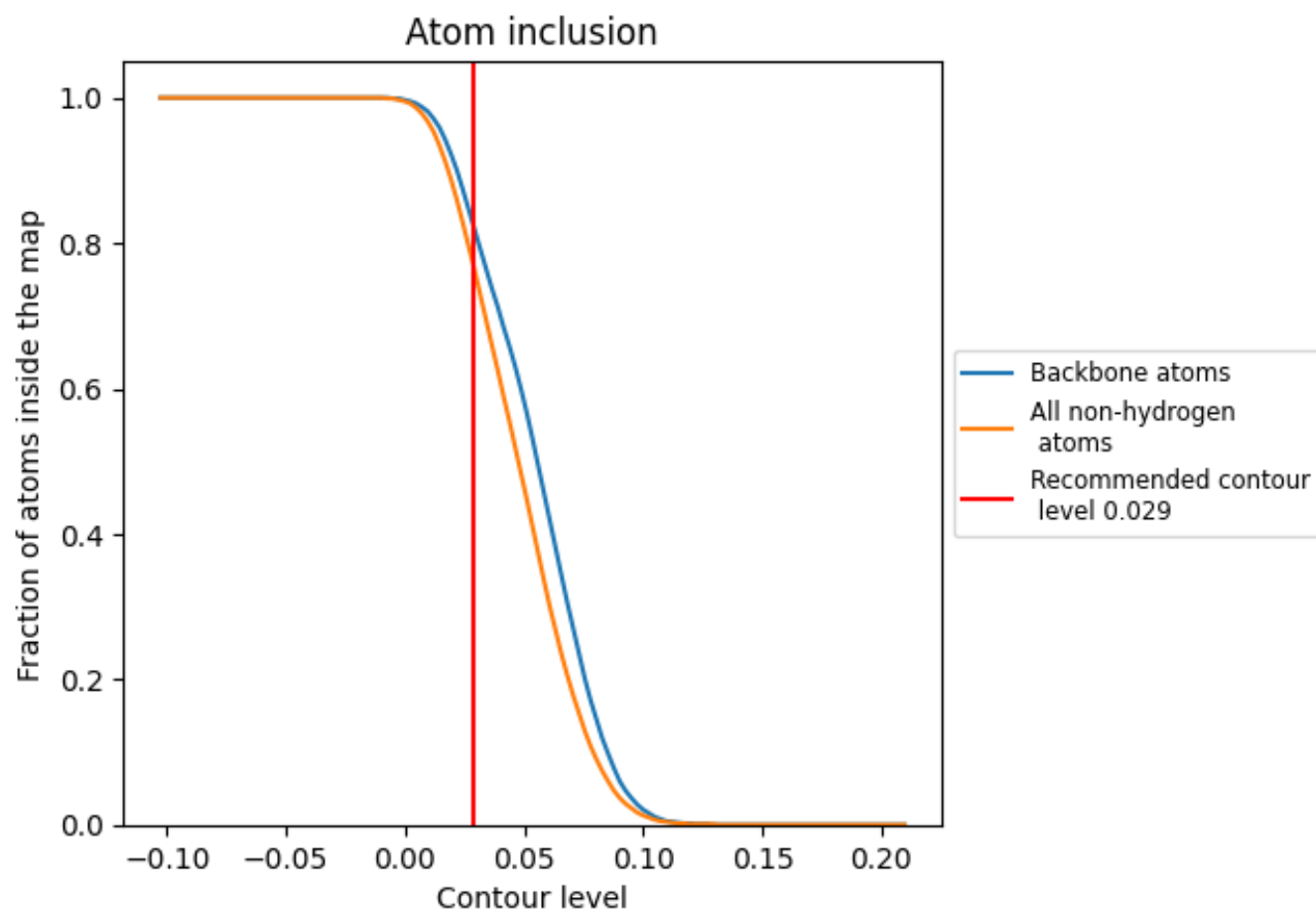
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.029).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 77% 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 (0.029) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7660	 0.5700
A	 0.7530	 0.5600
B	 0.8870	 0.6130
C	 0.8550	 0.6000
E	 0.7550	 0.5650
F	 0.6390	 0.4950
G	 0.5080	 0.4570
H	 0.7620	 0.5540
I	 0.7210	 0.5550
J	 0.7700	 0.5700
K	 0.5100	 0.4710
L	 0.8000	 0.5790
M	 0.7970	 0.5770
N	 0.6890	 0.5700
O	 0.6960	 0.5370
P	 0.8800	 0.6100
Q	 0.8640	 0.6070
S	 0.8240	 0.5800
T	 0.6620	 0.5580
U	 0.7300	 0.5600
V	 0.6460	 0.5500
W	 0.7620	 0.5690
X	 0.6850	 0.5460
Y	 0.6540	 0.5280
Z	 0.6260	 0.5090
a	 0.7720	 0.5860
b	 0.7120	 0.5410
c	 0.7700	 0.5680
d	 0.7290	 0.5540
e	 0.6840	 0.5530
f	 0.5890	 0.5050
g	 0.7960	 0.5790
h	 0.7620	 0.5560
i	 0.8460	 0.6000
j	 0.7300	 0.5790



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Chain	Atom inclusion	Q-score
k	 0.7670	 0.5880
l	 0.7760	 0.5840
m	 0.7100	 0.5380
n	 0.6150	 0.5120
o	 0.7470	 0.5620
p	 0.7790	 0.5750
r	 0.8260	 0.5960
s	 0.8410	 0.5920
u	 0.7720	 0.5600
v	 0.6530	 0.5160
w	 0.7240	 0.5530