



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:22 PM UTC

PDB ID : 7V33 / pdb_00007v33
EMDB ID : EMD-31651
Title : Active state complex I from rotenone-NADH dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-08-10
Resolution : 2.60 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

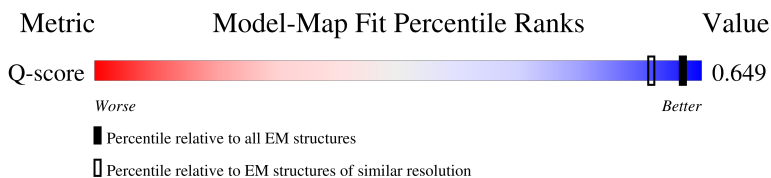
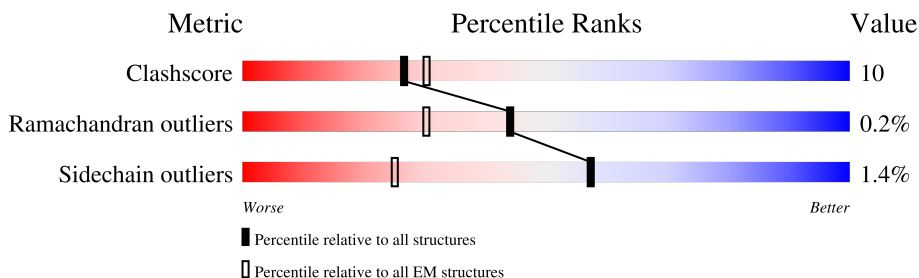
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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.



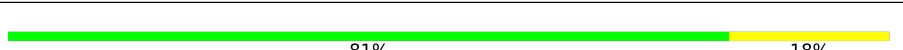
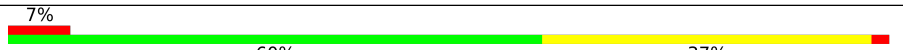
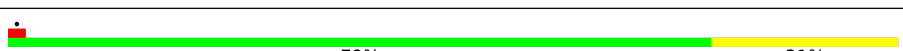
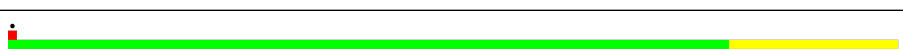
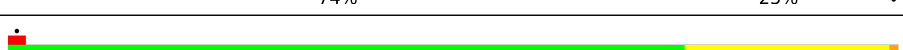
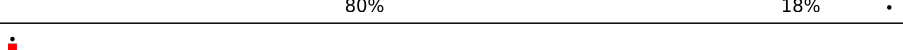
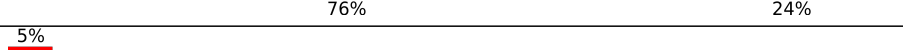
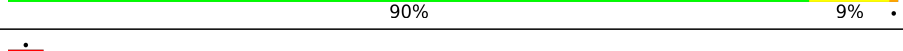
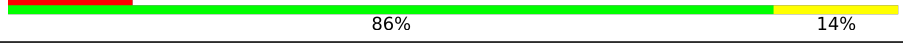
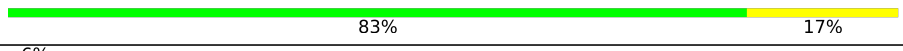
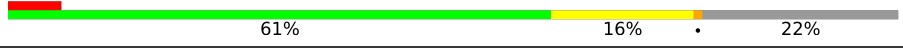
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	

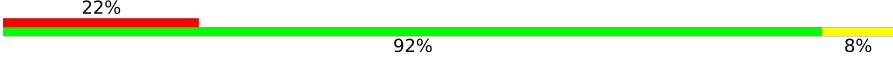
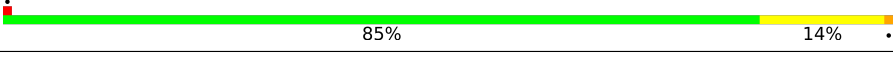
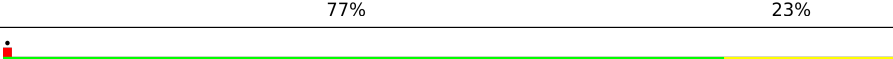
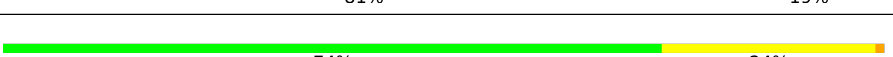
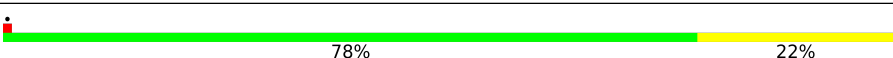
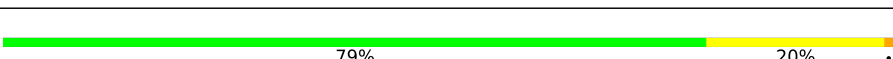
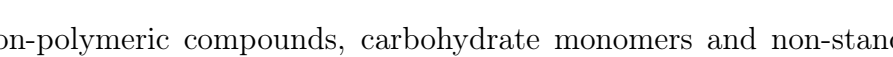
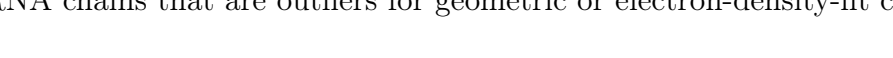
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Mol	Chain	Length	Quality of chain
5	F	86	
6	G	88	
6	X	88	
7	H	112	
8	I	112	
9	J	342	
10	K	43	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	67	
23	Z	80	
24	a	138	
25	b	126	
26	c	156	
27	d	175	
28	e	104	

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Mol	Chain	Length	Quality of chain
29	f	49	
30	g	122	
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	M	802	-	-	X	-
48	PEE	l	703	-	-	X	-
51	CDL	l	701	-	-	X	-

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 68246 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
			3330	2103	593	614	20		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	86	Total	C	N	O	S	0	0
			684	431	129	122	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			693	447	102	139	5		
6	X	88	Total	C	N	O	S	0	0
			696	449	103	139	5		

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

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

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

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

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

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

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

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
			5293	3319	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 NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	430	Total	C	N	O	S	0	0
			3459	2212	594	629	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
			643	417	110	115	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	142	Total	C	N	O	S	0	0
			1161	749	197	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 NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

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	122	Total	C	N	O	S	0	0
			1005	653	174	172	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
			4797	3181	743	822	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
			1276	850	187	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
			3624	2406	572	608	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
			2508	1678	385	424	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
			1036	646	196	185	9		

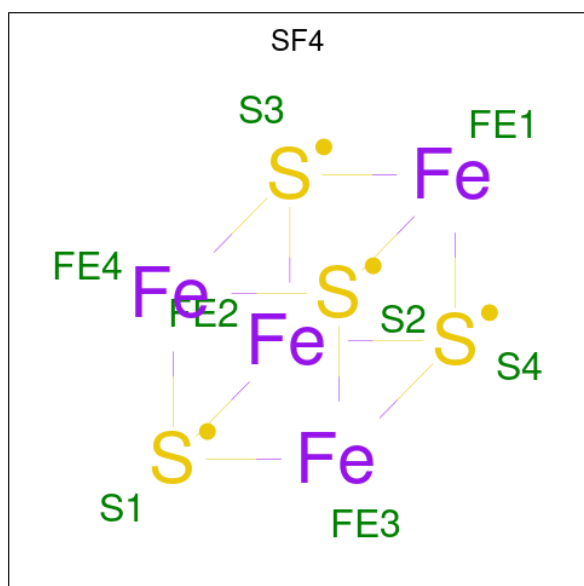
There is a discrepancy between the modelled and reference sequences:

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.

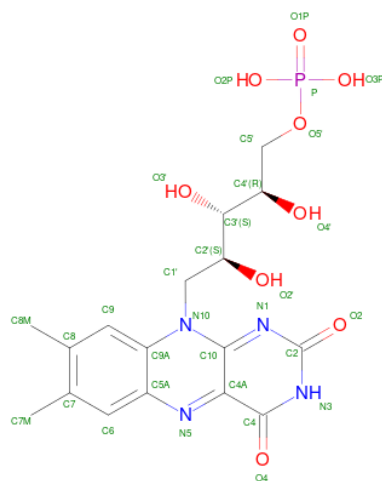
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2586	1646	439	491	10		

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



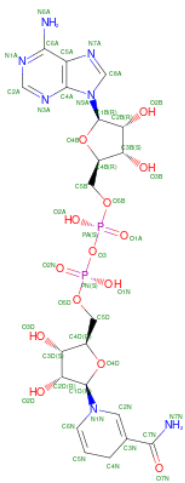
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

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



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

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



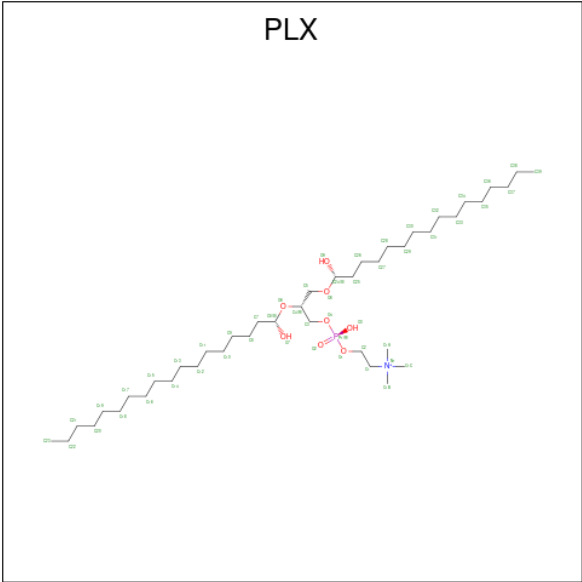
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total 44	C 21	N 7	O 14	P 2	0

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



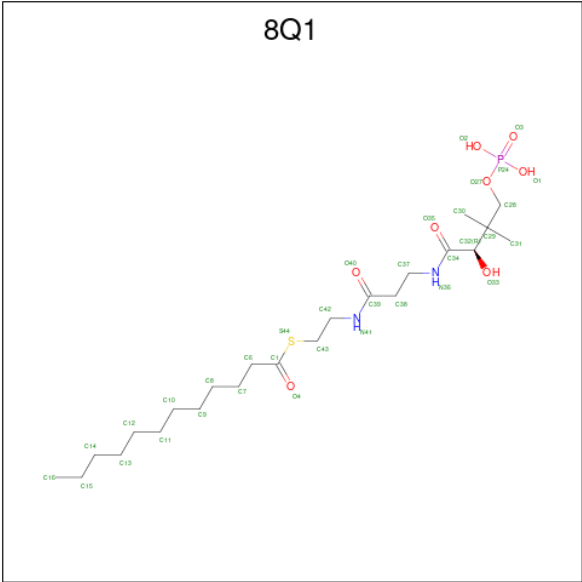
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	V	1	Total	N				0
			1	1				
48	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	j	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	l	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	l	1	Total	C	N	O	P	0
			50	40	1	8	1	
48	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	r	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



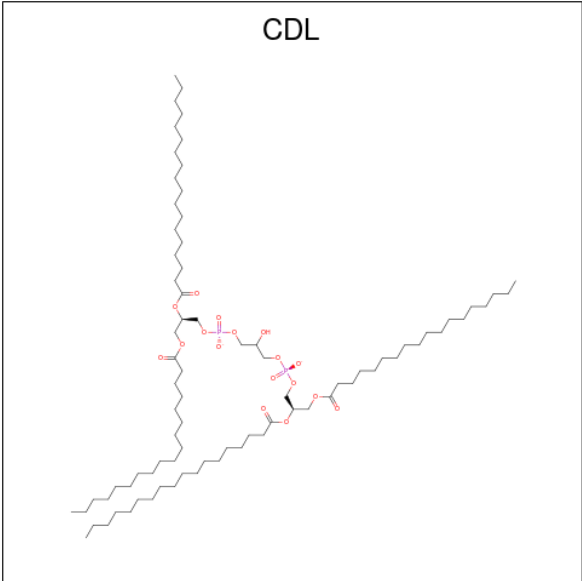
Mol	Chain	Residues	Atoms					AltConf
49	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	J	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42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

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



Mol	Chain	Residues	Atoms						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 CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



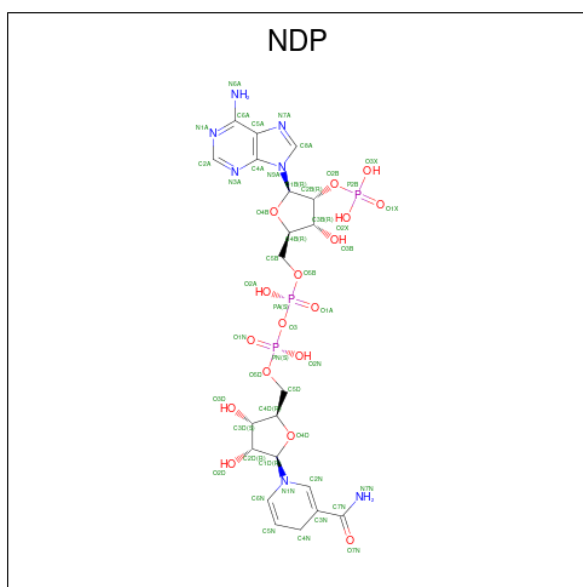
Mol	Chain	Residues	Atoms				AltConf
51	I	1	Total	C	O	P	0
			51	32	17	2	

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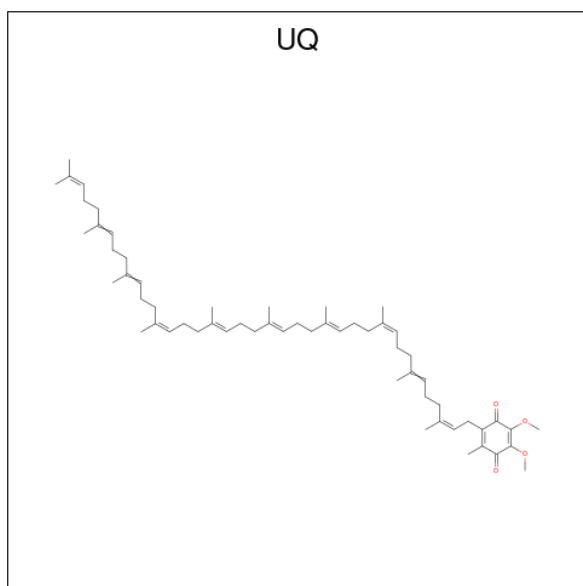
Mol	Chain	Residues	Atoms				AltConf
51	V	1	Total	C	O	P	0
			94	75	17	2	
51	a	1	Total	C	O	P	0
			100	81	17	2	
51	i	1	Total	C	O	P	0
			100	81	17	2	
51	k	1	Total	C	O	P	0
			78	59	17	2	
51	l	1	Total	C	O	P	0
			99	80	17	2	
51	l	1	Total	C	O	P	0
			100	81	17	2	
51	m	1	Total	C	O	P	0
			89	70	17	2	
51	o	1	Total	C	O	P	0
			100	81	17	2	
51	r	1	Total	C	O	P	0
			99	80	17	2	
51	u	1	Total	C	O	P	0
			55	36	17	2	

- Molecule 52 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).



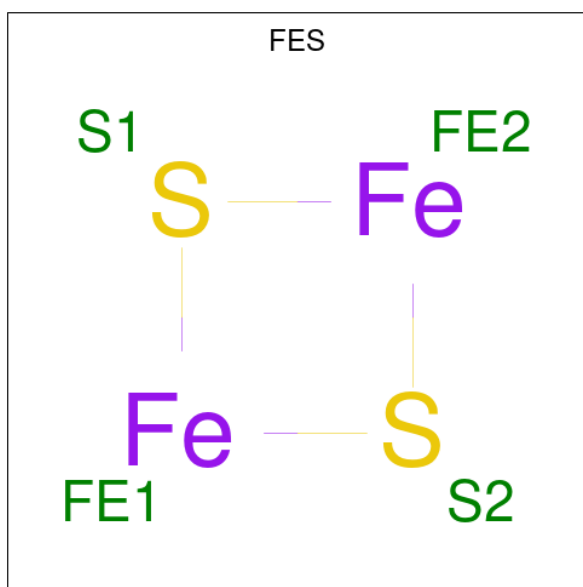
Mol	Chain	Residues	Atoms					AltConf
52	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 53 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

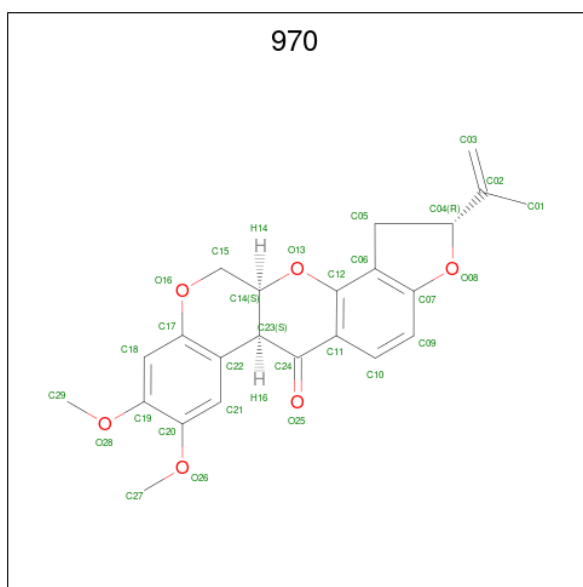


Mol	Chain	Residues	Atoms			AltConf
54	M	1	Total	Fe	S	0
			4	2	2	
54	O	1	Total	Fe	S	0
			4	2	2	

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 56 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).

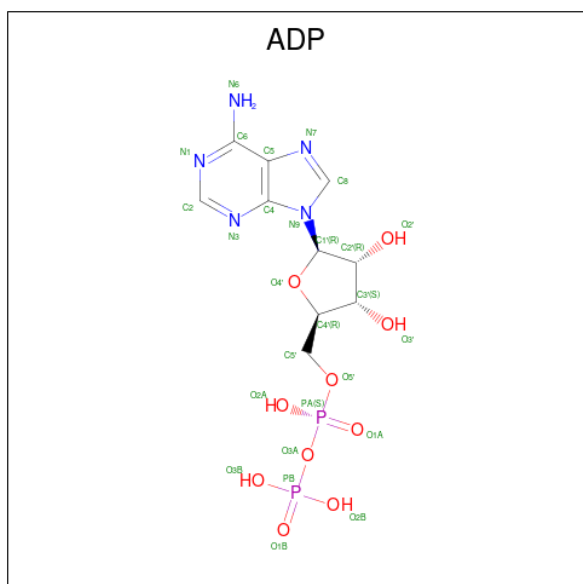


Mol	Chain	Residues	Atoms			AltConf
56	Q	1	Total	C	O	0
			29	23	6	

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 58 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

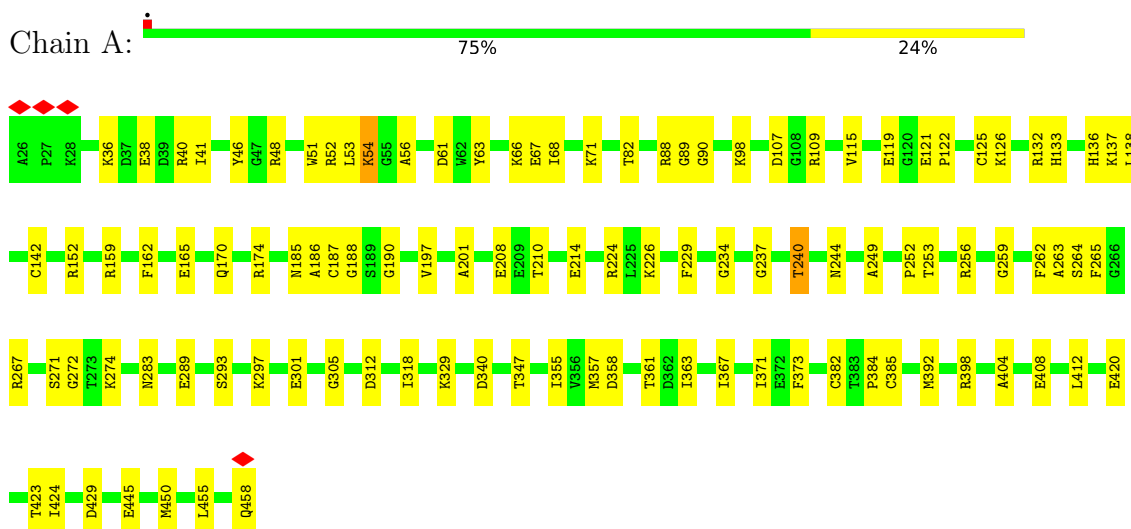


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	w	1	27	10	5	10	2	0

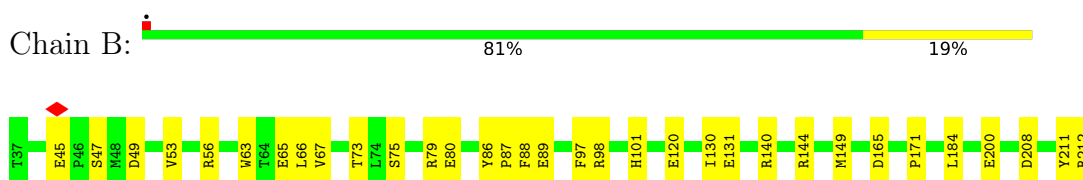
3 Residue-property plots

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

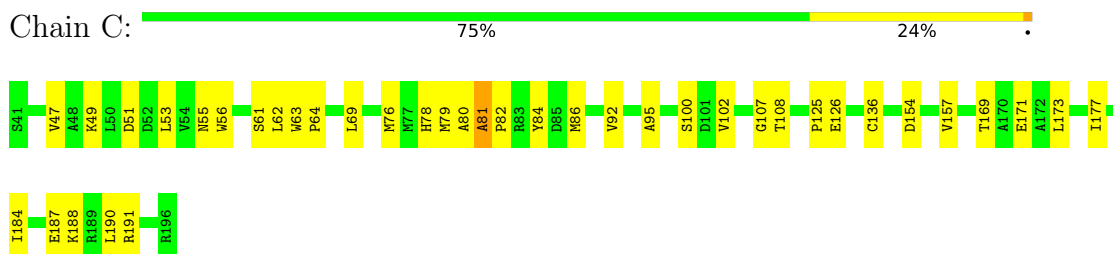
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



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



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



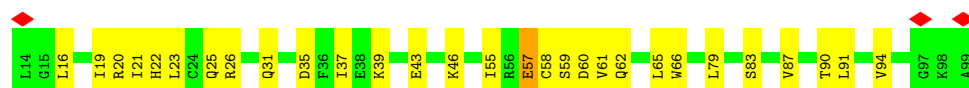
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain E:  84% 15%



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

Chain F:  66% 33%



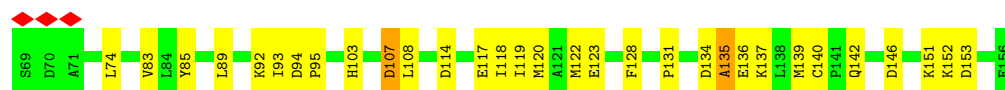
- Molecule 6: Acyl carrier protein, mitochondrial

Chain G:  17% 63% 33% 5%



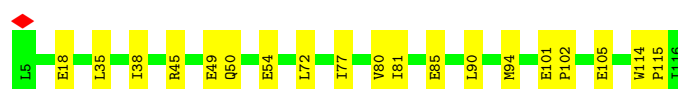
- Molecule 6: Acyl carrier protein, mitochondrial

Chain X:  65% 33%



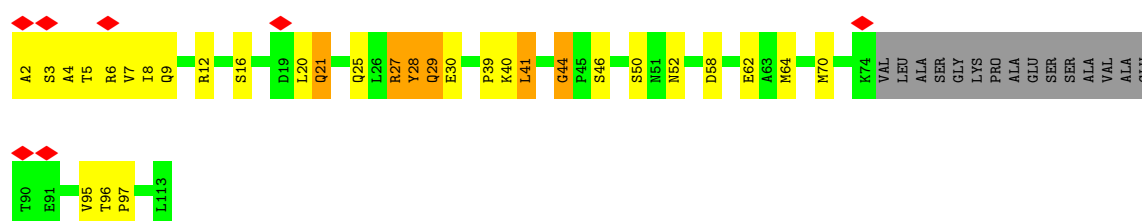
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain H:  83% 17%

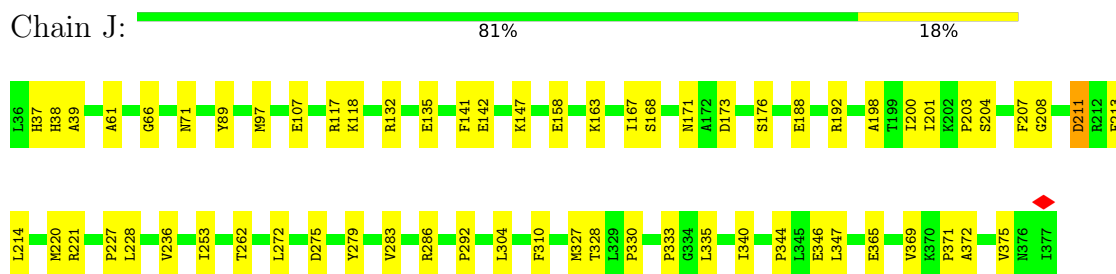


- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

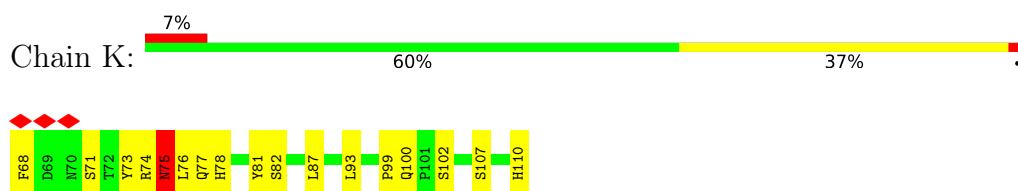
Chain I:  6% 59% 22% 5% 13%



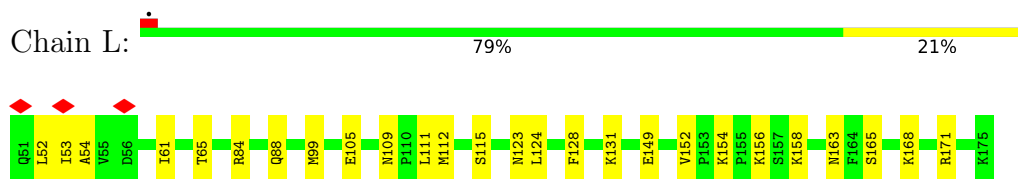
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



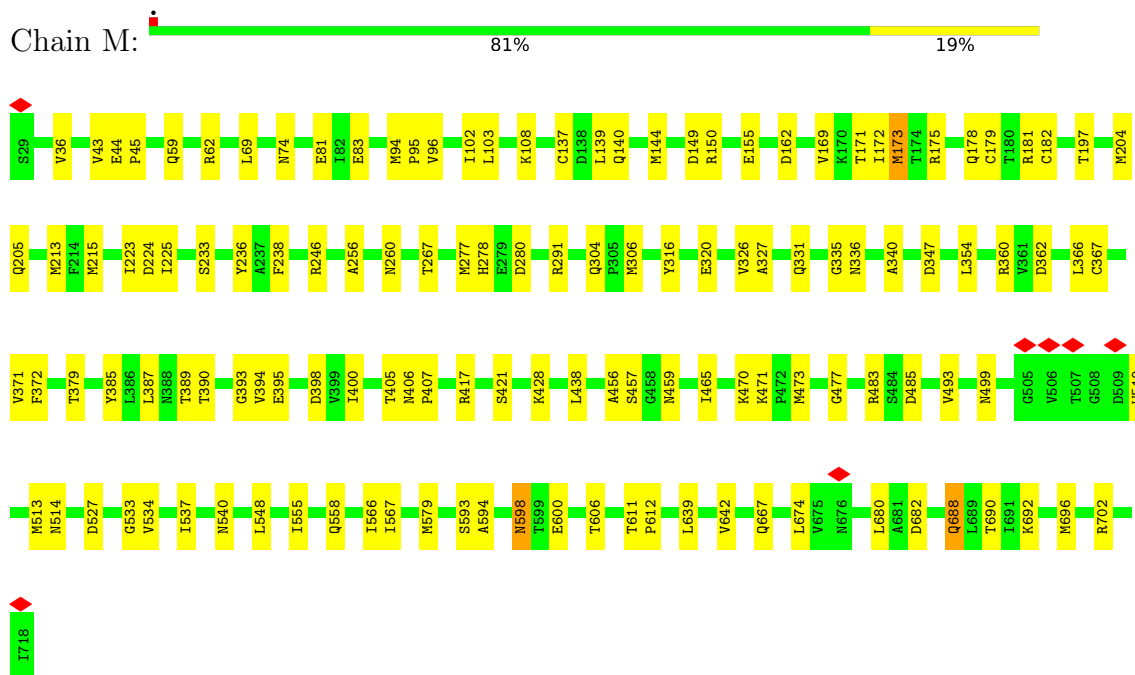
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



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

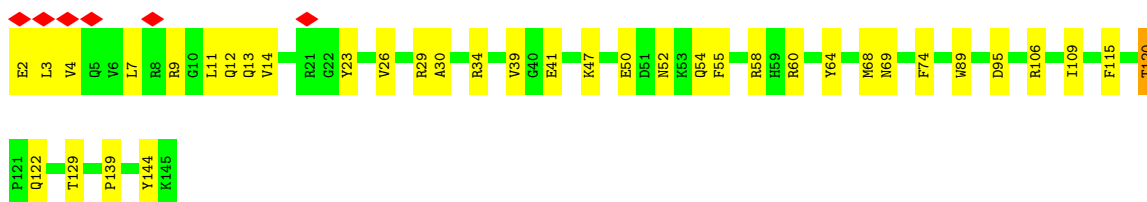


- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



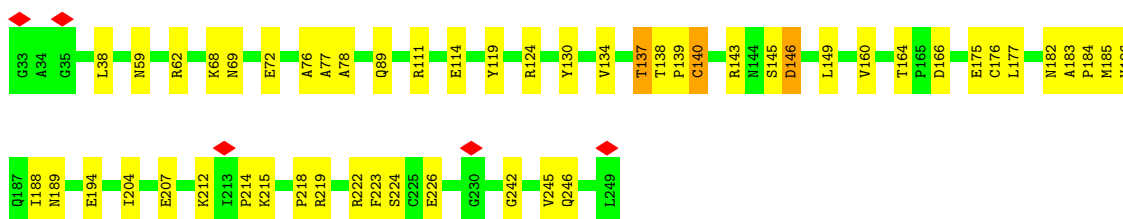
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain N:  74% 25%



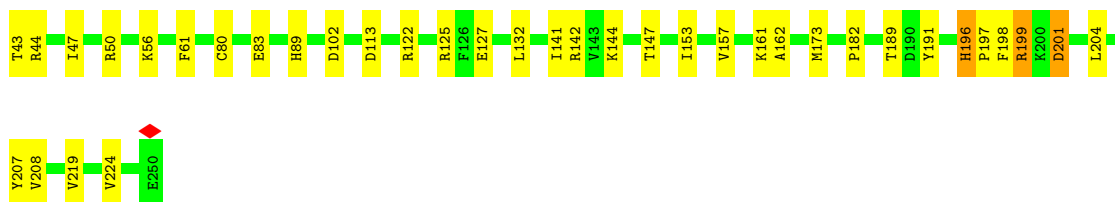
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain O:  76% 23%



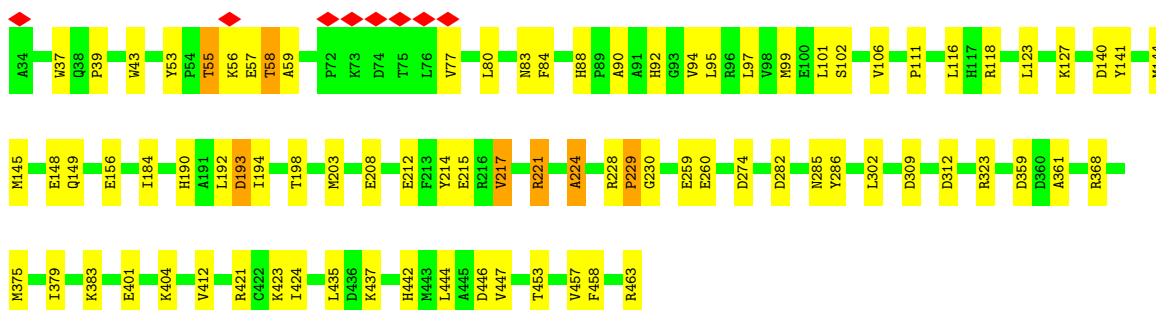
- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain P:  82% 16%



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

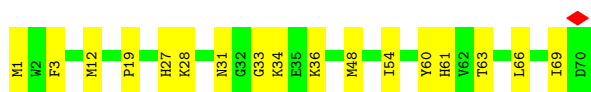
Chain Q:  80% 18%



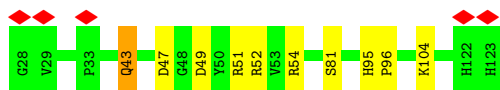
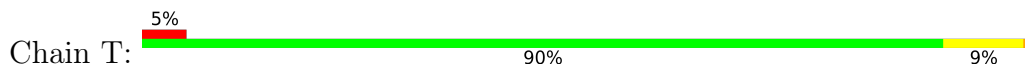
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S:  76% 24%

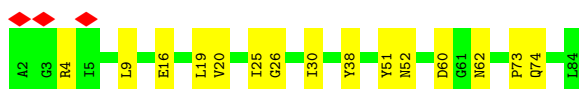
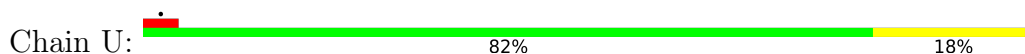




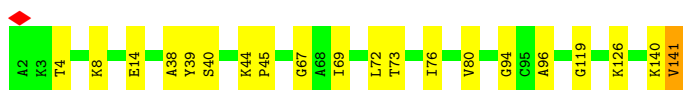
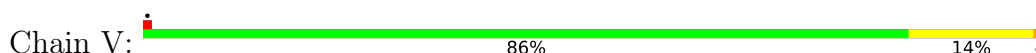
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



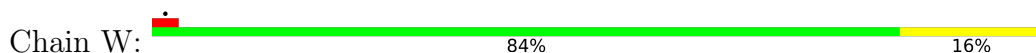
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



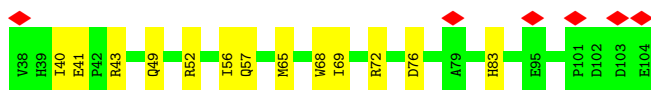
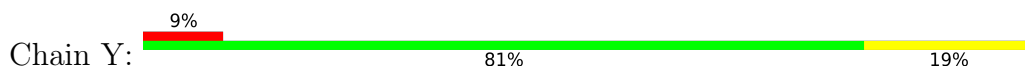
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



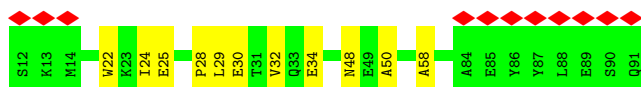
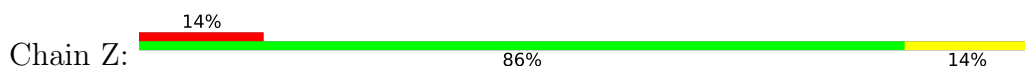
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



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



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



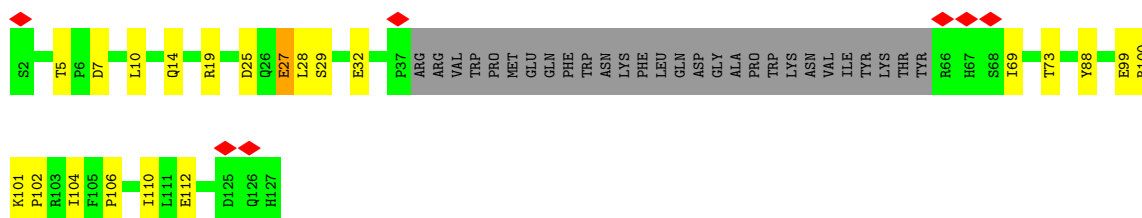
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a: 



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

Chain b: 



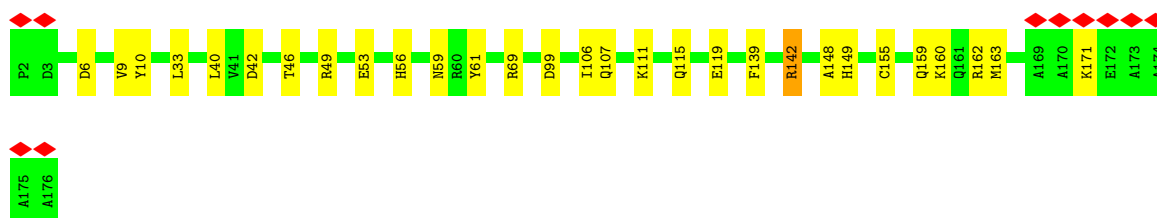
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c: 



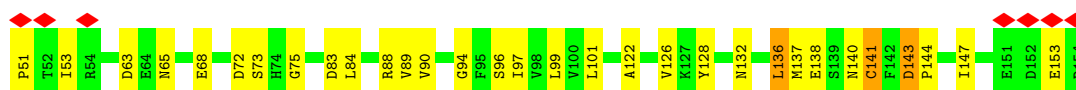
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d: 

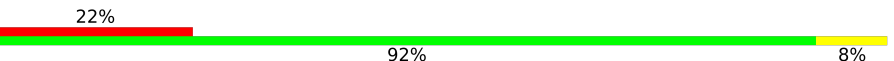


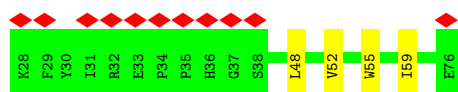
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e: 

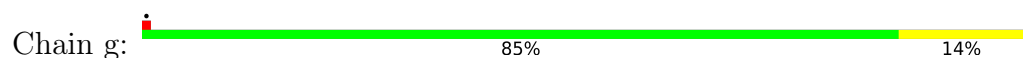


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

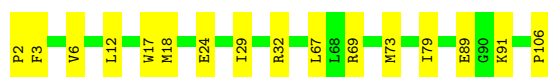
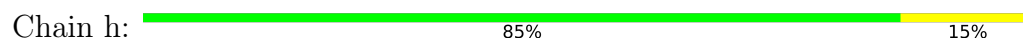
Chain f: 



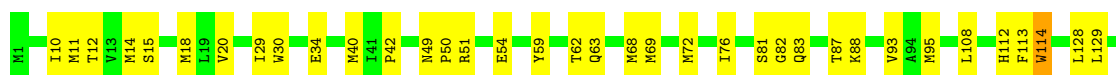
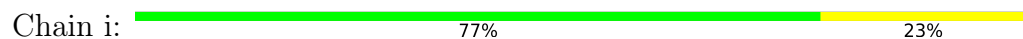
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



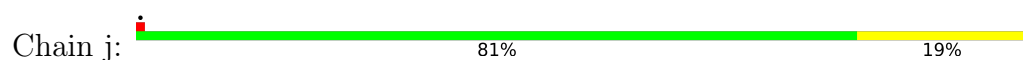
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



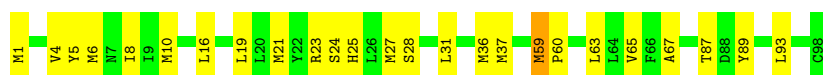
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



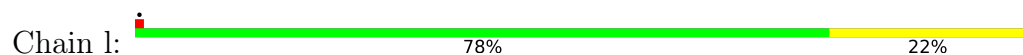
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

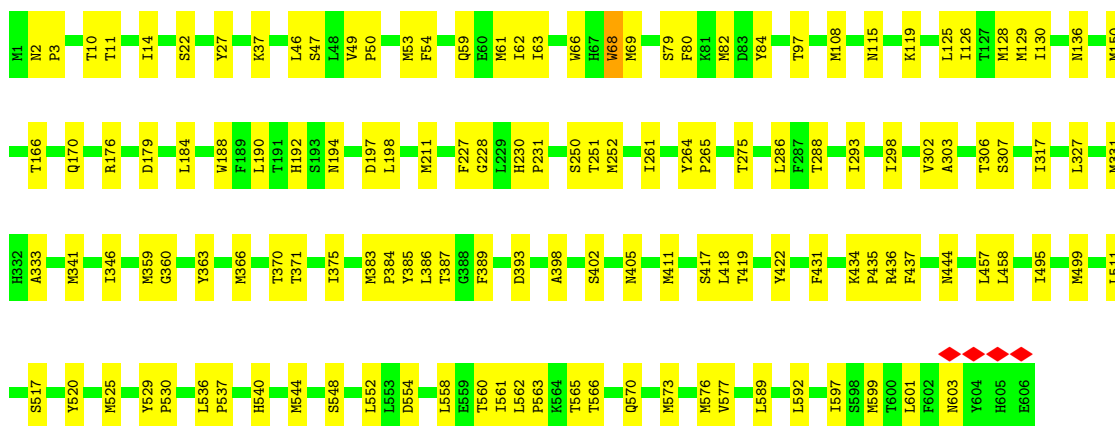


- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

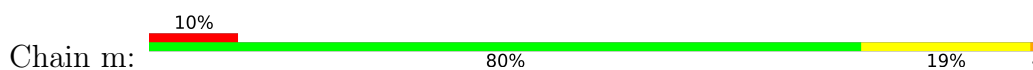


- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

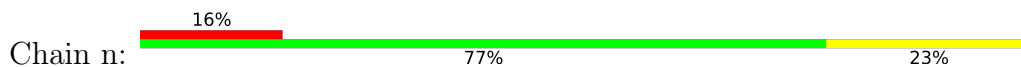




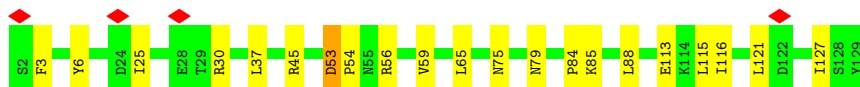
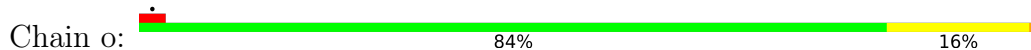
• Molecule 36: NADH-ubiquinone oxidoreductase chain 6



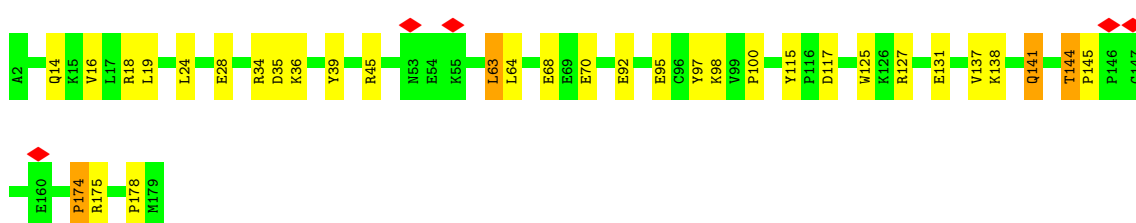
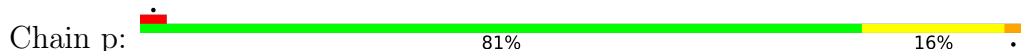
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



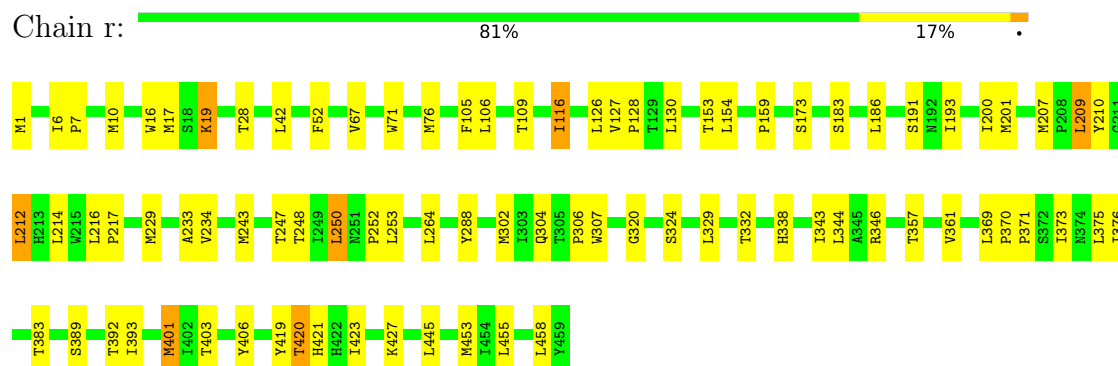
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



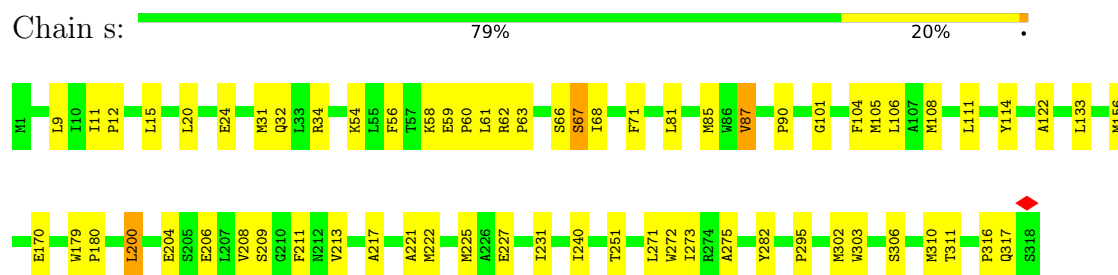
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



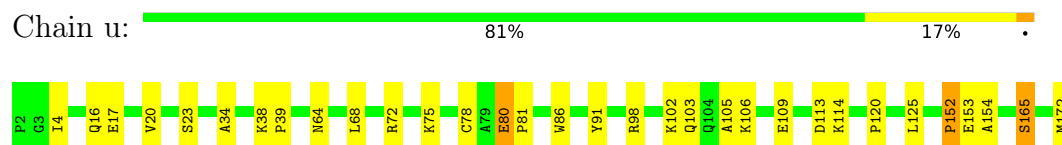
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4



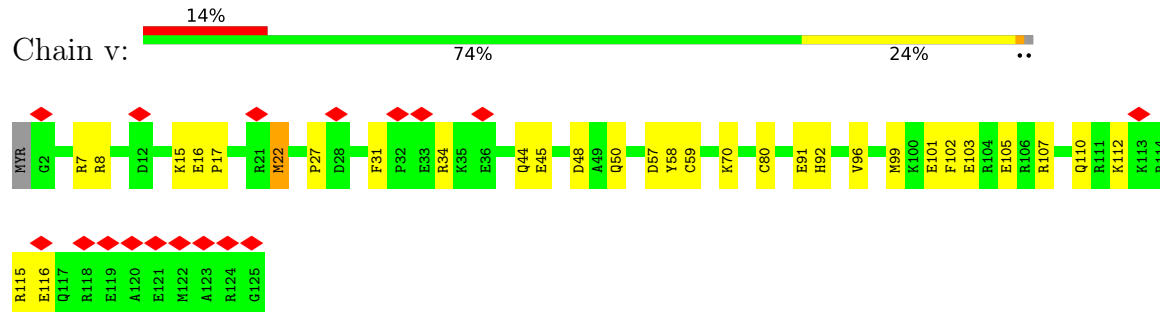
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1



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



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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	326044	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	0.248	Depositor
Minimum map value	-0.137	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0271	Depositor
Map size ($\text{\AA}$)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.24	0/3406	0.46	0/4603
2	B	0.26	0/1443	0.46	2/1952 (0.1%)
3	C	0.31	0/1279	0.52	2/1730 (0.1%)
4	E	0.22	0/995	0.44	1/1340 (0.1%)
5	F	0.27	0/695	0.56	1/936 (0.1%)
6	G	0.22	0/705	0.56	1/956 (0.1%)
6	X	0.26	0/708	0.70	2/959 (0.2%)
7	H	0.23	0/929	0.53	0/1258
8	I	0.29	0/798	0.72	3/1079 (0.3%)
9	J	0.23	0/2828	0.45	1/3834 (0.0%)
10	K	0.29	0/377	0.68	1/509 (0.2%)
11	L	0.24	0/1039	0.38	0/1403
12	M	0.29	0/5381	0.60	7/7291 (0.1%)
13	N	0.19	0/1245	0.38	0/1694
14	O	0.24	0/1711	0.53	0/2328
15	P	0.30	0/1789	0.58	3/2436 (0.1%)
16	Q	0.38	4/3538 (0.1%)	0.55	6/4796 (0.1%)
17	S	0.29	0/581	0.55	0/781
18	T	0.23	0/755	0.42	0/1018
19	U	0.18	0/664	0.33	0/912
20	V	0.22	0/1042	0.45	0/1411
21	W	0.22	0/1192	0.44	0/1610
22	Y	0.17	0/610	0.39	0/836
23	Z	0.15	0/660	0.34	0/892
24	a	0.24	0/1184	0.49	1/1603 (0.1%)
25	b	0.21	0/844	0.40	0/1149
26	c	0.27	0/1371	0.62	4/1875 (0.2%)
27	d	0.23	0/1494	0.48	1/2015 (0.0%)
28	e	0.23	0/891	0.63	2/1210 (0.2%)
29	f	0.18	0/385	0.38	0/522
30	g	0.22	0/1036	0.43	2/1401 (0.1%)
31	h	0.25	0/889	0.46	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.28	0/2773	0.53	3/3768 (0.1%)
33	j	0.24	0/938	0.40	0/1281
34	k	0.29	0/759	0.59	0/1029
35	l	0.23	0/4926	0.47	3/6700 (0.0%)
36	m	0.25	0/1307	0.60	2/1777 (0.1%)
37	n	0.17	0/491	0.35	0/663
38	o	0.24	0/1092	0.55	3/1481 (0.2%)
39	p	0.20	0/1590	0.43	2/2155 (0.1%)
40	r	0.26	0/3715	0.49	2/5067 (0.0%)
41	s	0.29	0/2581	0.60	6/3529 (0.2%)
42	u	0.26	0/1436	0.53	0/1938
43	v	0.19	0/1060	0.41	0/1421
44	w	0.18	0/2646	0.37	0/3584
All	All	0.26	4/67778 (0.0%)	0.51	61/91922 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	193	ASP	C-N	8.54	1.44	1.33
16	Q	141	TYR	C-N	-7.96	1.25	1.33
16	Q	140	ASP	C-N	6.68	1.45	1.33
16	Q	192	LEU	C-N	-5.05	1.27	1.33

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	74	ASN	N-CA-C	9.81	122.06	111.36
41	s	206	GLU	N-CA-C	9.80	122.05	111.36
28	e	143	ASP	CA-C-N	9.60	129.71	119.05
28	e	143	ASP	C-N-CA	9.60	129.71	119.05
36	m	23	LYS	CA-C-N	9.54	131.76	119.84
36	m	23	LYS	C-N-CA	9.54	131.76	119.84
8	I	28	TYR	N-CA-C	9.47	121.68	111.36
40	r	250	LEU	N-CA-C	8.05	120.06	111.28
9	J	213	PHE	N-CA-C	8.03	119.66	111.07
27	d	142	ARG	N-CA-C	7.77	119.53	111.14
24	a	163	ARG	N-CA-C	7.25	119.26	111.36
16	Q	193	ASP	O-C-N	7.16	129.83	122.09
6	G	106	LYS	N-CA-C	7.00	118.70	111.14
12	M	173	MET	N-CA-C	6.64	120.48	112.38
16	Q	102	SER	N-CA-C	-6.61	97.75	108.52
16	Q	224	ALA	N-CA-C	6.59	118.13	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	126	TRP	CA-C-N	6.56	134.08	121.54
26	c	126	TRP	C-N-CA	6.56	134.08	121.54
41	s	204	GLU	N-CA-C	6.49	118.01	111.07
38	o	53	ASP	CA-C-N	6.46	125.89	118.85
38	o	53	ASP	C-N-CA	6.46	125.89	118.85
40	r	421	HIS	N-CA-C	6.32	118.17	111.28
6	X	135	ALA	N-CA-C	6.31	118.16	111.28
32	i	112	HIS	N-CA-C	6.27	120.54	113.01
39	p	144	THR	CA-C-N	6.27	126.83	120.38
39	p	144	THR	C-N-CA	6.27	126.83	120.38
35	l	192	HIS	N-CA-C	6.21	118.12	111.36
8	I	44	GLY	CA-C-N	6.15	126.04	119.28
8	I	44	GLY	C-N-CA	6.15	126.04	119.28
16	Q	141	TYR	CA-C-N	-6.12	115.34	122.14
16	Q	141	TYR	C-N-CA	-6.12	115.34	122.14
26	c	44	THR	CA-C-N	6.08	125.80	119.05
26	c	44	THR	C-N-CA	6.08	125.80	119.05
4	E	97	TRP	N-CA-C	-6.05	104.77	111.36
41	s	211	PHE	N-CA-C	5.98	117.80	111.28
15	P	196	HIS	CA-C-N	5.67	125.35	119.05
15	P	196	HIS	C-N-CA	5.67	125.35	119.05
12	M	406	ASN	CA-C-N	5.65	125.32	119.05
12	M	406	ASN	C-N-CA	5.65	125.32	119.05
38	o	127	ILE	N-CA-C	5.61	116.34	110.62
41	s	200	LEU	N-CA-C	5.58	117.44	111.36
35	l	68	TRP	N-CA-C	5.51	117.09	111.14
2	B	45	GLU	CA-C-N	5.43	125.19	119.76
2	B	45	GLU	C-N-CA	5.43	125.19	119.76
12	M	371	VAL	N-CA-C	5.42	116.05	108.89
30	g	7	ARG	N-CA-C	-5.35	103.29	109.93
30	g	3	MET	N-CA-C	5.34	117.18	111.36
15	P	102	ASP	N-CA-C	5.34	120.07	113.50
5	F	25	GLN	N-CA-C	5.30	117.06	111.28
10	K	75	ASN	N-CA-C	5.30	122.09	110.80
32	i	113	PHE	N-CA-C	5.25	117.00	111.28
41	s	217	ALA	N-CA-C	5.23	116.91	108.08
35	l	198	LEU	N-CA-C	5.18	116.93	111.28
16	Q	217	VAL	N-CA-C	5.14	115.91	110.72
6	X	107	ASP	N-CA-C	5.13	116.95	111.36
12	M	612	PRO	CA-C-N	5.12	125.02	119.85
12	M	612	PRO	C-N-CA	5.12	125.02	119.85
3	C	81	ALA	CA-C-N	5.07	126.17	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	81	ALA	C-N-CA	5.07	126.17	119.84
32	i	114	TRP	N-CA-C	5.04	117.51	111.71
41	s	67	SER	N-CA-C	-5.02	100.54	108.73

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	3330	0	3292	82	0
2	B	1412	0	1363	25	0
3	C	1248	0	1254	40	0
4	E	971	0	975	17	0
5	F	684	0	700	23	0
6	G	693	0	671	35	0
6	X	696	0	680	25	0
7	H	910	0	950	12	0
8	I	780	0	808	35	0
9	J	2751	0	2773	43	0
10	K	366	0	338	16	0
11	L	1016	0	1016	21	0
12	M	5293	0	5326	92	0
13	N	1204	0	1162	30	0
14	O	1671	0	1674	42	0
15	P	1738	0	1693	34	0
16	Q	3459	0	3396	68	0
17	S	566	0	561	19	0
18	T	741	0	702	7	0
19	U	643	0	642	16	0
20	V	1021	0	1025	16	0
21	W	1161	0	1144	20	0
22	Y	584	0	529	14	0
23	Z	641	0	620	9	0
24	a	1151	0	1164	22	0
25	b	819	0	835	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	c	1315	0	1208	23	0
27	d	1461	0	1429	34	0
28	e	867	0	817	34	0
29	f	377	0	353	2	0
30	g	1005	0	999	25	0
31	h	867	0	871	15	0
32	i	2710	0	2874	68	0
33	j	914	0	951	29	0
34	k	748	0	799	26	0
35	l	4797	0	4935	107	0
36	m	1276	0	1243	43	0
37	n	479	0	486	14	0
38	o	1062	0	1072	19	0
39	p	1534	0	1470	31	0
40	r	3624	0	3832	62	0
41	s	2508	0	2607	67	0
42	u	1398	0	1374	26	0
43	v	1036	0	992	26	0
44	w	2586	0	2542	43	0
45	A	8	0	0	1	0
45	B	16	0	0	0	0
45	C	8	0	0	1	0
45	M	16	0	0	3	0
46	A	31	0	19	5	0
47	A	44	0	27	5	0
48	B	51	0	82	4	0
48	C	47	0	71	7	0
48	U	51	0	82	18	0
48	V	1	0	0	0	0
48	W	41	0	59	4	0
48	j	41	0	59	15	0
48	l	143	0	217	32	0
48	r	51	0	82	8	0
49	C	52	0	88	8	0
49	J	52	0	88	11	0
49	a	52	0	88	1	0
49	g	52	0	88	7	0
49	j	52	0	88	3	0
49	r	104	0	176	11	0
50	G	35	0	0	1	0
50	X	35	0	0	7	0
51	I	51	0	46	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	V	94	0	138	10	0
51	a	100	0	156	6	0
51	i	100	0	156	19	0
51	k	78	0	106	5	0
51	l	199	0	307	51	0
51	m	89	0	125	5	0
51	o	100	0	156	9	0
51	r	99	0	151	7	0
51	u	55	0	54	9	0
52	J	48	0	26	1	0
53	J	33	0	39	5	0
53	s	38	0	47	6	0
54	M	4	0	0	0	0
54	O	4	0	0	0	0
55	M	1	0	0	0	0
56	Q	29	0	0	0	0
57	T	1	0	0	0	0
58	w	27	0	11	8	0
All	All	68246	0	68979	1372	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (1372) 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)
9:J:220:MET:CE	9:J:227:PRO:HD2	1.58	1.32
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.22
6:G:105:MET:HG2	6:G:139:MET:CE	1.68	1.21
1:A:66:LYS:HE3	1:A:188:GLY:O	1.42	1.18
49:J:403:PLX:H131	48:j:201:PEE:C37	1.76	1.15
6:G:105:MET:HE2	6:G:139:MET:SD	1.88	1.14
30:g:2:THR:HG21	30:g:5:SER:CB	1.76	1.14
8:I:4:ALA:HA	51:I:201:CDL:OA2	1.50	1.10
9:J:220:MET:HE3	9:J:227:PRO:HD2	1.34	1.10
30:g:2:THR:CG2	30:g:5:SER:HB2	1.80	1.09
6:G:105:MET:HG2	6:G:139:MET:HE1	1.36	1.08
51:l:701:CDL:H541	51:l:701:CDL:HA62	1.38	1.05
44:w:139:ARG:HH12	58:w:401:ADP:N6	1.52	1.05
30:g:2:THR:HG21	30:g:5:SER:HB2	1.05	1.03
1:A:82:THR:HG23	1:A:259:GLY:HA3	1.37	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:l:703:PEE:H37	48:l:703:PEE:H60	1.41	1.02
38:o:45:ARG:HH12	39:p:144:THR:HG21	1.23	1.01
41:s:24:GLU:HG3	41:s:271:LEU:HD22	1.41	1.00
8:I:4:ALA:HA	51:l:201:CDL:CA2	1.92	1.00
48:l:703:PEE:H37	48:l:703:PEE:C37	1.92	0.99
34:k:21:MET:O	36:m:23:LYS:HE3	1.62	0.99
50:X:201:8Q1:C42	39:p:63:LEU:HB3	1.93	0.99
50:X:201:8Q1:C31	39:p:16:VAL:HG21	1.93	0.98
6:G:105:MET:CG	6:G:139:MET:CE	2.42	0.97
44:w:66:ILE:HG23	58:w:401:ADP:O2A	1.65	0.96
12:M:336:ASN:HD21	12:M:540:ASN:HB3	1.32	0.94
48:r:501:PEE:H79	48:r:501:PEE:H40	1.50	0.92
6:G:105:MET:HG2	6:G:139:MET:HE2	1.49	0.92
49:J:403:PLX:C13	48:j:201:PEE:C37	2.48	0.92
42:u:80:GLU:HB2	42:u:81:PRO:HD3	1.51	0.92
51:l:701:CDL:H541	51:l:701:CDL:CA6	2.00	0.90
51:l:701:CDL:H312	51:l:701:CDL:H742	1.53	0.90
12:M:179:CYS:HG	45:M:802:SF4:FE1	0.83	0.90
28:e:128:TYR:CE1	28:e:132:ASN:ND2	2.40	0.89
51:m:201:CDL:H381	51:m:201:CDL:H341	1.52	0.89
44:w:139:ARG:NH1	58:w:401:ADP:HN61	1.70	0.88
6:G:105:MET:CG	6:G:139:MET:HE1	2.02	0.87
35:l:520:TYR:HE1	51:l:702:CDL:OB4	1.57	0.87
44:w:139:ARG:HH12	58:w:401:ADP:HN61	0.92	0.86
17:S:31:ASN:ND2	17:S:60:TYR:OH	2.08	0.86
39:p:138:LYS:HD2	39:p:141:GLN:OE1	1.75	0.86
6:G:105:MET:CG	6:G:139:MET:HE2	2.03	0.86
30:g:2:THR:CG2	30:g:5:SER:CB	2.46	0.86
12:M:336:ASN:ND2	12:M:540:ASN:HB3	1.91	0.85
28:e:143:ASP:OD1	28:e:144:PRO:HD2	1.77	0.85
16:Q:53:TYR:CE1	48:l:703:PEE:H2	2.11	0.85
24:a:94:GLY:O	27:d:61:TYR:OH	1.92	0.85
19:U:30:ILE:HD12	48:U:101:PEE:H43	1.58	0.85
48:U:101:PEE:H37	41:s:302:MET:CE	2.07	0.84
32:i:236:LYS:HG3	32:i:237:MET:HG3	1.59	0.84
12:M:336:ASN:HD21	12:M:540:ASN:CB	1.89	0.84
6:X:136:GLU:O	6:X:139:MET:HE2	1.77	0.84
48:U:101:PEE:H37	41:s:302:MET:HE1	1.59	0.83
27:d:142:ARG:HH21	28:e:138:GLU:HB2	1.42	0.83
9:J:220:MET:HE2	9:J:227:PRO:HD2	1.59	0.83
16:Q:53:TYR:HE1	48:l:703:PEE:H2	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:162:ARG:NH1	28:e:140:ASN:OD1	2.11	0.83
35:l:520:TYR:CE1	51:l:702:CDL:OB4	2.32	0.83
35:l:190:LEU:HD23	40:r:383:THR:HG21	1.62	0.82
51:l:701:CDL:H742	51:l:701:CDL:C31	2.09	0.82
2:B:79:ARG:HH11	8:I:25:GLN:HE22	1.24	0.82
6:G:105:MET:HE2	6:G:139:MET:CE	2.09	0.82
15:P:125:ARG:NH2	15:P:199:ARG:HG2	1.95	0.82
51:l:702:CDL:H111	51:l:702:CDL:H152	1.59	0.82
15:P:161:LYS:HE3	16:Q:285:ASN:OD1	1.80	0.81
38:o:116:ILE:HG13	38:o:121:LEU:HD12	1.62	0.81
16:Q:99:MET:HE1	16:Q:444:LEU:HD11	1.60	0.81
12:M:44:GLU:OE1	12:M:45:PRO:HD2	1.80	0.81
12:M:485:ASP:OD1	12:M:680:LEU:HD12	1.81	0.80
33:j:11:VAL:HG22	48:j:201:PEE:H42	1.64	0.80
5:F:59:SER:O	5:F:61:VAL:N	2.14	0.80
51:i:401:CDL:H182	51:i:401:CDL:H222	1.64	0.79
11:L:109:ASN:ND2	11:L:111:LEU:O	2.15	0.78
35:l:190:LEU:HD21	40:r:307:TRP:CH2	2.19	0.78
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.66	0.78
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.17	0.78
32:i:14:MET:HB3	51:i:401:CDL:H602	1.64	0.78
53:J:402:UQ:H101	53:J:402:UQ:H152	1.66	0.77
33:j:18:VAL:HG12	48:j:201:PEE:H16	1.66	0.77
51:l:701:CDL:H451	51:l:701:CDL:H612	1.64	0.77
5:F:43:GLU:HA	5:F:46:LYS:HG3	1.65	0.77
34:k:37:MET:HE2	34:k:67:ALA:HB2	1.66	0.77
51:l:701:CDL:H312	51:l:701:CDL:C74	2.14	0.77
6:X:92:LYS:HD2	6:X:114:ASP:OD2	1.82	0.77
8:I:40:LYS:HB3	21:W:7:LYS:H	1.48	0.76
8:I:4:ALA:HA	51:I:201:CDL:HA22	1.67	0.76
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.19	0.76
2:B:79:ARG:HH11	8:I:25:GLN:NE2	1.84	0.76
12:M:483:ARG:HH22	12:M:682:ASP:HB3	1.51	0.76
17:S:34:LYS:CE	17:S:61:HIS:O	2.34	0.76
34:k:25:HIS:NE2	36:m:77:GLU:OE1	2.18	0.76
48:l:703:PEE:H34	48:l:703:PEE:H42	1.66	0.76
27:d:142:ARG:NE	28:e:138:GLU:O	2.19	0.76
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.68	0.76
27:d:142:ARG:NH2	28:e:138:GLU:HB2	2.01	0.75
10:K:100:GLN:NE2	14:O:69:ASN:O	2.19	0.75
9:J:135:GLU:OE2	9:J:141:PHE:N	2.18	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:l:705:PEE:H2	49:r:503:PLX:H21	1.67	0.74
14:O:207:GLU:HG3	14:O:212:LYS:HE2	1.67	0.74
34:k:21:MET:HE2	35:l:592:LEU:CD2	2.18	0.74
25:b:28:LEU:HD22	25:b:32:GLU:HG2	1.70	0.74
26:c:166:LEU:HD12	26:c:170:ARG:HH21	1.53	0.74
26:c:70:MET:HE2	38:o:85:LYS:NZ	2.02	0.74
1:A:89:GLY:O	47:A:503:NAI:H2N	1.88	0.73
13:N:120:THR:HG22	13:N:122:GLN:H	1.53	0.73
38:o:45:ARG:NH1	39:p:144:THR:HG21	2.00	0.73
12:M:327:ALA:O	12:M:331:GLN:HG3	1.88	0.73
50:X:201:8Q1:C31	39:p:16:VAL:CG2	2.67	0.73
5:F:20:ARG:HB2	5:F:66:TRP:HB2	1.71	0.73
11:L:123:ASN:OD1	12:M:246:ARG:NH2	2.22	0.73
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.71	0.73
34:k:59:MET:HG3	34:k:60:PRO:HD3	1.71	0.73
1:A:82:THR:CG2	1:A:259:GLY:HA3	2.16	0.73
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.71	0.72
19:U:16:GLU:HG3	48:U:101:PEE:H49	1.71	0.72
3:C:56:TRP:CH2	49:C:303:PLX:H112	2.23	0.72
48:C:302:PEE:C23	49:J:403:PLX:H161	2.19	0.72
10:K:78:HIS:HA	10:K:81:TYR:CD2	2.24	0.72
15:P:125:ARG:NH2	15:P:201:ASP:OD1	2.21	0.72
35:l:3:PRO:HG2	35:l:53:MET:HE1	1.69	0.72
6:G:108:LEU:HD12	6:G:108:LEU:N	2.04	0.72
51:a:201:CDL:HB21	48:l:705:PEE:H49	1.70	0.72
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.71	0.72
51:l:701:CDL:OB7	49:r:503:PLX:H222	1.90	0.72
48:C:302:PEE:O5	48:C:302:PEE:H52	1.90	0.72
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.71	0.72
44:w:66:ILE:HA	58:w:401:ADP:O2A	1.90	0.72
14:O:143:ARG:O	14:O:184:PRO:HG3	1.89	0.72
48:l:703:PEE:H37	48:l:703:PEE:C36	2.19	0.72
51:I:201:CDL:OA7	13:N:3:LEU:HD12	1.90	0.71
19:U:9:LEU:HD13	48:U:101:PEE:H79	1.71	0.71
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.72	0.71
32:i:68:MET:HE1	34:k:37:MET:SD	2.30	0.71
15:P:207:TYR:C	15:P:224:VAL:HG23	2.16	0.71
17:S:34:LYS:NZ	17:S:61:HIS:O	2.22	0.71
44:w:139:ARG:NH1	58:w:401:ADP:N6	2.33	0.71
6:G:105:MET:CE	6:G:139:MET:SD	2.75	0.71
12:M:335:GLY:HA2	12:M:362:ASP:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:23:LYS:N	36:m:24:PRO:HD3	2.05	0.70
51:u:201:CDL:H581	51:u:201:CDL:H541	1.72	0.70
51:I:201:CDL:OA9	51:I:201:CDL:H532	1.91	0.70
43:v:107:ARG:HA	43:v:110:GLN:HG2	1.72	0.70
21:W:57:ARG:HB3	41:s:316:PRO:HG3	1.73	0.70
15:P:173:MET:HE1	15:P:189:THR:HG23	1.74	0.70
33:j:108:GLN:HB2	36:m:169:MET:HE1	1.74	0.70
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.25	0.70
14:O:222:ARG:NH1	14:O:226:GLU:O	2.23	0.70
21:W:94:GLU:HG3	31:h:79:ILE:HD11	1.74	0.69
40:r:344:LEU:O	40:r:420:THR:HG21	1.92	0.69
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.26	0.69
51:l:701:CDL:H351	51:l:701:CDL:H401	1.75	0.69
51:l:701:CDL:H411	40:r:371:PRO:HD2	1.74	0.69
13:N:68:MET:HG3	13:N:69:ASN:H	1.56	0.69
41:s:209:SER:HB3	41:s:213:VAL:HA	1.75	0.69
12:M:400:ILE:HD12	12:M:473:MET:HE3	1.74	0.69
35:l:227:PHE:O	35:l:230:HIS:ND1	2.26	0.69
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.26	0.69
34:k:21:MET:HE2	35:l:592:LEU:HD21	1.75	0.69
3:C:188:LYS:HB2	3:C:191:ARG:HD2	1.74	0.68
48:r:501:PEE:H33	48:r:501:PEE:H71	1.74	0.68
10:K:102:SER:HB2	14:O:72:GLU:OE1	1.92	0.68
35:l:170:GLN:NE2	48:l:704:PEE:O1P	2.26	0.68
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.27	0.68
24:a:53:ARG:NH2	25:b:29:SER:O	2.26	0.68
35:l:558:LEU:HD21	51:o:201:CDL:H872	1.75	0.68
35:l:562:LEU:HG	48:l:703:PEE:H31	1.75	0.68
12:M:81:GLU:HG3	12:M:108:LYS:HD2	1.76	0.68
51:l:702:CDL:H371	51:l:702:CDL:H601	1.76	0.68
3:C:51:ASP:OD2	3:C:188:LYS:HA	1.93	0.68
12:M:534:VAL:HG21	12:M:555:ILE:CG1	2.24	0.68
28:e:63:ASP:OD2	40:r:338:HIS:NE2	2.27	0.67
51:I:201:CDL:H312	13:N:3:LEU:HD11	1.76	0.67
51:l:701:CDL:HA62	51:l:701:CDL:C54	2.19	0.67
8:I:2:ALA:N	8:I:21:GLN:OE1	2.27	0.67
9:J:208:GLY:N	9:J:211:ASP:HB3	2.09	0.67
32:i:129:LEU:HD13	51:i:401:CDL:H311	1.76	0.67
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.76	0.67
17:S:28:LYS:NZ	42:u:91:TYR:OH	2.27	0.67
32:i:40:MET:HE1	32:i:129:LEU:HD23	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:190:MET:HE2	32:i:205:LEU:HA	1.77	0.67
14:O:134:VAL:HG11	14:O:149:LEU:HD13	1.77	0.66
3:C:188:LYS:HB3	3:C:191:ARG:NH1	2.09	0.66
35:l:261:ILE:HG13	35:l:317:ILE:HD11	1.76	0.66
2:B:47:SER:O	2:B:56:ARG:NH2	2.28	0.66
9:J:220:MET:HE3	9:J:227:PRO:CD	2.21	0.66
12:M:534:VAL:HG21	12:M:555:ILE:HG12	1.77	0.66
5:F:59:SER:C	5:F:61:VAL:H	2.03	0.66
16:Q:99:MET:HE1	16:Q:444:LEU:CD1	2.25	0.66
22:Y:69:ILE:HD13	35:l:383:MET:HE2	1.77	0.66
9:J:208:GLY:H	9:J:211:ASP:HB3	1.60	0.66
14:O:38:LEU:O	14:O:124:ARG:NH2	2.28	0.66
6:G:105:MET:SD	6:G:139:MET:HE1	2.36	0.66
12:M:483:ARG:NH2	12:M:682:ASP:HB3	2.09	0.66
33:j:11:VAL:CG2	48:j:201:PEE:H42	2.25	0.66
6:G:105:MET:HE2	6:G:139:MET:HE1	1.78	0.66
32:i:129:LEU:HD12	51:i:401:CDL:H331	1.78	0.66
12:M:179:CYS:SG	45:M:802:SF4:FE1	1.86	0.65
26:c:116:ARG:HG2	48:l:704:PEE:H49	1.78	0.65
27:d:162:ARG:NH2	28:e:140:ASN:OD1	2.29	0.65
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.77	0.65
8:I:3:SER:C	51:I:201:CDL:HA22	2.21	0.65
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.77	0.65
1:A:159:ARG:NH2	14:O:176:CYS:O	2.29	0.65
4:E:64:ARG:NH2	6:G:117:GLU:OE1	2.25	0.65
5:F:31:GLN:NE2	5:F:35:ASP:OD1	2.29	0.65
38:o:56:ARG:HH11	38:o:56:ARG:HB3	1.60	0.65
24:a:106:VAL:HB	37:n:50:ARG:HH21	1.61	0.65
32:i:246:VAL:HG11	51:r:504:CDL:H392	1.79	0.65
32:i:254:LEU:HD21	40:r:154:LEU:HD11	1.79	0.65
44:w:125:ASP:O	44:w:130:ARG:NH2	2.30	0.65
26:c:124:VAL:HG23	35:l:525:MET:HE1	1.78	0.65
25:b:32:GLU:HG3	39:p:115:TYR:HD1	1.62	0.64
31:h:2:PRO:HA	32:i:140:SER:HB2	1.77	0.64
51:i:401:CDL:H182	51:i:401:CDL:C22	2.26	0.64
51:u:201:CDL:H581	51:u:201:CDL:C54	2.28	0.64
9:J:188:GLU:HG3	9:J:200:ILE:HD13	1.77	0.64
20:V:14:GLU:OE2	20:V:126:LYS:NZ	2.30	0.64
27:d:159:GLN:HG2	27:d:163:MET:HE2	1.79	0.64
43:v:27:PRO:O	43:v:34:ARG:NH1	2.30	0.64
1:A:36:LYS:H	1:A:36:LYS:HD3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:117:ARG:HH22	9:J:158:GLU:HG2	1.61	0.64
1:A:357:MET:HB3	1:A:361:THR:HG21	1.80	0.64
12:M:367:CYS:HB3	12:M:533:GLY:O	1.96	0.64
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.79	0.64
14:O:59:ASN:ND2	14:O:89:GLN:OE1	2.29	0.64
33:j:23:TRP:HE1	48:j:201:PEE:H1	1.61	0.64
48:l:703:PEE:H60	48:l:703:PEE:C23	2.23	0.64
42:u:103:GLN:N	42:u:103:GLN:OE1	2.28	0.64
32:i:146:SER:HA	32:i:149:ILE:HD12	1.79	0.64
3:C:188:LYS:HB3	3:C:191:ARG:HH11	1.61	0.64
36:m:33:LEU:HD23	36:m:64:MET:HE3	1.79	0.64
1:A:385:CYS:HB3	45:A:501:SF4:S2	2.38	0.64
5:F:21:ILE:HG12	5:F:65:LEU:HD12	1.80	0.64
5:F:23:LEU:HD23	5:F:23:LEU:H	1.63	0.64
12:M:456:ALA:O	12:M:499:ASN:ND2	2.31	0.64
8:I:8:ILE:HD11	51:I:201:CDL:H142	1.79	0.63
35:l:554:ASP:OD2	40:r:288:TYR:OH	2.16	0.63
39:p:16:VAL:HG12	39:p:64:LEU:HD13	1.79	0.63
48:l:703:PEE:H37	48:l:703:PEE:H59	1.79	0.63
48:l:705:PEE:H2	49:r:503:PLX:C2	2.28	0.63
34:k:23:ARG:HG3	36:m:23:LYS:HE2	1.81	0.63
41:s:62:ARG:HD2	41:s:68:ILE:HD11	1.80	0.63
9:J:171:ASN:HA	9:J:327:MET:HE3	1.81	0.63
42:u:172:MET:SD	51:u:201:CDL:HB31	2.39	0.63
1:A:61:ASP:OD1	1:A:137:LYS:HG2	1.99	0.63
26:c:85:GLU:OE2	26:c:119:THR:OG1	2.15	0.63
15:P:147:THR:HB	15:P:153:ILE:HD11	1.81	0.63
21:W:36:PHE:O	21:W:40:ILE:HG12	1.98	0.63
1:A:109:ARG:NH1	1:A:237:GLY:O	2.32	0.63
33:j:33:LYS:HD3	41:s:61:LEU:HD21	1.80	0.63
6:G:87:LEU:HD23	6:G:98:LEU:HD11	1.80	0.62
15:P:125:ARG:HH22	15:P:201:ASP:CG	2.06	0.62
12:M:162:ASP:O	18:T:104:LYS:NZ	2.31	0.62
23:Z:30:GLU:O	23:Z:34:GLU:HG3	1.99	0.62
51:l:701:CDL:H452	40:r:445:LEU:HB3	1.80	0.62
44:w:66:ILE:CG2	58:w:401:ADP:O2A	2.44	0.62
11:L:105:GLU:HA	12:M:611:THR:HG21	1.82	0.62
14:O:177:LEU:HD12	14:O:185:MET:SD	2.39	0.62
21:W:74:LEU:O	21:W:78:GLU:HG3	2.00	0.62
51:l:701:CDL:HA62	51:l:701:CDL:H522	1.79	0.62
48:l:703:PEE:H34	48:l:703:PEE:C25	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:v:112:LYS:O	43:v:116:GLU:HG3	1.99	0.62
4:E:96:VAL:HG12	4:E:96:VAL:O	1.99	0.62
35:l:370:THR:HG22	35:l:431:PHE:CD2	2.35	0.62
35:l:562:LEU:HB3	35:l:563:PRO:HD3	1.79	0.62
9:J:220:MET:CE	9:J:227:PRO:CD	2.55	0.62
50:X:201:8Q1:C13	39:p:70:GLU:OE2	2.47	0.62
32:i:15:SER:OG	51:i:401:CDL:H841	2.00	0.62
12:M:43:VAL:HG21	12:M:96:VAL:HG21	1.81	0.62
51:V:201:CDL:H521	35:l:577:VAL:HA	1.82	0.62
27:d:142:ARG:HH21	28:e:138:GLU:CB	2.10	0.62
32:i:68:MET:HE2	32:i:68:MET:HA	1.80	0.62
3:C:100:SER:O	41:s:58:LYS:NZ	2.33	0.61
6:X:93:ILE:HG23	6:X:108:LEU:CD1	2.29	0.61
34:k:87:THR:HG22	34:k:89:TYR:H	1.65	0.61
11:L:165:SER:OG	11:L:168:LYS:HB2	2.00	0.61
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.82	0.61
19:U:60:ASP:OD1	19:U:62:ASN:ND2	2.33	0.61
27:d:159:GLN:O	27:d:163:MET:HG3	1.99	0.61
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.82	0.61
4:E:92:GLU:OE1	15:P:191:TYR:HB3	1.99	0.61
8:I:27:ARG:NH2	16:Q:212:GLU:OE1	2.33	0.61
22:Y:52:ARG:HH11	22:Y:52:ARG:HB3	1.66	0.61
27:d:111:LYS:HE3	35:l:197:ASP:OD2	2.01	0.61
29:f:48:LEU:O	29:f:52:VAL:HG23	2.01	0.61
14:O:111:ARG:NH1	14:O:114:GLU:OE2	2.33	0.61
42:u:105:ALA:O	42:u:109:GLU:HG2	2.01	0.61
13:N:29:ARG:NH2	13:N:64:TYR:O	2.31	0.61
15:P:43:THR:HA	15:P:47:ILE:HD12	1.83	0.61
1:A:263:ALA:HA	1:A:271:SER:HB3	1.81	0.61
6:G:105:MET:CE	6:G:139:MET:CE	2.78	0.61
12:M:566:ILE:HD13	12:M:579:MET:HE3	1.83	0.61
38:o:56:ARG:HB3	38:o:56:ARG:NH1	2.15	0.61
31:h:3:PHE:HB2	32:i:144:GLN:NE2	2.15	0.61
9:J:207:PHE:HA	9:J:211:ASP:OD2	2.00	0.60
32:i:14:MET:CB	51:i:401:CDL:H602	2.31	0.60
34:k:65:VAL:HG11	36:m:157:THR:HG23	1.83	0.60
6:G:94:ASP:OD1	6:G:94:ASP:N	2.34	0.60
36:m:28:TYR:CE2	36:m:82:VAL:HG12	2.36	0.60
41:s:156:MET:HA	41:s:156:MET:HE2	1.83	0.60
1:A:40:ARG:NH1	1:A:289:GLU:O	2.34	0.60
3:C:81:ALA:HB1	3:C:82:PRO:HD2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:99:ASP:HB3	28:e:137:MET:HE1	1.83	0.60
51:i:401:CDL:OA7	51:i:401:CDL:HA62	2.01	0.60
36:m:61:LEU:O	41:s:114:TYR:OH	2.19	0.60
16:Q:53:TYR:CE1	48:l:703:PEE:O2P	2.54	0.60
35:l:228:GLY:HA3	48:l:704:PEE:H38	1.82	0.60
2:B:89:GLU:OE1	13:N:58:ARG:HD2	2.02	0.60
6:X:128:PHE:CD2	6:X:152:LYS:HE2	2.35	0.60
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.82	0.60
32:i:258:SER:OG	32:i:336:VAL:HG12	2.02	0.60
2:B:120:GLU:HB2	2:B:130:ILE:HD12	1.83	0.60
43:v:22:MET:HE1	43:v:102:PHE:HA	1.83	0.60
19:U:9:LEU:CD1	48:U:101:PEE:H79	2.32	0.60
27:d:69:ARG:NH2	37:n:46:LYS:O	2.35	0.60
30:g:4:MET:HE3	30:g:84:MET:CE	2.32	0.60
32:i:218:LEU:HB3	32:i:244:MET:HE2	1.82	0.60
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.37	0.60
35:l:563:PRO:HB3	48:l:703:PEE:H30	1.83	0.59
44:w:295:ARG:HA	44:w:298:VAL:HG22	1.84	0.59
53:J:402:UQ:HM23	53:J:402:UQ:O1	2.02	0.59
11:L:84:ARG:NH1	11:L:88:GLN:O	2.35	0.59
51:l:701:CDL:H622	51:l:701:CDL:C66	2.31	0.59
1:A:256:ARG:O	14:O:246:GLN:HG2	2.02	0.59
32:i:49:ASN:O	32:i:51:ARG:N	2.36	0.59
2:B:184:LEU:HB3	11:L:112:MET:HE2	1.84	0.59
25:b:99:GLU:HG2	35:l:61:MET:HE2	1.84	0.59
26:c:153:TYR:OH	43:v:8:ARG:NH1	2.34	0.59
33:j:19:LEU:HD11	48:j:201:PEE:H48	1.83	0.59
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.36	0.59
3:C:95:ALA:HB1	41:s:208:VAL:HG13	1.83	0.59
19:U:30:ILE:CD1	48:U:101:PEE:H43	2.32	0.59
22:Y:83:HIS:O	22:Y:83:HIS:ND1	2.34	0.59
32:i:95:MET:HE2	32:i:149:ILE:HG12	1.85	0.59
38:o:3:PHE:CE2	39:p:70:GLU:HG2	2.38	0.59
44:w:60:ILE:HG12	44:w:203:VAL:HB	1.82	0.59
36:m:23:LYS:N	36:m:24:PRO:CD	2.65	0.59
6:X:89:LEU:HD13	23:Z:48:ASN:HA	1.84	0.59
48:r:501:PEE:H40	48:r:501:PEE:C46	2.26	0.59
2:B:98:ARG:NH2	16:Q:224:ALA:O	2.34	0.59
44:w:95:ASP:OD1	44:w:95:ASP:N	2.36	0.59
1:A:90:GLY:HA3	47:A:503:NAI:H1D	1.84	0.59
32:i:11:MET:HG2	51:i:401:CDL:C56	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:g:2:THR:CG2	30:g:5:SER:HB3	2.30	0.58
32:i:222:SER:O	32:i:224:ALA:N	2.36	0.58
41:s:209:SER:HB3	41:s:213:VAL:CA	2.34	0.58
9:J:220:MET:HE1	9:J:227:PRO:HD2	1.75	0.58
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.84	0.58
44:w:72:ARG:NH1	44:w:76:GLU:OE1	2.36	0.58
10:K:73:TYR:HB2	14:O:223:PHE:CD1	2.39	0.58
12:M:149:ASP:OD2	12:M:150:ARG:NH1	2.36	0.58
20:V:69:ILE:HG22	20:V:96:ALA:HB1	1.83	0.58
27:d:139:PHE:HD2	28:e:137:MET:HE1	1.67	0.58
33:j:27:LEU:CD2	41:s:60:PRO:HD2	2.34	0.58
17:S:66:LEU:HD13	42:u:75:LYS:HB2	1.86	0.58
51:l:701:CDL:H611	51:l:701:CDL:H782	1.86	0.58
1:A:88:ARG:O	1:A:126:LYS:NZ	2.35	0.58
1:A:420:GLU:HG3	1:A:429:ASP:OD1	2.03	0.58
39:p:127:ARG:NH1	39:p:131:GLU:OE2	2.36	0.58
35:l:566:THR:CG2	48:l:703:PEE:H61	2.33	0.58
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.86	0.58
40:r:306:PRO:HB3	40:r:458:LEU:HD12	1.86	0.58
44:w:250:SER:O	44:w:280:LYS:NZ	2.36	0.58
7:H:81:ILE:O	7:H:85:GLU:HG3	2.04	0.58
27:d:6:ASP:HB3	27:d:9:VAL:HG22	1.86	0.58
6:X:119:ILE:O	6:X:123:GLU:HG3	2.04	0.57
25:b:100:ARG:NH2	27:d:119:GLU:HG2	2.18	0.57
35:l:150:MET:SD	51:l:701:CDL:H152	2.43	0.57
9:J:344:PRO:HG2	9:J:347:LEU:HD13	1.86	0.57
16:Q:94:VAL:O	16:Q:94:VAL:HG23	2.02	0.57
35:l:366:MET:O	35:l:370:THR:HG23	2.05	0.57
1:A:53:LEU:HB2	1:A:136:HIS:CE1	2.39	0.57
6:G:116:VAL:HG12	6:G:120:MET:HE2	1.86	0.57
7:H:105:GLU:HB3	15:P:89:HIS:CD2	2.40	0.57
53:J:402:UQ:H161	53:J:402:UQ:H203	1.84	0.57
5:F:57:GLU:OE2	5:F:57:GLU:N	2.37	0.57
12:M:83:GLU:HG3	12:M:103:LEU:HD11	1.87	0.57
17:S:12:MET:HE1	41:s:20:LEU:HA	1.86	0.57
12:M:696:MET:HE2	12:M:702:ARG:HA	1.86	0.57
24:a:106:VAL:O	37:n:50:ARG:NH2	2.38	0.57
51:k:101:CDL:H162	35:l:589:LEU:HD21	1.85	0.57
8:I:30:GLU:CD	8:I:30:GLU:H	2.12	0.57
14:O:242:GLY:HA2	14:O:245:VAL:HG13	1.87	0.57
27:d:160:LYS:NZ	30:g:114:ILE:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:320:THR:HG21	44:w:300:ASN:HA	1.86	0.57
35:l:126:ILE:HG21	51:l:701:CDL:H871	1.86	0.57
2:B:63:TRP:O	2:B:67:VAL:HG23	2.04	0.56
48:C:302:PEE:H32	49:C:303:PLX:H382	1.86	0.56
5:F:46:LYS:HE3	12:M:674:LEU:HD11	1.87	0.56
8:I:4:ALA:CA	51:I:201:CDL:HA22	2.33	0.56
16:Q:80:LEU:C	16:Q:80:LEU:HD23	2.30	0.56
6:G:105:MET:CE	6:G:139:MET:HE1	2.35	0.56
10:K:73:TYR:CZ	10:K:75:ASN:HB3	2.40	0.56
31:h:89:GLU:OE1	31:h:91:LYS:NZ	2.37	0.56
1:A:46:TYR:CE1	14:O:226:GLU:HA	2.39	0.56
1:A:382:CYS:HB3	1:A:424:ILE:HD12	1.87	0.56
11:L:165:SER:CB	11:L:168:LYS:HB2	2.35	0.56
14:O:130:TYR:HA	14:O:189:ASN:HD21	1.70	0.56
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.87	0.56
16:Q:88:HIS:HD2	16:Q:90:ALA:H	1.53	0.56
6:X:117:GLU:OE2	39:p:45:ARG:NH1	2.37	0.56
50:X:201:8Q1:C11	39:p:70:GLU:OE2	2.53	0.56
32:i:88:LYS:O	32:i:148:SER:CB	2.53	0.56
30:g:2:THR:HG21	30:g:5:SER:HB3	1.83	0.56
1:A:170:GLN:HE21	1:A:197:VAL:HB	1.71	0.56
3:C:80:ALA:HA	3:C:86:MET:HG2	1.86	0.56
27:d:160:LYS:HE2	28:e:147:ILE:HG23	1.87	0.56
35:l:570:GLN:HE22	48:l:703:PEE:H69	1.71	0.56
13:N:60:ARG:HH22	13:N:95:ASP:HA	1.70	0.56
31:h:106:PRO:HG2	42:u:17:GLU:HB3	1.87	0.56
34:k:10:MET:HE2	36:m:103:MET:SD	2.45	0.56
44:w:88:GLU:OE2	44:w:161:ARG:NH1	2.35	0.56
32:i:211:MET:HE3	32:i:251:MET:HA	1.87	0.56
51:l:701:CDL:H382	40:r:369:LEU:HB3	1.86	0.56
3:C:92:VAL:HG21	53:s:401:UQ:H103	1.88	0.56
5:F:23:LEU:HD23	5:F:23:LEU:N	2.21	0.56
35:l:495:ILE:O	35:l:499:MET:HG2	2.06	0.56
44:w:123:SER:OG	44:w:125:ASP:OD1	2.17	0.56
46:A:502:FMN:N5	47:A:503:NAI:H4N	2.21	0.56
6:G:105:MET:HG3	6:G:139:MET:HE2	1.85	0.56
39:p:137:VAL:O	39:p:141:GLN:HG2	2.06	0.56
25:b:110:ILE:HG22	25:b:112:GLU:H	1.69	0.55
41:s:222:MET:HA	41:s:225:MET:HE3	1.87	0.55
1:A:185:ASN:OD1	1:A:190:GLY:N	2.33	0.55
26:c:184:TYR:HB2	43:v:34:ARG:HH21	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:139:PHE:CD2	28:e:137:MET:HE1	2.41	0.55
1:A:312:ASP:HA	1:A:329:LYS:HE3	1.89	0.55
10:K:77:GLN:OE1	10:K:77:GLN:N	2.39	0.55
12:M:224:ASP:OD2	12:M:291:ARG:NH2	2.38	0.55
35:l:517:SER:OG	51:l:702:CDL:OA3	2.24	0.55
37:n:10:ASP:HB2	40:r:19:LYS:NZ	2.21	0.55
1:A:283:ASN:ND2	1:A:305:GLY:O	2.38	0.55
2:B:79:ARG:NH1	8:I:25:GLN:HE22	2.01	0.55
12:M:182:CYS:HG	45:M:802:SF4:FE3	1.24	0.55
3:C:126:GLU:HG2	9:J:89:TYR:OH	2.06	0.55
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.89	0.55
41:s:81:LEU:HD11	41:s:111:LEU:HG	1.89	0.55
17:S:34:LYS:HE3	17:S:61:HIS:O	2.07	0.55
48:U:101:PEE:H26	41:s:295:PRO:HB3	1.87	0.55
34:k:23:ARG:HD3	36:m:23:LYS:O	2.06	0.55
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.89	0.55
1:A:36:LYS:HG2	1:A:38:GLU:HG2	1.88	0.55
3:C:126:GLU:OE2	33:j:33:LYS:NZ	2.37	0.55
32:i:211:MET:HG3	32:i:333:SER:HB2	1.88	0.55
34:k:27:MET:HE1	36:m:70:TYR:HB3	1.89	0.55
35:l:363:TYR:HA	35:l:370:THR:HG21	1.89	0.55
51:l:702:CDL:H752	51:l:702:CDL:H132	1.89	0.55
37:n:12:TRP:O	37:n:15:ILE:HG13	2.07	0.55
22:Y:69:ILE:HD13	35:l:383:MET:CE	2.36	0.54
40:r:346:ARG:O	40:r:419:TYR:HA	2.07	0.54
7:H:105:GLU:HA	7:H:105:GLU:OE1	2.06	0.54
9:J:192:ARG:NH1	9:J:198:ALA:O	2.39	0.54
40:r:186:LEU:HD13	40:r:253:LEU:HD23	1.89	0.54
25:b:5:THR:OG1	25:b:7:ASP:OD1	2.24	0.54
32:i:88:LYS:O	32:i:148:SER:HB3	2.08	0.54
40:r:403:THR:HA	40:r:406:TYR:CE2	2.43	0.54
6:G:140:CYS:SG	6:G:143:GLU:HG3	2.47	0.54
27:d:162:ARG:CZ	28:e:140:ASN:OD1	2.55	0.54
1:A:185:ASN:O	1:A:187:CYS:N	2.41	0.54
3:C:188:LYS:CB	3:C:191:ARG:HD2	2.36	0.54
24:a:96:ALA:HB2	27:d:61:TYR:CE2	2.42	0.54
40:r:191:SER:HB3	48:r:501:PEE:H2	1.88	0.54
9:J:328:THR:HG22	9:J:330:PRO:HD3	1.89	0.54
49:g:201:PLX:H361	49:g:201:PLX:H311	1.89	0.54
31:h:69:ARG:O	31:h:73:MET:HG3	2.08	0.54
43:v:17:PRO:HB3	43:v:105:GLU:HG2	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:156:GLU:OE1	6:G:156:GLU:N	2.36	0.54
34:k:28:SER:HB3	36:m:23:LYS:HG2	1.90	0.54
38:o:37:LEU:O	38:o:37:LEU:HD12	2.07	0.54
12:M:407:PRO:HD2	12:M:438:LEU:HD21	1.90	0.54
33:j:67:LEU:HD22	36:m:59:ILE:HD12	1.89	0.54
26:c:70:MET:HE2	38:o:85:LYS:HZ1	1.72	0.54
32:i:221:HIS:HB2	32:i:323:MET:HE1	1.90	0.54
35:l:119:LYS:NZ	51:l:701:CDL:OA3	2.40	0.54
51:l:701:CDL:C66	51:l:701:CDL:C62	2.86	0.54
40:r:201:MET:HE2	48:r:501:PEE:H78	1.89	0.54
11:L:168:LYS:HE2	11:L:168:LYS:HA	1.88	0.53
25:b:100:ARG:HH22	27:d:119:GLU:HG2	1.74	0.53
51:m:201:CDL:H341	51:m:201:CDL:C38	2.27	0.53
32:i:11:MET:HG2	51:i:401:CDL:H562	1.89	0.53
32:i:129:LEU:CD1	51:i:401:CDL:H311	2.38	0.53
4:E:16:SER:HA	11:L:52:LEU:HD23	1.90	0.53
4:E:52:LEU:HD22	4:E:104:MET:HE3	1.90	0.53
6:X:137:LYS:O	6:X:139:MET:HG2	2.07	0.53
32:i:72:MET:HE2	32:i:76:ILE:HG12	1.91	0.53
9:J:304:LEU:HD11	49:J:403:PLX:H312	1.90	0.53
20:V:67:GLY:HA2	51:V:201:CDL:H221	1.90	0.53
22:Y:43:ARG:HH11	22:Y:49:GLN:HB2	1.73	0.53
51:l:702:CDL:H121	51:l:702:CDL:H732	1.89	0.53
39:p:92:GLU:HB3	39:p:95:GLU:HG3	1.91	0.53
43:v:57:ASP:O	43:v:59:CYS:N	2.42	0.53
1:A:115:VAL:HG11	1:A:138:LEU:HD11	1.91	0.53
3:C:53:LEU:HD22	49:C:303:PLX:H322	1.90	0.53
30:g:4:MET:CE	30:g:84:MET:HE3	2.39	0.53
41:s:209:SER:HB3	41:s:213:VAL:CB	2.39	0.53
1:A:132:ARG:HG3	1:A:133:HIS:CD2	2.44	0.53
1:A:152:ARG:NH2	10:K:99:PRO:O	2.39	0.53
8:I:4:ALA:N	51:I:201:CDL:HA22	2.23	0.53
32:i:93:VAL:HG13	35:l:599:MET:HE1	1.89	0.53
1:A:263:ALA:C	1:A:265:PHE:H	2.16	0.53
9:J:208:GLY:H	9:J:211:ASP:CB	2.20	0.53
12:M:485:ASP:CG	12:M:680:LEU:HD12	2.34	0.53
18:T:49:ASP:OD2	18:T:51:ARG:NH2	2.35	0.53
30:g:35:TYR:CE1	51:u:201:CDL:H771	2.44	0.53
32:i:62:THR:HG21	32:i:114:TRP:CD1	2.44	0.53
39:p:97:TYR:HB2	39:p:178:PRO:HG2	1.90	0.53
3:C:184:ILE:O	3:C:187:GLU:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:66:ARG:HH12	28:e:72:ASP:HB2	1.74	0.53
51:a:201:CDL:CB2	48:l:705:PEE:H49	2.39	0.53
6:G:119:ILE:O	6:G:123:GLU:HG3	2.09	0.53
6:G:141:PRO:O	6:G:145:VAL:HG23	2.08	0.53
12:M:354:LEU:HD22	12:M:548:LEU:HD22	1.90	0.53
1:A:119:GLU:O	1:A:159:ARG:NH1	2.43	0.53
6:G:93:ILE:HD13	6:G:108:LEU:CD2	2.38	0.53
27:d:148:ALA:O	27:d:149:HIS:HB2	2.09	0.52
9:J:168:SER:O	9:J:203:PRO:HD2	2.08	0.52
6:X:92:LYS:CD	6:X:114:ASP:OD2	2.55	0.52
32:i:258:SER:HB2	32:i:333:SER:O	2.09	0.52
33:j:95:LEU:HD13	41:s:302:MET:HG2	1.92	0.52
1:A:358:ASP:O	1:A:361:THR:HG22	2.10	0.52
9:J:335:LEU:HB3	9:J:340:ILE:HB	1.92	0.52
18:T:47:ASP:O	18:T:52:ARG:NH2	2.40	0.52
30:g:15:PHE:HB2	49:g:201:PLX:H6	1.90	0.52
37:n:30:ARG:NE	51:u:201:CDL:OA4	2.42	0.52
12:M:598:ASN:C	12:M:598:ASN:HD22	2.15	0.52
30:g:4:MET:HE3	30:g:84:MET:HE3	1.91	0.52
48:j:201:PEE:O1P	41:s:62:ARG:NH1	2.41	0.52
40:r:370:PRO:HG3	40:r:375:LEU:HG	1.92	0.52
4:E:117:ASP:OD1	4:E:120:SER:OG	2.25	0.52
27:d:33:LEU:HD13	35:l:49:VAL:HG13	1.91	0.52
35:l:66:TRP:CD1	48:l:705:PEE:H16	2.44	0.52
4:E:92:GLU:OE1	15:P:191:TYR:CB	2.57	0.52
9:J:283:VAL:HG22	9:J:369:VAL:HG11	1.90	0.52
6:X:120:MET:HE1	39:p:24:LEU:HB3	1.92	0.52
22:Y:76:ASP:O	35:l:385:TYR:OH	2.27	0.52
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.90	0.52
40:r:329:LEU:O	40:r:332:THR:OG1	2.27	0.52
6:G:144:ILE:O	6:G:148:ILE:HG13	2.09	0.52
14:O:182:ASN:HB3	14:O:194:GLU:CB	2.38	0.52
48:U:101:PEE:H33	41:s:302:MET:HE2	1.92	0.52
6:X:93:ILE:HG23	6:X:108:LEU:HD12	1.92	0.52
35:l:327:LEU:O	35:l:331:MET:HG2	2.09	0.52
4:E:19:PRO:HB3	11:L:53:ILE:HD13	1.92	0.52
12:M:379:THR:O	12:M:379:THR:HG22	2.09	0.52
16:Q:88:HIS:CE1	41:s:208:VAL:HG23	2.45	0.52
34:k:31:LEU:HD21	36:m:67:VAL:HG11	1.91	0.52
1:A:455:LEU:O	1:A:458:GLN:NE2	2.42	0.52
5:F:65:LEU:HB2	5:F:79:LEU:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:131:PRO:HG2	6:X:134:ASP:HB2	1.91	0.52
23:Z:25:GLU:HA	23:Z:30:GLU:OE2	2.10	0.52
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.91	0.52
51:u:201:CDL:H772	51:u:201:CDL:H731	1.92	0.52
3:C:62:LEU:HD22	3:C:102:VAL:CG2	2.40	0.51
4:E:92:GLU:OE1	15:P:191:TYR:HD1	1.93	0.51
6:G:92:LYS:HE2	6:G:114:ASP:OD1	2.10	0.51
8:I:12:ARG:HB3	8:I:20:LEU:HD12	1.92	0.51
20:V:141:VAL:O	24:a:161:ARG:NH1	2.42	0.51
43:v:57:ASP:OD2	43:v:91:GLU:OE2	2.28	0.51
8:I:8:ILE:HD11	51:I:201:CDL:C14	2.40	0.51
48:U:101:PEE:H53	48:U:101:PEE:O5	2.10	0.51
24:a:52:LYS:NZ	25:b:27:GLU:OE1	2.34	0.51
33:j:22:PHE:HB2	48:j:201:PEE:O4	2.10	0.51
51:l:701:CDL:H742	51:l:701:CDL:H311	1.92	0.51
1:A:404:ALA:HB3	1:A:450:MET:HE2	1.93	0.51
20:V:94:GLY:HA3	20:V:119:GLY:HA2	1.91	0.51
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.33	0.51
23:Z:28:PRO:O	23:Z:32:VAL:HG23	2.10	0.51
24:a:79:GLY:HA3	51:a:201:CDL:H222	1.91	0.51
25:b:106:PRO:HG3	43:v:45:GLU:HG2	1.92	0.51
27:d:155:CYS:SG	28:e:141:CYS:SG	3.08	0.51
51:l:701:CDL:H331	51:l:701:CDL:OA9	2.09	0.51
44:w:254:GLU:CD	44:w:254:GLU:H	2.16	0.51
1:A:263:ALA:O	1:A:265:PHE:N	2.44	0.51
6:G:108:LEU:N	6:G:108:LEU:CD1	2.73	0.51
49:J:403:PLX:H132	48:j:201:PEE:C37	2.38	0.51
30:g:35:TYR:HE1	51:u:201:CDL:H771	1.76	0.51
34:k:37:MET:HE1	34:k:63:LEU:HG	1.91	0.51
35:l:22:SER:OG	51:l:701:CDL:H512	2.10	0.51
51:l:701:CDL:H541	51:l:701:CDL:HA61	1.90	0.51
11:L:165:SER:OG	11:L:168:LYS:CB	2.59	0.51
50:X:201:8Q1:C30	50:X:201:8Q1:N36	2.73	0.51
1:A:262:PHE:CZ	1:A:272:GLY:HA3	2.45	0.51
53:J:402:UQ:O1	53:J:402:UQ:H8	2.09	0.51
12:M:256:ALA:O	12:M:598:ASN:HB2	2.11	0.51
16:Q:53:TYR:HE1	48:l:703:PEE:O2P	1.92	0.51
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.93	0.51
19:U:26:GLY:HA3	48:U:101:PEE:C23	2.41	0.51
32:i:12:THR:HG23	36:m:159:TRP:HE1	1.75	0.51
9:J:71:ASN:HA	9:J:97:MET:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:58:ALA:O	35:l:434:LYS:NZ	2.43	0.51
34:k:4:VAL:O	34:k:8:ILE:HG12	2.11	0.51
1:A:67:GLU:O	1:A:71:LYS:HG2	2.11	0.51
48:C:302:PEE:H81	41:s:56:PHE:CE2	2.46	0.51
20:V:76:ILE:O	20:V:80:VAL:HG22	2.10	0.51
44:w:108:LEU:HD13	44:w:331:PHE:HA	1.92	0.51
15:P:127:GLU:OE1	15:P:144:LYS:NZ	2.30	0.50
30:g:33:LEU:HD22	30:g:71:VAL:HG13	1.91	0.50
36:m:83:TRP:CE3	51:m:201:CDL:H732	2.46	0.50
40:r:6:ILE:O	40:r:10:MET:HG2	2.11	0.50
51:u:201:CDL:H772	51:u:201:CDL:C73	2.41	0.50
17:S:19:PRO:HB3	41:s:9:LEU:HD12	1.92	0.50
51:V:201:CDL:H402	51:V:201:CDL:H771	1.92	0.50
25:b:10:LEU:O	25:b:14:GLN:HG3	2.11	0.50
32:i:81:SER:O	32:i:83:GLN:N	2.39	0.50
35:l:68:TRP:CZ3	35:l:69:MET:HE2	2.47	0.50
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.47	0.50
12:M:407:PRO:HD2	12:M:438:LEU:CD2	2.42	0.50
20:V:40:SER:HA	51:V:201:CDL:HB61	1.93	0.50
48:l:703:PEE:H36	48:l:703:PEE:H28	1.94	0.50
5:F:61:VAL:HG13	5:F:62:GLN:H	1.76	0.50
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.46	0.50
12:M:405:THR:HB	12:M:477:GLY:HA3	1.94	0.50
14:O:188:ILE:O	14:O:189:ASN:C	2.55	0.50
33:j:23:TRP:CE2	48:j:201:PEE:H51	2.46	0.50
14:O:215:LYS:O	14:O:219:ARG:NH1	2.43	0.50
21:W:86:MET:HE1	21:W:125:TYR:CZ	2.47	0.50
37:n:47:ARG:NH1	37:n:53:GLU:OE2	2.43	0.50
41:s:170:GLU:OE2	42:u:98:ARG:NH1	2.42	0.50
3:C:69:LEU:HB2	3:C:107:GLY:HA3	1.94	0.50
35:l:599:MET:O	35:l:603:ASN:CB	2.59	0.50
12:M:385:TYR:OH	12:M:527:ASP:OD1	2.23	0.50
23:Z:24:ILE:HB	23:Z:29:LEU:HB2	1.93	0.50
26:c:62:TYR:OH	26:c:74:ASP:O	2.23	0.50
39:p:98:LYS:HG2	39:p:178:PRO:HG3	1.93	0.50
16:Q:145:MET:HG3	16:Q:214:TYR:OH	2.12	0.50
33:j:23:TRP:CZ2	48:j:201:PEE:H51	2.47	0.50
8:I:12:ARG:HD2	8:I:20:LEU:HD12	1.93	0.50
12:M:178:GLN:HG2	12:M:204:MET:CE	2.42	0.50
12:M:389:THR:HG21	12:M:473:MET:SD	2.52	0.50
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:26:GLY:HA3	48:U:101:PEE:H38	1.94	0.49
48:l:703:PEE:H36	48:l:703:PEE:C18	2.42	0.49
37:n:10:ASP:HB2	40:r:19:LYS:HZ3	1.76	0.49
17:S:34:LYS:O	42:u:91:TYR:O	2.29	0.49
24:a:83:ALA:O	24:a:87:THR:HG22	2.12	0.49
31:h:29:ILE:HG21	36:m:138:GLU:HG3	1.93	0.49
32:i:11:MET:HA	51:i:401:CDL:H582	1.93	0.49
41:s:63:PRO:HB2	41:s:66:SER:HB3	1.94	0.49
20:V:39:TYR:HB3	51:V:201:CDL:H712	1.95	0.49
20:V:141:VAL:HG22	24:a:157:ARG:HB3	1.94	0.49
51:i:401:CDL:OA7	51:i:401:CDL:H132	2.11	0.49
39:p:19:LEU:HD13	39:p:68:GLU:OE1	2.13	0.49
42:u:80:GLU:HB2	42:u:81:PRO:CD	2.35	0.49
3:C:56:TRP:CZ3	49:C:303:PLX:C11	2.95	0.49
11:L:131:LYS:NZ	11:L:149:GLU:OE2	2.43	0.49
12:M:360:ARG:HG2	12:M:360:ARG:HH11	1.77	0.49
13:N:34:ARG:NH1	13:N:54:GLN:OE1	2.37	0.49
26:c:167:TYR:CG	26:c:178:PRO:HG3	2.47	0.49
28:e:143:ASP:OD1	28:e:144:PRO:CD	2.56	0.49
41:s:15:LEU:HD12	53:s:401:UQ:C27	2.42	0.49
1:A:48:ARG:HH21	14:O:226:GLU:CD	2.21	0.49
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.46	0.49
12:M:400:ILE:CD1	12:M:473:MET:HE3	2.41	0.49
24:a:184:LYS:O	24:a:185:THR:HG22	2.12	0.49
35:l:389:PHE:HA	35:l:393:ASP:OD1	2.13	0.49
51:l:701:CDL:H572	51:l:701:CDL:H861	1.93	0.49
44:w:246:LEU:HD22	44:w:255:VAL:HG11	1.95	0.49
9:J:207:PHE:HB2	9:J:214:LEU:HG	1.95	0.49
14:O:218:PRO:HD2	14:O:223:PHE:HA	1.95	0.49
15:P:201:ASP:OD1	15:P:201:ASP:N	2.37	0.49
1:A:98:LYS:NZ	46:A:502:FMN:H5'2	2.27	0.49
6:G:128:PHE:HE2	6:G:147:TYR:HE1	1.61	0.49
8:I:5:THR:HG22	8:I:6:ARG:HD3	1.95	0.49
49:g:201:PLX:H342	32:i:261:MET:HE1	1.93	0.49
51:i:401:CDL:HB62	44:w:40:PRO:HB2	1.94	0.49
11:L:154:LYS:O	11:L:156:LYS:NZ	2.46	0.49
26:c:139:PHE:CE2	51:l:702:CDL:H842	2.47	0.49
39:p:28:GLU:OE2	39:p:34:ARG:NH1	2.44	0.49
39:p:68:GLU:OE1	39:p:68:GLU:HA	2.13	0.49
41:s:101:GLY:O	41:s:105:MET:HG2	2.13	0.49
44:w:243:LYS:HB2	44:w:243:LYS:NZ	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:TRP:CZ3	49:C:303:PLX:H111	2.48	0.49
12:M:457:SER:OG	12:M:459:ASN:OD1	2.26	0.49
33:j:87:MET:HG2	36:m:147:TYR:HB3	1.95	0.49
35:l:54:PHE:CZ	35:l:84:TYR:HB2	2.48	0.49
51:l:701:CDL:H432	51:l:701:CDL:H602	1.95	0.49
9:J:375:VAL:HG23	9:J:375:VAL:O	2.13	0.48
12:M:181:ARG:HB3	12:M:225:ILE:HD12	1.95	0.48
13:N:3:LEU:O	13:N:7:LEU:HG	2.13	0.48
14:O:137:THR:HG22	14:O:138:THR:H	1.77	0.48
15:P:113:ASP:OD1	16:Q:423:LYS:NZ	2.39	0.48
42:u:80:GLU:CB	42:u:81:PRO:HD3	2.33	0.48
32:i:128:LEU:HD12	32:i:216:PHE:HB3	1.95	0.48
40:r:159:PRO:HB3	48:r:501:PEE:H25	1.95	0.48
48:C:302:PEE:H58	48:C:302:PEE:H24	1.94	0.48
16:Q:144:MET:O	16:Q:148:GLU:HG3	2.13	0.48
34:k:19:LEU:C	34:k:19:LEU:HD13	2.37	0.48
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.95	0.48
8:I:44:GLY:HA3	16:Q:359:ASP:OD2	2.12	0.48
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.48	0.48
6:X:153:ASP:OD1	25:b:19:ARG:NH2	2.33	0.48
22:Y:56:ILE:HG13	22:Y:57:GLN:N	2.28	0.48
5:F:59:SER:C	5:F:61:VAL:N	2.67	0.48
48:W:201:PEE:H32	48:W:201:PEE:H38	1.60	0.48
24:a:66:ARG:NH1	28:e:72:ASP:HB2	2.28	0.48
24:a:134:GLU:OE1	37:n:57:TRP:NE1	2.31	0.48
35:l:130:ILE:HD13	51:l:701:CDL:H252	1.94	0.48
36:m:31:LEU:HD21	51:m:201:CDL:H562	1.94	0.48
8:I:96:THR:HB	8:I:97:PRO:HD2	1.95	0.48
16:Q:94:VAL:HG21	16:Q:116:LEU:HB2	1.95	0.48
20:V:38:ALA:HA	51:k:101:CDL:H201	1.94	0.48
35:l:63:ILE:O	35:l:79:SER:HA	2.13	0.48
35:l:383:MET:HB3	35:l:386:LEU:HD12	1.95	0.48
51:l:701:CDL:C66	51:l:701:CDL:H232	2.42	0.48
51:l:702:CDL:H651	51:l:702:CDL:H451	1.96	0.48
10:K:74:ARG:O	10:K:76:LEU:N	2.47	0.48
12:M:390:THR:HB	12:M:600:GLU:OE2	2.14	0.48
13:N:55:PHE:CZ	13:N:58:ARG:HG3	2.48	0.48
22:Y:65:MET:SD	35:l:375:ILE:HG12	2.53	0.48
23:Z:22:TRP:HB3	23:Z:50:ALA:HB3	1.95	0.48
27:d:115:GLN:HG2	35:l:62:ILE:HG12	1.96	0.48
48:r:501:PEE:H52	48:r:501:PEE:H59	1.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ALA:O	1:A:252:PRO:HD2	2.13	0.48
2:B:49:ASP:O	2:B:53:VAL:HG23	2.14	0.48
16:Q:184:ILE:HG23	16:Q:203:MET:HB3	1.96	0.48
19:U:20:VAL:HG13	48:U:101:PEE:H67	1.95	0.48
48:W:201:PEE:H50	36:m:45:LEU:HD11	1.96	0.48
28:e:143:ASP:HA	28:e:144:PRO:HD3	1.64	0.48
35:l:548:SER:HA	35:l:552:LEU:HB3	1.95	0.48
12:M:372:PHE:CZ	12:M:385:TYR:HB3	2.49	0.48
15:P:157:VAL:HG21	15:P:182:PRO:HD3	1.94	0.48
16:Q:53:TYR:H	32:i:171:ASN:ND2	2.11	0.48
12:M:340:ALA:HB3	12:M:366:LEU:HD23	1.95	0.48
12:M:558:GLN:N	12:M:558:GLN:OE1	2.46	0.48
21:W:88:ARG:O	21:W:92:GLU:HG2	2.14	0.48
34:k:21:MET:O	36:m:23:LYS:CE	2.49	0.48
3:C:64:PRO:HD2	3:C:92:VAL:O	2.13	0.47
8:I:64:MET:HE2	15:P:80:CYS:SG	2.53	0.47
13:N:29:ARG:HD2	13:N:74:PHE:O	2.13	0.47
35:l:125:LEU:O	35:l:129:MET:HG2	2.14	0.47
35:l:286:LEU:HD13	35:l:411:MET:HG3	1.95	0.47
36:m:78:MET:O	36:m:80:PRO:HD3	2.14	0.47
32:i:254:LEU:CD2	40:r:154:LEU:HD11	2.43	0.47
35:l:298:ILE:O	35:l:302:VAL:HG23	2.14	0.47
36:m:86:ASN:OD1	36:m:87:LYS:N	2.46	0.47
4:E:92:GLU:OE1	15:P:191:TYR:CD1	2.67	0.47
10:K:78:HIS:HA	10:K:81:TYR:CE2	2.48	0.47
15:P:204:LEU:HD11	16:Q:123:LEU:HD23	1.95	0.47
22:Y:52:ARG:HB3	22:Y:52:ARG:NH1	2.30	0.47
31:h:32:ARG:HH11	31:h:32:ARG:HG2	1.79	0.47
35:l:540:HIS:O	35:l:544:MET:HG2	2.13	0.47
37:n:30:ARG:NH2	51:u:201:CDL:OA4	2.47	0.47
41:s:306:SER:HB3	41:s:310:MET:HE2	1.96	0.47
44:w:300:ASN:OD1	44:w:303:GLU:HB2	2.14	0.47
12:M:395:GLU:OE1	12:M:417:ARG:NH1	2.38	0.47
12:M:398:ASP:N	12:M:398:ASP:OD1	2.46	0.47
13:N:39:VAL:HG23	13:N:50:GLU:HG2	1.95	0.47
16:Q:144:MET:SD	16:Q:144:MET:N	2.83	0.47
20:V:45:PRO:HB3	51:k:101:CDL:H111	1.97	0.47
21:W:121:MET:HB2	36:m:130:THR:HG22	1.97	0.47
35:l:293:ILE:HD13	35:l:418:LEU:HD22	1.95	0.47
35:l:517:SER:OG	51:l:702:CDL:PA1	2.72	0.47
3:C:92:VAL:HG21	53:s:401:UQ:C10	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:493:VAL:HG12	12:M:513:MET:HE1	1.96	0.47
16:Q:156:GLU:HG3	16:Q:229:PRO:O	2.15	0.47
21:W:70:ALA:HB2	42:u:125:LEU:HD13	1.96	0.47
6:X:118:ILE:O	6:X:122:MET:HG2	2.15	0.47
27:d:171:LYS:NZ	28:e:153:GLU:HB2	2.29	0.47
35:l:27:TYR:O	35:l:115:ASN:ND2	2.38	0.47
43:v:103:GLU:O	43:v:107:ARG:HG2	2.15	0.47
44:w:118:TYR:OH	58:w:401:ADP:O2'	2.32	0.47
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.95	0.47
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.71	0.47
23:Z:32:VAL:HG13	39:p:39:TYR:HB2	1.96	0.47
28:e:153:GLU:CD	28:e:153:GLU:H	2.23	0.47
51:l:702:CDL:H521	51:l:702:CDL:CB6	2.43	0.47
40:r:16:TRP:CZ2	51:r:504:CDL:C26	2.97	0.47
40:r:126:LEU:HD21	40:r:153:THR:HG21	1.97	0.47
1:A:122:PRO:HA	14:O:176:CYS:SG	2.55	0.47
1:A:201:ALA:O	14:O:119:TYR:HB3	2.15	0.47
1:A:373:PHE:HD1	14:O:175:GLU:HB3	1.80	0.47
3:C:108:THR:HA	3:C:136:CYS:HB3	1.95	0.47
4:E:101:THR:OG1	15:P:219:VAL:O	2.22	0.47
12:M:598:ASN:C	12:M:598:ASN:ND2	2.73	0.47
17:S:12:MET:CE	41:s:20:LEU:HA	2.45	0.47
19:U:19:LEU:HD12	48:U:101:PEE:H48	1.97	0.47
51:l:702:CDL:HA31	51:l:702:CDL:H712	1.96	0.47
37:n:21:PHE:HA	40:r:7:PRO:HG3	1.95	0.47
1:A:107:ASP:OD1	1:A:107:ASP:N	2.48	0.47
2:B:208:ASP:OD2	2:B:212:ARG:NE	2.47	0.47
49:J:403:PLX:H272	49:J:403:PLX:H301	1.50	0.47
27:d:148:ALA:O	27:d:149:HIS:CB	2.63	0.47
40:r:302:MET:HE2	40:r:302:MET:HA	1.97	0.47
43:v:44:GLN:OE1	43:v:44:GLN:HA	2.15	0.47
11:L:115:SER:HB2	12:M:267:THR:HB	1.97	0.47
12:M:393:GLY:O	12:M:394:VAL:C	2.58	0.47
32:i:11:MET:HG2	51:i:401:CDL:H561	1.96	0.47
32:i:246:VAL:HG21	51:r:504:CDL:H362	1.97	0.47
51:r:504:CDL:H473	51:r:504:CDL:H191	1.97	0.47
53:s:401:UQ:H221	53:s:401:UQ:H262	1.58	0.47
1:A:56:ALA:HB1	1:A:61:ASP:HB2	1.97	0.47
12:M:144:MET:HG3	16:Q:383:LYS:HG3	1.97	0.47
51:l:701:CDL:H822	51:l:701:CDL:H631	1.96	0.47
13:N:9:ARG:O	13:N:12:GLN:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:101:LEU:HD23	16:Q:106:VAL:HA	1.97	0.46
16:Q:145:MET:HG3	16:Q:214:TYR:CZ	2.50	0.46
28:e:122:ALA:O	28:e:126:VAL:HG23	2.15	0.46
51:l:702:CDL:H111	51:l:702:CDL:C15	2.38	0.46
40:r:210:TYR:O	40:r:264:LEU:HD22	2.16	0.46
1:A:367:ILE:O	1:A:371:ILE:HG12	2.14	0.46
3:C:84:TYR:OH	3:C:171:GLU:OE2	2.30	0.46
21:W:120:MET:O	21:W:121:MET:HB3	2.16	0.46
26:c:81:ARG:NH1	26:c:85:GLU:OE1	2.45	0.46
26:c:127:ASN:O	26:c:131:LYS:HG3	2.16	0.46
30:g:13:LEU:HA	49:g:201:PLX:H32	1.97	0.46
51:i:401:CDL:C22	51:i:401:CDL:C18	2.93	0.46
51:l:701:CDL:H401	51:l:701:CDL:C35	2.44	0.46
40:r:76:MET:HG2	40:r:229:MET:HE2	1.96	0.46
51:r:504:CDL:H861	51:r:504:CDL:H832	1.58	0.46
42:u:113:ASP:OD1	42:u:114:LYS:HD3	2.15	0.46
43:v:70:LYS:HG2	43:v:80:CYS:SG	2.54	0.46
44:w:65:ASN:HD22	44:w:238:GLU:HG2	1.80	0.46
14:O:164:THR:OG1	14:O:166:ASP:OD1	2.32	0.46
33:j:66:ASP:O	33:j:69:ILE:HG12	2.16	0.46
44:w:96:SER:HA	44:w:101:GLY:HA2	1.97	0.46
1:A:185:ASN:C	1:A:187:CYS:H	2.22	0.46
3:C:107:GLY:HA2	45:C:301:SF4:S1	2.55	0.46
12:M:44:GLU:OE1	12:M:45:PRO:CD	2.60	0.46
6:X:83:VAL:HG22	6:X:122:MET:HE2	1.97	0.46
40:r:106:LEU:HD13	40:r:234:VAL:HG11	1.97	0.46
4:E:14:GLY:O	11:L:54:ALA:HA	2.14	0.46
15:P:196:HIS:HA	15:P:197:PRO:HD3	1.79	0.46
24:a:184:LYS:C	24:a:186:THR:H	2.22	0.46
37:n:54:GLU:OE2	37:n:54:GLU:N	2.45	0.46
41:s:209:SER:CB	41:s:213:VAL:HA	2.45	0.46
43:v:15:LYS:HE3	43:v:15:LYS:HB3	1.64	0.46
44:w:110:GLY:HA2	44:w:134:TRP:CE2	2.51	0.46
34:k:16:LEU:HD13	34:k:36:MET:HE1	1.98	0.46
10:K:100:GLN:HG3	14:O:68:LYS:O	2.15	0.46
11:L:99:MET:HE3	11:L:128:PHE:CE1	2.51	0.46
12:M:395:GLU:HA	12:M:421:SER:OG	2.16	0.46
12:M:667:GLN:OE1	12:M:667:GLN:N	2.49	0.46
17:S:69:ILE:HD11	42:u:20:VAL:HG13	1.96	0.46
33:j:80:GLN:NE2	41:s:317:GLN:O	2.49	0.46
35:l:190:LEU:CD2	40:r:383:THR:HG21	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:435:PRO:HB3	35:l:437:PHE:CZ	2.50	0.46
51:o:201:CDL:H871	40:r:210:TYR:CE2	2.50	0.46
40:r:357:THR:O	40:r:361:VAL:HG23	2.15	0.46
1:A:48:ARG:NH2	14:O:226:GLU:OE1	2.40	0.46
48:B:303:PEE:H38	19:U:25:ILE:CD1	2.46	0.46
51:a:201:CDL:H512	51:a:201:CDL:HB4	1.83	0.46
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.51	0.46
41:s:15:LEU:HD12	53:s:401:UQ:H272	1.98	0.46
41:s:81:LEU:O	41:s:85:MET:HG2	2.16	0.46
44:w:72:ARG:HA	44:w:75:ARG:NH1	2.30	0.46
48:C:302:PEE:C23	49:J:403:PLX:C16	2.90	0.46
51:I:201:CDL:H511	51:I:201:CDL:H542	1.63	0.46
12:M:471:LYS:HB3	12:M:510:TRP:CZ2	2.51	0.46
12:M:688:GLN:H	12:M:688:GLN:HG2	1.60	0.46
25:b:69:ILE:O	25:b:73:THR:HG22	2.15	0.46
26:c:70:MET:HE2	38:o:85:LYS:HZ2	1.78	0.46
31:h:24:GLU:HG3	31:h:24:GLU:O	2.15	0.46
35:l:346:ILE:HD11	35:l:431:PHE:CZ	2.50	0.46
35:l:597:ILE:HG23	35:l:601:LEU:HD22	1.98	0.46
40:r:42:LEU:HB3	40:r:453:MET:HE2	1.98	0.46
43:v:92:HIS:O	43:v:96:VAL:HG12	2.16	0.46
44:w:54:THR:C	44:w:56:THR:H	2.24	0.46
44:w:65:ASN:OD1	44:w:66:ILE:N	2.38	0.46
1:A:63:TYR:O	1:A:256:ARG:HD3	2.15	0.46
2:B:101:HIS:ND1	2:B:149:MET:HE1	2.30	0.46
48:B:303:PEE:H38	19:U:25:ILE:HD11	1.97	0.46
3:C:56:TRP:CZ2	49:C:303:PLX:H112	2.50	0.46
5:F:61:VAL:HG13	5:F:62:GLN:N	2.31	0.46
8:I:4:ALA:CA	51:I:201:CDL:OA2	2.42	0.46
49:J:403:PLX:H252	49:J:403:PLX:H281	1.79	0.46
12:M:197:THR:HA	12:M:205:GLN:O	2.16	0.46
14:O:140:CYS:HA	14:O:183:ALA:HB1	1.97	0.46
35:l:252:MET:HE2	35:l:252:MET:HB3	1.84	0.46
35:l:529:TYR:HB3	35:l:530:PRO:HD3	1.97	0.46
41:s:66:SER:HB2	41:s:122:ALA:O	2.16	0.46
41:s:221:ALA:O	41:s:225:MET:HG3	2.16	0.46
1:A:234:GLY:HA3	1:A:240:THR:OG1	2.16	0.45
1:A:267:ARG:HG3	1:A:293:SER:OG	2.16	0.45
3:C:78:HIS:HD1	16:Q:208:GLU:HG2	1.81	0.45
5:F:65:LEU:HD11	5:F:91:LEU:HD13	1.97	0.45
51:I:201:CDL:H722	17:S:3:PHE:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:534:VAL:HG21	12:M:555:ILE:HG13	1.95	0.45
15:P:50:ARG:NH2	15:P:80:CYS:SG	2.90	0.45
16:Q:55:THR:O	16:Q:58:THR:N	2.49	0.45
26:c:186:ILE:HG21	43:v:101:GLU:HG2	1.98	0.45
28:e:65:ASN:HB3	28:e:68:GLU:HG2	1.97	0.45
9:J:208:GLY:H	9:J:211:ASP:CG	2.24	0.45
12:M:169:VAL:HG22	12:M:223:ILE:HD11	1.97	0.45
16:Q:198:THR:OG1	41:s:275:ALA:O	2.24	0.45
48:U:101:PEE:H67	48:U:101:PEE:H73	1.74	0.45
22:Y:40:ILE:HD11	35:l:444:ASN:HB2	1.98	0.45
35:l:560:THR:O	35:l:565:THR:OG1	2.28	0.45
40:r:216:LEU:HB3	40:r:217:PRO:HD3	1.97	0.45
3:C:95:ALA:CB	41:s:208:VAL:HG13	2.44	0.45
16:Q:208:GLU:CD	16:Q:221:ARG:HH22	2.23	0.45
19:U:38:TYR:HB2	41:s:310:MET:O	2.16	0.45
21:W:55:ARG:NH2	41:s:311:THR:O	2.49	0.45
32:i:243:LEU:HD23	51:r:504:CDL:H361	1.97	0.45
35:l:230:HIS:N	35:l:231:PRO:HD3	2.30	0.45
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.52	0.45
11:L:165:SER:OG	11:L:168:LYS:CG	2.65	0.45
13:N:7:LEU:O	13:N:11:LEU:HD23	2.17	0.45
32:i:278:MET:HB3	32:i:279:PRO:HD3	1.98	0.45
33:j:22:PHE:HA	41:s:60:PRO:HG3	1.99	0.45
33:j:23:TRP:NE1	48:j:201:PEE:C1	2.80	0.45
35:l:566:THR:HG21	48:l:703:PEE:H61	1.97	0.45
3:C:61:SER:O	41:s:54:LYS:HE2	2.17	0.45
24:a:147:ALA:HB2	40:r:173:SER:HB2	1.98	0.45
26:c:40:PRO:O	26:c:74:ASP:HB3	2.16	0.45
26:c:63:GLU:HA	26:c:63:GLU:OE1	2.16	0.45
27:d:42:ASP:O	27:d:46:THR:HG23	2.16	0.45
35:l:49:VAL:HB	35:l:50:PRO:HD3	1.99	0.45
40:r:127:VAL:HB	40:r:128:PRO:HD3	1.98	0.45
41:s:32:GLN:OE1	41:s:34:ARG:NH2	2.48	0.45
7:H:50:GLN:O	7:H:54:GLU:HG3	2.16	0.45
9:J:221:ARG:HD2	9:J:286:ARG:HD2	1.98	0.45
35:l:419:THR:HA	35:l:422:TYR:CE2	2.51	0.45
36:m:31:LEU:C	36:m:31:LEU:HD23	2.41	0.45
15:P:125:ARG:CZ	15:P:199:ARG:HG2	2.46	0.45
30:g:2:THR:HG22	30:g:5:SER:CB	2.41	0.45
35:l:11:THR:HG21	35:l:47:SER:HB3	1.99	0.45
35:l:37:LYS:HE3	35:l:37:LYS:HB3	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:31:MET:HE1	41:s:272:TRP:CD1	2.51	0.45
1:A:214:GLU:OE2	1:A:224:ARG:NH2	2.45	0.45
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.52	0.45
48:B:303:PEE:H64	41:s:273:ILE:HD11	1.99	0.45
3:C:154:ASP:HA	3:C:157:VAL:O	2.17	0.45
8:I:4:ALA:O	8:I:9:GLN:NE2	2.45	0.45
12:M:94:MET:HA	12:M:95:PRO:HD3	1.88	0.45
13:N:4:VAL:HA	13:N:7:LEU:HD12	1.99	0.45
14:O:224:SER:HB2	14:O:226:GLU:HG2	1.99	0.45
18:T:43:GLN:CD	18:T:43:GLN:C	2.85	0.45
25:b:10:LEU:HG	25:b:14:GLN:HE21	1.82	0.45
32:i:339:MET:HE3	32:i:339:MET:HB3	1.75	0.45
42:u:152:PRO:O	42:u:153:GLU:HB2	2.16	0.45
5:F:16:LEU:HD21	5:F:19:ILE:HD11	1.99	0.45
12:M:690:THR:HG23	12:M:692:LYS:HG2	1.98	0.45
35:l:136:ASN:OD1	35:l:136:ASN:N	2.49	0.45
51:o:201:CDL:H812	51:o:201:CDL:H781	1.70	0.45
39:p:35:ASP:OD1	39:p:36:LYS:N	2.48	0.45
40:r:389:SER:O	40:r:392:THR:OG1	2.32	0.45
51:r:504:CDL:H541	51:r:504:CDL:H511	1.56	0.45
2:B:80:GLU:HG3	17:S:1:MET:SD	2.57	0.45
9:J:167:ILE:HD13	9:J:201:ILE:HB	1.98	0.45
49:J:403:PLX:H6	49:J:403:PLX:H32	1.47	0.45
10:K:68:PHE:O	10:K:68:PHE:CD2	2.70	0.45
19:U:73:PRO:HG2	19:U:74:GLN:NE2	2.32	0.45
20:V:69:ILE:O	20:V:73:THR:HG23	2.17	0.45
51:V:201:CDL:H322	51:V:201:CDL:H352	1.60	0.45
28:e:72:ASP:OD1	28:e:72:ASP:N	2.48	0.45
33:j:71:LEU:O	36:m:147:TYR:OH	2.26	0.45
44:w:85:HIS:NE2	44:w:160:GLU:OE2	2.40	0.45
5:F:90:THR:O	5:F:94:VAL:HG12	2.18	0.44
9:J:37:HIS:O	9:J:39:ALA:N	2.50	0.44
12:M:304:GLN:HB2	12:M:316:TYR:CD1	2.52	0.44
13:N:68:MET:HG2	13:N:115:PHE:CD2	2.52	0.44
26:c:148:GLU:HG2	35:l:405:ASN:HD22	1.82	0.44
28:e:97:ILE:O	28:e:101:LEU:HB2	2.17	0.44
32:i:14:MET:SD	51:i:401:CDL:H571	2.57	0.44
34:k:59:MET:HG3	34:k:60:PRO:CD	2.45	0.44
35:l:383:MET:SD	35:l:384:PRO:HD2	2.57	0.44
42:u:38:LYS:HB3	42:u:39:PRO:HD3	1.99	0.44
44:w:132:GLN:NE2	44:w:166:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.47	0.44
30:g:32:ARG:O	30:g:36:MET:HG2	2.16	0.44
42:u:34:ALA:HB2	42:u:120:PRO:HG3	1.98	0.44
43:v:7:ARG:NE	43:v:16:GLU:OE2	2.48	0.44
1:A:68:ILE:HD11	1:A:256:ARG:HG3	2.00	0.44
1:A:445:GLU:OE1	1:A:445:GLU:N	2.49	0.44
8:I:70:MET:O	8:I:70:MET:SD	2.75	0.44
14:O:146:ASP:OD1	14:O:146:ASP:N	2.49	0.44
20:V:8:LYS:HB3	20:V:8:LYS:HE3	1.79	0.44
25:b:88:TYR:CE1	27:d:49:ARG:HG2	2.53	0.44
33:j:57:LEU:HD21	36:m:169:MET:SD	2.58	0.44
36:m:129:ASP:O	36:m:130:THR:OG1	2.28	0.44
41:s:209:SER:HB3	41:s:213:VAL:HB	1.99	0.44
44:w:209:VAL:HG22	44:w:260:ALA:HB2	1.99	0.44
9:J:173:ASP:HB3	9:J:176:SER:HB3	1.99	0.44
13:N:144:TYR:HD1	13:N:144:TYR:H	1.65	0.44
16:Q:123:LEU:O	16:Q:127:LYS:HG2	2.17	0.44
35:l:119:LYS:CE	51:l:701:CDL:OA3	2.65	0.44
51:l:702:CDL:H521	51:l:702:CDL:HB62	2.00	0.44
39:p:100:PRO:HD3	40:r:419:TYR:CZ	2.53	0.44
41:s:303:TRP:CZ3	41:s:310:MET:HE1	2.53	0.44
43:v:57:ASP:C	43:v:59:CYS:N	2.74	0.44
3:C:63:TRP:CD1	3:C:92:VAL:HG22	2.52	0.44
4:E:104:MET:HE2	4:E:104:MET:HA	1.99	0.44
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.98	0.44
24:a:67:PHE:CZ	24:a:71:MET:HE2	2.52	0.44
51:l:701:CDL:H272	51:l:701:CDL:H241	1.80	0.44
40:r:193:ILE:HD13	49:r:502:PLX:H102	2.00	0.44
49:r:503:PLX:H221	49:r:503:PLX:H191	1.83	0.44
42:u:153:GLU:HG3	42:u:154:ALA:N	2.33	0.44
43:v:57:ASP:C	43:v:59:CYS:H	2.26	0.44
9:J:236:VAL:HG22	9:J:272:LEU:HD23	1.99	0.44
12:M:59:GLN:HG3	12:M:62:ARG:NH2	2.32	0.44
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.50	0.44
15:P:44:ARG:HB2	15:P:44:ARG:CZ	2.48	0.44
16:Q:282:ASP:OD2	16:Q:437:LYS:NZ	2.51	0.44
21:W:133:ILE:HD13	36:m:125:TRP:CH2	2.53	0.44
33:j:73:LEU:N	33:j:74:PRO:HD2	2.33	0.44
51:l:702:CDL:H601	51:l:702:CDL:C37	2.44	0.44
51:l:702:CDL:H732	51:l:702:CDL:C12	2.48	0.44
3:C:56:TRP:CZ3	49:C:303:PLX:H112	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:30:TRP:O	32:i:34:GLU:HG2	2.17	0.44
32:i:194:LEU:HD12	32:i:201:THR:HG21	1.99	0.44
38:o:53:ASP:HA	38:o:54:PRO:HD3	1.77	0.44
49:r:502:PLX:H72	49:r:502:PLX:H101	1.74	0.44
42:u:16:GLN:HB3	42:u:68:LEU:HD11	1.99	0.44
44:w:57:SER:HB3	44:w:150:LEU:HD11	1.99	0.44
49:J:403:PLX:H371	49:J:403:PLX:H342	1.83	0.44
12:M:639:LEU:O	12:M:642:VAL:HG12	2.17	0.44
13:N:14:VAL:HA	13:N:23:TYR:CD1	2.52	0.44
35:l:150:MET:HE3	35:l:150:MET:HA	2.00	0.44
38:o:113:GLU:OE1	38:o:113:GLU:HA	2.18	0.44
40:r:200:ILE:HD11	40:r:250:LEU:CD1	2.47	0.44
40:r:401:MET:HE3	40:r:401:MET:HB3	1.67	0.44
1:A:355:ILE:HD13	14:O:139:PRO:HG3	2.00	0.44
1:A:384:PRO:HB2	1:A:423:THR:CG2	2.45	0.44
3:C:169:THR:HG22	16:Q:221:ARG:HD2	2.00	0.44
4:E:48:HIS:NE2	9:J:365:GLU:OE1	2.44	0.44
8:I:97:PRO:HD3	15:P:61:PHE:CE1	2.53	0.44
12:M:172:ILE:HD12	12:M:175:ARG:NH1	2.33	0.44
16:Q:55:THR:O	16:Q:56:LYS:C	2.60	0.44
32:i:245:MET:HB3	32:i:245:MET:HE3	1.78	0.44
32:i:325:LEU:HD12	51:i:401:CDL:H151	1.99	0.44
35:l:188:TRP:CD1	35:l:211:MET:HE3	2.53	0.44
44:w:354:LEU:HD23	44:w:354:LEU:HA	1.81	0.44
2:B:88:PHE:CZ	13:N:30:ALA:HA	2.53	0.43
2:B:97:PHE:HB2	16:Q:215:GLU:OE2	2.18	0.43
3:C:49:LYS:HA	3:C:49:LYS:HD3	1.71	0.43
3:C:173:LEU:O	3:C:177:ILE:HG12	2.18	0.43
16:Q:83:ASN:N	33:j:38:GLU:OE1	2.47	0.43
21:W:58:ARG:HD2	21:W:58:ARG:HA	1.79	0.43
28:e:84:LEU:O	28:e:88:ARG:HG3	2.18	0.43
32:i:20:VAL:HG13	32:i:29:ILE:HG23	2.00	0.43
34:k:16:LEU:HD13	34:k:36:MET:CE	2.48	0.43
35:l:562:LEU:HB3	35:l:563:PRO:CD	2.46	0.43
40:r:214:LEU:O	40:r:217:PRO:HD2	2.18	0.43
44:w:143:TYR:OH	44:w:199:LEU:O	2.29	0.43
7:H:35:LEU:HD13	7:H:49:GLU:HG3	2.00	0.43
12:M:213:MET:HB3	12:M:215:MET:HG2	2.00	0.43
16:Q:53:TYR:H	32:i:171:ASN:HD21	1.65	0.43
16:Q:94:VAL:CG2	16:Q:116:LEU:HB2	2.49	0.43
16:Q:259:GLU:OE1	21:W:23:ARG:NH1	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:404:LYS:HE2	16:Q:457:VAL:HB	2.00	0.43
21:W:94:GLU:HG3	31:h:79:ILE:CD1	2.44	0.43
28:e:136:LEU:HD12	28:e:136:LEU:HA	1.74	0.43
30:g:13:LEU:HD11	31:h:6:VAL:HG12	2.01	0.43
39:p:14:GLN:HB3	39:p:18:ARG:NH1	2.33	0.43
42:u:165:SER:HB3	42:u:172:MET:O	2.18	0.43
5:F:83:SER:O	5:F:87:VAL:HG23	2.18	0.43
8:I:39:PRO:HB2	8:I:41:LEU:HD13	1.99	0.43
16:Q:37:TRP:O	16:Q:37:TRP:CE3	2.71	0.43
16:Q:375:MET:HE3	16:Q:379:ILE:HG13	2.01	0.43
20:V:44:LYS:HB2	20:V:44:LYS:HE2	1.74	0.43
30:g:2:THR:HG22	30:g:5:SER:H	1.83	0.43
51:k:101:CDL:OB9	36:m:23:LYS:NZ	2.47	0.43
40:r:105:PHE:O	40:r:109:THR:OG1	2.27	0.43
44:w:72:ARG:NH2	44:w:264:GLU:HA	2.33	0.43
1:A:41:ILE:HG12	1:A:253:THR:HG21	1.99	0.43
5:F:26:ARG:HB3	5:F:26:ARG:NH1	2.33	0.43
12:M:137:CYS:SG	12:M:139:LEU:HB3	2.58	0.43
14:O:76:ALA:C	14:O:78:ALA:N	2.74	0.43
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.99	0.43
51:V:201:CDL:H582	51:V:201:CDL:H611	1.70	0.43
6:X:136:GLU:O	6:X:139:MET:CE	2.58	0.43
27:d:9:VAL:HG23	27:d:10:TYR:CD2	2.54	0.43
35:l:68:TRP:CD2	48:l:705:PEE:H42	2.53	0.43
35:l:359:MET:O	35:l:436:ARG:NH2	2.51	0.43
49:C:303:PLX:H1C3	49:C:303:PLX:O1	2.17	0.43
9:J:132:ARG:NH1	52:J:401:NDP:O3X	2.44	0.43
21:W:121:MET:HB2	36:m:130:THR:CG2	2.48	0.43
6:X:122:MET:HA	6:X:122:MET:HE3	1.99	0.43
24:a:170:GLN:HB2	30:g:6:GLY:O	2.19	0.43
27:d:106:ILE:HD11	28:e:136:LEU:HD21	2.00	0.43
27:d:107:GLN:OE1	35:l:194:ASN:ND2	2.52	0.43
30:g:85:TYR:CZ	32:i:344:SER:HB3	2.54	0.43
32:i:95:MET:CE	32:i:149:ILE:HG12	2.48	0.43
35:l:511:LEU:HD12	35:l:511:LEU:HA	1.81	0.43
35:l:566:THR:O	35:l:570:GLN:HG2	2.18	0.43
40:r:373:ILE:HA	40:r:376:ILE:HD12	2.00	0.43
41:s:200:LEU:HG	41:s:282:TYR:HB3	2.00	0.43
9:J:163:LYS:NZ	9:J:253:ILE:O	2.40	0.43
53:J:402:UQ:H71	53:J:402:UQ:HM53	1.78	0.43
12:M:306:MET:HE1	13:N:139:PRO:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:28:LYS:O	17:S:33:GLY:N	2.52	0.43
51:V:201:CDL:H322	35:l:576:MET:HE1	2.00	0.43
50:X:201:8Q1:C11	39:p:70:GLU:HB3	2.48	0.43
35:l:108:MET:HE3	35:l:108:MET:HB3	1.94	0.43
35:l:176:ARG:HA	35:l:179:ASP:HB2	2.00	0.43
41:s:15:LEU:CD1	53:s:401:UQ:H272	2.49	0.43
1:A:98:LYS:HZ3	46:A:502:FMN:H5'2	1.82	0.43
8:I:30:GLU:OE1	8:I:30:GLU:N	2.47	0.43
9:J:262:THR:O	9:J:333:PRO:HD2	2.19	0.43
22:Y:52:ARG:O	22:Y:56:ILE:HG23	2.18	0.43
49:j:202:PLX:H72	49:j:202:PLX:H4	1.63	0.43
35:l:46:LEU:HD12	35:l:46:LEU:HA	1.87	0.43
37:n:9:ARG:HD2	37:n:9:ARG:HA	1.66	0.43
38:o:25:ILE:HG21	38:o:30:ARG:NH1	2.34	0.43
44:w:244:THR:O	44:w:248:GLU:HG3	2.18	0.43
1:A:48:ARG:NH1	10:K:71:SER:HA	2.34	0.43
4:E:87:LYS:HB2	4:E:87:LYS:HE2	1.73	0.43
5:F:37:ILE:HD13	5:F:55:ILE:HG21	2.01	0.43
11:L:105:GLU:HA	12:M:611:THR:CG2	2.47	0.43
18:T:95:HIS:ND1	18:T:96:PRO:O	2.44	0.43
31:h:18:MET:O	31:h:18:MET:HG2	2.19	0.43
49:j:202:PLX:H191	49:j:202:PLX:H222	1.80	0.43
35:l:128:MET:HG2	35:l:251:THR:HG22	2.00	0.43
41:s:68:ILE:HD12	41:s:68:ILE:HA	1.74	0.43
6:G:147:TYR:CD1	6:G:147:TYR:C	2.97	0.43
15:P:125:ARG:NH1	15:P:199:ARG:HD3	2.33	0.43
20:V:141:VAL:HG22	24:a:157:ARG:CB	2.49	0.43
24:a:74:TYR:O	28:e:96:SER:OG	2.26	0.43
25:b:101:LYS:O	43:v:50:GLN:NE2	2.39	0.43
51:l:701:CDL:H351	51:l:701:CDL:C40	2.48	0.43
41:s:11:ILE:HB	41:s:12:PRO:HD3	2.00	0.43
44:w:345:GLU:HA	44:w:345:GLU:OE1	2.19	0.43
3:C:55:ASN:ND2	3:C:187:GLU:O	2.45	0.43
16:Q:228:ARG:O	16:Q:230:GLY:N	2.51	0.43
32:i:14:MET:O	32:i:18:MET:HG2	2.19	0.43
32:i:255:PRO:HG3	32:i:260:PHE:CD1	2.54	0.43
33:j:27:LEU:HA	41:s:59:GLU:HG3	2.01	0.43
34:k:59:MET:HE2	34:k:59:MET:HB2	1.81	0.43
35:l:375:ILE:HD12	35:l:458:LEU:HD11	2.00	0.43
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.32	0.42
3:C:190:LEU:HD22	48:C:302:PEE:H13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:I:201:CDL:C31	13:N:3:LEU:HD11	2.45	0.42
13:N:11:LEU:HA	13:N:14:VAL:HG12	2.01	0.42
48:W:201:PEE:H42	48:W:201:PEE:H33	2.01	0.42
6:X:103:HIS:O	6:X:107:ASP:HB2	2.19	0.42
26:c:156:VAL:HG12	43:v:99:MET:HG3	2.00	0.42
32:i:54:GLU:HG3	34:k:93:LEU:HB3	2.00	0.42
35:l:2:ASN:ND2	35:l:59:GLN:OE1	2.51	0.42
35:l:80:PHE:HB3	35:l:82:MET:HE2	2.01	0.42
51:l:701:CDL:H202	51:l:701:CDL:H231	1.76	0.42
48:l:703:PEE:H42	48:l:703:PEE:C21	2.37	0.42
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.54	0.42
38:o:75:ASN:O	38:o:79:ASN:ND2	2.51	0.42
44:w:93:TYR:O	44:w:96:SER:OG	2.35	0.42
7:H:105:GLU:HB3	15:P:89:HIS:NE2	2.34	0.42
19:U:51:TYR:HB3	36:m:136:PHE:HE2	1.84	0.42
6:X:142:GLN:NE2	6:X:146:ASP:OD1	2.52	0.42
35:l:288:THR:HG21	35:l:307:SER:OG	2.19	0.42
51:o:201:CDL:H111	51:o:201:CDL:H142	1.75	0.42
40:r:427:LYS:HD3	40:r:427:LYS:HA	1.73	0.42
41:s:20:LEU:HD12	41:s:20:LEU:O	2.19	0.42
1:A:340:ASP:OD1	1:A:340:ASP:N	2.51	0.42
3:C:125:PRO:HG2	41:s:58:LYS:NZ	2.34	0.42
8:I:6:ARG:HG2	8:I:7:VAL:N	2.33	0.42
10:K:107:SER:HB3	10:K:110:HIS:ND1	2.35	0.42
48:U:101:PEE:H50	48:U:101:PEE:H57	1.77	0.42
20:V:4:THR:O	20:V:8:LYS:HG3	2.20	0.42
21:W:105:LYS:HG2	42:u:4:ILE:HD11	2.00	0.42
22:Y:68:TRP:CZ2	22:Y:72:ARG:HD2	2.54	0.42
51:a:201:CDL:H372	51:a:201:CDL:H342	1.50	0.42
31:h:12:LEU:HD12	31:h:12:LEU:HA	1.88	0.42
38:o:59:VAL:HG22	40:r:423:ILE:HG12	2.00	0.42
51:o:201:CDL:H601	51:o:201:CDL:H742	2.00	0.42
1:A:51:TRP:CE3	1:A:51:TRP:O	2.72	0.42
11:L:61:ILE:O	11:L:65:THR:HG23	2.19	0.42
16:Q:55:THR:HG22	16:Q:57:GLU:H	1.84	0.42
29:f:55:TRP:O	29:f:59:ILE:HG12	2.19	0.42
35:l:250:SER:HB2	35:l:333:ALA:HA	2.00	0.42
36:m:82:VAL:HG22	36:m:85:SER:HB3	2.00	0.42
1:A:88:ARG:HD2	1:A:274:LYS:HE2	2.01	0.42
1:A:115:VAL:HG21	1:A:142:CYS:SG	2.60	0.42
2:B:65:GLU:H	2:B:65:GLU:HG3	1.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:4:ALA:CA	51:I:201:CDL:CA2	2.79	0.42
8:I:46:SER:O	8:I:52:ASN:ND2	2.50	0.42
12:M:233:SER:HB3	12:M:236:TYR:HB3	2.00	0.42
34:k:1:MET:HE3	34:k:5:TYR:HB3	2.02	0.42
35:l:166:THR:CG2	48:l:704:PEE:H2	2.49	0.42
41:s:179:TRP:CG	41:s:180:PRO:HD3	2.55	0.42
43:v:31:PHE:CD2	43:v:34:ARG:HD3	2.54	0.42
16:Q:99:MET:CE	16:Q:444:LEU:HD11	2.42	0.42
17:S:63:THR:HG21	42:u:86:TRP:CZ3	2.55	0.42
17:S:66:LEU:HD23	17:S:66:LEU:HA	1.86	0.42
27:d:49:ARG:O	27:d:53:GLU:HG3	2.20	0.42
51:k:101:CDL:H161	51:k:101:CDL:H191	1.79	0.42
40:r:209:LEU:HD23	40:r:212:LEU:HD12	2.02	0.42
41:s:104:PHE:O	41:s:108:MET:HG2	2.20	0.42
1:A:392:MET:HG2	1:A:412:LEU:HD11	2.00	0.42
7:H:90:LEU:O	7:H:94:MET:HG2	2.19	0.42
12:M:428:LYS:HE2	12:M:465:ILE:HD13	2.02	0.42
16:Q:92:HIS:NE2	16:Q:193:ASP:OD2	2.50	0.42
49:j:202:PLX:H22	49:j:202:PLX:H1C3	1.65	0.42
2:B:75:SER:OG	8:I:16:SER:HB3	2.20	0.42
8:I:28:TYR:O	8:I:29:GLN:OE1	2.37	0.42
9:J:228:LEU:O	9:J:292:PRO:HA	2.20	0.42
12:M:36:VAL:HG22	12:M:102:ILE:HD12	2.01	0.42
48:W:201:PEE:H7	36:m:45:LEU:HD22	2.01	0.42
22:Y:41:GLU:OE2	22:Y:41:GLU:N	2.50	0.42
25:b:25:ASP:OD2	39:p:125:TRP:NE1	2.43	0.42
31:h:17:TRP:CD1	31:h:17:TRP:H	2.38	0.42
49:r:502:PLX:H51	49:r:502:PLX:H6	1.47	0.42
41:s:227:GLU:O	41:s:231:ILE:HG12	2.20	0.42
1:A:53:LEU:O	1:A:54:LYS:C	2.63	0.42
6:G:84:LEU:HD13	6:G:84:LEU:HA	1.94	0.42
8:I:58:ASP:O	8:I:62:GLU:HG3	2.20	0.42
15:P:162:ALA:HB2	16:Q:286:TYR:C	2.45	0.42
30:g:56:VAL:HG21	40:r:17:MET:HE1	2.00	0.42
51:o:201:CDL:H811	51:o:201:CDL:H842	1.91	0.42
40:r:186:LEU:O	40:r:252:PRO:HD2	2.19	0.42
48:r:501:PEE:H68	48:r:501:PEE:H62	1.72	0.42
41:s:24:GLU:HA	41:s:271:LEU:HD13	2.02	0.42
1:A:226:LYS:HD2	1:A:229:PHE:CD2	2.55	0.42
1:A:363:ILE:HD12	1:A:363:ILE:HA	1.89	0.42
6:G:107:ASP:HB2	6:G:108:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:g:85:TYR:CE2	42:u:165:SER:HB2	2.55	0.42
49:g:201:PLX:H91	49:g:201:PLX:H122	1.71	0.42
35:l:184:LEU:HD13	40:r:393:ILE:HG21	2.02	0.42
35:l:393:ASP:OD1	35:l:393:ASP:N	2.53	0.42
6:G:89:LEU:HD12	6:G:89:LEU:HA	1.81	0.41
8:I:8:ILE:HG21	51:I:201:CDL:OA4	2.20	0.41
14:O:204:ILE:HG23	14:O:214:PRO:HG3	2.02	0.41
17:S:48:MET:HB3	17:S:48:MET:HE2	1.83	0.41
48:U:101:PEE:H58	48:U:101:PEE:H64	1.43	0.41
30:g:15:PHE:CD1	49:g:201:PLX:H71	2.55	0.41
37:n:24:GLY:HA2	40:r:6:ILE:HD12	2.01	0.41
49:r:502:PLX:H6	49:r:502:PLX:H261	2.01	0.41
9:J:142:GLU:OE1	9:J:147:LYS:HE3	2.20	0.41
11:L:158:LYS:NZ	12:M:69:LEU:O	2.44	0.41
16:Q:302:LEU:HD23	16:Q:302:LEU:HA	1.95	0.41
16:Q:312:ASP:OD1	16:Q:312:ASP:N	2.52	0.41
32:i:254:LEU:HA	32:i:255:PRO:HD3	1.93	0.41
51:l:701:CDL:H242	48:l:705:PEE:H34	2.01	0.41
41:s:133:LEU:HD13	41:s:133:LEU:HA	1.89	0.41
48:B:303:PEE:H55	48:B:303:PEE:H61	1.69	0.41
6:G:93:ILE:HG12	6:G:108:LEU:HD23	2.01	0.41
11:L:163:ASN:O	11:L:171:ARG:HA	2.20	0.41
12:M:278:HIS:CE1	12:M:280:ASP:HB2	2.55	0.41
15:P:208:VAL:N	15:P:224:VAL:HG23	2.35	0.41
17:S:31:ASN:ND2	17:S:36:LYS:HA	2.35	0.41
6:X:94:ASP:HA	6:X:95:PRO:HD3	1.87	0.41
26:c:139:PHE:O	26:c:143:MET:HG2	2.20	0.41
28:e:73:SER:C	28:e:75:GLY:H	2.27	0.41
33:j:23:TRP:NE1	48:j:201:PEE:H1	2.33	0.41
41:s:85:MET:HE3	41:s:85:MET:HB3	1.91	0.41
42:u:78:CYS:HB2	42:u:81:PRO:HD2	2.02	0.41
1:A:373:PHE:CD1	14:O:175:GLU:HB3	2.55	0.41
2:B:171:PRO:HG3	2:B:200:GLU:HG2	2.02	0.41
3:C:79:MET:HE2	3:C:79:MET:HB3	1.94	0.41
5:F:39:LYS:HE2	5:F:39:LYS:HB2	1.70	0.41
6:G:74:LEU:HD23	6:G:154:VAL:HG21	2.01	0.41
6:G:113:LEU:HD23	6:G:113:LEU:HA	1.85	0.41
21:W:131:GLU:OE2	21:W:131:GLU:N	2.51	0.41
26:c:125:SER:HB3	38:o:6:TYR:CD1	2.56	0.41
32:i:10:ILE:HG21	51:i:401:CDL:H531	2.03	0.41
51:o:201:CDL:H151	51:o:201:CDL:H362	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:67:VAL:HG12	49:r:503:PLX:H362	2.03	0.41
3:C:47:VAL:O	3:C:51:ASP:HB2	2.20	0.41
9:J:204:SER:O	9:J:204:SER:OG	2.37	0.41
10:K:87:LEU:HB3	14:O:62:ARG:HD3	2.02	0.41
15:P:207:TYR:O	15:P:224:VAL:HG23	2.20	0.41
16:Q:190:HIS:O	16:Q:194:ILE:HG12	2.20	0.41
51:V:201:CDL:H372	51:V:201:CDL:H341	1.60	0.41
22:Y:41:GLU:N	22:Y:41:GLU:CD	2.79	0.41
26:c:54:LYS:NZ	26:c:74:ASP:OD2	2.54	0.41
35:l:398:ALA:O	35:l:402:SER:OG	2.34	0.41
35:l:561:ILE:HG13	35:l:562:LEU:N	2.35	0.41
40:r:247:THR:HB	40:r:304:GLN:HE22	1.86	0.41
12:M:260:ASN:ND2	12:M:278:HIS:HD2	2.19	0.41
6:X:136:GLU:OE1	39:p:18:ARG:NH1	2.52	0.41
24:a:75:ILE:HD13	51:a:201:CDL:H841	2.03	0.41
31:h:67:LEU:HD11	32:i:82:GLY:H	1.86	0.41
39:p:141:GLN:HG2	39:p:141:GLN:H	1.70	0.41
40:r:71:TRP:CD2	49:r:503:PLX:H341	2.56	0.41
1:A:89:GLY:HA2	1:A:244:ASN:ND2	2.36	0.41
9:J:310:PHE:CG	49:J:403:PLX:H1C2	2.56	0.41
13:N:2:GLU:HG2	13:N:3:LEU:H	1.86	0.41
16:Q:53:TYR:HE1	48:l:703:PEE:C1	2.24	0.41
16:Q:228:ARG:C	16:Q:230:GLY:H	2.28	0.41
21:W:101:VAL:HG13	21:W:102:PRO:HD2	2.03	0.41
25:b:101:LYS:HA	25:b:102:PRO:HD3	1.97	0.41
49:g:201:PLX:H71	49:g:201:PLX:H102	1.98	0.41
32:i:294:MET:HE1	40:r:130:LEU:HD21	2.03	0.41
38:o:84:PRO:O	38:o:88:LEU:HB2	2.20	0.41
43:v:112:LYS:O	43:v:115:ARG:HG2	2.20	0.41
44:w:72:ARG:HH22	44:w:264:GLU:HA	1.85	0.41
12:M:390:THR:HA	12:M:600:GLU:HG2	2.03	0.41
12:M:593:SER:HA	12:M:606:THR:O	2.21	0.41
14:O:182:ASN:CB	14:O:194:GLU:HB3	2.44	0.41
15:P:173:MET:HB3	15:P:198:PHE:HB2	2.01	0.41
19:U:4:ARG:C	19:U:4:ARG:HD2	2.46	0.41
26:c:184:TYR:HB2	43:v:34:ARG:NH2	2.36	0.41
32:i:307:SER:OG	32:i:308:THR:N	2.54	0.41
35:l:303:ALA:O	35:l:306:THR:HG22	2.21	0.41
51:o:201:CDL:H752	51:o:201:CDL:H721	1.84	0.41
40:r:116:ILE:HD13	40:r:116:ILE:HA	1.94	0.41
1:A:36:LYS:H	1:A:36:LYS:CD	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LYS:HA	1:A:71:LYS:HD2	1.91	0.41
1:A:263:ALA:C	1:A:265:PHE:N	2.75	0.41
4:E:68:MET:SD	50:G:201:8Q1:C30	3.09	0.41
7:H:18:GLU:OE1	7:H:18:GLU:N	2.45	0.41
7:H:101:GLU:HB3	7:H:102:PRO:HD2	2.02	0.41
12:M:81:GLU:OE2	12:M:103:LEU:HD12	2.20	0.41
12:M:534:VAL:HG22	12:M:537:ILE:HB	2.02	0.41
13:N:68:MET:HG2	13:N:115:PHE:HD2	1.85	0.41
13:N:129:THR:HA	18:T:43:GLN:HG2	2.03	0.41
14:O:149:LEU:HD11	14:O:160:VAL:HG12	2.02	0.41
14:O:185:MET:SD	14:O:185:MET:C	3.04	0.41
16:Q:260:GLU:HG2	21:W:25:LEU:HD22	2.02	0.41
48:U:101:PEE:C21	41:s:302:MET:HE2	2.51	0.41
49:a:202:PLX:O3	49:a:202:PLX:H52	2.21	0.41
28:e:94:GLY:O	28:e:99:LEU:HB2	2.21	0.41
28:e:128:TYR:CD1	28:e:132:ASN:ND2	2.86	0.41
34:k:6:MET:HE3	36:m:119:PHE:CB	2.51	0.41
40:r:229:MET:HG2	40:r:324:SER:OG	2.20	0.41
40:r:233:ALA:HA	40:r:320:GLY:HA2	2.02	0.41
41:s:85:MET:SD	41:s:108:MET:HB2	2.60	0.41
42:u:86:TRP:CE3	42:u:86:TRP:C	2.98	0.41
7:H:38:ILE:O	7:H:45:ARG:NH1	2.52	0.41
9:J:107:GLU:O	9:J:118:LYS:NZ	2.54	0.41
13:N:3:LEU:HD23	13:N:7:LEU:HD11	2.02	0.41
28:e:51:PRO:C	28:e:53:ILE:H	2.27	0.41
32:i:59:TYR:O	32:i:63:GLN:HG2	2.21	0.41
33:j:23:TRP:NE1	48:j:201:PEE:H51	2.35	0.41
35:l:10:THR:O	35:l:14:ILE:HG23	2.21	0.41
48:l:703:PEE:C23	48:l:703:PEE:H59	2.49	0.41
36:m:20:PHE:CE2	36:m:33:LEU:HD13	2.56	0.41
38:o:65:LEU:HD11	40:r:343:ILE:HD11	2.03	0.41
15:P:122:ARG:NH1	15:P:127:GLU:OE2	2.50	0.40
51:V:201:CDL:H472	51:V:201:CDL:H442	1.85	0.40
36:m:101:PHE:N	36:m:101:PHE:CD1	2.89	0.40
51:o:201:CDL:H742	51:o:201:CDL:H622	2.02	0.40
41:s:67:SER:O	41:s:71:PHE:HB2	2.20	0.40
44:w:39:GLY:HA2	44:w:296:MET:SD	2.61	0.40
44:w:295:ARG:O	44:w:299:GLN:HG2	2.21	0.40
1:A:297:LYS:HE3	1:A:301:GLU:OE2	2.21	0.40
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.57	0.40
51:I:201:CDL:H142	51:I:201:CDL:H111	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:277:MET:HE3	12:M:277:MET:HB3	1.94	0.40
13:N:41:GLU:HG3	13:N:47:LYS:HG2	2.03	0.40
13:N:60:ARG:NH1	13:N:89:TRP:O	2.51	0.40
16:Q:274:ASP:CG	16:Q:323:ARG:HH12	2.28	0.40
25:b:104:ILE:HB	43:v:48:ASP:HB3	2.02	0.40
40:r:1:MET:HB2	40:r:52:PHE:CD2	2.56	0.40
41:s:106:LEU:HD23	41:s:106:LEU:HA	1.95	0.40
9:J:61:ALA:HA	9:J:66:GLY:HA3	2.03	0.40
16:Q:442:HIS:HB3	16:Q:446:ASP:HB2	2.02	0.40
6:X:83:VAL:HA	6:X:122:MET:HE1	2.02	0.40
24:a:168:TRP:HA	30:g:3:MET:O	2.21	0.40
28:e:90:VAL:HG22	40:r:28:THR:HG21	2.03	0.40
32:i:95:MET:HE2	32:i:149:ILE:CG1	2.49	0.40
35:l:341:MET:HE2	35:l:457:LEU:HD12	2.03	0.40
35:l:573:MET:HE3	35:l:573:MET:HA	2.04	0.40
49:r:502:PLX:H92	49:r:502:PLX:H121	1.71	0.40
42:u:72:ARG:HG3	42:u:72:ARG:NH1	2.37	0.40
43:v:7:ARG:HB2	43:v:16:GLU:OE2	2.22	0.40
3:C:64:PRO:HA	3:C:102:VAL:O	2.21	0.40
7:H:72:LEU:HD13	7:H:80:VAL:HG11	2.03	0.40
12:M:326:VAL:HG13	12:M:567:ILE:HD13	2.02	0.40
14:O:76:ALA:C	14:O:78:ALA:H	2.30	0.40
16:Q:55:THR:O	16:Q:59:ALA:N	2.51	0.40
17:S:27:HIS:O	17:S:31:ASN:HB2	2.22	0.40
6:X:119:ILE:HG21	6:X:135:ALA:HB1	2.03	0.40
6:X:151:LYS:HD2	6:X:151:LYS:HA	1.96	0.40
33:j:27:LEU:HD21	41:s:60:PRO:HD2	2.01	0.40
51:l:702:CDL:H172	51:l:702:CDL:H201	1.66	0.40
51:m:201:CDL:H141	51:m:201:CDL:H171	1.72	0.40
38:o:115:LEU:HD23	38:o:115:LEU:HA	1.89	0.40
39:p:144:THR:HA	39:p:145:PRO:HD3	1.76	0.40
39:p:174:PRO:O	39:p:175:ARG:HB2	2.22	0.40
1:A:318:ILE:HG13	1:A:357:MET:HE2	2.03	0.40
5:F:22:HIS:HB3	5:F:58:CYS:HB3	2.04	0.40
5:F:23:LEU:HD13	5:F:37:ILE:HD12	2.03	0.40
10:K:87:LEU:HD13	10:K:87:LEU:HA	1.92	0.40
14:O:76:ALA:O	14:O:78:ALA:N	2.54	0.40
16:Q:111:PRO:HG3	16:Q:435:LEU:HD23	2.04	0.40
18:T:51:ARG:HG2	18:T:54:ARG:HH21	1.86	0.40
27:d:56:HIS:O	27:d:59:ASN:O	2.40	0.40
33:j:60:ILE:HG22	36:m:168:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:370:THR:HG22	35:l:431:PHE:HD2	1.83	0.40
40:r:455:LEU:HD23	40:r:455:LEU:HA	1.91	0.40
41:s:90:PRO:HD2	41:s:240:ILE:HD13	2.03	0.40
44:w:215:GLN:O	44:w:219:GLN:HG2	2.21	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%)	414 (96%)	15 (4%)	2 (0%)	24	46
2	B	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
3	C	154/156 (99%)	144 (94%)	10 (6%)	0	100	100
4	E	113/115 (98%)	108 (96%)	4 (4%)	1 (1%)	14	30
5	F	84/86 (98%)	81 (96%)	2 (2%)	1 (1%)	10	23
6	G	86/88 (98%)	80 (93%)	6 (7%)	0	100	100
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	105 (96%)	4 (4%)	1 (1%)	14	30
8	I	93/112 (83%)	84 (90%)	7 (8%)	2 (2%)	5	10
9	J	340/342 (99%)	329 (97%)	10 (3%)	1 (0%)	36	58
10	K	41/43 (95%)	39 (95%)	1 (2%)	1 (2%)	4	9
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	665 (97%)	23 (3%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	204 (95%)	10 (5%)	1 (0%)	24	46
15	P	206/208 (99%)	198 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Q	427/430 (99%)	410 (96%)	16 (4%)	1 (0%)	43	66
17	S	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
18	T	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
19	U	81/83 (98%)	77 (95%)	4 (5%)	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%)	62 (95%)	3 (5%)	0	100	100
23	Z	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
24	a	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
25	b	94/126 (75%)	88 (94%)	6 (6%)	0	100	100
26	c	154/156 (99%)	143 (93%)	10 (6%)	1 (1%)	21	42
27	d	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
28	e	102/104 (98%)	97 (95%)	5 (5%)	0	100	100
29	f	47/49 (96%)	42 (89%)	5 (11%)	0	100	100
30	g	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	97 (94%)	6 (6%)	0	100	100
32	i	345/347 (99%)	332 (96%)	12 (4%)	1 (0%)	36	58
33	j	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
34	k	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
35	l	604/606 (100%)	587 (97%)	17 (3%)	0	100	100
36	m	173/175 (99%)	154 (89%)	19 (11%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	119 (94%)	7 (6%)	0	100	100
39	p	176/178 (99%)	171 (97%)	4 (2%)	1 (1%)	21	42
40	r	457/459 (100%)	451 (99%)	6 (1%)	0	100	100
41	s	316/318 (99%)	305 (96%)	11 (4%)	0	100	100
42	u	169/171 (99%)	163 (96%)	5 (3%)	1 (1%)	21	42
43	v	122/125 (98%)	117 (96%)	4 (3%)	1 (1%)	16	34
44	w	318/320 (99%)	309 (97%)	9 (3%)	0	100	100
All	All	8175/8314 (98%)	7857 (96%)	302 (4%)	16 (0%)	44	66

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	60	ASP
10	K	75	ASN
1	A	264	SER
8	I	29	GLN
9	J	38	HIS
7	H	77	ILE
14	O	77	ALA
16	Q	229	PRO
43	v	58	TYR
8	I	41	LEU
26	c	127	ASN
32	i	50	PRO
42	u	152	PRO
1	A	186	ALA
4	E	96	VAL
39	p	174	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/346 (100%)	341 (99%)	5 (1%)	59	81
2	B	151/151 (100%)	150 (99%)	1 (1%)	76	89
3	C	132/132 (100%)	131 (99%)	1 (1%)	73	88
4	E	107/107 (100%)	105 (98%)	2 (2%)	50	75
5	F	74/76 (97%)	73 (99%)	1 (1%)	59	81
6	G	76/81 (94%)	69 (91%)	7 (9%)	8	19
6	X	77/81 (95%)	75 (97%)	2 (3%)	40	68
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	83 (95%)	4 (5%)	24	49
9	J	296/296 (100%)	294 (99%)	2 (1%)	76	89
10	K	42/42 (100%)	41 (98%)	1 (2%)	43	70
11	L	113/113 (100%)	111 (98%)	2 (2%)	51	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	M	579/580 (100%)	574 (99%)	5 (1%)	70	87
13	N	130/130 (100%)	126 (97%)	4 (3%)	35	63
14	O	183/183 (100%)	178 (97%)	5 (3%)	39	67
15	P	190/190 (100%)	187 (98%)	3 (2%)	55	79
16	Q	370/370 (100%)	364 (98%)	6 (2%)	55	79
17	S	57/58 (98%)	56 (98%)	1 (2%)	51	76
18	T	79/79 (100%)	77 (98%)	2 (2%)	42	69
19	U	69/69 (100%)	68 (99%)	1 (1%)	59	81
20	V	101/101 (100%)	98 (97%)	3 (3%)	36	64
21	W	121/123 (98%)	121 (100%)	0	100	100
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%)	89 (99%)	1 (1%)	65	84
26	c	141/141 (100%)	140 (99%)	1 (1%)	76	89
27	d	155/155 (100%)	154 (99%)	1 (1%)	78	91
28	e	96/96 (100%)	92 (96%)	4 (4%)	26	52
29	f	35/45 (78%)	35 (100%)	0	100	100
30	g	108/109 (99%)	107 (99%)	1 (1%)	70	87
31	h	93/93 (100%)	93 (100%)	0	100	100
32	i	311/311 (100%)	306 (98%)	5 (2%)	55	79
33	j	100/100 (100%)	99 (99%)	1 (1%)	68	86
34	k	85/85 (100%)	83 (98%)	2 (2%)	43	70
35	l	536/540 (99%)	532 (99%)	4 (1%)	76	89
36	m	127/141 (90%)	127 (100%)	0	100	100
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	113/113 (100%)	113 (100%)	0	100	100
39	p	159/159 (100%)	156 (98%)	3 (2%)	50	75
40	r	409/410 (100%)	399 (98%)	10 (2%)	43	70
41	s	275/275 (100%)	273 (99%)	2 (1%)	76	89
42	u	153/153 (100%)	147 (96%)	6 (4%)	28	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	v	106/111 (96%)	105 (99%)	1 (1%)	70	87
44	w	282/283 (100%)	279 (99%)	3 (1%)	65	84
All	All	7151/7241 (99%)	7048 (99%)	103 (1%)	57	81

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	54	LYS
1	A	125	CYS
1	A	240	THR
1	A	347	THR
2	B	73	THR
3	C	76	MET
4	E	45	ASN
4	E	116	THR
5	F	57	GLU
6	G	75	THR
6	G	87	LEU
6	G	94	ASP
6	G	98	LEU
6	G	99	SER
6	G	102	SER
6	G	108	LEU
8	I	21	GLN
8	I	27	ARG
8	I	50	SER
8	I	95	VAL
9	J	211	ASP
9	J	275	ASP
10	K	82	SER
11	L	124	LEU
11	L	152	VAL
12	M	171	THR
12	M	173	MET
12	M	470	LYS
12	M	598	ASN
12	M	688	GLN
13	N	13	GLN
13	N	26	VAL
13	N	52	ASN

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Mol	Chain	Res	Type
13	N	120	THR
14	O	137	THR
14	O	140	CYS
14	O	145	SER
14	O	146	ASP
14	O	186	VAL
15	P	56	LYS
15	P	199	ARG
15	P	201	ASP
16	Q	55	THR
16	Q	58	THR
16	Q	77	VAL
16	Q	217	VAL
16	Q	221	ARG
16	Q	453	THR
17	S	54	ILE
18	T	43	GLN
18	T	81	SER
19	U	52	ASN
20	V	72	LEU
20	V	140	LYS
20	V	141	VAL
6	X	74	LEU
6	X	140	CYS
25	b	27	GLU
26	c	159	LYS
27	d	40	LEU
28	e	83	ASP
28	e	89	VAL
28	e	136	LEU
28	e	141	CYS
30	g	69	SER
32	i	69	MET
32	i	87	THR
32	i	147	GLN
32	i	223	SER
32	i	336	VAL
33	j	5	LEU
34	k	24	SER
34	k	59	MET
35	l	275	THR
35	l	371	THR

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Mol	Chain	Res	Type
35	l	387	THR
35	l	417	SER
39	p	63	LEU
39	p	117	ASP
39	p	141	GLN
40	r	19	LYS
40	r	116	ILE
40	r	183	SER
40	r	207	MET
40	r	209	LEU
40	r	212	LEU
40	r	243	MET
40	r	248	THR
40	r	401	MET
40	r	420	THR
41	s	87	VAL
41	s	251	THR
42	u	23	SER
42	u	64	ASN
42	u	80	GLU
42	u	102	LYS
42	u	106	LYS
42	u	165	SER
43	v	22	MET
44	w	49	THR
44	w	95	ASP
44	w	116	LYS

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

Mol	Chain	Res	Type
1	A	170	GLN
1	A	393	ASN
3	C	111	ASN
4	E	26	ASN
4	E	126	HIS
5	F	25	GLN
5	F	48	ASN
5	F	93	ASN
6	G	142	GLN
8	I	21	GLN
8	I	25	GLN

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Mol	Chain	Res	Type
8	I	29	GLN
8	I	110	GLN
10	K	79	HIS
11	L	71	HIS
12	M	278	HIS
12	M	300	GLN
12	M	304	GLN
12	M	336	ASN
12	M	406	ASN
12	M	425	ASN
12	M	540	ASN
12	M	598	ASN
12	M	604	GLN
13	N	52	ASN
13	N	123	GLN
14	O	90	ASN
14	O	131	HIS
14	O	133	GLN
15	P	228	GLN
16	Q	87	GLN
16	Q	88	HIS
16	Q	147	ASN
16	Q	149	GLN
16	Q	233	HIS
16	Q	454	GLN
17	S	27	HIS
17	S	31	ASN
18	T	43	GLN
18	T	117	GLN
18	T	123	HIS
19	U	71	GLN
19	U	74	GLN
20	V	7	HIS
6	X	142	GLN
22	Y	46	GLN
23	Z	21	GLN
24	a	170	GLN
26	c	132	HIS
27	d	134	GLN
30	g	63	GLN
31	h	34	HIS
32	i	36	ASN

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Mol	Chain	Res	Type
32	i	77	ASN
32	i	134	GLN
32	i	144	GLN
32	i	171	ASN
32	i	172	GLN
32	i	273	ASN
33	j	108	GLN
34	k	57	ASN
34	k	92	ASN
35	l	56	HIS
35	l	109	HIS
35	l	192	HIS
35	l	270	ASN
35	l	274	GLN
35	l	405	ASN
35	l	446	ASN
35	l	470	ASN
35	l	570	GLN
37	n	14	HIS
38	o	52	ASN
40	r	20	HIS
40	r	43	ASN
40	r	81	GLN
40	r	180	HIS
40	r	184	HIS
40	r	304	GLN
44	w	124	ASN
44	w	132	GLN
44	w	223	ASN
44	w	299	GLN
44	w	300	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	2MR	Q	118	16	10,12,13	2.04	2 (20%)	5,13,15	6.14	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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.63	1.46	1.34
16	Q	118	2MR	CQ2-NH2	-2.08	1.41	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	12.39	130.84	119.48
16	Q	118	2MR	CD-NE-CZ	4.46	131.74	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.43	131.01	123.65

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 47 ligands modelled in this entry, 1 is modelled with single atom and 2 are monoatomic - leaving 44 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
51	CDL	a	201	-	99,99,99	1.11	8 (8%)	105,111,111	0.90	4 (3%)
46	FMN	A	502	-	33,33,33	1.10	2 (6%)	48,50,50	1.28	8 (16%)
51	CDL	l	702	-	99,99,99	0.92	4 (4%)	105,111,111	1.11	8 (7%)
48	PEE	r	501	-	50,50,50	1.17	6 (12%)	53,55,55	0.97	2 (3%)
50	8Q1	G	201	-	32,34,34	2.29	7 (21%)	39,43,43	1.84	12 (30%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
52	NDP	J	401	-	51,52,52	1.18	5 (9%)	71,80,80	1.53	10 (14%)
56	970	Q	501	-	33,33,33	4.85	14 (42%)	48,50,50	2.44	22 (45%)
48	PEE	l	704	-	49,49,50	1.18	6 (12%)	52,54,55	0.97	2 (3%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-
49	PLX	C	303	-	51,51,51	0.61	0	53,59,59	0.75	1 (1%)
51	CDL	I	201	-	50,50,99	1.29	4 (8%)	56,62,111	1.37	6 (10%)
45	SF4	C	301	3	0,12,12	-	-	-	-	-
45	SF4	B	302	2	0,12,12	-	-	-	-	-
49	PLX	a	202	-	51,51,51	1.21	4 (7%)	53,59,59	0.64	1 (1%)
51	CDL	r	504	-	98,98,99	1.10	8 (8%)	104,110,111	0.87	4 (3%)
48	PEE	C	302	-	46,46,50	1.21	6 (13%)	49,51,55	1.01	2 (4%)
53	UQ	J	402	-	33,33,63	3.50	8 (24%)	42,43,79	2.80	14 (33%)
49	PLX	J	403	-	51,51,51	1.18	4 (7%)	53,59,59	0.64	1 (1%)
48	PEE	l	705	-	45,45,50	1.25	6 (13%)	48,50,55	1.00	2 (4%)
51	CDL	o	201	-	99,99,99	1.10	9 (9%)	105,111,111	0.89	5 (4%)
49	PLX	r	502	-	51,51,51	1.20	5 (9%)	53,59,59	0.64	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	8Q1	X	201	-	32,34,34	2.29	7 (21%)	39,43,43	1.73	11 (28%)
48	PEE	W	201	-	40,40,50	1.16	5 (12%)	43,45,55	1.04	2 (4%)
49	PLX	g	201	-	51,51,51	1.18	3 (5%)	53,59,59	0.69	1 (1%)
51	CDL	i	401	-	99,99,99	0.93	4 (4%)	105,111,111	1.02	4 (3%)
54	FES	M	803	12	0,4,4	-	-	-		
54	FES	O	301	14	0,4,4	-	-	-		
51	CDL	u	201	-	54,54,99	1.23	4 (7%)	60,66,111	1.26	5 (8%)
48	PEE	B	303	-	50,50,50	1.17	6 (12%)	53,55,55	1.01	2 (3%)
45	SF4	A	501	1	0,12,12	-	-	-		
51	CDL	V	201	-	93,93,99	1.14	9 (9%)	99,105,111	0.87	4 (4%)
51	CDL	k	101	-	77,77,99	1.20	7 (9%)	83,89,111	0.96	4 (4%)
48	PEE	U	101	-	50,50,50	1.17	5 (10%)	53,55,55	0.94	2 (3%)
48	PEE	l	703	-	46,46,50	1.21	6 (13%)	49,51,55	1.05	3 (6%)
53	UQ	s	401	-	38,38,63	3.64	11 (28%)	48,49,79	2.77	17 (35%)
47	NAI	A	503	-	47,48,48	3.98	22 (46%)	64,73,73	1.69	12 (18%)
49	PLX	j	202	-	51,51,51	1.19	4 (7%)	53,59,59	0.61	1 (1%)
51	CDL	l	701	-	98,98,99	0.92	4 (4%)	104,110,111	1.10	8 (7%)
49	PLX	r	503	-	51,51,51	1.20	5 (9%)	53,59,59	0.56	1 (1%)
51	CDL	m	201	-	88,88,99	0.98	4 (4%)	94,100,111	1.11	6 (6%)
58	ADP	w	401	-	28,29,29	3.18	9 (32%)	43,45,45	1.87	8 (18%)
45	SF4	B	301	2	0,12,12	-	-	-		
48	PEE	j	201	-	40,40,50	1.18	5 (12%)	43,45,55	1.06	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	CDL	a	201	-	-	60/110/110/110	-
46	FMN	A	502	-	-	8/18/18/18	0/3/3/3
51	CDL	l	702	-	-	38/110/110/110	-
48	PEE	r	501	-	-	33/54/54/54	-
50	8Q1	G	201	-	-	17/41/41/41	-
52	NDP	J	401	-	-	7/34/77/77	0/5/5/5
45	SF4	M	802	12	-	-	0/6/5/5
56	970	Q	501	-	-	7/8/41/41	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PEE	l	704	-	-	22/53/53/54	-
45	SF4	M	801	12	-	-	0/6/5/5
49	PLX	C	303	-	-	19/55/55/55	-
51	CDL	I	201	-	-	27/61/61/110	-
45	SF4	B	302	2	-	-	0/6/5/5
45	SF4	C	301	3	-	-	0/6/5/5
49	PLX	a	202	-	-	32/55/55/55	-
51	CDL	r	504	-	-	58/109/109/110	-
48	PEE	C	302	-	-	27/50/50/54	-
53	UQ	J	402	-	-	14/27/51/87	0/1/1/1
49	PLX	J	403	-	-	27/55/55/55	-
48	PEE	l	705	-	-	21/49/49/54	-
51	CDL	o	201	-	-	56/110/110/110	-
49	PLX	r	502	-	-	29/55/55/55	-
50	8Q1	X	201	-	-	28/41/41/41	-
48	PEE	W	201	-	-	23/44/44/54	-
49	PLX	g	201	-	-	37/55/55/55	-
51	CDL	i	401	-	-	35/110/110/110	-
54	FES	M	803	12	-	-	0/1/1/1
54	FES	O	301	14	-	-	0/1/1/1
51	CDL	u	201	-	-	17/65/65/110	-
48	PEE	B	303	-	-	25/54/54/54	-
45	SF4	A	501	1	-	-	0/6/5/5
51	CDL	V	201	-	-	58/104/104/110	-
51	CDL	k	101	-	-	40/88/88/110	-
48	PEE	U	101	-	-	27/54/54/54	-
48	PEE	l	703	-	-	25/50/50/54	-
53	UQ	s	401	-	-	13/33/57/87	0/1/1/1
47	NAI	A	503	-	-	4/29/72/72	0/5/5/5
49	PLX	j	202	-	-	33/55/55/55	-
51	CDL	l	701	-	-	38/109/109/110	-
49	PLX	r	503	-	-	38/55/55/55	-
51	CDL	m	201	-	-	34/99/99/110	-
58	ADP	w	401	-	-	6/16/32/32	0/3/3/3
45	SF4	B	301	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PEE	j	201	-	-	17/44/44/54	-

All (226) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Q	501	970	O16-C17	18.66	1.58	1.37
56	Q	501	970	C14-C23	-12.07	1.41	1.52
47	A	503	NAI	C3D-C4D	-10.53	1.26	1.53
53	s	401	UQ	C18-C19	9.98	1.56	1.33
53	J	402	UQ	C18-C19	9.92	1.55	1.33
53	s	401	UQ	C13-C14	9.65	1.55	1.33
53	J	402	UQ	C13-C14	9.53	1.55	1.33
53	s	401	UQ	C23-C24	9.43	1.54	1.33
47	A	503	NAI	O4B-C1B	9.34	1.63	1.42
53	s	401	UQ	C8-C9	9.32	1.54	1.33
53	J	402	UQ	C8-C9	9.24	1.54	1.33
58	w	401	ADP	C3'-C4'	-9.13	1.29	1.53
56	Q	501	970	O13-C12	8.34	1.50	1.37
47	A	503	NAI	O4B-C4B	-8.28	1.26	1.45
58	w	401	ADP	O4'-C4'	7.81	1.62	1.45
50	X	201	8Q1	P24-O27	7.80	1.84	1.60
47	A	503	NAI	C2D-C1D	-7.76	1.29	1.53
50	G	201	8Q1	P24-O27	7.69	1.84	1.60
53	J	402	UQ	C23-C24	7.49	1.54	1.32
47	A	503	NAI	C2B-C1B	-7.39	1.30	1.53
53	s	401	UQ	C28-C29	7.37	1.54	1.32
56	Q	501	970	O08-C07	7.00	1.47	1.37
47	A	503	NAI	O4D-C4D	6.82	1.60	1.45
58	w	401	ADP	PA-O3A	6.40	1.66	1.59
47	A	503	NAI	PA-O3	5.93	1.65	1.59
47	A	503	NAI	C2D-C3D	5.90	1.69	1.53
56	Q	501	970	C23-C24	-5.87	1.46	1.52
56	Q	501	970	C22-C23	-5.55	1.43	1.51
47	A	503	NAI	O4D-C1D	5.47	1.54	1.42
50	X	201	8Q1	C28-C29	5.43	1.61	1.52
58	w	401	ADP	C6-N6	5.42	1.48	1.34
47	A	503	NAI	C7N-N7N	5.30	1.48	1.33
47	A	503	NAI	C4N-C3N	-5.26	1.40	1.50
47	A	503	NAI	PN-O3	5.22	1.65	1.59
50	G	201	8Q1	C28-C29	5.14	1.61	1.52
47	A	503	NAI	C6A-N6A	5.07	1.47	1.34
58	w	401	ADP	O4'-C1'	-4.36	1.31	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	I	201	CDL	OB8-CB7	4.36	1.46	1.33
51	l	701	CDL	OA8-CA7	4.34	1.46	1.33
51	m	201	CDL	OA8-CA7	4.33	1.46	1.33
51	i	401	CDL	OA8-CA7	4.31	1.45	1.33
51	l	702	CDL	OB8-CB7	4.28	1.45	1.33
47	A	503	NAI	O2B-C2B	4.28	1.53	1.43
51	l	701	CDL	OB8-CB7	4.27	1.45	1.33
51	I	201	CDL	OA8-CA7	4.26	1.45	1.33
51	m	201	CDL	OA6-CA5	4.25	1.46	1.34
51	i	401	CDL	OB8-CB7	4.22	1.45	1.33
52	J	401	NDP	C5A-C4A	4.20	1.46	1.39
51	u	201	CDL	OA8-CA7	4.19	1.45	1.33
51	i	401	CDL	OB6-CB5	4.17	1.46	1.34
51	l	702	CDL	OA8-CA7	4.15	1.45	1.33
51	i	401	CDL	OA6-CA5	4.13	1.46	1.34
51	u	201	CDL	OB8-CB7	4.12	1.45	1.33
51	m	201	CDL	OB8-CB7	4.10	1.45	1.33
51	u	201	CDL	OA6-CA5	4.10	1.45	1.34
51	l	701	CDL	OA6-CA5	4.09	1.45	1.34
51	u	201	CDL	OB6-CB5	4.09	1.45	1.34
51	I	201	CDL	OA6-CA5	4.05	1.45	1.34
51	I	201	CDL	OB6-CB5	4.03	1.45	1.34
50	G	201	8Q1	C1-S44	4.01	1.85	1.76
51	l	702	CDL	OA6-CA5	3.99	1.45	1.34
51	m	201	CDL	OB6-CB5	3.98	1.45	1.34
50	G	201	8Q1	C6-C1	3.92	1.54	1.50
56	Q	501	970	C05-C04	-3.92	1.48	1.54
51	l	702	CDL	OB6-CB5	3.92	1.45	1.34
50	X	201	8Q1	C1-S44	3.91	1.85	1.76
51	l	701	CDL	OB6-CB5	3.90	1.45	1.34
48	l	705	PEE	C18-C19	3.82	1.53	1.31
48	l	704	PEE	C18-C19	3.81	1.53	1.31
48	C	302	PEE	C18-C19	3.81	1.53	1.31
48	j	201	PEE	C18-C19	3.81	1.53	1.31
48	B	303	PEE	C18-C19	3.79	1.53	1.31
48	W	201	PEE	C18-C19	3.78	1.53	1.31
48	r	501	PEE	C18-C19	3.78	1.53	1.31
48	l	703	PEE	C18-C19	3.77	1.53	1.31
48	U	101	PEE	C18-C19	3.76	1.53	1.31
48	r	501	PEE	C39-C38	3.74	1.52	1.31
48	B	303	PEE	C39-C38	3.73	1.52	1.31
48	U	101	PEE	C39-C38	3.71	1.52	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	l	705	PEE	C39-C38	3.71	1.52	1.31
48	l	703	PEE	C39-C38	3.70	1.52	1.31
48	C	302	PEE	C39-C38	3.70	1.52	1.31
48	l	704	PEE	C39-C38	3.69	1.52	1.31
56	Q	501	970	O13-C14	3.57	1.49	1.45
47	A	503	NAI	C7N-C3N	3.52	1.56	1.48
51	V	201	CDL	OA8-CA7	3.50	1.43	1.33
50	G	201	8Q1	O27-C28	-3.44	1.32	1.43
51	o	201	CDL	OA8-CA7	3.43	1.43	1.33
51	a	201	CDL	OA8-CA7	3.39	1.43	1.33
47	A	503	NAI	C4N-C5N	-3.39	1.40	1.49
58	w	401	ADP	C8-N9	-3.37	1.31	1.37
51	r	504	CDL	OA8-CA7	3.35	1.43	1.33
51	k	101	CDL	OA8-CA7	3.34	1.43	1.33
50	X	201	8Q1	O27-C28	-3.30	1.33	1.43
56	Q	501	970	O16-C15	3.29	1.52	1.44
51	k	101	CDL	OA6-CA5	3.26	1.43	1.34
50	G	201	8Q1	C34-N36	3.23	1.41	1.33
46	A	502	FMN	C4A-N5	3.22	1.37	1.30
50	X	201	8Q1	C6-C1	3.19	1.54	1.50
58	w	401	ADP	O2'-C2'	-3.18	1.35	1.43
50	X	201	8Q1	C34-N36	3.13	1.41	1.33
51	a	201	CDL	OB6-CB5	3.12	1.43	1.34
49	a	202	PLX	O6-C4	-3.06	1.40	1.44
50	X	201	8Q1	C39-N41	3.04	1.40	1.33
51	V	201	CDL	OA6-CA5	3.04	1.42	1.34
51	r	504	CDL	OB8-CB7	3.03	1.42	1.33
58	w	401	ADP	O3'-C3'	3.00	1.50	1.43
51	V	201	CDL	OB6-CB5	2.98	1.42	1.34
49	g	201	PLX	O6-C4	-2.96	1.40	1.44
51	o	201	CDL	OA6-CA5	2.96	1.42	1.34
56	Q	501	970	O25-C24	-2.93	1.18	1.22
51	V	201	CDL	OB8-CB7	2.93	1.41	1.33
51	k	101	CDL	OB8-CB7	2.91	1.41	1.33
51	k	101	CDL	OB6-CB5	2.90	1.42	1.34
51	a	201	CDL	OB8-CB7	2.89	1.41	1.33
51	o	201	CDL	OB6-CB5	2.87	1.42	1.34
56	Q	501	970	C10-C11	2.85	1.44	1.39
51	r	504	CDL	OB6-CB5	2.84	1.42	1.34
49	r	503	PLX	O6-C4	-2.83	1.41	1.44
50	G	201	8Q1	C39-N41	2.80	1.40	1.33
51	a	201	CDL	OA6-CA5	2.80	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	C8A-N9A	-2.78	1.32	1.37
53	s	401	UQ	C6-C1	2.78	1.54	1.46
51	r	504	CDL	OA6-CA5	2.76	1.42	1.34
51	o	201	CDL	OB8-CB7	2.75	1.41	1.33
51	a	201	CDL	OA6-CA4	-2.75	1.40	1.46
48	C	302	PEE	O2-C2	-2.70	1.40	1.46
53	J	402	UQ	C6-C1	2.70	1.54	1.46
48	l	703	PEE	O2-C2	-2.67	1.40	1.46
48	U	101	PEE	O3-C30	2.65	1.41	1.33
49	j	202	PLX	O6-C4	-2.64	1.41	1.44
48	W	201	PEE	O2-C2	-2.63	1.40	1.46
51	r	504	CDL	OA6-CA4	-2.63	1.40	1.46
52	J	401	NDP	C5A-N7A	-2.61	1.34	1.39
56	Q	501	970	C12-C06	2.61	1.43	1.39
48	U	101	PEE	O2-C2	-2.59	1.40	1.46
48	l	704	PEE	O2-C2	-2.58	1.40	1.46
49	r	502	PLX	O6-C4	-2.58	1.41	1.44
48	j	201	PEE	O3-C30	2.57	1.40	1.33
48	j	201	PEE	O2-C2	-2.57	1.40	1.46
51	o	201	CDL	OA6-CA4	-2.56	1.40	1.46
52	J	401	NDP	C5A-C6A	2.55	1.48	1.41
48	r	501	PEE	O2-C2	-2.55	1.40	1.46
48	l	705	PEE	O2-C2	-2.54	1.40	1.46
51	k	101	CDL	OB6-CB4	-2.53	1.40	1.46
48	B	303	PEE	O2-C2	-2.53	1.40	1.46
48	l	705	PEE	O3-C30	2.49	1.40	1.33
48	l	704	PEE	O3-C30	2.49	1.40	1.33
51	r	504	CDL	OB6-CB4	-2.49	1.40	1.46
49	j	202	PLX	C7-C6	2.48	1.55	1.50
47	A	503	NAI	C6N-C5N	2.48	1.40	1.33
56	Q	501	970	C05-C06	-2.47	1.48	1.51
49	r	502	PLX	C7-C6	2.44	1.55	1.50
51	o	201	CDL	OB6-CB4	-2.43	1.40	1.46
49	J	403	PLX	C7-C6	2.42	1.55	1.50
51	V	201	CDL	OA6-CA4	-2.42	1.40	1.46
47	A	503	NAI	O3B-C3B	-2.42	1.37	1.43
58	w	401	ADP	C5-N7	-2.41	1.34	1.39
53	s	401	UQ	C7-C8	2.40	1.54	1.50
49	J	403	PLX	O6-C4	-2.37	1.41	1.44
51	V	201	CDL	OB6-CB4	-2.37	1.41	1.46
49	a	202	PLX	C7-C6	2.36	1.55	1.50
48	l	703	PEE	O3-C30	2.34	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	W	201	PEE	O3-C30	2.33	1.40	1.33
49	r	503	PLX	C7-C6	2.33	1.55	1.50
51	a	201	CDL	OB6-CB4	-2.33	1.41	1.46
48	W	201	PEE	O3-C3	-2.33	1.40	1.45
48	C	302	PEE	O3-C30	2.32	1.40	1.33
51	V	201	CDL	PB2-OB2	2.32	1.68	1.59
46	A	502	FMN	C10-N1	2.30	1.37	1.33
49	g	201	PLX	C7-C6	2.30	1.55	1.50
51	V	201	CDL	PB2-OB5	2.30	1.68	1.59
48	l	705	PEE	O2-C10	2.29	1.40	1.34
48	j	201	PEE	O2-C10	2.29	1.40	1.34
48	B	303	PEE	O3-C30	2.29	1.40	1.33
48	r	501	PEE	O3-C30	2.27	1.40	1.33
51	o	201	CDL	PB2-OB2	2.26	1.68	1.59
47	A	503	NAI	C5B-C4B	2.26	1.58	1.51
48	l	703	PEE	O2-C10	2.24	1.40	1.34
51	a	201	CDL	PB2-OB5	2.24	1.68	1.59
48	r	501	PEE	O3-C3	-2.23	1.40	1.45
48	W	201	PEE	O2-C10	2.23	1.40	1.34
51	a	201	CDL	PB2-OB2	2.23	1.68	1.59
48	C	302	PEE	O3-C3	-2.22	1.40	1.45
47	A	503	NAI	PN-O5D	2.21	1.68	1.59
53	J	402	UQ	C7-C8	2.20	1.54	1.50
48	U	101	PEE	O2-C10	2.20	1.40	1.34
49	r	502	PLX	P1-O4	2.20	1.68	1.59
47	A	503	NAI	C5A-N7A	-2.19	1.35	1.39
48	l	704	PEE	O3-C3	-2.19	1.40	1.45
49	j	202	PLX	P1-O4	2.17	1.67	1.59
48	r	501	PEE	O2-C10	2.17	1.40	1.34
53	s	401	UQ	O4-C4	-2.17	1.18	1.23
51	o	201	CDL	PB2-OB5	2.16	1.67	1.59
53	J	402	UQ	O4-C4	-2.15	1.18	1.23
52	J	401	NDP	C4A-N9A	-2.15	1.33	1.37
48	B	303	PEE	O2-C10	2.15	1.40	1.34
49	a	202	PLX	P1-O4	2.15	1.67	1.59
48	B	303	PEE	O3-C3	-2.15	1.40	1.45
48	l	704	PEE	O2-C10	2.14	1.40	1.34
51	r	504	CDL	PB2-OB2	2.14	1.67	1.59
49	r	502	PLX	P1-O1	2.13	1.67	1.59
53	J	402	UQ	O3-CM3	-2.10	1.40	1.45
56	Q	501	970	C04-C02	2.10	1.52	1.50
49	g	201	PLX	P1-O4	2.10	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	l	703	PEE	O3-C3	-2.10	1.40	1.45
48	C	302	PEE	O2-C10	2.10	1.40	1.34
49	r	503	PLX	P1-O4	2.10	1.67	1.59
51	k	101	CDL	PB2-OB5	2.10	1.67	1.59
51	r	504	CDL	PB2-OB5	2.09	1.67	1.59
49	r	502	PLX	C25-C24	2.09	1.55	1.50
53	s	401	UQ	C21-C19	2.09	1.55	1.51
53	s	401	UQ	O3-CM3	-2.08	1.40	1.45
51	o	201	CDL	C11-CA5	2.07	1.56	1.50
49	a	202	PLX	P1-O1	2.07	1.67	1.59
49	j	202	PLX	P1-O1	2.06	1.67	1.59
52	J	401	NDP	C6N-C5N	2.05	1.39	1.33
49	r	503	PLX	P1-O1	2.04	1.67	1.59
49	J	403	PLX	P1-O4	2.04	1.67	1.59
48	l	705	PEE	O3-C3	-2.03	1.40	1.45
48	j	201	PEE	O3-C3	-2.02	1.40	1.45
51	k	101	CDL	C11-CA5	2.01	1.56	1.50
53	s	401	UQ	O1-C1	-2.01	1.18	1.23
49	r	503	PLX	C1-C2	2.01	1.57	1.51
51	V	201	CDL	C11-CA5	2.00	1.56	1.50
49	J	403	PLX	P1-O1	2.00	1.67	1.59

All (198) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	J	402	UQ	C7-C8-C9	-7.93	113.16	126.83
56	Q	501	970	O08-C07-C06	-7.79	108.35	112.99
53	s	401	UQ	C7-C8-C9	-7.60	113.74	126.83
53	J	402	UQ	C12-C13-C14	-6.74	112.19	127.62
53	J	402	UQ	C17-C18-C19	-6.63	112.44	127.62
53	s	401	UQ	C22-C23-C24	-6.26	113.30	127.62
53	s	401	UQ	C12-C13-C14	-6.06	113.75	127.62
53	s	401	UQ	C17-C18-C19	-6.00	113.89	127.62
56	Q	501	970	C15-C14-C23	5.75	115.31	110.65
52	J	401	NDP	C5A-C4A-N3A	-5.66	118.92	126.72
58	w	401	ADP	C5-C4-N3	-5.56	119.06	126.72
47	A	503	NAI	C5A-C4A-N3A	-5.49	119.16	126.72
50	G	201	8Q1	C6-C1-S44	5.17	119.56	113.40
51	l	702	CDL	OA6-CA5-C11	4.65	121.55	111.48
58	w	401	ADP	N3-C2-N1	-4.64	121.56	128.58
51	l	701	CDL	OA6-CA5-C11	4.58	121.38	111.48
51	a	201	CDL	OB6-CB5-C51	4.55	121.32	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	J	401	NDP	N3A-C4A-N9A	4.54	134.89	127.17
53	J	402	UQ	C22-C23-C24	-4.51	112.61	127.64
53	s	401	UQ	C10-C9-C8	-4.45	112.20	123.63
47	A	503	NAI	N3A-C2A-N1A	-4.44	121.85	128.58
58	w	401	ADP	N3-C4-N9	4.40	134.65	127.17
50	X	201	8Q1	C6-C1-S44	4.37	118.61	113.40
48	j	201	PEE	O2-C10-C11	4.36	120.91	111.48
53	J	402	UQ	C20-C19-C18	-4.33	112.51	123.63
53	s	401	UQ	C27-C28-C29	-4.32	113.23	127.64
56	Q	501	970	C05-C04-C02	-4.28	109.00	115.53
53	J	402	UQ	C10-C9-C8	-4.28	112.65	123.63
51	m	201	CDL	OB6-CB5-C51	4.25	120.68	111.48
53	s	401	UQ	C25-C24-C23	-4.24	112.74	123.63
48	B	303	PEE	O2-C10-C11	4.23	120.64	111.48
51	i	401	CDL	OA6-CA5-C11	4.23	120.63	111.48
53	J	402	UQ	C15-C14-C13	-4.21	112.81	123.63
51	m	201	CDL	OA6-CA5-C11	4.21	120.58	111.48
51	r	504	CDL	OA6-CA5-C11	4.15	120.46	111.48
48	l	705	PEE	O2-C10-C11	4.10	120.35	111.48
51	l	702	CDL	OB6-CB5-C51	4.10	120.35	111.48
50	X	201	8Q1	C43-S44-C1	4.09	113.92	101.84
56	Q	501	970	O08-C07-C09	4.08	131.89	123.85
48	r	501	PEE	O2-C10-C11	4.07	120.28	111.48
51	u	201	CDL	OA6-CA5-C11	4.02	120.19	111.48
51	I	201	CDL	OA6-CA5-C11	4.00	120.14	111.48
51	o	201	CDL	OB6-CB5-C51	3.98	120.08	111.48
51	u	201	CDL	OB6-CB5-C51	3.97	120.07	111.48
51	l	701	CDL	OB6-CB5-C51	3.96	120.06	111.48
50	G	201	8Q1	C43-S44-C1	3.95	113.53	101.84
51	i	401	CDL	OB6-CB5-C51	3.93	119.98	111.48
47	A	503	NAI	N3A-C4A-N9A	3.92	133.84	127.17
48	W	201	PEE	O2-C10-C11	3.92	119.96	111.48
53	s	401	UQ	C20-C19-C18	-3.90	113.61	123.63
51	I	201	CDL	OB6-CB5-C51	3.90	119.91	111.48
53	s	401	UQ	C21-C19-C18	-3.87	112.47	121.17
48	C	302	PEE	O2-C10-C11	3.87	119.86	111.48
53	s	401	UQ	C15-C14-C13	-3.87	113.70	123.63
53	J	402	UQ	C11-C9-C8	-3.86	112.50	121.17
53	J	402	UQ	C21-C19-C18	-3.84	112.55	121.17
51	V	201	CDL	OB6-CB5-C51	3.82	119.74	111.48
48	l	703	PEE	O2-C10-C11	3.80	119.70	111.48
51	o	201	CDL	OA6-CA5-C11	3.80	119.70	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	s	401	UQ	C11-C9-C8	-3.80	112.65	121.17
51	r	504	CDL	OB6-CB5-C51	3.78	119.67	111.48
53	s	401	UQ	C16-C14-C13	-3.77	112.71	121.17
51	V	201	CDL	OA6-CA5-C11	3.76	119.61	111.48
51	a	201	CDL	OA6-CA5-C11	3.75	119.59	111.48
51	k	101	CDL	OB6-CB5-C51	3.74	119.56	111.48
52	J	401	NDP	C2A-N3A-C4A	3.68	120.81	111.83
47	A	503	NAI	C2A-N3A-C4A	3.68	120.81	111.83
56	Q	501	970	O28-C19-C20	3.66	120.37	115.40
53	J	402	UQ	C16-C14-C13	-3.66	112.95	121.17
48	U	101	PEE	O2-C10-C11	3.64	119.36	111.48
58	w	401	ADP	C2-N3-C4	3.63	120.69	111.83
48	l	704	PEE	O2-C10-C11	3.61	119.29	111.48
53	s	401	UQ	C26-C24-C23	-3.55	113.21	121.17
56	Q	501	970	C22-C23-C14	3.53	114.69	109.64
51	k	101	CDL	OA6-CA5-C11	3.51	119.08	111.48
50	X	201	8Q1	O35-C34-N36	-3.50	115.57	122.98
52	J	401	NDP	C4A-C5A-N7A	-3.47	106.61	110.58
58	w	401	ADP	N9-C8-N7	-3.45	109.05	113.94
56	Q	501	970	C06-C05-C04	3.41	104.44	101.45
47	A	503	NAI	C4A-C5A-N7A	-3.38	106.72	110.58
47	A	503	NAI	C5A-N7A-C8A	3.37	108.75	103.45
46	A	502	FMN	C4-N3-C2	-3.36	119.68	125.64
53	s	401	UQ	C30-C29-C28	-3.30	112.76	122.66
50	G	201	8Q1	O35-C34-N36	-3.29	116.02	122.98
47	A	503	NAI	N9A-C8A-N7A	-3.28	109.28	113.94
52	J	401	NDP	N3A-C2A-N1A	-3.27	123.63	128.58
53	J	402	UQ	C25-C24-C23	-3.27	112.85	122.66
53	J	402	UQ	C26-C24-C23	-3.27	112.85	122.66
56	Q	501	970	C09-C07-C06	-3.25	119.76	123.21
51	l	701	CDL	OB8-CB7-C71	3.18	121.52	111.83
58	w	401	ADP	C5-N7-C8	3.16	108.41	103.45
51	u	201	CDL	OB8-CB7-C71	3.16	121.46	111.83
53	s	401	UQ	C31-C29-C28	-3.13	113.26	122.66
51	l	701	CDL	OA8-CA7-C31	3.12	121.35	111.83
58	w	401	ADP	C4-N9-C8	3.11	109.00	105.74
47	A	503	NAI	C4D-O4D-C1D	-3.08	102.66	109.47
56	Q	501	970	C07-C06-C12	3.08	121.66	118.72
51	l	702	CDL	OB8-CB7-C71	3.06	121.16	111.83
51	k	101	CDL	OB8-CB7-C71	3.05	121.12	111.83
51	I	201	CDL	CA6-CA4-CA3	-3.03	104.71	111.78
51	l	702	CDL	CA4-OA6-CA5	-3.01	110.60	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Q	501	970	O26-C20-C19	2.99	119.46	115.40
48	l	704	PEE	O3-C30-C31	2.98	120.93	111.83
48	U	101	PEE	O3-C30-C31	2.94	120.79	111.83
50	G	201	8Q1	O4-C1-S44	-2.93	118.95	122.68
58	w	401	ADP	C4-C5-N7	-2.92	107.24	110.58
50	G	201	8Q1	O2-P24-O27	-2.92	99.06	106.67
51	a	201	CDL	OB8-CB7-C71	2.90	120.66	111.83
51	I	201	CDL	OB8-CB7-C71	2.87	120.57	111.83
50	G	201	8Q1	C37-C38-C39	2.86	117.15	112.39
51	l	702	CDL	CB4-OB6-CB5	-2.85	110.97	117.80
48	B	303	PEE	O3-C30-C31	2.84	120.50	111.83
52	J	401	NDP	C4A-N9A-C8A	2.84	108.72	105.74
51	I	201	CDL	OA8-CA7-C31	2.83	120.45	111.83
47	A	503	NAI	C3D-C2D-C1D	2.82	106.80	101.46
50	X	201	8Q1	C37-C38-C39	2.82	117.09	112.39
51	m	201	CDL	OB8-CB7-C71	2.82	120.42	111.83
51	I	201	CDL	CB4-OB6-CB5	-2.79	111.11	117.80
48	l	703	PEE	O3-C30-C31	2.78	120.30	111.83
51	V	201	CDL	OB8-CB7-C71	2.77	120.28	111.83
51	l	701	CDL	CA4-OA6-CA5	-2.77	111.17	117.80
51	o	201	CDL	OA8-CA7-C31	2.77	120.27	111.83
50	G	201	8Q1	C32-C34-N36	2.76	121.72	116.48
51	m	201	CDL	OA8-CA7-C31	2.75	120.21	111.83
48	j	201	PEE	O3-C30-C31	2.74	120.19	111.83
56	Q	501	970	C11-C24-C23	2.74	119.61	115.89
56	Q	501	970	C29-O28-C19	-2.73	113.50	117.51
51	o	201	CDL	OB8-CB7-C71	2.73	120.16	111.83
51	i	401	CDL	OA8-CA7-C31	2.71	120.10	111.83
56	Q	501	970	O28-C19-C18	-2.71	119.41	124.08
47	A	503	NAI	C2D-C3D-C4D	2.71	107.84	102.61
46	A	502	FMN	C4A-C4-N3	2.71	120.14	113.25
51	i	401	CDL	OB8-CB7-C71	2.69	120.03	111.83
51	k	101	CDL	OA8-CA7-C31	2.69	120.03	111.83
51	a	201	CDL	OA8-CA7-C31	2.65	119.92	111.83
51	u	201	CDL	OA8-CA7-C31	2.65	119.19	111.15
51	r	504	CDL	OB8-CB7-C71	2.65	119.90	111.83
52	J	401	NDP	C5A-N7A-C8A	2.64	107.60	103.45
48	r	501	PEE	O3-C30-C31	2.63	119.84	111.83
51	l	702	CDL	OA8-CA7-C31	2.61	119.80	111.83
53	J	402	UQ	CM5-C5-C6	-2.60	120.18	124.45
48	W	201	PEE	O3-C30-C31	2.60	119.75	111.83
56	Q	501	970	C11-C12-C06	-2.59	119.22	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	C	302	PEE	O3-C30-C31	2.59	119.74	111.83
53	J	402	UQ	C7-C6-C5	-2.59	120.45	124.89
46	A	502	FMN	O4-C4-C4A	-2.58	119.72	126.53
49	g	201	PLX	C1A-N1-C1	2.57	120.14	109.91
48	l	703	PEE	C2-O2-C10	-2.56	111.67	117.80
50	X	201	8Q1	O2-P24-O27	-2.55	100.02	106.67
51	r	504	CDL	OA8-CA7-C31	2.55	119.60	111.83
50	G	201	8Q1	O40-C39-N41	-2.54	118.05	123.03
51	V	201	CDL	OA8-CA7-C31	2.53	119.54	111.83
50	X	201	8Q1	C32-C34-N36	2.52	121.26	116.48
50	X	201	8Q1	O27-P24-O3	-2.49	99.70	106.44
48	l	705	PEE	O3-C30-C31	2.49	119.43	111.83
49	a	202	PLX	C1A-N1-C1	2.47	119.75	109.91
52	J	401	NDP	C2B-C1B-N9A	-2.47	109.68	113.75
49	r	502	PLX	C1A-N1-C1	2.45	119.66	109.91
51	l	702	CDL	OA6-CA5-OA7	-2.41	118.08	123.70
49	J	403	PLX	C1A-N1-C1	2.41	119.47	109.91
46	A	502	FMN	C5A-C9A-N10	2.39	120.13	117.97
47	A	503	NAI	C4A-N9A-C8A	2.39	108.25	105.74
49	j	202	PLX	C1A-N1-C1	2.37	119.32	109.91
56	Q	501	970	C05-C06-C12	-2.36	127.24	131.52
56	Q	501	970	C15-O16-C17	-2.36	110.59	115.29
46	A	502	FMN	C9A-C5A-N5	-2.35	119.96	122.45
56	Q	501	970	C12-O13-C14	-2.34	112.26	116.07
56	Q	501	970	C27-O26-C20	-2.32	114.11	117.51
53	s	401	UQ	C7-C6-C5	-2.32	120.92	124.89
46	A	502	FMN	C4A-C10-N10	2.32	119.80	116.48
51	l	701	CDL	CB4-OB6-CB5	-2.31	112.27	117.80
50	G	201	8Q1	O1-P24-O2	2.31	116.45	107.80
50	X	201	8Q1	O1-P24-O2	2.26	116.28	107.80
50	X	201	8Q1	O4-C1-S44	-2.25	119.82	122.68
51	u	201	CDL	OB8-CB7-OB9	-2.25	118.00	123.63
46	A	502	FMN	C4A-C10-N1	-2.22	119.14	124.59
56	Q	501	970	O26-C20-C21	-2.22	120.25	124.08
53	s	401	UQ	CM5-C5-C6	-2.22	120.80	124.45
51	m	201	CDL	CB4-OB6-CB5	-2.19	112.55	117.80
50	G	201	8Q1	O27-P24-O3	-2.19	100.52	106.44
50	X	201	8Q1	O40-C39-N41	-2.17	118.78	123.03
46	A	502	FMN	C10-C4A-N5	-2.17	120.39	124.81
50	G	201	8Q1	O4-C1-C6	-2.16	121.49	123.98
52	J	401	NDP	N9A-C8A-N7A	-2.15	110.89	113.94
51	m	201	CDL	OB8-CB7-OB9	-2.15	118.26	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Q	501	970	C05-C06-C07	2.14	111.10	108.58
56	Q	501	970	O13-C14-C23	2.13	114.56	112.44
52	J	401	NDP	C6A-C5A-N7A	2.12	136.18	132.09
51	l	701	CDL	OA6-CA5-OA7	-2.11	118.78	123.70
47	A	503	NAI	C6N-N1N-C2N	2.11	121.57	119.32
51	l	701	CDL	OB8-CB7-OB9	-2.10	118.37	123.63
50	X	201	8Q1	O4-C1-C6	-2.09	121.57	123.98
50	G	201	8Q1	C38-C39-N41	2.09	120.14	116.34
51	o	201	CDL	CB4-OB6-CB5	-2.06	112.86	117.80
51	l	702	CDL	OB6-CB5-OB7	-2.05	118.90	123.70
56	Q	501	970	O13-C12-C06	2.04	119.82	116.29
49	C	303	PLX	C6-O6-C4	-2.04	111.13	115.20
49	r	503	PLX	C1A-N1-C1	2.04	118.01	109.91

There are no chirality outliers.

All (1000) 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	C3'-C4'-C5'-O5'
46	A	502	FMN	O4'-C4'-C5'-O5'
47	A	503	NAI	C5B-O5B-PA-O1A
48	B	303	PEE	C4-O4P-P-O3P
48	B	303	PEE	C4-O4P-P-O2P
48	C	302	PEE	C1-O3P-P-O2P
48	C	302	PEE	C1-O3P-P-O1P
48	C	302	PEE	C1-O3P-P-O4P
48	C	302	PEE	O4P-C4-C5-N
48	W	201	PEE	C1-O3P-P-O2P
48	W	201	PEE	C1-O3P-P-O1P
48	W	201	PEE	C1-O3P-P-O4P
48	W	201	PEE	C4-O4P-P-O3P
48	W	201	PEE	C4-O4P-P-O2P
48	W	201	PEE	O4P-C4-C5-N
48	j	201	PEE	C11-C10-O2-C2
48	j	201	PEE	O4P-C4-C5-N
48	l	703	PEE	C11-C10-O2-C2
48	l	703	PEE	C1-O3P-P-O1P
48	l	703	PEE	C4-O4P-P-O3P
48	l	703	PEE	C4-O4P-P-O2P
48	l	703	PEE	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
48	l	703	PEE	C5-C4-O4P-P
48	l	703	PEE	O4P-C4-C5-N
48	l	704	PEE	C11-C10-O2-C2
48	l	704	PEE	O4P-C4-C5-N
48	l	705	PEE	C1-O3P-P-O2P
48	l	705	PEE	C1-O3P-P-O1P
48	l	705	PEE	C1-O3P-P-O4P
48	l	705	PEE	O4P-C4-C5-N
48	r	501	PEE	C1-O3P-P-O2P
48	r	501	PEE	C1-O3P-P-O4P
48	r	501	PEE	C4-O4P-P-O3P
48	r	501	PEE	C4-O4P-P-O1P
49	C	303	PLX	C3-O4-P1-O1
49	C	303	PLX	C3-O4-P1-O3
49	C	303	PLX	O9-C24-O8-C5
49	J	403	PLX	O7-C6-O6-C4
49	J	403	PLX	C3-C4-O6-C6
49	J	403	PLX	C2-O1-P1-O4
49	J	403	PLX	C2-O1-P1-O2
49	J	403	PLX	N1-C1-C2-O1
49	a	202	PLX	O7-C6-O6-C4
49	a	202	PLX	C3-O4-P1-O1
49	a	202	PLX	C3-O4-P1-O3
49	a	202	PLX	C2-O1-P1-O4
49	a	202	PLX	C2-O1-P1-O2
49	a	202	PLX	C2-O1-P1-O3
49	a	202	PLX	O9-C24-O8-C5
49	a	202	PLX	O9-C24-C25-C26
49	g	201	PLX	O7-C6-C7-C8
49	g	201	PLX	O7-C6-O6-C4
49	g	201	PLX	C3-O4-P1-O1
49	g	201	PLX	C3-O4-P1-O2
49	g	201	PLX	C3-O4-P1-O3
49	g	201	PLX	C2-O1-P1-O4
49	g	201	PLX	C2-O1-P1-O2
49	g	201	PLX	C2-O1-P1-O3
49	j	202	PLX	O7-C6-C7-C8
49	j	202	PLX	C7-C6-O6-C4
49	j	202	PLX	C3-O4-P1-O1
49	j	202	PLX	C3-O4-P1-O2
49	j	202	PLX	C3-O4-P1-O3
49	j	202	PLX	O9-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
49	r	502	PLX	O6-C6-C7-C8
49	r	502	PLX	O7-C6-O6-C4
49	r	502	PLX	C5-C4-O6-C6
49	r	502	PLX	C3-O4-P1-O1
49	r	502	PLX	C3-O4-P1-O2
49	r	502	PLX	C3-O4-P1-O3
49	r	502	PLX	O9-C24-C25-C26
49	r	503	PLX	O7-C6-O6-C4
49	r	503	PLX	C3-O4-P1-O2
49	r	503	PLX	C2-O1-P1-O4
49	r	503	PLX	O9-C24-C25-C26
50	G	201	8Q1	C1-C6-C7-C8
50	G	201	8Q1	O27-C28-C29-C30
50	G	201	8Q1	O27-C28-C29-C31
50	G	201	8Q1	O27-C28-C29-C32
50	G	201	8Q1	C28-C29-C32-C34
50	G	201	8Q1	C28-C29-C32-O33
50	G	201	8Q1	C30-C29-C32-C34
50	G	201	8Q1	C30-C29-C32-O33
50	G	201	8Q1	C31-C29-C32-C34
50	G	201	8Q1	C31-C29-C32-O33
50	G	201	8Q1	C28-O27-P24-O2
50	G	201	8Q1	C28-O27-P24-O1
50	X	201	8Q1	C1-C6-C7-C8
50	X	201	8Q1	O4-C1-S44-C43
50	X	201	8Q1	C6-C1-S44-C43
50	X	201	8Q1	C28-C29-C32-C34
50	X	201	8Q1	C28-C29-C32-O33
50	X	201	8Q1	C30-C29-C32-C34
50	X	201	8Q1	C30-C29-C32-O33
50	X	201	8Q1	C31-C29-C32-C34
50	X	201	8Q1	C31-C29-C32-O33
50	X	201	8Q1	C29-C32-C34-N36
50	X	201	8Q1	C29-C32-C34-O35
50	X	201	8Q1	N41-C42-C43-S44
50	X	201	8Q1	C43-C42-N41-C39
50	X	201	8Q1	C28-O27-P24-O3
50	X	201	8Q1	C28-O27-P24-O2
50	X	201	8Q1	C28-O27-P24-O1
51	I	201	CDL	CA2-OA2-PA1-OA3
51	I	201	CDL	CA2-OA2-PA1-OA5
51	I	201	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
51	I	201	CDL	CA3-OA5-PA1-OA4
51	I	201	CDL	CB3-OB5-PB2-OB2
51	I	201	CDL	CB3-OB5-PB2-OB4
51	V	201	CDL	CA2-OA2-PA1-OA3
51	V	201	CDL	CA2-OA2-PA1-OA5
51	a	201	CDL	CB2-C1-CA2-OA2
51	a	201	CDL	CA2-OA2-PA1-OA3
51	a	201	CDL	CA2-OA2-PA1-OA5
51	a	201	CDL	CB2-OB2-PB2-OB3
51	a	201	CDL	CB2-OB2-PB2-OB5
51	a	201	CDL	OB7-CB5-OB6-CB4
51	a	201	CDL	C51-CB5-OB6-CB4
51	i	401	CDL	CA2-OA2-PA1-OA4
51	i	401	CDL	CA2-OA2-PA1-OA5
51	i	401	CDL	CA3-OA5-PA1-OA2
51	i	401	CDL	CA3-OA5-PA1-OA3
51	i	401	CDL	CA3-OA5-PA1-OA4
51	i	401	CDL	CB3-OB5-PB2-OB2
51	i	401	CDL	CB3-OB5-PB2-OB3
51	k	101	CDL	CA2-OA2-PA1-OA4
51	k	101	CDL	OA5-CA3-CA4-OA6
51	k	101	CDL	CB2-OB2-PB2-OB3
51	k	101	CDL	CB2-OB2-PB2-OB5
51	l	701	CDL	CA2-OA2-PA1-OA5
51	l	701	CDL	CB3-OB5-PB2-OB2
51	l	701	CDL	CB3-OB5-PB2-OB3
51	l	701	CDL	CB3-OB5-PB2-OB4
51	l	702	CDL	CA2-OA2-PA1-OA3
51	l	702	CDL	CA3-OA5-PA1-OA2
51	l	702	CDL	CA3-OA5-PA1-OA3
51	l	702	CDL	CA3-OA5-PA1-OA4
51	l	702	CDL	CB2-OB2-PB2-OB4
51	l	702	CDL	CB2-OB2-PB2-OB5
51	l	702	CDL	C51-CB5-OB6-CB4
51	m	201	CDL	CA2-OA2-PA1-OA3
51	m	201	CDL	CA3-OA5-PA1-OA3
51	m	201	CDL	CB2-OB2-PB2-OB3
51	m	201	CDL	CB2-OB2-PB2-OB4
51	m	201	CDL	CB2-OB2-PB2-OB5
51	m	201	CDL	C51-CB5-OB6-CB4
51	o	201	CDL	CA2-OA2-PA1-OA3
51	o	201	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
51	o	201	CDL	CA2-OA2-PA1-OA5
51	o	201	CDL	CA3-OA5-PA1-OA3
51	o	201	CDL	CB3-OB5-PB2-OB2
51	o	201	CDL	CB3-OB5-PB2-OB3
51	o	201	CDL	CB3-OB5-PB2-OB4
51	o	201	CDL	C51-CB5-OB6-CB4
51	r	504	CDL	CA3-OA5-PA1-OA2
51	r	504	CDL	CA3-OA5-PA1-OA3
51	r	504	CDL	CB2-OB2-PB2-OB3
51	r	504	CDL	CB3-OB5-PB2-OB2
51	r	504	CDL	CB3-OB5-PB2-OB3
51	r	504	CDL	CB3-OB5-PB2-OB4
51	r	504	CDL	C51-CB5-OB6-CB4
51	u	201	CDL	CA2-OA2-PA1-OA3
51	u	201	CDL	CA2-OA2-PA1-OA5
51	u	201	CDL	CA3-OA5-PA1-OA2
51	u	201	CDL	CB3-OB5-PB2-OB2
51	u	201	CDL	CB3-OB5-PB2-OB3
52	J	401	NDP	C5D-O5D-PN-O1N
53	J	402	UQ	C1-C6-C7-C8
53	J	402	UQ	C7-C8-C9-C11
53	J	402	UQ	C12-C13-C14-C16
53	s	401	UQ	C7-C8-C9-C10
53	s	401	UQ	C7-C8-C9-C11
56	Q	501	970	C03-C02-C04-C05
56	Q	501	970	C03-C02-C04-O08
58	w	401	ADP	C5'-O5'-PA-O2A
48	U	101	PEE	O5-C30-O3-C3
48	l	703	PEE	O4-C10-O2-C2
48	l	704	PEE	O4-C10-O2-C2
51	l	702	CDL	OB7-CB5-OB6-CB4
51	m	201	CDL	OB7-CB5-OB6-CB4
51	o	201	CDL	OB7-CB5-OB6-CB4
51	r	504	CDL	OB7-CB5-OB6-CB4
48	U	101	PEE	C31-C30-O3-C3
53	s	401	UQ	C18-C19-C21-C22
53	J	402	UQ	C22-C23-C24-C26
48	l	705	PEE	C2-C3-O3-C30
51	V	201	CDL	C31-CA7-OA8-CA6
53	J	402	UQ	C7-C8-C9-C10
53	J	402	UQ	C17-C18-C19-C21
53	s	401	UQ	C17-C18-C19-C21

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Mol	Chain	Res	Type	Atoms
53	s	401	UQ	C22-C23-C24-C26
51	V	201	CDL	OA9-CA7-OA8-CA6
51	l	702	CDL	OB9-CB7-OB8-CB6
48	j	201	PEE	O4-C10-O2-C2
51	V	201	CDL	OA7-CA5-OA6-CA4
49	r	502	PLX	C9-C10-C11-C12
51	V	201	CDL	C11-C12-C13-C14
51	a	201	CDL	O1-C1-CB2-OB2
51	l	701	CDL	O1-C1-CA2-OA2
51	l	702	CDL	O1-C1-CA2-OA2
51	m	201	CDL	O1-C1-CA2-OA2
51	o	201	CDL	O1-C1-CA2-OA2
51	o	201	CDL	O1-C1-CB2-OB2
51	r	504	CDL	O1-C1-CA2-OA2
51	u	201	CDL	O1-C1-CB2-OB2
51	i	401	CDL	C31-CA7-OA8-CA6
51	l	702	CDL	C71-CB7-OB8-CB6
51	i	401	CDL	OA9-CA7-OA8-CA6
48	C	302	PEE	C11-C10-O2-C2
51	I	201	CDL	C11-CA5-OA6-CA4
51	V	201	CDL	C11-CA5-OA6-CA4
49	J	403	PLX	C25-C26-C27-C28
48	l	704	PEE	C31-C30-O3-C3
49	J	403	PLX	C27-C28-C29-C30
48	l	704	PEE	O5-C30-O3-C3
51	k	101	CDL	C73-C74-C75-C76
51	l	701	CDL	C31-CA7-OA8-CA6
51	r	504	CDL	C71-CB7-OB8-CB6
51	l	701	CDL	OA9-CA7-OA8-CA6
51	r	504	CDL	OB9-CB7-OB8-CB6
51	a	201	CDL	CA2-C1-CB2-OB2
51	l	701	CDL	CB2-C1-CA2-OA2
51	o	201	CDL	CA2-C1-CB2-OB2
48	W	201	PEE	C31-C30-O3-C3
51	I	201	CDL	C31-CA7-OA8-CA6
51	a	201	CDL	C31-CA7-OA8-CA6
48	B	303	PEE	C34-C35-C36-C37
49	j	202	PLX	C13-C14-C15-C16
49	r	502	PLX	C11-C12-C13-C14
49	r	502	PLX	C7-C8-C9-C10
51	V	201	CDL	C62-C63-C64-C65
49	g	201	PLX	C2-C1-N1-C1A

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Mol	Chain	Res	Type	Atoms
51	r	504	CDL	C83-C84-C85-C86
53	J	402	UQ	C12-C11-C9-C8
48	l	705	PEE	C34-C35-C36-C37
51	l	702	CDL	O1-C1-CB2-OB2
48	B	303	PEE	C31-C30-O3-C3
51	I	201	CDL	OA9-CA7-OA8-CA6
51	a	201	CDL	OA9-CA7-OA8-CA6
51	V	201	CDL	C32-C33-C34-C35
51	a	201	CDL	C34-C35-C36-C37
51	V	201	CDL	OB5-CB3-CB4-OB6
51	V	201	CDL	OB6-CB4-CB6-OB8
51	i	401	CDL	OB6-CB4-CB6-OB8
53	s	401	UQ	C22-C23-C24-C25
48	B	303	PEE	C17-C18-C19-C20
51	r	504	CDL	C51-C52-C53-C54
51	i	401	CDL	CA7-C31-C32-C33
49	a	202	PLX	C12-C13-C14-C15
53	s	401	UQ	C27-C28-C29-C31
48	C	302	PEE	O4-C10-O2-C2
51	I	201	CDL	OA7-CA5-OA6-CA4
53	J	402	UQ	C9-C11-C12-C13
53	s	401	UQ	C14-C16-C17-C18
49	g	201	PLX	C2-C1-N1-C1B
48	r	501	PEE	C10-C11-C12-C13
51	l	701	CDL	CB7-C71-C72-C73
51	a	201	CDL	CA5-C11-C12-C13
51	u	201	CDL	CB7-C71-C72-C73
48	r	501	PEE	C33-C34-C35-C36
49	g	201	PLX	C7-C8-C9-C10
51	a	201	CDL	C36-C37-C38-C39
51	a	201	CDL	O1-C1-CA2-OA2
51	k	101	CDL	O1-C1-CA2-OA2
51	V	201	CDL	C71-CB7-OB8-CB6
48	W	201	PEE	O5-C30-O3-C3
51	l	701	CDL	CB5-C51-C52-C53
51	r	504	CDL	CA5-C11-C12-C13
48	W	201	PEE	C17-C18-C19-C20
51	r	504	CDL	CB7-C71-C72-C73
51	V	201	CDL	C51-CB5-OB6-CB4
48	B	303	PEE	O5-C30-O3-C3
51	l	702	CDL	CB7-C71-C72-C73
51	l	702	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
51	V	201	CDL	OB7-CB5-OB6-CB4
51	k	101	CDL	CB2-C1-CA2-OA2
51	l	702	CDL	CB2-C1-CA2-OA2
51	o	201	CDL	CB2-C1-CA2-OA2
51	r	504	CDL	CB2-C1-CA2-OA2
48	j	201	PEE	C31-C30-O3-C3
48	l	705	PEE	C21-C22-C23-C24
53	s	401	UQ	C23-C24-C26-C27
48	l	705	PEE	C11-C10-O2-C2
51	l	702	CDL	C11-CA5-OA6-CA4
48	W	201	PEE	C22-C23-C24-C25
48	l	705	PEE	O4-C10-O2-C2
48	l	705	PEE	C37-C38-C39-C40
49	j	202	PLX	C19-C20-C21-C22
48	j	201	PEE	O5-C30-O3-C3
49	g	201	PLX	C9-C10-C11-C12
51	I	201	CDL	C51-C52-C53-C54
48	U	101	PEE	C19-C20-C21-C22
51	o	201	CDL	C11-C12-C13-C14
51	I	201	CDL	C51-CB5-OB6-CB4
51	m	201	CDL	CA5-C11-C12-C13
49	a	202	PLX	C34-C35-C36-C37
48	W	201	PEE	C12-C13-C14-C15
49	J	403	PLX	C14-C15-C16-C17
49	J	403	PLX	C34-C35-C36-C37
49	j	202	PLX	C33-C34-C35-C36
50	G	201	8Q1	C10-C11-C12-C13
51	o	201	CDL	C14-C15-C16-C17
51	o	201	CDL	C59-C60-C61-C62
48	C	302	PEE	C17-C18-C19-C20
48	U	101	PEE	C22-C23-C24-C25
49	a	202	PLX	C9-C10-C11-C12
49	a	202	PLX	C33-C34-C35-C36
51	V	201	CDL	OB9-CB7-OB8-CB6
49	C	303	PLX	O9-C24-C25-C26
49	r	502	PLX	O7-C6-C7-C8
49	J	403	PLX	C28-C29-C30-C31
49	J	403	PLX	C31-C32-C33-C34
49	a	202	PLX	C10-C11-C12-C13
49	j	202	PLX	C27-C28-C29-C30
51	a	201	CDL	C39-C40-C41-C42
51	a	201	CDL	C62-C63-C64-C65

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Mol	Chain	Res	Type	Atoms
51	l	701	CDL	C73-C74-C75-C76
51	o	201	CDL	C54-C55-C56-C57
51	l	702	CDL	OA7-CA5-OA6-CA4
48	W	201	PEE	C13-C14-C15-C16
49	r	503	PLX	C34-C35-C36-C37
48	j	201	PEE	C12-C13-C14-C15
48	r	501	PEE	C11-C12-C13-C14
49	g	201	PLX	C30-C31-C32-C33
51	V	201	CDL	C31-C32-C33-C34
51	V	201	CDL	C56-C57-C58-C59
51	o	201	CDL	C60-C61-C62-C63
48	B	303	PEE	C35-C36-C37-C38
48	B	303	PEE	C13-C14-C15-C16
48	C	302	PEE	C34-C35-C36-C37
49	g	201	PLX	C11-C10-C9-C8
51	a	201	CDL	C35-C36-C37-C38
48	B	303	PEE	C11-C10-O2-C2
49	r	502	PLX	C11-C10-C9-C8
51	o	201	CDL	C37-C38-C39-C40
48	l	704	PEE	C21-C22-C23-C24
49	J	403	PLX	C13-C14-C15-C16
49	r	503	PLX	C32-C33-C34-C35
49	r	503	PLX	C10-C11-C12-C13
51	i	401	CDL	C38-C39-C40-C41
51	V	201	CDL	C35-C36-C37-C38
48	j	201	PEE	C23-C24-C25-C26
49	r	502	PLX	C25-C26-C27-C28
51	o	201	CDL	C82-C83-C84-C85
48	r	501	PEE	C1-C2-C3-O3
51	o	201	CDL	CB3-CB4-CB6-OB8
48	C	302	PEE	C13-C14-C15-C16
49	J	403	PLX	C33-C34-C35-C36
49	j	202	PLX	C11-C12-C13-C14
49	j	202	PLX	C25-C26-C27-C28
51	V	201	CDL	C71-C72-C73-C74
51	o	201	CDL	C74-C75-C76-C77
51	u	201	CDL	CB5-C51-C52-C53
48	B	303	PEE	C23-C24-C25-C26
48	l	704	PEE	C31-C32-C33-C34
48	r	501	PEE	C40-C41-C42-C43
49	J	403	PLX	C7-C8-C9-C10
49	g	201	PLX	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
49	g	201	PLX	C13-C14-C15-C16
51	V	201	CDL	C34-C35-C36-C37
51	a	201	CDL	C17-C18-C19-C20
51	a	201	CDL	C60-C61-C62-C63
51	r	504	CDL	C80-C81-C82-C83
48	r	501	PEE	C21-C22-C23-C24
49	a	202	PLX	C7-C8-C9-C10
51	V	201	CDL	C75-C76-C77-C78
51	a	201	CDL	C22-C23-C24-C25
51	a	201	CDL	C75-C76-C77-C78
51	r	504	CDL	C14-C15-C16-C17
49	C	303	PLX	C25-C26-C27-C28
49	J	403	PLX	C30-C31-C32-C33
49	g	201	PLX	C2-C1-N1-C1C
49	g	201	PLX	C27-C28-C29-C30
51	V	201	CDL	C58-C59-C60-C61
51	k	101	CDL	C11-C12-C13-C14
51	m	201	CDL	C16-C17-C18-C19
51	r	504	CDL	C43-C44-C45-C46
49	C	303	PLX	C15-C16-C17-C18
51	o	201	CDL	C35-C36-C37-C38
48	r	501	PEE	C11-C10-O2-C2
48	U	101	PEE	C21-C22-C23-C24
48	l	705	PEE	C20-C21-C22-C23
51	k	101	CDL	C17-C18-C19-C20
49	C	303	PLX	C9-C10-C11-C12
49	r	503	PLX	C7-C8-C9-C10
51	o	201	CDL	C83-C84-C85-C86
48	W	201	PEE	C24-C25-C26-C27
49	r	503	PLX	C25-C26-C27-C28
51	I	201	CDL	C11-C12-C13-C14
51	I	201	CDL	OB7-CB5-OB6-CB4
49	j	202	PLX	C16-C17-C18-C19
49	j	202	PLX	C10-C11-C12-C13
49	r	502	PLX	C33-C34-C35-C36
51	k	101	CDL	C71-C72-C73-C74
51	r	504	CDL	C41-C42-C43-C44
48	U	101	PEE	C41-C42-C43-C44
51	i	401	CDL	C14-C15-C16-C17
51	V	201	CDL	C40-C41-C42-C43
51	V	201	CDL	C78-C79-C80-C81
51	a	201	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
51	l	701	CDL	C11-C12-C13-C14
51	l	702	CDL	C33-C34-C35-C36
50	G	201	8Q1	C12-C13-C14-C15
49	j	202	PLX	C14-C15-C16-C17
51	o	201	CDL	C17-C18-C19-C20
51	o	201	CDL	C75-C76-C77-C78
48	U	101	PEE	C30-C31-C32-C33
51	V	201	CDL	CB5-C51-C52-C53
51	l	702	CDL	CB5-C51-C52-C53
48	B	303	PEE	C38-C39-C40-C41
49	a	202	PLX	C30-C31-C32-C33
49	g	201	PLX	C28-C29-C30-C31
51	V	201	CDL	C72-C73-C74-C75
49	J	403	PLX	C26-C27-C28-C29
48	W	201	PEE	C11-C10-O2-C2
51	i	401	CDL	C11-CA5-OA6-CA4
48	B	303	PEE	O4-C10-O2-C2
48	W	201	PEE	O4-C10-O2-C2
48	l	704	PEE	C15-C16-C17-C18
48	l	705	PEE	C15-C16-C17-C18
56	Q	501	970	C20-C19-O28-C29
51	V	201	CDL	C43-C44-C45-C46
51	l	702	CDL	C12-C13-C14-C15
49	g	201	PLX	C10-C11-C12-C13
51	o	201	CDL	C51-C52-C53-C54
51	i	401	CDL	C77-C78-C79-C80
53	J	402	UQ	C5-C6-C7-C8
51	V	201	CDL	C59-C60-C61-C62
48	U	101	PEE	C17-C18-C19-C20
49	g	201	PLX	C32-C33-C34-C35
51	a	201	CDL	C80-C81-C82-C83
48	r	501	PEE	C13-C14-C15-C16
48	r	501	PEE	C20-C21-C22-C23
49	r	502	PLX	C27-C28-C29-C30
49	r	502	PLX	C19-C20-C21-C22
48	W	201	PEE	C21-C22-C23-C24
49	r	502	PLX	C12-C13-C14-C15
48	r	501	PEE	O4-C10-O2-C2
51	i	401	CDL	OA7-CA5-OA6-CA4
51	o	201	CDL	OB5-CB3-CB4-OB6
51	r	504	CDL	C55-C56-C57-C58
53	s	401	UQ	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
51	l	701	CDL	C81-C82-C83-C84
51	r	504	CDL	C31-C32-C33-C34
48	l	703	PEE	C10-C11-C12-C13
48	l	705	PEE	C30-C31-C32-C33
51	a	201	CDL	CB5-C51-C52-C53
51	o	201	CDL	OA6-CA4-CA6-OA8
51	o	201	CDL	OB6-CB4-CB6-OB8
49	r	502	PLX	C28-C29-C30-C31
49	a	202	PLX	C19-C20-C21-C22
49	j	202	PLX	C11-C10-C9-C8
49	r	503	PLX	C16-C17-C18-C19
51	a	201	CDL	C11-C12-C13-C14
48	l	705	PEE	C13-C14-C15-C16
51	V	201	CDL	C73-C74-C75-C76
51	a	201	CDL	C52-C53-C54-C55
49	r	503	PLX	C29-C30-C31-C32
51	r	504	CDL	CB5-C51-C52-C53
51	u	201	CDL	CA2-C1-CB2-OB2
51	r	504	CDL	C21-C22-C23-C24
48	l	703	PEE	C31-C30-O3-C3
51	r	504	CDL	C17-C18-C19-C20
51	r	504	CDL	C13-C14-C15-C16
51	r	504	CDL	C32-C33-C34-C35
49	r	503	PLX	C13-C14-C15-C16
49	r	503	PLX	C11-C10-C9-C8
51	o	201	CDL	C72-C73-C74-C75
49	a	202	PLX	C13-C14-C15-C16
51	o	201	CDL	C32-C33-C34-C35
48	C	302	PEE	C19-C20-C21-C22
48	C	302	PEE	C44-C45-C46-C47
51	V	201	CDL	OB5-CB3-CB4-CB6
48	j	201	PEE	C11-C12-C13-C14
49	r	502	PLX	C18-C19-C20-C21
48	r	501	PEE	C30-C31-C32-C33
48	j	201	PEE	C13-C14-C15-C16
48	r	501	PEE	C34-C35-C36-C37
51	m	201	CDL	C12-C13-C14-C15
49	g	201	PLX	C25-C26-C27-C28
51	r	504	CDL	C82-C83-C84-C85
48	W	201	PEE	C20-C21-C22-C23
51	o	201	CDL	C12-C13-C14-C15
51	V	201	CDL	C61-C62-C63-C64

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Mol	Chain	Res	Type	Atoms
49	r	503	PLX	C17-C18-C19-C20
51	l	701	CDL	C35-C36-C37-C38
49	C	303	PLX	C10-C11-C12-C13
48	W	201	PEE	C1-C2-C3-O3
51	V	201	CDL	CB3-CB4-CB6-OB8
51	V	201	CDL	C79-C80-C81-C82
51	k	101	CDL	C23-C24-C25-C26
48	U	101	PEE	C35-C36-C37-C38
49	g	201	PLX	C12-C13-C14-C15
51	o	201	CDL	C36-C37-C38-C39
51	k	101	CDL	C76-C77-C78-C79
51	r	504	CDL	C72-C73-C74-C75
51	r	504	CDL	C52-C53-C54-C55
49	r	502	PLX	C13-C14-C15-C16
46	A	502	FMN	C5'-O5'-P-O1P
50	G	201	8Q1	C28-O27-P24-O3
49	r	503	PLX	C28-C29-C30-C31
48	l	703	PEE	O5-C30-O3-C3
51	I	201	CDL	CA6-CA4-OA6-CA5
51	V	201	CDL	CA6-CA4-OA6-CA5
51	i	401	CDL	CA6-CA4-OA6-CA5
48	l	703	PEE	C35-C36-C37-C38
48	l	703	PEE	C32-C33-C34-C35
51	r	504	CDL	C59-C60-C61-C62
49	j	202	PLX	C7-C8-C9-C10
48	l	704	PEE	O3P-C1-C2-O2
49	j	202	PLX	O4-C3-C4-O6
51	l	702	CDL	C17-C18-C19-C20
51	k	101	CDL	C81-C82-C83-C84
51	i	401	CDL	C13-C14-C15-C16
48	r	501	PEE	C42-C43-C44-C45
51	o	201	CDL	C77-C78-C79-C80
51	r	504	CDL	C71-C72-C73-C74
51	V	201	CDL	C15-C16-C17-C18
51	l	702	CDL	C15-C16-C17-C18
48	l	704	PEE	O2-C2-C3-O3
49	J	403	PLX	O6-C4-C5-O8
51	k	101	CDL	OA6-CA4-CA6-OA8
48	C	302	PEE	C12-C13-C14-C15
51	a	201	CDL	C57-C58-C59-C60
51	a	201	CDL	C44-C45-C46-C47
48	l	704	PEE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
51	k	101	CDL	C75-C76-C77-C78
48	B	303	PEE	C44-C45-C46-C47
51	o	201	CDL	C32-C31-CA7-OA8
51	a	201	CDL	C71-C72-C73-C74
51	l	701	CDL	C37-C38-C39-C40
48	r	501	PEE	C39-C40-C41-C42
52	J	401	NDP	PN-O3-PA-O1A
51	a	201	CDL	C71-CB7-OB8-CB6
51	k	101	CDL	C31-CA7-OA8-CA6
51	V	201	CDL	C52-C53-C54-C55
51	i	401	CDL	C82-C83-C84-C85
51	o	201	CDL	C57-C58-C59-C60
48	l	704	PEE	C24-C25-C26-C27
48	r	501	PEE	C17-C18-C19-C20
51	r	504	CDL	C73-C74-C75-C76
48	l	703	PEE	C13-C14-C15-C16
49	r	503	PLX	C11-C12-C13-C14
48	l	703	PEE	C18-C19-C20-C21
48	r	501	PEE	C38-C39-C40-C41
48	U	101	PEE	C12-C13-C14-C15
48	l	703	PEE	C2-C1-O3P-P
51	k	101	CDL	C84-C85-C86-C87
48	C	302	PEE	C42-C43-C44-C45
49	r	502	PLX	C30-C31-C32-C33
51	l	701	CDL	C75-C76-C77-C78
51	l	702	CDL	C39-C40-C41-C42
51	o	201	CDL	C64-C65-C66-C67
51	l	702	CDL	C11-C12-C13-C14
49	r	503	PLX	C14-C15-C16-C17
50	G	201	8Q1	C11-C12-C13-C14
50	X	201	8Q1	C7-C8-C9-C10
48	U	101	PEE	C32-C33-C34-C35
49	C	303	PLX	C32-C33-C34-C35
49	r	503	PLX	C26-C27-C28-C29
48	C	302	PEE	O3P-C1-C2-C3
49	C	303	PLX	O4-C3-C4-C5
49	J	403	PLX	O4-C3-C4-C5
51	i	401	CDL	OB5-CB3-CB4-CB6
51	k	101	CDL	OA5-CA3-CA4-CA6
51	o	201	CDL	OB5-CB3-CB4-CB6
51	a	201	CDL	C84-C85-C86-C87
49	r	502	PLX	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
51	V	201	CDL	CA7-C31-C32-C33
51	l	701	CDL	C51-C52-C53-C54
49	r	503	PLX	C12-C13-C14-C15
50	X	201	8Q1	C12-C13-C14-C15
49	j	202	PLX	C29-C30-C31-C32
51	k	101	CDL	C52-C53-C54-C55
48	l	704	PEE	C42-C43-C44-C45
49	j	202	PLX	C34-C35-C36-C37
49	g	201	PLX	C16-C17-C18-C19
49	g	201	PLX	C36-C37-C38-C39
49	j	202	PLX	C12-C13-C14-C15
51	a	201	CDL	C76-C77-C78-C79
48	C	302	PEE	C1-C2-C3-O3
48	l	703	PEE	C1-C2-C3-O3
48	l	705	PEE	C1-C2-C3-O3
49	a	202	PLX	C3-C4-C5-O8
49	r	503	PLX	C3-C4-C5-O8
51	i	401	CDL	CB3-CB4-CB6-OB8
51	o	201	CDL	CA3-CA4-CA6-OA8
49	r	502	PLX	C14-C15-C16-C17
51	k	101	CDL	C14-C15-C16-C17
48	l	703	PEE	C14-C15-C16-C17
51	r	504	CDL	C62-C63-C64-C65
48	l	704	PEE	C13-C14-C15-C16
49	a	202	PLX	C11-C10-C9-C8
51	V	201	CDL	C33-C34-C35-C36
48	r	501	PEE	O3P-C1-C2-O2
49	C	303	PLX	O4-C3-C4-O6
49	J	403	PLX	C12-C13-C14-C15
51	I	201	CDL	C1-CA2-OA2-PA1
48	U	101	PEE	C44-C45-C46-C47
48	l	705	PEE	C11-C12-C13-C14
51	o	201	CDL	C84-C85-C86-C87
51	i	401	CDL	C76-C77-C78-C79
51	m	201	CDL	C33-C34-C35-C36
48	B	303	PEE	O2-C2-C3-O3
48	C	302	PEE	O2-C2-C3-O3
51	k	101	CDL	OB6-CB4-CB6-OB8
51	l	702	CDL	OB6-CB4-CB6-OB8
51	m	201	CDL	C52-C53-C54-C55
49	J	403	PLX	C16-C17-C18-C19
49	a	202	PLX	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
48	C	302	PEE	C31-C32-C33-C34
51	k	101	CDL	C80-C81-C82-C83
51	m	201	CDL	C51-C52-C53-C54
49	J	403	PLX	O8-C24-C25-C26
49	a	202	PLX	O8-C24-C25-C26
49	j	202	PLX	O6-C6-C7-C8
49	r	502	PLX	O8-C24-C25-C26
49	r	503	PLX	O8-C24-C25-C26
49	J	403	PLX	C10-C11-C12-C13
51	l	702	CDL	C16-C17-C18-C19
51	k	101	CDL	C12-C13-C14-C15
51	V	201	CDL	C64-C65-C66-C67
51	m	201	CDL	C72-C73-C74-C75
49	j	202	PLX	C20-C21-C22-C23
50	X	201	8Q1	C11-C10-C9-C8
51	o	201	CDL	C34-C35-C36-C37
51	l	701	CDL	C51-CB5-OB6-CB4
49	C	303	PLX	C11-C12-C13-C14
51	l	702	CDL	C79-C80-C81-C82
48	j	201	PEE	C24-C25-C26-C27
51	m	201	CDL	CB2-C1-CA2-OA2
51	V	201	CDL	C14-C15-C16-C17
56	Q	501	970	C18-C19-O28-C29
48	l	703	PEE	C34-C35-C36-C37
51	k	101	CDL	C18-C19-C20-C21
46	A	502	FMN	C1'-C2'-C3'-O3'
48	l	704	PEE	O3P-C1-C2-C3
51	V	201	CDL	OA5-CA3-CA4-CA6
51	m	201	CDL	OA5-CA3-CA4-CA6
49	a	202	PLX	C27-C28-C29-C30
50	G	201	8Q1	C13-C14-C15-C16
51	o	201	CDL	C79-C80-C81-C82
51	V	201	CDL	C17-C18-C19-C20
51	l	701	CDL	C11-CA5-OA6-CA4
58	w	401	ADP	PA-O3A-PB-O1B
51	r	504	CDL	C37-C38-C39-C40
51	a	201	CDL	OB9-CB7-OB8-CB6
51	a	201	CDL	C43-C44-C45-C46
49	a	202	PLX	C11-C12-C13-C14
51	r	504	CDL	C78-C79-C80-C81
48	U	101	PEE	C38-C39-C40-C41
48	B	303	PEE	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
51	V	201	CDL	C55-C56-C57-C58
51	k	101	CDL	OA9-CA7-OA8-CA6
48	U	101	PEE	C34-C35-C36-C37
49	C	303	PLX	C11-C10-C9-C8
51	a	201	CDL	C82-C83-C84-C85
51	m	201	CDL	C35-C36-C37-C38
51	a	201	CDL	C20-C21-C22-C23
48	B	303	PEE	O3P-C1-C2-O2
48	C	302	PEE	O3P-C1-C2-O2
51	i	401	CDL	OB5-CB3-CB4-OB6
51	m	201	CDL	OA5-CA3-CA4-OA6
51	o	201	CDL	OA5-CA3-CA4-OA6
51	r	504	CDL	OB5-CB3-CB4-OB6
51	i	401	CDL	C71-C72-C73-C74
51	m	201	CDL	C54-C55-C56-C57
48	j	201	PEE	C34-C35-C36-C37
53	J	402	UQ	C20-C19-C21-C22
51	r	504	CDL	C15-C16-C17-C18
48	l	705	PEE	C5-C4-O4P-P
48	r	501	PEE	C5-C4-O4P-P
51	I	201	CDL	CA7-C31-C32-C33
48	W	201	PEE	O2-C2-C3-O3
48	r	501	PEE	O2-C2-C3-O3
49	a	202	PLX	O6-C4-C5-O8
51	a	201	CDL	C37-C38-C39-C40
48	r	501	PEE	C14-C15-C16-C17
49	r	503	PLX	C33-C34-C35-C36
51	u	201	CDL	C72-C73-C74-C75
51	l	701	CDL	C78-C79-C80-C81
51	r	504	CDL	C39-C40-C41-C42
48	U	101	PEE	C11-C12-C13-C14
49	r	502	PLX	N1-C1-C2-O1
51	V	201	CDL	C44-C45-C46-C47
48	C	302	PEE	C31-C30-O3-C3
49	g	201	PLX	O9-C24-C25-C26
49	J	403	PLX	C25-C24-O8-C5
51	r	504	CDL	C22-C23-C24-C25
49	g	201	PLX	C20-C21-C22-C23
48	r	501	PEE	C41-C42-C43-C44
51	r	504	CDL	C56-C57-C58-C59
50	X	201	8Q1	C13-C14-C15-C16
48	B	303	PEE	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
48	l	703	PEE	O3P-C1-C2-C3
49	j	202	PLX	O4-C3-C4-C5
49	r	503	PLX	O4-C3-C4-C5
51	o	201	CDL	OA5-CA3-CA4-CA6
51	r	504	CDL	OB5-CB3-CB4-CB6
51	l	701	CDL	OA7-CA5-OA6-CA4
51	l	701	CDL	OB7-CB5-OB6-CB4
51	a	201	CDL	C83-C84-C85-C86
50	X	201	8Q1	O27-C28-C29-C31
56	Q	501	970	C01-C02-C04-C05
51	a	201	CDL	C14-C15-C16-C17
51	a	201	CDL	C51-C52-C53-C54
51	m	201	CDL	O1-C1-CB2-OB2
51	r	504	CDL	C1-CB2-OB2-PB2
56	Q	501	970	C01-C02-C04-O08
49	g	201	PLX	O8-C24-C25-C26
49	J	403	PLX	O4-C3-C4-O6
49	r	503	PLX	O4-C3-C4-O6
51	i	401	CDL	C59-C60-C61-C62
48	C	302	PEE	O5-C30-O3-C3
49	r	502	PLX	O6-C4-C5-O8
49	r	503	PLX	O6-C4-C5-O8
51	r	504	CDL	OB6-CB4-CB6-OB8
51	u	201	CDL	C73-C74-C75-C76
49	g	201	PLX	C3-C4-C5-O8
51	k	101	CDL	CB3-CB4-CB6-OB8
51	l	702	CDL	CB3-CB4-CB6-OB8
51	V	201	CDL	C57-C58-C59-C60
50	X	201	8Q1	O27-C28-C29-C32
48	r	501	PEE	C12-C13-C14-C15
51	m	201	CDL	C37-C38-C39-C40
51	V	201	CDL	C54-C55-C56-C57
48	C	302	PEE	C4-O4P-P-O3P
48	C	302	PEE	C4-O4P-P-O2P
48	C	302	PEE	C4-O4P-P-O1P
48	U	101	PEE	C1-O3P-P-O1P
48	l	705	PEE	C4-O4P-P-O1P
48	r	501	PEE	C4-O4P-P-O2P
49	J	403	PLX	C2-O1-P1-O3
49	r	503	PLX	C3-C4-O6-C6
49	r	503	PLX	C5-C4-O6-C6
51	I	201	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
51	V	201	CDL	CA3-OA5-PA1-OA3
51	V	201	CDL	CB3-OB5-PB2-OB2
51	V	201	CDL	CB3-OB5-PB2-OB3
51	a	201	CDL	CA2-OA2-PA1-OA4
51	a	201	CDL	CA3-OA5-PA1-OA2
51	a	201	CDL	CA3-OA5-PA1-OA3
51	a	201	CDL	CA3-OA5-PA1-OA4
51	a	201	CDL	CB2-OB2-PB2-OB4
51	i	401	CDL	CB3-OB5-PB2-OB4
51	k	101	CDL	CA2-OA2-PA1-OA3
51	k	101	CDL	CA2-OA2-PA1-OA5
51	k	101	CDL	CB2-OB2-PB2-OB4
51	l	701	CDL	CA2-OA2-PA1-OA3
51	l	701	CDL	CB2-OB2-PB2-OB3
51	l	702	CDL	CB2-OB2-PB2-OB3
51	m	201	CDL	CB3-OB5-PB2-OB3
51	r	504	CDL	CA2-OA2-PA1-OA4
51	r	504	CDL	CA2-OA2-PA1-OA5
51	r	504	CDL	CB2-OB2-PB2-OB5
51	u	201	CDL	CA2-OA2-PA1-OA4
51	u	201	CDL	CA3-OA5-PA1-OA3
51	u	201	CDL	CB2-OB2-PB2-OB3
52	J	401	NDP	C5D-O5D-PN-O3
53	J	402	UQ	C3-C2-O2-CM2
58	w	401	ADP	C5'-O5'-PA-O1A
58	w	401	ADP	C5'-O5'-PA-O3A
51	l	701	CDL	CA4-CA3-OA5-PA1
51	o	201	CDL	C1-CB2-OB2-PB2
51	o	201	CDL	C55-C56-C57-C58
51	V	201	CDL	C22-C23-C24-C25
51	m	201	CDL	CB7-C71-C72-C73
51	i	401	CDL	C12-C13-C14-C15
48	j	201	PEE	C21-C22-C23-C24
51	k	101	CDL	C16-C17-C18-C19
51	k	101	CDL	CA6-CA4-OA6-CA5
49	j	202	PLX	C30-C31-C32-C33
49	g	201	PLX	C33-C34-C35-C36
51	r	504	CDL	C79-C80-C81-C82
48	U	101	PEE	C16-C17-C18-C19
51	r	504	CDL	C34-C35-C36-C37
51	V	201	CDL	OA5-CA3-CA4-OA6
51	o	201	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
51	l	701	CDL	C36-C37-C38-C39
51	l	702	CDL	CA7-C31-C32-C33
49	r	503	PLX	C18-C19-C20-C21
49	a	202	PLX	C28-C29-C30-C31
49	j	202	PLX	C9-C10-C11-C12
53	J	402	UQ	C4-C3-O3-CM3
49	r	503	PLX	C24-C25-C26-C27
49	C	303	PLX	C19-C20-C21-C22
51	k	101	CDL	C53-C54-C55-C56
48	l	703	PEE	O2-C2-C3-O3
48	l	705	PEE	O2-C2-C3-O3
51	a	201	CDL	OA6-CA4-CA6-OA8
51	m	201	CDL	OB6-CB4-CB6-OB8
48	U	101	PEE	C43-C44-C45-C46
48	r	501	PEE	C37-C38-C39-C40
51	l	701	CDL	C84-C85-C86-C87
48	C	302	PEE	C15-C16-C17-C18
49	J	403	PLX	C3-C4-C5-O8
49	r	502	PLX	C3-C4-C5-O8
52	J	401	NDP	PN-O3-PA-O2A
46	A	502	FMN	O2'-C2'-C3'-C4'
51	a	201	CDL	C40-C41-C42-C43
51	a	201	CDL	C53-C54-C55-C56
51	i	401	CDL	C36-C37-C38-C39
49	C	303	PLX	C14-C15-C16-C17
49	r	502	PLX	C4-C3-O4-P1
51	V	201	CDL	C38-C39-C40-C41
48	r	501	PEE	C36-C37-C38-C39
51	l	701	CDL	C58-C59-C60-C61
49	j	202	PLX	C28-C29-C30-C31
51	V	201	CDL	O1-C1-CA2-OA2
49	C	303	PLX	C27-C28-C29-C30
51	l	701	CDL	C24-C25-C26-C27
49	r	502	PLX	C31-C32-C33-C34
51	k	101	CDL	OB9-CB7-OB8-CB6
48	j	201	PEE	O2-C2-C3-O3
49	C	303	PLX	O6-C4-C5-O8
48	U	101	PEE	C20-C21-C22-C23
51	r	504	CDL	C54-C55-C56-C57
49	a	202	PLX	C24-C25-C26-C27
51	o	201	CDL	C32-C31-CA7-OA9
52	J	401	NDP	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
49	J	403	PLX	C18-C19-C20-C21
51	u	201	CDL	C1-CB2-OB2-PB2
51	l	701	CDL	C33-C34-C35-C36
51	V	201	CDL	CB2-C1-CA2-OA2
48	l	705	PEE	C38-C39-C40-C41
50	X	201	8Q1	O33-C32-C34-N36
51	I	201	CDL	CA3-CA4-CA6-OA8
51	l	701	CDL	C82-C83-C84-C85
50	X	201	8Q1	C10-C11-C12-C13
48	U	101	PEE	C1-C2-O2-C10
47	A	503	NAI	O4D-C1D-N1N-C2N
51	a	201	CDL	C33-C34-C35-C36
51	l	702	CDL	C38-C39-C40-C41
51	a	201	CDL	CA7-C31-C32-C33
51	o	201	CDL	C18-C19-C20-C21
49	r	503	PLX	C2-C1-N1-C1B
51	m	201	CDL	C14-C15-C16-C17
51	k	101	CDL	C32-C33-C34-C35
51	I	201	CDL	OA5-CA3-CA4-OA6
51	l	701	CDL	OA5-CA3-CA4-OA6
48	W	201	PEE	C16-C17-C18-C19
49	a	202	PLX	C6-C7-C8-C9
51	r	504	CDL	C33-C34-C35-C36
48	l	705	PEE	C2-C1-O3P-P
49	a	202	PLX	C25-C26-C27-C28
49	r	503	PLX	C31-C32-C33-C34
48	l	703	PEE	C21-C22-C23-C24
48	C	302	PEE	C41-C42-C43-C44
48	j	201	PEE	C18-C19-C20-C21
49	g	201	PLX	O6-C4-C5-O8
47	A	503	NAI	C2D-C1D-N1N-C2N
52	J	401	NDP	C2B-O2B-P2B-O1X
53	J	402	UQ	C13-C14-C16-C17
48	C	302	PEE	C38-C39-C40-C41
49	a	202	PLX	O6-C6-C7-C8
49	j	202	PLX	O8-C24-C25-C26
49	C	303	PLX	C17-C18-C19-C20
51	r	504	CDL	C42-C43-C44-C45
51	l	701	CDL	C74-C75-C76-C77
51	r	504	CDL	C12-C13-C14-C15
51	k	101	CDL	C71-CB7-OB8-CB6
48	U	101	PEE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
48	l	704	PEE	C2-C1-O3P-P
48	j	201	PEE	C32-C33-C34-C35
49	j	202	PLX	C15-C16-C17-C18
51	u	201	CDL	C55-C56-C57-C58
48	U	101	PEE	C40-C41-C42-C43
49	r	503	PLX	C19-C20-C21-C22
48	B	303	PEE	C42-C43-C44-C45
48	B	303	PEE	C1-C2-C3-O3
48	l	704	PEE	C1-C2-C3-O3
51	k	101	CDL	CA3-CA4-CA6-OA8
51	m	201	CDL	CB3-CB4-CB6-OB8
51	r	504	CDL	CB3-CB4-CB6-OB8
51	l	701	CDL	C31-C32-C33-C34
51	r	504	CDL	C60-C61-C62-C63
51	m	201	CDL	C75-C76-C77-C78
49	C	303	PLX	O7-C6-C7-C8
51	r	504	CDL	C76-C77-C78-C79
48	B	303	PEE	C11-C12-C13-C14
49	g	201	PLX	C35-C36-C37-C38
49	g	201	PLX	O4-C3-C4-O6
53	s	401	UQ	C6-C7-C8-C9
48	W	201	PEE	C23-C24-C25-C26
48	U	101	PEE	C36-C37-C38-C39
48	l	704	PEE	C38-C39-C40-C41
49	r	503	PLX	C27-C28-C29-C30
49	j	202	PLX	C17-C18-C19-C20
51	a	201	CDL	C56-C57-C58-C59
48	r	501	PEE	O3P-C1-C2-C3
51	I	201	CDL	OA5-CA3-CA4-CA6
51	I	201	CDL	OA6-CA4-CA6-OA8
51	V	201	CDL	OA6-CA4-CA6-OA8
51	a	201	CDL	OB6-CB4-CB6-OB8
48	B	303	PEE	C2-C1-O3P-P
51	m	201	CDL	C78-C79-C80-C81
51	l	701	CDL	C20-C21-C22-C23
51	l	702	CDL	C40-C41-C42-C43
51	o	201	CDL	C78-C79-C80-C81
48	C	302	PEE	C18-C19-C20-C21
48	l	704	PEE	C36-C37-C38-C39
51	l	702	CDL	C53-C54-C55-C56
51	V	201	CDL	C32-C31-CA7-OA8
46	A	502	FMN	O2'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
48	l	704	PEE	C11-C12-C13-C14
58	w	401	ADP	PA-O3A-PB-O2B
58	w	401	ADP	PA-O3A-PB-O3B
51	I	201	CDL	O1-C1-CB2-OB2
51	l	702	CDL	C31-CA7-OA8-CA6
53	s	401	UQ	C12-C13-C14-C16
49	r	503	PLX	C2-C1-N1-C1C
49	r	503	PLX	C2-C1-N1-C1A
51	i	401	CDL	CA3-CA4-CA6-OA8
51	o	201	CDL	C21-C22-C23-C24
51	l	702	CDL	OA9-CA7-OA8-CA6
51	i	401	CDL	C39-C40-C41-C42
51	l	701	CDL	C80-C81-C82-C83
51	o	201	CDL	C40-C41-C42-C43
49	r	503	PLX	C30-C31-C32-C33
49	g	201	PLX	O6-C6-C7-C8
51	l	701	CDL	C71-C72-C73-C74
51	l	702	CDL	C12-C11-CA5-OA6
49	j	202	PLX	O6-C4-C5-O8
51	i	401	CDL	OA6-CA4-CA6-OA8
48	B	303	PEE	C18-C19-C20-C21
48	l	704	PEE	C18-C19-C20-C21
48	U	101	PEE	O2-C10-C11-C12
51	I	201	CDL	C52-C51-CB5-OB6
51	o	201	CDL	C15-C16-C17-C18
51	u	201	CDL	C57-C58-C59-C60
48	W	201	PEE	C33-C34-C35-C36
48	B	303	PEE	C16-C17-C18-C19
51	m	201	CDL	C36-C37-C38-C39
48	r	501	PEE	O2-C10-C11-C12
51	o	201	CDL	C81-C82-C83-C84
51	a	201	CDL	C64-C65-C66-C67
49	a	202	PLX	C14-C15-C16-C17
48	l	703	PEE	C22-C23-C24-C25
51	i	401	CDL	C18-C19-C20-C21
53	s	401	UQ	C13-C14-C16-C17
51	m	201	CDL	C74-C75-C76-C77
51	V	201	CDL	C41-C42-C43-C44
51	l	702	CDL	C13-C14-C15-C16
52	J	401	NDP	C2B-O2B-P2B-O3X
48	r	501	PEE	C31-C32-C33-C34
48	j	201	PEE	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
49	j	202	PLX	C3-C4-C5-O8
51	V	201	CDL	CA3-CA4-CA6-OA8
49	j	202	PLX	C25-C24-O8-C5
51	i	401	CDL	C51-C52-C53-C54
51	a	201	CDL	C32-C31-CA7-OA8
51	i	401	CDL	C52-C51-CB5-OB6
51	m	201	CDL	C12-C11-CA5-OA6
51	i	401	CDL	C53-C54-C55-C56
51	l	702	CDL	C78-C79-C80-C81
48	l	704	PEE	C40-C41-C42-C43
49	g	201	PLX	C15-C16-C17-C18
49	g	201	PLX	C11-C12-C13-C14
50	X	201	8Q1	O27-C28-C29-C30
51	I	201	CDL	C72-C71-CB7-OB8
50	X	201	8Q1	C6-C7-C8-C9
48	U	101	PEE	C13-C14-C15-C16
53	J	402	UQ	C2-C3-O3-CM3
48	l	703	PEE	C19-C20-C21-C22
50	X	201	8Q1	C11-C12-C13-C14
51	l	701	CDL	C72-C73-C74-C75
49	a	202	PLX	C17-C18-C19-C20
48	j	201	PEE	O3-C30-C31-C32
51	k	101	CDL	C32-C31-CA7-OA8
49	a	202	PLX	C4-C3-O4-P1
49	r	503	PLX	C6-C7-C8-C9
51	a	201	CDL	C21-C22-C23-C24
51	a	201	CDL	C58-C59-C60-C61
48	U	101	PEE	O3P-C1-C2-O2
47	A	503	NAI	C2D-C1D-N1N-C6N
50	X	201	8Q1	C9-C10-C11-C12
48	l	703	PEE	C36-C37-C38-C39
48	B	303	PEE	C12-C13-C14-C15
51	I	201	CDL	C52-C51-CB5-OB7
49	g	201	PLX	O9-C24-O8-C5
49	r	503	PLX	O9-C24-O8-C5
48	W	201	PEE	C18-C19-C20-C21
48	r	501	PEE	O4-C10-C11-C12
48	B	303	PEE	C20-C21-C22-C23
51	I	201	CDL	C72-C71-CB7-OB9
51	k	101	CDL	C21-C22-C23-C24
48	U	101	PEE	O4-C10-C11-C12
56	Q	501	970	C19-C20-O26-C27

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Mol	Chain	Res	Type	Atoms
51	r	504	CDL	C19-C20-C21-C22
51	o	201	CDL	C63-C64-C65-C66
51	m	201	CDL	C12-C11-CA5-OA7
51	k	101	CDL	C12-C11-CA5-OA6
51	r	504	CDL	C72-C71-CB7-OB8
51	k	101	CDL	C32-C31-CA7-OA9
51	a	201	CDL	C31-C32-C33-C34
51	a	201	CDL	C12-C11-CA5-OA6
51	m	201	CDL	C58-C59-C60-C61
51	a	201	CDL	C32-C31-CA7-OA9

There are no ring outliers.

38 monomers are involved in 298 short contacts:

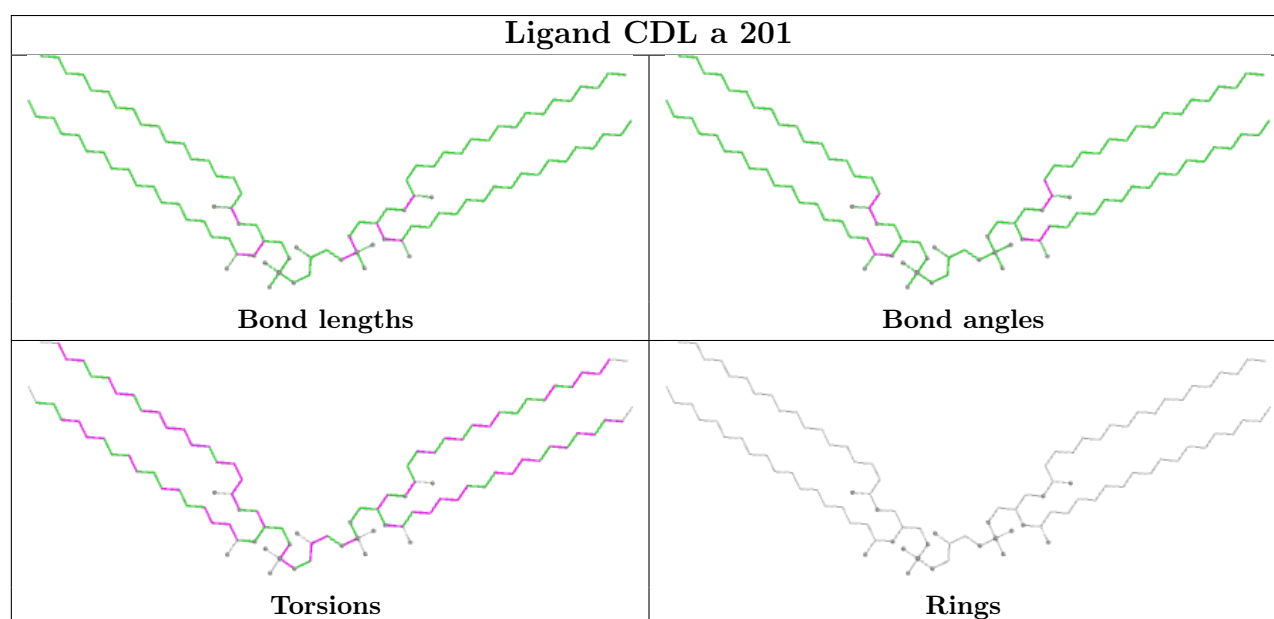
Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	a	201	CDL	6	0
46	A	502	FMN	5	0
51	l	702	CDL	17	0
48	r	501	PEE	8	0
50	G	201	8Q1	1	0
45	M	802	SF4	3	0
52	J	401	NDP	1	0
48	l	704	PEE	4	0
49	C	303	PLX	8	0
51	I	201	CDL	18	0
45	C	301	SF4	1	0
49	a	202	PLX	1	0
51	r	504	CDL	7	0
48	C	302	PEE	7	0
53	J	402	UQ	5	0
49	J	403	PLX	11	0
48	l	705	PEE	7	0
51	o	201	CDL	9	0
49	r	502	PLX	5	0
50	X	201	8Q1	7	0
48	W	201	PEE	4	0
49	g	201	PLX	7	0
51	i	401	CDL	19	0
51	u	201	CDL	9	0
48	B	303	PEE	4	0
45	A	501	SF4	1	0
51	V	201	CDL	10	0

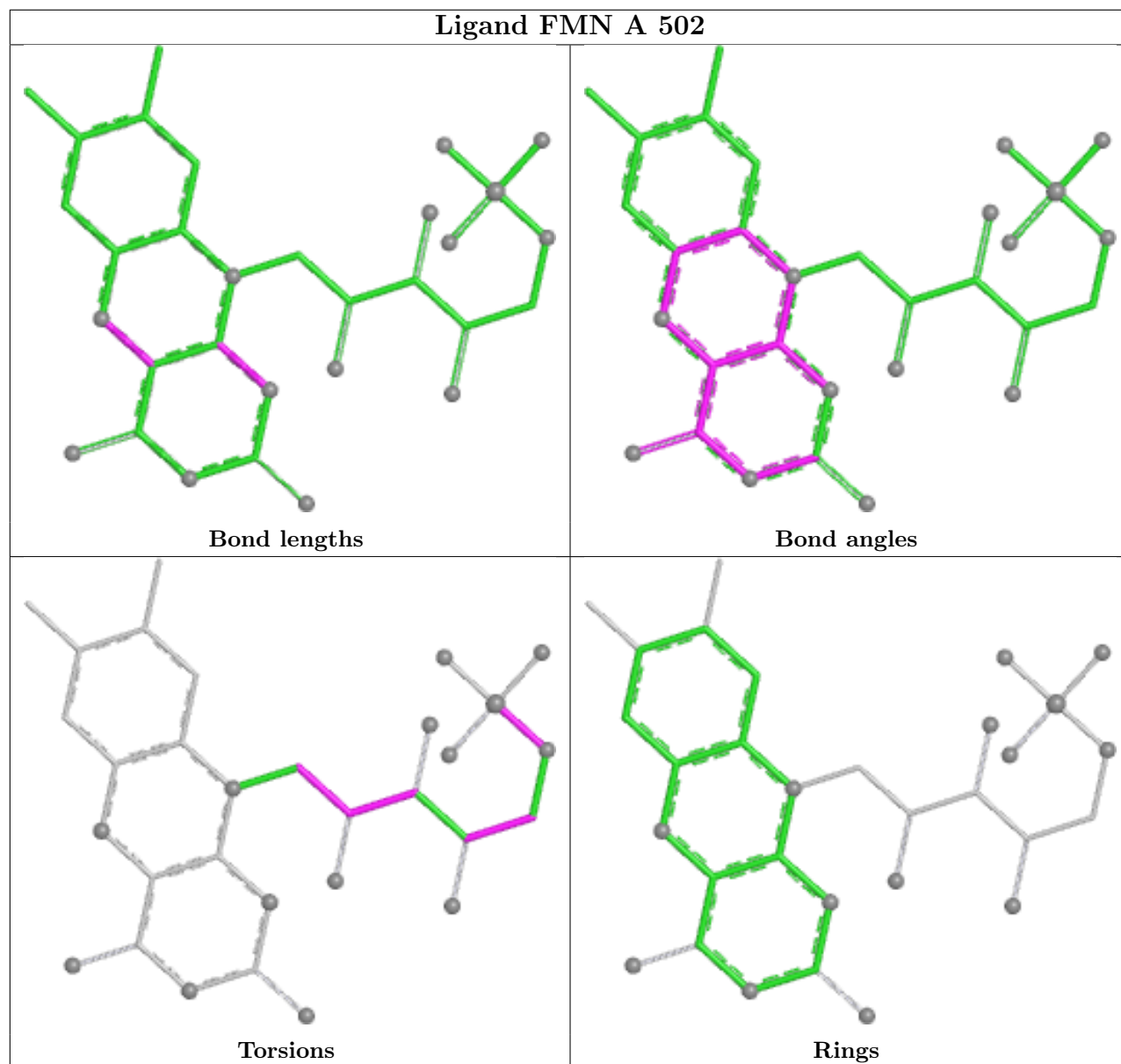
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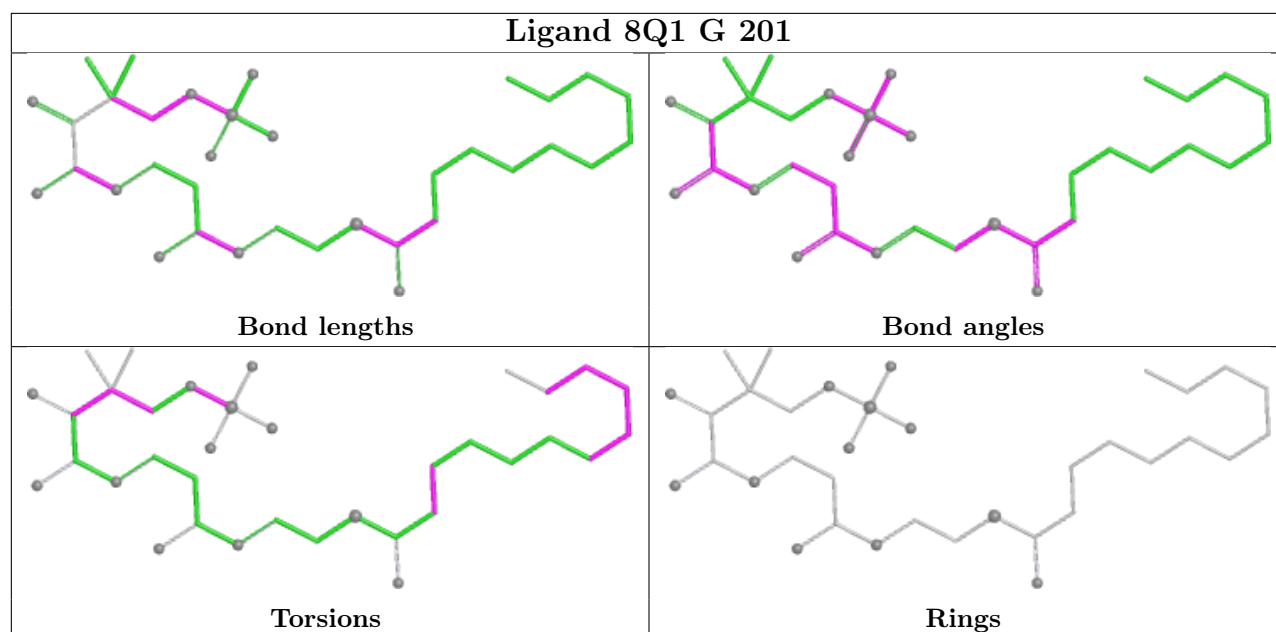
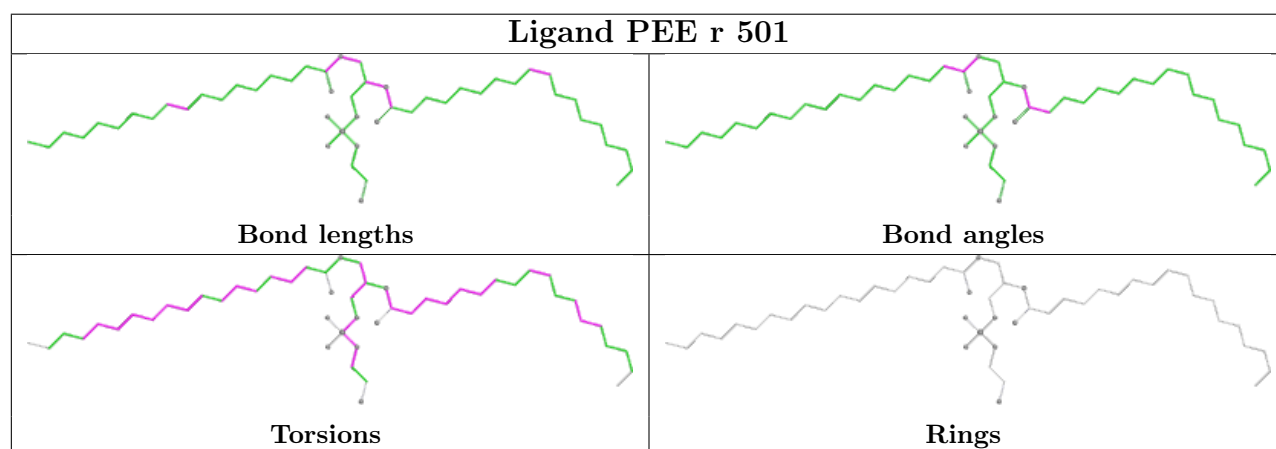
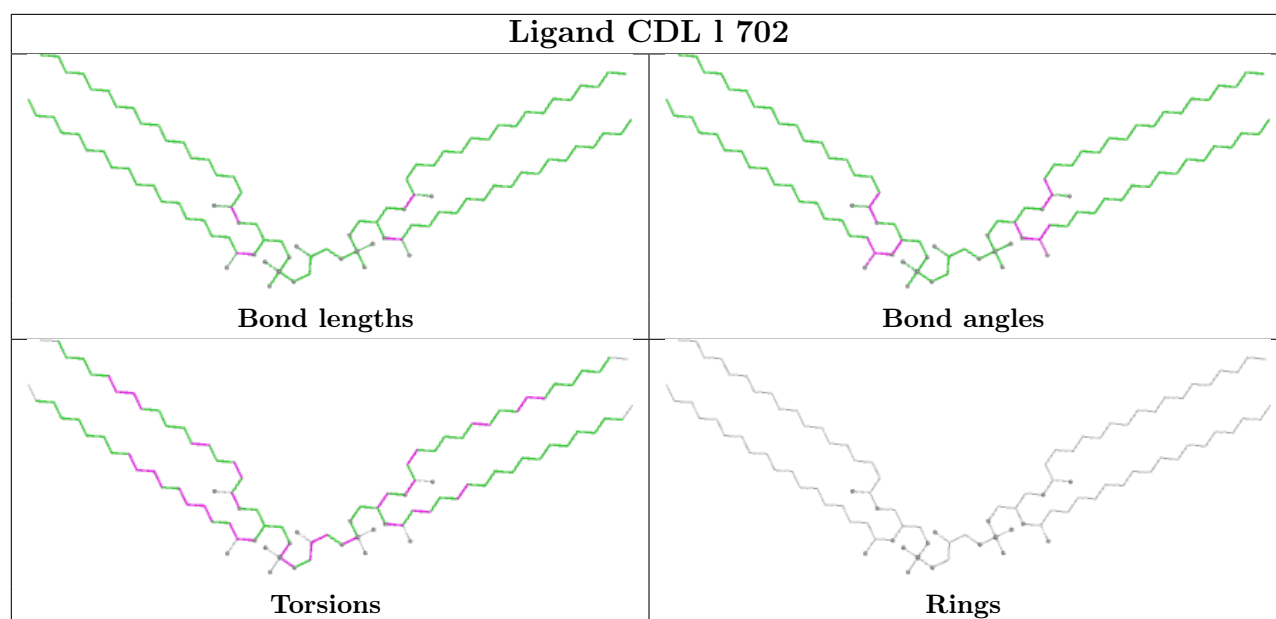
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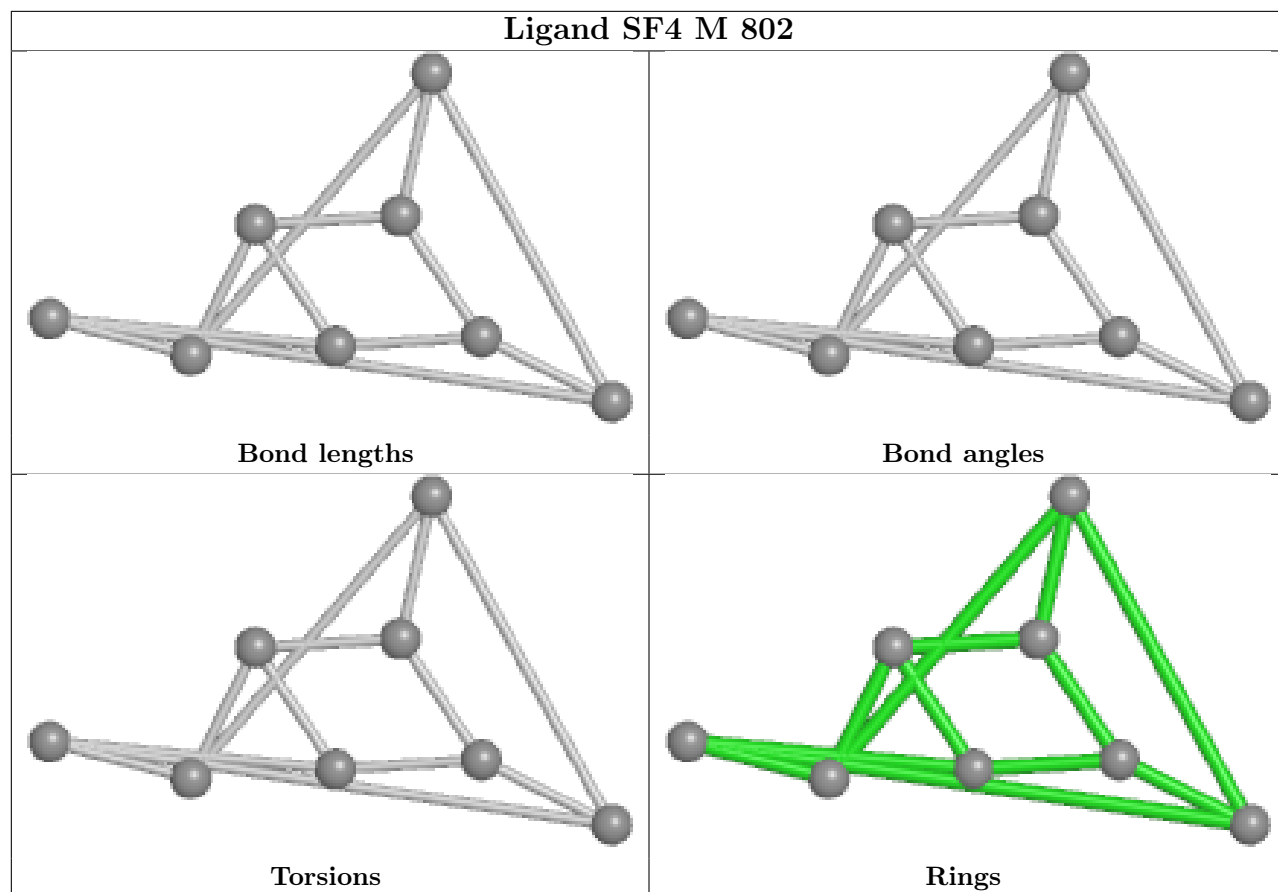
Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	k	101	CDL	5	0
48	U	101	PEE	18	0
48	l	703	PEE	21	0
53	s	401	UQ	6	0
47	A	503	NAI	5	0
49	j	202	PLX	3	0
51	l	701	CDL	34	0
49	r	503	PLX	6	0
51	m	201	CDL	5	0
58	w	401	ADP	8	0
48	j	201	PEE	15	0

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.

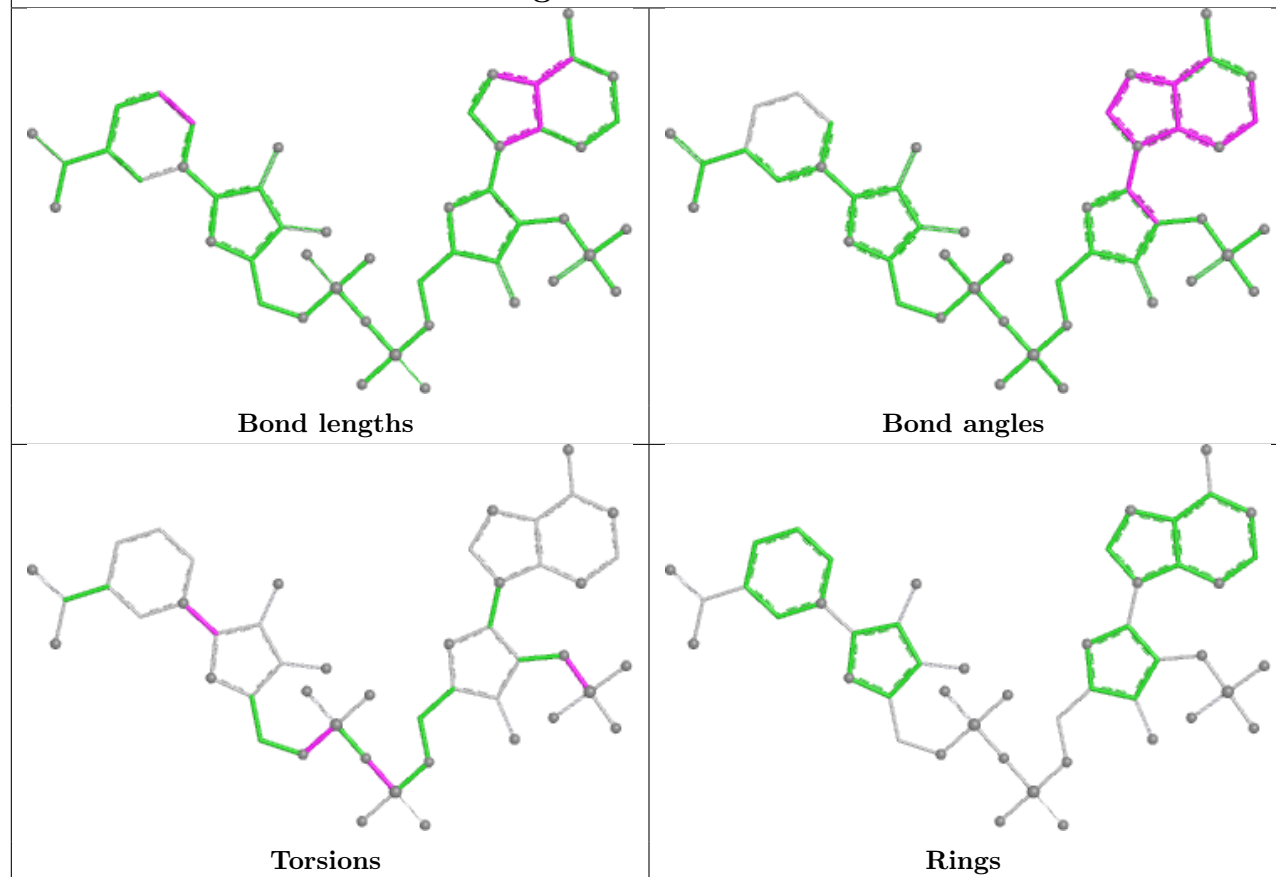




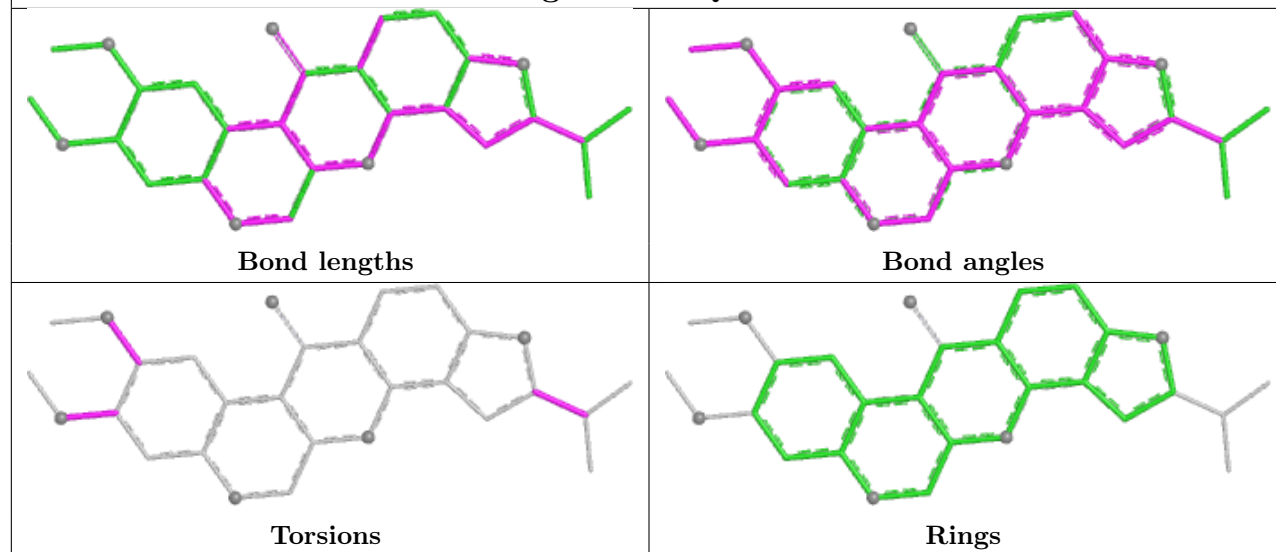


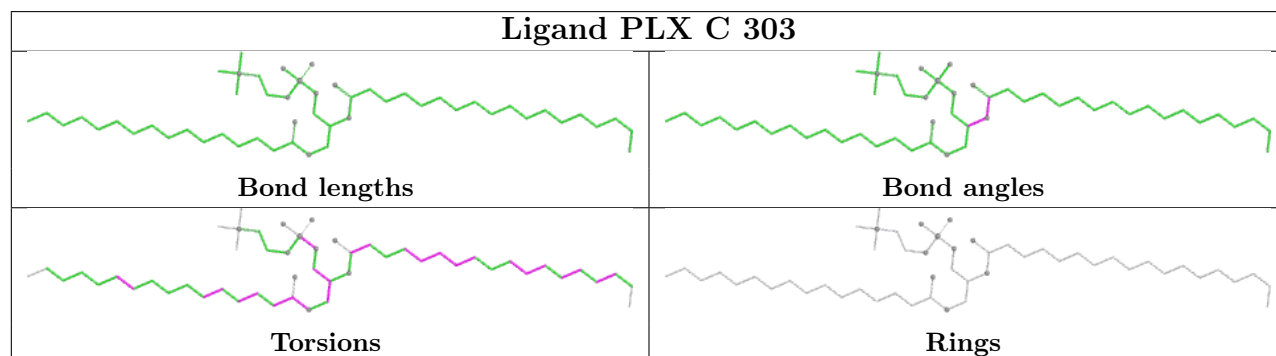
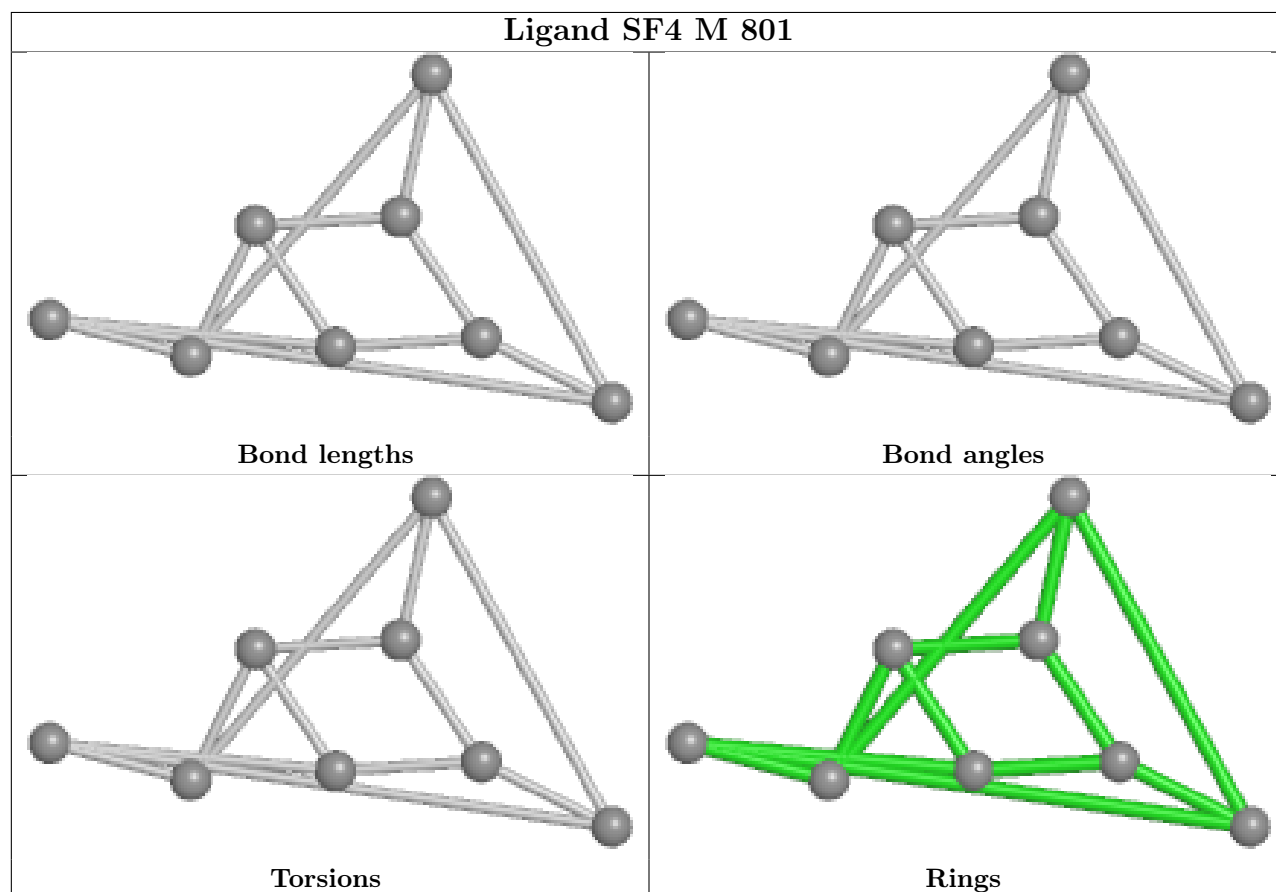
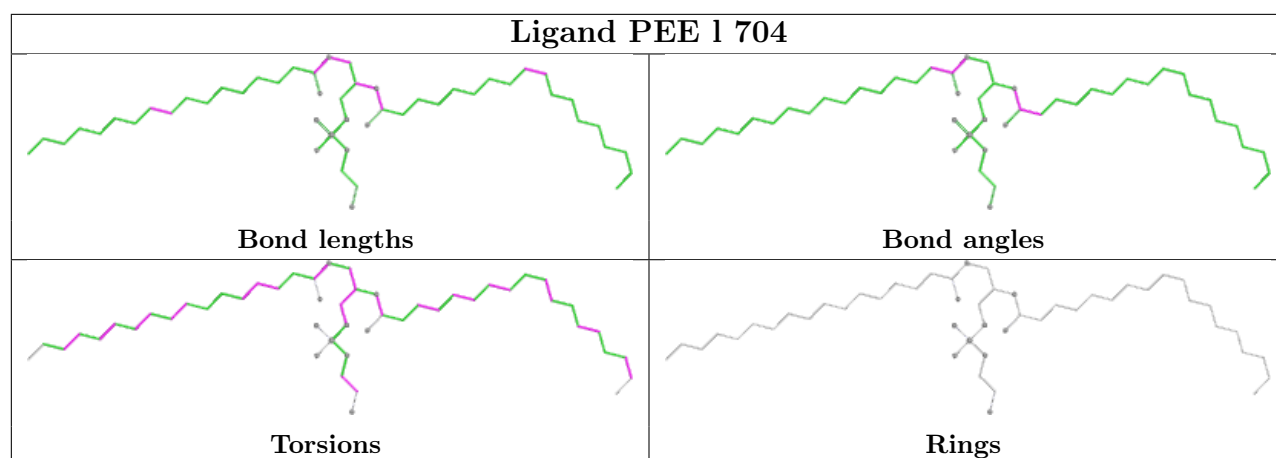


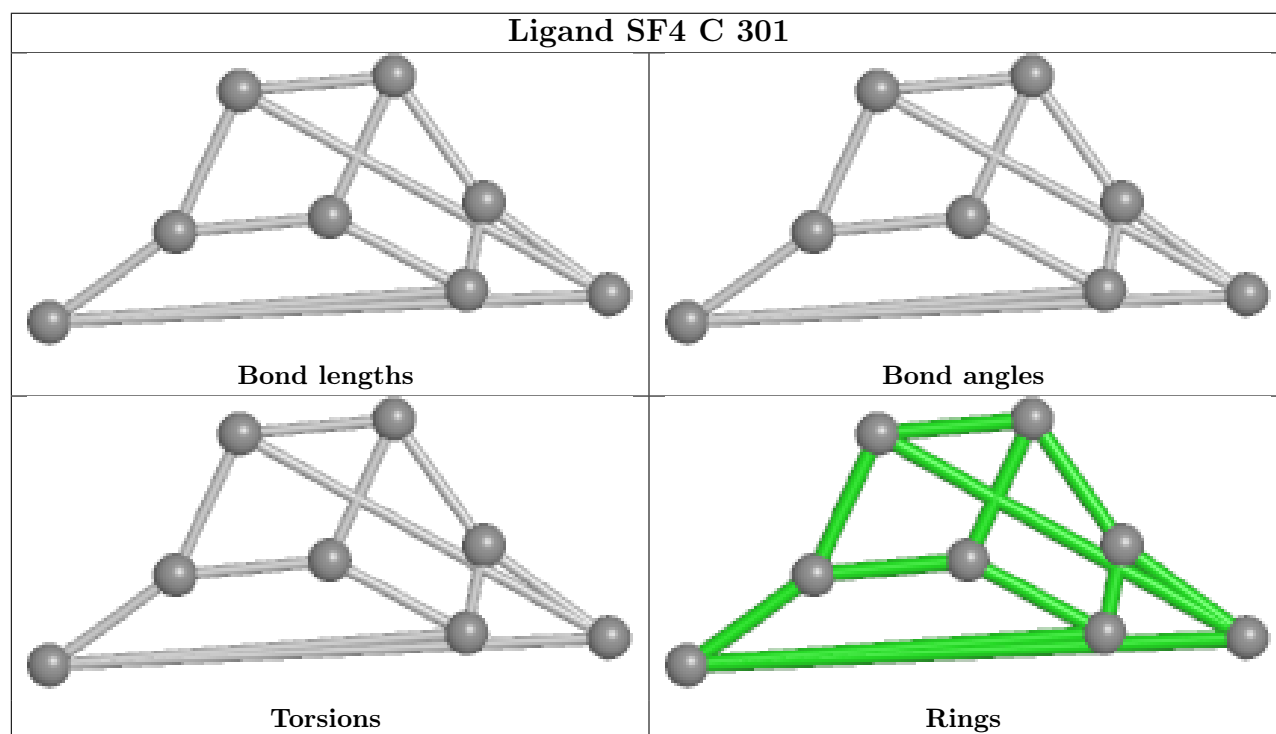
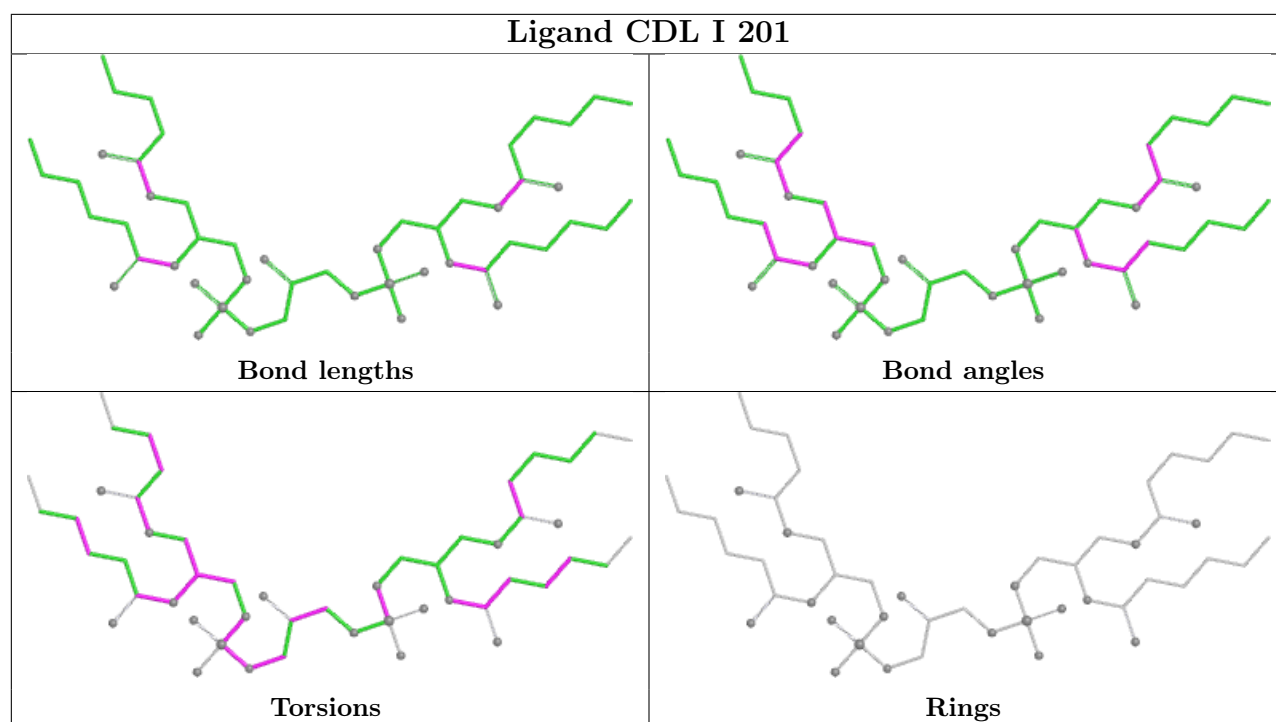
Ligand NDP J 401

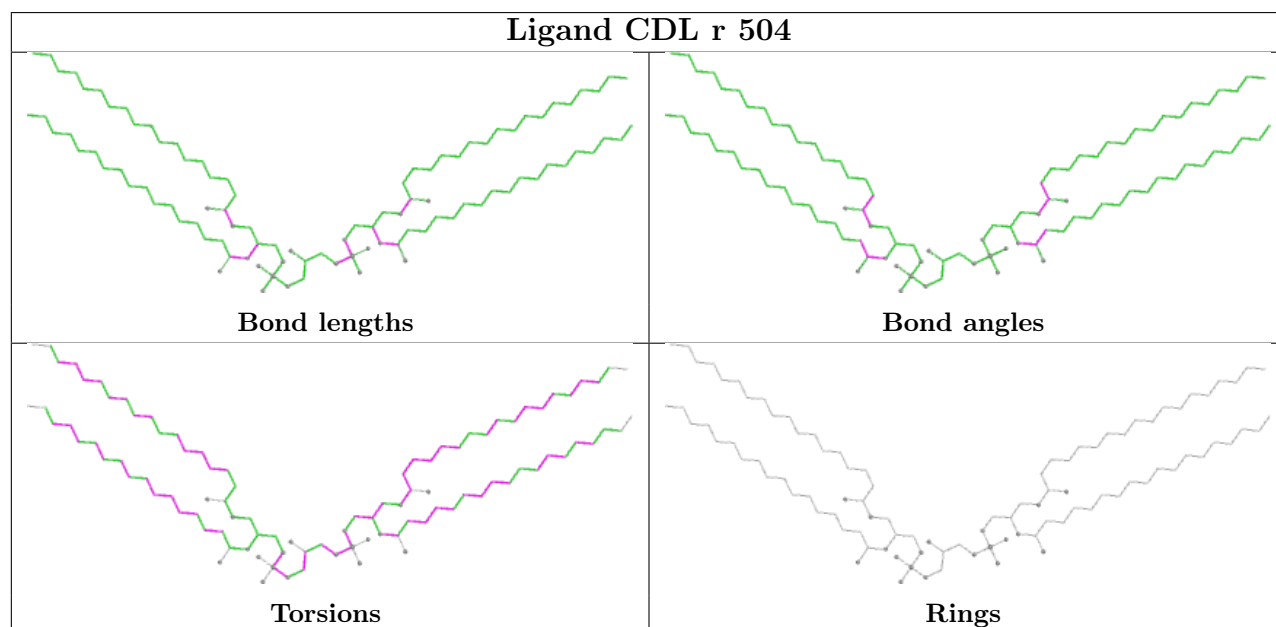
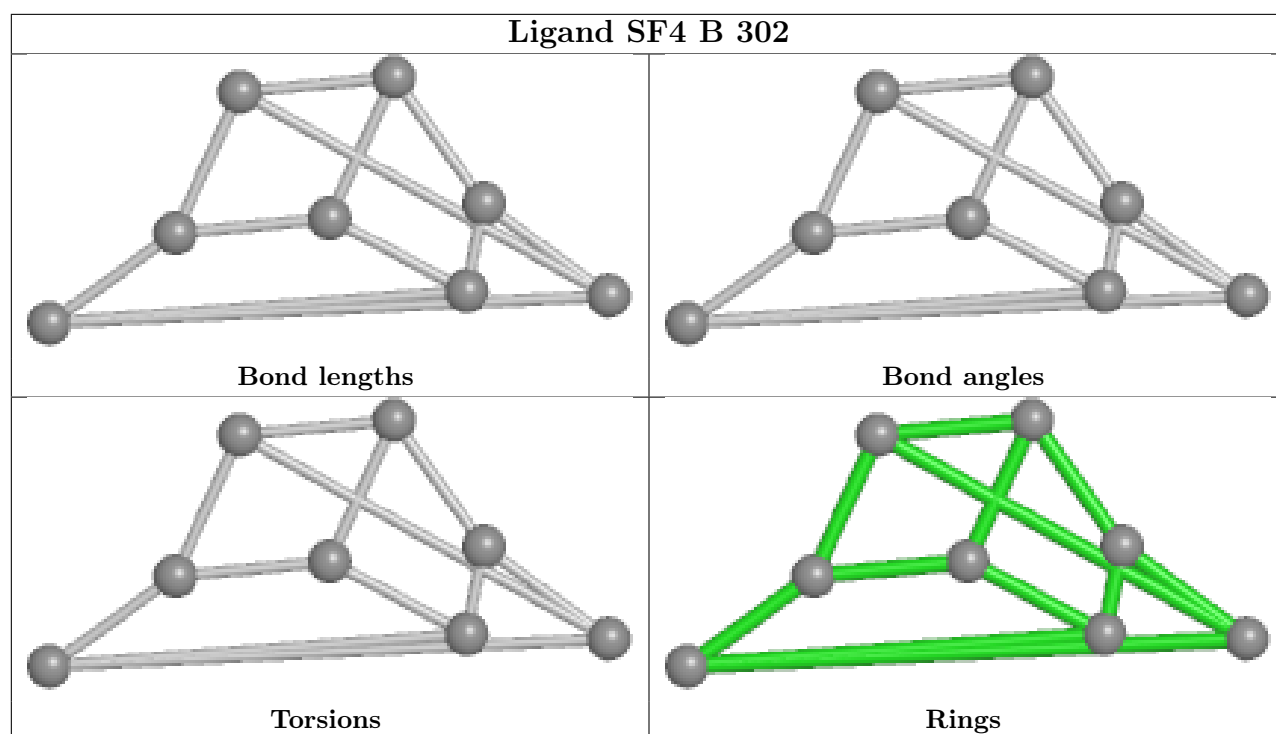


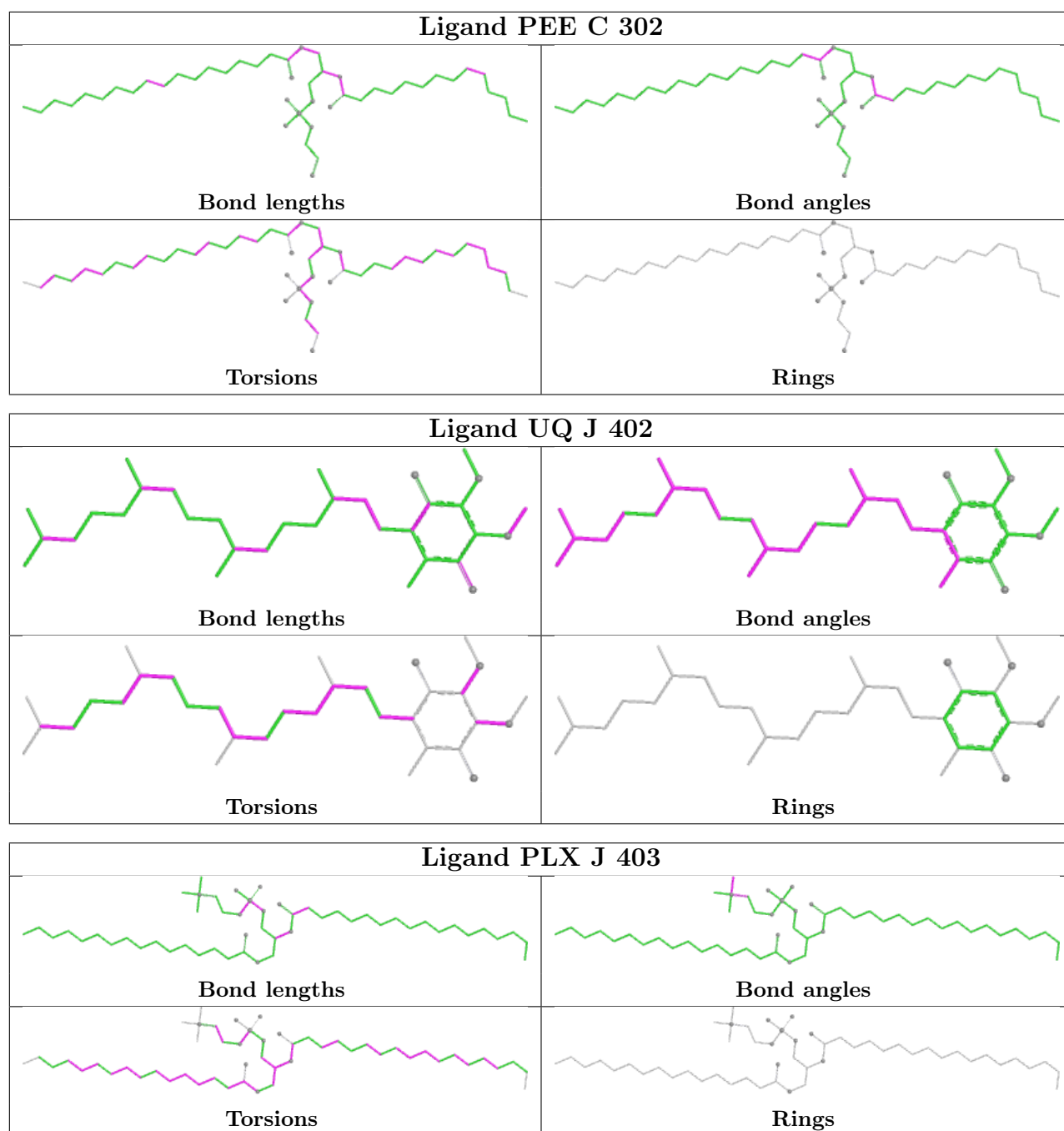
Ligand 970 Q 501

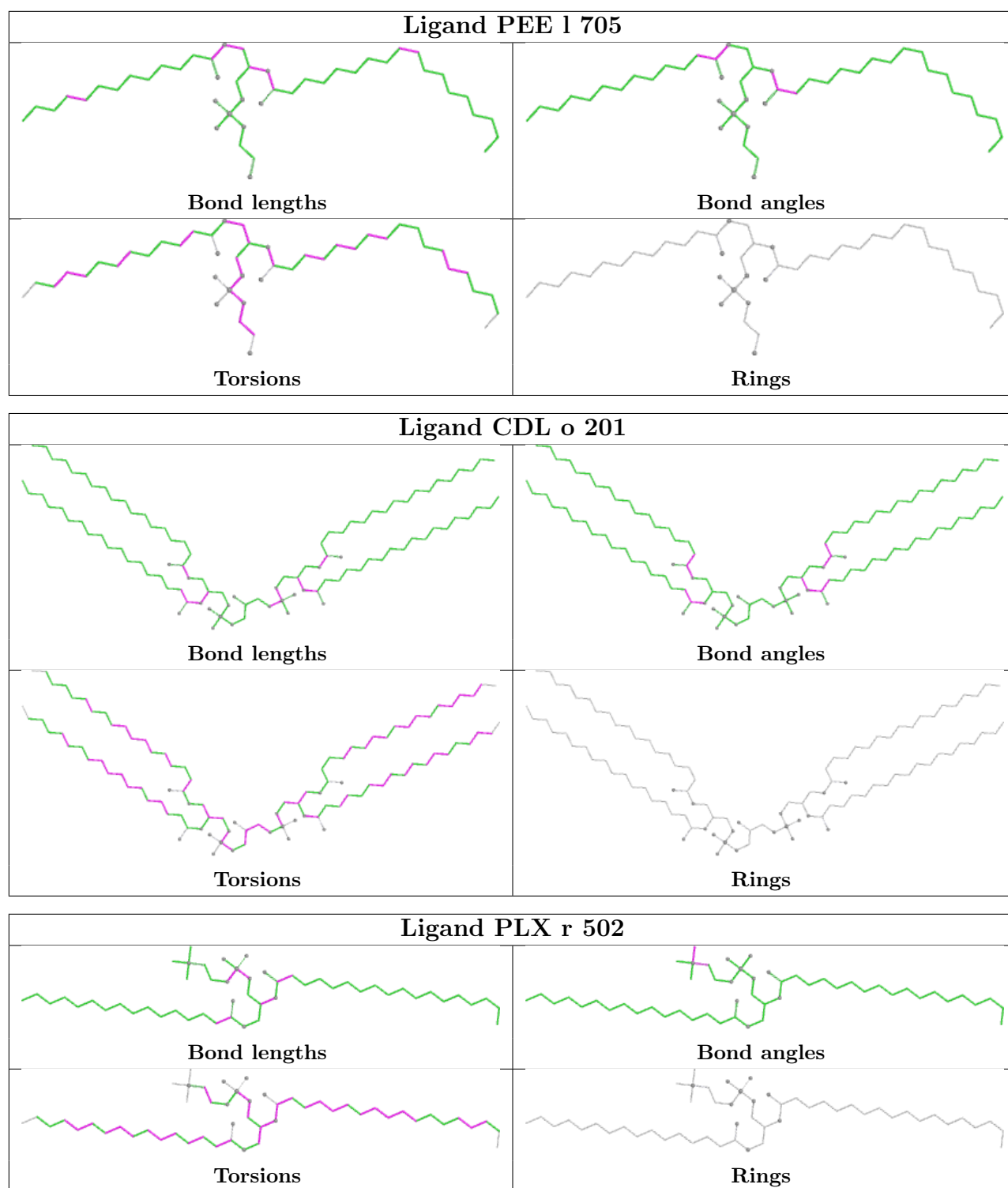


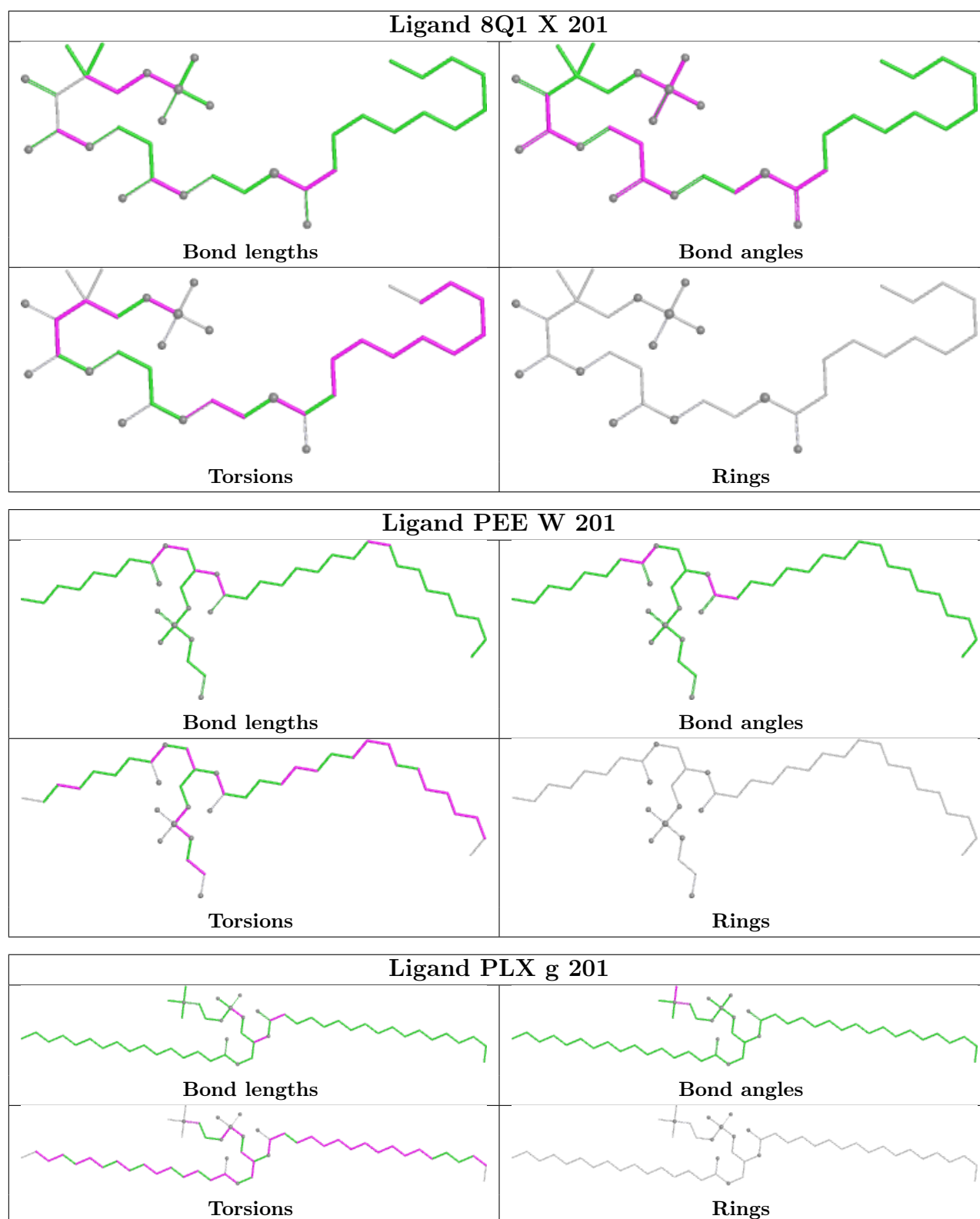


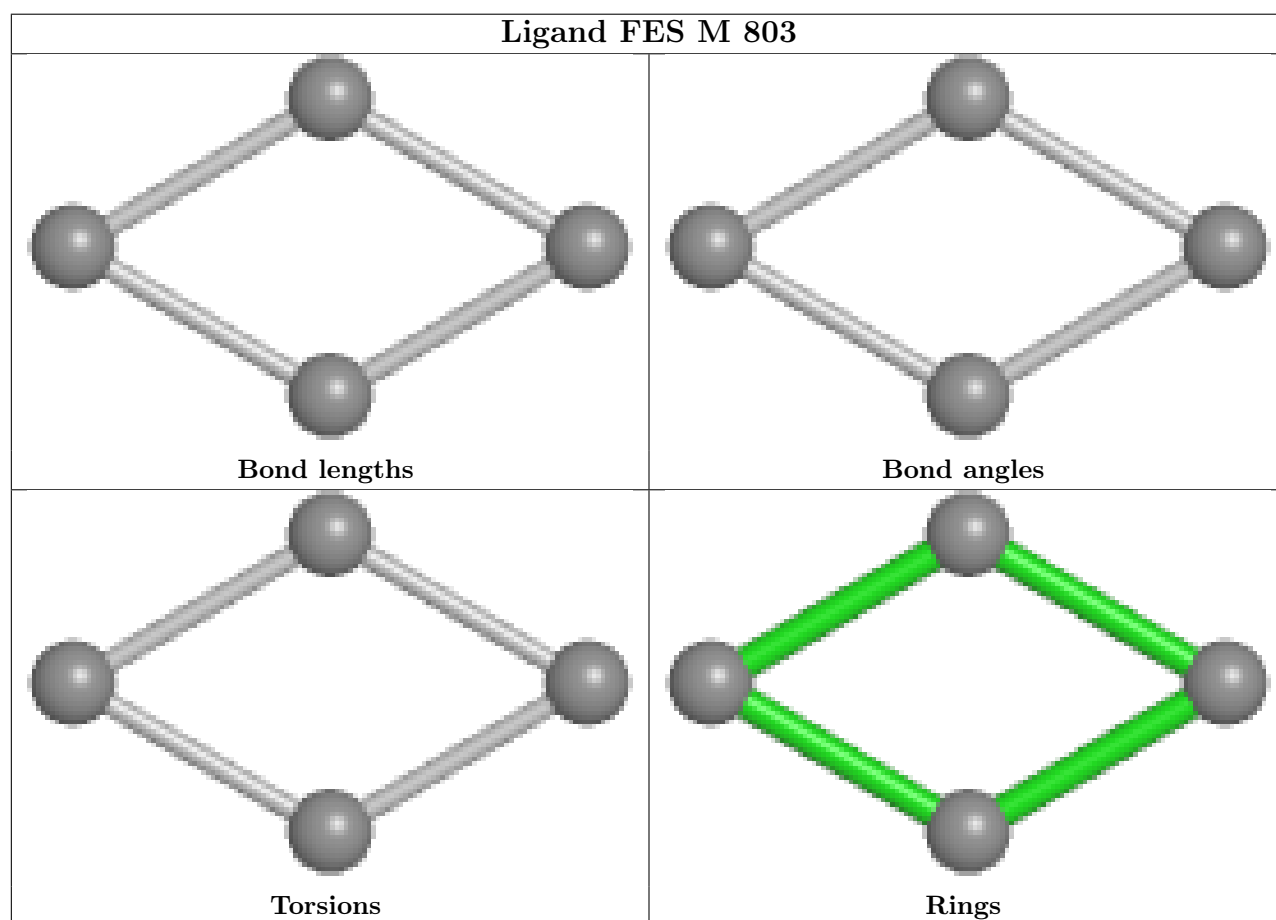
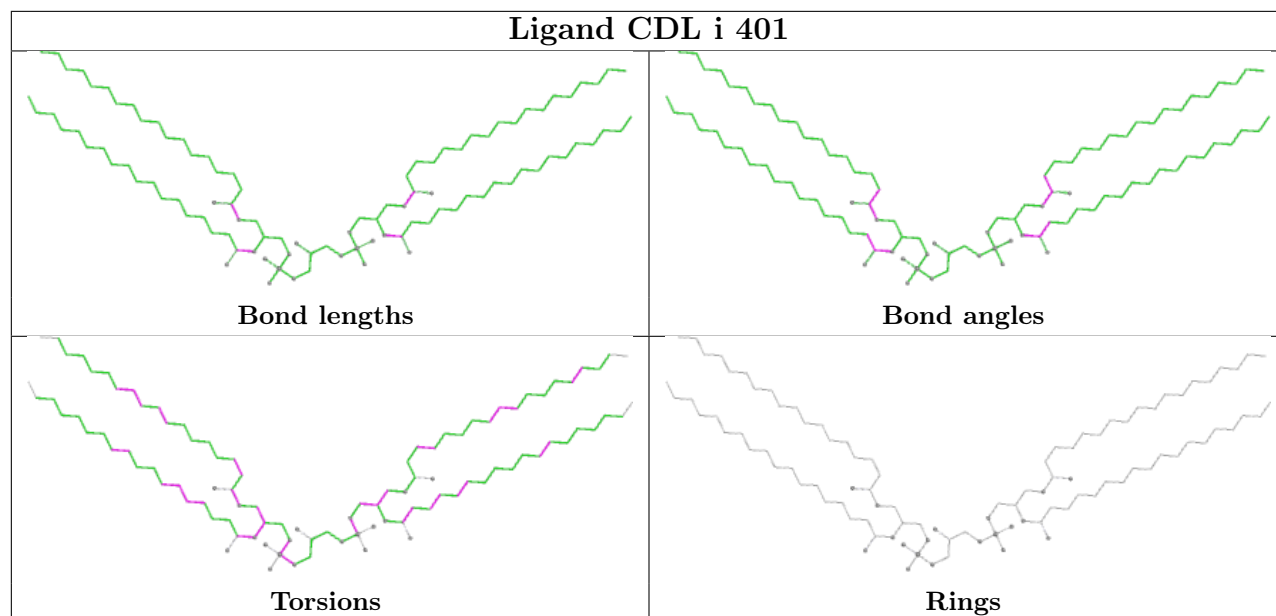


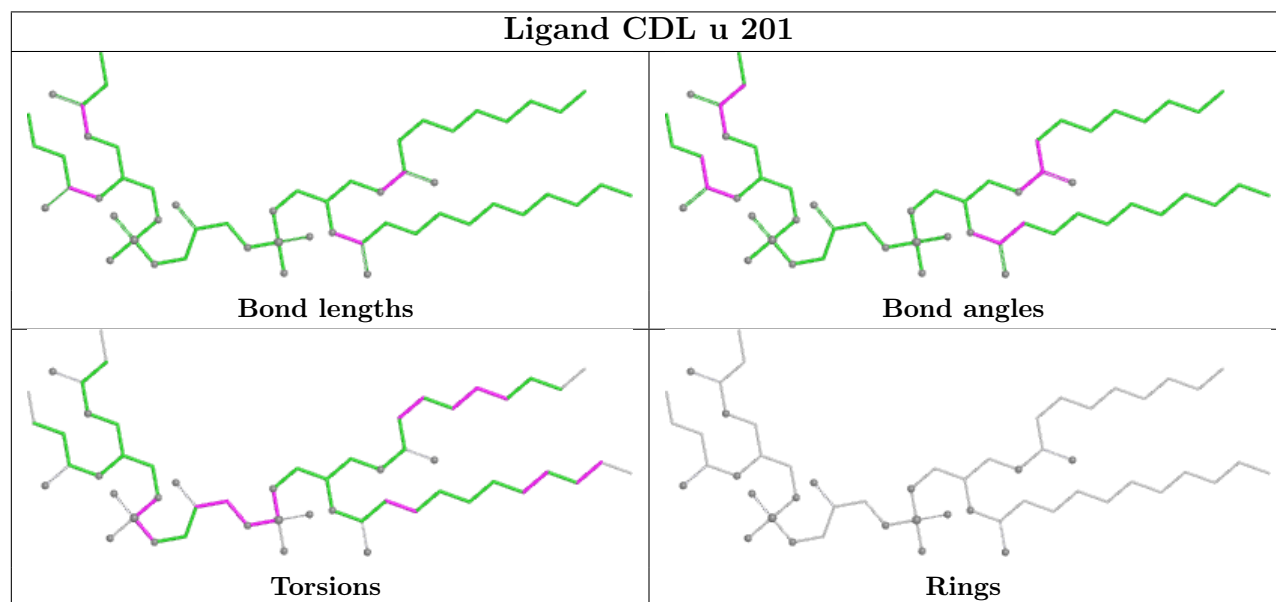
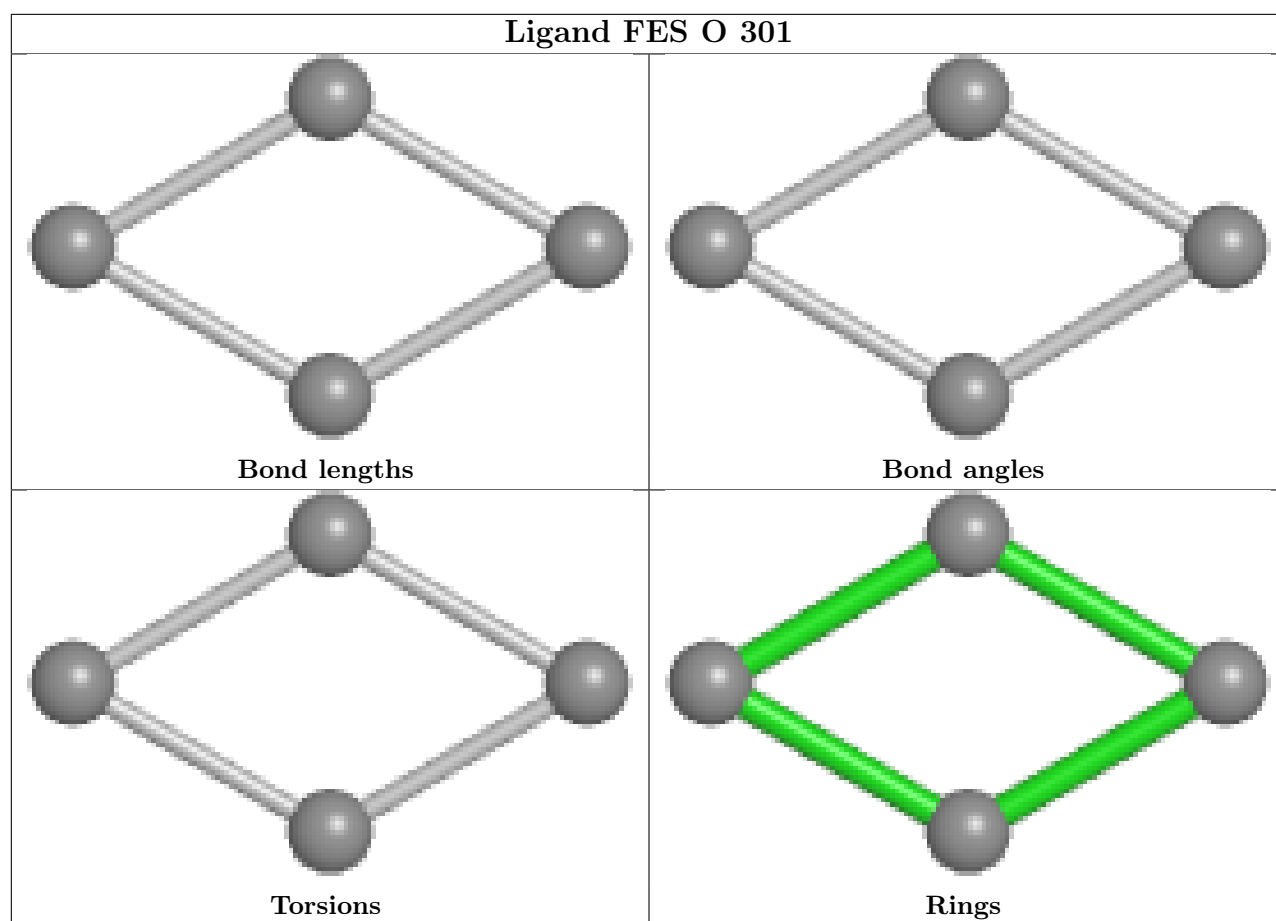


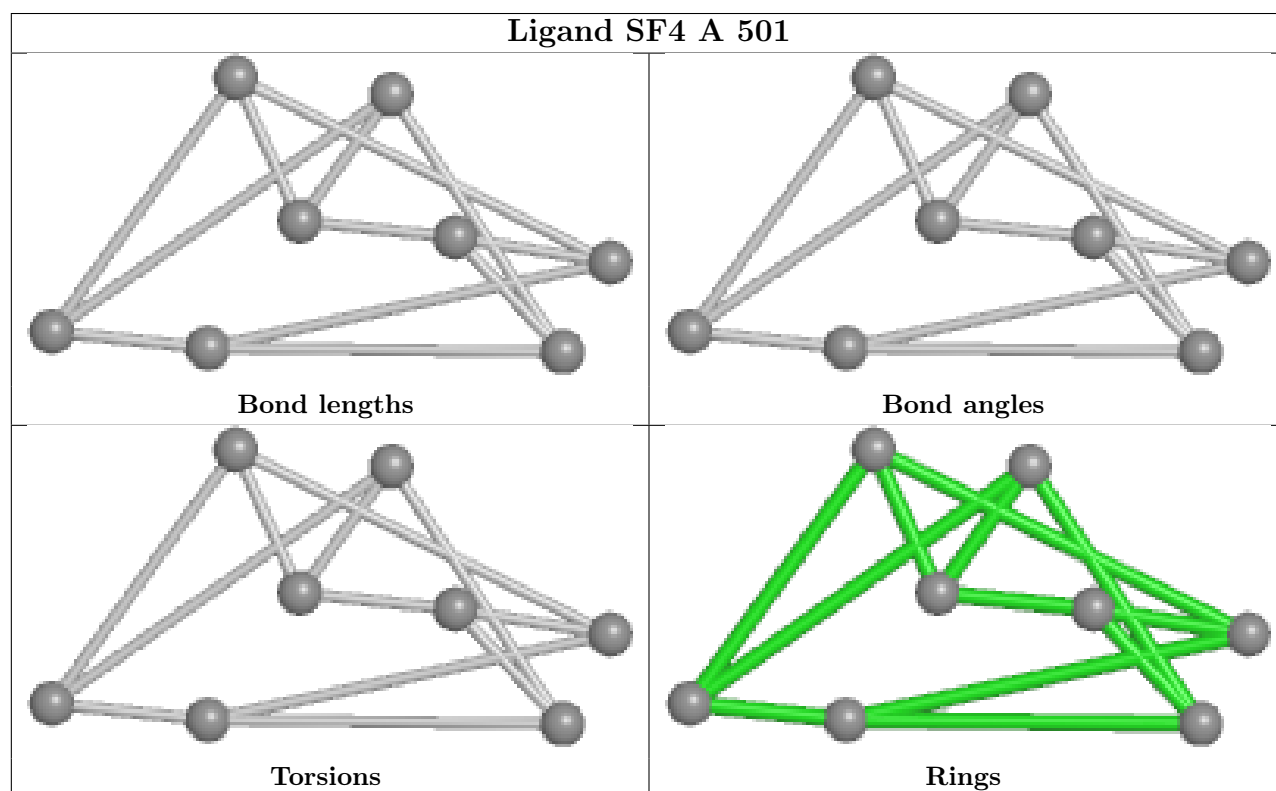
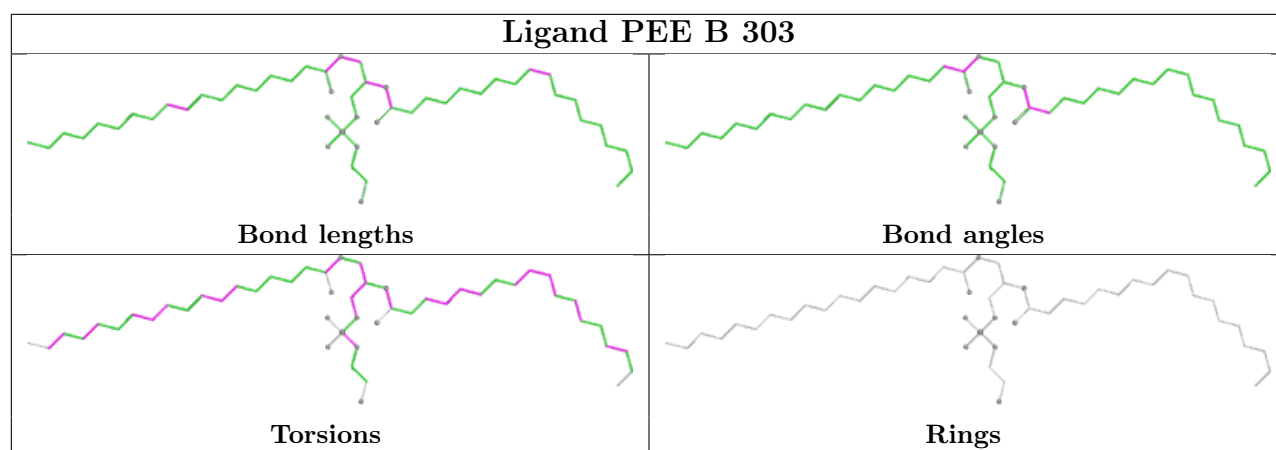


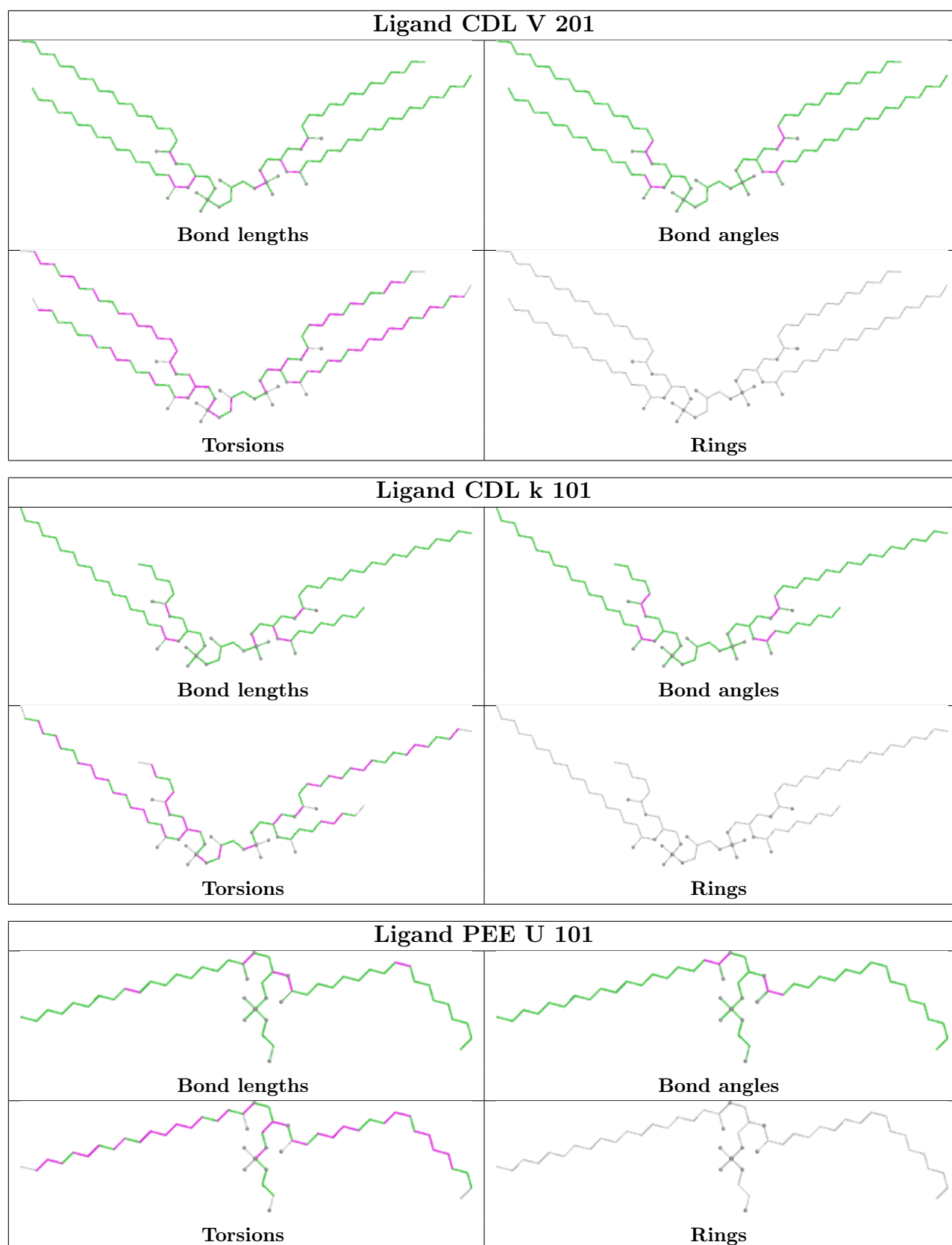


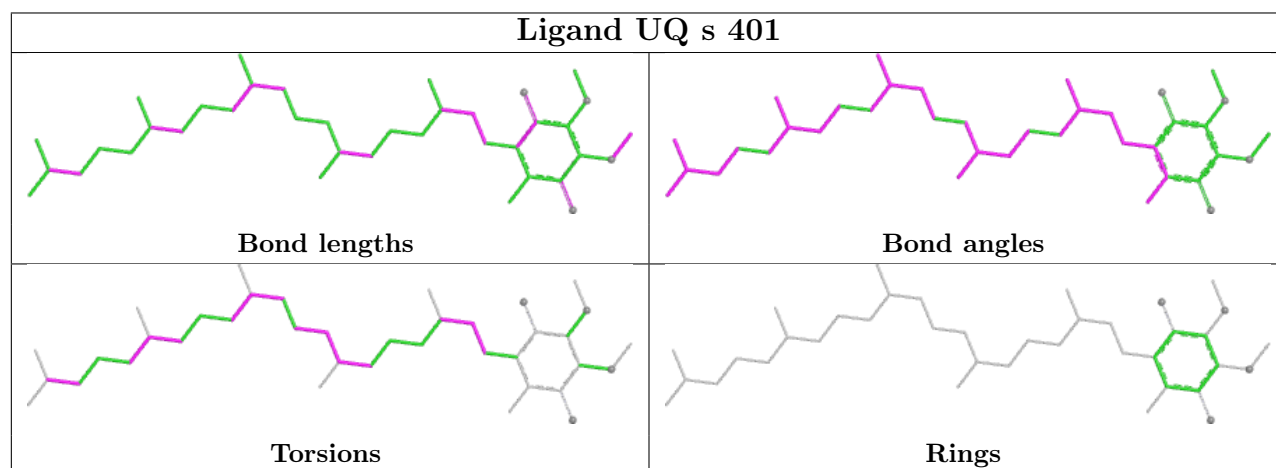
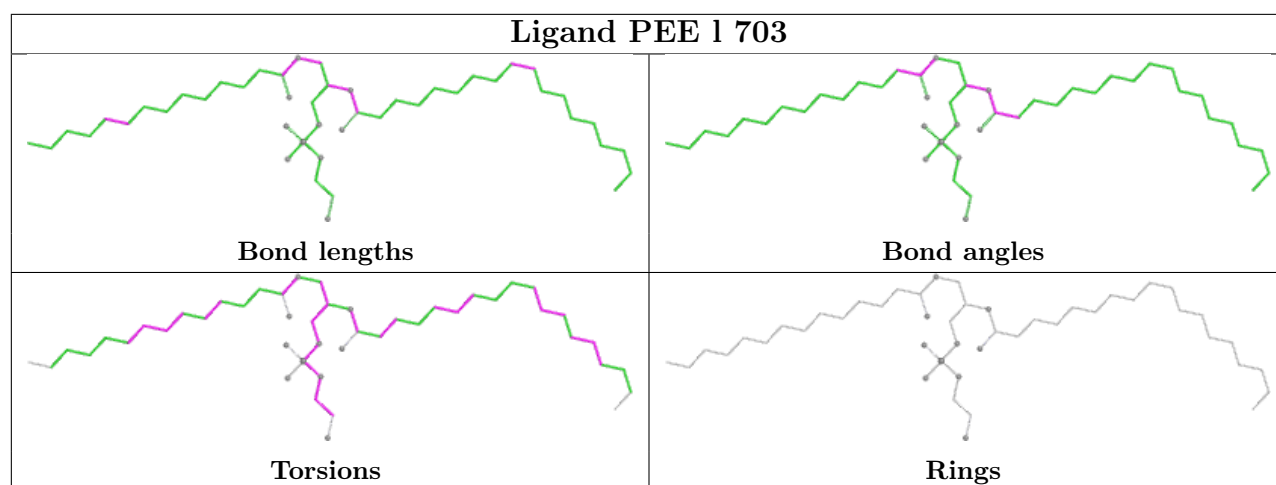


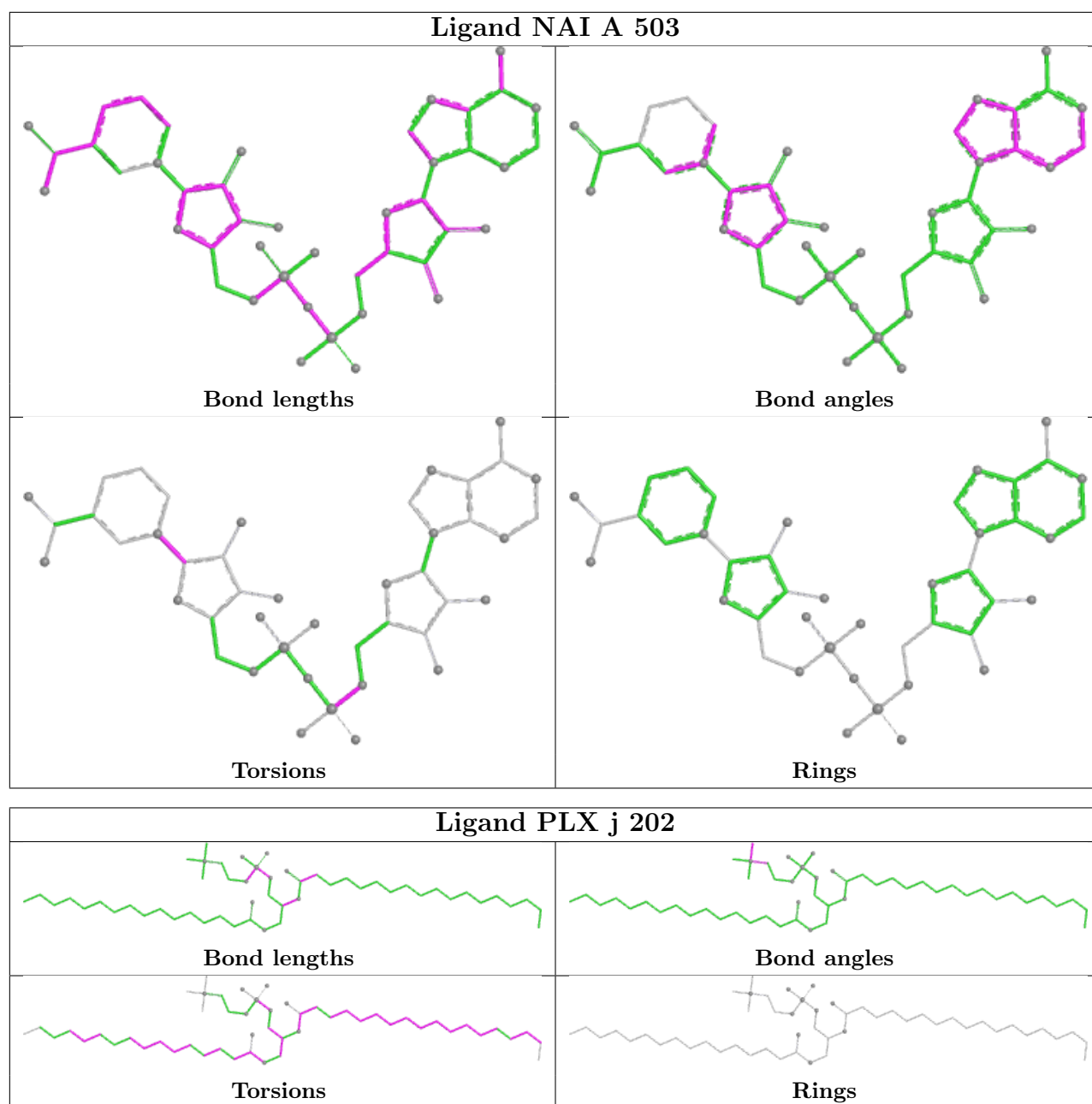


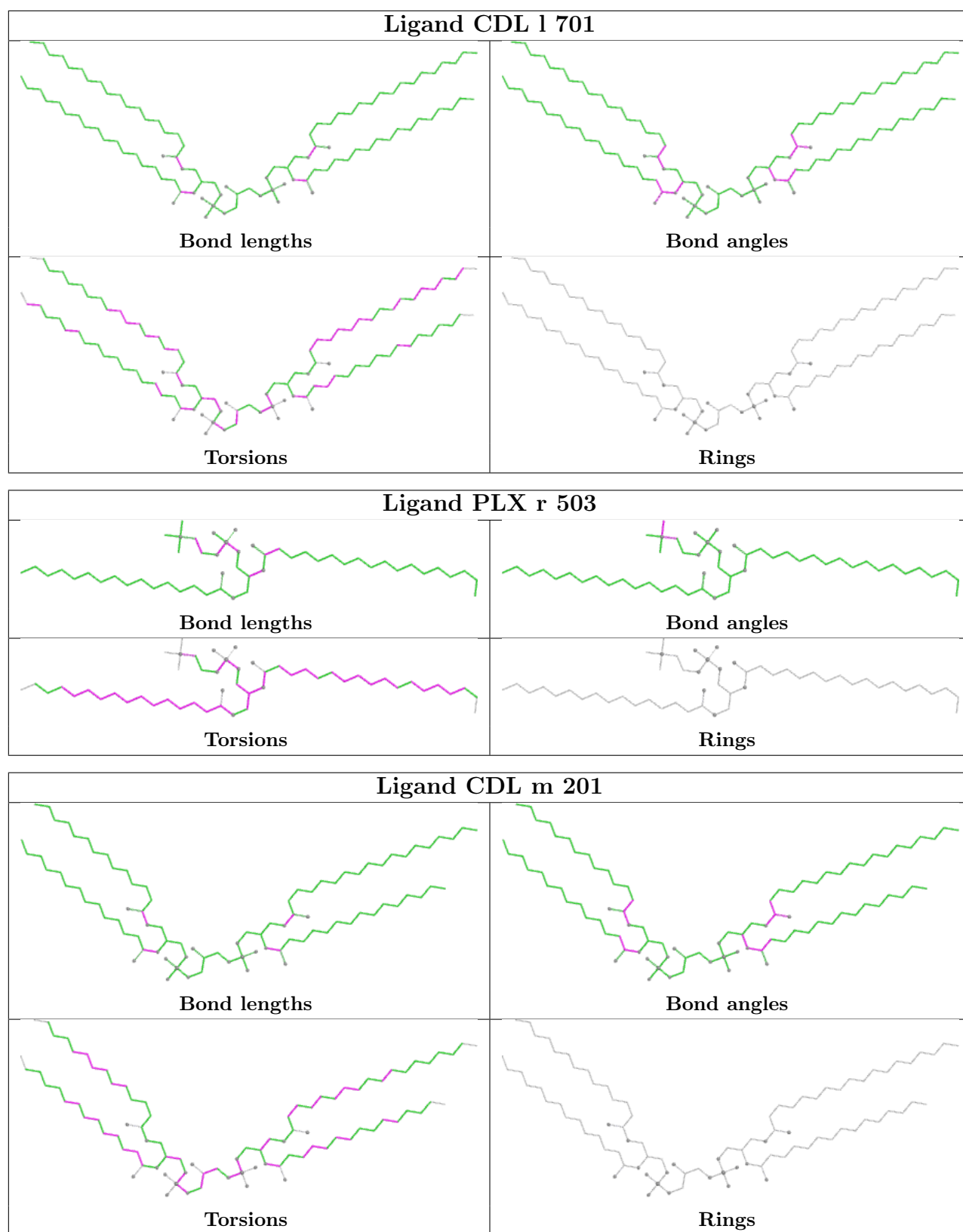


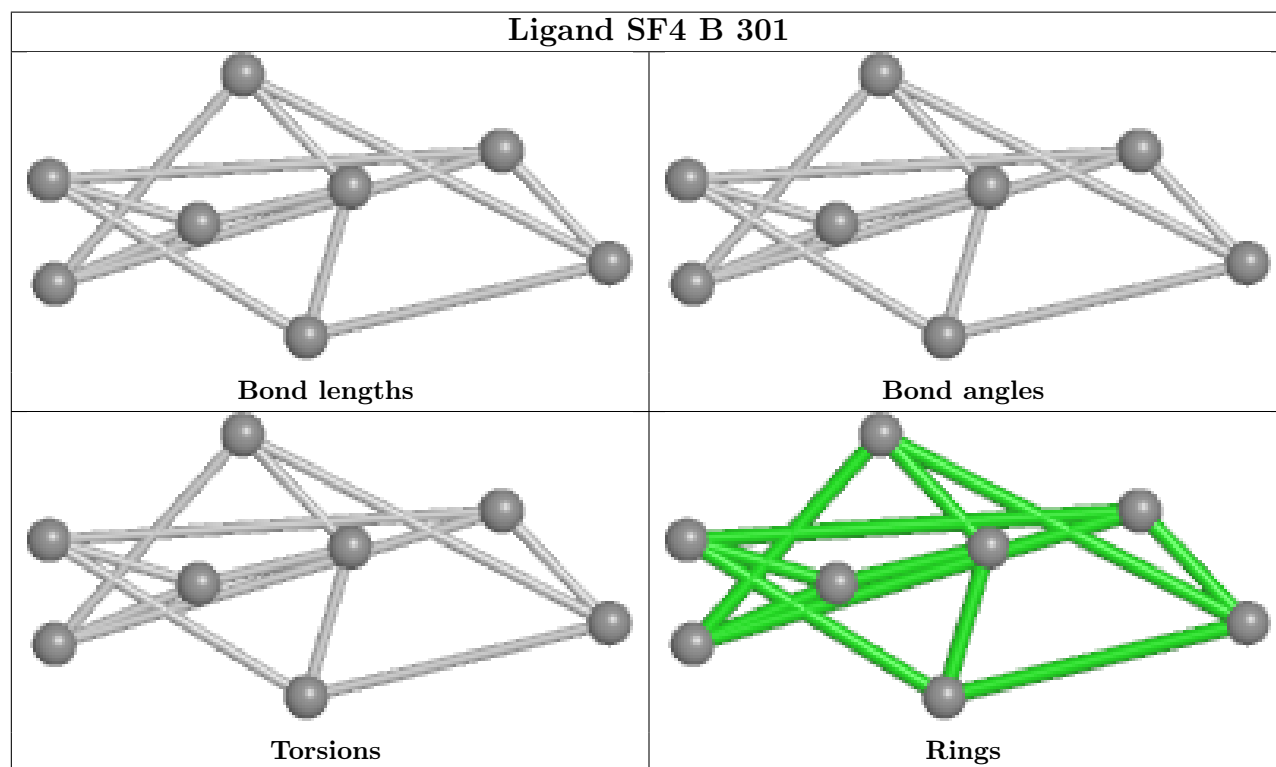
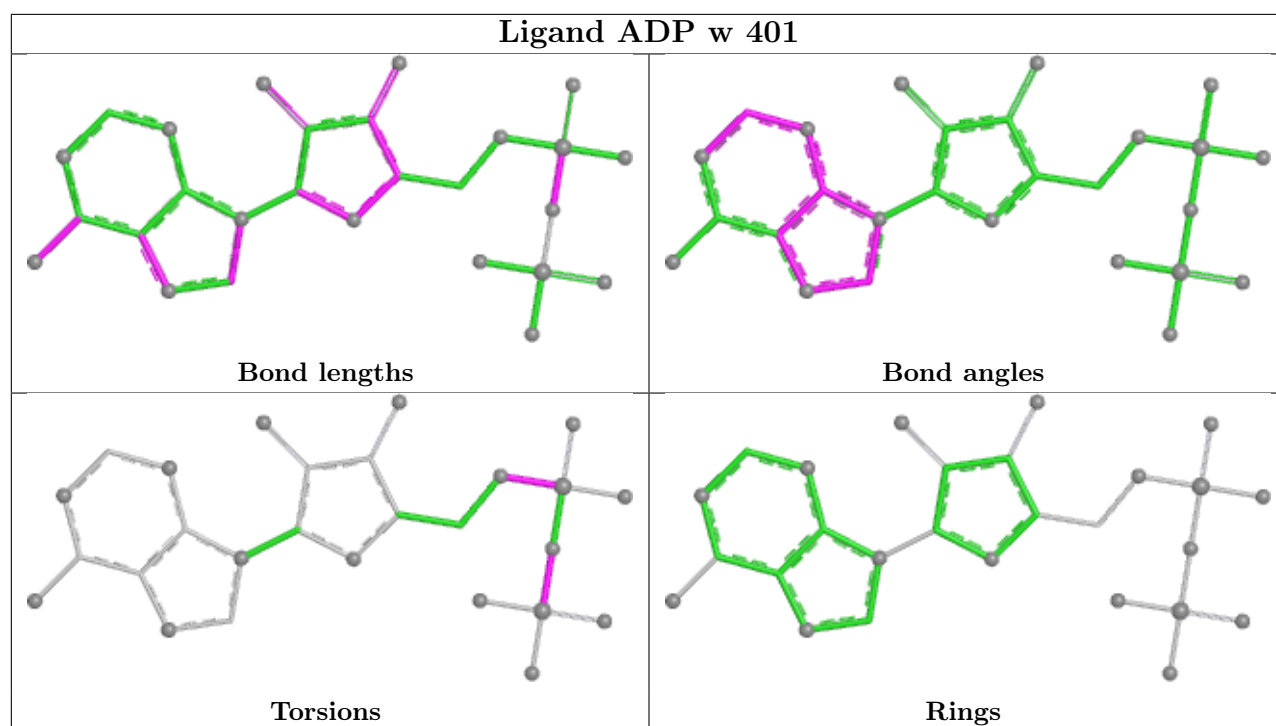


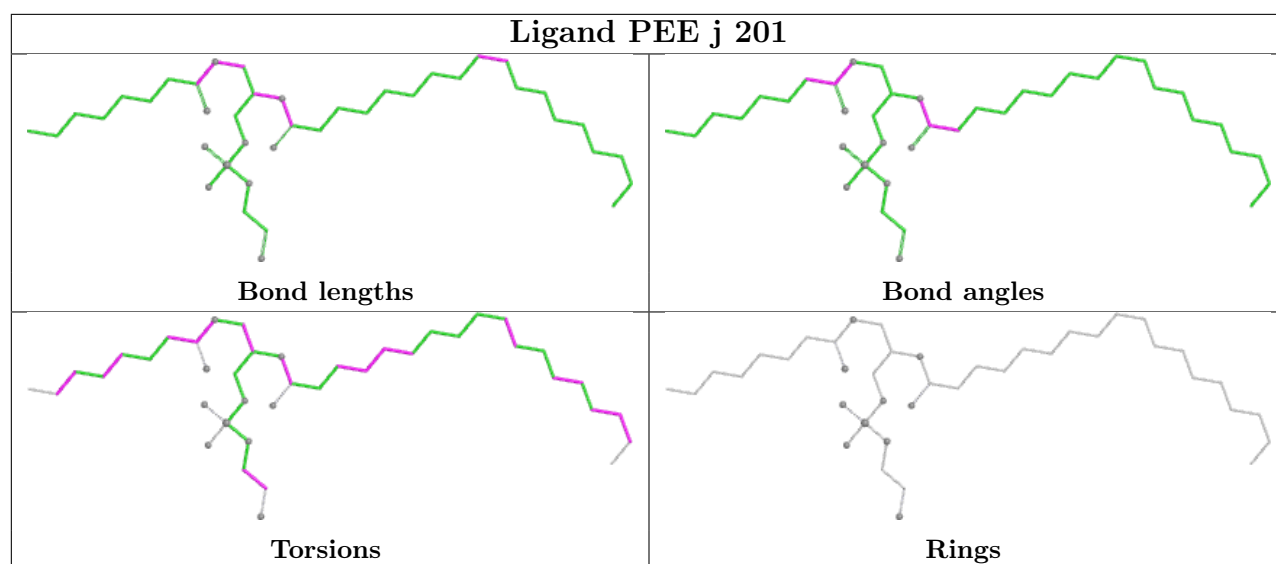












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

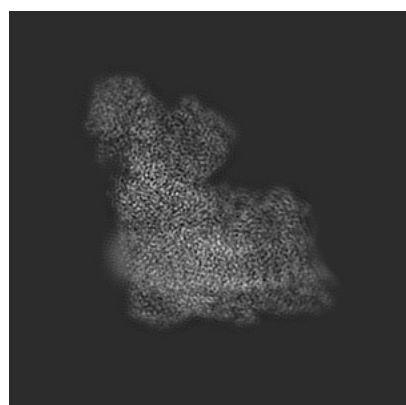
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31651. These allow visual inspection of the internal detail of the map and identification of artifacts.

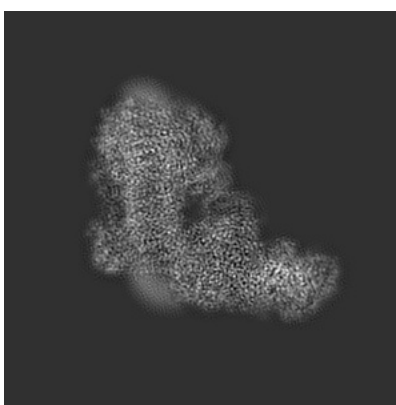
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

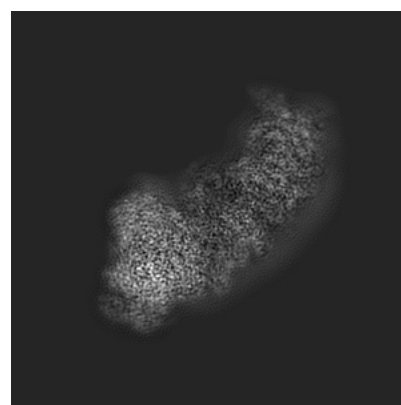
6.1.1 Primary map



X



Y

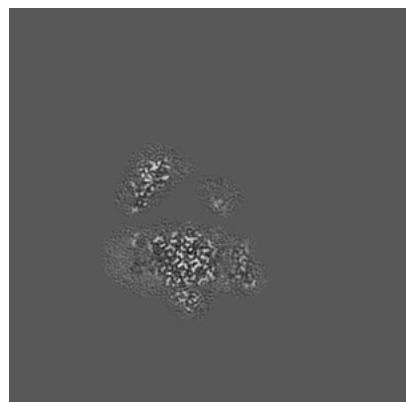


Z

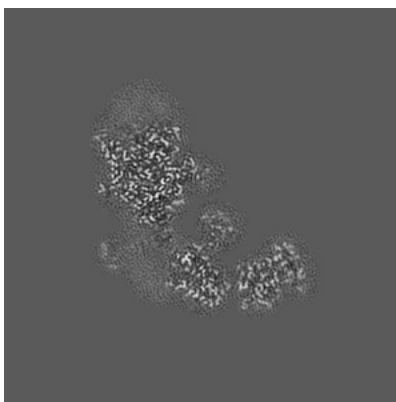
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

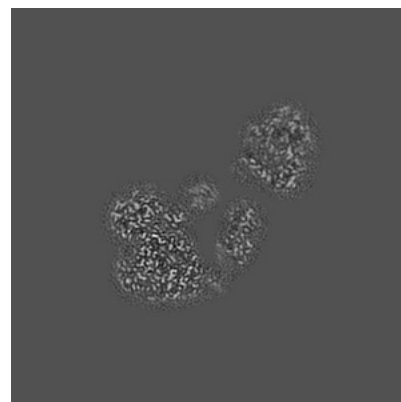
6.2.1 Primary map



X Index: 155



Y Index: 155

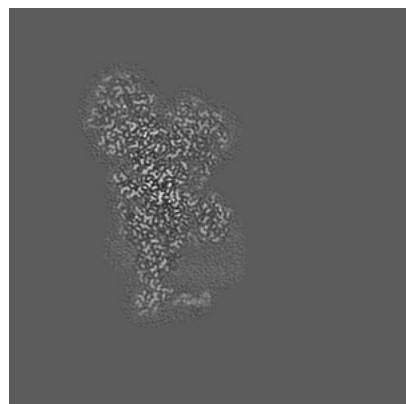


Z Index: 155

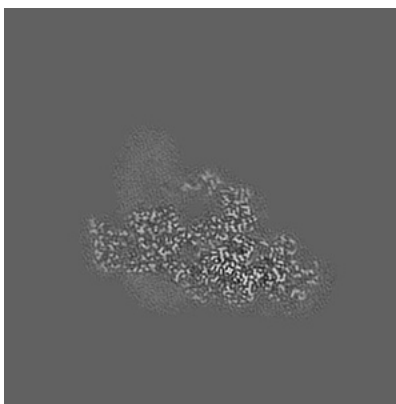
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

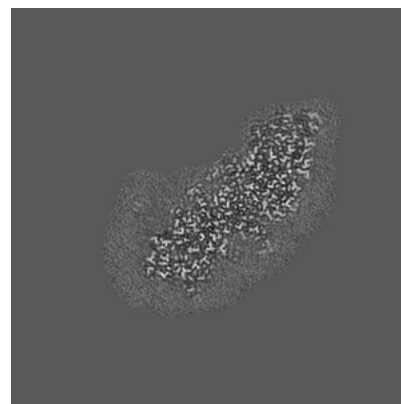
6.3.1 Primary map



X Index: 109



Y Index: 112

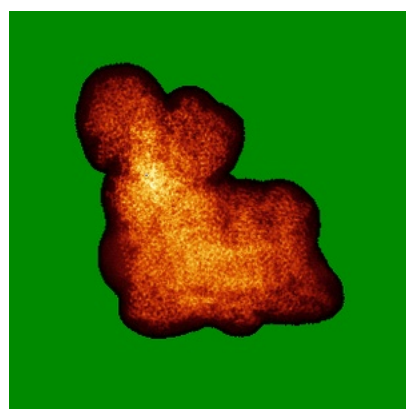


Z Index: 124

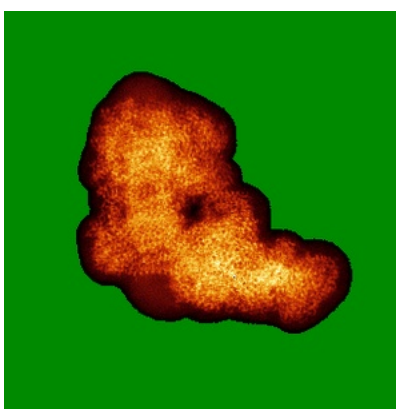
The images above show the largest variance slices of the map in three orthogonal directions.

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

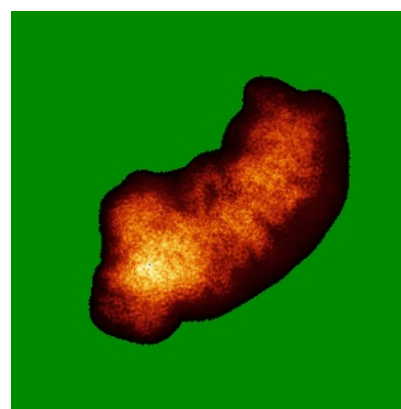
6.4.1 Primary map



X



Y

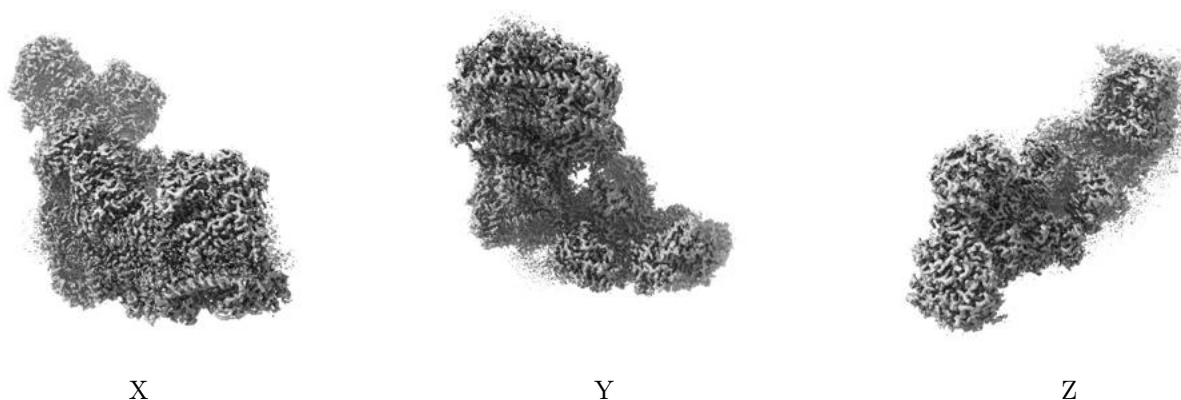


Z

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 0.0271. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

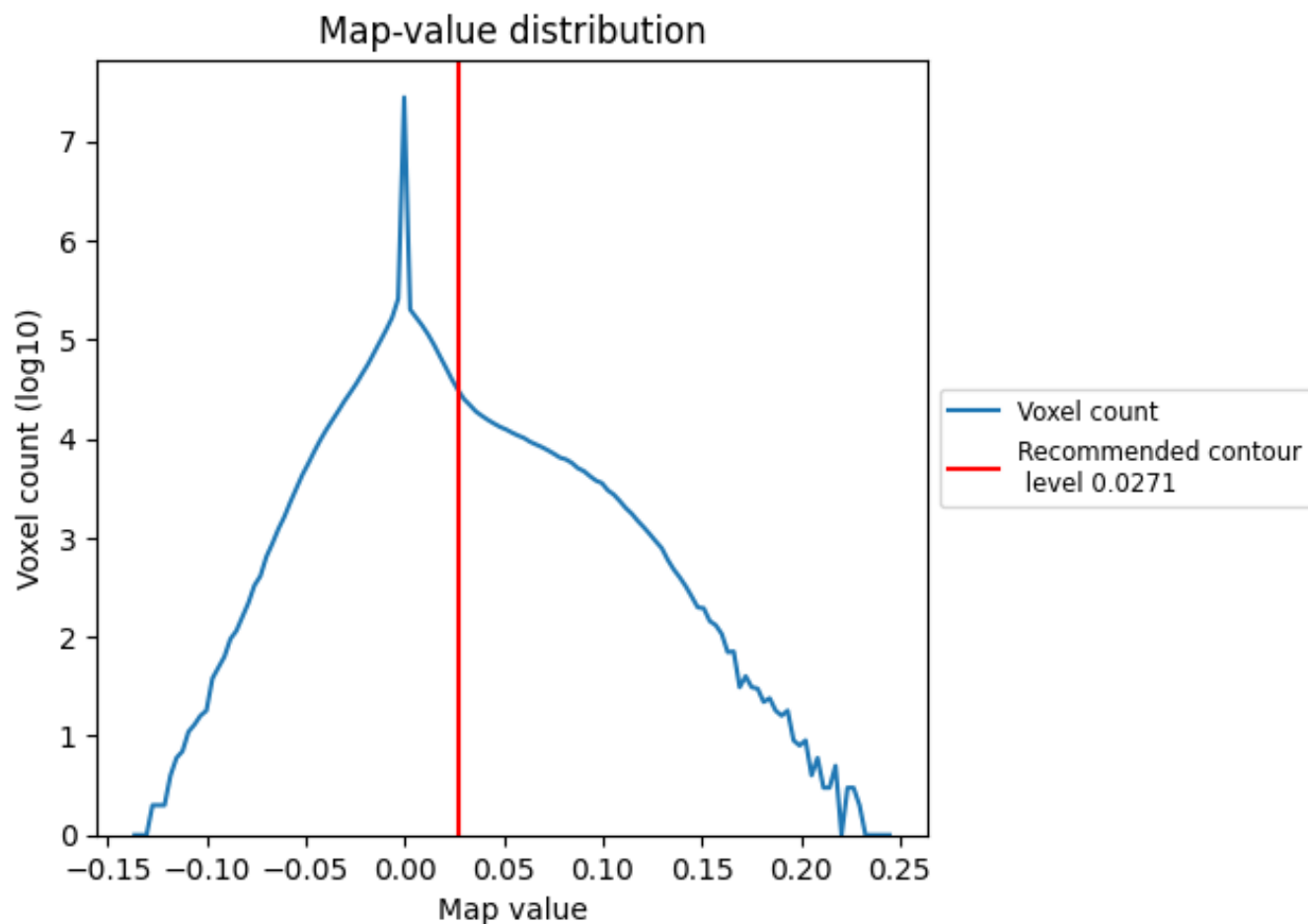
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

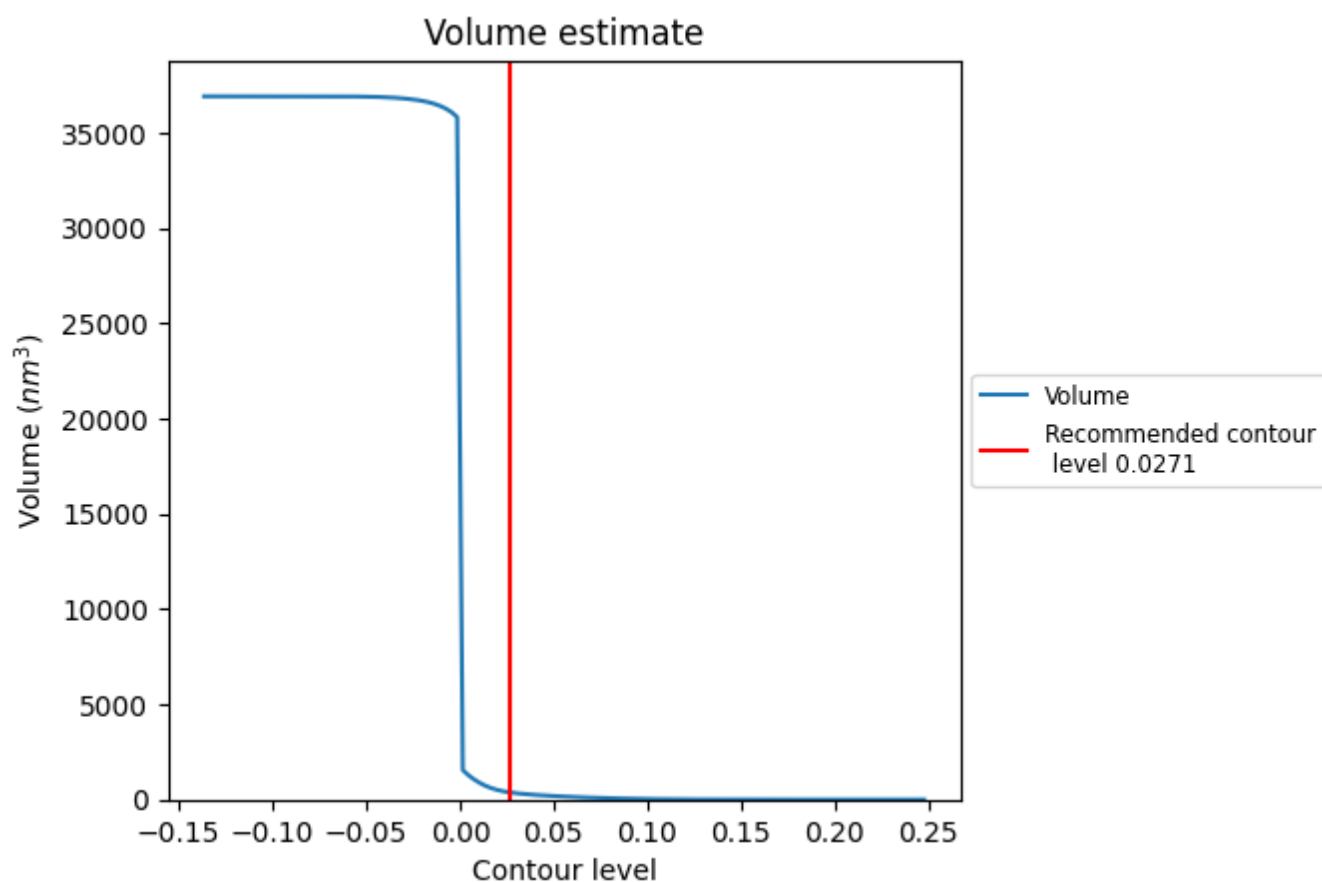
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

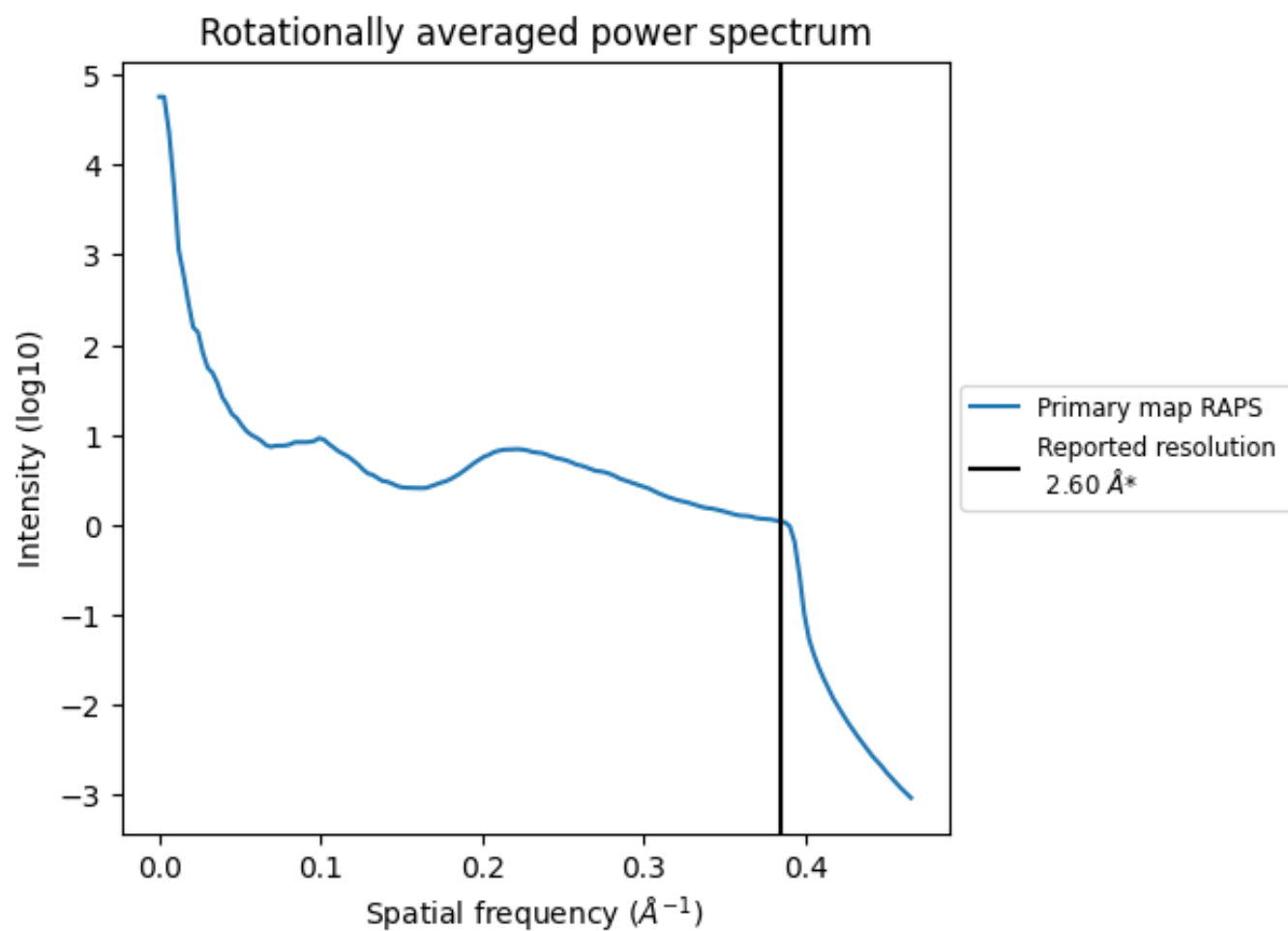
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 371 nm^3 ; this corresponds to an approximate mass of 335 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

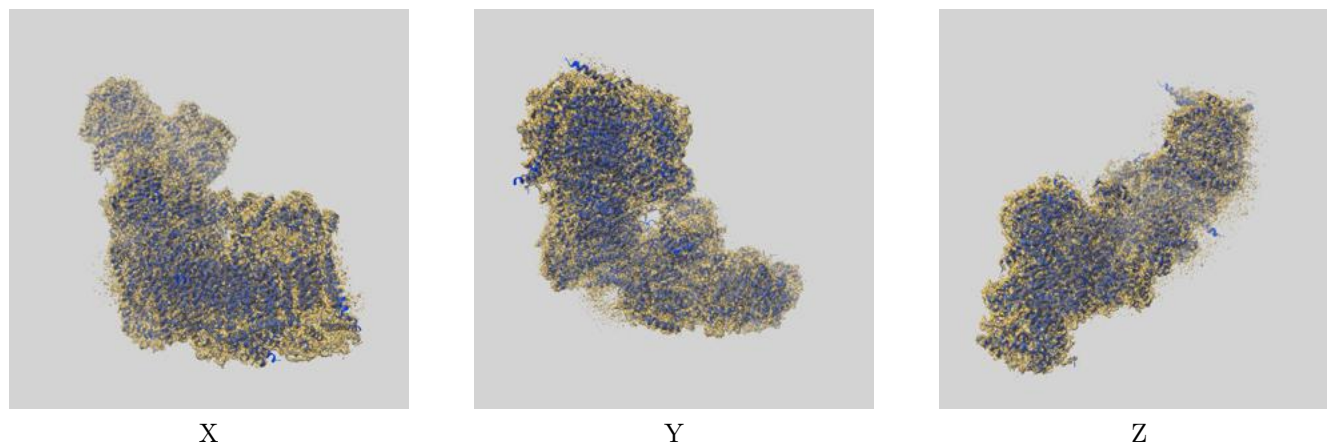
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

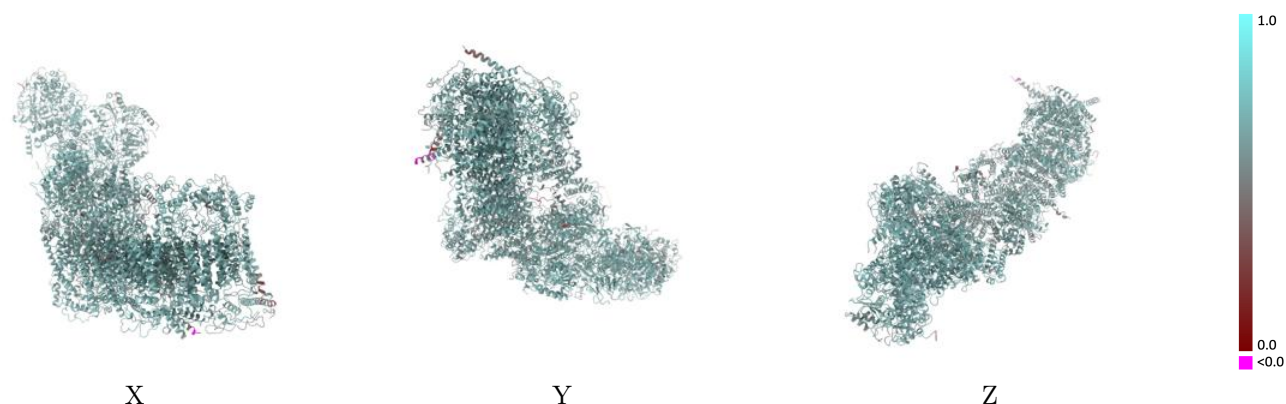
This section contains information regarding the fit between EMDB map EMD-31651 and PDB model 7V33. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

9.1 Map-model overlay [i](#)



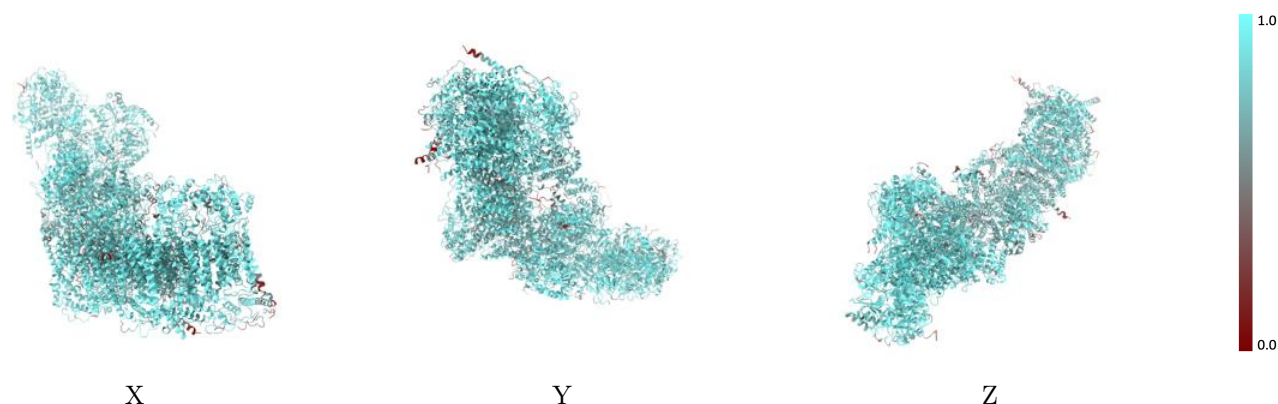
The images above show the 3D surface view of the map at the recommended contour level 0.0271 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



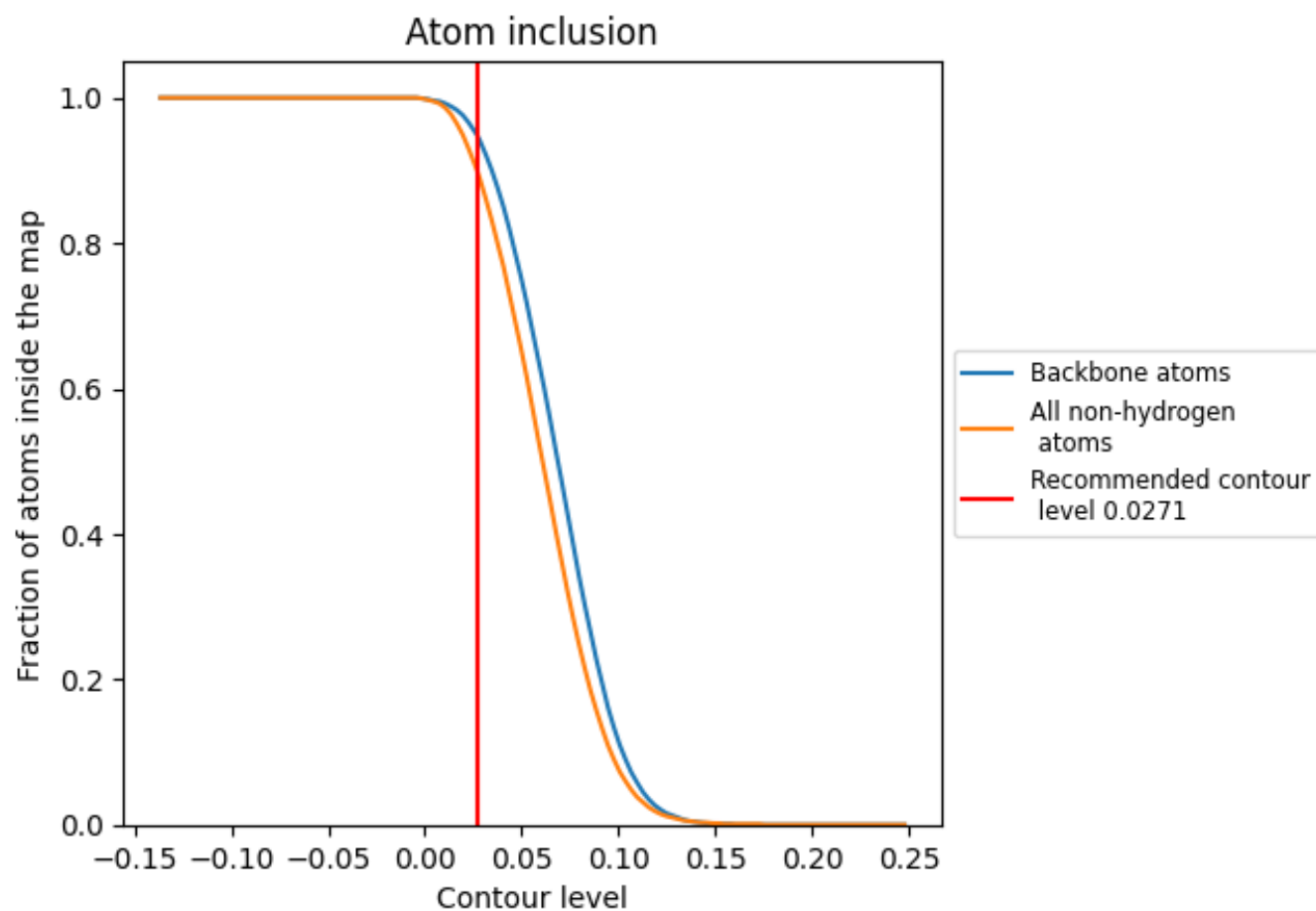
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0271).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 90% 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 (0.0271) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8990	 0.6490
A	 0.9060	 0.6390
B	 0.9650	 0.6870
C	 0.9600	 0.6870
E	 0.9080	 0.6600
F	 0.8290	 0.5970
G	 0.6930	 0.5290
H	 0.9170	 0.6420
I	 0.8040	 0.6240
J	 0.9200	 0.6570
K	 0.8230	 0.6020
L	 0.9210	 0.6720
M	 0.9310	 0.6570
N	 0.8840	 0.6480
O	 0.8670	 0.6220
P	 0.9680	 0.6890
Q	 0.9610	 0.6850
S	 0.9580	 0.6650
T	 0.8890	 0.6610
U	 0.8720	 0.6430
V	 0.8590	 0.6340
W	 0.8970	 0.6460
X	 0.8080	 0.6030
Y	 0.7730	 0.5930
Z	 0.7360	 0.5720
a	 0.8990	 0.6580
b	 0.8260	 0.6170
c	 0.8600	 0.6320
d	 0.8480	 0.6230
e	 0.8490	 0.6280
f	 0.7510	 0.5920
g	 0.9130	 0.6550
h	 0.8910	 0.6410
i	 0.9450	 0.6770
j	 0.8980	 0.6650



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Chain	Atom inclusion	Q-score
k	 0.9400	 0.6740
l	 0.9100	 0.6560
m	 0.8500	 0.6310
n	 0.7500	 0.5980
o	 0.8260	 0.6290
p	 0.8730	 0.6350
r	 0.9530	 0.6750
s	 0.9610	 0.6780
u	 0.9040	 0.6500
v	 0.7460	 0.5730
w	 0.8640	 0.6270