



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 11:35 AM JST

PDB ID : 7W1O / pdb_00007w1o
EMDB ID : EMD-32253
Title : Deactive state CI from Q10-NADH dataset, Subclass 1
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-19
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

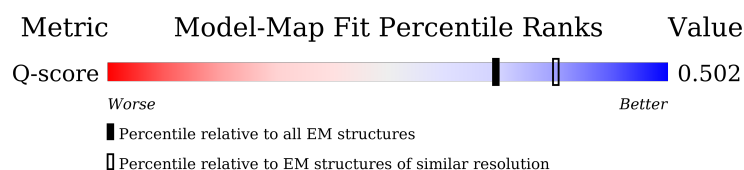
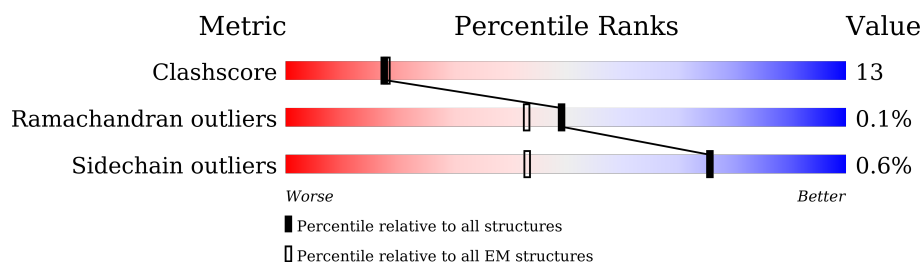
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	431	14% 64% 36%
2	B	176	69% 30%
3	C	156	70% 30%
4	E	115	13% 82% 18%

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Mol	Chain	Length	Quality of chain
5	F	86	
6	G	88	
6	X	88	
7	H	112	
8	I	112	
9	J	341	
10	K	42	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	70	
23	Z	84	
24	a	140	
25	b	126	
26	c	156	
27	d	175	
28	e	107	

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Mol	Chain	Length	Quality of chain
29	f	42	
30	g	121	
31	h	105	
32	i	347	
33	j	113	
34	k	98	
35	l	603	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	125	
44	w	320	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	A	501	-	-	X	-

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 66536 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3315	2094	590	611	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
			1405	881	243	268	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
			1239	790	224	211	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
			959	614	176	164	5		

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

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

- Molecule 6 is a protein called Acyl carrier protein.

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
			697	448	103	141	5		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	297	Total	C	N	O	S	0	0
			2337	1502	419	408	8		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	217	Total	C	N	O	S	0	0
			1668	1064	280	314	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1731	1121	298	310	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	419	Total	C	N	O	S	0	0
			3362	2155	578	605	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
			560	359	104	92	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 Complex I-B16.6.

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

- Molecule 22 is a protein called Complex I-AGGG.

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

- Molecule 23 is a protein called Complex I-B12.

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

- Molecule 24 is a protein called Complex I-SGDH.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	156	Total	C	N	O	S	0	0
			1311	851	213	239	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
			1441	903	260	270	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	107	Total	C	N	O	S	0	0
			889	568	145	172	4		

- Molecule 29 is a protein called Complex I-KFYI.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	347	Total	C	N	O	S	0	0
			2707	1781	419	461	46		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	603	Total	C	N	O	S	0	0
			4784	3173	741	819	51		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	128	Total	C	N	O	S	0	0
			1045	679	182	184			

- 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
			3628	2411	571	608	38		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	303	Total	C	N	O	S	0	0
			2394	1607	369	397	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	171	Total	C	N	O	S	0	0
			1378	878	244	246	10		

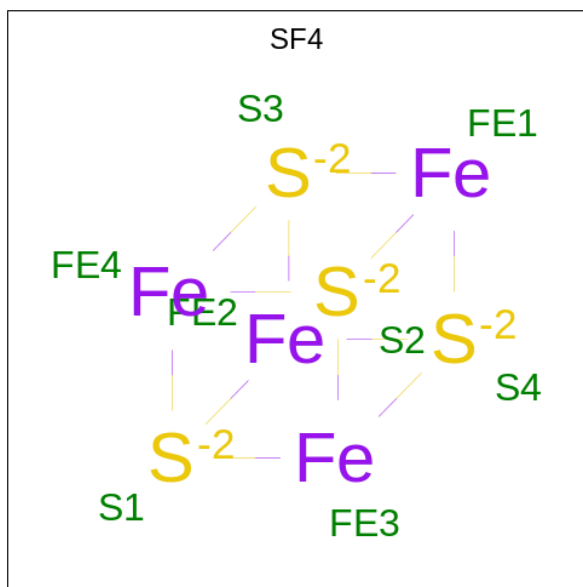
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			1012	633	188	182	9		

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

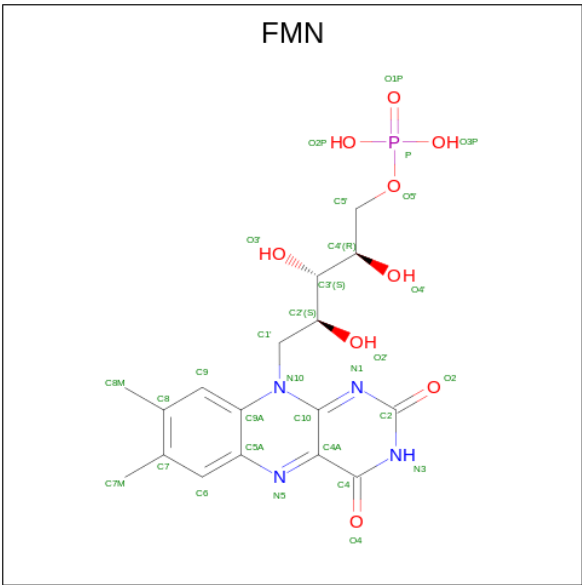
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2583	1646	437	491	9		

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



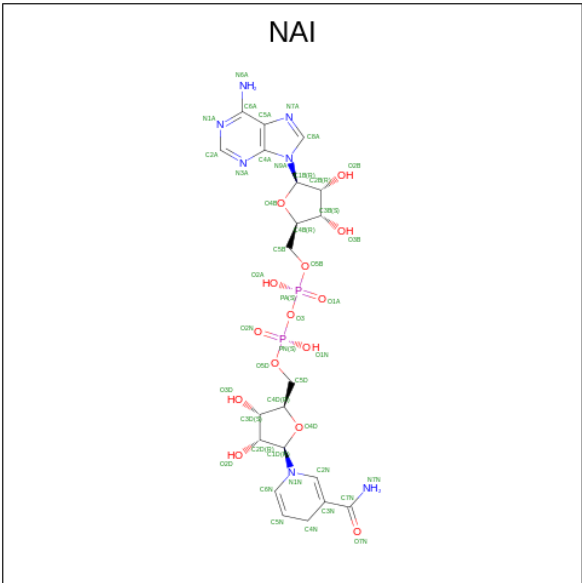
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



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

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



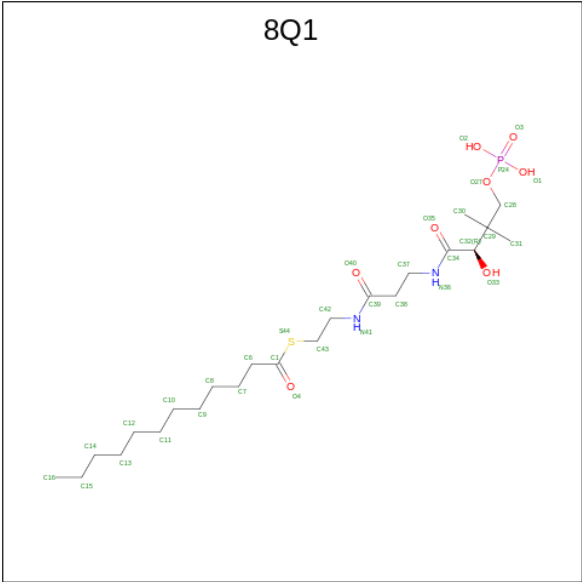
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

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



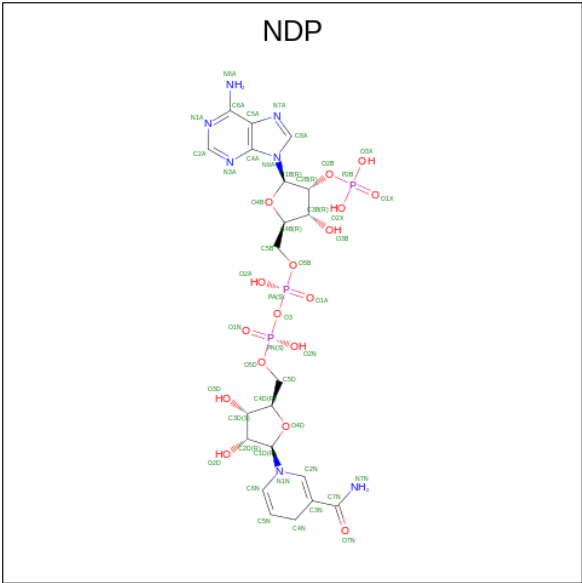
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	Q	1	Total	N				0
			1	1				
48	V	1	Total	C	N	O	P	0
			40	30	1	8	1	
48	j	1	Total	N				0
			1	1				
48	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	r	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



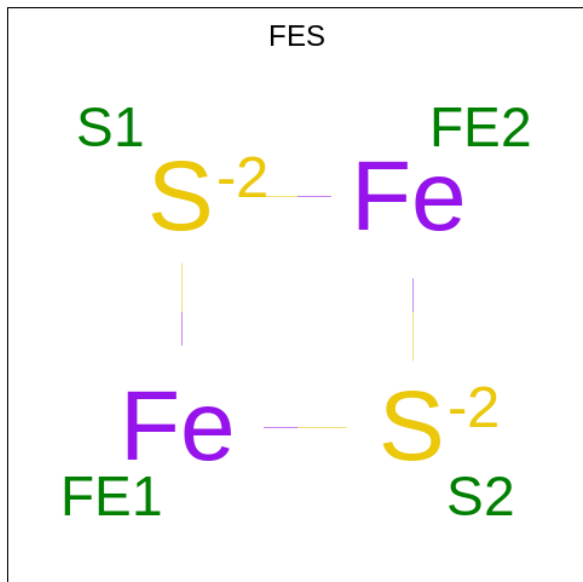
Mol	Chain	Residues	Atoms						AltConf
49	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
49	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 50 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
50	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 51 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



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

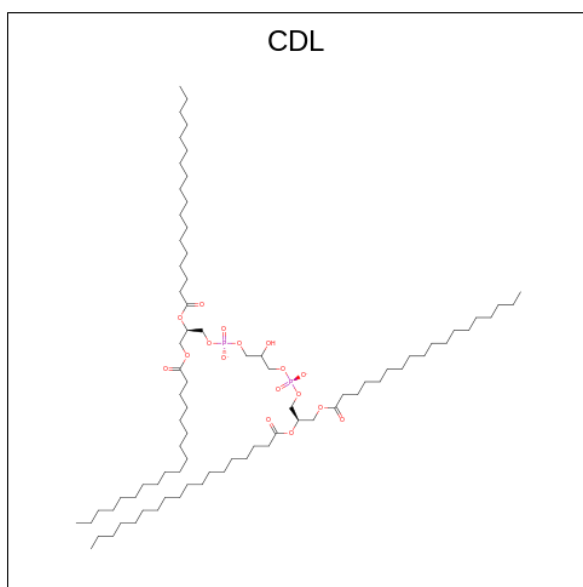
- Molecule 52 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

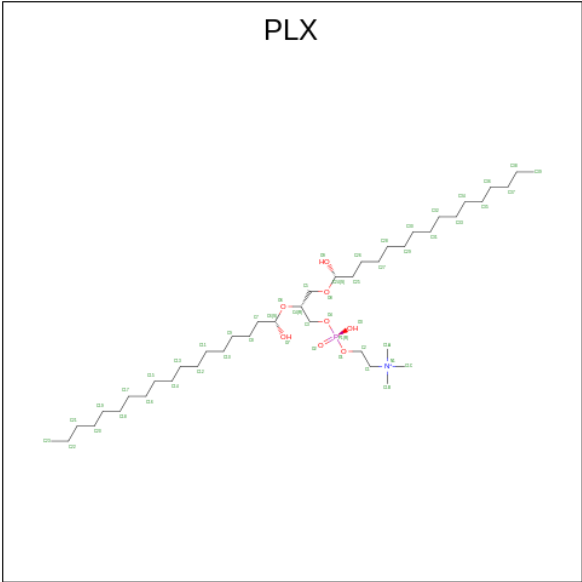
Mol	Chain	Residues	Atoms		AltConf
53	T	1	Total	Zn	0
			1	1	

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



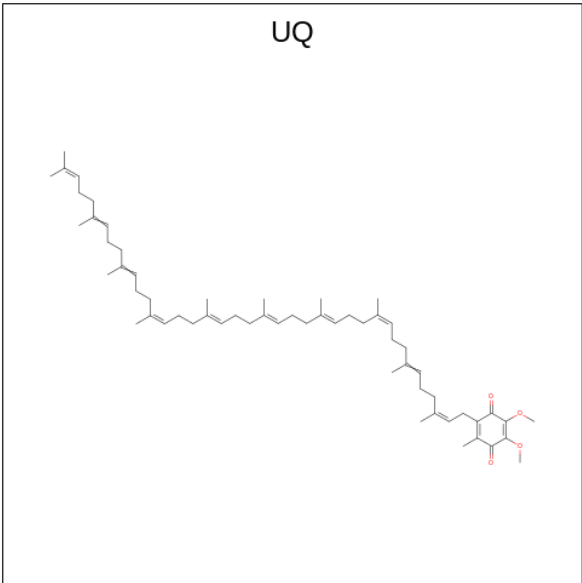
Mol	Chain	Residues	Atoms				AltConf
54	V	1	Total	C	O	P	0
			94	75	17	2	
54	V	1	Total	C	O	P	0
			68	49	17	2	
54	a	1	Total	C	O	P	0
			91	72	17	2	
54	g	1	Total	C	O	P	0
			97	78	17	2	
54	i	1	Total	C	O	P	0
			66	47	17	2	
54	l	1	Total	C	O	P	0
			99	80	17	2	
54	l	1	Total	C	O	P	0
			100	81	17	2	
54	u	1	Total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

- Molecule 55 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-TRIOX (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



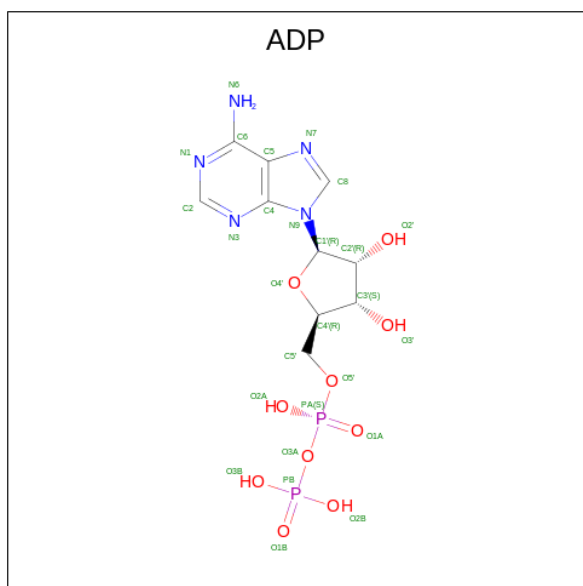
Mol	Chain	Residues	Atoms					AltConf
55	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
55	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
55	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
55	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

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



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

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

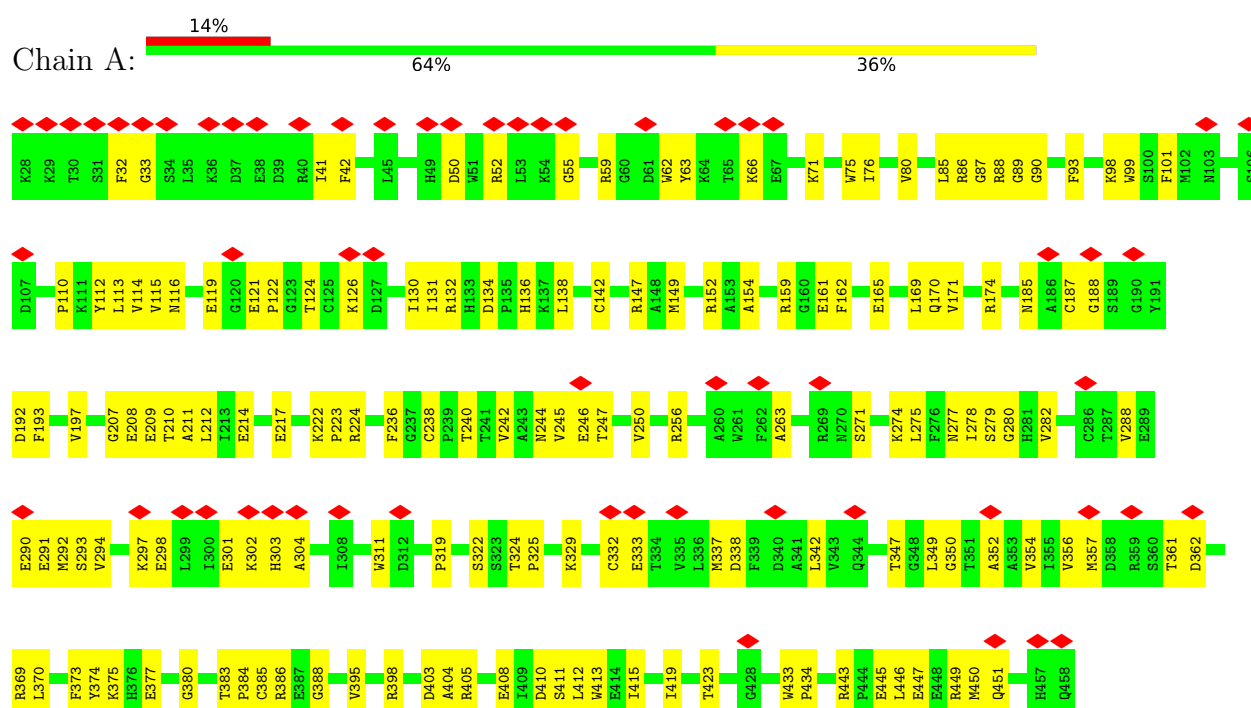


Mol	Chain	Residues	Atoms					AltConf
57	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

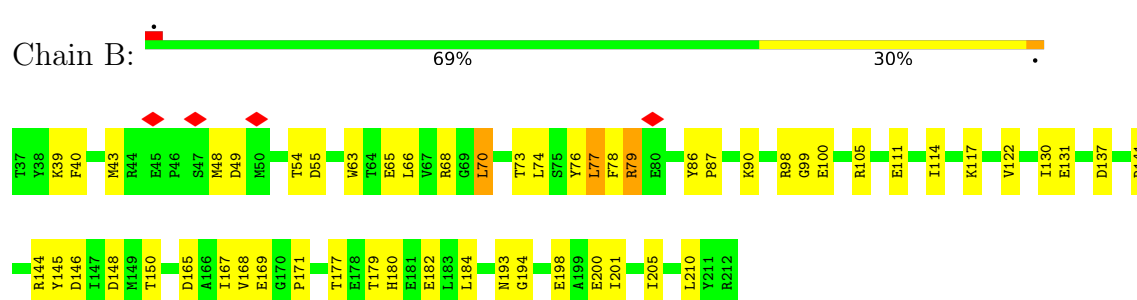
3 Residue-property plots

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

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

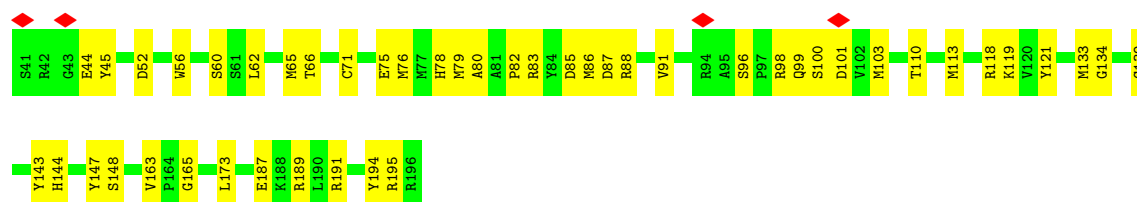


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

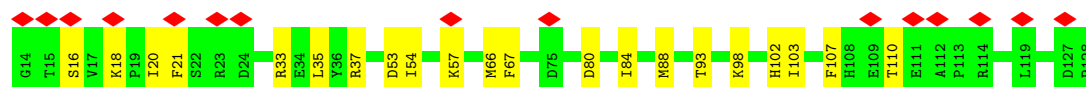
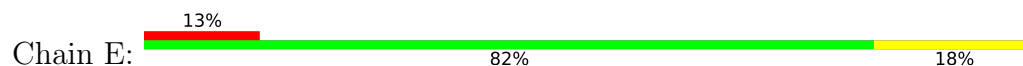


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

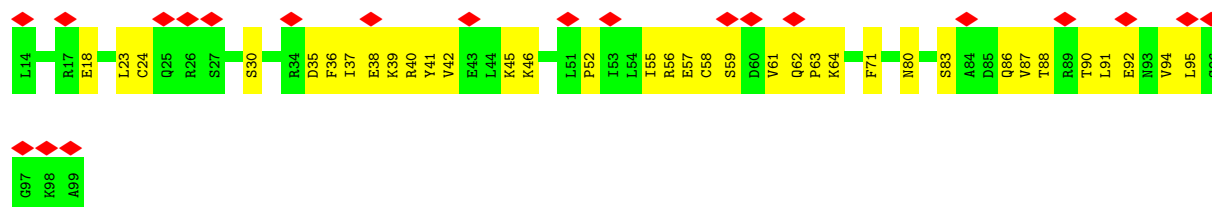




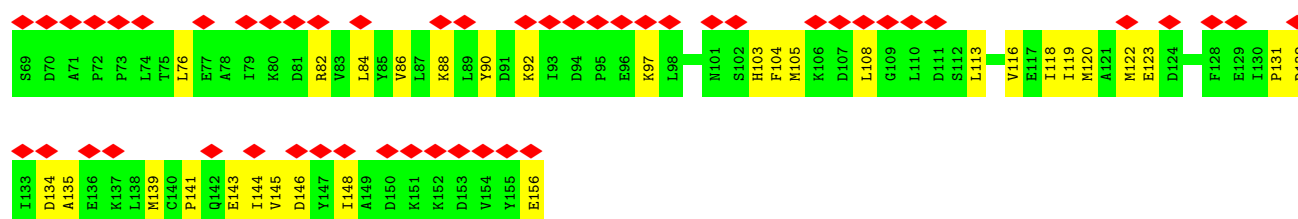
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



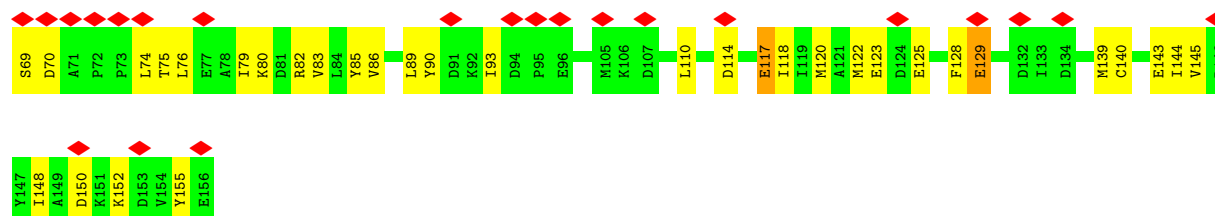
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



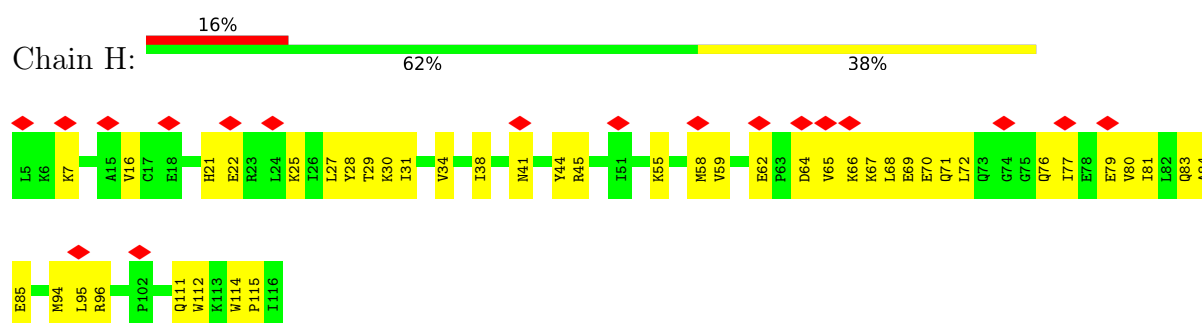
- Molecule 6: Acyl carrier protein



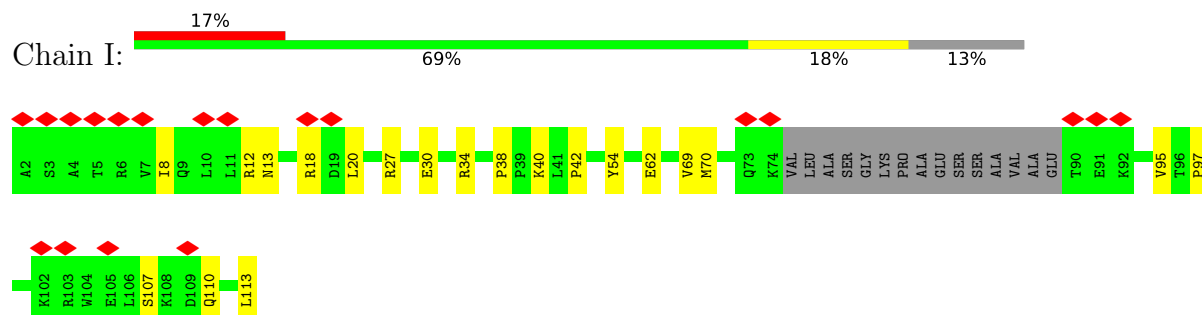
- Molecule 6: Acyl carrier protein



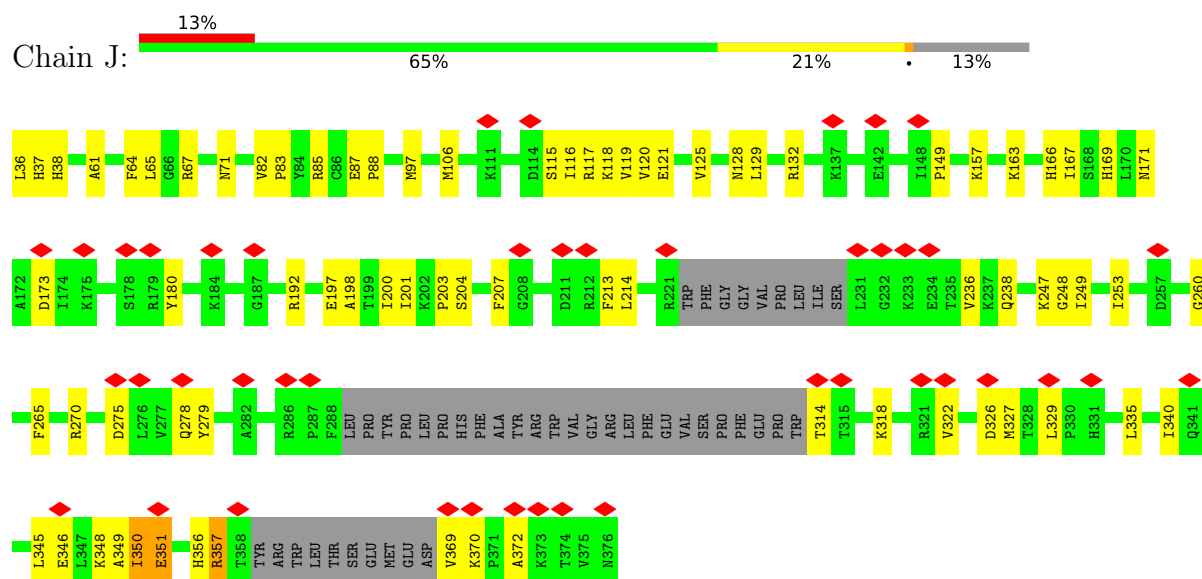
- Molecule 7: Complex I subunit B13



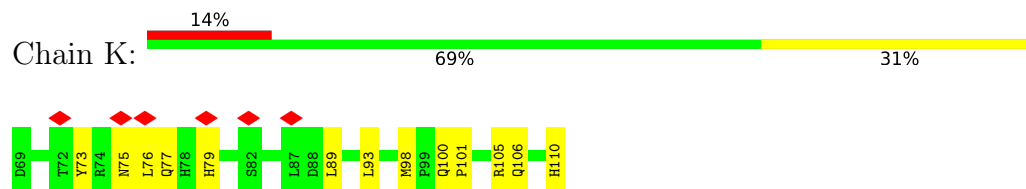
- Molecule 8: Complex I-B14.5a



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

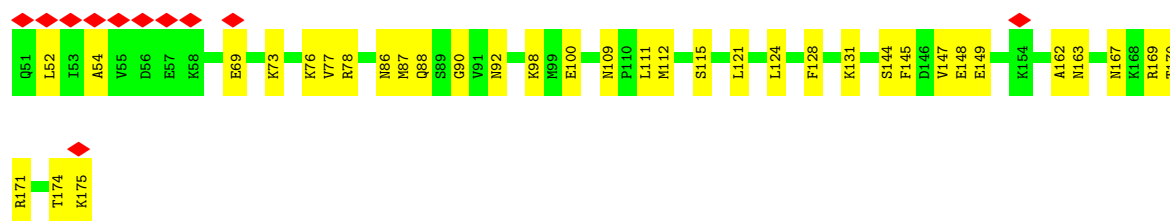


- Molecule 10: Complex I-9kD

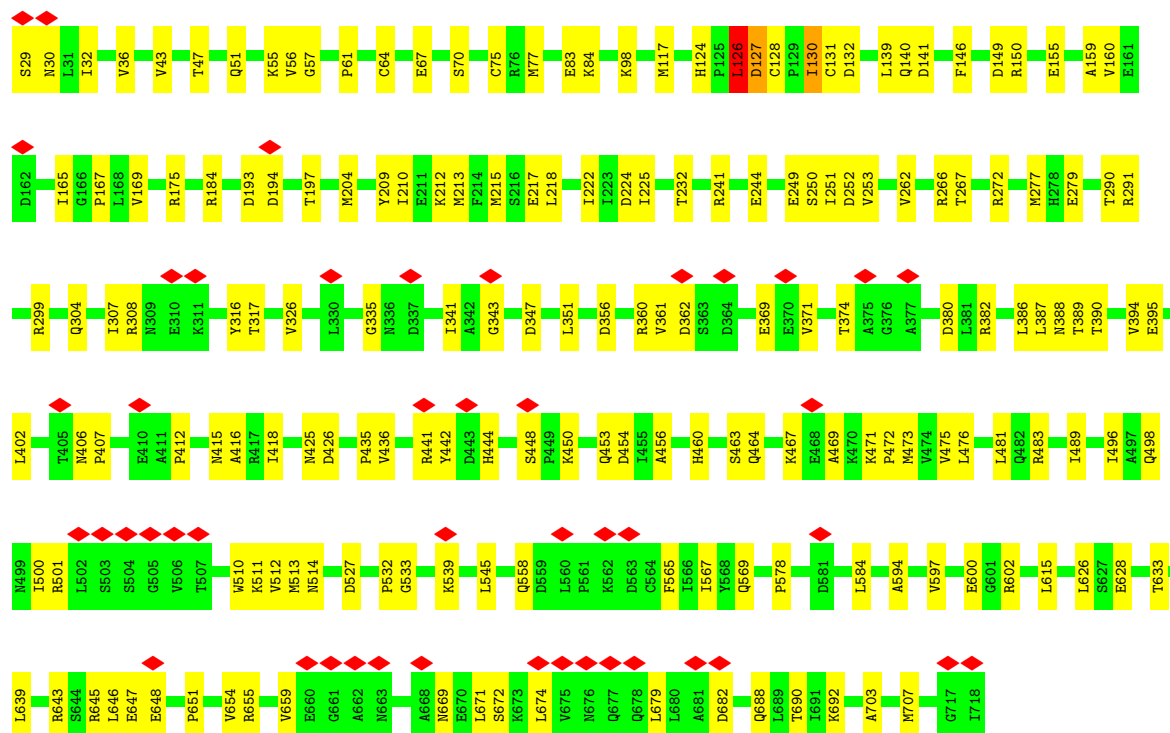
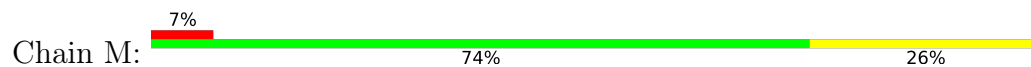


- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

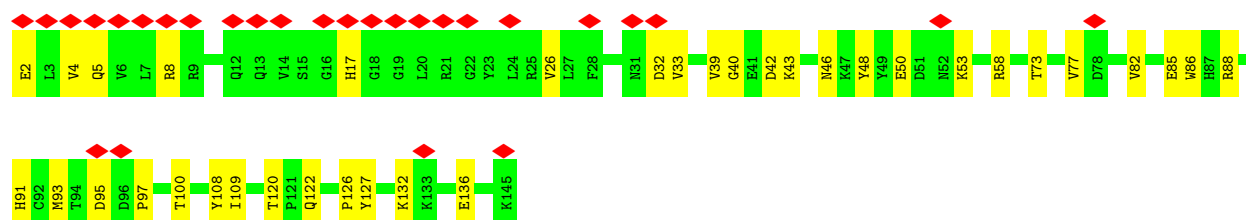
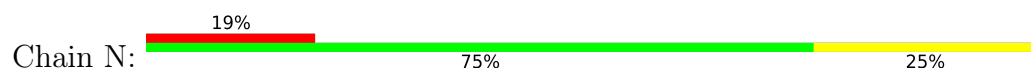




- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

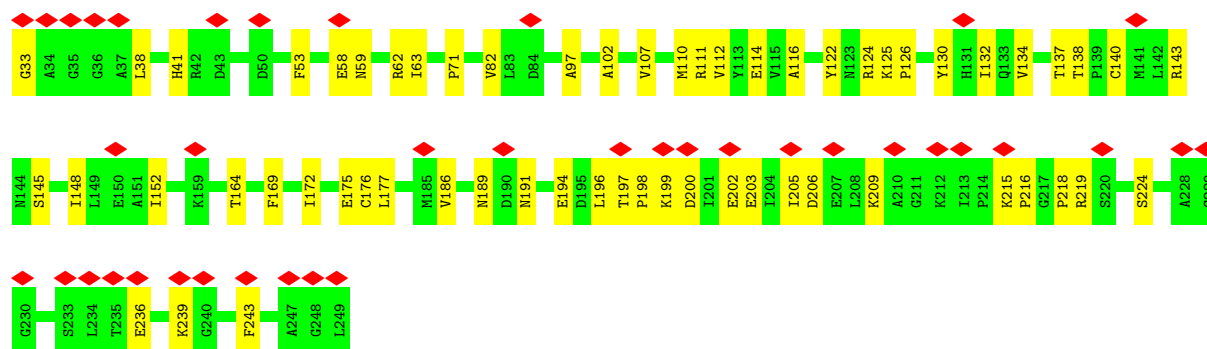


- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

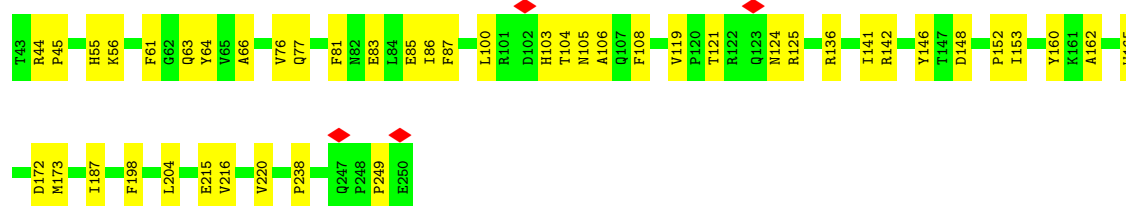
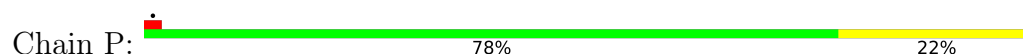


- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

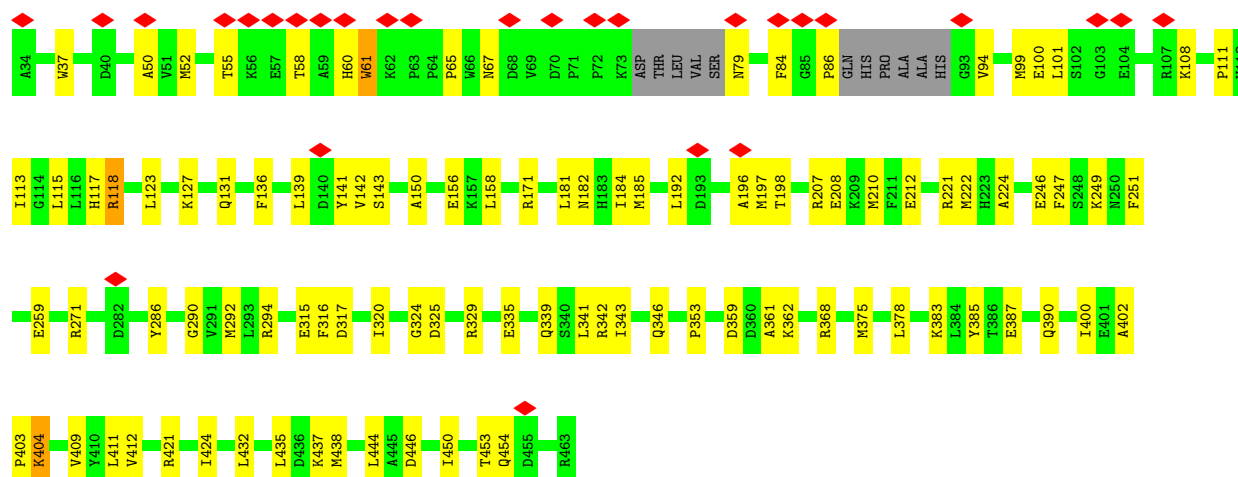
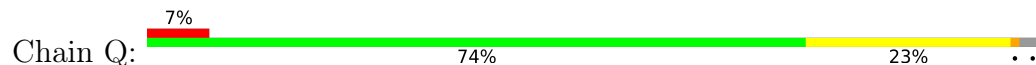




• Molecule 15: Complex I-30kD



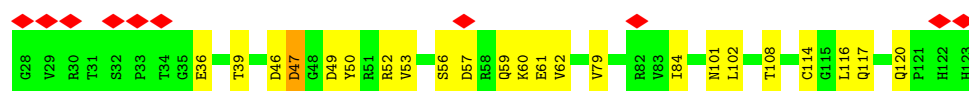
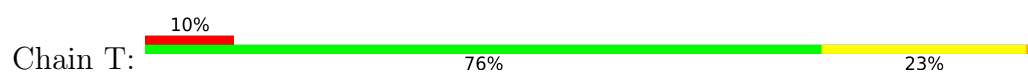
• Molecule 16: Complex I-49kD



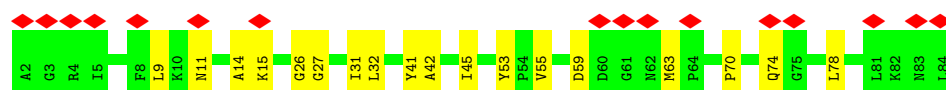
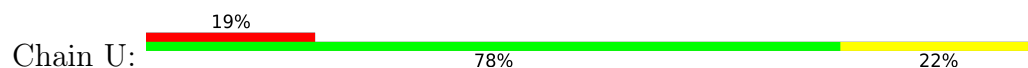
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



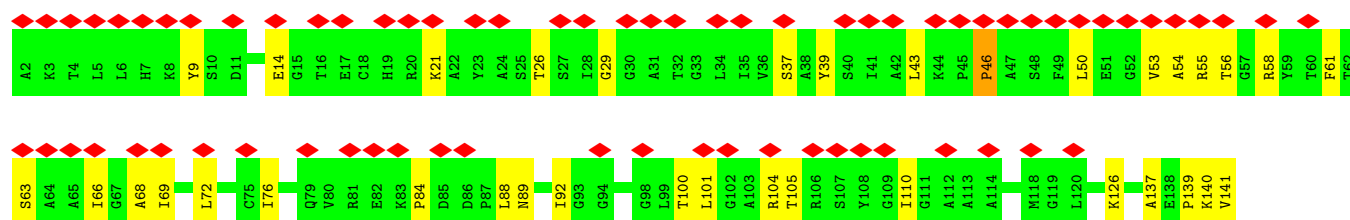
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



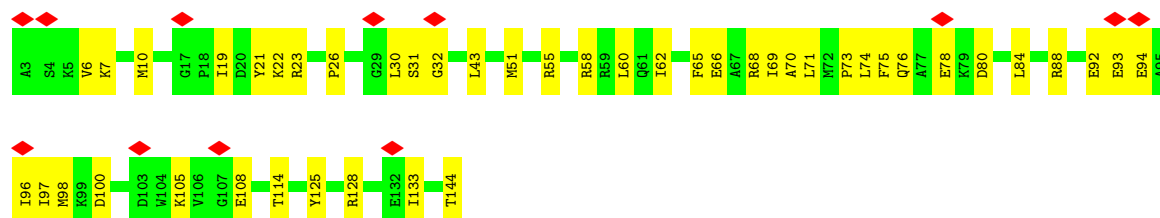
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



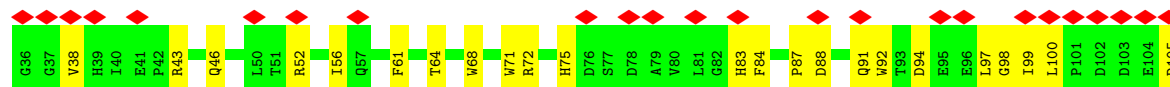
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



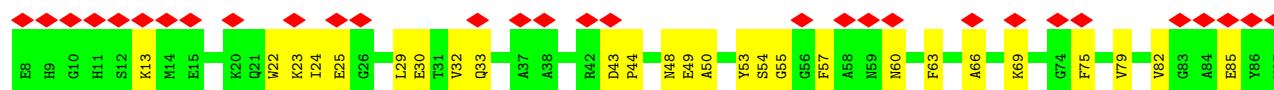
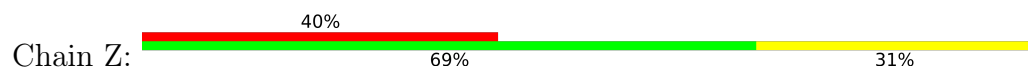
- Molecule 21: Complex I-B16.6



- Molecule 22: Complex I-AGGG

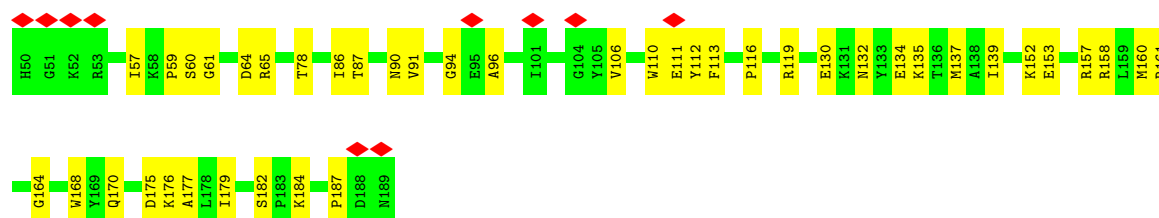


- Molecule 23: Complex I-B12

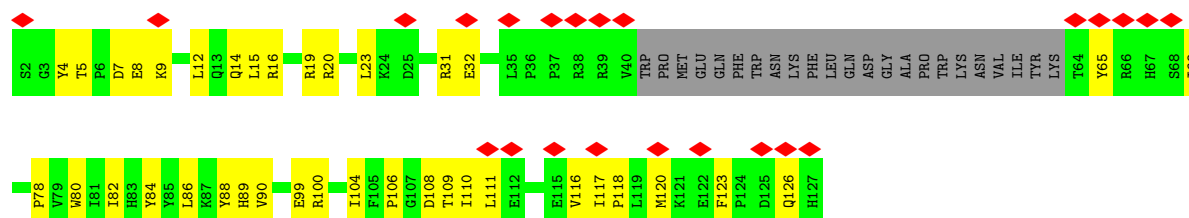




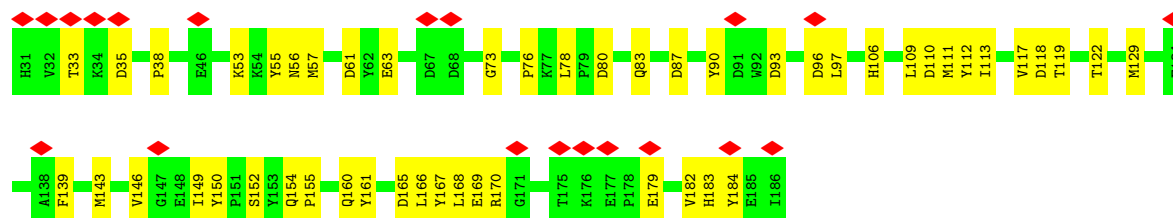
• Molecule 24: Complex I-SGDH



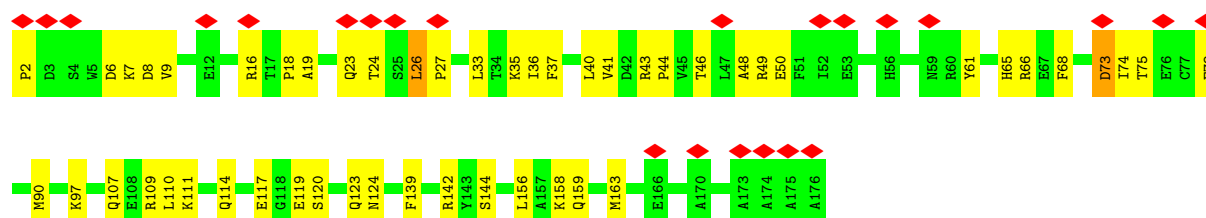
• Molecule 25: Complex I-B17



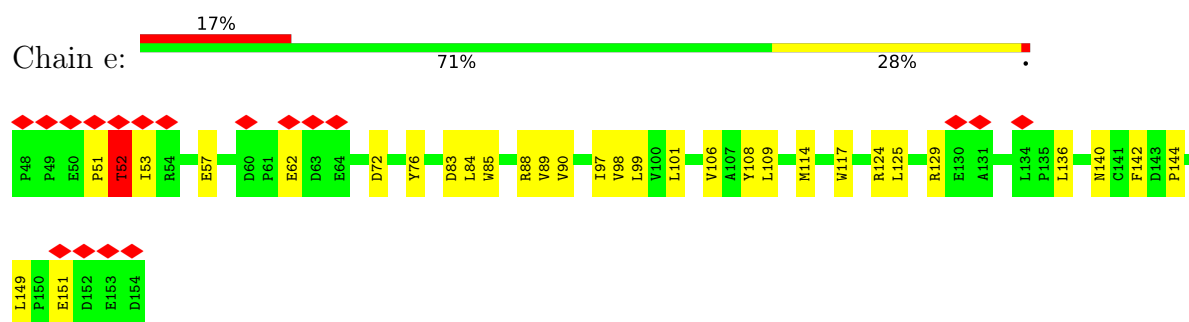
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



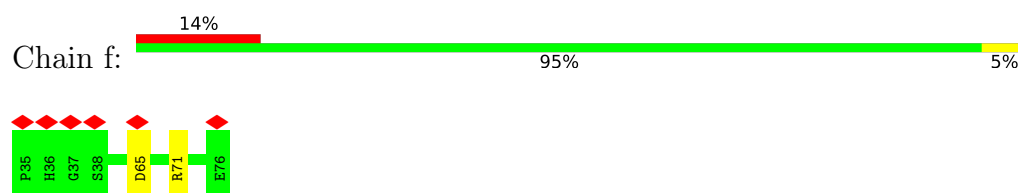
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



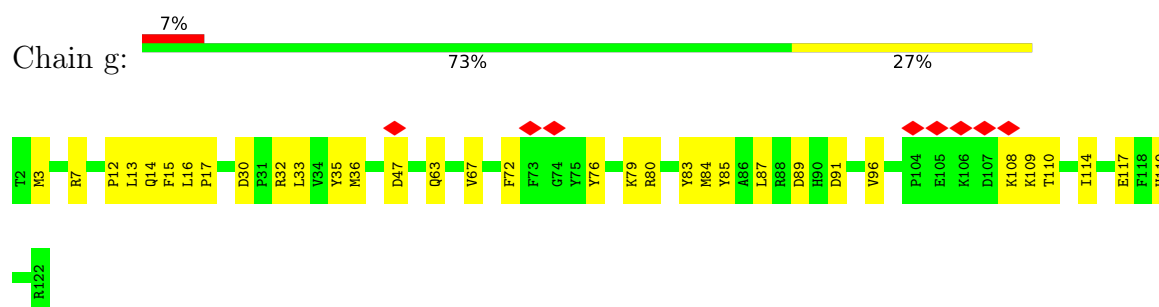
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



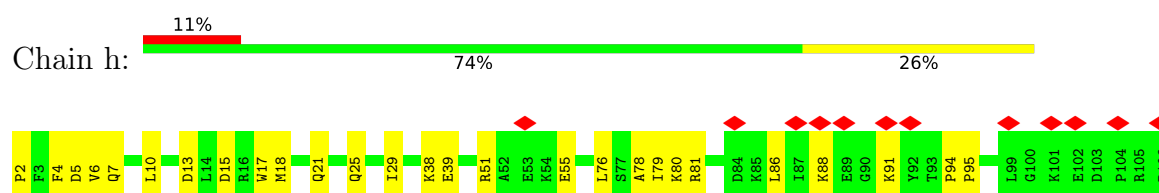
- Molecule 29: Complex I-KFYI



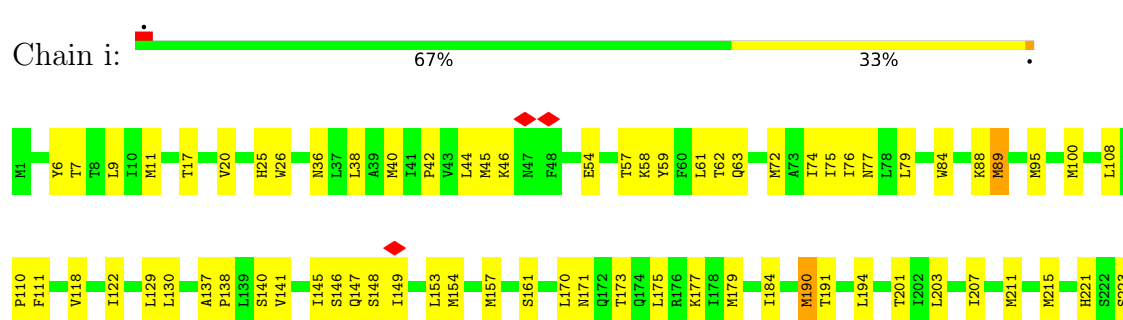
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



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

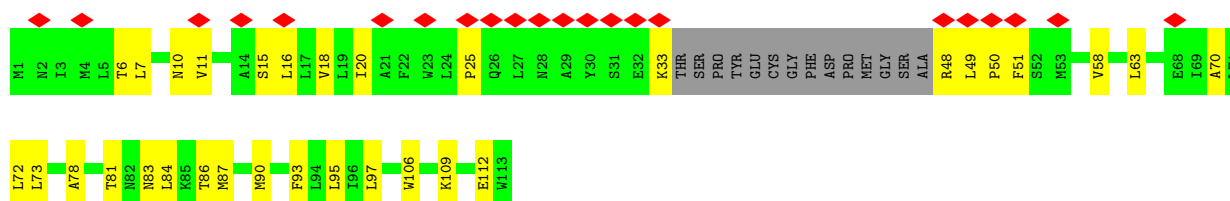


- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

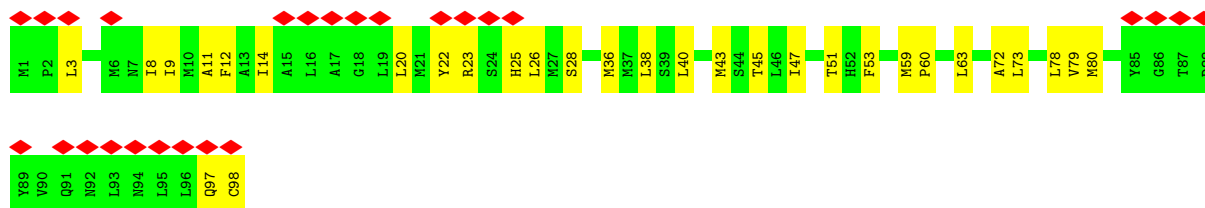




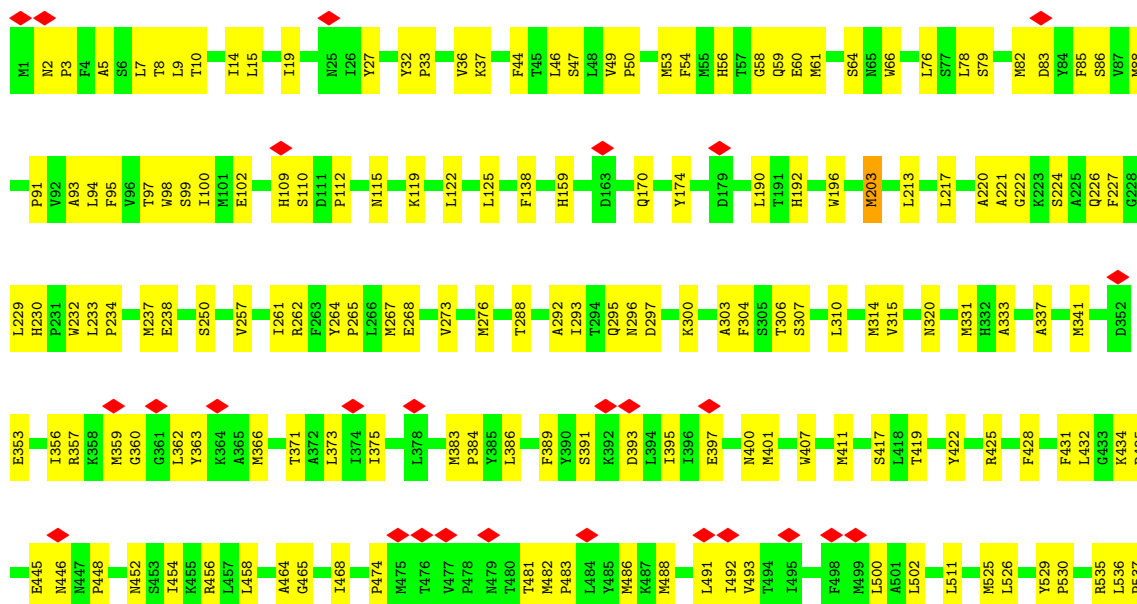
• Molecule 33: NADH-ubiquinone oxidoreductase chain 3

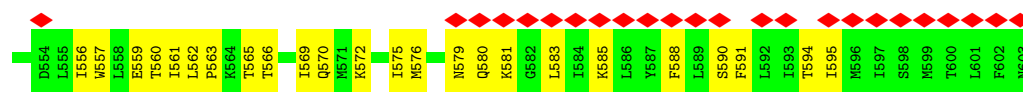


• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

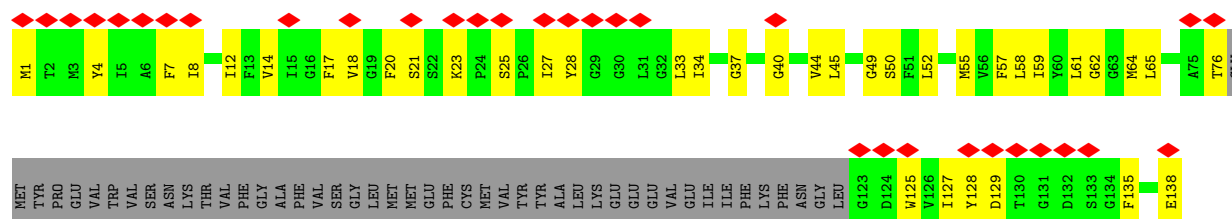


• Molecule 35: NADH-ubiquinone oxidoreductase chain 5

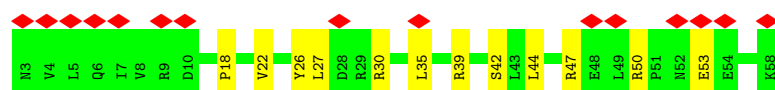
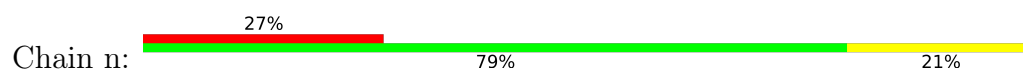




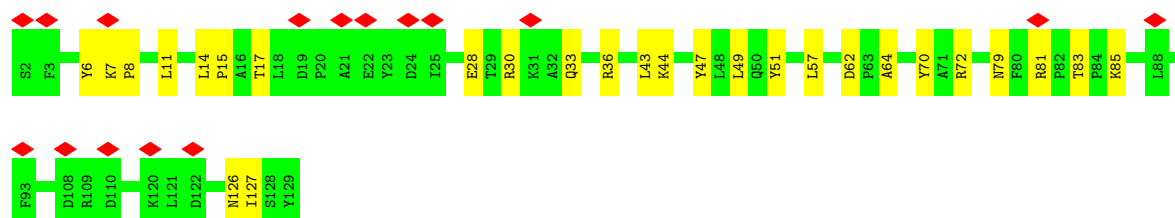
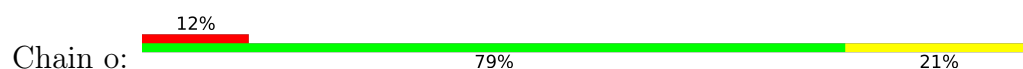
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6



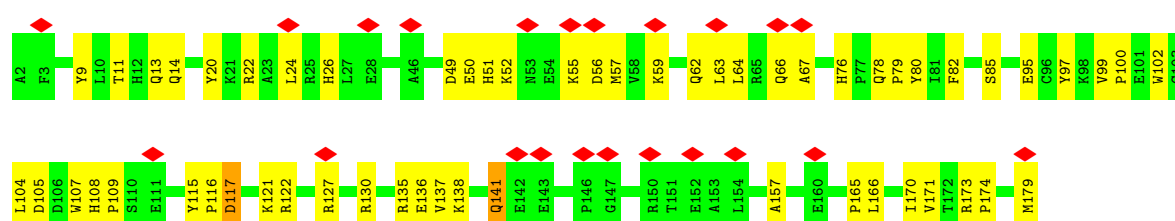
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



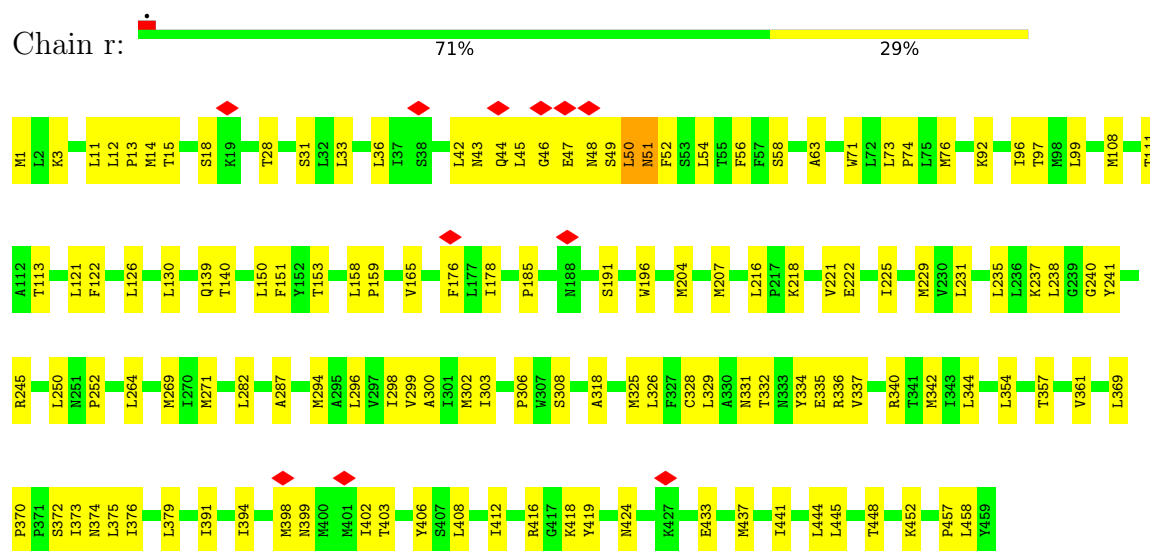
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



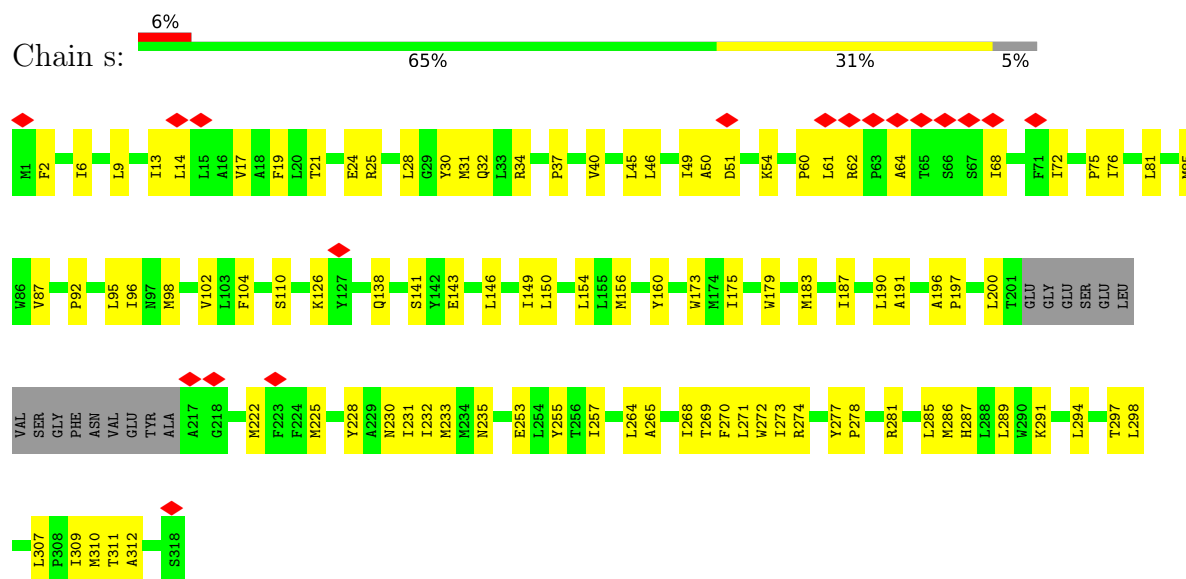
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



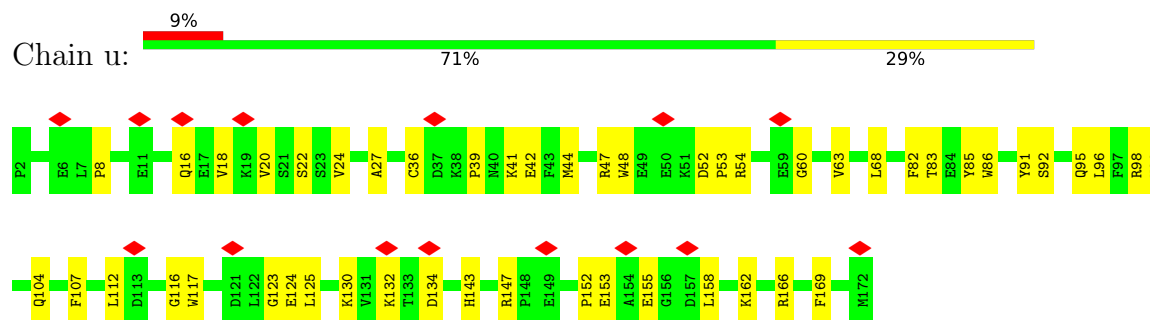
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4



- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

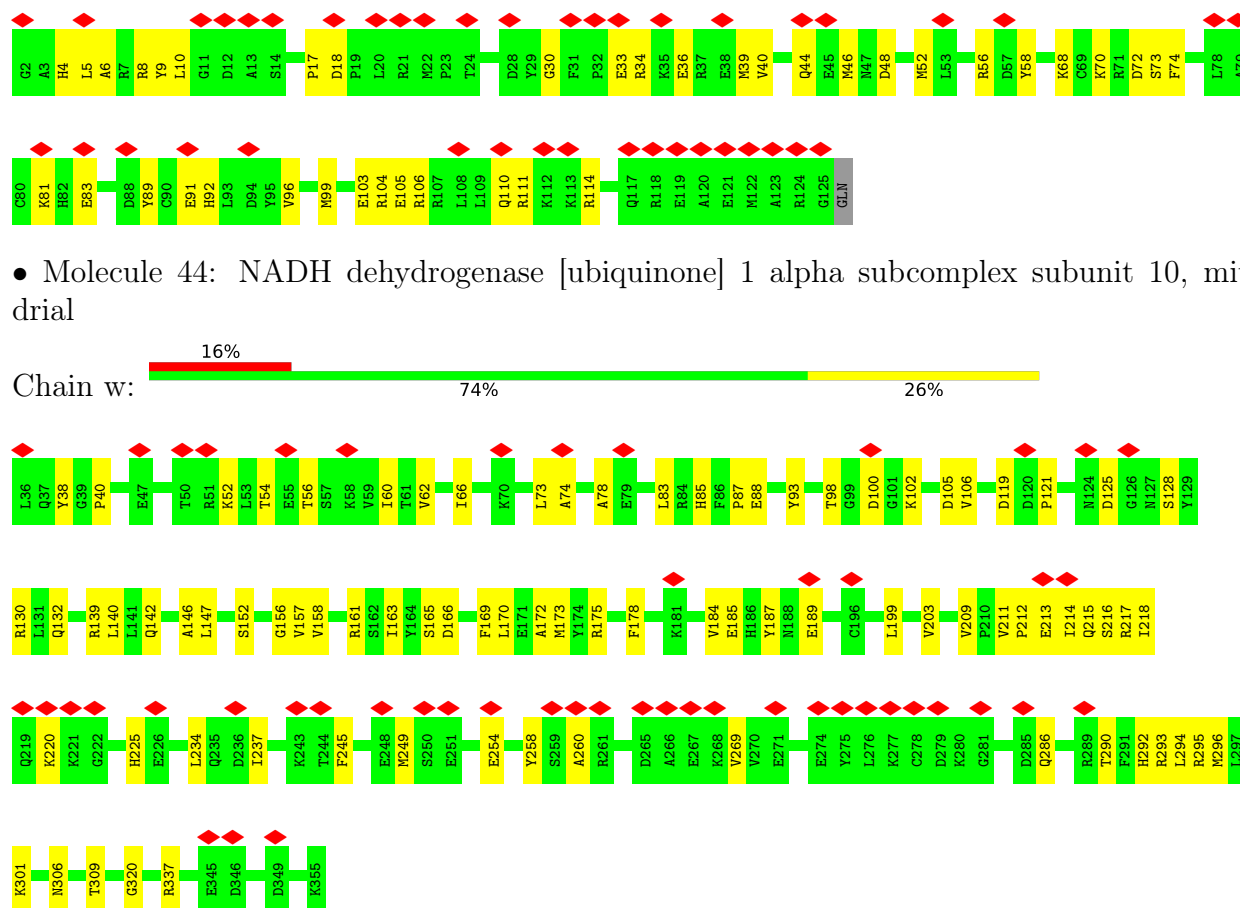


- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



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





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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24886	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	0.239	Depositor
Minimum map value	-0.085	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0267	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.16	0/3390	0.37	0/4580
2	B	0.18	0/1435	0.43	0/1941
3	C	0.21	0/1270	0.48	0/1719
4	E	0.15	0/983	0.36	0/1325
5	F	0.19	0/702	0.47	0/945
6	G	0.18	0/705	0.51	0/956
6	X	0.18	0/709	0.46	0/960
7	H	0.20	0/929	0.49	0/1258
8	I	0.17	0/798	0.39	0/1079
9	J	0.18	0/2388	0.48	0/3225
10	K	0.11	0/365	0.33	0/493
11	L	0.17	0/1039	0.40	0/1403
12	M	0.15	0/5384	0.39	0/7295
13	N	0.14	0/1245	0.37	0/1694
14	O	0.15	0/1708	0.40	0/2324
15	P	0.16	0/1782	0.43	0/2427
16	Q	0.20	0/3436	0.41	0/4653
17	S	0.24	0/575	0.56	0/774
18	T	0.15	0/755	0.36	0/1018
19	U	0.17	0/664	0.41	0/912
20	V	0.16	0/1042	0.35	0/1411
21	W	0.18	0/1198	0.37	0/1617
22	Y	0.22	0/626	0.51	0/857
23	Z	0.15	0/695	0.38	0/939
24	a	0.18	0/1199	0.39	0/1623
25	b	0.18	0/906	0.41	0/1232
26	c	0.16	0/1367	0.41	0/1870
27	d	0.20	0/1473	0.50	3/1989 (0.2%)
28	e	0.18	0/915	0.44	0/1245
29	f	0.13	0/350	0.28	0/473
30	g	0.14	0/1031	0.33	0/1394
31	h	0.15	0/889	0.38	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.19	0/2770	0.45	1/3764 (0.0%)
33	j	0.22	0/819	0.49	0/1117
34	k	0.20	0/759	0.44	0/1029
35	l	0.19	0/4913	0.43	0/6682
36	m	0.18	0/973	0.44	0/1320
37	n	0.14	0/491	0.34	0/663
38	o	0.20	0/1074	0.47	0/1457
39	p	0.19	0/1590	0.43	0/2155
40	r	0.18	0/3720	0.45	1/5074 (0.0%)
41	s	0.18	0/2464	0.43	0/3369
42	u	0.22	0/1416	0.50	0/1913
43	v	0.17	0/1036	0.44	0/1393
44	w	0.16	0/2643	0.38	0/3580
All	All	0.18	0/66621	0.42	5/90337 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	r	48	ASN	N-CA-C	9.71	121.46	111.07
27	d	26	LEU	CA-C-N	6.91	126.83	119.85
27	d	26	LEU	C-N-CA	6.91	126.83	119.85
27	d	142	ARG	N-CA-C	5.33	117.17	111.36
32	i	89	MET	N-CA-C	5.05	116.79	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3315	0	3276	115	0
2	B	1405	0	1356	63	0
3	C	1239	0	1241	38	0
4	E	959	0	954	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	691	0	704	37	0
6	G	693	0	671	21	0
6	X	697	0	669	27	0
7	H	910	0	950	34	0
8	I	780	0	808	23	0
9	J	2337	0	2370	70	0
10	K	355	0	329	15	0
11	L	1016	0	1016	30	0
12	M	5296	0	5327	141	0
13	N	1204	0	1162	29	0
14	O	1668	0	1669	47	0
15	P	1731	0	1687	44	0
16	Q	3362	0	3306	95	0
17	S	560	0	552	17	0
18	T	741	0	702	18	0
19	U	643	0	642	18	0
20	V	1021	0	1027	25	0
21	W	1167	0	1155	44	0
22	Y	600	0	539	19	0
23	Z	674	0	643	24	0
24	a	1165	0	1174	39	0
25	b	879	0	899	48	0
26	c	1311	0	1204	42	0
27	d	1441	0	1396	56	0
28	e	889	0	834	27	0
29	f	342	0	341	2	0
30	g	1000	0	994	26	0
31	h	867	0	871	20	0
32	i	2707	0	2870	104	0
33	j	800	0	855	33	0
34	k	748	0	799	31	0
35	l	4784	0	4930	157	0
36	m	951	0	962	42	0
37	n	479	0	486	13	0
38	o	1045	0	1050	31	0
39	p	1534	0	1470	56	0
40	r	3628	0	3835	108	0
41	s	2394	0	2508	92	0
42	u	1378	0	1345	80	0
43	v	1012	0	947	44	0
44	w	2583	0	2539	64	0
45	A	8	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	B	16	0	0	0	0
45	C	8	0	0	0	0
45	M	16	0	0	1	0
46	A	31	0	19	3	0
47	A	44	0	27	5	0
48	B	51	0	82	0	0
48	Q	1	0	0	0	0
48	V	40	0	54	1	0
48	j	52	0	82	5	0
48	l	92	0	138	4	0
48	m	41	0	59	2	0
48	r	51	0	82	3	0
49	G	35	0	0	0	0
49	X	35	0	0	4	0
50	J	48	0	25	5	0
51	M	4	0	0	0	0
51	O	4	0	0	1	0
52	M	1	0	0	0	0
53	T	1	0	0	0	0
54	V	162	0	221	10	0
54	a	91	0	132	3	0
54	g	97	0	147	9	0
54	i	66	0	76	4	0
54	l	199	0	307	22	0
54	u	78	0	103	8	0
55	a	52	0	88	1	0
55	g	52	0	88	4	0
55	j	52	0	88	3	0
55	r	52	0	88	6	0
56	s	28	0	31	6	0
57	w	27	0	11	2	0
All	All	66536	0	67012	1799	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 13.

All (1799) 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)
42:u:82:PHE:HB2	42:u:107:PHE:CE1	1.41	1.48
27:d:26:LEU:CD1	27:d:27:PRO:HD2	1.59	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:95:MET:CE	32:i:149:ILE:HG12	1.59	1.32
27:d:26:LEU:HD12	27:d:27:PRO:CD	1.60	1.31
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.20
50:J:401:NDP:C4D	50:J:401:NDP:O4D	1.68	1.17
42:u:82:PHE:CB	42:u:107:PHE:CE1	2.27	1.16
12:M:388:ASN:HB3	12:M:511:LYS:HE2	1.20	1.15
9:J:248:GLY:HA2	9:J:340:ILE:HD11	1.30	1.10
27:d:114:GLN:HB2	35:l:203:MET:HE1	1.37	1.06
6:X:83:VAL:HG13	6:X:122:MET:HE1	1.39	1.05
42:u:82:PHE:CB	42:u:107:PHE:HE1	1.67	1.03
32:i:95:MET:CE	32:i:149:ILE:CG1	2.38	1.00
42:u:82:PHE:HB2	42:u:107:PHE:CD1	1.96	0.99
42:u:82:PHE:HA	42:u:107:PHE:CD1	1.98	0.97
27:d:24:THR:HG23	43:v:73:SER:CB	1.96	0.96
32:i:95:MET:HE2	32:i:149:ILE:HG12	1.49	0.94
27:d:24:THR:CG2	43:v:73:SER:HB2	1.97	0.94
9:J:248:GLY:HA2	9:J:340:ILE:CD1	1.97	0.94
32:i:95:MET:HE1	32:i:149:ILE:HG12	1.48	0.94
9:J:248:GLY:CA	9:J:340:ILE:HD11	1.97	0.94
9:J:125:VAL:HG22	9:J:163:LYS:HB2	1.50	0.93
9:J:248:GLY:CA	9:J:340:ILE:CD1	2.46	0.93
12:M:126:LEU:H	12:M:126:LEU:HD12	1.34	0.92
42:u:85:TYR:CE1	42:u:104:GLN:HB2	2.05	0.92
32:i:95:MET:HE2	32:i:149:ILE:CG1	1.99	0.91
12:M:389:THR:HG21	12:M:473:MET:HE3	1.53	0.90
42:u:82:PHE:CA	42:u:107:PHE:CD1	2.53	0.90
9:J:116:ILE:O	9:J:120:VAL:HG22	1.72	0.90
9:J:279:TYR:CE2	9:J:346:GLU:OE1	2.25	0.90
32:i:95:MET:HE2	32:i:149:ILE:HA	1.56	0.88
38:o:30:ARG:NH1	39:p:9:TYR:CG	2.41	0.88
42:u:85:TYR:HE1	42:u:104:GLN:HB2	1.38	0.88
16:Q:143:SER:CB	16:Q:403:PRO:HG2	2.03	0.87
16:Q:402:ALA:HB1	16:Q:403:PRO:HD2	1.56	0.87
16:Q:79:ASN:HA	16:Q:101:LEU:O	1.74	0.87
9:J:248:GLY:N	9:J:340:ILE:CD1	2.40	0.85
42:u:82:PHE:CA	42:u:107:PHE:HD1	1.89	0.84
9:J:345:LEU:O	9:J:345:LEU:HD23	1.78	0.84
35:l:288:THR:HG21	35:l:307:SER:HB3	1.59	0.84
40:r:44:GLN:HE22	40:r:50:LEU:HD23	1.41	0.84
27:d:24:THR:CG2	43:v:73:SER:CB	2.55	0.83
24:a:134:GLU:OE1	37:n:39:ARG:HA	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:89:LEU:HD23	23:Z:48:ASN:HA	1.60	0.83
40:r:370:PRO:HB3	40:r:375:LEU:HD22	1.59	0.82
6:X:123:GLU:HG2	6:X:129:GLU:HA	1.61	0.82
42:u:82:PHE:CB	42:u:107:PHE:CD1	2.59	0.82
27:d:23:GLN:HA	27:d:23:GLN:HE21	1.45	0.82
16:Q:402:ALA:HB1	16:Q:403:PRO:CD	2.10	0.81
42:u:96:LEU:HB2	42:u:99:HIS:HD2	1.46	0.81
27:d:24:THR:HG21	43:v:73:SER:HB2	1.60	0.81
32:i:149:ILE:HD13	32:i:154:MET:HE2	1.61	0.81
16:Q:143:SER:HB3	16:Q:403:PRO:HG2	1.62	0.80
25:b:32:GLU:HG3	39:p:115:TYR:HA	1.64	0.80
40:r:44:GLN:NE2	40:r:50:LEU:CD2	2.45	0.80
26:c:154:GLN:HE21	35:l:401:MET:HA	1.47	0.80
12:M:389:THR:HG21	12:M:473:MET:CE	2.12	0.80
42:u:82:PHE:CD1	42:u:107:PHE:CE1	2.71	0.79
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.64	0.79
27:d:24:THR:HG23	43:v:73:SER:HB3	1.62	0.79
6:G:141:PRO:HA	6:G:144:ILE:HD12	1.66	0.78
17:S:1:MET:O	41:s:30:TYR:CE2	2.36	0.78
9:J:265:PHE:CD1	9:J:335:LEU:HD23	2.19	0.77
12:M:388:ASN:HB3	12:M:511:LYS:CE	2.09	0.77
36:m:57:PHE:HA	36:m:61:LEU:HD23	1.67	0.77
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.65	0.76
4:E:57:LYS:NZ	4:E:57:LYS:O	2.18	0.76
2:B:114:ILE:HD12	12:M:130:ILE:HG22	1.68	0.76
40:r:44:GLN:NE2	40:r:50:LEU:HD21	2.01	0.76
10:K:106:GLN:HB2	10:K:110:HIS:HD2	1.52	0.75
35:l:119:LYS:NZ	54:l:701:CDL:OA3	2.20	0.75
23:Z:66:ALA:HA	35:l:363:TYR:HE2	1.52	0.75
24:a:94:GLY:HA2	24:a:116:PRO:HG3	1.67	0.75
2:B:177:THR:HG21	2:B:182:GLU:HB2	1.69	0.74
12:M:382:ARG:HE	12:M:386:LEU:HD11	1.52	0.74
32:i:95:MET:HE1	32:i:149:ILE:CG1	2.13	0.74
1:A:66:LYS:NZ	1:A:188:GLY:O	2.20	0.74
5:F:58:CYS:HB2	5:F:61:VAL:HG23	1.68	0.74
22:Y:94:ASP:HB3	22:Y:99:ILE:HB	1.70	0.74
12:M:389:THR:CB	12:M:473:MET:CE	2.65	0.74
16:Q:208:GLU:OE2	16:Q:221:ARG:NH2	2.20	0.74
44:w:60:ILE:HB	44:w:158:VAL:HG12	1.70	0.74
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.20	0.74
20:V:140:LYS:HG2	20:V:141:VAL:HG13	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:122:MET:HE3	6:X:144:ILE:HG21	1.69	0.73
24:a:179:ILE:HG21	31:h:38:LYS:HG3	1.69	0.73
32:i:283:ALA:HB1	40:r:158:LEU:HD12	1.69	0.73
12:M:389:THR:HB	12:M:473:MET:HE2	1.69	0.73
41:s:25:ARG:NH2	41:s:51:ASP:OD2	2.22	0.73
40:r:44:GLN:HE22	40:r:50:LEU:CD2	2.02	0.73
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.70	0.73
21:W:51:MET:HE2	41:s:311:THR:HB	1.68	0.73
12:M:389:THR:CB	12:M:473:MET:HE2	2.18	0.72
2:B:70:LEU:HD11	41:s:273:ILE:HG13	1.70	0.72
12:M:210:ILE:HD11	12:M:212:LYS:HE2	1.71	0.72
12:M:389:THR:HB	12:M:473:MET:CE	2.19	0.72
25:b:111:LEU:HD11	27:d:19:ALA:HA	1.71	0.72
24:a:132:ASN:ND2	40:r:50:LEU:HA	2.04	0.72
27:d:23:GLN:HA	27:d:23:GLN:NE2	2.05	0.72
28:e:125:LEU:HD12	28:e:129:ARG:HE	1.55	0.72
40:r:50:LEU:HD22	40:r:50:LEU:N	2.05	0.72
44:w:87:PRO:O	44:w:142:GLN:NE2	2.21	0.72
3:C:44:GLU:HG2	3:C:194:TYR:HE2	1.55	0.72
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.72	0.72
25:b:123:PHE:HB3	43:v:40:VAL:HG21	1.71	0.72
40:r:45:LEU:HD13	40:r:50:LEU:HD11	1.72	0.72
42:u:82:PHE:HA	42:u:107:PHE:HD1	1.51	0.72
4:E:37:ARG:NH2	6:G:123:GLU:OE2	2.22	0.72
42:u:16:GLN:OE1	42:u:68:LEU:HD13	1.90	0.72
9:J:37:HIS:CE1	18:T:49:ASP:HA	2.24	0.71
1:A:375:LYS:NZ	14:O:33:GLY:O	2.23	0.71
25:b:99:GLU:OE1	35:l:59:GLN:NE2	2.22	0.71
12:M:131:CYS:O	12:M:241:ARG:NH1	2.21	0.71
10:K:105:ARG:NH1	11:L:167:ASN:O	2.23	0.71
2:B:144:ARG:NH1	2:B:146:ASP:OD2	2.23	0.71
1:A:154:ALA:HB2	1:A:193:PHE:CZ	2.26	0.71
42:u:112:LEU:HD23	42:u:112:LEU:C	2.16	0.71
12:M:224:ASP:OD2	12:M:291:ARG:NH2	2.21	0.71
54:g:202:CDL:H581	40:r:13:PRO:HB3	1.72	0.71
12:M:382:ARG:NH1	12:M:527:ASP:OD1	2.24	0.71
2:B:100:GLU:OE2	2:B:193:ASN:ND2	2.23	0.70
9:J:71:ASN:HB2	9:J:97:MET:HE2	1.74	0.70
42:u:82:PHE:HB2	42:u:107:PHE:HE1	0.79	0.70
10:K:100:GLN:HB3	14:O:71:PRO:HA	1.72	0.70
11:L:77:VAL:HG13	11:L:145:PHE:HB3	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:LEU:O	2:B:74:LEU:HD12	1.92	0.70
4:E:53:ASP:OD1	9:J:351:GLU:HB2	1.91	0.70
39:p:11:THR:HG22	39:p:14:GLN:HG3	1.74	0.70
1:A:282:VAL:HG13	1:A:356:VAL:HG21	1.74	0.70
1:A:33:GLY:HA2	1:A:294:VAL:HG12	1.74	0.70
12:M:374:THR:HG22	12:M:532:PRO:HG2	1.73	0.70
12:M:36:VAL:HB	12:M:56:VAL:HG21	1.75	0.69
25:b:19:ARG:NH1	39:p:171:VAL:O	2.26	0.69
40:r:221:VAL:O	40:r:340:ARG:NH1	2.26	0.69
27:d:2:PRO:O	27:d:7:LYS:NZ	2.25	0.69
42:u:85:TYR:CE1	42:u:104:GLN:CB	2.74	0.69
42:u:96:LEU:HB2	42:u:99:HIS:CD2	2.26	0.69
43:v:8:ARG:NH2	43:v:18:ASP:OD1	2.25	0.69
26:c:165:ASP:OD2	26:c:170:ARG:NH2	2.25	0.69
42:u:82:PHE:HD1	42:u:107:PHE:CE1	2.10	0.69
9:J:265:PHE:CG	9:J:335:LEU:HD21	2.28	0.69
21:W:114:THR:OG1	42:u:143:HIS:ND1	2.24	0.69
6:X:155:TYR:HE1	25:b:23:LEU:HB3	1.57	0.69
27:d:23:GLN:HG2	43:v:72:ASP:HB3	1.73	0.69
35:l:425:ARG:NH2	54:l:702:CDL:OB5	2.25	0.69
27:d:68:PHE:HD1	37:n:44:LEU:HD21	1.57	0.69
41:s:200:LEU:HD11	41:s:285:LEU:HD21	1.74	0.69
1:A:214:GLU:OE2	11:L:175:LYS:NZ	2.26	0.69
22:Y:84:PHE:HE2	43:v:89:TYR:HA	1.58	0.69
35:l:78:LEU:HD11	54:l:701:CDL:H251	1.73	0.69
1:A:154:ALA:HB2	1:A:193:PHE:HZ	1.58	0.68
27:d:97:LYS:NZ	40:r:47:GLU:OE2	2.25	0.68
32:i:268:GLN:HA	40:r:165:VAL:HG11	1.75	0.68
8:I:110:GLN:HG3	21:W:22:LYS:HE3	1.74	0.68
25:b:78:PRO:O	25:b:82:ILE:HG12	1.93	0.68
11:L:131:LYS:NZ	11:L:149:GLU:OE2	2.26	0.68
33:j:78:ALA:O	33:j:87:MET:HG3	1.94	0.68
40:r:191:SER:HB3	48:r:501:PEE:H3	1.74	0.68
9:J:345:LEU:HD23	9:J:345:LEU:C	2.19	0.68
35:l:159:HIS:HB2	40:r:416:ARG:HG2	1.74	0.68
2:B:77:LEU:HD23	41:s:30:TYR:HB3	1.75	0.68
27:d:139:PHE:HD1	38:o:127:ILE:HD12	1.59	0.68
44:w:62:VAL:HG21	44:w:74:ALA:HB2	1.76	0.68
12:M:472:PRO:O	12:M:510:TRP:NE1	2.26	0.67
44:w:132:GLN:OE1	57:w:401:ADP:N6	2.27	0.67
28:e:109:LEU:HD22	40:r:43:ASN:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:88:GLU:OE2	44:w:161:ARG:NH1	2.27	0.67
12:M:395:GLU:O	12:M:425:ASN:ND2	2.27	0.67
15:P:77:GLN:HG3	15:P:87:PHE:HE1	1.59	0.67
32:i:211:MET:HE3	32:i:251:MET:HA	1.76	0.67
40:r:325:MET:HE1	40:r:441:ILE:HD13	1.76	0.67
14:O:38:LEU:O	14:O:124:ARG:NH2	2.28	0.67
21:W:60:LEU:HD11	42:u:98:ARG:HB3	1.75	0.67
41:s:62:ARG:HH21	41:s:68:ILE:HB	1.60	0.67
19:U:26:GLY:HA3	48:j:202:PEE:H37	1.76	0.67
1:A:388:GLY:HA3	1:A:419:ILE:HD11	1.77	0.67
3:C:44:GLU:HG2	3:C:194:TYR:CE2	2.30	0.67
12:M:389:THR:CG2	12:M:473:MET:CE	2.72	0.67
20:V:69:ILE:HG13	20:V:100:THR:HG21	1.77	0.67
20:V:72:LEU:O	20:V:76:ILE:HG12	1.95	0.67
26:c:110:ASP:OD2	38:o:72:ARG:NH2	2.25	0.67
43:v:111:ARG:HA	43:v:114:ARG:HH11	1.58	0.67
24:a:152:LYS:HD3	30:g:96:VAL:HG21	1.76	0.66
2:B:111:GLU:O	2:B:141:ARG:NH1	2.28	0.66
13:N:42:ASP:OD1	13:N:43:LYS:N	2.29	0.66
14:O:132:ILE:HD11	14:O:169:PHE:CD1	2.30	0.66
6:X:79:ILE:O	6:X:83:VAL:HG23	1.94	0.66
5:F:18:GLU:HB3	5:F:52:PRO:HG2	1.76	0.66
27:d:9:VAL:O	27:d:109:ARG:NH2	2.29	0.66
32:i:95:MET:HE3	32:i:149:ILE:HG12	1.73	0.66
1:A:337:MET:HE1	1:A:354:VAL:HG21	1.78	0.66
12:M:131:CYS:HG	45:M:801:SF4:FE1	1.12	0.66
21:W:71:LEU:HB3	21:W:75:PHE:HE2	1.61	0.66
35:l:112:PRO:HB3	39:p:179:MET:HE1	1.76	0.66
35:l:357:ARG:HH12	39:p:76:HIS:HE1	1.42	0.66
2:B:98:ARG:NH2	16:Q:224:ALA:O	2.29	0.66
1:A:41:ILE:HG21	1:A:250:VAL:HG12	1.77	0.66
20:V:37:SER:HB2	20:V:56:THR:HG22	1.78	0.66
1:A:290:GLU:HG2	1:A:294:VAL:HG11	1.78	0.65
5:F:36:PHE:HE2	5:F:91:LEU:HD12	1.61	0.65
6:G:122:MET:HE3	6:G:144:ILE:HD13	1.78	0.65
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.78	0.65
14:O:132:ILE:HD11	14:O:169:PHE:HD1	1.60	0.65
33:j:86:THR:O	33:j:90:MET:HG2	1.95	0.65
17:S:1:MET:C	41:s:30:TYR:CE2	2.74	0.65
32:i:252:GLY:HA3	32:i:290:LEU:HD13	1.78	0.65
43:v:39:MET:SD	43:v:39:MET:N	2.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:88:GLN:NE2	12:M:141:ASP:OD2	2.30	0.65
40:r:241:TYR:OH	40:r:245:ARG:NH1	2.28	0.65
44:w:214:ILE:O	44:w:218:ILE:HG12	1.96	0.65
9:J:356:HIS:O	9:J:357:ARG:O	2.15	0.65
12:M:308:ARG:NH2	12:M:578:PRO:O	2.30	0.65
16:Q:387:GLU:OE2	16:Q:390:GLN:NE2	2.30	0.65
24:a:187:PRO:HA	42:u:48:TRP:CD1	2.32	0.65
26:c:96:ASP:OD1	26:c:97:LEU:N	2.29	0.65
9:J:132:ARG:NH2	50:J:401:NDP:O2X	2.30	0.65
26:c:179:GLU:N	26:c:179:GLU:OE2	2.30	0.65
36:m:58:LEU:HG	36:m:59:ILE:HD12	1.78	0.65
42:u:20:VAL:HB	42:u:24:VAL:HG21	1.79	0.65
15:P:172:ASP:OD2	15:P:187:ILE:N	2.29	0.65
42:u:82:PHE:CG	42:u:107:PHE:CE1	2.84	0.65
26:c:155:PRO:HD3	43:v:4:HIS:CE1	2.32	0.65
41:s:40:VAL:HG12	41:s:46:LEU:HB3	1.79	0.65
43:v:33:GLU:OE1	43:v:33:GLU:N	2.30	0.65
25:b:100:ARG:HE	35:l:60:GLU:HG3	1.62	0.64
9:J:163:LYS:NZ	9:J:253:ILE:O	2.29	0.64
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.30	0.64
32:i:61:LEU:HD11	34:k:26:LEU:HD11	1.78	0.64
35:l:391:SER:O	35:l:395:ILE:HG12	1.97	0.64
35:l:464:ALA:O	35:l:468:ILE:HG12	1.98	0.64
2:B:200:GLU:HG3	13:N:88:ARG:HB2	1.79	0.64
1:A:33:GLY:O	1:A:302:LYS:NZ	2.30	0.64
12:M:77:MET:HE1	12:M:117:MET:HG2	1.79	0.64
9:J:248:GLY:N	9:J:340:ILE:HD13	2.13	0.64
19:U:53:TYR:HB3	42:u:48:TRP:HH2	1.61	0.64
6:X:155:TYR:CE1	25:b:23:LEU:HB3	2.32	0.64
25:b:99:GLU:HG2	35:l:61:MET:HG2	1.79	0.64
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.80	0.64
42:u:24:VAL:HG12	42:u:86:TRP:CG	2.32	0.64
11:L:78:ARG:NH2	12:M:249:GLU:OE1	2.26	0.64
16:Q:292:MET:HE1	16:Q:438:MET:HE1	1.80	0.64
35:l:83:ASP:OD2	35:l:262:ARG:NH1	2.30	0.64
42:u:85:TYR:CE1	42:u:104:GLN:CA	2.81	0.64
32:i:84:TRP:HH2	34:k:59:MET:HE2	1.62	0.64
1:A:50:ASP:O	1:A:59:ARG:NH2	2.30	0.64
35:l:356:ILE:HG22	35:l:359:MET:HE1	1.79	0.64
39:p:117:ASP:O	39:p:121:LYS:HG3	1.98	0.64
42:u:85:TYR:CD1	42:u:104:GLN:HA	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:ARG:HA	8:I:12:ARG:NH2	2.12	0.64
42:u:112:LEU:O	42:u:116:GLY:HA2	1.98	0.64
44:w:78:ALA:HB2	44:w:158:VAL:HG21	1.80	0.63
9:J:117:ARG:O	9:J:121:GLU:HB2	1.97	0.63
6:X:150:ASP:OD2	25:b:16:ARG:NH1	2.32	0.63
19:U:27:GLY:O	19:U:31:ILE:HG13	1.98	0.63
7:H:21:HIS:O	7:H:25:LYS:HG3	1.98	0.63
32:i:278:MET:O	32:i:282:MET:HG3	1.98	0.63
54:u:201:CDL:H531	54:u:201:CDL:H191	1.79	0.63
44:w:98:THR:OG1	44:w:337:ARG:NH2	2.27	0.63
44:w:185:GLU:O	44:w:189:GLU:HG3	1.99	0.63
20:V:66:ILE:HD11	20:V:101:LEU:HD13	1.80	0.63
44:w:169:PHE:O	44:w:173:MET:HG3	1.99	0.63
38:o:7:LYS:HA	38:o:7:LYS:HE3	1.80	0.63
40:r:176:PHE:CZ	40:r:245:ARG:HD3	2.34	0.63
54:g:202:CDL:H391	32:i:334:THR:HG21	1.79	0.63
1:A:98:LYS:NZ	47:A:503:NAI:O3B	2.32	0.62
4:E:37:ARG:NH1	6:G:132:ASP:OD1	2.31	0.62
12:M:645:ARG:NH1	12:M:648:GLU:OE1	2.33	0.62
25:b:109:THR:HG22	25:b:116:VAL:HG12	1.82	0.62
27:d:139:PHE:CD1	38:o:127:ILE:HD12	2.34	0.62
22:Y:84:PHE:CE2	43:v:89:TYR:HA	2.34	0.62
23:Z:29:LEU:HA	23:Z:32:VAL:HG12	1.81	0.62
35:l:288:THR:HG23	35:l:304:PHE:HD1	1.63	0.62
44:w:105:ASP:OD1	44:w:106:VAL:N	2.33	0.62
14:O:200:ASP:OD2	14:O:219:ARG:HG3	1.99	0.62
54:g:202:CDL:H791	54:g:202:CDL:H251	1.81	0.62
12:M:126:LEU:H	12:M:126:LEU:CD1	2.12	0.62
49:X:201:8Q1:O27	49:X:201:8Q1:O33	2.18	0.62
32:i:100:MET:HE3	35:l:595:ILE:HG12	1.80	0.62
33:j:25:PRO:HB2	41:s:60:PRO:HD3	1.81	0.62
35:l:428:PHE:HA	35:l:432:LEU:HD22	1.81	0.62
16:Q:294:ARG:HG2	16:Q:320:ILE:HD13	1.82	0.62
21:W:80:ASP:OD2	42:u:47:ARG:NE	2.28	0.62
33:j:58:VAL:HG21	41:s:286:MET:HE1	1.82	0.62
35:l:250:SER:HB2	35:l:333:ALA:HA	1.82	0.62
36:m:45:LEU:HD23	36:m:50:SER:HA	1.80	0.62
17:S:1:MET:C	41:s:30:TYR:HE2	2.07	0.62
33:j:90:MET:HE2	36:m:151:THR:HA	1.82	0.62
35:l:227:PHE:O	35:l:230:HIS:ND1	2.26	0.62
40:r:108:MET:HB3	40:r:121:LEU:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:403:THR:HA	40:r:406:TYR:CE2	2.35	0.62
41:s:196:ALA:HB3	41:s:274:ARG:HA	1.81	0.62
5:F:40:ARG:NH1	5:F:88:THR:OG1	2.32	0.62
36:m:17:PHE:O	36:m:21:SER:HB2	1.99	0.62
1:A:398:ARG:HG2	1:A:403:ASP:HB3	1.82	0.61
2:B:79:ARG:NH2	8:I:20:LEU:HD21	2.15	0.61
9:J:265:PHE:CE1	9:J:335:LEU:HD23	2.35	0.61
28:e:72:ASP:OD1	39:p:108:HIS:NE2	2.33	0.61
41:s:85:MET:HB3	41:s:233:MET:HE3	1.82	0.61
14:O:116:ALA:HA	14:O:122:TYR:HD2	1.64	0.61
6:G:103:HIS:NE2	6:G:139:MET:SD	2.72	0.61
26:c:63:GLU:N	26:c:63:GLU:OE2	2.33	0.61
16:Q:156:GLU:OE2	16:Q:171:ARG:NH2	2.31	0.61
35:l:37:LYS:HD3	35:l:98:TRP:HE1	1.65	0.61
13:N:120:THR:HG22	13:N:122:GLN:H	1.64	0.61
25:b:126:GLN:OE1	25:b:126:GLN:N	2.33	0.61
12:M:304:GLN:HG2	12:M:615:LEU:HD12	1.83	0.61
12:M:463:SER:O	12:M:467:LYS:HG3	2.00	0.61
32:i:276:ILE:HG21	48:r:501:PEE:H7	1.83	0.61
34:k:25:HIS:O	34:k:28:SER:N	2.26	0.61
36:m:8:ILE:O	36:m:12:ILE:HG13	1.99	0.61
40:r:269:MET:HE1	40:r:296:LEU:HD13	1.82	0.61
41:s:264:LEU:O	41:s:268:ILE:HG12	2.00	0.61
17:S:11:VAL:HG11	41:s:19:PHE:CZ	2.34	0.61
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.36	0.61
5:F:91:LEU:O	5:F:95:LEU:HG	2.00	0.61
14:O:125:LYS:HG2	14:O:126:PRO:HD2	1.81	0.61
19:U:32:LEU:HB3	41:s:310:MET:SD	2.41	0.61
35:l:221:ALA:HA	35:l:226:GLN:HG2	1.82	0.61
15:P:85:GLU:OE2	15:P:142:ARG:NH1	2.33	0.61
16:Q:184:ILE:HD11	16:Q:251:PHE:HZ	1.65	0.61
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.81	0.60
23:Z:33:GLN:NE2	23:Z:43:ASP:OD1	2.34	0.60
6:G:141:PRO:O	6:G:145:VAL:HG23	2.01	0.60
32:i:95:MET:HE2	32:i:149:ILE:CA	2.29	0.60
33:j:112:GLU:OE1	41:s:291:LYS:NZ	2.34	0.60
35:l:407:TRP:O	35:l:411:MET:HG2	2.01	0.60
7:H:69:GLU:HG2	7:H:77:ILE:HG12	1.83	0.60
1:A:447:GLU:O	1:A:451:GLN:HG2	2.01	0.60
9:J:265:PHE:CD1	9:J:335:LEU:CD2	2.85	0.60
40:r:231:LEU:HD23	40:r:235:LEU:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.83	0.60
21:W:65:PHE:O	21:W:69:ILE:HG12	2.00	0.60
25:b:99:GLU:OE1	35:l:2:ASN:ND2	2.34	0.60
32:i:298:TYR:O	32:i:303:THR:OG1	2.20	0.60
42:u:112:LEU:O	42:u:116:GLY:N	2.34	0.60
19:U:78:LEU:HD12	42:u:123:GLY:HA3	1.82	0.60
35:l:3:PRO:HG2	35:l:53:MET:HE1	1.83	0.60
35:l:7:LEU:HA	35:l:10:THR:HG22	1.83	0.60
1:A:325:PRO:HG3	1:A:433:TRP:HB3	1.83	0.60
20:V:54:ALA:O	20:V:58:ARG:HG2	2.02	0.60
32:i:177:LYS:NZ	34:k:97:GLN:O	2.23	0.60
35:l:226:GLN:HG3	35:l:314:MET:HE2	1.84	0.60
1:A:98:LYS:HA	1:A:101:PHE:HD2	1.67	0.60
12:M:64:CYS:O	12:M:184:ARG:NH2	2.31	0.60
35:l:27:TYR:O	35:l:115:ASN:ND2	2.33	0.60
39:p:137:VAL:O	39:p:141:GLN:HG2	2.01	0.60
12:M:213:MET:HG2	12:M:215:MET:HG2	1.84	0.60
16:Q:198:THR:HG23	41:s:32:GLN:HG2	1.82	0.60
33:j:18:VAL:HB	41:s:222:MET:HE1	1.83	0.60
36:m:14:VAL:O	36:m:18:VAL:HG23	2.02	0.60
2:B:167:ILE:HG23	2:B:167:ILE:O	2.02	0.60
33:j:18:VAL:HG11	41:s:76:ILE:HD11	1.82	0.60
35:l:170:GLN:NE2	48:l:703:PEE:O1P	2.35	0.60
40:r:398:MET:O	40:r:402:ILE:HG13	2.02	0.60
11:L:77:VAL:O	11:L:145:PHE:HA	2.01	0.59
12:M:197:THR:HB	12:M:204:MET:HE2	1.84	0.59
41:s:156:MET:HE1	41:s:307:LEU:HD23	1.84	0.59
11:L:111:LEU:HG	11:L:112:MET:HG2	1.84	0.59
12:M:47:THR:HG23	12:M:51:GLN:HB2	1.84	0.59
15:P:173:MET:HB3	15:P:198:PHE:HB2	1.85	0.59
33:j:7:LEU:HD21	48:m:201:PEE:H59	1.84	0.59
37:n:27:LEU:HD21	54:u:201:CDL:H112	1.84	0.59
7:H:64:ASP:OD1	7:H:65:VAL:N	2.36	0.59
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.85	0.59
16:Q:182:ASN:OD1	16:Q:404:LYS:NZ	2.31	0.59
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.36	0.59
16:Q:446:ASP:OD2	41:s:281:ARG:NH1	2.35	0.59
6:X:90:TYR:OH	6:X:114:ASP:OD2	2.20	0.59
32:i:203:LEU:HB2	32:i:347:ASN:HD21	1.66	0.59
35:l:357:ARG:NH1	39:p:76:HIS:HE1	2.00	0.59
5:F:90:THR:O	5:F:94:VAL:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:107:SER:OG	16:Q:317:ASP:OD2	2.20	0.59
6:X:120:MET:HE1	39:p:24:LEU:HD23	1.85	0.59
44:w:60:ILE:HD12	44:w:203:VAL:HB	1.83	0.59
11:L:163:ASN:O	11:L:171:ARG:HA	2.03	0.59
6:X:76:LEU:HD21	25:b:20:ARG:HH21	1.67	0.59
24:a:111:GLU:OE1	24:a:119:ARG:NH2	2.35	0.59
35:l:112:PRO:HB3	39:p:179:MET:CE	2.33	0.59
14:O:110:MET:O	14:O:114:GLU:HG3	2.03	0.59
6:X:69:SER:OG	6:X:70:ASP:N	2.34	0.59
27:d:68:PHE:CD1	37:n:44:LEU:HD21	2.37	0.59
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.84	0.59
14:O:63:ILE:HD12	14:O:82:VAL:HG22	1.85	0.59
39:p:105:ASP:OD1	39:p:122:ARG:NH2	2.31	0.59
12:M:193:ASP:OD1	14:O:111:ARG:NH2	2.31	0.59
32:i:190:MET:HG2	32:i:201:THR:HG23	1.85	0.59
44:w:66:ILE:HD12	44:w:234:LEU:HD23	1.85	0.59
32:i:58:LYS:O	32:i:62:THR:HG23	2.03	0.58
3:C:80:ALA:HB2	3:C:86:MET:HE2	1.85	0.58
13:N:5:GLN:O	13:N:8:ARG:HG2	2.03	0.58
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.36	0.58
25:b:104:ILE:CD1	27:d:18:PRO:HG3	2.33	0.58
10:K:106:GLN:HB2	10:K:110:HIS:CD2	2.37	0.58
12:M:126:LEU:HD12	12:M:126:LEU:N	2.14	0.58
40:r:331:ASN:ND2	40:r:335:GLU:OE2	2.36	0.58
1:A:446:LEU:O	1:A:450:MET:HG3	2.03	0.58
3:C:101:ASP:OD2	41:s:54:LYS:HD2	2.04	0.58
16:Q:60:HIS:O	16:Q:61:TRP:C	2.46	0.58
1:A:159:ARG:NH2	14:O:176:CYS:O	2.37	0.58
9:J:248:GLY:CA	9:J:340:ILE:HD12	2.32	0.58
16:Q:210:MET:HE3	16:Q:247:PHE:CZ	2.38	0.58
24:a:135:LYS:HZ2	24:a:135:LYS:HB3	1.68	0.58
3:C:113:MET:HE1	16:Q:86:PRO:HB2	1.85	0.58
35:l:474:PRO:HD3	43:v:70:LYS:HE3	1.84	0.58
42:u:85:TYR:CE1	42:u:104:GLN:HA	2.39	0.58
21:W:76:GLN:NE2	21:W:80:ASP:OD1	2.36	0.58
35:l:590:SER:O	35:l:594:THR:HG23	2.04	0.58
40:r:318:ALA:HB1	40:r:374:ASN:OD1	2.03	0.58
44:w:203:VAL:HG22	44:w:254:GLU:HB2	1.86	0.58
9:J:369:VAL:HG12	9:J:370:LYS:HG2	1.85	0.58
36:m:21:SER:O	36:m:23:LYS:NZ	2.31	0.58
40:r:1:MET:HB2	40:r:52:PHE:CD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.22	0.58
11:L:92:ASN:HB3	15:P:238:PRO:HA	1.85	0.58
19:U:63:MET:O	42:u:130:LYS:NZ	2.37	0.58
26:c:119:THR:HG22	38:o:11:LEU:HA	1.86	0.58
1:A:113:LEU:HD13	1:A:149:MET:HE1	1.86	0.58
46:A:502:FMN:O4'	46:A:502:FMN:O2'	2.22	0.58
13:N:42:ASP:OD2	13:N:46:ASN:ND2	2.32	0.58
54:V:201:CDL:H452	54:V:201:CDL:H211	1.85	0.58
2:B:99:GLY:H	2:B:169:GLU:HG2	1.69	0.57
12:M:389:THR:O	12:M:390:THR:OG1	2.20	0.57
12:M:647:GLU:HB2	12:M:654:VAL:HG21	1.86	0.57
28:e:51:PRO:O	28:e:53:ILE:HG13	2.04	0.57
9:J:157:LYS:NZ	9:J:197:GLU:OE2	2.36	0.57
31:h:21:GLN:O	31:h:25:GLN:NE2	2.37	0.57
20:V:61:PHE:HD2	20:V:104:ARG:HH12	1.52	0.57
20:V:88:LEU:O	20:V:92:ILE:HG13	2.04	0.57
35:l:562:LEU:HB3	35:l:563:PRO:HD3	1.86	0.57
42:u:82:PHE:HD1	42:u:107:PHE:CZ	2.22	0.57
30:g:117:GLU:OE1	30:g:117:GLU:N	2.29	0.57
40:r:328:CYS:O	40:r:332:THR:HG23	2.03	0.57
2:B:179:THR:OG1	2:B:182:GLU:OE2	2.23	0.57
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.87	0.57
35:l:102:GLU:OE1	35:l:456:ARG:NH2	2.34	0.57
1:A:159:ARG:NE	1:A:161:GLU:OE2	2.38	0.57
15:P:86:ILE:HD12	15:P:141:ILE:HD11	1.86	0.57
41:s:287:HIS:HD1	41:s:291:LYS:HD2	1.70	0.57
15:P:64:TYR:OH	15:P:103:HIS:NE2	2.30	0.57
8:I:13:ASN:ND2	8:I:20:LEU:H	2.03	0.57
25:b:14:GLN:HE22	39:p:157:ALA:HB3	1.70	0.57
30:g:63:GLN:O	30:g:67:VAL:HG23	2.05	0.57
32:i:75:ILE:HG21	34:k:43:MET:HG2	1.86	0.57
16:Q:86:PRO:HB3	16:Q:94:VAL:HG23	1.87	0.57
27:d:107:GLN:O	27:d:111:LYS:HG3	2.04	0.57
36:m:25:SER:O	36:m:28:TYR:N	2.35	0.57
2:B:70:LEU:HD21	41:s:277:TYR:CZ	2.40	0.57
5:F:62:GLN:OE1	5:F:80:ASN:ND2	2.38	0.57
21:W:74:LEU:O	21:W:78:GLU:HG3	2.05	0.57
35:l:36:VAL:HG13	35:l:122:LEU:HD22	1.85	0.57
1:A:209:GLU:HB2	1:A:242:VAL:HG21	1.85	0.56
9:J:248:GLY:N	9:J:340:ILE:HD11	2.12	0.56
35:l:190:LEU:HD12	35:l:196:TRP:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ILE:HD11	1:A:245:VAL:HG12	1.87	0.56
8:I:30:GLU:OE1	8:I:30:GLU:N	2.31	0.56
33:j:7:LEU:O	33:j:11:VAL:HG23	2.05	0.56
35:l:483:PRO:HG2	35:l:486:MET:HE3	1.86	0.56
16:Q:182:ASN:CG	16:Q:403:PRO:CB	2.78	0.56
17:S:13:ALA:HB2	41:s:264:LEU:HD11	1.87	0.56
17:S:44:GLN:O	17:S:48:MET:HG3	2.06	0.56
1:A:244:ASN:N	46:A:502:FMN:O1P	2.37	0.56
24:a:96:ALA:HB2	27:d:61:TYR:CE1	2.40	0.56
32:i:221:HIS:HB2	32:i:323:MET:HE1	1.86	0.56
35:l:37:LYS:HE2	35:l:102:GLU:HG3	1.86	0.56
36:m:34:ILE:HD13	36:m:61:LEU:HD12	1.88	0.56
41:s:253:GLU:O	41:s:257:ILE:HG12	2.06	0.56
44:w:85:HIS:HA	44:w:158:VAL:HG23	1.86	0.56
44:w:217:ARG:HA	44:w:220:LYS:HG2	1.88	0.56
4:E:16:SER:HA	11:L:54:ALA:HA	1.88	0.56
12:M:356:ASP:O	12:M:360:ARG:HG2	2.05	0.56
21:W:144:THR:HB	41:s:96:ILE:HG23	1.86	0.56
29:f:65:ASP:OD2	30:g:79:LYS:NZ	2.38	0.56
1:A:288:VAL:HG21	1:A:303:HIS:ND1	2.20	0.56
2:B:114:ILE:HD12	12:M:130:ILE:CG2	2.35	0.56
6:G:143:GLU:HA	6:G:146:ASP:OD1	2.04	0.56
37:n:26:TYR:CZ	37:n:30:ARG:HD2	2.41	0.56
37:n:47:ARG:NH2	37:n:53:GLU:OE2	2.31	0.56
2:B:201:ILE:O	2:B:205:ILE:HG13	2.05	0.56
22:Y:97:LEU:HD12	43:v:104:ARG:HB2	1.88	0.56
12:M:194:ASP:OD1	12:M:212:LYS:NZ	2.34	0.56
44:w:172:ALA:HB2	44:w:237:ILE:HG13	1.88	0.56
32:i:38:LEU:HD12	34:k:73:LEU:HD22	1.88	0.56
7:H:76:GLN:HB2	7:H:79:GLU:HG2	1.86	0.56
11:L:78:ARG:NE	11:L:148:GLU:OE1	2.20	0.56
33:j:16:LEU:O	33:j:20:ILE:HG22	2.06	0.56
41:s:98:MET:HE1	41:s:104:PHE:CG	2.42	0.55
4:E:110:THR:HG21	15:P:220:VAL:HG11	1.87	0.55
5:F:36:PHE:CE2	5:F:91:LEU:HD12	2.41	0.55
25:b:84:TYR:OH	27:d:49:ARG:NH1	2.39	0.55
26:c:169:GLU:HA	27:d:123:GLN:HB2	1.86	0.55
35:l:293:ILE:HD12	35:l:422:TYR:HB3	1.87	0.55
9:J:327:MET:HE3	9:J:329:LEU:HD11	1.89	0.55
35:l:341:MET:HE2	35:l:454:ILE:HD13	1.89	0.55
38:o:6:TYR:HE2	38:o:15:PRO:HD3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:399:ASN:O	40:r:403:THR:HG22	2.07	0.55
42:u:112:LEU:HA	42:u:117:TRP:H	1.70	0.55
7:H:30:LYS:O	7:H:34:VAL:HG23	2.05	0.55
19:U:74:GLN:OE1	19:U:74:GLN:N	2.40	0.55
6:G:118:ILE:O	6:G:122:MET:HG2	2.06	0.55
39:p:95:GLU:HG3	40:r:418:LYS:HD3	1.89	0.55
3:C:96:SER:HB3	3:C:99:GLN:NE2	2.22	0.55
35:l:448:PRO:O	35:l:452:ASN:ND2	2.26	0.55
40:r:44:GLN:NE2	40:r:50:LEU:HD23	2.11	0.55
1:A:395:VAL:HG11	1:A:412:LEU:HD13	1.88	0.55
12:M:498:GLN:HE22	12:M:501:ARG:HH21	1.53	0.55
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.89	0.55
35:l:7:LEU:HD22	35:l:46:LEU:HD11	1.89	0.55
42:u:82:PHE:N	42:u:107:PHE:HD1	2.05	0.55
8:I:95:VAL:O	15:P:105:ASN:ND2	2.37	0.55
9:J:65:LEU:HD22	9:J:129:LEU:HD22	1.89	0.55
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.88	0.55
28:e:85:TRP:O	28:e:89:VAL:HG13	2.07	0.55
32:i:291:TYR:HA	40:r:151:PHE:HZ	1.72	0.55
40:r:14:MET:O	40:r:18:SER:OG	2.23	0.55
12:M:496:ILE:O	12:M:500:ILE:HG12	2.06	0.55
32:i:7:THR:HG21	54:i:401:CDL:H731	1.88	0.55
1:A:114:VAL:HG23	1:A:242:VAL:HA	1.89	0.54
3:C:71:CYS:HB3	16:Q:141:TYR:HB2	1.89	0.54
9:J:171:ASN:HA	9:J:327:MET:HE2	1.89	0.54
9:J:265:PHE:CG	9:J:335:LEU:CD2	2.90	0.54
12:M:124:HIS:HB3	16:Q:375:MET:HE3	1.87	0.54
12:M:126:LEU:HB3	16:Q:378:LEU:CD2	2.37	0.54
26:c:118:ASP:N	26:c:118:ASP:OD1	2.40	0.54
32:i:72:MET:HE3	34:k:9:ILE:HD13	1.88	0.54
33:j:70:ALA:HA	33:j:73:LEU:HD12	1.89	0.54
44:w:125:ASP:O	44:w:130:ARG:NH2	2.40	0.54
2:B:77:LEU:HG	41:s:31:MET:HG3	1.88	0.54
2:B:78:PHE:O	8:I:12:ARG:NH2	2.33	0.54
25:b:15:LEU:HD13	39:p:170:ILE:HG21	1.88	0.54
40:r:340:ARG:O	40:r:340:ARG:HG2	2.07	0.54
7:H:38:ILE:O	7:H:45:ARG:NH1	2.37	0.54
31:h:78:ALA:HA	31:h:81:ARG:HD3	1.89	0.54
35:l:559:GLU:O	35:l:563:PRO:HD2	2.06	0.54
42:u:112:LEU:O	42:u:116:GLY:CA	2.56	0.54
2:B:168:VAL:HG21	2:B:201:ILE:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:83:ARG:NH1	16:Q:212:GLU:OE2	2.32	0.54
14:O:59:ASN:O	14:O:63:ILE:HG12	2.08	0.54
24:a:87:THR:O	24:a:91:VAL:HG22	2.08	0.54
24:a:175:ASP:OD1	24:a:177:ALA:N	2.22	0.54
32:i:146:SER:O	32:i:149:ILE:HB	2.06	0.54
32:i:281:LEU:O	32:i:285:THR:OG1	2.21	0.54
1:A:116:ASN:ND2	1:A:212:LEU:HD13	2.23	0.54
3:C:44:GLU:CG	3:C:194:TYR:HE2	2.20	0.54
7:H:28:TYR:HA	7:H:31:ILE:HD12	1.88	0.54
7:H:112:TRP:CE2	15:P:87:PHE:HB3	2.42	0.54
12:M:371:VAL:HG22	12:M:533:GLY:HA2	1.89	0.54
33:j:15:SER:O	33:j:18:VAL:HG12	2.08	0.54
1:A:169:LEU:HD22	1:A:197:VAL:HG21	1.89	0.54
2:B:171:PRO:HB2	13:N:93:MET:HE1	1.90	0.54
3:C:191:ARG:O	3:C:195:ARG:HG3	2.08	0.54
5:F:23:LEU:O	5:F:57:GLU:HA	2.08	0.54
16:Q:139:LEU:HD11	16:Q:424:ILE:HD13	1.88	0.54
19:U:55:VAL:HG13	42:u:48:TRP:HE3	1.71	0.54
25:b:104:ILE:HB	43:v:48:ASP:HB3	1.89	0.54
40:r:326:LEU:HA	40:r:329:LEU:HD12	1.90	0.54
20:V:14:GLU:HG3	20:V:84:PRO:HB3	1.89	0.54
55:g:201:PLX:H232	32:i:332:LEU:HB3	1.90	0.54
54:l:701:CDL:H652	55:r:502:PLX:H122	1.90	0.54
41:s:28:LEU:O	41:s:32:GLN:HG3	2.07	0.54
1:A:357:MET:HB3	1:A:361:THR:HG21	1.90	0.54
4:E:18:LYS:NZ	15:P:152:PRO:HG2	2.23	0.54
14:O:102:ALA:HB2	14:O:112:VAL:HG21	1.90	0.54
32:i:161:SER:OG	32:i:184:ILE:O	2.26	0.54
5:F:57:GLU:OE1	5:F:57:GLU:N	2.40	0.54
40:r:159:PRO:HG2	48:r:501:PEE:H35	1.90	0.54
40:r:391:ILE:O	40:r:394:ILE:HG22	2.08	0.54
2:B:43:MET:HG3	2:B:43:MET:O	2.08	0.54
22:Y:100:LEU:O	43:v:111:ARG:NH1	2.41	0.54
35:l:76:LEU:HD21	35:l:196:TRP:HE3	1.73	0.54
36:m:168:ILE:HG13	36:m:169:MET:N	2.21	0.54
2:B:168:VAL:HG23	2:B:168:VAL:O	2.07	0.53
15:P:55:HIS:HB3	15:P:56:LYS:NZ	2.22	0.53
18:T:102:LEU:HB2	18:T:120:GLN:HG3	1.90	0.53
32:i:153:LEU:O	32:i:157:MET:HG3	2.08	0.53
35:l:383:MET:HB3	35:l:386:LEU:HD12	1.89	0.53
40:r:139:GLN:HE22	40:r:340:ARG:NH1	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:60:GLY:O	42:u:63:VAL:HG12	2.08	0.53
1:A:52:ARG:HE	10:K:77:GLN:NE2	2.06	0.53
1:A:385:CYS:HB3	45:A:501:SF4:S2	2.48	0.53
18:T:60:LYS:HG2	18:T:62:VAL:HG23	1.89	0.53
38:o:30:ARG:NH1	39:p:9:TYR:CD1	2.76	0.53
7:H:96:ARG:NH1	7:H:96:ARG:HB2	2.24	0.53
9:J:61:ALA:HB3	9:J:82:VAL:HG13	1.90	0.53
25:b:31:ARG:NH2	39:p:117:ASP:OD1	2.39	0.53
54:g:202:CDL:H271	54:g:202:CDL:H742	1.90	0.53
32:i:146:SER:HA	32:i:149:ILE:HD12	1.89	0.53
35:l:488:MET:O	35:l:492:ILE:HG12	2.09	0.53
35:l:556:ILE:O	35:l:560:THR:OG1	2.26	0.53
44:w:38:TYR:OH	44:w:292:HIS:ND1	2.26	0.53
14:O:58:GLU:OE1	14:O:62:ARG:NH1	2.41	0.53
22:Y:83:HIS:CE1	22:Y:84:PHE:HE1	2.26	0.53
24:a:90:ASN:HD22	54:a:201:CDL:CA5	2.21	0.53
34:k:8:ILE:HG21	34:k:43:MET:HB2	1.90	0.53
54:l:701:CDL:H871	54:l:701:CDL:H642	1.89	0.53
42:u:91:TYR:CD1	42:u:91:TYR:C	2.86	0.53
3:C:82:PRO:HA	41:s:34:ARG:HB3	1.90	0.53
6:G:120:MET:HA	6:G:123:GLU:HG3	1.90	0.53
10:K:76:LEU:HD12	10:K:79:HIS:CD2	2.44	0.53
12:M:628:GLU:OE1	12:M:633:THR:OG1	2.27	0.53
13:N:97:PRO:HG2	13:N:100:THR:HG23	1.90	0.53
23:Z:25:GLU:HA	23:Z:30:GLU:OE2	2.08	0.53
24:a:175:ASP:OD1	24:a:176:LYS:N	2.42	0.53
39:p:66:GLN:OE1	39:p:66:GLN:N	2.41	0.53
8:I:54:TYR:CZ	16:Q:362:LYS:HD2	2.44	0.53
9:J:87:GLU:HG3	9:J:88:PRO:HD2	1.91	0.53
11:L:162:ALA:O	11:L:170:THR:OG1	2.25	0.53
19:U:55:VAL:HG13	42:u:48:TRP:CE3	2.44	0.53
40:r:271:MET:HE2	40:r:271:MET:HA	1.90	0.53
2:B:105:ARG:HD2	13:N:108:TYR:CG	2.44	0.53
9:J:166:HIS:HB3	9:J:200:ILE:HD13	1.91	0.53
16:Q:251:PHE:HB3	16:Q:341:LEU:HD11	1.90	0.53
21:W:62:ILE:O	21:W:66:GLU:HG2	2.09	0.53
15:P:165:TRP:CZ2	16:Q:111:PRO:HG2	2.44	0.53
24:a:130:GLU:O	24:a:134:GLU:HG3	2.09	0.53
28:e:97:ILE:O	28:e:101:LEU:HB2	2.09	0.53
36:m:125:TRP:HA	36:m:128:TYR:CD2	2.43	0.53
6:G:144:ILE:O	6:G:148:ILE:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:47:ASP:N	18:T:47:ASP:OD1	2.41	0.53
23:Z:24:ILE:HG23	23:Z:29:LEU:HB2	1.91	0.53
44:w:258:TYR:HE2	44:w:269:VAL:HG13	1.74	0.53
44:w:40:PRO:HD3	44:w:296:MET:CE	2.39	0.52
12:M:406:ASN:ND2	12:M:688:GLN:O	2.41	0.52
14:O:148:ILE:O	14:O:152:ILE:HG13	2.10	0.52
14:O:236:GLU:OE1	14:O:239:LYS:NZ	2.40	0.52
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.91	0.52
35:l:5:ALA:HA	35:l:61:MET:HE1	1.91	0.52
35:l:86:SER:OG	35:l:262:ARG:NH2	2.42	0.52
40:r:54:LEU:O	40:r:113:THR:HG21	2.09	0.52
44:w:175:ARG:HG2	44:w:175:ARG:HH11	1.75	0.52
5:F:39:LYS:HB3	5:F:40:ARG:HG3	1.92	0.52
25:b:88:TYR:CZ	27:d:49:ARG:HG2	2.44	0.52
24:a:64:ASP:OD2	40:r:354:LEU:HB2	2.09	0.52
24:a:187:PRO:HA	42:u:48:TRP:HD1	1.74	0.52
36:m:62:GLY:HA3	41:s:110:SER:OG	2.08	0.52
40:r:76:MET:HE3	40:r:99:LEU:HD22	1.90	0.52
1:A:185:ASN:C	1:A:187:CYS:H	2.18	0.52
2:B:54:THR:HG22	21:W:32:GLY:HA3	1.91	0.52
3:C:133:MET:HE3	3:C:173:LEU:HB2	1.92	0.52
5:F:57:GLU:O	12:M:655:ARG:NH2	2.43	0.52
19:U:11:ASN:OD1	19:U:15:LYS:NZ	2.42	0.52
25:b:106:PRO:O	43:v:68:LYS:NZ	2.31	0.52
35:l:19:ILE:HG21	54:l:701:CDL:H852	1.91	0.52
35:l:60:GLU:OE2	35:l:83:ASP:HA	2.10	0.52
35:l:359:MET:O	35:l:436:ARG:NH2	2.43	0.52
44:w:213:GLU:OE2	44:w:217:ARG:HD2	2.09	0.52
9:J:85:ARG:HH21	50:J:401:NDP:C5A	2.23	0.52
13:N:17:HIS:CE1	13:N:26:VAL:HG11	2.45	0.52
15:P:108:PHE:O	15:P:160:TYR:OH	2.24	0.52
27:d:73:ASP:OD1	27:d:75:THR:OG1	2.28	0.52
55:g:201:PLX:H301	32:i:347:ASN:HB3	1.92	0.52
39:p:64:LEU:HA	39:p:67:ALA:HB3	1.92	0.52
40:r:51:ASN:HD22	40:r:51:ASN:N	2.07	0.52
44:w:213:GLU:O	44:w:216:SER:OG	2.24	0.52
54:g:202:CDL:H162	32:i:245:MET:HE1	1.91	0.52
16:Q:182:ASN:HB3	16:Q:403:PRO:HB3	1.92	0.52
41:s:17:VAL:HG12	41:s:232:ILE:HD12	1.92	0.52
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.92	0.52
6:X:90:TYR:HE1	23:Z:44:PRO:HB2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:23:ARG:HG2	36:m:23:LYS:HE2	1.91	0.52
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.91	0.52
35:l:306:THR:O	35:l:310:LEU:HG	2.10	0.52
1:A:380:GLY:HA2	1:A:386:ARG:HB2	1.92	0.52
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.33	0.52
40:r:457:PRO:HG2	40:r:458:LEU:HD12	1.91	0.52
42:u:162:LYS:HE2	42:u:162:LYS:HA	1.92	0.52
1:A:42:PHE:CE2	1:A:275:LEU:HD11	2.46	0.51
12:M:167:PRO:HD2	12:M:215:MET:HE1	1.92	0.51
17:S:47:LEU:HD22	42:u:22:SER:HB2	1.90	0.51
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.45	0.51
54:l:701:CDL:HA62	54:l:701:CDL:H511	1.92	0.51
42:u:92:SER:OG	42:u:95:GLN:HA	2.10	0.51
2:B:90:LYS:HG3	13:N:91:HIS:CE1	2.45	0.51
12:M:70:SER:O	12:M:184:ARG:NH1	2.43	0.51
12:M:252:ASP:OD1	12:M:253:VAL:N	2.42	0.51
13:N:17:HIS:ND1	13:N:26:VAL:HG11	2.25	0.51
13:N:122:GLN:HA	18:T:59:GLN:HG2	1.91	0.51
21:W:70:ALA:HB2	42:u:125:LEU:HD13	1.91	0.51
3:C:71:CYS:HB3	16:Q:141:TYR:CB	2.41	0.51
12:M:565:PHE:CD2	12:M:567:ILE:HD11	2.45	0.51
14:O:206:ASP:OD1	14:O:206:ASP:N	2.43	0.51
15:P:148:ASP:OD1	15:P:148:ASP:N	2.44	0.51
22:Y:105:ASP:OD1	43:v:111:ARG:NH2	2.44	0.51
32:i:211:MET:CE	32:i:251:MET:HA	2.40	0.51
32:i:280:THR:O	32:i:284:MET:HG2	2.09	0.51
34:k:14:ILE:HD13	36:m:18:VAL:HG22	1.91	0.51
35:l:482:MET:HE3	35:l:486:MET:HG2	1.92	0.51
36:m:1:MET:SD	36:m:4:TYR:N	2.77	0.51
3:C:139:GLY:O	3:C:144:HIS:ND1	2.43	0.51
9:J:192:ARG:NH1	9:J:198:ALA:O	2.44	0.51
12:M:388:ASN:ND2	12:M:513:MET:O	2.41	0.51
28:e:108:TYR:HE1	55:r:502:PLX:H11	1.76	0.51
37:n:47:ARG:HH22	37:n:53:GLU:CD	2.17	0.51
43:v:5:LEU:HD22	43:v:9:TYR:HE2	1.76	0.51
1:A:410:ASP:O	1:A:413:TRP:HB3	2.10	0.51
9:J:106:MET:HE1	18:T:56:SER:HB2	1.91	0.51
12:M:83:GLU:HG2	12:M:84:LYS:HG3	1.92	0.51
12:M:126:LEU:HB3	16:Q:378:LEU:HD22	1.93	0.51
12:M:476:LEU:HD21	12:M:481:LEU:HD21	1.91	0.51
13:N:39:VAL:HG23	13:N:50:GLU:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:315:GLU:O	16:Q:346:GLN:NE2	2.41	0.51
36:m:40:GLY:O	36:m:44:VAL:HG23	2.10	0.51
44:w:139:ARG:NH1	44:w:166:ASP:OD1	2.44	0.51
1:A:282:VAL:O	14:O:143:ARG:NH2	2.44	0.51
18:T:79:VAL:HG21	18:T:84:ILE:HD13	1.93	0.51
24:a:137:MET:HE2	37:n:42:SER:HB3	1.92	0.51
26:c:87:ASP:OD2	26:c:90:TYR:N	2.43	0.51
54:g:202:CDL:H242	40:r:97:THR:HG21	1.91	0.51
32:i:110:PRO:HB2	35:l:594:THR:HG21	1.91	0.51
35:l:213:LEU:HB3	35:l:273:VAL:HG11	1.93	0.51
40:r:354:LEU:O	40:r:357:THR:HG22	2.10	0.51
2:B:63:TRP:CH2	41:s:183:MET:HE3	2.45	0.51
9:J:207:PHE:HB2	9:J:214:LEU:HD13	1.93	0.51
11:L:90:GLY:HA3	15:P:238:PRO:HB2	1.91	0.51
12:M:539:LYS:HA	12:M:539:LYS:HE3	1.93	0.51
17:S:55:SER:O	17:S:64:LYS:NZ	2.44	0.51
34:k:98:CYS:HB2	35:l:580:GLN:HB2	1.93	0.51
14:O:102:ALA:HA	14:O:107:VAL:HG12	1.93	0.51
14:O:137:THR:HG22	14:O:138:THR:H	1.76	0.51
32:i:44:LEU:HD22	32:i:122:ILE:HD13	1.93	0.51
35:l:138:PHE:HE1	40:r:379:LEU:HD23	1.76	0.51
40:r:122:PHE:HD1	40:r:238:LEU:HD13	1.75	0.51
5:F:58:CYS:HB2	5:F:61:VAL:CG2	2.40	0.51
12:M:382:ARG:HD3	12:M:527:ASP:OD1	2.11	0.51
25:b:110:ILE:HG21	27:d:16:ARG:HB3	1.92	0.51
26:c:143:MET:HA	26:c:143:MET:HE3	1.93	0.51
33:j:73:LEU:O	41:s:160:TYR:OH	2.29	0.51
55:j:203:PLX:H151	55:j:203:PLX:H341	1.92	0.51
44:w:146:ALA:HB1	44:w:157:VAL:HG21	1.92	0.51
1:A:322:SER:HG	1:A:374:TYR:HH	1.55	0.51
2:B:49:ASP:OD1	2:B:49:ASP:N	2.39	0.51
3:C:66:THR:HG21	3:C:76:MET:SD	2.51	0.51
18:T:114:CYS:SG	18:T:116:LEU:HG	2.51	0.51
23:Z:25:GLU:OE2	23:Z:25:GLU:N	2.42	0.51
35:l:10:THR:O	35:l:14:ILE:HG23	2.11	0.51
42:u:85:TYR:CD1	42:u:104:GLN:CA	2.94	0.51
4:E:80:ASP:O	4:E:84:ILE:HG13	2.11	0.50
6:G:104:PHE:O	6:G:108:LEU:HB2	2.11	0.50
11:L:174:THR:HG21	14:O:114:GLU:OE1	2.11	0.50
14:O:239:LYS:HG3	14:O:243:PHE:CE2	2.47	0.50
15:P:119:VAL:HG12	15:P:121:THR:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:38:LEU:HD21	36:m:37:GLY:HA2	1.92	0.50
36:m:168:ILE:O	36:m:172:THR:OG1	2.29	0.50
1:A:244:ASN:OD1	1:A:245:VAL:N	2.41	0.50
3:C:147:TYR:CD1	3:C:148:SER:N	2.79	0.50
8:I:70:MET:HG3	15:P:66:ALA:HB1	1.92	0.50
16:Q:182:ASN:ND2	16:Q:403:PRO:HB3	2.26	0.50
54:V:201:CDL:H342	48:V:203:PEE:H25	1.93	0.50
6:X:117:GLU:OE1	39:p:20:TYR:OH	2.27	0.50
25:b:86:LEU:HD11	35:l:9:LEU:HD12	1.91	0.50
28:e:140:ASN:HD22	28:e:144:PRO:HG3	1.76	0.50
40:r:225:ILE:O	40:r:229:MET:HG3	2.11	0.50
41:s:62:ARG:HH11	41:s:64:ALA:HA	1.76	0.50
41:s:287:HIS:ND1	41:s:291:LYS:HD2	2.25	0.50
2:B:70:LEU:HD21	41:s:277:TYR:CE2	2.46	0.50
6:G:84:LEU:O	6:G:88:LYS:HG2	2.11	0.50
12:M:117:MET:HE1	12:M:139:LEU:HD12	1.93	0.50
28:e:114:MET:N	28:e:114:MET:SD	2.84	0.50
32:i:100:MET:HE1	35:l:595:ILE:HG23	1.94	0.50
32:i:191:THR:HA	32:i:194:LEU:HD23	1.92	0.50
34:k:23:ARG:HD3	36:m:23:LYS:HB2	1.94	0.50
35:l:357:ARG:HH12	39:p:76:HIS:CE1	2.26	0.50
7:H:55:LYS:HD3	7:H:72:LEU:HD22	1.93	0.50
13:N:32:ASP:OD2	13:N:58:ARG:NH2	2.44	0.50
21:W:84:LEU:HD12	42:u:8:PRO:HD2	1.92	0.50
26:c:83:GLN:HG3	26:c:112:TYR:O	2.12	0.50
31:h:86:LEU:HD22	31:h:91:LYS:HG2	1.93	0.50
32:i:310:ASN:HB2	44:w:309:THR:HG22	1.92	0.50
35:l:481:THR:HB	43:v:92:HIS:ND1	2.26	0.50
39:p:57:MET:HE2	39:p:57:MET:HA	1.94	0.50
42:u:155:GLU:N	42:u:155:GLU:OE2	2.45	0.50
16:Q:210:MET:HE3	16:Q:247:PHE:HZ	1.75	0.50
54:l:701:CDL:H801	55:r:502:PLX:H211	1.93	0.50
44:w:245:PHE:O	44:w:249:MET:HG2	2.12	0.50
1:A:222:LYS:NZ	12:M:204:MET:HE1	2.26	0.50
1:A:298:GLU:HG2	1:A:302:LYS:HE2	1.93	0.50
2:B:148:ASP:OD1	2:B:150:THR:OG1	2.30	0.50
25:b:117:ILE:HG22	25:b:118:PRO:HD2	1.93	0.50
33:j:90:MET:CE	36:m:151:THR:HA	2.41	0.50
1:A:50:ASP:HB3	1:A:55:GLY:HA3	1.93	0.50
2:B:168:VAL:HG11	2:B:205:ILE:HD11	1.94	0.50
7:H:81:ILE:O	7:H:85:GLU:OE1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:96:ARG:HB2	7:H:96:ARG:CZ	2.41	0.50
9:J:167:ILE:HD13	9:J:201:ILE:HB	1.92	0.50
15:P:215:GLU:OE2	15:P:216:VAL:HG13	2.12	0.50
33:j:63:LEU:HD23	34:k:72:ALA:HB2	1.94	0.50
11:L:121:LEU:HD22	11:L:124:LEU:HD22	1.93	0.50
55:g:201:PLX:H322	32:i:347:ASN:HD22	1.75	0.50
14:O:53:PHE:CD2	14:O:97:ALA:HA	2.47	0.50
14:O:194:GLU:N	14:O:194:GLU:OE1	2.45	0.50
16:Q:52:MET:O	32:i:171:ASN:OD1	2.30	0.50
16:Q:259:GLU:CD	21:W:23:ARG:HH21	2.20	0.50
23:Z:49:GLU:N	23:Z:49:GLU:OE2	2.44	0.50
26:c:57:MET:HE1	26:c:78:LEU:HD21	1.92	0.50
32:i:88:LYS:HA	32:i:148:SER:OG	2.11	0.50
33:j:49:LEU:N	33:j:50:PRO:HD2	2.27	0.50
35:l:44:PHE:HB2	35:l:94:LEU:HB3	1.94	0.50
1:A:380:GLY:O	1:A:386:ARG:NH1	2.43	0.49
10:K:76:LEU:O	10:K:79:HIS:HB2	2.12	0.49
16:Q:182:ASN:CG	16:Q:403:PRO:HB3	2.36	0.49
18:T:39:THR:HG22	18:T:62:VAL:HG22	1.94	0.49
32:i:223:SER:OG	44:w:306:ASN:ND2	2.42	0.49
36:m:25:SER:O	36:m:27:ILE:N	2.45	0.49
2:B:66:LEU:HB3	41:s:277:TYR:OH	2.12	0.49
2:B:77:LEU:O	2:B:77:LEU:HD22	2.12	0.49
9:J:345:LEU:C	9:J:345:LEU:CD2	2.85	0.49
14:O:197:THR:HG23	14:O:200:ASP:H	1.78	0.49
26:c:152:SER:HA	43:v:5:LEU:HD11	1.93	0.49
27:d:36:ILE:O	27:d:40:LEU:HB2	2.12	0.49
42:u:16:GLN:CD	42:u:68:LEU:HD13	2.36	0.49
16:Q:182:ASN:CG	16:Q:403:PRO:HB2	2.38	0.49
54:V:202:CDL:H732	54:V:202:CDL:H562	1.94	0.49
6:X:76:LEU:O	6:X:80:LYS:HG2	2.11	0.49
27:d:119:GLU:HG2	43:v:52:MET:HA	1.93	0.49
28:e:52:THR:O	28:e:52:THR:OG1	2.30	0.49
28:e:151:GLU:N	28:e:151:GLU:OE1	2.43	0.49
35:l:566:THR:O	35:l:570:GLN:HG2	2.12	0.49
40:r:50:LEU:CD2	40:r:50:LEU:N	2.73	0.49
42:u:24:VAL:HG12	42:u:86:TRP:CD2	2.47	0.49
44:w:119:ASP:OD1	44:w:225:HIS:ND1	2.39	0.49
44:w:245:PHE:HE1	44:w:249:MET:HE2	1.77	0.49
35:l:400:ASN:HB3	35:l:486:MET:SD	2.52	0.49
9:J:36:LEU:N	12:M:304:GLN:HE22	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:87:MET:HE2	12:M:272:ARG:NH1	2.27	0.49
12:M:127:ASP:OD2	12:M:175:ARG:NH2	2.45	0.49
28:e:62:GLU:H	28:e:62:GLU:CD	2.21	0.49
40:r:207:MET:SD	40:r:240:GLY:N	2.85	0.49
43:v:103:GLU:HA	43:v:103:GLU:OE2	2.13	0.49
7:H:22:GLU:OE1	7:H:22:GLU:N	2.44	0.49
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.47	0.49
12:M:159:ALA:O	18:T:101:ASN:ND2	2.45	0.49
13:N:26:VAL:HG13	13:N:33:VAL:HG12	1.95	0.49
54:a:201:CDL:H382	27:d:48:ALA:HB2	1.95	0.49
31:h:18:MET:HE3	32:i:25:HIS:CE1	2.46	0.49
44:w:209:VAL:HG22	44:w:260:ALA:HB2	1.94	0.49
1:A:217:GLU:OE2	1:A:236:PHE:N	2.40	0.49
1:A:319:PRO:HA	1:A:354:VAL:HG22	1.93	0.49
7:H:59:VAL:HG23	7:H:68:LEU:HD21	1.94	0.49
8:I:18:ARG:HH12	21:W:26:PRO:HD3	1.76	0.49
12:M:299:ARG:HH21	12:M:703:ALA:HA	1.78	0.49
22:Y:84:PHE:HD2	43:v:92:HIS:CG	2.30	0.49
35:l:66:TRP:O	35:l:78:LEU:N	2.38	0.49
35:l:557:TRP:O	35:l:561:ILE:HG12	2.11	0.49
1:A:88:ARG:HG3	1:A:246:GLU:HG2	1.93	0.49
3:C:147:TYR:CD1	3:C:148:SER:HB3	2.47	0.49
8:I:97:PRO:HD3	15:P:61:PHE:CE2	2.47	0.49
6:X:118:ILE:O	6:X:122:MET:HG2	2.13	0.49
28:e:98:VAL:HG22	40:r:36:LEU:HB2	1.95	0.49
9:J:318:LYS:O	9:J:322:VAL:HG12	2.13	0.49
20:V:137:ALA:HB3	32:i:275:SER:HB2	1.93	0.49
27:d:43:ARG:HB3	27:d:44:PRO:HD3	1.95	0.49
27:d:110:LEU:HD11	35:l:203:MET:HG2	1.95	0.49
35:l:393:ASP:O	35:l:397:GLU:HG3	2.12	0.49
41:s:85:MET:HB3	41:s:233:MET:CE	2.42	0.49
43:v:46:MET:SD	43:v:56:ARG:HG2	2.53	0.49
1:A:126:LYS:HG2	1:A:277:ASN:HD21	1.76	0.49
9:J:203:PRO:HB2	50:J:401:NDP:H5N	1.94	0.49
11:L:111:LEU:HD11	13:N:126:PRO:HG2	1.95	0.49
12:M:690:THR:HG23	12:M:692:LYS:HG2	1.93	0.49
25:b:106:PRO:HG2	25:b:120:MET:SD	2.52	0.49
35:l:66:TRP:CZ3	48:l:704:PEE:H32	2.48	0.49
40:r:204:MET:HE2	40:r:302:MET:HE3	1.95	0.49
44:w:290:THR:HA	44:w:293:ARG:HD2	1.95	0.49
2:B:70:LEU:HD11	41:s:273:ILE:CG1	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:85:ARG:NH2	50:J:401:NDP:O2X	2.45	0.48
12:M:453:GLN:O	12:M:456:ALA:HB3	2.13	0.48
25:b:7:ASP:OD1	25:b:8:GLU:N	2.45	0.48
40:r:139:GLN:HE22	40:r:340:ARG:CZ	2.26	0.48
1:A:89:GLY:O	47:A:503:NAI:H2N	2.13	0.48
1:A:373:PHE:O	1:A:377:GLU:HG2	2.13	0.48
5:F:62:GLN:CD	5:F:80:ASN:HD21	2.20	0.48
16:Q:84:PHE:HE2	16:Q:444:LEU:HD11	1.78	0.48
27:d:6:ASP:OD1	27:d:8:ASP:N	2.23	0.48
35:l:384:PRO:HG3	35:l:491:LEU:HD21	1.94	0.48
41:s:197:PRO:HB3	41:s:278:PRO:O	2.12	0.48
4:E:33:ARG:O	4:E:37:ARG:HG3	2.13	0.48
5:F:83:SER:OG	5:F:86:GLN:HG3	2.14	0.48
15:P:103:HIS:CD2	15:P:105:ASN:HB2	2.49	0.48
24:a:135:LYS:HB3	24:a:135:LYS:NZ	2.26	0.48
25:b:108:ASP:O	25:b:117:ILE:HG13	2.13	0.48
26:c:165:ASP:O	26:c:170:ARG:NH2	2.46	0.48
38:o:30:ARG:NH1	39:p:9:TYR:CD2	2.75	0.48
38:o:83:THR:HG22	38:o:85:LYS:H	1.78	0.48
43:v:83:GLU:OE2	43:v:83:GLU:N	2.29	0.48
8:I:34:ARG:HB2	13:N:95:ASP:OD1	2.12	0.48
9:J:192:ARG:NH1	9:J:260:GLY:O	2.47	0.48
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.44	0.48
21:W:74:LEU:HD21	42:u:18:VAL:HG21	1.94	0.48
27:d:23:GLN:HE21	27:d:23:GLN:CA	2.13	0.48
30:g:15:PHE:HB3	30:g:16:LEU:HD12	1.94	0.48
3:C:56:TRP:CH2	41:s:50:ALA:HB2	2.48	0.48
4:E:98:LYS:HB3	4:E:102:HIS:HB2	1.95	0.48
12:M:326:VAL:HG23	12:M:567:ILE:HG12	1.94	0.48
40:r:329:LEU:HG	40:r:437:MET:HE2	1.93	0.48
11:L:109:ASN:ND2	11:L:111:LEU:O	2.46	0.48
12:M:307:ILE:HD11	12:M:317:THR:HG21	1.95	0.48
27:d:144:SER:O	27:d:158:LYS:NZ	2.28	0.48
32:i:17:THR:HG23	32:i:36:ASN:ND2	2.28	0.48
40:r:11:LEU:O	40:r:15:THR:HG22	2.13	0.48
41:s:62:ARG:HD3	41:s:64:ALA:H	1.79	0.48
9:J:314:THR:HA	9:J:318:LYS:HB3	1.95	0.48
13:N:39:VAL:CG2	13:N:50:GLU:HG2	2.44	0.48
17:S:11:VAL:HG21	41:s:45:LEU:HD22	1.95	0.48
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.78	0.48
25:b:12:LEU:HD23	25:b:16:ARG:HH22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:72:MET:O	32:i:76:ILE:HG13	2.13	0.48
54:l:701:CDL:H801	55:r:502:PLX:H233	1.95	0.48
39:p:26:HIS:CD2	39:p:79:PRO:HB3	2.49	0.48
44:w:147:LEU:HB3	44:w:298:VAL:HG11	1.95	0.48
5:F:37:ILE:HA	5:F:41:TYR:HB2	1.96	0.48
19:U:53:TYR:HB3	42:u:48:TRP:CH2	2.46	0.48
7:H:76:GLN:O	7:H:79:GLU:N	2.46	0.48
12:M:464:GLN:HA	12:M:467:LYS:HD3	1.96	0.48
26:c:117:VAL:HG12	35:l:538:THR:OG1	2.13	0.48
31:h:51:ARG:O	31:h:55:GLU:HG3	2.14	0.48
40:r:52:PHE:HB2	40:r:56:PHE:O	2.14	0.48
1:A:98:LYS:HA	1:A:101:PHE:CD2	2.49	0.48
15:P:162:ALA:HB2	16:Q:286:TYR:C	2.39	0.48
26:c:33:THR:OG1	26:c:35:ASP:OD1	2.31	0.48
28:e:76:TYR:HB2	28:e:83:ASP:OD1	2.14	0.48
35:l:66:TRP:HZ3	48:l:704:PEE:H32	1.78	0.48
40:r:44:GLN:HE21	40:r:50:LEU:HD21	1.74	0.48
7:H:38:ILE:HD13	7:H:95:LEU:HD13	1.96	0.47
7:H:72:LEU:HD13	7:H:80:VAL:HG11	1.96	0.47
12:M:250:SER:OG	12:M:251:ILE:N	2.46	0.47
26:c:167:TYR:HD2	26:c:168:LEU:HD22	1.79	0.47
54:i:401:CDL:HB62	44:w:40:PRO:HB2	1.96	0.47
41:s:46:LEU:HD12	41:s:49:ILE:HG21	1.96	0.47
20:V:141:VAL:HG12	24:a:158:ARG:HB2	1.96	0.47
24:a:106:VAL:HG23	37:n:50:ARG:HH21	1.79	0.47
30:g:12:PRO:HB3	31:h:5:ASP:HB3	1.95	0.47
33:j:6:THR:O	33:j:10:ASN:ND2	2.47	0.47
35:l:373:LEU:HD13	35:l:431:PHE:CE2	2.50	0.47
2:B:48:MET:HG3	2:B:48:MET:O	2.13	0.47
8:I:27:ARG:NH1	16:Q:212:GLU:OE1	2.45	0.47
11:L:131:LYS:HE3	11:L:147:VAL:HG11	1.96	0.47
14:O:199:LYS:O	14:O:203:GLU:HG3	2.14	0.47
16:Q:182:ASN:ND2	16:Q:403:PRO:CB	2.77	0.47
21:W:84:LEU:HD21	42:u:53:PRO:HB2	1.97	0.47
21:W:88:ARG:O	21:W:92:GLU:HG2	2.14	0.47
25:b:80:TRP:HD1	27:d:41:VAL:HG13	1.79	0.47
38:o:33:GLN:OE1	39:p:9:TYR:HB3	2.14	0.47
40:r:369:LEU:HD12	40:r:370:PRO:HD2	1.95	0.47
5:F:30:SER:OG	5:F:63:PRO:HG3	2.14	0.47
21:W:94:GLU:HA	21:W:97:ILE:HG22	1.96	0.47
54:g:202:CDL:H362	54:g:202:CDL:H392	1.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:h:88:LYS:HE2	31:h:88:LYS:HB3	1.58	0.47
39:p:135:ARG:O	39:p:138:LYS:HG3	2.15	0.47
40:r:328:CYS:HB2	40:r:437:MET:HE1	1.96	0.47
2:B:40:PHE:HB3	2:B:43:MET:HB3	1.96	0.47
2:B:184:LEU:HD23	11:L:112:MET:HG3	1.97	0.47
4:E:35:LEU:HG	4:E:67:PHE:HZ	1.79	0.47
5:F:71:PHE:CD1	12:M:362:ASP:HB2	2.49	0.47
9:J:236:VAL:HG11	9:J:270:ARG:HE	1.79	0.47
16:Q:325:ASP:OD1	16:Q:325:ASP:N	2.44	0.47
21:W:105:LYS:HD3	21:W:108:GLU:CD	2.40	0.47
25:b:31:ARG:NH1	25:b:31:ARG:HB3	2.29	0.47
26:c:56:ASN:ND2	38:o:43:LEU:HD21	2.30	0.47
28:e:57:GLU:OE1	44:w:320:GLY:HA3	2.15	0.47
32:i:9:LEU:HD13	32:i:42:PRO:HB2	1.96	0.47
34:k:80:MET:N	34:k:80:MET:SD	2.87	0.47
35:l:174:TYR:CD2	35:l:232:TRP:HB3	2.49	0.47
43:v:17:PRO:HB3	43:v:105:GLU:HG2	1.96	0.47
43:v:39:MET:HE3	43:v:58:TYR:HE1	1.79	0.47
1:A:119:GLU:OE2	1:A:124:THR:HG22	2.15	0.47
1:A:134:ASP:OD1	1:A:134:ASP:N	2.44	0.47
3:C:98:ARG:HG2	41:s:61:LEU:HD12	1.96	0.47
9:J:249:ILE:O	9:J:253:ILE:HD12	2.14	0.47
16:Q:37:TRP:CE2	40:r:140:THR:HG22	2.49	0.47
17:S:11:VAL:HG11	41:s:19:PHE:CE2	2.50	0.47
33:j:84:LEU:HD13	41:s:309:ILE:HG23	1.95	0.47
35:l:384:PRO:HA	35:l:389:PHE:CG	2.50	0.47
1:A:170:GLN:HB3	10:K:89:LEU:HD13	1.96	0.47
1:A:211:ALA:HB2	1:A:223:PRO:HG3	1.96	0.47
2:B:117:LYS:HD3	12:M:244:GLU:OE2	2.14	0.47
5:F:42:VAL:HG22	5:F:46:LYS:HZ2	1.79	0.47
5:F:88:THR:O	5:F:92:GLU:HG2	2.15	0.47
9:J:204:SER:OG	9:J:238:GLN:O	2.29	0.47
12:M:483:ARG:HH22	12:M:682:ASP:HB2	1.80	0.47
16:Q:65:PRO:HB2	16:Q:67:ASN:O	2.13	0.47
25:b:5:THR:OG1	25:b:8:GLU:HG3	2.14	0.47
25:b:104:ILE:HG13	27:d:16:ARG:HH22	1.78	0.47
26:c:117:VAL:HG11	35:l:539:TYR:HA	1.97	0.47
26:c:146:VAL:O	26:c:149:ILE:HG22	2.15	0.47
30:g:72:PHE:CE2	30:g:76:TYR:HE2	2.32	0.47
30:g:109:LYS:HD2	30:g:114:ILE:HD11	1.96	0.47
32:i:149:ILE:HD13	32:i:154:MET:CE	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:12:PHE:CD1	34:k:36:MET:HG2	2.50	0.47
39:p:63:LEU:HD23	39:p:63:LEU:HA	1.79	0.47
39:p:82:PHE:HB2	39:p:85:SER:OG	2.15	0.47
43:v:44:GLN:OE1	43:v:44:GLN:HA	2.15	0.47
5:F:36:PHE:C	5:F:36:PHE:CD1	2.91	0.47
21:W:68:ARG:HD2	36:m:135:PHE:HD2	1.80	0.47
6:X:140:CYS:HB3	6:X:143:GLU:HG3	1.97	0.47
27:d:37:PHE:CD2	35:l:3:PRO:HB3	2.49	0.47
44:w:73:LEU:HD11	44:w:269:VAL:HG21	1.95	0.47
44:w:165:SER:HB3	44:w:245:PHE:CZ	2.50	0.47
31:h:7:GLN:NE2	31:h:15:ASP:OD1	2.42	0.47
34:k:26:LEU:HD23	34:k:78:LEU:HD13	1.97	0.47
40:r:185:PRO:HB3	40:r:252:PRO:HD3	1.97	0.47
2:B:177:THR:HG22	2:B:179:THR:H	1.80	0.47
4:E:16:SER:HB3	11:L:52:LEU:HB3	1.97	0.47
4:E:93:THR:HG23	4:E:103:ILE:HD11	1.96	0.47
20:V:39:TYR:OH	35:l:594:THR:HG22	2.15	0.47
49:X:201:8Q1:S44	39:p:63:LEU:HB3	2.54	0.47
23:Z:13:LYS:HD2	23:Z:13:LYS:HA	1.66	0.47
32:i:221:HIS:O	32:i:319:HIS:NE2	2.45	0.47
54:l:701:CDL:H742	54:l:701:CDL:H312	1.96	0.47
36:m:27:ILE:HG23	36:m:28:TYR:HD1	1.80	0.47
40:r:300:ALA:O	40:r:308:SER:HB3	2.15	0.47
1:A:278:ILE:HD12	1:A:354:VAL:HB	1.97	0.46
2:B:130:ILE:HG12	2:B:145:TYR:CD1	2.51	0.46
5:F:56:ARG:HB3	12:M:651:PRO:HD2	1.96	0.46
12:M:436:VAL:O	12:M:442:TYR:OH	2.22	0.46
14:O:191:ASN:ND2	14:O:216:PRO:HG3	2.30	0.46
22:Y:68:TRP:CH2	22:Y:72:ARG:HD3	2.50	0.46
26:c:160:GLN:HG2	26:c:183:HIS:CE1	2.50	0.46
31:h:2:PRO:HA	32:i:140:SER:HB2	1.96	0.46
35:l:222:GLY:HA2	35:l:229:LEU:HD12	1.98	0.46
54:l:701:CDL:H421	54:l:701:CDL:H602	1.96	0.46
39:p:62:GLN:NE2	39:p:66:GLN:HE22	2.12	0.46
41:s:13:ILE:O	41:s:17:VAL:HG13	2.15	0.46
42:u:112:LEU:C	42:u:112:LEU:CD2	2.85	0.46
44:w:139:ARG:HD2	44:w:166:ASP:OD1	2.14	0.46
3:C:110:THR:OG1	16:Q:115:LEU:O	2.20	0.46
9:J:173:ASP:OD1	9:J:173:ASP:N	2.48	0.46
15:P:100:LEU:O	15:P:108:PHE:N	2.38	0.46
21:W:93:GLU:O	21:W:96:ILE:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:128:PHE:HZ	6:X:148:ILE:HG12	1.79	0.46
28:e:90:VAL:HG22	40:r:28:THR:HG21	1.97	0.46
42:u:83:THR:HA	42:u:86:TRP:CD1	2.51	0.46
54:u:201:CDL:H781	54:u:201:CDL:H752	1.67	0.46
43:v:30:GLY:H	43:v:104:ARG:HH22	1.63	0.46
13:N:127:TYR:OH	18:T:61:GLU:O	2.23	0.46
15:P:77:GLN:HG3	15:P:87:PHE:CE1	2.45	0.46
16:Q:286:TYR:HE2	16:Q:437:LYS:HG2	1.80	0.46
26:c:122:THR:HB	26:c:129:MET:HE1	1.96	0.46
32:i:7:THR:O	32:i:11:MET:HG2	2.15	0.46
42:u:169:PHE:HE1	54:u:201:CDL:H521	1.80	0.46
43:v:81:LYS:HB3	43:v:81:LYS:HE2	1.58	0.46
2:B:171:PRO:HG2	2:B:200:GLU:OE1	2.16	0.46
7:H:27:LEU:O	7:H:31:ILE:HD12	2.15	0.46
9:J:83:PRO:HG3	9:J:119:VAL:HG11	1.96	0.46
12:M:98:LYS:HE3	12:M:98:LYS:HB3	1.76	0.46
12:M:252:ASP:OD2	12:M:290:THR:OG1	2.21	0.46
12:M:394:VAL:HG11	12:M:418:ILE:HG12	1.97	0.46
14:O:198:PRO:O	14:O:202:GLU:HG2	2.16	0.46
18:T:46:ASP:OD1	18:T:46:ASP:N	2.45	0.46
30:g:14:GLN:NE2	30:g:17:PRO:HA	2.30	0.46
42:u:52:ASP:OD1	42:u:54:ARG:NE	2.48	0.46
11:L:98:LYS:HA	11:L:98:LYS:HD3	1.70	0.46
33:j:109:LYS:NZ	33:j:109:LYS:HB3	2.31	0.46
35:l:535:ARG:O	35:l:539:TYR:HB3	2.16	0.46
36:m:49:GLY:HA2	36:m:139:GLU:OE2	2.15	0.46
39:p:100:PRO:HG3	40:r:419:TYR:CE1	2.51	0.46
44:w:100:ASP:HB2	44:w:102:LYS:HE2	1.96	0.46
44:w:175:ARG:HG2	44:w:175:ARG:NH1	2.31	0.46
1:A:115:VAL:HG21	1:A:142:CYS:SG	2.56	0.46
3:C:143:TYR:CD2	16:Q:118:2MR:HB2	2.50	0.46
5:F:36:PHE:CD2	5:F:87:VAL:HG13	2.51	0.46
16:Q:353:PRO:HB3	21:W:10:MET:HE2	1.96	0.46
17:S:6:LEU:HD23	17:S:9:ILE:HD12	1.97	0.46
54:V:201:CDL:H352	54:V:201:CDL:H322	1.41	0.46
49:X:201:8Q1:O3	39:p:13:GLN:NE2	2.49	0.46
33:j:93:PHE:CZ	33:j:97:LEU:HD11	2.51	0.46
48:j:202:PEE:H35	48:j:202:PEE:H30	1.70	0.46
1:A:297:LYS:O	1:A:301:GLU:HG2	2.15	0.46
1:A:322:SER:HB2	1:A:370:LEU:HD22	1.97	0.46
3:C:75:GLU:O	3:C:78:HIS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:275:ASP:O	9:J:278:GLN:HB2	2.15	0.46
16:Q:139:LEU:HD23	16:Q:139:LEU:HA	1.78	0.46
54:V:202:CDL:H873	40:r:264:LEU:HD21	1.97	0.46
21:W:55:ARG:NH2	41:s:311:THR:O	2.48	0.46
35:l:64:SER:HA	35:l:79:SER:HA	1.98	0.46
43:v:6:ALA:O	43:v:10:LEU:HB2	2.16	0.46
4:E:18:LYS:HZ3	15:P:152:PRO:HG2	1.81	0.46
12:M:347:ASP:O	12:M:351:LEU:HG	2.16	0.46
24:a:57:ILE:HG23	39:p:104:LEU:HD21	1.98	0.46
24:a:132:ASN:HD22	40:r:50:LEU:HA	1.80	0.46
31:h:29:ILE:HG21	36:m:138:GLU:HG2	1.97	0.46
32:i:141:VAL:O	32:i:145:ILE:HG12	2.16	0.46
2:B:150:THR:HG21	2:B:180:HIS:CD2	2.50	0.46
7:H:7:LYS:HA	7:H:16:VAL:HG21	1.98	0.46
11:L:69:GLU:OE2	11:L:73:LYS:HD3	2.16	0.46
23:Z:82:VAL:HA	23:Z:85:GLU:HG2	1.98	0.46
41:s:102:VAL:HG21	41:s:154:LEU:HD11	1.98	0.46
43:v:34:ARG:NH1	43:v:36:GLU:OE2	2.49	0.46
18:T:36:GLU:HG3	18:T:52:ARG:HH12	1.81	0.46
26:c:184:TYR:HA	43:v:34:ARG:NH1	2.31	0.46
31:h:6:VAL:HG13	31:h:10:LEU:HD13	1.97	0.46
32:i:77:ASN:OD1	32:i:89:MET:O	2.34	0.46
35:l:417:SER:HB3	35:l:493:VAL:HG22	1.98	0.46
36:m:129:ASP:OD1	36:m:129:ASP:N	2.48	0.46
42:u:112:LEU:HD23	42:u:112:LEU:O	2.15	0.46
9:J:207:PHE:HB3	9:J:213:PHE:HD2	1.82	0.45
9:J:247:LYS:C	9:J:340:ILE:CD1	2.88	0.45
19:U:41:TYR:O	19:U:45:ILE:HG13	2.16	0.45
22:Y:71:TRP:HE1	22:Y:75:HIS:CE1	2.33	0.45
30:g:85:TYR:CZ	32:i:344:SER:HB3	2.52	0.45
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.98	0.45
35:l:526:LEU:HD12	35:l:530:PRO:HG2	1.99	0.45
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.97	0.45
37:n:30:ARG:HG2	37:n:30:ARG:NH1	2.31	0.45
40:r:130:LEU:HD13	40:r:150:LEU:HD13	1.97	0.45
41:s:14:LEU:HA	41:s:17:VAL:HG22	1.98	0.45
42:u:39:PRO:HA	42:u:42:GLU:HG2	1.97	0.45
42:u:82:PHE:CD1	42:u:107:PHE:CZ	3.00	0.45
1:A:443:ARG:O	1:A:447:GLU:HG3	2.15	0.45
2:B:55:ASP:OD1	21:W:31:SER:HA	2.17	0.45
2:B:137:ASP:OD1	2:B:137:ASP:N	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:134:GLY:HA2	3:C:165:GLY:O	2.17	0.45
4:E:53:ASP:CG	9:J:351:GLU:HB2	2.40	0.45
7:H:83:GLN:NE2	15:P:104:THR:HA	2.31	0.45
12:M:382:ARG:NE	12:M:386:LEU:HD11	2.26	0.45
25:b:84:TYR:CD1	25:b:88:TYR:HD2	2.33	0.45
26:c:160:GLN:HB3	26:c:183:HIS:CD2	2.51	0.45
39:p:170:ILE:O	39:p:173:ARG:HG3	2.16	0.45
1:A:349:LEU:HD11	1:A:352:ALA:HB2	1.97	0.45
4:E:20:ILE:HG22	4:E:21:PHE:CD1	2.51	0.45
16:Q:182:ASN:CB	16:Q:403:PRO:HB3	2.46	0.45
23:Z:54:SER:OG	23:Z:55:GLY:N	2.49	0.45
25:b:104:ILE:HG13	27:d:16:ARG:NH2	2.30	0.45
42:u:16:GLN:OE1	42:u:68:LEU:CD1	2.63	0.45
1:A:369:ARG:NH2	14:O:175:GLU:OE2	2.46	0.45
9:J:247:LYS:C	9:J:340:ILE:HD11	2.40	0.45
12:M:639:LEU:O	12:M:643:ARG:HG3	2.17	0.45
14:O:177:LEU:N	51:O:301:FES:S1	2.81	0.45
15:P:81:PHE:CD1	15:P:83:GLU:HG3	2.52	0.45
16:Q:286:TYR:CE2	16:Q:437:LYS:HG2	2.52	0.45
23:Z:53:TYR:CE2	35:l:434:LYS:HG3	2.51	0.45
23:Z:60:ASN:OD1	23:Z:60:ASN:N	2.44	0.45
24:a:61:GLY:O	24:a:65:ARG:HG3	2.17	0.45
30:g:80:ARG:O	30:g:84:MET:HG2	2.16	0.45
32:i:40:MET:HE1	32:i:129:LEU:HB3	1.98	0.45
32:i:215:MET:HE1	32:i:244:MET:HG3	1.98	0.45
35:l:292:ALA:HB2	35:l:304:PHE:HB3	1.97	0.45
54:l:702:CDL:H591	54:l:702:CDL:H622	1.44	0.45
40:r:12:LEU:HB2	40:r:13:PRO:HD3	1.98	0.45
1:A:112:TYR:O	1:A:240:THR:HA	2.17	0.45
1:A:147:ARG:HA	1:A:147:ARG:HD2	1.82	0.45
8:I:40:LYS:HB3	21:W:7:LYS:H	1.81	0.45
16:Q:127:LYS:HB3	16:Q:131:GLN:HB2	1.99	0.45
17:S:14:ALA:O	17:S:17:PHE:HB2	2.17	0.45
26:c:73:GLY:HA3	38:o:79:ASN:HD22	1.82	0.45
29:f:71:ARG:HB3	29:f:71:ARG:CZ	2.46	0.45
35:l:54:PHE:O	35:l:58:GLY:N	2.50	0.45
35:l:233:LEU:HB3	35:l:234:PRO:HD3	1.99	0.45
39:p:97:TYR:HB3	39:p:179:MET:HB2	1.98	0.45
14:O:140:CYS:O	14:O:145:SER:OG	2.33	0.45
16:Q:316:PHE:CG	16:Q:343:ILE:HD11	2.52	0.45
54:a:201:CDL:H342	54:a:201:CDL:H372	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:14:GLN:NE2	39:p:157:ALA:HB3	2.32	0.45
41:s:24:GLU:OE1	41:s:228:TYR:OH	2.24	0.45
42:u:134:ASP:OD1	42:u:134:ASP:N	2.35	0.45
1:A:110:PRO:O	1:A:238:CYS:HB3	2.17	0.45
1:A:222:LYS:HZ1	12:M:204:MET:HE1	1.82	0.45
3:C:88:ARG:HA	41:s:37:PRO:HA	1.99	0.45
12:M:707:MET:HE2	12:M:707:MET:HA	1.99	0.45
13:N:73:THR:HG22	13:N:77:VAL:HG12	1.97	0.45
14:O:130:TYR:HA	14:O:189:ASN:ND2	2.32	0.45
15:P:55:HIS:HB3	15:P:56:LYS:HZ2	1.80	0.45
16:Q:142:VAL:HG11	16:Q:185:MET:HG2	1.99	0.45
25:b:86:LEU:HA	25:b:90:VAL:HB	1.99	0.45
28:e:99:LEU:HD23	28:e:99:LEU:HA	1.85	0.45
31:h:76:LEU:O	31:h:80:LYS:HG3	2.17	0.45
38:o:47:TYR:O	38:o:51:TYR:HB2	2.17	0.45
2:B:70:LEU:O	41:s:272:TRP:CZ2	2.69	0.45
12:M:469:ALA:CB	12:M:472:PRO:HB3	2.47	0.45
16:Q:99:MET:HE1	16:Q:444:LEU:HD12	1.98	0.45
16:Q:249:LYS:HA	21:W:19:ILE:HG23	1.99	0.45
26:c:139:PHE:CE2	54:l:702:CDL:H842	2.51	0.45
30:g:36:MET:HE3	30:g:36:MET:HB3	1.80	0.45
32:i:149:ILE:HG21	32:i:154:MET:HE2	1.99	0.45
33:j:48:ARG:C	33:j:50:PRO:HD2	2.42	0.45
38:o:57:LEU:HG	38:o:57:LEU:O	2.16	0.45
40:r:204:MET:HE1	40:r:298:ILE:HG23	1.98	0.45
42:u:36:CYS:O	42:u:39:PRO:HD2	2.17	0.45
12:M:266:ARG:HG2	12:M:267:THR:HG23	1.99	0.45
13:N:48:TYR:OH	13:N:82:VAL:HG13	2.16	0.45
21:W:71:LEU:HB3	21:W:75:PHE:CE2	2.48	0.45
23:Z:22:TRP:HB3	23:Z:50:ALA:HB3	1.99	0.45
23:Z:75:PHE:O	23:Z:79:VAL:HG23	2.17	0.45
24:a:112:TYR:HE2	27:d:66:ARG:HA	1.82	0.45
31:h:39:GLU:OE2	42:u:147:ARG:NH2	2.38	0.45
41:s:183:MET:O	41:s:187:ILE:HG12	2.17	0.45
1:A:87:GLY:N	1:A:93:PHE:O	2.48	0.45
2:B:70:LEU:HD11	41:s:273:ILE:CD1	2.47	0.45
9:J:356:HIS:C	9:J:357:ARG:O	2.60	0.45
16:Q:196:ALA:O	16:Q:197:MET:HG3	2.17	0.45
20:V:101:LEU:O	20:V:105:THR:HG22	2.17	0.45
25:b:4:TYR:HB2	25:b:9:LYS:HE3	1.99	0.45
30:g:89:ASP:CG	42:u:166:ARG:HH12	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:l:702:CDL:H572	54:l:702:CDL:H541	1.52	0.45
40:r:433:GLU:O	40:r:437:MET:HG2	2.17	0.45
3:C:45:TYR:CD1	3:C:45:TYR:C	2.95	0.44
6:G:97:LYS:HE3	6:G:108:LEU:HD22	1.99	0.44
6:G:105:MET:N	6:G:105:MET:SD	2.90	0.44
7:H:58:MET:HE1	7:H:71:GLN:C	2.42	0.44
10:K:110:HIS:ND1	12:M:441:ARG:HG3	2.33	0.44
12:M:510:TRP:CD2	12:M:510:TRP:O	2.70	0.44
17:S:59:ARG:HB2	17:S:62:VAL:HG23	1.99	0.44
24:a:59:PRO:HD3	39:p:99:VAL:HG21	1.98	0.44
24:a:110:TRP:O	24:a:119:ARG:HG2	2.17	0.44
54:i:401:CDL:H312	54:i:401:CDL:H342	1.39	0.44
38:o:79:ASN:OD1	38:o:79:ASN:N	2.50	0.44
40:r:282:LEU:HG	40:r:342:MET:HG3	1.98	0.44
41:s:9:LEU:O	41:s:13:ILE:HG13	2.18	0.44
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.98	0.44
44:w:54:THR:C	44:w:56:THR:H	2.26	0.44
1:A:383:THR:HG23	12:M:75:CYS:HA	1.99	0.44
12:M:402:LEU:HD23	12:M:475:VAL:HB	1.99	0.44
12:M:569:GLN:HA	12:M:584:LEU:O	2.17	0.44
17:S:69:ILE:HD12	17:S:69:ILE:HA	1.88	0.44
54:V:202:CDL:H781	54:V:202:CDL:H812	1.57	0.44
54:l:701:CDL:H772	54:l:701:CDL:H601	1.99	0.44
44:w:211:VAL:O	44:w:214:ILE:HG22	2.18	0.44
2:B:168:VAL:HG21	2:B:201:ILE:CG2	2.47	0.44
3:C:163:VAL:HG21	3:C:173:LEU:HD12	1.98	0.44
8:I:54:TYR:CE2	16:Q:362:LYS:HD2	2.52	0.44
12:M:165:ILE:HD11	12:M:169:VAL:HG11	1.98	0.44
12:M:335:GLY:H	12:M:361:VAL:HG12	1.81	0.44
19:U:42:ALA:HB2	41:s:312:ALA:HA	1.99	0.44
24:a:86:ILE:CD1	28:e:108:TYR:HE2	2.30	0.44
32:i:26:TRP:HB3	32:i:74:ILE:HD13	1.99	0.44
32:i:54:GLU:O	32:i:57:THR:HG22	2.17	0.44
32:i:59:TYR:CE1	32:i:130:LEU:HD11	2.52	0.44
32:i:95:MET:CE	32:i:149:ILE:HG13	2.38	0.44
32:i:170:LEU:O	32:i:295:ARG:NH2	2.45	0.44
34:k:11:ALA:HB2	36:m:14:VAL:HG12	2.00	0.44
34:k:20:LEU:HD12	35:l:588:PHE:HD2	1.82	0.44
34:k:22:TYR:O	35:l:585:LYS:HG2	2.17	0.44
40:r:452:LYS:HE2	40:r:452:LYS:HB3	1.82	0.44
1:A:263:ALA:HA	1:A:271:SER:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ILE:HG21	1:A:304:ALA:HB2	1.99	0.44
2:B:39:LYS:NZ	16:Q:335:GLU:OE1	2.36	0.44
7:H:44:TYR:HE2	7:H:94:MET:HB2	1.82	0.44
15:P:44:ARG:HB3	15:P:45:PRO:CD	2.47	0.44
15:P:152:PRO:O	15:P:153:ILE:HD13	2.17	0.44
16:Q:139:LEU:CD1	16:Q:424:ILE:HG21	2.48	0.44
17:S:44:GLN:H	17:S:44:GLN:HG2	1.62	0.44
19:U:70:PRO:HB3	42:u:124:GLU:O	2.18	0.44
26:c:38:PRO:HD2	38:o:70:TYR:CD2	2.52	0.44
30:g:7:ARG:NH1	30:g:91:ASP:OD1	2.51	0.44
32:i:72:MET:HB2	34:k:40:LEU:HD21	1.99	0.44
32:i:243:LEU:O	32:i:246:VAL:HG12	2.17	0.44
35:l:264:TYR:HA	35:l:267:MET:HB2	2.00	0.44
54:l:701:CDL:H212	54:l:701:CDL:H181	1.79	0.44
41:s:265:ALA:O	41:s:269:THR:OG1	2.34	0.44
44:w:165:SER:HB3	44:w:245:PHE:CE1	2.52	0.44
1:A:119:GLU:O	1:A:159:ARG:NH1	2.50	0.44
1:A:185:ASN:O	1:A:187:CYS:N	2.49	0.44
12:M:32:ILE:HG23	12:M:98:LYS:HG2	2.00	0.44
13:N:53:LYS:HA	13:N:53:LYS:HD3	1.82	0.44
14:O:186:VAL:HG22	14:O:196:LEU:HD11	2.00	0.44
21:W:125:TYR:HA	21:W:128:ARG:HG3	2.00	0.44
32:i:6:TYR:CE2	32:i:46:LYS:HE2	2.52	0.44
32:i:95:MET:HE2	32:i:149:ILE:HG13	1.90	0.44
35:l:99:SER:HA	35:l:456:ARG:HH21	1.83	0.44
35:l:303:ALA:O	35:l:306:THR:HG22	2.17	0.44
39:p:127:ARG:HG2	39:p:130:ARG:NH2	2.32	0.44
41:s:92:PRO:HB3	41:s:255:TYR:CD1	2.52	0.44
41:s:230:ASN:O	41:s:233:MET:HG3	2.18	0.44
7:H:21:HIS:HE1	7:H:65:VAL:HG22	1.83	0.44
7:H:62:GLU:OE2	7:H:67:LYS:HD3	2.17	0.44
20:V:43:LEU:HD22	35:l:580:GLN:NE2	2.33	0.44
54:V:202:CDL:H872	54:V:202:CDL:H841	1.76	0.44
21:W:80:ASP:OD2	42:u:47:ARG:NH2	2.51	0.44
25:b:106:PRO:HB3	25:b:118:PRO:O	2.17	0.44
55:j:203:PLX:H342	55:j:203:PLX:H372	1.61	0.44
35:l:268:GLU:HB2	35:l:320:ASN:HD21	1.82	0.44
35:l:502:LEU:HD23	35:l:502:LEU:HA	1.81	0.44
40:r:42:LEU:HD23	40:r:42:LEU:HA	1.80	0.44
56:s:401:UQ:H101	56:s:401:UQ:H121	1.68	0.44
44:w:293:ARG:HG2	44:w:294:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:HD21	1:A:247:THR:HG23	1.99	0.44
3:C:62:LEU:O	3:C:91:VAL:HA	2.17	0.44
7:H:79:GLU:OE1	15:P:136:ARG:NH2	2.50	0.44
16:Q:432:LEU:HD12	16:Q:432:LEU:HA	1.79	0.44
24:a:187:PRO:HB2	42:u:47:ARG:NH1	2.33	0.44
32:i:175:LEU:O	32:i:179:MET:HG2	2.18	0.44
37:n:18:PRO:O	37:n:22:VAL:HG13	2.17	0.44
41:s:51:ASP:HB3	56:s:401:UQ:H8	1.99	0.44
1:A:121:GLU:HG3	1:A:122:PRO:HD2	2.00	0.44
5:F:35:ASP:O	5:F:36:PHE:C	2.60	0.44
8:I:42:PRO:HD3	21:W:6:VAL:HG13	2.00	0.44
9:J:350:ILE:O	9:J:350:ILE:HD12	2.18	0.44
10:K:79:HIS:ND1	14:O:215:LYS:HE3	2.32	0.44
20:V:46:PRO:HB3	20:V:55:ARG:NH2	2.32	0.44
22:Y:61:PHE:HA	22:Y:64:THR:HG22	2.00	0.44
25:b:100:ARG:HB3	35:l:60:GLU:HB2	1.99	0.44
26:c:129:MET:HE2	35:l:525:MET:HE1	1.98	0.44
32:i:59:TYR:O	32:i:63:GLN:HG2	2.18	0.44
33:j:106:TRP:CE3	48:j:202:PEE:H20	2.53	0.44
35:l:49:VAL:HB	35:l:50:PRO:HD3	2.00	0.44
7:H:41:ASN:OD1	7:H:41:ASN:N	2.42	0.44
7:H:81:ILE:O	7:H:84:ALA:HB3	2.18	0.44
12:M:454:ASP:OD1	12:M:460:HIS:N	2.51	0.44
14:O:239:LYS:HG3	14:O:243:PHE:CD2	2.52	0.44
27:d:78:GLU:OE2	30:g:108:LYS:HE3	2.18	0.44
35:l:47:SER:O	35:l:50:PRO:HD2	2.18	0.44
40:r:221:VAL:HG13	40:r:340:ARG:HH11	1.82	0.44
11:L:128:PHE:HD1	15:P:121:THR:HA	1.83	0.43
14:O:215:LYS:HA	14:O:215:LYS:HD2	1.77	0.43
32:i:75:ILE:HD11	34:k:59:MET:HE1	1.99	0.43
48:m:201:PEE:H25	48:m:201:PEE:H56	2.00	0.43
39:p:49:ASP:HB2	39:p:52:LYS:HE2	1.99	0.43
39:p:100:PRO:HG3	40:r:419:TYR:CZ	2.52	0.43
39:p:108:HIS:CD2	39:p:109:PRO:HD2	2.52	0.43
40:r:44:GLN:OE1	40:r:63:ALA:HB2	2.18	0.43
44:w:83:LEU:HD22	44:w:156:GLY:HA3	2.00	0.43
44:w:173:MET:HB3	44:w:178:PHE:HB2	2.01	0.43
2:B:65:GLU:HA	2:B:68:ARG:HD2	1.99	0.43
14:O:152:ILE:HG23	14:O:205:ILE:HD11	2.00	0.43
32:i:247:THR:O	32:i:251:MET:HG3	2.18	0.43
34:k:3:LEU:HG	36:m:7:PHE:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:192:HIS:HA	38:o:126:ASN:OD1	2.17	0.43
35:l:238:GLU:HA	35:l:238:GLU:OE2	2.18	0.43
35:l:337:ALA:O	35:l:341:MET:HG3	2.18	0.43
54:l:701:CDL:H381	40:r:372:SER:HB3	2.00	0.43
40:r:357:THR:O	40:r:361:VAL:HG23	2.19	0.43
40:r:361:VAL:HG11	40:r:441:ILE:HG12	2.00	0.43
3:C:187:GLU:OE2	3:C:189:ARG:NH1	2.52	0.43
9:J:149:PRO:HB3	9:J:166:HIS:CE1	2.52	0.43
11:L:76:LYS:NZ	11:L:144:SER:OG	2.39	0.43
19:U:63:MET:HE3	42:u:130:LYS:HD2	2.00	0.43
22:Y:52:ARG:HG3	22:Y:56:ILE:HD11	1.99	0.43
26:c:55:TYR:CE2	26:c:76:PRO:HD3	2.53	0.43
30:g:119:HIS:CE1	40:r:252:PRO:HG3	2.53	0.43
32:i:325:LEU:O	32:i:329:MET:HG2	2.19	0.43
54:i:401:CDL:H142	54:i:401:CDL:H171	1.64	0.43
33:j:81:THR:C	33:j:83:ASN:H	2.25	0.43
35:l:511:LEU:HD23	35:l:511:LEU:HA	1.85	0.43
41:s:102:VAL:HG11	41:s:154:LEU:HD11	1.99	0.43
42:u:27:ALA:HB1	42:u:85:TYR:CD2	2.52	0.43
1:A:99:TRP:N	1:A:99:TRP:CD1	2.86	0.43
1:A:116:ASN:ND2	1:A:207:GLY:O	2.49	0.43
1:A:408:GLU:O	1:A:411:SER:HB3	2.18	0.43
12:M:209:TYR:CZ	14:O:41:HIS:HB2	2.54	0.43
14:O:218:PRO:HG3	14:O:224:SER:H	1.83	0.43
16:Q:402:ALA:CB	16:Q:403:PRO:CD	2.84	0.43
20:V:139:PRO:O	24:a:161:ARG:HD3	2.19	0.43
27:d:6:ASP:OD1	27:d:6:ASP:C	2.61	0.43
35:l:292:ALA:HB2	35:l:304:PHE:CB	2.49	0.43
39:p:136:GLU:HG2	39:p:165:PRO:HA	1.99	0.43
1:A:171:VAL:HG12	10:K:89:LEU:HD21	2.01	0.43
1:A:338:ASP:O	1:A:342:LEU:HB2	2.18	0.43
1:A:388:GLY:HA3	1:A:419:ILE:CD1	2.46	0.43
13:N:42:ASP:HB2	13:N:48:TYR:HE1	1.83	0.43
16:Q:100:GLU:HB2	16:Q:108:LYS:HB3	2.01	0.43
16:Q:450:ILE:O	16:Q:453:THR:HG22	2.19	0.43
21:W:73:PRO:HA	42:u:44:MET:HE1	2.01	0.43
6:X:83:VAL:HG21	6:X:145:VAL:HG22	2.00	0.43
23:Z:57:PHE:CG	35:l:435:PRO:HG3	2.53	0.43
26:c:182:VAL:HB	43:v:36:GLU:OE1	2.18	0.43
32:i:111:PHE:HA	35:l:591:PHE:CE1	2.54	0.43
32:i:226:THR:HG23	32:i:229:SER:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:295:GLN:O	35:l:425:ARG:NH1	2.51	0.43
35:l:296:ASN:O	35:l:356:ILE:HG12	2.18	0.43
38:o:8:PRO:HG3	38:o:14:LEU:HD13	2.00	0.43
40:r:326:LEU:HD23	40:r:329:LEU:HD12	2.01	0.43
41:s:190:LEU:HD23	41:s:270:PHE:CE2	2.53	0.43
56:s:401:UQ:H72	56:s:401:UQ:H111	1.86	0.43
44:w:199:LEU:HD21	44:w:286:GLN:OE1	2.19	0.43
1:A:63:TYR:O	1:A:256:ARG:HD3	2.18	0.43
5:F:40:ARG:HH22	5:F:88:THR:HG23	1.84	0.43
9:J:64:PHE:O	9:J:67:ARG:HG2	2.18	0.43
20:V:29:GLY:O	20:V:63:SER:OG	2.30	0.43
22:Y:87:PRO:HG3	43:v:96:VAL:HG22	2.00	0.43
24:a:153:GLU:O	24:a:157:ARG:HG3	2.19	0.43
33:j:90:MET:HE1	36:m:151:THR:HG23	2.00	0.43
34:k:45:THR:HG23	36:m:52:LEU:HD13	2.01	0.43
35:l:384:PRO:HA	35:l:389:PHE:CD1	2.54	0.43
35:l:419:THR:HA	35:l:422:TYR:CE2	2.53	0.43
36:m:33:LEU:HD23	36:m:65:LEU:HD11	2.00	0.43
40:r:218:LYS:O	40:r:222:GLU:HG2	2.18	0.43
40:r:334:TYR:CD1	40:r:340:ARG:HB2	2.53	0.43
44:w:40:PRO:HD3	44:w:296:MET:HE1	1.99	0.43
1:A:405:ARG:N	1:A:408:GLU:OE1	2.32	0.43
14:O:137:THR:HG22	14:O:138:THR:N	2.33	0.43
19:U:14:ALA:O	19:U:15:LYS:HG2	2.18	0.43
20:V:50:LEU:O	20:V:53:VAL:HG12	2.18	0.43
23:Z:69:LYS:HD2	35:l:363:TYR:OH	2.18	0.43
35:l:383:MET:SD	35:l:384:PRO:HD2	2.59	0.43
35:l:579:ASN:O	35:l:579:ASN:OD1	2.35	0.43
40:r:403:THR:HA	40:r:406:TYR:CD2	2.53	0.43
1:A:404:ALA:HB1	1:A:408:GLU:OE1	2.18	0.43
2:B:194:GLY:O	2:B:198:GLU:HB2	2.19	0.43
12:M:407:PRO:HB2	12:M:415:ASN:HB2	2.01	0.43
16:Q:136:PHE:HE2	16:Q:409:VAL:HG11	1.84	0.43
21:W:133:ILE:HD13	36:m:125:TRP:CH2	2.54	0.43
6:X:90:TYR:CE1	23:Z:44:PRO:HB2	2.53	0.43
25:b:12:LEU:HD23	25:b:16:ARG:NH2	2.33	0.43
27:d:33:LEU:HD23	27:d:33:LEU:HA	1.88	0.43
30:g:33:LEU:HD23	30:g:33:LEU:HA	1.85	0.43
54:g:202:CDL:H212	54:g:202:CDL:H461	2.01	0.43
32:i:84:TRP:CD1	34:k:53:PHE:HE2	2.37	0.43
35:l:83:ASP:OD1	35:l:85:PHE:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:33:LEU:HD23	36:m:65:LEU:HD21	2.01	0.43
39:p:138:LYS:HA	39:p:141:GLN:CG	2.48	0.43
42:u:96:LEU:HD12	42:u:99:HIS:NE2	2.33	0.43
44:w:121:PRO:O	44:w:128:SER:OG	2.36	0.43
2:B:76:TYR:HA	2:B:79:ARG:HE	1.84	0.43
5:F:63:PRO:O	5:F:64:LYS:HD2	2.19	0.43
12:M:43:VAL:HA	12:M:55:LYS:NZ	2.34	0.43
13:N:2:GLU:HG3	13:N:4:VAL:HG22	2.01	0.43
34:k:60:PRO:O	34:k:63:LEU:HB3	2.18	0.43
40:r:31:SER:HB3	40:r:73:LEU:HD23	2.00	0.43
40:r:337:VAL:HG11	40:r:344:LEU:HD22	2.01	0.43
1:A:76:ILE:O	1:A:80:VAL:HG22	2.18	0.43
1:A:210:THR:HB	1:A:224:ARG:HG2	2.01	0.43
2:B:39:LYS:HG3	16:Q:317:ASP:HB3	2.01	0.43
2:B:210:LEU:HD12	8:I:38:PRO:HB3	2.01	0.43
4:E:54:ILE:HD13	4:E:107:PHE:CZ	2.54	0.43
5:F:45:LYS:HE3	12:M:380:ASP:OD2	2.18	0.43
5:F:55:ILE:O	5:F:56:ARG:NH1	2.52	0.43
54:V:202:CDL:H721	54:V:202:CDL:H752	1.78	0.43
26:c:149:ILE:HG23	26:c:150:TYR:CD1	2.53	0.43
27:d:90:MET:N	27:d:90:MET:SD	2.92	0.43
35:l:366:MET:HB2	35:l:445:GLU:OE2	2.18	0.43
1:A:398:ARG:NH2	1:A:408:GLU:OE2	2.52	0.42
4:E:84:ILE:HG22	4:E:88:MET:HE3	2.00	0.42
8:I:18:ARG:HH12	21:W:26:PRO:CD	2.32	0.42
9:J:204:SER:OG	9:J:204:SER:O	2.36	0.42
11:L:174:THR:CG2	14:O:111:ARG:HD2	2.49	0.42
13:N:132:LYS:NZ	13:N:136:GLU:OE2	2.48	0.42
20:V:126:LYS:HA	20:V:126:LYS:HD2	1.73	0.42
21:W:30:LEU:HD12	21:W:30:LEU:HA	1.85	0.42
21:W:68:ARG:HD2	36:m:135:PHE:CD2	2.53	0.42
6:X:75:THR:O	6:X:79:ILE:HG13	2.19	0.42
24:a:60:SER:HB2	39:p:107:TRP:HA	2.01	0.42
54:l:701:CDL:H822	54:l:701:CDL:H631	2.00	0.42
36:m:55:MET:HE2	36:m:55:MET:HB2	1.85	0.42
54:u:201:CDL:H741	54:u:201:CDL:H712	1.47	0.42
1:A:329:LYS:HA	1:A:332:CYS:SG	2.59	0.42
2:B:78:PHE:HB3	8:I:8:ILE:HG23	2.01	0.42
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.54	0.42
20:V:9:TYR:CE1	20:V:21:LYS:HE2	2.53	0.42
25:b:16:ARG:HD3	25:b:20:ARG:HH12	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:53:LYS:HB3	26:c:53:LYS:HE2	1.70	0.42
27:d:46:THR:O	27:d:50:GLU:HG2	2.19	0.42
32:i:207:ILE:O	32:i:211:MET:HB2	2.19	0.42
33:j:33:LYS:HD2	33:j:33:LYS:HA	1.84	0.42
35:l:93:ALA:O	35:l:97:THR:OG1	2.26	0.42
35:l:264:TYR:CG	35:l:265:PRO:HD3	2.53	0.42
54:l:701:CDL:H632	55:r:502:PLX:H122	2.01	0.42
41:s:21:THR:HG21	56:s:401:UQ:H103	2.01	0.42
42:u:158:LEU:HD23	42:u:158:LEU:HA	1.86	0.42
44:w:40:PRO:HD3	44:w:296:MET:HE2	2.01	0.42
3:C:79:MET:CE	3:C:173:LEU:HD23	2.49	0.42
3:C:103:MET:HE1	3:C:121:TYR:HB2	2.00	0.42
12:M:388:ASN:CB	12:M:511:LYS:HB3	2.49	0.42
49:X:201:8Q1:S44	39:p:63:LEU:HD13	2.59	0.42
26:c:93:ASP:OD1	38:o:44:LYS:NZ	2.52	0.42
27:d:74:ILE:HG23	27:d:156:LEU:HD22	2.01	0.42
32:i:211:MET:HG3	32:i:333:SER:HB2	2.00	0.42
54:l:701:CDL:H751	54:l:701:CDL:H722	1.62	0.42
40:r:373:ILE:HD11	40:r:444:LEU:HD23	2.01	0.42
42:u:169:PHE:CE1	54:u:201:CDL:H521	2.55	0.42
44:w:132:GLN:OE1	44:w:132:GLN:HA	2.19	0.42
44:w:170:LEU:HD21	44:w:184:VAL:HG23	2.01	0.42
1:A:131:ILE:HG12	1:A:138:LEU:HD22	2.02	0.42
3:C:65:MET:HB3	3:C:100:SER:HB3	2.01	0.42
5:F:46:LYS:HE3	12:M:674:LEU:HD21	2.00	0.42
17:S:31:ASN:O	17:S:34:LYS:HG2	2.19	0.42
22:Y:92:TRP:HH2	43:v:99:MET:HB3	1.85	0.42
33:j:95:LEU:HA	33:j:95:LEU:HD23	1.75	0.42
38:o:127:ILE:HD13	38:o:127:ILE:HA	1.90	0.42
41:s:141:SER:HB3	41:s:289:LEU:HD22	1.99	0.42
41:s:149:ILE:HG13	41:s:297:THR:HG23	2.01	0.42
1:A:311:TRP:NE1	1:A:333:GLU:OE1	2.53	0.42
1:A:445:GLU:OE2	1:A:449:ARG:NH2	2.44	0.42
2:B:200:GLU:CG	13:N:88:ARG:HB2	2.48	0.42
3:C:119:LYS:HB3	3:C:119:LYS:HE2	1.62	0.42
4:E:57:LYS:HA	4:E:57:LYS:HD2	1.83	0.42
12:M:326:VAL:HG13	12:M:626:LEU:HD13	2.02	0.42
12:M:448:SER:OG	12:M:450:LYS:HE2	2.19	0.42
24:a:135:LYS:HZ1	37:n:35:LEU:HD12	1.83	0.42
27:d:163:MET:HE2	28:e:149:LEU:HD11	2.01	0.42
30:g:30:ASP:OD2	30:g:32:ARG:NH2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:51:PHE:HZ	34:k:79:VAL:HG22	1.85	0.42
41:s:173:TRP:HB2	41:s:175:ILE:HG22	2.02	0.42
44:w:170:LEU:HD22	44:w:187:TYR:CD1	2.53	0.42
1:A:71:LYS:HD2	1:A:75:TRP:CD1	2.54	0.42
1:A:324:THR:HB	1:A:347:THR:HG23	2.02	0.42
4:E:20:ILE:HG12	15:P:152:PRO:HG3	2.02	0.42
9:J:129:LEU:HD23	9:J:167:ILE:HG13	2.01	0.42
9:J:169:HIS:HD2	9:J:180:TYR:HE2	1.66	0.42
16:Q:404:LYS:H	16:Q:404:LYS:HG2	1.69	0.42
24:a:78:THR:HG21	28:e:101:LEU:HD21	2.02	0.42
25:b:84:TYR:HD1	25:b:88:TYR:HD2	1.67	0.42
32:i:147:GLN:CD	32:i:147:GLN:H	2.27	0.42
48:j:202:PEE:H59	48:j:202:PEE:H64	1.85	0.42
40:r:49:SER:HB2	40:r:58:SER:O	2.19	0.42
41:s:231:ILE:O	41:s:235:ASN:ND2	2.50	0.42
1:A:274:LYS:HB2	1:A:292:MET:SD	2.60	0.42
3:C:56:TRP:O	3:C:60:SER:OG	2.36	0.42
6:G:131:PRO:HD2	6:G:134:ASP:OD1	2.19	0.42
9:J:115:SER:HA	9:J:118:LYS:HG2	2.00	0.42
12:M:128:CYS:SG	12:M:140:GLN:NE2	2.83	0.42
12:M:343:GLY:HA2	12:M:369:GLU:OE2	2.20	0.42
12:M:467:LYS:HB3	12:M:467:LYS:HE3	1.85	0.42
16:Q:150:ALA:HB2	16:Q:400:ILE:HG12	2.01	0.42
16:Q:324:GLY:O	16:Q:329:ARG:NH2	2.53	0.42
20:V:43:LEU:HD22	35:l:580:GLN:HE22	1.84	0.42
21:W:58:ARG:HD2	21:W:58:ARG:HA	1.80	0.42
23:Z:63:PHE:HB3	35:l:502:LEU:HD11	2.01	0.42
27:d:159:GLN:NE2	28:e:142:PHE:O	2.36	0.42
32:i:317:PHE:CD2	44:w:301:LYS:HB2	2.55	0.42
35:l:8:THR:HB	35:l:82:MET:HE3	2.01	0.42
35:l:32:TYR:HB3	35:l:33:PRO:HD3	2.02	0.42
35:l:220:ALA:O	35:l:224:SER:HB2	2.19	0.42
36:m:64:MET:HB2	36:m:64:MET:HE3	1.75	0.42
40:r:375:LEU:O	40:r:375:LEU:HG	2.19	0.42
41:s:102:VAL:HG13	41:s:150:LEU:HD21	2.01	0.42
44:w:295:ARG:HA	44:w:298:VAL:HG22	2.00	0.42
3:C:85:ASP:CG	41:s:34:ARG:HD2	2.44	0.42
5:F:41:TYR:CE1	5:F:55:ILE:HD11	2.55	0.42
5:F:45:LYS:HD2	5:F:45:LYS:HA	1.88	0.42
14:O:134:VAL:HG23	14:O:186:VAL:HG12	2.02	0.42
16:Q:158:LEU:HD12	16:Q:411:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:38:VAL:CG2	35:l:446:ASN:HD22	2.33	0.42
23:Z:66:ALA:HA	35:l:363:TYR:CE2	2.43	0.42
24:a:160:MET:SD	24:a:168:TRP:HB2	2.59	0.42
25:b:31:ARG:O	25:b:31:ARG:HG2	2.19	0.42
32:i:344:SER:C	32:i:346:LEU:H	2.27	0.42
33:j:72:LEU:HD21	33:j:95:LEU:HG	2.02	0.42
48:j:202:PEE:H67	48:j:202:PEE:H73	1.91	0.42
37:n:30:ARG:HG2	37:n:30:ARG:HH11	1.85	0.42
40:r:3:LYS:HE2	40:r:3:LYS:HB3	1.87	0.42
40:r:445:LEU:O	40:r:448:THR:HG22	2.20	0.42
44:w:212:PRO:HA	44:w:215:GLN:OE1	2.20	0.42
6:G:113:LEU:O	6:G:116:VAL:HG12	2.20	0.42
9:J:37:HIS:NE2	18:T:49:ASP:HA	2.35	0.42
10:K:73:TYR:CZ	10:K:75:ASN:HB2	2.54	0.42
11:L:115:SER:HB2	12:M:267:THR:HB	2.02	0.42
12:M:61:PRO:HG3	12:M:146:PHE:CE2	2.55	0.42
12:M:67:GLU:H	12:M:67:GLU:HG3	1.69	0.42
12:M:277:MET:SD	12:M:279:GLU:HG2	2.60	0.42
12:M:326:VAL:CG2	12:M:567:ILE:HG12	2.49	0.42
16:Q:383:LYS:HA	16:Q:383:LYS:HD2	1.86	0.42
6:X:152:LYS:HB3	6:X:152:LYS:HE2	1.93	0.42
27:d:74:ILE:HD12	27:d:74:ILE:HA	1.89	0.42
35:l:109:HIS:ND1	35:l:110:SER:N	2.67	0.42
36:m:57:PHE:O	36:m:61:LEU:HB2	2.19	0.42
38:o:62:ASP:C	38:o:62:ASP:OD1	2.62	0.42
41:s:81:LEU:O	41:s:85:MET:HG2	2.20	0.42
6:G:76:LEU:HG	6:G:156:GLU:C	2.44	0.42
7:H:66:LYS:O	7:H:70:GLU:HG2	2.20	0.42
12:M:57:GLY:HA3	15:P:249:PRO:HG3	2.02	0.42
12:M:388:ASN:HB2	12:M:511:LYS:HB3	2.02	0.42
14:O:202:GLU:O	14:O:206:ASP:OD1	2.38	0.42
16:Q:271:ARG:HD2	16:Q:271:ARG:HA	1.82	0.42
24:a:182:SER:O	24:a:184:LYS:HG2	2.20	0.42
25:b:65:TYR:O	25:b:69:ILE:HG22	2.20	0.42
27:d:117:GLU:HG3	27:d:124:ASN:HB2	2.02	0.42
32:i:278:MET:HB2	32:i:278:MET:HE2	1.82	0.42
35:l:297:ASP:HB3	35:l:300:LYS:HB2	2.00	0.42
35:l:331:MET:SD	35:l:465:GLY:HA2	2.60	0.42
35:l:500:LEU:HD22	54:l:702:CDL:H551	2.02	0.42
36:m:127:ILE:H	36:m:127:ILE:HG12	1.68	0.42
38:o:81:ARG:NH1	38:o:81:ARG:HG2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:138:GLN:NE2	41:s:191:ALA:O	2.53	0.42
44:w:93:TYR:CE2	44:w:142:GLN:HB2	2.55	0.42
1:A:89:GLY:HA2	1:A:244:ASN:HD22	1.85	0.41
6:G:119:ILE:O	6:G:123:GLU:HG3	2.19	0.41
12:M:341:ILE:HG13	12:M:545:LEU:HD11	2.02	0.41
20:V:26:THR:CG2	20:V:68:ALA:HB2	2.50	0.41
6:X:86:VAL:HG21	6:X:125:GLU:HG3	2.01	0.41
24:a:164:GLY:O	24:a:170:GLN:NE2	2.51	0.41
55:a:202:PLX:H31	55:a:202:PLX:H6	1.87	0.41
25:b:89:HIS:CE1	48:l:704:PEE:H50	2.55	0.41
30:g:3:MET:HE2	30:g:3:MET:HB2	1.91	0.41
30:g:35:TYR:HD2	32:i:339:MET:SD	2.43	0.41
55:g:201:PLX:H201	32:i:332:LEU:HD13	2.02	0.41
35:l:565:THR:O	35:l:569:ILE:HG12	2.20	0.41
36:m:17:PHE:HA	36:m:20:PHE:CD1	2.54	0.41
39:p:50:GLU:C	39:p:51:HIS:HD2	2.28	0.41
40:r:408:LEU:O	40:r:412:ILE:HG13	2.19	0.41
56:s:401:UQ:H72	56:s:401:UQ:HM53	1.71	0.41
42:u:85:TYR:CD1	42:u:104:GLN:N	2.87	0.41
7:H:111:GLN:HG2	15:P:146:TYR:CD2	2.55	0.41
12:M:669:ASN:O	12:M:672:SER:OG	2.30	0.41
16:Q:222:MET:O	16:Q:224:ALA:N	2.54	0.41
16:Q:290:GLY:C	16:Q:294:ARG:HH21	2.27	0.41
26:c:61:ASP:OD2	38:o:36:ARG:NE	2.44	0.41
27:d:120:SER:O	27:d:120:SER:OG	2.32	0.41
32:i:79:LEU:HB2	34:k:47:ILE:CD1	2.51	0.41
32:i:137:ALA:HB3	32:i:138:PRO:HD3	2.02	0.41
40:r:306:PRO:HA	40:r:458:LEU:HD22	2.02	0.41
1:A:32:PHE:HB2	1:A:293:SER:O	2.20	0.41
1:A:116:ASN:O	1:A:245:VAL:HG23	2.20	0.41
10:K:98:MET:HE2	10:K:98:MET:N	2.35	0.41
14:O:164:THR:CG2	14:O:169:PHE:H	2.33	0.41
17:S:21:MET:HE2	17:S:21:MET:HB3	1.82	0.41
19:U:59:ASP:HB3	42:u:132:LYS:HG2	2.02	0.41
21:W:98:MET:HE3	31:h:79:ILE:HA	2.02	0.41
40:r:92:LYS:O	40:r:96:ILE:HG13	2.20	0.41
41:s:143:GLU:HA	41:s:146:LEU:HB2	2.03	0.41
41:s:294:LEU:O	41:s:298:LEU:HG	2.20	0.41
54:u:201:CDL:H601	54:u:201:CDL:H572	1.87	0.41
5:F:42:VAL:HG23	12:M:671:LEU:HD22	2.02	0.41
9:J:197:GLU:OE1	9:J:197:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:238:GLN:N	9:J:326:ASP:OD2	2.40	0.41
12:M:390:THR:HG22	12:M:600:GLU:HB3	2.03	0.41
12:M:510:TRP:CD1	12:M:512:VAL:HG22	2.55	0.41
12:M:602:ARG:HB2	12:M:659:VAL:HG23	2.02	0.41
15:P:63:GLN:OE1	15:P:63:GLN:HA	2.20	0.41
16:Q:317:ASP:O	16:Q:339:GLN:HG3	2.20	0.41
23:Z:23:LYS:HB3	23:Z:25:GLU:OE2	2.20	0.41
26:c:80:ASP:HA	26:c:106:HIS:HE2	1.84	0.41
30:g:47:ASP:HB2	32:i:327:PRO:HG2	2.02	0.41
39:p:136:GLU:OE1	39:p:166:LEU:N	2.52	0.41
40:r:126:LEU:HD11	40:r:153:THR:HG21	2.02	0.41
40:r:237:LYS:HE2	40:r:294:MET:HE3	2.02	0.41
40:r:336:ARG:HG2	40:r:336:ARG:HH11	1.85	0.41
44:w:132:GLN:CD	57:w:401:ADP:HN62	2.26	0.41
1:A:362:ASP:OD1	1:A:449:ARG:NH2	2.46	0.41
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.53	0.41
7:H:58:MET:HE1	7:H:71:GLN:HB3	2.02	0.41
7:H:83:GLN:HE21	15:P:104:THR:HA	1.86	0.41
8:I:8:ILE:HD13	8:I:8:ILE:HA	1.94	0.41
13:N:40:GLY:HA3	13:N:86:TRP:CH2	2.55	0.41
18:T:50:TYR:O	18:T:53:VAL:HG12	2.21	0.41
21:W:100:ASP:OD1	21:W:100:ASP:N	2.54	0.41
22:Y:43:ARG:O	22:Y:46:GLN:NE2	2.53	0.41
27:d:97:LYS:HZ1	40:r:46:GLY:C	2.27	0.41
28:e:136:LEU:HD13	28:e:136:LEU:HA	1.98	0.41
30:g:110:THR:O	30:g:114:ILE:HG12	2.20	0.41
54:g:202:CDL:H322	54:g:202:CDL:H722	2.02	0.41
31:h:78:ALA:O	31:h:81:ARG:HG2	2.20	0.41
32:i:257:LEU:HD12	32:i:334:THR:HG23	2.02	0.41
34:k:47:ILE:O	34:k:51:THR:HG23	2.21	0.41
34:k:59:MET:HB3	34:k:60:PRO:HD3	2.02	0.41
35:l:529:TYR:HB3	35:l:530:PRO:HD3	2.02	0.41
38:o:49:LEU:HD23	38:o:49:LEU:HA	1.88	0.41
38:o:81:ARG:NH2	38:o:83:THR:OG1	2.54	0.41
41:s:2:PHE:CE2	41:s:6:ILE:HD11	2.56	0.41
41:s:225:MET:SD	56:s:401:UQ:H153	2.59	0.41
1:A:433:TRP:HB2	1:A:434:PRO:HD3	2.03	0.41
3:C:87:ASP:HA	3:C:91:VAL:O	2.21	0.41
3:C:148:SER:OG	16:Q:117:HIS:O	2.34	0.41
8:I:113:LEU:HD13	16:Q:335:GLU:OE1	2.20	0.41
20:V:69:ILE:HG21	20:V:100:THR:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:V:201:CDL:H592	54:V:201:CDL:H622	1.71	0.41
6:X:82:ARG:NE	6:X:125:GLU:OE2	2.50	0.41
22:Y:88:ASP:HB3	22:Y:91:GLN:HG2	2.03	0.41
27:d:35:LYS:HD3	27:d:35:LYS:HA	1.67	0.41
32:i:79:LEU:HB2	34:k:47:ILE:HD11	2.01	0.41
55:j:203:PLX:H182	55:j:203:PLX:H152	1.94	0.41
35:l:371:THR:O	35:l:375:ILE:HG13	2.20	0.41
35:l:572:LYS:HD2	35:l:572:LYS:HA	1.82	0.41
35:l:576:MET:HA	35:l:579:ASN:ND2	2.36	0.41
39:p:56:ASP:OD1	39:p:59:LYS:HB3	2.21	0.41
44:w:60:ILE:CD1	44:w:203:VAL:HB	2.49	0.41
1:A:90:GLY:HA2	1:A:350:GLY:O	2.20	0.41
12:M:149:ASP:OD2	12:M:150:ARG:NH1	2.54	0.41
14:O:58:GLU:HG3	14:O:59:ASN:OD1	2.20	0.41
15:P:106:ALA:HB1	15:P:108:PHE:HD1	1.85	0.41
15:P:187:ILE:HD11	16:Q:113:ILE:HG12	2.01	0.41
6:X:74:LEU:HD21	6:X:152:LYS:NZ	2.36	0.41
25:b:31:ARG:HH21	39:p:116:PRO:HG2	1.86	0.41
30:g:32:ARG:O	30:g:36:MET:HG2	2.21	0.41
32:i:231:SER:O	32:i:234:TRP:HD1	2.02	0.41
39:p:102:TRP:CZ2	40:r:424:ASN:HA	2.56	0.41
41:s:96:ILE:HG22	41:s:98:MET:HG2	2.03	0.41
41:s:294:LEU:HD12	41:s:294:LEU:HA	1.80	0.41
12:M:132:ASP:HB2	12:M:232:THR:HG21	2.02	0.41
12:M:435:PRO:HB3	12:M:444:HIS:CE1	2.55	0.41
14:O:206:ASP:HA	14:O:209:LYS:HD3	2.02	0.41
15:P:204:LEU:HD11	16:Q:123:LEU:HD23	2.03	0.41
16:Q:50:ALA:O	32:i:173:THR:OG1	2.38	0.41
20:V:14:GLU:H	20:V:14:GLU:CD	2.24	0.41
22:Y:98:GLY:HA3	43:v:104:ARG:HH12	1.86	0.41
26:c:111:MET:HE3	26:c:112:TYR:CE1	2.56	0.41
27:d:65:HIS:CD2	28:e:124:ARG:HH22	2.39	0.41
28:e:84:LEU:HD21	28:e:88:ARG:CZ	2.50	0.41
31:h:4:PHE:O	31:h:6:VAL:N	2.53	0.41
35:l:237:MET:SD	35:l:303:ALA:HB2	2.61	0.41
35:l:581:LYS:HB3	35:l:583:LEU:HD23	2.02	0.41
54:l:701:CDL:H631	54:l:701:CDL:H842	2.02	0.41
38:o:81:ARG:HG2	38:o:81:ARG:HH11	1.86	0.41
40:r:49:SER:C	40:r:50:LEU:HD22	2.46	0.41
1:A:297:LYS:HG3	1:A:298:GLU:N	2.36	0.41
46:A:502:FMN:N5	47:A:503:NAI:H4N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:LEU:O	41:s:272:TRP:NE1	2.54	0.41
5:F:91:LEU:HD23	5:F:91:LEU:HA	1.81	0.41
8:I:69:VAL:O	15:P:76:VAL:HB	2.21	0.41
9:J:128:ASN:C	9:J:129:LEU:HG	2.46	0.41
9:J:279:TYR:HB2	9:J:372:ALA:HB2	2.02	0.41
19:U:59:ASP:HA	19:U:63:MET:CE	2.51	0.41
6:X:93:ILE:HD11	6:X:110:LEU:HD11	2.03	0.41
26:c:166:LEU:HD22	26:c:169:GLU:OE1	2.21	0.41
30:g:47:ASP:C	30:g:47:ASP:OD1	2.64	0.41
30:g:83:TYR:CZ	30:g:87:LEU:HD11	2.56	0.41
31:h:13:ASP:OD1	31:h:17:TRP:HD1	2.04	0.41
31:h:86:LEU:HD23	31:h:86:LEU:HA	1.88	0.41
32:i:270:MET:HE2	32:i:279:PRO:HG3	2.02	0.41
33:j:48:ARG:HE	41:s:126:LYS:HD3	1.85	0.41
35:l:363:TYR:C	35:l:363:TYR:CD1	2.99	0.41
38:o:6:TYR:CE2	38:o:15:PRO:HD3	2.53	0.41
38:o:28:GLU:H	38:o:28:GLU:HG2	1.68	0.41
39:p:55:LYS:HD3	39:p:55:LYS:HA	1.69	0.41
39:p:76:HIS:O	39:p:78:GLN:N	2.54	0.41
43:v:91:GLU:HA	43:v:91:GLU:OE1	2.20	0.41
44:w:172:ALA:CB	44:w:237:ILE:HG13	2.50	0.41
1:A:86:ARG:H	1:A:88:ARG:NH2	2.19	0.41
1:A:279:SER:OG	1:A:280:GLY:N	2.54	0.41
12:M:29:SER:OG	12:M:30:ASN:N	2.43	0.41
12:M:304:GLN:HB2	12:M:316:TYR:CD1	2.55	0.41
12:M:558:GLN:N	12:M:558:GLN:OE1	2.54	0.41
18:T:57:ASP:OD1	18:T:57:ASP:C	2.64	0.41
22:Y:88:ASP:CG	22:Y:91:GLN:HG2	2.46	0.41
24:a:113:PHE:HB2	24:a:119:ARG:HG3	2.02	0.41
24:a:139:ILE:HG23	40:r:54:LEU:HD23	2.03	0.41
33:j:87:MET:HE1	41:s:309:ILE:HD11	2.03	0.41
35:l:15:LEU:HD12	35:l:15:LEU:HA	1.82	0.41
35:l:257:VAL:O	35:l:261:ILE:HG13	2.20	0.41
54:u:201:CDL:H132	54:u:201:CDL:H762	2.02	0.41
44:w:140:LEU:HD13	44:w:163:ILE:HG21	2.02	0.41
1:A:62:TRP:HE1	1:A:136:HIS:HB3	1.86	0.40
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.61	0.40
1:A:415:ILE:O	1:A:419:ILE:HG12	2.20	0.40
3:C:85:ASP:OD2	41:s:34:ARG:HB2	2.21	0.40
6:G:119:ILE:HG21	6:G:135:ALA:HB1	2.02	0.40
9:J:207:PHE:HE2	9:J:348:LYS:CB	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:646:LEU:HD23	12:M:646:LEU:HA	1.91	0.40
16:Q:246:GLU:OE2	16:Q:249:LYS:NZ	2.36	0.40
16:Q:342:ARG:HD2	21:W:21:TYR:CZ	2.56	0.40
23:Z:57:PHE:CD2	35:l:435:PRO:HG3	2.56	0.40
24:a:86:ILE:HD12	28:e:108:TYR:HE2	1.86	0.40
26:c:109:LEU:O	26:c:113:ILE:HG23	2.21	0.40
26:c:161:TYR:HB3	26:c:166:LEU:HG	2.03	0.40
30:g:13:LEU:HD12	30:g:13:LEU:HA	1.91	0.40
32:i:20:VAL:HG11	32:i:137:ALA:HB1	2.04	0.40
35:l:353:GLU:OE2	39:p:80:TYR:HE1	2.04	0.40
39:p:62:GLN:HE21	39:p:66:GLN:HE22	1.69	0.40
44:w:52:LYS:NZ	44:w:152:SER:O	2.44	0.40
1:A:246:GLU:O	1:A:250:VAL:HG22	2.20	0.40
11:L:77:VAL:HG23	11:L:100:GLU:O	2.21	0.40
12:M:299:ARG:NE	12:M:703:ALA:O	2.54	0.40
13:N:85:GLU:HG2	13:N:86:TRP:H	1.86	0.40
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	2.02	0.40
35:l:217:LEU:HD23	35:l:276:MET:HE2	2.02	0.40
35:l:362:LEU:HD12	35:l:366:MET:SD	2.61	0.40
35:l:575:ILE:O	35:l:579:ASN:ND2	2.54	0.40
36:m:65:LEU:HD13	36:m:65:LEU:HA	1.87	0.40
40:r:71:TRP:O	40:r:74:PRO:HD2	2.22	0.40
40:r:299:VAL:O	40:r:303:ILE:HG12	2.21	0.40
1:A:152:ARG:CZ	10:K:101:PRO:HD3	2.52	0.40
1:A:290:GLU:HG3	1:A:291:GLU:H	1.87	0.40
3:C:118:ARG:HA	3:C:118:ARG:HD2	1.93	0.40
5:F:35:ASP:O	5:F:38:GLU:HG3	2.21	0.40
6:G:82:ARG:O	6:G:86:VAL:HG13	2.22	0.40
7:H:25:LYS:O	7:H:29:THR:HG23	2.21	0.40
7:H:111:GLN:OE1	15:P:124:ASN:HB2	2.21	0.40
12:M:124:HIS:CD2	16:Q:375:MET:HE3	2.56	0.40
12:M:249:GLU:HG2	12:M:262:VAL:HG22	2.04	0.40
12:M:489:ILE:HG13	12:M:679:LEU:HD21	2.03	0.40
15:P:165:TRP:HZ2	16:Q:111:PRO:HG2	1.83	0.40
20:V:105:THR:HG21	20:V:110:ILE:HD13	2.02	0.40
21:W:93:GLU:O	21:W:97:ILE:HG22	2.21	0.40
27:d:110:LEU:CD1	35:l:203:MET:HE3	2.52	0.40
35:l:88:MET:O	35:l:91:PRO:HD2	2.20	0.40
38:o:17:THR:HG21	39:p:22:ARG:HH22	1.86	0.40
40:r:216:LEU:HD23	40:r:287:ALA:HB1	2.03	0.40
40:r:373:ILE:HG22	40:r:376:ILE:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:41:LYS:HA	42:u:41:LYS:HD3	1.76	0.40
42:u:152:PRO:C	42:u:153:GLU:HG3	2.45	0.40
43:v:106:ARG:O	43:v:110:GLN:HG2	2.21	0.40
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.86	0.40
6:G:90:TYR:HD1	6:G:92:LYS:H	1.70	0.40
9:J:345:LEU:HD23	9:J:349:ALA:HB2	2.03	0.40
16:Q:208:GLU:O	16:Q:212:GLU:HG3	2.21	0.40
16:Q:435:LEU:HB2	16:Q:454:GLN:HE22	1.85	0.40
28:e:106:VAL:HG11	55:r:502:PLX:H271	2.04	0.40
32:i:45:MET:HE2	32:i:45:MET:HB3	1.92	0.40
35:l:293:ILE:HD12	35:l:293:ILE:HA	1.89	0.40
35:l:458:LEU:HD23	35:l:458:LEU:HA	1.82	0.40
41:s:72:ILE:O	41:s:75:PRO:HD2	2.22	0.40
41:s:95:LEU:HG	41:s:96:ILE:HG13	2.04	0.40
44:w:132:GLN:HE21	44:w:170:LEU:HB2	1.85	0.40
2:B:198:GLU:HB3	13:N:109:ILE:HG12	2.04	0.40
5:F:24:CYS:HB2	5:F:30:SER:OG	2.21	0.40
5:F:56:ARG:NH1	12:M:382:ARG:HG2	2.37	0.40
5:F:59:SER:O	5:F:61:VAL:HG22	2.21	0.40
11:L:169:ARG:HD2	12:M:426:ASP:OD1	2.20	0.40
12:M:160:VAL:HA	18:T:101:ASN:HD22	1.87	0.40
12:M:218:LEU:HD11	12:M:416:ALA:HB2	2.03	0.40
18:T:108:THR:OG1	18:T:117:GLN:HG2	2.22	0.40
54:V:201:CDL:H341	54:V:201:CDL:H371	1.73	0.40
21:W:125:TYR:HB3	21:W:133:ILE:HG12	2.04	0.40
26:c:184:TYR:HA	43:v:34:ARG:HH12	1.86	0.40
27:d:68:PHE:HD2	28:e:117:TRP:CZ2	2.39	0.40
31:h:94:PRO:HA	31:h:95:PRO:HD3	1.95	0.40
32:i:118:VAL:O	32:i:122:ILE:HG12	2.21	0.40
33:j:84:LEU:HD23	33:j:84:LEU:HA	1.83	0.40
35:l:56:HIS:HA	43:v:74:PHE:CD1	2.56	0.40
35:l:95:PHE:HE1	35:l:456:ARG:HD2	1.86	0.40
38:o:62:ASP:OD1	38:o:64:ALA:N	2.53	0.40
40:r:1:MET:SD	40:r:111:THR:HG21	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	414 (96%)	15 (4%)	0	100	100
2	B	174/176 (99%)	167 (96%)	7 (4%)	0	100	100
3	C	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
4	E	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
5	F	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
6	G	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
6	X	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
7	H	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
8	I	93/112 (83%)	82 (88%)	11 (12%)	0	100	100
9	J	289/341 (85%)	267 (92%)	20 (7%)	2 (1%)	18	51
10	K	40/42 (95%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
12	M	688/690 (100%)	663 (96%)	24 (4%)	1 (0%)	48	79
13	N	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
14	O	215/217 (99%)	205 (95%)	10 (5%)	0	100	100
15	P	206/208 (99%)	186 (90%)	19 (9%)	1 (0%)	24	57
16	Q	412/430 (96%)	399 (97%)	11 (3%)	2 (0%)	24	57
17	S	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
18	T	94/96 (98%)	89 (95%)	5 (5%)	0	100	100
19	U	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
20	V	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	18	51
21	W	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
22	Y	68/70 (97%)	62 (91%)	6 (9%)	0	100	100
23	Z	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
24	a	138/140 (99%)	135 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	b	99/126 (79%)	97 (98%)	2 (2%)	0	100	100
26	c	154/156 (99%)	141 (92%)	13 (8%)	0	100	100
27	d	173/175 (99%)	171 (99%)	2 (1%)	0	100	100
28	e	105/107 (98%)	98 (93%)	6 (6%)	1 (1%)	12	44
29	f	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
30	g	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
32	i	345/347 (99%)	328 (95%)	17 (5%)	0	100	100
33	j	95/113 (84%)	91 (96%)	4 (4%)	0	100	100
34	k	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
35	l	601/603 (100%)	567 (94%)	34 (6%)	0	100	100
36	m	125/175 (71%)	109 (87%)	16 (13%)	0	100	100
37	n	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
38	o	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
39	p	176/178 (99%)	165 (94%)	10 (6%)	1 (1%)	21	54
40	r	457/459 (100%)	445 (97%)	12 (3%)	0	100	100
41	s	299/318 (94%)	279 (93%)	20 (7%)	0	100	100
42	u	169/171 (99%)	161 (95%)	8 (5%)	0	100	100
43	v	122/125 (98%)	117 (96%)	5 (4%)	0	100	100
44	w	318/320 (99%)	301 (95%)	17 (5%)	0	100	100
All	All	8029/8309 (97%)	7637 (95%)	383 (5%)	9 (0%)	49	79

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	357	ARG
28	e	52	THR
15	P	125	ARG
12	M	126	LEU
16	Q	61	TRP
20	V	46	PRO
9	J	38	HIS
16	Q	404	LYS
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	344/345 (100%)	343 (100%)	1 (0%)	86	83
2	B	150/151 (99%)	146 (97%)	4 (3%)	39	62
3	C	130/132 (98%)	129 (99%)	1 (1%)	73	77
4	E	103/107 (96%)	102 (99%)	1 (1%)	68	75
5	F	76/76 (100%)	76 (100%)	0	100	100
6	G	76/81 (94%)	76 (100%)	0	100	100
6	X	76/81 (94%)	73 (96%)	3 (4%)	28	54
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	86 (99%)	1 (1%)	65	74
9	J	248/295 (84%)	246 (99%)	2 (1%)	73	77
10	K	41/41 (100%)	41 (100%)	0	100	100
11	L	113/113 (100%)	112 (99%)	1 (1%)	70	76
12	M	580/580 (100%)	575 (99%)	5 (1%)	70	76
13	N	130/130 (100%)	130 (100%)	0	100	100
14	O	182/183 (100%)	181 (100%)	1 (0%)	81	80
15	P	188/190 (99%)	188 (100%)	0	100	100
16	Q	357/370 (96%)	354 (99%)	3 (1%)	73	77
17	S	56/58 (97%)	56 (100%)	0	100	100
18	T	79/79 (100%)	78 (99%)	1 (1%)	61	72
19	U	69/69 (100%)	68 (99%)	1 (1%)	59	71
20	V	101/101 (100%)	100 (99%)	1 (1%)	68	75
21	W	122/123 (99%)	122 (100%)	0	100	100
22	Y	63/63 (100%)	63 (100%)	0	100	100
23	Z	65/65 (100%)	65 (100%)	0	100	100
24	a	122/122 (100%)	122 (100%)	0	100	100
25	b	98/119 (82%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	c	140/141 (99%)	140 (100%)	0	100	100
27	d	151/155 (97%)	150 (99%)	1 (1%)	76	78
28	e	98/99 (99%)	97 (99%)	1 (1%)	68	75
29	f	35/38 (92%)	35 (100%)	0	100	100
30	g	108/108 (100%)	108 (100%)	0	100	100
31	h	93/93 (100%)	93 (100%)	0	100	100
32	i	310/311 (100%)	308 (99%)	2 (1%)	78	79
33	j	88/99 (89%)	88 (100%)	0	100	100
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	536/537 (100%)	533 (99%)	3 (1%)	78	79
36	m	99/141 (70%)	97 (98%)	2 (2%)	48	67
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	109/113 (96%)	109 (100%)	0	100	100
39	p	159/159 (100%)	157 (99%)	2 (1%)	61	72
40	r	409/410 (100%)	405 (99%)	4 (1%)	68	75
41	s	263/275 (96%)	263 (100%)	0	100	100
42	u	148/153 (97%)	148 (100%)	0	100	100
43	v	101/112 (90%)	101 (100%)	0	100	100
44	w	281/283 (99%)	281 (100%)	0	100	100
All	All	7021/7235 (97%)	6980 (99%)	41 (1%)	76	79

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	ASP
2	B	70	LEU
2	B	73	THR
2	B	77	LEU
2	B	79	ARG
3	C	52	ASP
4	E	66	MET
8	I	62	GLU
9	J	350	ILE
9	J	351	GLU
11	L	86	ASN

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Mol	Chain	Res	Type
12	M	126	LEU
12	M	127	ASP
12	M	130	ILE
12	M	471	LYS
12	M	597	VAL
14	O	172	ILE
16	Q	55	THR
16	Q	58	THR
16	Q	192	LEU
18	T	47	ASP
19	U	9	LEU
20	V	89	ASN
6	X	117	GLU
6	X	129	GLU
6	X	139	MET
27	d	73	ASP
28	e	52	THR
32	i	190	MET
32	i	308	THR
35	l	100	ILE
35	l	203	MET
35	l	315	VAL
36	m	76	THR
36	m	139	GLU
39	p	117	ASP
39	p	141	GLN
40	r	33	LEU
40	r	50	LEU
40	r	51	ASN
40	r	178	ILE

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

Mol	Chain	Res	Type
1	A	164	ASN
1	A	170	GLN
1	A	220	GLN
4	E	45	ASN
5	F	48	ASN
6	G	142	GLN
7	H	21	HIS
8	I	21	GLN

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Mol	Chain	Res	Type
8	I	25	GLN
9	J	37	HIS
9	J	109	ASN
9	J	122	HIS
9	J	128	ASN
10	K	75	ASN
11	L	86	ASN
12	M	66	HIS
12	M	123	ASN
12	M	278	HIS
12	M	300	GLN
12	M	336	ASN
12	M	498	GLN
12	M	540	ASN
13	N	31	ASN
13	N	54	GLN
13	N	91	HIS
13	N	112	ASN
13	N	123	GLN
13	N	135	GLN
14	O	69	ASN
14	O	191	ASN
15	P	181	HIS
15	P	247	GLN
16	Q	147	ASN
16	Q	431	HIS
22	Y	46	GLN
22	Y	83	HIS
23	Z	9	HIS
23	Z	11	HIS
24	a	90	ASN
24	a	132	ASN
24	a	181	HIS
25	b	14	GLN
26	c	84	GLN
26	c	154	GLN
26	c	183	HIS
27	d	23	GLN
27	d	161	GLN
30	g	119	HIS
32	i	63	GLN
32	i	174	GLN

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Mol	Chain	Res	Type
32	i	309	ASN
32	i	316	GLN
32	i	347	ASN
33	j	10	ASN
34	k	52	HIS
34	k	57	ASN
35	l	170	GLN
35	l	309	GLN
35	l	321	GLN
35	l	447	ASN
35	l	580	GLN
37	n	3	ASN
37	n	11	HIS
38	o	75	ASN
39	p	26	HIS
39	p	62	GLN
39	p	75	GLN
40	r	44	GLN
40	r	51	ASN
40	r	168	GLN
40	r	188	ASN
41	s	5	ASN
41	s	38	ASN
41	s	47	GLN
41	s	317	GLN
42	u	30	HIS
44	w	85	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	2MR	Q	118	16	10,12,13	1.99	1 (10%)	5,13,15	6.32	3 (60%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.61	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	13.00	131.40	119.48
16	Q	118	2MR	CD-NE-CZ	4.76	132.32	123.41
16	Q	118	2MR	CQ2-NH2-CZ	2.73	129.91	123.86

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 2 are modelled with single atom and 2 are monoatomic - leaving 34 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	CDL	i	401	-	65,65,99	1.27	8 (12%)	71,77,111	1.03	5 (7%)
49	8Q1	X	201	-	31,34,34	1.69	6 (19%)	40,43,43	1.56	8 (20%)
56	UQ	s	401	-	28,28,63	3.30	7 (25%)	34,37,79	2.99	11 (32%)
54	CDL	a	201	-	90,90,99	1.12	8 (8%)	96,102,111	0.94	4 (4%)
45	SF4	B	302	2	0,12,12	-	-	-		
51	FES	O	301	14	0,4,4	-	-	-		
57	ADP	w	401	-	27,29,29	2.96	8 (29%)	42,45,45	2.04	11 (26%)
54	CDL	l	702	-	99,99,99	1.09	8 (8%)	105,111,111	0.87	4 (3%)
48	PEE	V	203	-	39,39,50	1.31	6 (15%)	41,44,55	1.02	2 (4%)
46	FMN	A	502	-	33,33,33	1.10	2 (6%)	48,50,50	1.22	8 (16%)
48	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	1.00	2 (3%)
55	PLX	a	202	-	51,51,51	1.16	5 (9%)	55,59,59	0.62	1 (1%)
55	PLX	j	203	-	51,51,51	1.16	4 (7%)	55,59,59	0.58	1 (1%)
48	PEE	j	202	-	50,50,50	1.16	6 (12%)	53,55,55	0.96	2 (3%)
55	PLX	g	201	-	51,51,51	1.14	3 (5%)	55,59,59	0.63	1 (1%)
45	SF4	A	501	1	0,12,12	-	-	-		
54	CDL	u	201	-	77,77,99	1.19	8 (10%)	83,89,111	0.94	4 (4%)
45	SF4	M	801	12	0,12,12	-	-	-		
48	PEE	B	303	-	50,50,50	1.16	6 (12%)	53,55,55	1.02	2 (3%)
51	FES	M	803	12	0,4,4	-	-	-		
54	CDL	V	202	-	67,67,99	1.25	9 (13%)	73,79,111	1.00	4 (5%)
48	PEE	l	703	-	45,45,50	1.22	6 (13%)	48,50,55	1.00	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	8Q1	G	201	6	31,34,34	1.70	6 (19%)	40,43,43	1.60	5 (12%)
50	NDP	J	401	-	49,52,52	4.40	23 (46%)	66,80,80	2.15	16 (24%)
54	CDL	V	201	-	93,93,99	1.12	9 (9%)	99,105,111	0.91	4 (4%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
54	CDL	l	701	-	98,98,99	1.08	8 (8%)	104,110,111	0.93	5 (4%)
55	PLX	r	502	-	51,51,51	1.14	3 (5%)	55,59,59	0.65	1 (1%)
45	SF4	C	301	3,16	0,12,12	-	-	-	-	-
47	NAI	A	503	-	45,48,48	3.92	20 (44%)	60,73,73	1.74	11 (18%)
54	CDL	g	202	-	96,96,99	1.10	8 (8%)	102,108,111	0.85	4 (3%)
48	PEE	l	704	-	45,45,50	1.22	6 (13%)	48,50,55	0.96	2 (4%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
48	PEE	m	201	-	40,40,50	1.14	5 (12%)	43,45,55	1.04	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	CDL	i	401	-	-	45/76/76/110	-
49	8Q1	X	201	-	-	7/41/41/41	-
56	UQ	s	401	-	-	12/21/45/87	0/1/1/1
54	CDL	a	201	-	-	50/101/101/110	-
45	SF4	B	302	2	-	-	0/6/5/5
57	ADP	w	401	-	-	2/16/32/32	0/3/3/3
51	FES	O	301	14	-	-	0/1/1/1
54	CDL	l	702	-	-	69/110/110/110	-
48	PEE	V	203	-	-	19/43/43/54	-
46	FMN	A	502	-	-	5/18/18/18	0/3/3/3
48	PEE	r	501	-	-	22/54/54/54	-
55	PLX	a	202	-	-	25/55/55/55	-
55	PLX	j	203	-	-	26/55/55/55	-
48	PEE	j	202	-	-	28/54/54/54	-
55	PLX	g	201	-	-	21/55/55/55	-
45	SF4	A	501	1	-	-	0/6/5/5
54	CDL	u	201	-	-	42/88/88/110	-
54	CDL	V	202	-	-	45/78/78/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PEE	B	303	-	-	28/54/54/54	-
45	SF4	M	801	12	-	-	0/6/5/5
51	FES	M	803	12	-	-	0/1/1/1
48	PEE	l	703	-	-	27/49/49/54	-
49	8Q1	G	201	6	-	18/41/41/41	-
50	NDP	J	401	-	-	10/34/77/77	0/4/5/5
54	CDL	V	201	-	-	62/104/104/110	-
54	CDL	l	701	-	-	56/109/109/110	-
55	PLX	r	502	-	-	35/55/55/55	-
45	SF4	M	802	12	-	-	0/6/5/5
45	SF4	C	301	3,16	-	-	0/6/5/5
47	NAI	A	503	-	-	7/29/72/72	0/5/5/5
54	CDL	g	202	-	-	60/107/107/110	-
48	PEE	l	704	-	-	31/49/49/54	-
45	SF4	B	301	2	-	-	0/6/5/5
48	PEE	m	201	-	-	22/44/44/54	-

All (194) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	J	401	NDP	C3B-C2B	-12.80	1.24	1.52
50	J	401	NDP	C6N-C5N	12.50	1.55	1.33
50	J	401	NDP	O4D-C4D	10.56	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.29	1.26	1.53
50	J	401	NDP	C3D-C4D	-9.85	1.27	1.53
56	s	401	UQ	C13-C14	9.27	1.55	1.33
47	A	503	NAI	O4B-C1B	9.20	1.63	1.42
56	s	401	UQ	C8-C9	9.07	1.54	1.33
57	w	401	ADP	C3'-C4'	-8.82	1.30	1.53
56	s	401	UQ	C18-C19	8.22	1.56	1.32
47	A	503	NAI	O4B-C4B	-8.17	1.26	1.45
50	J	401	NDP	O4B-C4B	-7.87	1.27	1.45
57	w	401	ADP	O4'-C4'	7.78	1.62	1.45
50	J	401	NDP	C2N-C3N	7.53	1.56	1.34
47	A	503	NAI	C2D-C1D	-7.51	1.29	1.53
47	A	503	NAI	C2B-C1B	-7.30	1.30	1.53
47	A	503	NAI	O4D-C4D	7.00	1.60	1.45
47	A	503	NAI	C2D-C3D	5.99	1.69	1.53
50	J	401	NDP	C6A-N6A	5.96	1.49	1.34
47	A	503	NAI	C7N-N7N	5.79	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	J	401	NDP	P2B-O2B	5.74	1.70	1.59
47	A	503	NAI	O4D-C1D	5.59	1.55	1.42
57	w	401	ADP	C6-N6	5.49	1.47	1.34
49	G	201	8Q1	C34-N36	5.48	1.45	1.33
49	X	201	8Q1	C39-N41	5.43	1.45	1.33
49	X	201	8Q1	C34-N36	5.41	1.45	1.33
50	J	401	NDP	C3B-C4B	5.40	1.66	1.53
49	G	201	8Q1	C39-N41	5.33	1.45	1.33
47	A	503	NAI	C6A-N6A	5.21	1.47	1.34
47	A	503	NAI	C4N-C3N	-5.03	1.40	1.49
50	J	401	NDP	C6N-N1N	4.96	1.49	1.37
50	J	401	NDP	O4D-C1D	-4.93	1.30	1.42
50	J	401	NDP	O4B-C1B	4.66	1.53	1.42
47	A	503	NAI	O2B-C2B	4.53	1.53	1.43
57	w	401	ADP	O4'-C1'	-4.42	1.31	1.42
50	J	401	NDP	C1B-N9A	-4.38	1.33	1.46
50	J	401	NDP	C7N-N7N	4.22	1.44	1.33
50	J	401	NDP	O2D-C2D	-4.15	1.33	1.43
46	A	502	FMN	C4A-N5	4.01	1.38	1.30
47	A	503	NAI	C6N-C5N	3.97	1.40	1.33
48	r	501	PEE	C18-C19	3.75	1.53	1.31
48	l	704	PEE	C18-C19	3.75	1.53	1.31
48	B	303	PEE	C18-C19	3.74	1.53	1.31
48	l	703	PEE	C18-C19	3.74	1.53	1.31
48	V	203	PEE	C18-C19	3.73	1.53	1.31
48	j	202	PEE	C18-C19	3.73	1.53	1.31
48	m	201	PEE	C18-C19	3.72	1.53	1.31
47	A	503	NAI	C7N-C3N	3.69	1.56	1.48
48	l	704	PEE	C39-C38	3.66	1.53	1.31
48	j	202	PEE	C39-C38	3.65	1.53	1.31
48	V	203	PEE	C39-C38	3.65	1.52	1.31
48	r	501	PEE	C39-C38	3.65	1.52	1.31
48	B	303	PEE	C39-C38	3.64	1.52	1.31
48	l	703	PEE	C39-C38	3.63	1.52	1.31
54	i	401	CDL	OA8-CA7	3.52	1.43	1.33
54	l	702	CDL	OA8-CA7	3.48	1.43	1.33
54	a	201	CDL	OA8-CA7	3.45	1.43	1.33
54	u	201	CDL	OA8-CA7	3.42	1.43	1.33
54	V	202	CDL	OA8-CA7	3.39	1.43	1.33
54	V	201	CDL	OA8-CA7	3.39	1.43	1.33
54	g	202	CDL	OA8-CA7	3.36	1.43	1.33
47	A	503	NAI	C4N-C5N	-3.34	1.40	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	l	701	CDL	OA8-CA7	3.33	1.43	1.33
57	w	401	ADP	O2'-C2'	-3.33	1.35	1.43
57	w	401	ADP	C8-N9	-3.12	1.31	1.37
50	J	401	NDP	C7N-C3N	3.11	1.55	1.48
54	a	201	CDL	OA6-CA5	3.09	1.43	1.34
54	l	702	CDL	OB6-CB5	3.09	1.43	1.34
50	J	401	NDP	O3D-C3D	3.09	1.50	1.43
57	w	401	ADP	O3'-C3'	3.08	1.50	1.43
54	V	201	CDL	OA6-CA5	3.08	1.43	1.34
54	g	202	CDL	OB6-CB5	3.06	1.42	1.34
54	u	201	CDL	OB6-CB5	3.05	1.42	1.34
54	i	401	CDL	OB6-CB5	3.02	1.42	1.34
54	V	201	CDL	OB6-CB5	3.02	1.42	1.34
54	g	202	CDL	OB8-CB7	3.01	1.42	1.33
54	V	202	CDL	OA6-CA5	3.00	1.42	1.34
54	V	201	CDL	OB8-CB7	2.99	1.42	1.33
54	g	202	CDL	OA6-CA5	2.99	1.42	1.34
50	J	401	NDP	C8A-N9A	-2.99	1.32	1.37
54	l	702	CDL	OB8-CB7	2.99	1.42	1.33
54	u	201	CDL	OB8-CB7	2.99	1.42	1.33
54	i	401	CDL	OB8-CB7	2.99	1.42	1.33
54	V	202	CDL	OB6-CB5	2.99	1.42	1.34
54	l	701	CDL	OB8-CB7	2.97	1.42	1.33
54	a	201	CDL	OB6-CB5	2.95	1.42	1.34
54	V	202	CDL	OB8-CB7	2.95	1.41	1.33
54	l	701	CDL	OA6-CA5	2.94	1.42	1.34
55	r	502	PLX	O6-C4	-2.93	1.40	1.44
54	l	701	CDL	OB6-CB5	2.92	1.42	1.34
54	l	702	CDL	OA6-CA5	2.92	1.42	1.34
54	a	201	CDL	OB8-CB7	2.91	1.41	1.33
50	J	401	NDP	C5A-N7A	-2.91	1.33	1.39
54	u	201	CDL	OA6-CA5	2.87	1.42	1.34
54	i	401	CDL	OA6-CA5	2.86	1.42	1.34
55	a	202	PLX	O6-C4	-2.83	1.40	1.44
55	g	201	PLX	O6-C4	-2.77	1.40	1.44
56	s	401	UQ	C6-C1	2.74	1.54	1.46
55	j	203	PLX	O6-C4	-2.58	1.41	1.44
47	A	503	NAI	C8A-N9A	-2.56	1.32	1.37
48	l	704	PEE	O3-C30	2.51	1.40	1.33
50	J	401	NDP	C2D-C3D	2.50	1.60	1.53
47	A	503	NAI	PN-O5D	2.49	1.69	1.59
54	i	401	CDL	OA6-CA4	-2.48	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	O3B-C3B	-2.48	1.37	1.43
50	J	401	NDP	O2B-C2B	2.47	1.53	1.44
48	l	703	PEE	O2-C2	-2.46	1.40	1.46
48	B	303	PEE	O3-C30	2.46	1.40	1.33
49	G	201	8Q1	C1-S44	2.45	1.82	1.76
48	r	501	PEE	O3-C30	2.45	1.40	1.33
54	u	201	CDL	OA6-CA4	-2.45	1.40	1.46
48	l	703	PEE	O3-C30	2.44	1.40	1.33
54	l	701	CDL	OA6-CA4	-2.43	1.40	1.46
48	j	202	PEE	O3-C30	2.42	1.40	1.33
48	l	704	PEE	O2-C2	-2.42	1.40	1.46
48	r	501	PEE	O2-C2	-2.42	1.40	1.46
48	j	202	PEE	O2-C2	-2.42	1.40	1.46
48	V	203	PEE	O2-C2	-2.40	1.40	1.46
54	l	702	CDL	OA6-CA4	-2.40	1.40	1.46
54	g	202	CDL	OA6-CA4	-2.39	1.40	1.46
48	m	201	PEE	O2-C10	2.39	1.41	1.34
47	A	503	NAI	C5B-C4B	2.39	1.59	1.51
48	B	303	PEE	O2-C10	2.38	1.41	1.34
55	j	203	PLX	C7-C6	2.38	1.55	1.50
46	A	502	FMN	C10-N1	2.37	1.38	1.33
48	V	203	PEE	O3-C30	2.36	1.40	1.33
49	X	201	8Q1	C1-S44	2.36	1.81	1.76
48	m	201	PEE	O3-C30	2.35	1.40	1.33
48	V	203	PEE	O2-C10	2.33	1.40	1.34
55	g	201	PLX	C7-C6	2.33	1.55	1.50
57	w	401	ADP	C5-N7	-2.33	1.34	1.39
54	V	202	CDL	OA6-CA4	-2.32	1.40	1.46
48	B	303	PEE	O2-C2	-2.31	1.40	1.46
48	m	201	PEE	O2-C2	-2.30	1.40	1.46
49	G	201	8Q1	C6-C1	2.29	1.53	1.50
55	r	502	PLX	C7-C6	2.29	1.55	1.50
48	r	501	PEE	O2-C10	2.26	1.40	1.34
54	a	201	CDL	OA6-CA4	-2.25	1.41	1.46
48	l	703	PEE	O2-C10	2.25	1.40	1.34
48	l	704	PEE	O2-C10	2.25	1.40	1.34
54	V	202	CDL	PB2-OB2	2.25	1.68	1.59
54	V	201	CDL	PB2-OB2	2.24	1.68	1.59
55	a	202	PLX	C7-C6	2.24	1.55	1.50
56	s	401	UQ	O4-C4	-2.23	1.18	1.23
48	j	202	PEE	O2-C10	2.22	1.40	1.34
54	a	201	CDL	OB6-CB4	-2.22	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	g	202	CDL	PB2-OB5	2.21	1.68	1.59
54	V	202	CDL	OB6-CB4	-2.21	1.41	1.46
54	l	701	CDL	OB6-CB4	-2.21	1.41	1.46
56	s	401	UQ	C7-C8	2.21	1.53	1.50
54	g	202	CDL	PB2-OB2	2.21	1.68	1.59
54	l	701	CDL	PB2-OB2	2.21	1.68	1.59
54	l	702	CDL	PB2-OB2	2.21	1.68	1.59
49	X	201	8Q1	O35-C34	-2.20	1.19	1.23
55	j	203	PLX	P1-O4	2.20	1.68	1.59
54	V	201	CDL	PB2-OB5	2.20	1.68	1.59
49	X	201	8Q1	O40-C39	-2.19	1.18	1.23
48	j	202	PEE	O3-C3	-2.19	1.40	1.45
54	u	201	CDL	PB2-OB2	2.18	1.68	1.59
54	V	201	CDL	OB6-CB4	-2.18	1.41	1.46
49	G	201	8Q1	O40-C39	-2.18	1.18	1.23
54	i	401	CDL	OB6-CB4	-2.18	1.41	1.46
48	V	203	PEE	O3-C3	-2.18	1.40	1.45
54	i	401	CDL	PB2-OB5	2.18	1.68	1.59
54	a	201	CDL	PB2-OB2	2.18	1.68	1.59
48	m	201	PEE	O3-C3	-2.18	1.40	1.45
49	G	201	8Q1	O35-C34	-2.18	1.19	1.23
54	V	202	CDL	PB2-OB5	2.18	1.68	1.59
49	X	201	8Q1	C6-C1	2.17	1.53	1.50
56	s	401	UQ	O1-C1	-2.16	1.18	1.23
54	i	401	CDL	PB2-OB2	2.16	1.68	1.59
54	u	201	CDL	OB6-CB4	-2.16	1.41	1.46
54	l	702	CDL	PB2-OB5	2.15	1.68	1.59
50	J	401	NDP	PA-O5B	2.15	1.68	1.59
54	u	201	CDL	PB2-OB5	2.15	1.68	1.59
54	l	701	CDL	PB2-OB5	2.12	1.67	1.59
54	l	702	CDL	OB6-CB4	-2.12	1.41	1.46
48	B	303	PEE	O3-C3	-2.12	1.40	1.45
54	a	201	CDL	PB2-OB5	2.11	1.67	1.59
50	J	401	NDP	O7N-C7N	-2.10	1.19	1.24
54	V	201	CDL	C11-CA5	2.10	1.56	1.50
48	l	704	PEE	O3-C3	-2.10	1.40	1.45
47	A	503	NAI	C2N-C3N	2.09	1.40	1.34
55	j	203	PLX	P1-O1	2.09	1.67	1.59
48	l	703	PEE	O3-C3	-2.09	1.40	1.45
55	g	201	PLX	P1-O4	2.08	1.67	1.59
48	r	501	PEE	O3-C3	-2.08	1.40	1.45
55	a	202	PLX	P1-O1	2.08	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	a	202	PLX	P1-O4	2.08	1.67	1.59
54	V	201	CDL	OA6-CA4	-2.06	1.41	1.46
54	g	202	CDL	OB6-CB4	-2.06	1.41	1.46
55	a	202	PLX	C25-C24	2.05	1.55	1.50
54	V	202	CDL	C11-CA5	2.04	1.56	1.50
55	r	502	PLX	P1-O1	2.02	1.67	1.59

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	s	401	UQ	C7-C8-C9	-10.56	109.22	126.79
50	J	401	NDP	C3N-C2N-N1N	-7.77	112.01	123.10
50	J	401	NDP	C1D-N1N-C2N	-6.35	110.54	121.11
49	G	201	8Q1	C6-C1-S44	6.05	120.50	113.46
50	J	401	NDP	C5A-C4A-N3A	-6.03	118.88	126.75
49	X	201	8Q1	C6-C1-S44	5.82	120.23	113.46
57	w	401	ADP	C5-C4-N3	-5.77	119.22	126.75
47	A	503	NAI	C5A-C4A-N3A	-5.73	119.27	126.75
56	s	401	UQ	C12-C13-C14	-5.65	114.06	127.66
50	J	401	NDP	C1D-N1N-C6N	-5.06	109.94	120.83
56	s	401	UQ	C11-C9-C8	-4.82	111.37	121.12
56	s	401	UQ	C10-C9-C8	-4.53	112.07	123.68
57	w	401	ADP	N3-C4-N9	4.47	134.44	127.08
57	w	401	ADP	N3-C2-N1	-4.45	121.64	128.60
48	B	303	PEE	O2-C10-C11	4.40	120.99	111.50
54	l	701	CDL	OB6-CB5-C51	4.36	120.90	111.50
47	A	503	NAI	N3A-C2A-N1A	-4.29	121.89	128.60
54	V	202	CDL	OA6-CA5-C11	4.25	120.66	111.50
50	J	401	NDP	N3A-C4A-N9A	4.17	133.96	127.08
54	i	401	CDL	OA6-CA5-C11	4.17	120.49	111.50
54	a	201	CDL	OA6-CA5-C11	4.15	120.44	111.50
56	s	401	UQ	C17-C18-C19	-4.13	113.62	127.75
56	s	401	UQ	C16-C14-C13	-4.12	112.78	121.12
54	V	201	CDL	OB6-CB5-C51	4.09	120.31	111.50
54	a	201	CDL	OB6-CB5-C51	4.09	120.31	111.50
54	l	702	CDL	OA6-CA5-C11	4.07	120.28	111.50
54	l	701	CDL	OA6-CA5-C11	4.07	120.26	111.50
54	g	202	CDL	OB6-CB5-C51	4.06	120.25	111.50
48	r	501	PEE	O2-C10-C11	4.02	120.16	111.50
48	m	201	PEE	O2-C10-C11	4.01	120.14	111.50
54	V	201	CDL	OA6-CA5-C11	4.01	120.13	111.50
47	A	503	NAI	N3A-C4A-N9A	4.00	133.68	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	u	201	CDL	OA6-CA5-C11	3.97	120.06	111.50
54	l	702	CDL	OB6-CB5-C51	3.95	120.01	111.50
50	J	401	NDP	N3A-C2A-N1A	-3.90	122.50	128.60
48	j	202	PEE	O2-C10-C11	3.88	119.87	111.50
56	s	401	UQ	C15-C14-C13	-3.85	113.79	123.68
48	V	203	PEE	O2-C10-C11	3.85	119.80	111.50
48	l	703	PEE	O2-C10-C11	3.84	119.78	111.50
54	V	202	CDL	OB6-CB5-C51	3.82	119.74	111.50
48	l	704	PEE	O2-C10-C11	3.81	119.72	111.50
47	A	503	NAI	C2A-N3A-C4A	3.81	120.75	111.75
56	s	401	UQ	C7-C6-C1	3.80	123.05	118.48
50	J	401	NDP	C2A-N3A-C4A	3.76	120.64	111.75
57	w	401	ADP	C2-N3-C4	3.72	120.53	111.75
54	i	401	CDL	OB6-CB5-C51	3.71	119.51	111.50
54	u	201	CDL	OB6-CB5-C51	3.64	119.35	111.50
49	G	201	8Q1	C37-C38-C39	3.61	118.37	112.36
47	A	503	NAI	C5A-N7A-C8A	3.61	108.64	103.51
54	g	202	CDL	OA6-CA5-C11	3.61	119.28	111.50
57	w	401	ADP	N9-C8-N7	-3.60	108.99	113.91
49	G	201	8Q1	O4-C1-C6	-3.45	119.91	123.99
56	s	401	UQ	C21-C19-C18	-3.44	112.69	122.65
57	w	401	ADP	C5-N7-C8	3.44	108.40	103.51
49	X	201	8Q1	O4-C1-C6	-3.41	119.96	123.99
47	A	503	NAI	N9A-C8A-N7A	-3.30	109.40	113.91
56	s	401	UQ	CM5-C5-C6	-3.30	119.02	124.40
47	A	503	NAI	C3D-C2D-C1D	3.29	107.68	101.43
56	s	401	UQ	C20-C19-C18	-3.29	113.14	122.65
46	A	502	FMN	C4-N3-C2	-3.22	119.70	125.64
47	A	503	NAI	C4A-C5A-N7A	-3.20	106.73	110.62
50	J	401	NDP	C5A-N7A-C8A	3.18	108.03	103.51
47	A	503	NAI	C4D-O4D-C1D	-3.09	102.65	109.47
57	w	401	ADP	C4-N9-C8	3.04	109.02	105.73
50	J	401	NDP	N9A-C8A-N7A	-3.04	109.76	113.91
50	J	401	NDP	PN-O3-PA	-3.03	122.44	132.83
50	J	401	NDP	C4A-C5A-N7A	-3.00	106.96	110.62
49	X	201	8Q1	C37-C38-C39	2.93	117.23	112.36
54	V	201	CDL	OB8-CB7-C71	2.90	121.02	111.91
48	r	501	PEE	O3-C30-C31	2.88	120.93	111.91
57	w	401	ADP	C4'-O4'-C1'	-2.85	103.18	109.47
46	A	502	FMN	C4A-C4-N3	2.77	120.21	113.19
57	w	401	ADP	C4-C5-N7	-2.75	107.26	110.62
48	B	303	PEE	O3-C30-C31	2.73	120.48	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	i	401	CDL	OB8-CB7-C71	2.71	120.42	111.91
48	l	703	PEE	O3-C30-C31	2.69	120.33	111.91
55	r	502	PLX	C1A-N1-C1	2.65	120.77	109.92
54	V	202	CDL	OB8-CB7-C71	2.64	120.21	111.91
54	i	401	CDL	OA8-CA7-C31	2.62	120.14	111.91
54	l	702	CDL	OB8-CB7-C71	2.59	120.03	111.91
54	u	201	CDL	OB8-CB7-C71	2.58	120.02	111.91
48	m	201	PEE	O3-C30-C31	2.57	119.98	111.91
54	l	701	CDL	OB8-CB7-C71	2.56	119.94	111.91
57	w	401	ADP	PA-O3A-PB	-2.55	124.09	132.83
54	a	201	CDL	OB8-CB7-C71	2.53	119.86	111.91
54	u	201	CDL	OA8-CA7-C31	2.53	119.85	111.91
54	g	202	CDL	OA8-CA7-C31	2.53	119.83	111.91
54	a	201	CDL	OA8-CA7-C31	2.52	119.82	111.91
48	j	202	PEE	O3-C30-C31	2.52	119.81	111.91
48	m	201	PEE	C3-C2-C1	-2.51	105.84	111.79
48	l	704	PEE	O3-C30-C31	2.51	119.79	111.91
54	l	701	CDL	CB4-OB6-CB5	-2.51	111.62	117.79
54	g	202	CDL	OB8-CB7-C71	2.48	119.70	111.91
54	l	701	CDL	OA8-CA7-C31	2.47	119.64	111.91
46	A	502	FMN	C4A-C10-N10	2.43	120.04	116.48
54	V	201	CDL	OA8-CA7-C31	2.43	119.55	111.91
54	l	702	CDL	OA8-CA7-C31	2.42	119.51	111.91
46	A	502	FMN	O4-C4-C4A	-2.42	120.18	126.60
55	g	201	PLX	C1A-N1-C1	2.41	119.76	109.92
49	X	201	8Q1	C32-C34-N36	2.37	121.30	116.58
46	A	502	FMN	C9A-C5A-N5	-2.36	119.87	122.43
47	A	503	NAI	C2D-C3D-C4D	2.35	107.20	102.64
55	j	203	PLX	C1A-N1-C1	2.33	119.46	109.92
46	A	502	FMN	C10-C4A-N5	-2.33	119.91	124.86
49	G	201	8Q1	O4-C1-S44	-2.33	119.59	122.61
50	J	401	NDP	C2B-C3B-C4B	2.32	107.04	101.99
48	V	203	PEE	O3-C30-C31	2.32	119.18	111.91
55	a	202	PLX	C1A-N1-C1	2.29	119.27	109.92
54	V	202	CDL	OA8-CA7-C31	2.28	119.05	111.91
47	A	503	NAI	C4A-N9A-C8A	2.26	108.18	105.73
49	G	201	8Q1	C43-S44-C1	2.23	108.80	101.87
50	J	401	NDP	C4A-N9A-C8A	2.18	108.09	105.73
49	X	201	8Q1	C43-S44-C1	2.17	108.62	101.87
49	X	201	8Q1	O4-C1-S44	-2.16	119.80	122.61
54	i	401	CDL	CA4-OA6-CA5	-2.16	112.48	117.79
57	w	401	ADP	O4'-C1'-C2'	-2.11	102.03	106.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	J	401	NDP	C2D-C3D-C4D	2.10	106.73	102.64
46	A	502	FMN	C4A-C10-N1	-2.10	119.87	124.73
49	X	201	8Q1	C37-N36-C34	-2.09	118.86	122.59
49	X	201	8Q1	C38-C39-N41	2.09	119.93	116.42
50	J	401	NDP	C2B-C1B-N9A	-2.08	110.03	113.53
46	A	502	FMN	C5A-C9A-N10	2.03	120.05	117.95
50	J	401	NDP	C3D-C2D-C1D	2.01	105.25	101.43

There are no chirality outliers.

All (774) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
47	A	503	NAI	PN-O3-PA-O5B
47	A	503	NAI	C5D-O5D-PN-O3
47	A	503	NAI	O4D-C4D-C5D-O5D
47	A	503	NAI	C3D-C4D-C5D-O5D
48	B	303	PEE	C11-C10-O2-C2
48	B	303	PEE	C4-O4P-P-O2P
48	V	203	PEE	C11-C10-O2-C2
48	V	203	PEE	C1-O3P-P-O2P
48	V	203	PEE	C1-O3P-P-O1P
48	V	203	PEE	C1-O3P-P-O4P
48	V	203	PEE	C4-O4P-P-O1P
48	j	202	PEE	C4-O4P-P-O3P
48	j	202	PEE	C4-O4P-P-O2P
48	l	703	PEE	C11-C10-O2-C2
48	l	703	PEE	C4-O4P-P-O2P
48	l	703	PEE	O4P-C4-C5-N
48	l	704	PEE	C1-O3P-P-O1P
48	l	704	PEE	O4P-C4-C5-N
48	l	704	PEE	C37-C38-C39-C40
48	m	201	PEE	C4-O4P-P-O1P
48	r	501	PEE	C11-C10-O2-C2
49	G	201	8Q1	C1-C6-C7-C8
49	G	201	8Q1	O4-C1-S44-C43
49	G	201	8Q1	C6-C1-S44-C43
49	G	201	8Q1	C28-C29-C32-C34
49	G	201	8Q1	C28-C29-C32-O33
49	G	201	8Q1	C31-C29-C32-O33
49	G	201	8Q1	C28-O27-P24-O2

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Mol	Chain	Res	Type	Atoms
49	G	201	8Q1	C28-O27-P24-O1
49	X	201	8Q1	O4-C1-S44-C43
49	X	201	8Q1	C6-C1-S44-C43
49	X	201	8Q1	C42-C43-S44-C1
50	J	401	NDP	C5D-O5D-PN-O1N
50	J	401	NDP	O4D-C4D-C5D-O5D
50	J	401	NDP	C2N-C3N-C7N-N7N
54	V	201	CDL	O1-C1-CA2-OA2
54	V	201	CDL	CA2-C1-CB2-OB2
54	V	201	CDL	CA2-OA2-PA1-OA3
54	V	201	CDL	CA2-OA2-PA1-OA4
54	V	201	CDL	CA3-OA5-PA1-OA2
54	V	201	CDL	CA3-OA5-PA1-OA3
54	V	201	CDL	CA3-OA5-PA1-OA4
54	V	201	CDL	OA7-CA5-OA6-CA4
54	V	201	CDL	C11-CA5-OA6-CA4
54	V	201	CDL	CB2-OB2-PB2-OB3
54	V	201	CDL	CB2-OB2-PB2-OB4
54	V	201	CDL	CB2-OB2-PB2-OB5
54	V	201	CDL	CB3-OB5-PB2-OB3
54	V	201	CDL	CB3-OB5-PB2-OB4
54	V	202	CDL	CA2-C1-CB2-OB2
54	V	202	CDL	CB2-OB2-PB2-OB3
54	V	202	CDL	CB3-OB5-PB2-OB2
54	V	202	CDL	CB3-OB5-PB2-OB3
54	V	202	CDL	CB3-OB5-PB2-OB4
54	a	201	CDL	CA2-OA2-PA1-OA3
54	a	201	CDL	CA2-OA2-PA1-OA4
54	a	201	CDL	CB2-OB2-PB2-OB3
54	a	201	CDL	CB3-OB5-PB2-OB4
54	g	202	CDL	CA2-OA2-PA1-OA3
54	g	202	CDL	CA2-OA2-PA1-OA4
54	g	202	CDL	OA6-CA4-CA6-OA8
54	g	202	CDL	CB3-OB5-PB2-OB3
54	i	401	CDL	CA2-OA2-PA1-OA5
54	i	401	CDL	CA3-OA5-PA1-OA2
54	i	401	CDL	CA3-OA5-PA1-OA3
54	i	401	CDL	CA3-OA5-PA1-OA4
54	i	401	CDL	CB2-OB2-PB2-OB3
54	i	401	CDL	CB2-OB2-PB2-OB4
54	i	401	CDL	CB2-OB2-PB2-OB5
54	i	401	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
54	l	701	CDL	O1-C1-CA2-OA2
54	l	701	CDL	CB2-OB2-PB2-OB3
54	l	701	CDL	CB2-OB2-PB2-OB4
54	l	701	CDL	CB3-OB5-PB2-OB2
54	l	701	CDL	CB3-OB5-PB2-OB3
54	l	701	CDL	CB3-OB5-PB2-OB4
54	l	702	CDL	O1-C1-CA2-OA2
54	l	702	CDL	CA2-OA2-PA1-OA3
54	l	702	CDL	CA2-OA2-PA1-OA4
54	l	702	CDL	CA2-OA2-PA1-OA5
54	l	702	CDL	CB2-OB2-PB2-OB4
54	l	702	CDL	OB6-CB4-CB6-OB8
54	u	201	CDL	O1-C1-CA2-OA2
54	u	201	CDL	CB2-C1-CA2-OA2
54	u	201	CDL	CA2-OA2-PA1-OA5
54	u	201	CDL	CB2-OB2-PB2-OB3
54	u	201	CDL	CB3-OB5-PB2-OB3
54	u	201	CDL	CB3-OB5-PB2-OB4
55	a	202	PLX	O7-C6-O6-C4
55	a	202	PLX	C3-O4-P1-O2
55	a	202	PLX	C2-O1-P1-O2
55	a	202	PLX	N1-C1-C2-O1
55	g	201	PLX	O7-C6-O6-C4
55	g	201	PLX	C3-O4-P1-O2
55	g	201	PLX	C3-O4-P1-O3
55	j	203	PLX	O7-C6-C7-C8
55	j	203	PLX	O7-C6-O6-C4
55	j	203	PLX	O9-C24-C25-C26
55	r	502	PLX	O7-C6-O6-C4
55	r	502	PLX	C3-O4-P1-O1
55	r	502	PLX	C2-O1-P1-O3
55	r	502	PLX	O9-C24-C25-C26
56	s	401	UQ	C7-C8-C9-C10
56	s	401	UQ	C7-C8-C9-C11
56	s	401	UQ	C12-C11-C9-C8
56	s	401	UQ	C12-C13-C14-C16
56	s	401	UQ	C13-C14-C16-C17
56	s	401	UQ	C14-C16-C17-C18
56	s	401	UQ	C17-C18-C19-C21
48	l	704	PEE	O5-C30-O3-C3
54	i	401	CDL	OA9-CA7-OA8-CA6
48	B	303	PEE	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
48	V	203	PEE	O4-C10-O2-C2
48	j	202	PEE	O4-C10-O2-C2
48	l	703	PEE	O4-C10-O2-C2
48	r	501	PEE	O4-C10-O2-C2
48	j	202	PEE	C11-C10-O2-C2
54	l	701	CDL	OA9-CA7-OA8-CA6
56	s	401	UQ	C12-C11-C9-C10
54	V	201	CDL	OA9-CA7-OA8-CA6
48	l	703	PEE	C31-C30-O3-C3
48	l	704	PEE	C31-C30-O3-C3
54	g	202	CDL	C71-CB7-OB8-CB6
54	i	401	CDL	C31-CA7-OA8-CA6
54	l	701	CDL	C31-CA7-OA8-CA6
48	j	202	PEE	C17-C18-C19-C20
54	V	201	CDL	C59-C60-C61-C62
48	l	703	PEE	O5-C30-O3-C3
54	g	202	CDL	OB9-CB7-OB8-CB6
54	l	702	CDL	C11-C12-C13-C14
54	V	201	CDL	C32-C33-C34-C35
54	V	202	CDL	C51-CB5-OB6-CB4
54	g	202	CDL	C51-CB5-OB6-CB4
48	j	202	PEE	C30-C31-C32-C33
50	J	401	NDP	C2D-C1D-N1N-C6N
54	V	202	CDL	C80-C81-C82-C83
54	l	701	CDL	C14-C15-C16-C17
54	l	701	CDL	C58-C59-C60-C61
55	j	203	PLX	C28-C29-C30-C31
54	V	202	CDL	C32-C33-C34-C35
54	l	702	CDL	C59-C60-C61-C62
54	i	401	CDL	C31-C32-C33-C34
54	l	702	CDL	C75-C76-C77-C78
55	r	502	PLX	C30-C31-C32-C33
54	V	201	CDL	C31-CA7-OA8-CA6
54	V	202	CDL	OB7-CB5-OB6-CB4
54	l	702	CDL	C39-C40-C41-C42
55	g	201	PLX	C7-C8-C9-C10
54	u	201	CDL	C71-C72-C73-C74
54	V	201	CDL	C11-C12-C13-C14
54	g	202	CDL	C78-C79-C80-C81
54	V	201	CDL	CB2-C1-CA2-OA2
54	a	201	CDL	CB2-C1-CA2-OA2
54	a	201	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
54	g	202	CDL	CB2-C1-CA2-OA2
54	i	401	CDL	CA2-C1-CB2-OB2
54	l	701	CDL	CB2-C1-CA2-OA2
54	l	701	CDL	CA2-C1-CB2-OB2
54	l	702	CDL	CB2-C1-CA2-OA2
54	g	202	CDL	OB7-CB5-OB6-CB4
54	l	701	CDL	OB9-CB7-OB8-CB6
54	l	701	CDL	C71-CB7-OB8-CB6
54	l	702	CDL	C71-CB7-OB8-CB6
54	V	201	CDL	C62-C63-C64-C65
48	m	201	PEE	C31-C32-C33-C34
54	a	201	CDL	C34-C35-C36-C37
54	i	401	CDL	C14-C15-C16-C17
55	r	502	PLX	C35-C36-C37-C38
48	V	203	PEE	O3P-C1-C2-O2
48	m	201	PEE	C13-C14-C15-C16
54	V	201	CDL	C34-C35-C36-C37
54	l	701	CDL	C55-C56-C57-C58
54	l	702	CDL	C35-C36-C37-C38
54	l	702	CDL	C54-C55-C56-C57
54	a	201	CDL	O1-C1-CB2-OB2
54	l	702	CDL	O1-C1-CB2-OB2
54	V	201	CDL	OB6-CB4-CB6-OB8
54	V	202	CDL	OB6-CB4-CB6-OB8
48	m	201	PEE	C33-C34-C35-C36
54	l	701	CDL	C72-C73-C74-C75
55	r	502	PLX	C12-C13-C14-C15
54	u	201	CDL	CB7-C71-C72-C73
54	l	702	CDL	OB9-CB7-OB8-CB6
54	l	702	CDL	CB5-C51-C52-C53
48	B	303	PEE	C17-C18-C19-C20
54	V	202	CDL	CB7-C71-C72-C73
54	g	202	CDL	CA5-C11-C12-C13
54	g	202	CDL	CA7-C31-C32-C33
54	g	202	CDL	CB7-C71-C72-C73
54	i	401	CDL	CA7-C31-C32-C33
54	i	401	CDL	CB7-C71-C72-C73
54	l	701	CDL	CB5-C51-C52-C53
54	l	701	CDL	CB7-C71-C72-C73
54	u	201	CDL	CB5-C51-C52-C53
54	u	201	CDL	C52-C53-C54-C55
55	g	201	PLX	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
50	J	401	NDP	C3D-C4D-C5D-O5D
48	V	203	PEE	C31-C30-O3-C3
54	g	202	CDL	C57-C58-C59-C60
54	u	201	CDL	C75-C76-C77-C78
55	r	502	PLX	C2-C1-N1-C1C
55	r	502	PLX	C2-C1-N1-C1A
54	a	201	CDL	CA7-C31-C32-C33
54	g	202	CDL	CB5-C51-C52-C53
54	l	702	CDL	CB7-C71-C72-C73
54	g	202	CDL	C23-C24-C25-C26
48	l	703	PEE	C30-C31-C32-C33
54	V	202	CDL	O1-C1-CB2-OB2
54	a	201	CDL	O1-C1-CA2-OA2
54	g	202	CDL	O1-C1-CA2-OA2
54	i	401	CDL	O1-C1-CB2-OB2
54	l	701	CDL	O1-C1-CB2-OB2
54	V	201	CDL	CB7-C71-C72-C73
48	V	203	PEE	C17-C18-C19-C20
48	l	703	PEE	C37-C38-C39-C40
48	m	201	PEE	C17-C18-C19-C20
54	u	201	CDL	C11-CA5-OA6-CA4
54	l	701	CDL	C20-C21-C22-C23
48	l	703	PEE	C4-O4P-P-O3P
48	m	201	PEE	C4-O4P-P-O3P
48	r	501	PEE	C4-O4P-P-O3P
54	V	201	CDL	CA2-OA2-PA1-OA5
54	V	202	CDL	CA2-OA2-PA1-OA5
54	V	202	CDL	CB2-OB2-PB2-OB5
54	a	201	CDL	CA2-OA2-PA1-OA5
54	a	201	CDL	CA3-OA5-PA1-OA2
54	a	201	CDL	CB2-OB2-PB2-OB5
54	a	201	CDL	CB3-OB5-PB2-OB2
54	g	202	CDL	CA2-OA2-PA1-OA5
54	g	202	CDL	CB2-OB2-PB2-OB5
54	g	202	CDL	CB3-OB5-PB2-OB2
54	l	701	CDL	CB2-OB2-PB2-OB5
54	l	702	CDL	CB2-OB2-PB2-OB5
54	l	702	CDL	CB3-OB5-PB2-OB2
54	u	201	CDL	CB2-OB2-PB2-OB5
54	u	201	CDL	CB3-OB5-PB2-OB2
55	a	202	PLX	C2-O1-P1-O4
55	g	201	PLX	C3-O4-P1-O1

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Mol	Chain	Res	Type	Atoms
55	r	502	PLX	C2-O1-P1-O4
54	V	201	CDL	C71-CB7-OB8-CB6
54	u	201	CDL	OA7-CA5-OA6-CA4
54	l	701	CDL	C42-C43-C44-C45
55	j	203	PLX	C34-C35-C36-C37
54	V	202	CDL	C71-CB7-OB8-CB6
54	V	202	CDL	C78-C79-C80-C81
54	l	701	CDL	C23-C24-C25-C26
48	l	704	PEE	C33-C34-C35-C36
54	V	201	CDL	C74-C75-C76-C77
54	l	702	CDL	C55-C56-C57-C58
55	g	201	PLX	C28-C29-C30-C31
54	V	201	CDL	C31-C32-C33-C34
54	V	201	CDL	C52-C53-C54-C55
54	g	202	CDL	C60-C61-C62-C63
54	u	201	CDL	C59-C60-C61-C62
55	a	202	PLX	C12-C13-C14-C15
55	g	201	PLX	C32-C33-C34-C35
55	r	502	PLX	C33-C34-C35-C36
48	l	704	PEE	C22-C23-C24-C25
54	g	202	CDL	C43-C44-C45-C46
54	g	202	CDL	C75-C76-C77-C78
54	u	201	CDL	C55-C56-C57-C58
55	a	202	PLX	C33-C34-C35-C36
55	g	201	PLX	C11-C10-C9-C8
55	j	203	PLX	C13-C14-C15-C16
48	r	501	PEE	C20-C21-C22-C23
54	a	201	CDL	C17-C18-C19-C20
54	a	201	CDL	C73-C74-C75-C76
55	a	202	PLX	C34-C35-C36-C37
55	r	502	PLX	C28-C29-C30-C31
48	V	203	PEE	O5-C30-O3-C3
48	B	303	PEE	C21-C22-C23-C24
48	l	704	PEE	C31-C32-C33-C34
54	g	202	CDL	C12-C13-C14-C15
54	i	401	CDL	C73-C74-C75-C76
54	l	701	CDL	C73-C74-C75-C76
54	l	702	CDL	C72-C73-C74-C75
55	j	203	PLX	C7-C8-C9-C10
54	V	201	CDL	O1-C1-CB2-OB2
54	V	201	CDL	C72-C73-C74-C75
54	g	202	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
54	V	202	CDL	C31-CA7-OA8-CA6
54	V	202	CDL	C79-C80-C81-C82
54	a	201	CDL	C75-C76-C77-C78
54	g	202	CDL	C32-C33-C34-C35
54	g	202	CDL	C63-C64-C65-C66
54	g	202	CDL	C73-C74-C75-C76
55	j	203	PLX	C12-C13-C14-C15
55	r	502	PLX	C15-C16-C17-C18
54	V	202	CDL	C52-C53-C54-C55
54	i	401	CDL	C32-C33-C34-C35
54	l	702	CDL	C40-C41-C42-C43
55	r	502	PLX	C13-C14-C15-C16
49	G	201	8Q1	C7-C8-C9-C10
54	l	702	CDL	C52-C53-C54-C55
54	l	702	CDL	C56-C57-C58-C59
55	g	201	PLX	C33-C34-C35-C36
48	l	703	PEE	C31-C32-C33-C34
48	l	704	PEE	C13-C14-C15-C16
48	m	201	PEE	O4-C10-O2-C2
48	m	201	PEE	C11-C10-O2-C2
54	a	201	CDL	C71-C72-C73-C74
55	a	202	PLX	C7-C8-C9-C10
55	r	502	PLX	C32-C33-C34-C35
54	V	201	CDL	CA7-C31-C32-C33
48	l	704	PEE	C14-C15-C16-C17
54	g	202	CDL	C62-C63-C64-C65
54	u	201	CDL	C13-C14-C15-C16
55	r	502	PLX	C10-C11-C12-C13
54	V	202	CDL	OB9-CB7-OB8-CB6
48	B	303	PEE	C14-C15-C16-C17
55	g	201	PLX	C9-C10-C11-C12
55	r	502	PLX	C11-C10-C9-C8
48	r	501	PEE	C12-C13-C14-C15
54	V	202	CDL	C75-C76-C77-C78
54	g	202	CDL	C71-C72-C73-C74
54	l	701	CDL	C39-C40-C41-C42
54	l	702	CDL	C60-C61-C62-C63
54	l	702	CDL	C81-C82-C83-C84
54	V	202	CDL	C81-C82-C83-C84
54	i	401	CDL	C74-C75-C76-C77
55	j	203	PLX	C27-C28-C29-C30
55	j	203	PLX	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
54	a	201	CDL	C22-C23-C24-C25
54	l	701	CDL	C35-C36-C37-C38
54	l	701	CDL	C56-C57-C58-C59
55	a	202	PLX	C19-C20-C21-C22
54	V	201	CDL	OB9-CB7-OB8-CB6
55	g	201	PLX	C15-C16-C17-C18
55	j	203	PLX	C26-C27-C28-C29
54	V	201	CDL	C37-C38-C39-C40
54	i	401	CDL	C52-C53-C54-C55
55	r	502	PLX	C14-C15-C16-C17
54	a	201	CDL	C37-C38-C39-C40
54	l	701	CDL	C52-C53-C54-C55
54	l	701	CDL	C75-C76-C77-C78
48	l	704	PEE	C11-C10-O2-C2
55	r	502	PLX	O7-C6-C7-C8
48	l	703	PEE	C21-C22-C23-C24
54	i	401	CDL	C37-C38-C39-C40
54	u	201	CDL	C14-C15-C16-C17
54	u	201	CDL	CA7-C31-C32-C33
48	B	303	PEE	C35-C36-C37-C38
55	j	203	PLX	C14-C15-C16-C17
54	l	702	CDL	C53-C54-C55-C56
55	j	203	PLX	C25-C26-C27-C28
48	V	203	PEE	C11-C12-C13-C14
48	l	704	PEE	O4-C10-O2-C2
54	i	401	CDL	C11-C12-C13-C14
54	V	202	CDL	CB5-C51-C52-C53
54	a	201	CDL	CB7-C71-C72-C73
54	a	201	CDL	C32-C33-C34-C35
54	g	202	CDL	C74-C75-C76-C77
54	V	202	CDL	OA9-CA7-OA8-CA6
48	m	201	PEE	C22-C23-C24-C25
54	V	201	CDL	C54-C55-C56-C57
54	g	202	CDL	C13-C14-C15-C16
48	B	303	PEE	C37-C38-C39-C40
48	l	703	PEE	C19-C20-C21-C22
54	a	201	CDL	C71-CB7-OB8-CB6
55	j	203	PLX	C15-C16-C17-C18
55	j	203	PLX	C10-C11-C12-C13
54	g	202	CDL	C61-C62-C63-C64
55	r	502	PLX	C31-C32-C33-C34
54	a	201	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
54	V	202	CDL	C71-C72-C73-C74
48	j	202	PEE	C32-C33-C34-C35
48	j	202	PEE	C41-C42-C43-C44
54	l	701	CDL	C59-C60-C61-C62
54	V	201	CDL	C51-CB5-OB6-CB4
48	l	703	PEE	O3P-C1-C2-O2
54	a	201	CDL	OA5-CA3-CA4-OA6
49	X	201	8Q1	C9-C10-C11-C12
54	g	202	CDL	OB6-CB4-CB6-OB8
54	i	401	CDL	OB6-CB4-CB6-OB8
55	r	502	PLX	C2-C1-N1-C1B
48	m	201	PEE	C12-C13-C14-C15
54	V	201	CDL	C14-C15-C16-C17
54	l	701	CDL	C81-C82-C83-C84
48	V	203	PEE	C12-C13-C14-C15
54	a	201	CDL	C43-C44-C45-C46
54	V	202	CDL	C55-C56-C57-C58
54	l	702	CDL	C32-C33-C34-C35
54	V	201	CDL	OB7-CB5-OB6-CB4
54	l	701	CDL	C74-C75-C76-C77
54	l	702	CDL	C37-C38-C39-C40
48	B	303	PEE	C4-O4P-P-O3P
48	V	203	PEE	C4-O4P-P-O3P
54	V	201	CDL	CB3-OB5-PB2-OB2
54	i	401	CDL	CB3-OB5-PB2-OB2
48	l	704	PEE	O3P-C1-C2-C3
48	r	501	PEE	C42-C43-C44-C45
55	r	502	PLX	C9-C10-C11-C12
54	u	201	CDL	C19-C20-C21-C22
54	l	701	CDL	C82-C83-C84-C85
54	l	702	CDL	C43-C44-C45-C46
55	a	202	PLX	C11-C12-C13-C14
54	a	201	CDL	OB9-CB7-OB8-CB6
48	B	303	PEE	C33-C34-C35-C36
54	V	201	CDL	CA3-CA4-CA6-OA8
54	V	202	CDL	CB3-CB4-CB6-OB8
54	g	202	CDL	CA3-CA4-CA6-OA8
54	g	202	CDL	CB3-CB4-CB6-OB8
54	l	702	CDL	C33-C34-C35-C36
55	j	203	PLX	C3-C4-C5-O8
48	l	704	PEE	C10-C11-C12-C13
56	s	401	UQ	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
54	u	201	CDL	C78-C79-C80-C81
55	r	502	PLX	C16-C17-C18-C19
55	a	202	PLX	O6-C6-C7-C8
48	B	303	PEE	C44-C45-C46-C47
48	r	501	PEE	C19-C20-C21-C22
54	V	202	CDL	C84-C85-C86-C87
54	l	702	CDL	C64-C65-C66-C67
55	g	201	PLX	C13-C14-C15-C16
55	r	502	PLX	C7-C8-C9-C10
54	l	702	CDL	C14-C15-C16-C17
54	u	201	CDL	C53-C54-C55-C56
48	V	203	PEE	C30-C31-C32-C33
48	j	202	PEE	C31-C30-O3-C3
54	l	702	CDL	C31-CA7-OA8-CA6
56	s	401	UQ	C1-C6-C7-C8
48	B	303	PEE	C12-C13-C14-C15
54	u	201	CDL	C11-C12-C13-C14
49	G	201	8Q1	C28-O27-P24-O3
54	l	701	CDL	C11-C12-C13-C14
54	l	701	CDL	C79-C80-C81-C82
54	V	201	CDL	OB5-CB3-CB4-OB6
54	V	202	CDL	OB5-CB3-CB4-OB6
48	l	703	PEE	C33-C34-C35-C36
54	V	201	CDL	C13-C14-C15-C16
54	g	202	CDL	C59-C60-C61-C62
48	r	501	PEE	C10-C11-C12-C13
54	u	201	CDL	C73-C74-C75-C76
54	i	401	CDL	OA6-CA4-CA6-OA8
54	l	701	CDL	C37-C38-C39-C40
49	G	201	8Q1	C30-C29-C32-O33
54	V	201	CDL	C33-C34-C35-C36
54	a	201	CDL	CB5-C51-C52-C53
55	a	202	PLX	C10-C11-C12-C13
48	l	704	PEE	C23-C24-C25-C26
54	V	201	CDL	C71-C72-C73-C74
54	a	201	CDL	C24-C25-C26-C27
54	i	401	CDL	C36-C37-C38-C39
54	g	202	CDL	C39-C40-C41-C42
54	g	202	CDL	C42-C43-C44-C45
48	B	303	PEE	C31-C30-O3-C3
48	r	501	PEE	C17-C18-C19-C20
48	j	202	PEE	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
50	J	401	NDP	O4B-C4B-C5B-O5B
48	V	203	PEE	O3P-C1-C2-C3
48	l	703	PEE	O3P-C1-C2-C3
54	V	201	CDL	OA5-CA3-CA4-CA6
54	V	201	CDL	OB5-CB3-CB4-CB6
54	a	201	CDL	OA5-CA3-CA4-CA6
54	g	202	CDL	OA5-CA3-CA4-CA6
54	i	401	CDL	OB5-CB3-CB4-CB6
56	s	401	UQ	C9-C11-C12-C13
54	g	202	CDL	C54-C55-C56-C57
48	B	303	PEE	C22-C23-C24-C25
54	l	702	CDL	C73-C74-C75-C76
48	l	704	PEE	C32-C33-C34-C35
55	a	202	PLX	C27-C28-C29-C30
48	l	704	PEE	C12-C13-C14-C15
48	j	202	PEE	C36-C37-C38-C39
54	i	401	CDL	C12-C13-C14-C15
55	j	203	PLX	C9-C10-C11-C12
56	s	401	UQ	C17-C18-C19-C20
48	j	202	PEE	C19-C20-C21-C22
48	m	201	PEE	C31-C30-O3-C3
54	i	401	CDL	C71-CB7-OB8-CB6
48	l	703	PEE	C1-C2-C3-O3
48	l	704	PEE	C1-C2-C3-O3
48	m	201	PEE	C1-C2-C3-O3
54	i	401	CDL	CB3-CB4-CB6-OB8
54	u	201	CDL	CA3-CA4-CA6-OA8
55	r	502	PLX	C3-C4-C5-O8
48	l	704	PEE	C17-C18-C19-C20
54	l	702	CDL	OA9-CA7-OA8-CA6
54	V	201	CDL	C22-C23-C24-C25
49	X	201	8Q1	C7-C8-C9-C10
55	j	203	PLX	C33-C34-C35-C36
48	j	202	PEE	O5-C30-O3-C3
49	G	201	8Q1	C11-C10-C9-C8
54	l	702	CDL	C12-C13-C14-C15
55	a	202	PLX	C5-C4-O6-C6
55	r	502	PLX	C5-C4-O6-C6
54	l	701	CDL	C84-C85-C86-C87
54	u	201	CDL	C54-C55-C56-C57
48	l	704	PEE	O3P-C1-C2-O2
54	V	201	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
54	i	401	CDL	OB5-CB3-CB4-OB6
48	j	202	PEE	C24-C25-C26-C27
54	l	702	CDL	C51-C52-C53-C54
48	l	704	PEE	O2-C2-C3-O3
48	r	501	PEE	O2-C2-C3-O3
54	V	202	CDL	OA6-CA4-CA6-OA8
54	a	201	CDL	OB6-CB4-CB6-OB8
54	l	702	CDL	OA6-CA4-CA6-OA8
55	j	203	PLX	O6-C4-C5-O8
54	l	702	CDL	C20-C21-C22-C23
54	i	401	CDL	CB2-C1-CA2-OA2
54	l	702	CDL	CA2-C1-CB2-OB2
54	u	201	CDL	C22-C23-C24-C25
48	m	201	PEE	O3-C30-C31-C32
54	a	201	CDL	C14-C15-C16-C17
54	l	701	CDL	CA7-C31-C32-C33
55	g	201	PLX	C34-C35-C36-C37
48	m	201	PEE	C23-C24-C25-C26
54	a	201	CDL	C52-C53-C54-C55
54	l	701	CDL	C18-C19-C20-C21
54	l	702	CDL	C74-C75-C76-C77
54	V	202	CDL	OB5-CB3-CB4-CB6
54	i	401	CDL	OA5-CA3-CA4-CA6
48	j	202	PEE	C38-C39-C40-C41
48	V	203	PEE	C10-C11-C12-C13
48	B	303	PEE	O5-C30-O3-C3
54	a	201	CDL	C36-C37-C38-C39
54	i	401	CDL	C51-C52-C53-C54
54	V	201	CDL	CA6-CA4-OA6-CA5
54	V	202	CDL	C33-C34-C35-C36
48	l	703	PEE	C14-C15-C16-C17
48	r	501	PEE	C1-C2-C3-O3
54	V	201	CDL	CB3-CB4-CB6-OB8
54	g	202	CDL	CB4-CB3-OB5-PB2
54	l	702	CDL	CB3-CB4-CB6-OB8
54	u	201	CDL	CB4-CB3-OB5-PB2
48	r	501	PEE	O3P-C1-C2-O2
54	g	202	CDL	OA5-CA3-CA4-OA6
54	i	401	CDL	OA5-CA3-CA4-OA6
48	B	303	PEE	C36-C37-C38-C39
49	G	201	8Q1	C31-C29-C32-C34
54	i	401	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
54	i	401	CDL	C13-C14-C15-C16
48	l	703	PEE	O2-C2-C3-O3
48	m	201	PEE	O2-C2-C3-O3
54	V	201	CDL	OA6-CA4-CA6-OA8
54	a	201	CDL	OA6-CA4-CA6-OA8
57	w	401	ADP	C5'-O5'-PA-O3A
48	m	201	PEE	O5-C30-O3-C3
55	r	502	PLX	C24-C25-C26-C27
54	V	201	CDL	C64-C65-C66-C67
48	l	704	PEE	C11-C12-C13-C14
54	a	201	CDL	C39-C40-C41-C42
54	a	201	CDL	C60-C61-C62-C63
46	A	502	FMN	O2'-C2'-C3'-C4'
48	j	202	PEE	C1-O3P-P-O4P
54	l	702	CDL	CA3-OA5-PA1-OA2
54	u	201	CDL	CA3-OA5-PA1-OA2
55	a	202	PLX	C3-O4-P1-O1
48	r	501	PEE	C13-C14-C15-C16
47	A	503	NAI	C5D-O5D-PN-O1N
48	B	303	PEE	C4-O4P-P-O1P
48	V	203	PEE	C4-O4P-P-O2P
48	j	202	PEE	C1-O3P-P-O2P
48	j	202	PEE	C1-O3P-P-O1P
48	j	202	PEE	C4-O4P-P-O1P
48	r	501	PEE	C4-O4P-P-O2P
54	V	202	CDL	CA2-OA2-PA1-OA4
54	V	202	CDL	CB2-OB2-PB2-OB4
54	a	201	CDL	CA3-OA5-PA1-OA4
54	a	201	CDL	CB2-OB2-PB2-OB4
54	a	201	CDL	CB3-OB5-PB2-OB3
54	g	202	CDL	CB2-OB2-PB2-OB3
54	g	202	CDL	CB2-OB2-PB2-OB4
54	i	401	CDL	CA2-OA2-PA1-OA4
54	i	401	CDL	CB3-OB5-PB2-OB4
54	l	702	CDL	CB2-OB2-PB2-OB3
54	l	702	CDL	CB3-OB5-PB2-OB3
54	l	702	CDL	CB3-OB5-PB2-OB4
54	u	201	CDL	CA3-OA5-PA1-OA3
54	u	201	CDL	CA3-OA5-PA1-OA4
54	u	201	CDL	CB2-OB2-PB2-OB4
55	a	202	PLX	C2-O1-P1-O3
55	r	502	PLX	C3-O4-P1-O3

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Mol	Chain	Res	Type	Atoms
55	r	502	PLX	C2-O1-P1-O2
48	B	303	PEE	C31-C32-C33-C34
48	B	303	PEE	O3P-C1-C2-C3
48	r	501	PEE	O3P-C1-C2-C3
54	a	201	CDL	OB5-CB3-CB4-CB6
54	l	702	CDL	OA5-CA3-CA4-CA6
55	j	203	PLX	O4-C3-C4-C5
48	j	202	PEE	O4P-C4-C5-N
48	B	303	PEE	C23-C24-C25-C26
46	A	502	FMN	C1'-C2'-C3'-O3'
55	a	202	PLX	C25-C24-O8-C5
55	g	201	PLX	C25-C24-O8-C5
55	j	203	PLX	C25-C24-O8-C5
55	r	502	PLX	C25-C24-O8-C5
48	l	703	PEE	C23-C24-C25-C26
48	B	303	PEE	C15-C16-C17-C18
54	V	202	CDL	CB2-C1-CA2-OA2
48	m	201	PEE	C20-C21-C22-C23
48	B	303	PEE	O3P-C1-C2-O2
54	a	201	CDL	OB5-CB3-CB4-OB6
54	l	702	CDL	OA5-CA3-CA4-OA6
55	j	203	PLX	O4-C3-C4-O6
54	V	201	CDL	C38-C39-C40-C41
48	r	501	PEE	C36-C37-C38-C39
54	V	202	CDL	C83-C84-C85-C86
55	r	502	PLX	C25-C26-C27-C28
54	l	701	CDL	C51-CB5-OB6-CB4
55	r	502	PLX	C18-C19-C20-C21
54	V	202	CDL	C72-C73-C74-C75
50	J	401	NDP	C2N-C3N-C7N-O7N
54	a	201	CDL	CA3-CA4-CA6-OA8
54	i	401	CDL	CA3-CA4-CA6-OA8
54	u	201	CDL	OA6-CA4-CA6-OA8
55	r	502	PLX	O6-C4-C5-O8
54	g	202	CDL	C37-C38-C39-C40
48	r	501	PEE	C23-C24-C25-C26
54	g	202	CDL	C56-C57-C58-C59
48	B	303	PEE	C34-C35-C36-C37
54	l	702	CDL	C58-C59-C60-C61
55	r	502	PLX	C26-C27-C28-C29
54	a	201	CDL	C55-C56-C57-C58
48	r	501	PEE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
54	l	702	CDL	C15-C16-C17-C18
55	r	502	PLX	O8-C24-C25-C26
54	g	202	CDL	C41-C42-C43-C44
54	V	202	CDL	C32-C31-CA7-OA8
48	l	704	PEE	C16-C17-C18-C19
55	a	202	PLX	O9-C24-C25-C26
48	B	303	PEE	C39-C40-C41-C42
48	m	201	PEE	C19-C20-C21-C22
55	a	202	PLX	C11-C10-C9-C8
54	l	701	CDL	C71-C72-C73-C74
48	B	303	PEE	C42-C43-C44-C45
54	l	701	CDL	C54-C55-C56-C57
54	V	201	CDL	C75-C76-C77-C78
54	V	201	CDL	C80-C81-C82-C83
54	l	701	CDL	CA4-CA3-OA5-PA1
54	l	701	CDL	C40-C41-C42-C43
54	a	201	CDL	C13-C14-C15-C16
48	l	704	PEE	C1-O3P-P-O4P
54	l	701	CDL	CA2-OA2-PA1-OA5
55	j	203	PLX	C3-O4-P1-O1
54	l	702	CDL	C57-C58-C59-C60
54	l	702	CDL	CA3-CA4-CA6-OA8
48	l	703	PEE	C18-C19-C20-C21
48	m	201	PEE	C16-C17-C18-C19
54	l	702	CDL	C11-CA5-OA6-CA4
48	j	202	PEE	C10-C11-C12-C13
54	V	201	CDL	C1-CB2-OB2-PB2
55	a	202	PLX	C13-C14-C15-C16
54	l	702	CDL	C77-C78-C79-C80
55	a	202	PLX	C18-C19-C20-C21
48	j	202	PEE	C13-C14-C15-C16
48	l	704	PEE	C18-C19-C20-C21
55	a	202	PLX	C29-C30-C31-C32
54	l	701	CDL	OB7-CB5-OB6-CB4
55	g	201	PLX	C36-C37-C38-C39
48	l	704	PEE	C36-C37-C38-C39
54	V	201	CDL	C78-C79-C80-C81
54	g	202	CDL	C64-C65-C66-C67
54	u	201	CDL	C18-C19-C20-C21
48	l	704	PEE	C39-C40-C41-C42
55	j	203	PLX	O8-C24-C25-C26
54	l	702	CDL	C62-C63-C64-C65

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Mol	Chain	Res	Type	Atoms
55	g	201	PLX	C26-C27-C28-C29
54	g	202	CDL	CA4-CA3-OA5-PA1
49	G	201	8Q1	N41-C42-C43-S44
48	V	203	PEE	C13-C14-C15-C16
54	l	702	CDL	OA7-CA5-OA6-CA4
54	V	202	CDL	C53-C54-C55-C56
47	A	503	NAI	O4D-C1D-N1N-C2N
54	i	401	CDL	C33-C34-C35-C36
55	g	201	PLX	C31-C32-C33-C34
48	r	501	PEE	C21-C22-C23-C24
54	a	201	CDL	C53-C54-C55-C56
54	g	202	CDL	C17-C18-C19-C20
54	g	202	CDL	C36-C37-C38-C39
54	l	702	CDL	C84-C85-C86-C87
55	a	202	PLX	C15-C16-C17-C18
55	g	201	PLX	C27-C28-C29-C30
54	V	202	CDL	CB4-CB3-OB5-PB2
54	u	201	CDL	C61-C62-C63-C64
55	g	201	PLX	C30-C31-C32-C33
48	l	703	PEE	C15-C16-C17-C18
54	V	202	CDL	C77-C78-C79-C80
48	j	202	PEE	C21-C22-C23-C24
54	l	701	CDL	C34-C35-C36-C37
54	i	401	CDL	O1-C1-CA2-OA2
54	a	201	CDL	C58-C59-C60-C61
54	i	401	CDL	C15-C16-C17-C18
47	A	503	NAI	C2D-C1D-N1N-C2N
48	l	703	PEE	C13-C14-C15-C16
54	l	702	CDL	C44-C45-C46-C47
54	V	202	CDL	C12-C11-CA5-OA6
54	V	201	CDL	C58-C59-C60-C61
48	V	203	PEE	C38-C39-C40-C41
54	V	202	CDL	OA5-CA3-CA4-OA6
48	B	303	PEE	C20-C21-C22-C23
54	l	702	CDL	C61-C62-C63-C64
48	m	201	PEE	C21-C22-C23-C24
55	j	203	PLX	O6-C6-C7-C8
48	B	303	PEE	C24-C25-C26-C27
55	j	203	PLX	C11-C10-C9-C8
54	l	701	CDL	C61-C62-C63-C64
46	A	502	FMN	O2'-C2'-C3'-O3'
49	G	201	8Q1	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
54	l	702	CDL	C32-C31-CA7-OA8
50	J	401	NDP	C3B-C4B-C5B-O5B
54	V	201	CDL	C43-C44-C45-C46
48	l	703	PEE	O2-C10-C11-C12
49	X	201	8Q1	O27-C28-C29-C30
54	l	701	CDL	C12-C11-CA5-OA6
48	j	202	PEE	C16-C17-C18-C19
48	l	703	PEE	C16-C17-C18-C19
49	G	201	8Q1	C6-C7-C8-C9
49	X	201	8Q1	C13-C14-C15-C16
48	j	202	PEE	C40-C41-C42-C43
54	a	201	CDL	C41-C42-C43-C44
54	l	701	CDL	C51-C52-C53-C54
54	l	702	CDL	C41-C42-C43-C44
48	l	703	PEE	C36-C37-C38-C39
54	V	202	CDL	CA3-CA4-CA6-OA8
54	a	201	CDL	CB3-CB4-CB6-OB8
55	a	202	PLX	C7-C6-O6-C4
54	l	701	CDL	OB5-CB3-CB4-OB6
48	j	202	PEE	C37-C38-C39-C40
48	j	202	PEE	O2-C10-C11-C12
54	l	701	CDL	C16-C17-C18-C19
54	g	202	CDL	C12-C11-CA5-OA6
48	m	201	PEE	C18-C19-C20-C21
49	G	201	8Q1	C30-C29-C32-C34
54	l	702	CDL	C12-C11-CA5-OA6
49	G	201	8Q1	C13-C14-C15-C16
48	m	201	PEE	O5-C30-C31-C32
50	J	401	NDP	C5D-O5D-PN-O3
54	u	201	CDL	C31-CA7-OA8-CA6
54	u	201	CDL	OA9-CA7-OA8-CA6
48	l	704	PEE	C30-C31-C32-C33
54	l	701	CDL	C72-C71-CB7-OB8
54	l	702	CDL	C32-C31-CA7-OA9
54	l	701	CDL	C12-C11-CA5-OA7
48	l	703	PEE	O4-C10-C11-C12
48	l	704	PEE	C38-C39-C40-C41
54	g	202	CDL	C53-C54-C55-C56
54	l	702	CDL	C17-C18-C19-C20
48	r	501	PEE	C30-C31-C32-C33
54	i	401	CDL	C53-C54-C55-C56
48	B	303	PEE	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
48	l	703	PEE	C4-O4P-P-O1P
50	J	401	NDP	C5B-O5B-PA-O2A
54	l	701	CDL	CA2-OA2-PA1-OA3
57	w	401	ADP	C5'-O5'-PA-O2A
54	V	201	CDL	C21-C22-C23-C24
54	g	202	CDL	C12-C11-CA5-OA7
54	l	702	CDL	C12-C11-CA5-OA7
54	V	201	CDL	C55-C56-C57-C58
54	g	202	CDL	C34-C35-C36-C37
54	l	702	CDL	C31-C32-C33-C34
48	l	704	PEE	C5-C4-O4P-P
54	u	201	CDL	CA3-CA4-OA6-CA5
54	u	201	CDL	CA6-CA4-OA6-CA5
48	j	202	PEE	O4-C10-C11-C12
54	l	702	CDL	C21-C22-C23-C24
48	r	501	PEE	C16-C17-C18-C19
54	V	201	CDL	C17-C18-C19-C20
55	g	201	PLX	C25-C26-C27-C28
48	l	704	PEE	O3-C30-C31-C32
54	u	201	CDL	CA2-C1-CB2-OB2
54	g	202	CDL	OB5-CB3-CB4-OB6
54	g	202	CDL	C33-C34-C35-C36
54	g	202	CDL	C72-C71-CB7-OB8
54	i	401	CDL	C52-C51-CB5-OB6
54	u	201	CDL	C72-C71-CB7-OB8
54	l	701	CDL	C72-C71-CB7-OB9
54	V	202	CDL	O1-C1-CA2-OA2
54	a	201	CDL	C16-C17-C18-C19
54	g	202	CDL	C72-C71-CB7-OB9
48	r	501	PEE	C33-C34-C35-C36

There are no ring outliers.

27 monomers are involved in 108 short contacts:

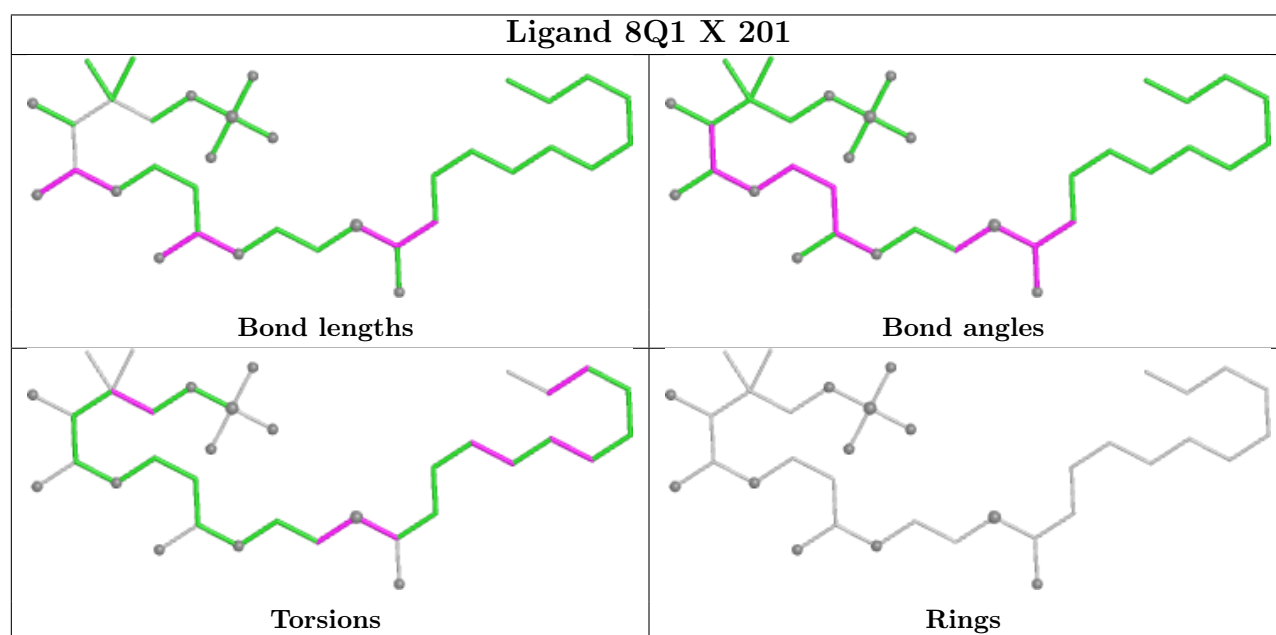
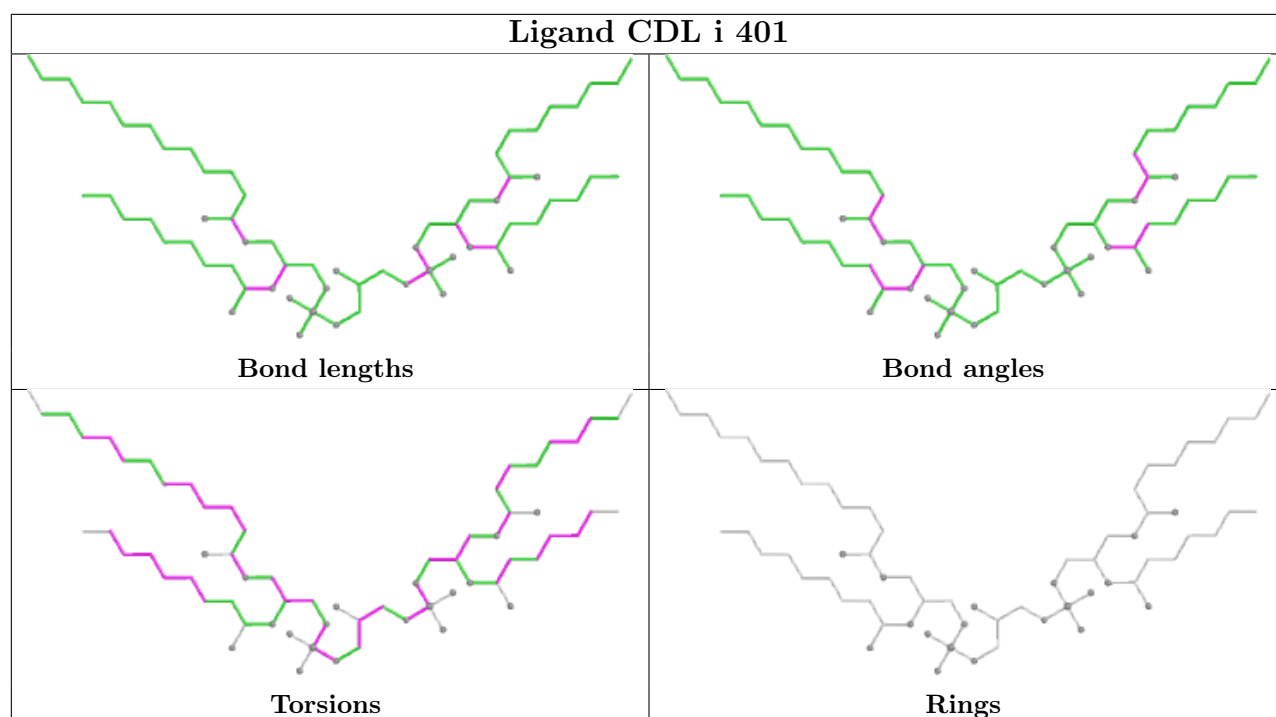
Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	i	401	CDL	4	0
49	X	201	8Q1	4	0
56	s	401	UQ	6	0
54	a	201	CDL	3	0
51	O	301	FES	1	0
57	w	401	ADP	2	0
54	l	702	CDL	5	0

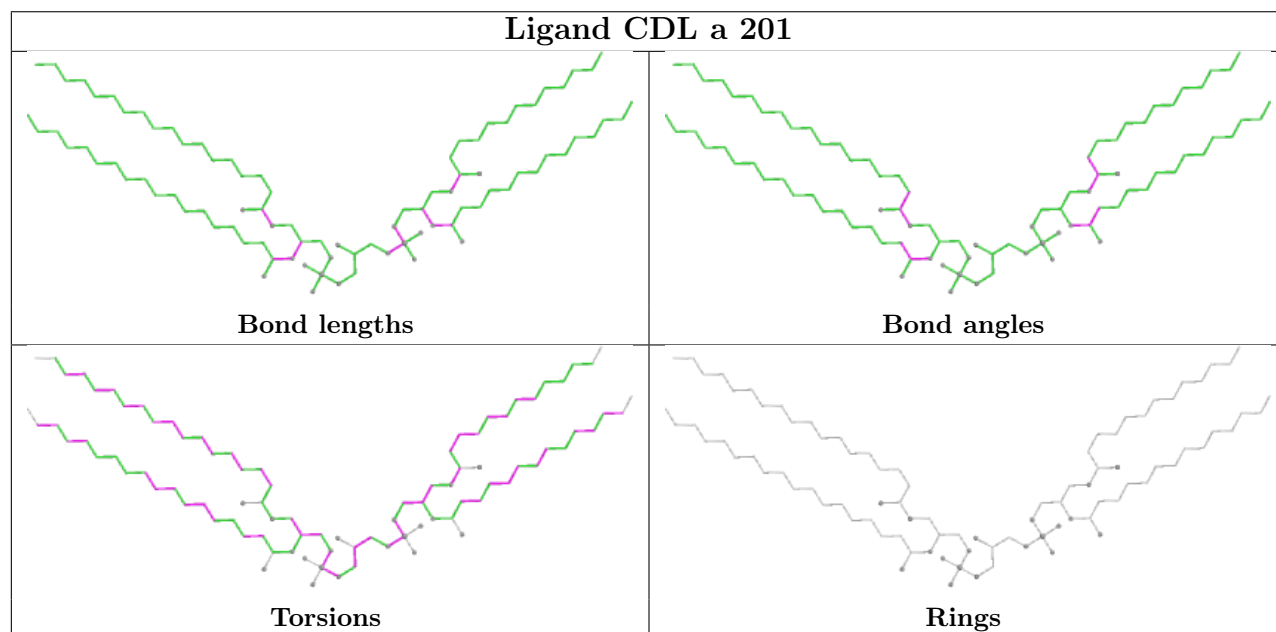
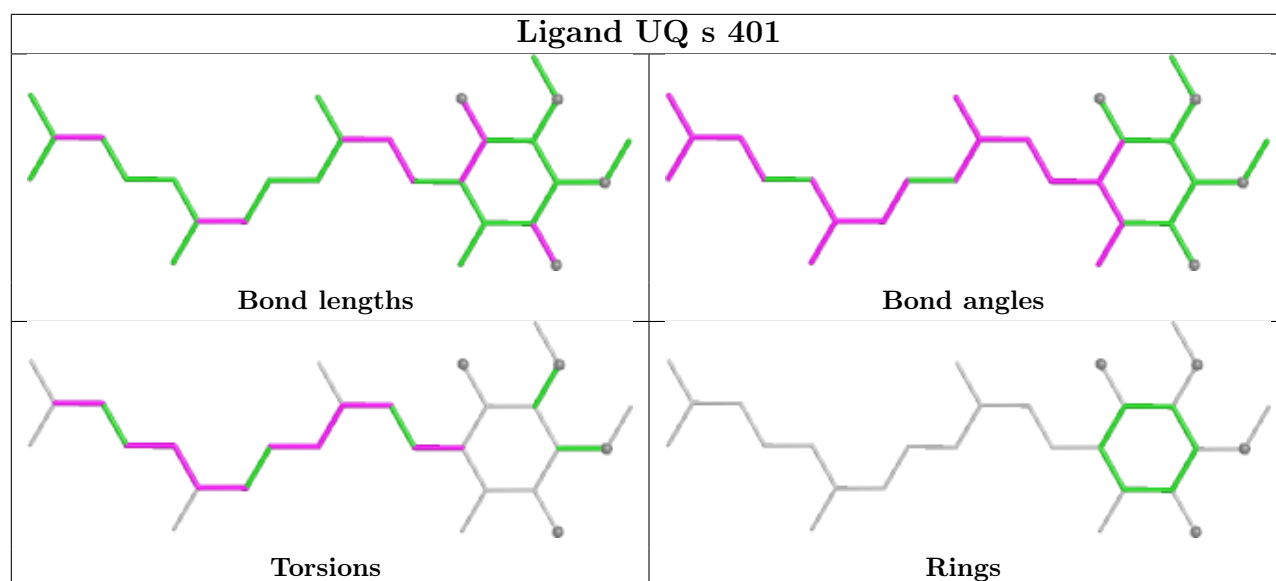
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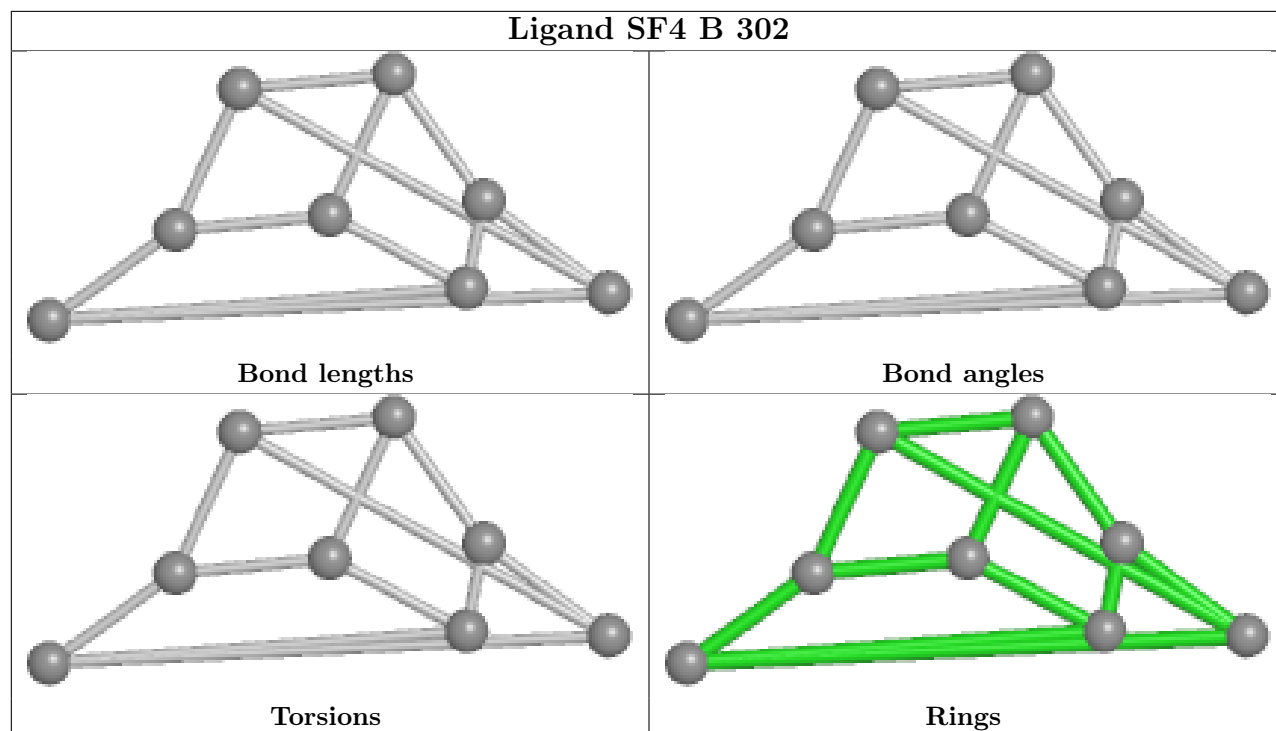
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	V	203	PEE	1	0
46	A	502	FMN	3	0
48	r	501	PEE	3	0
55	a	202	PLX	1	0
55	j	203	PLX	3	0
48	j	202	PEE	5	0
55	g	201	PLX	4	0
45	A	501	SF4	2	0
54	u	201	CDL	8	0
45	M	801	SF4	1	0
54	V	202	CDL	5	0
48	l	703	PEE	1	0
50	J	401	NDP	5	0
54	V	201	CDL	5	0
54	l	701	CDL	17	0
55	r	502	PLX	6	0
47	A	503	NAI	5	0
54	g	202	CDL	9	0
48	l	704	PEE	3	0
48	m	201	PEE	2	0

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

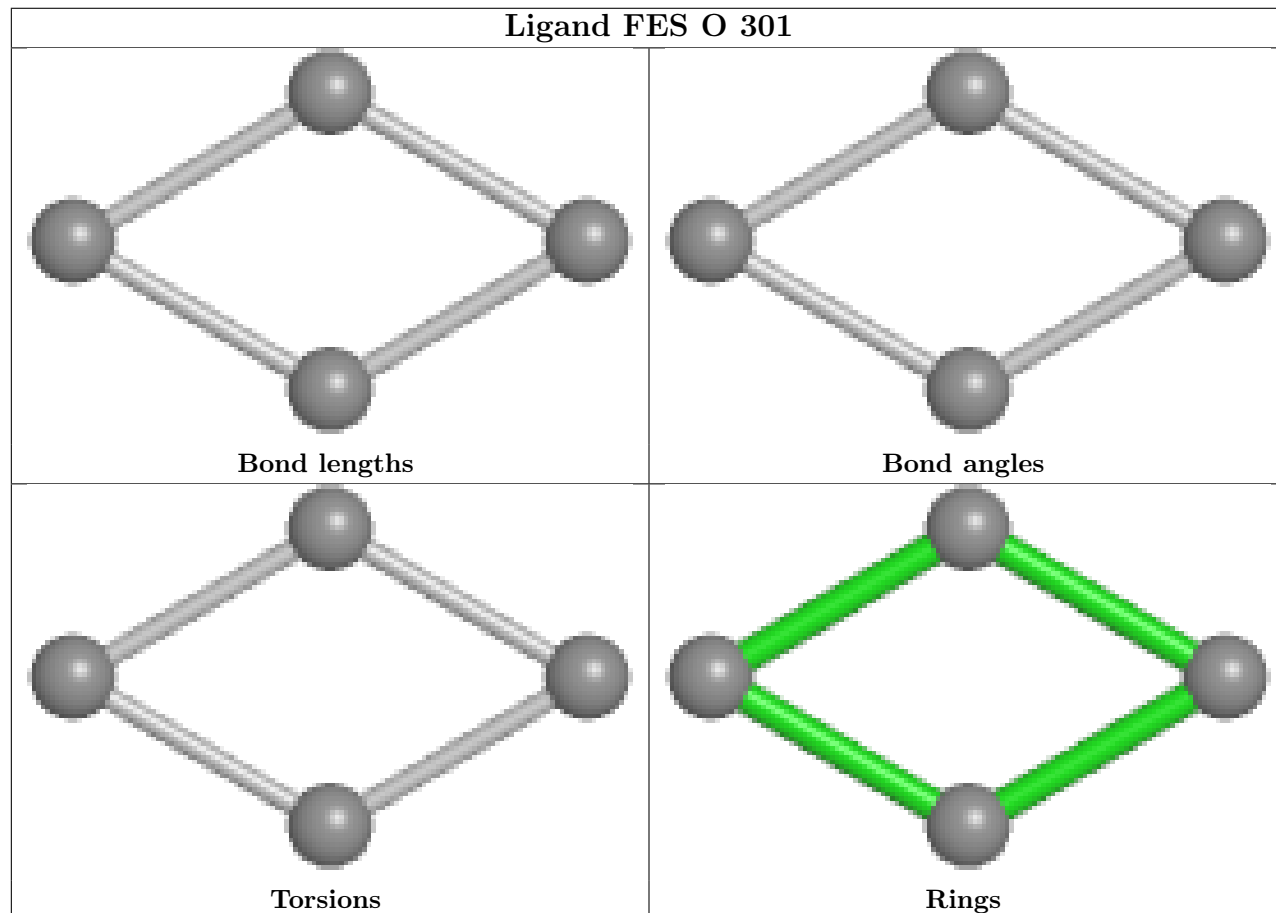


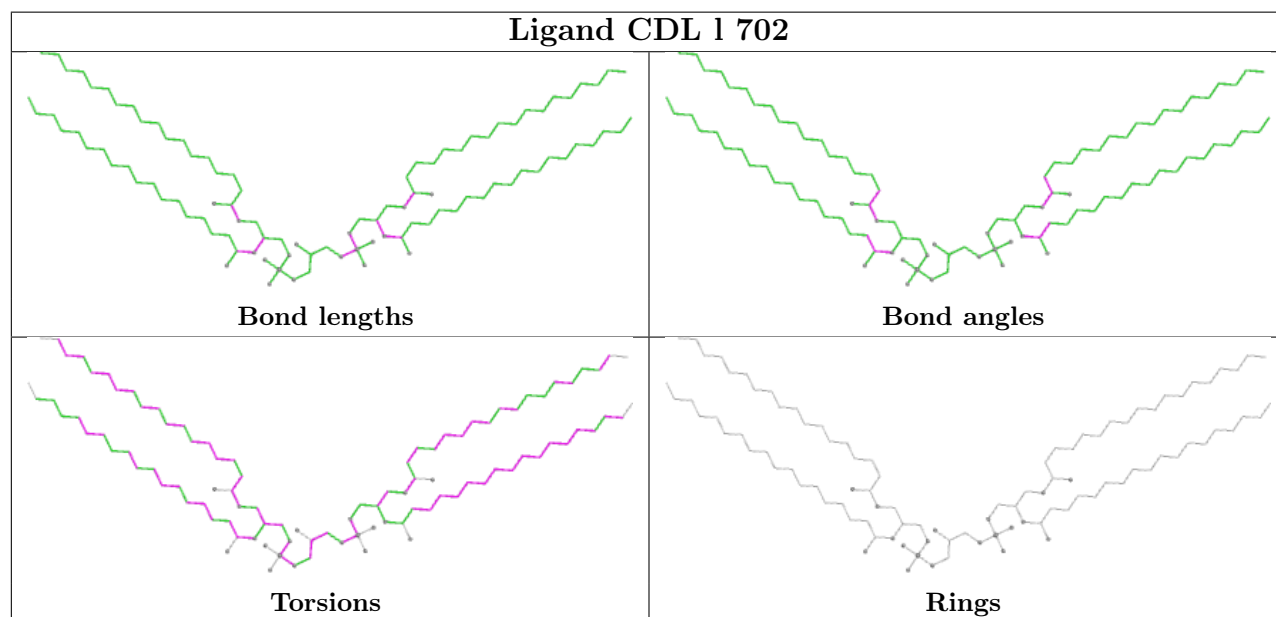
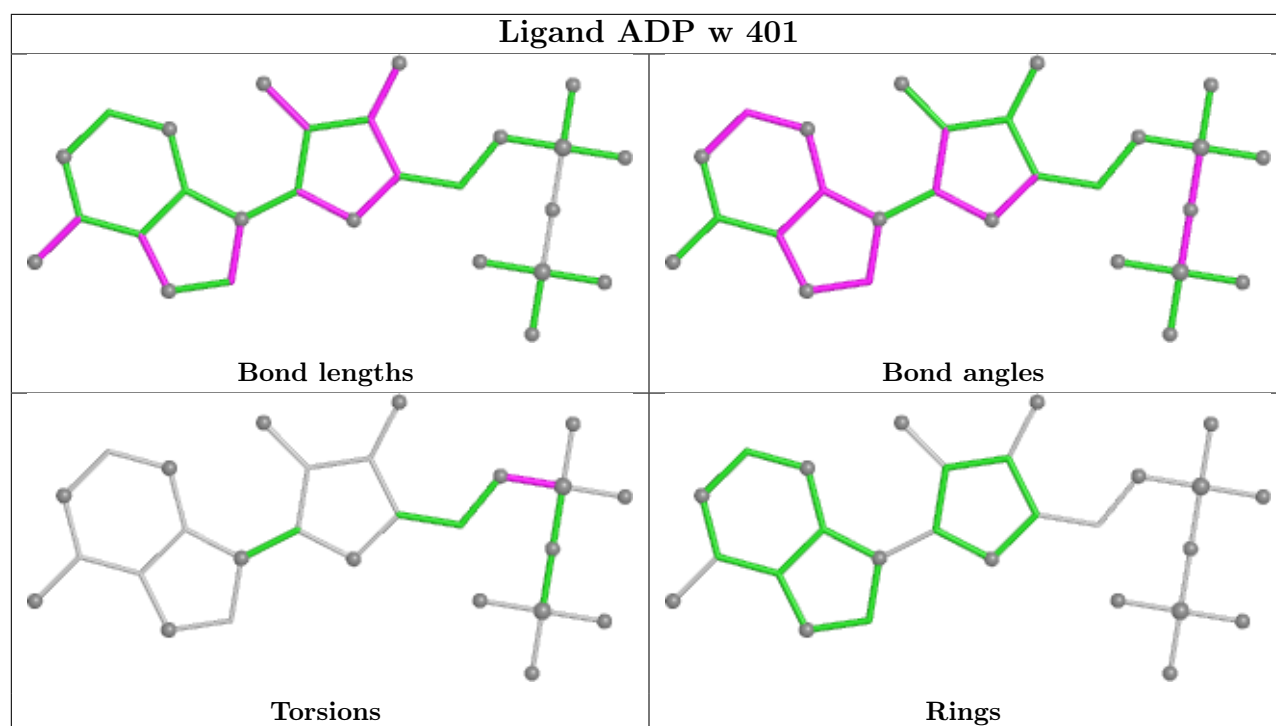


Ligand SF4 B 302

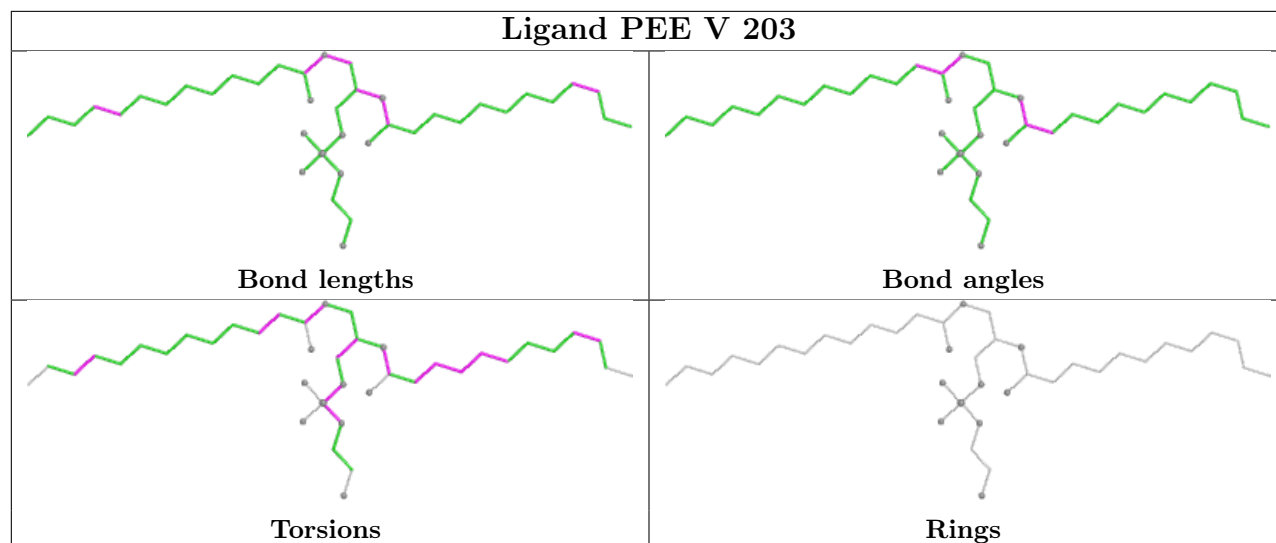


Ligand FES O 301

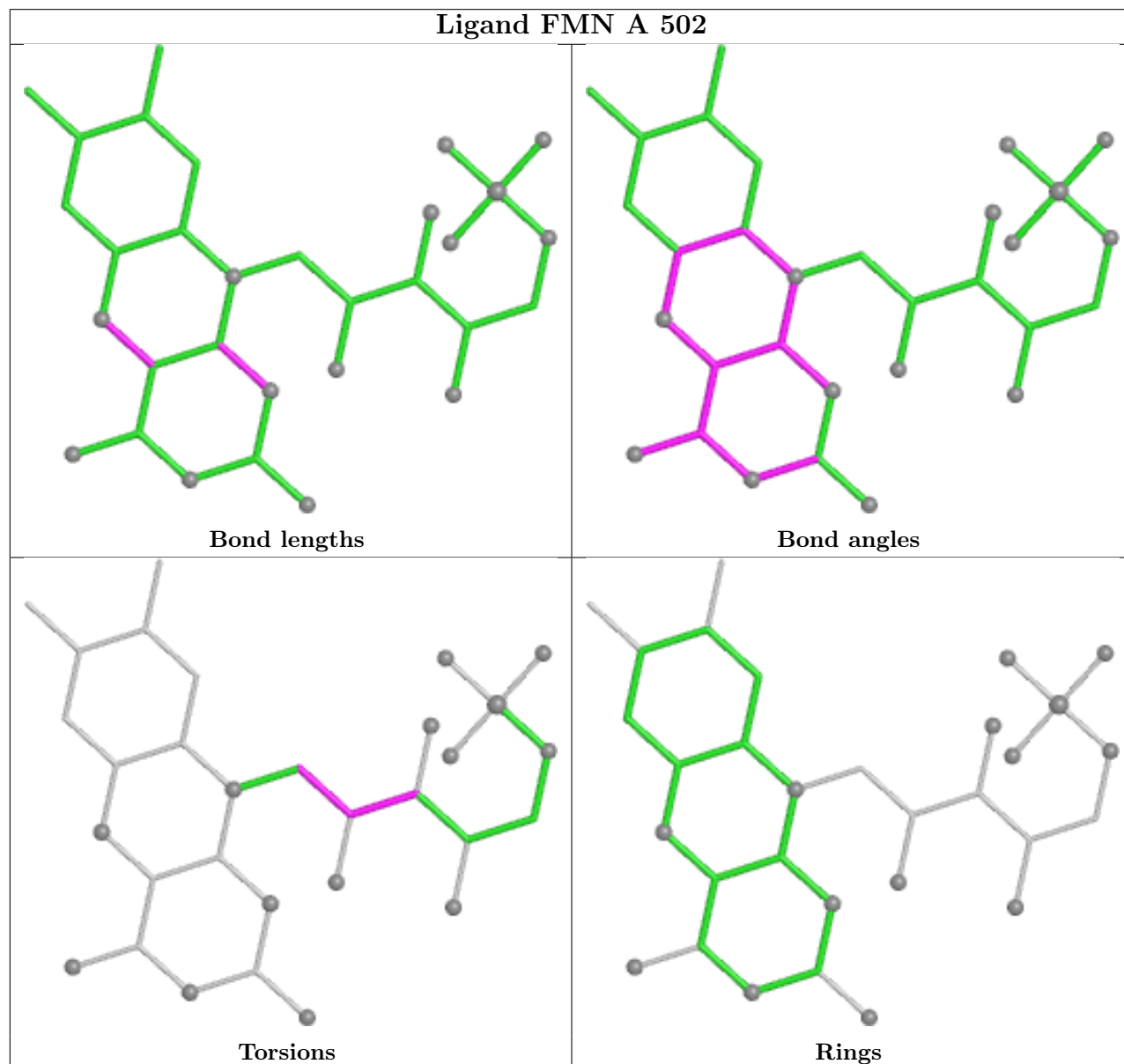


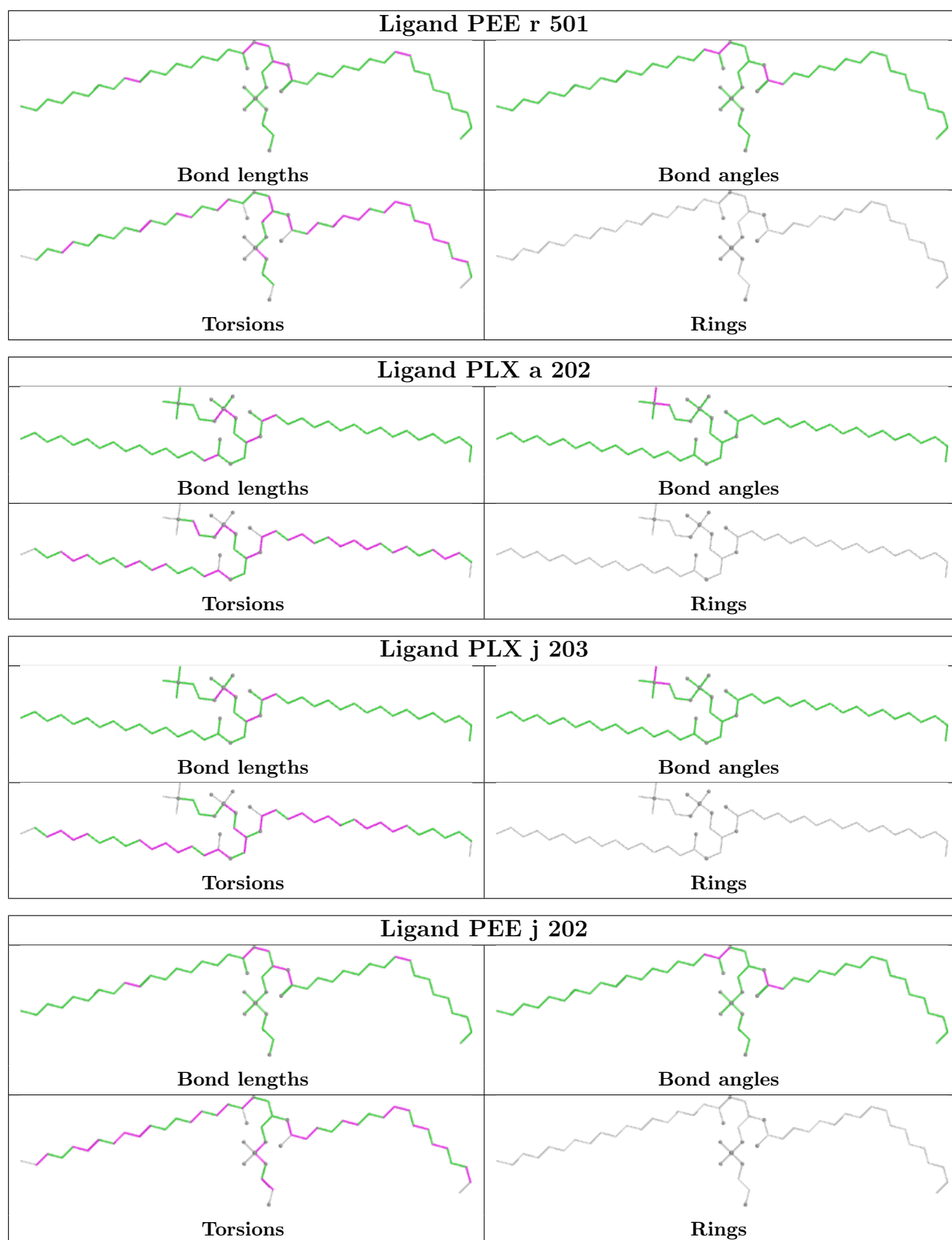


Ligand PEE V 203

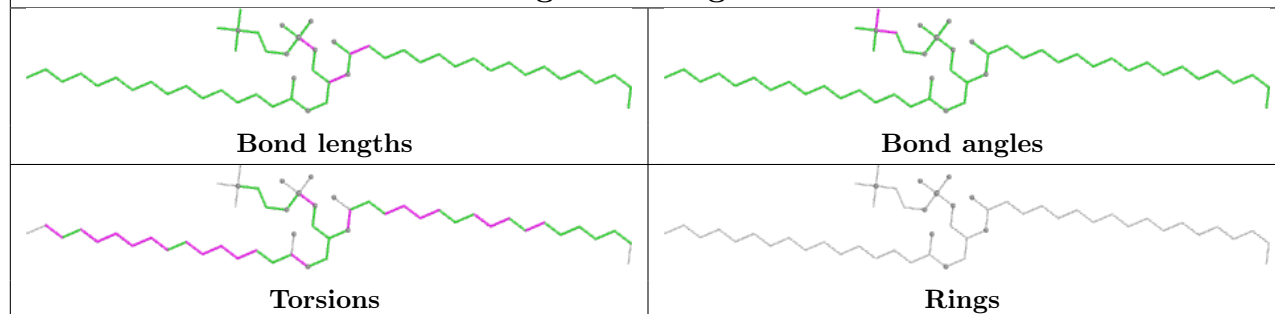


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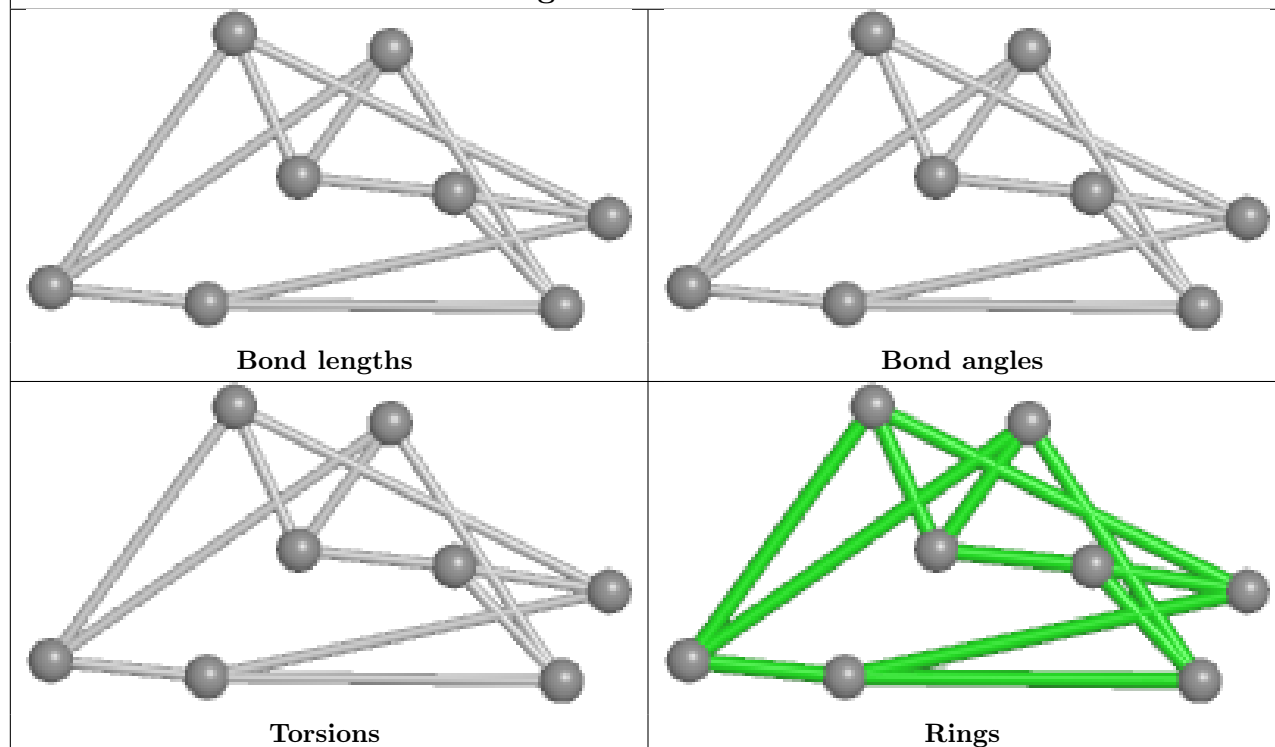




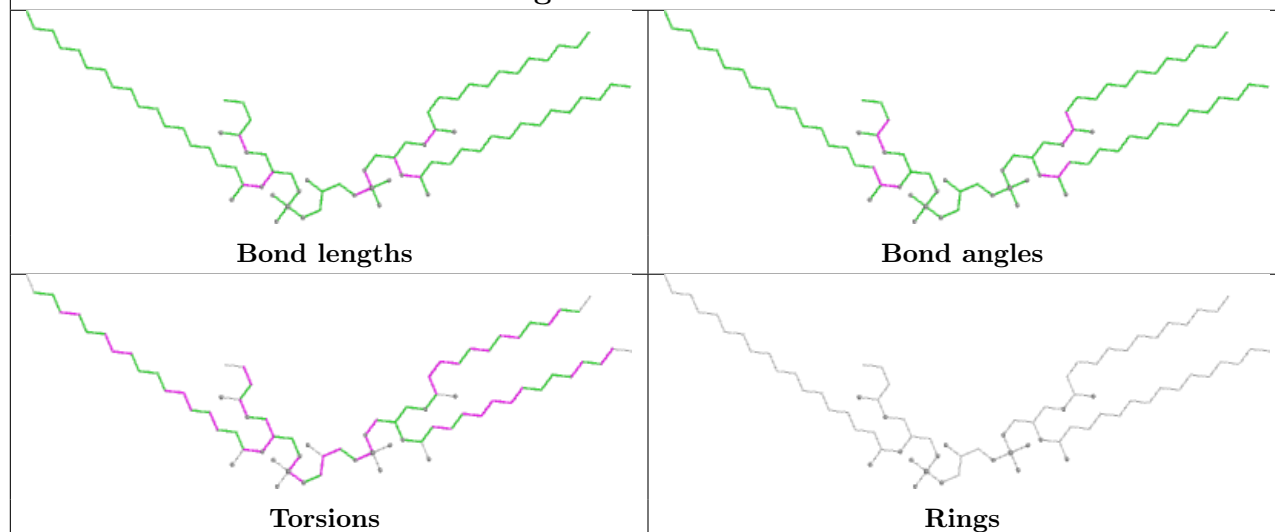
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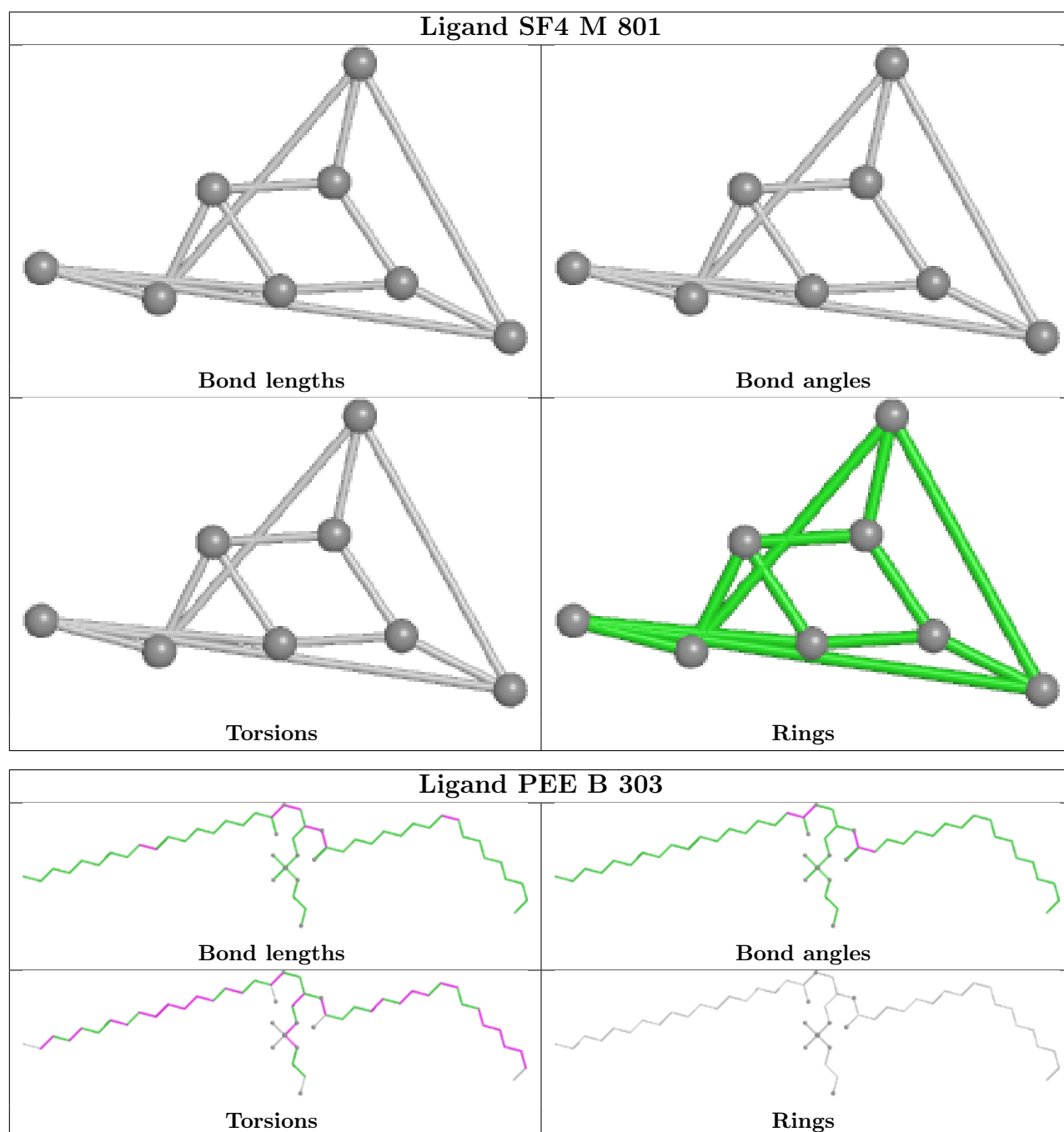


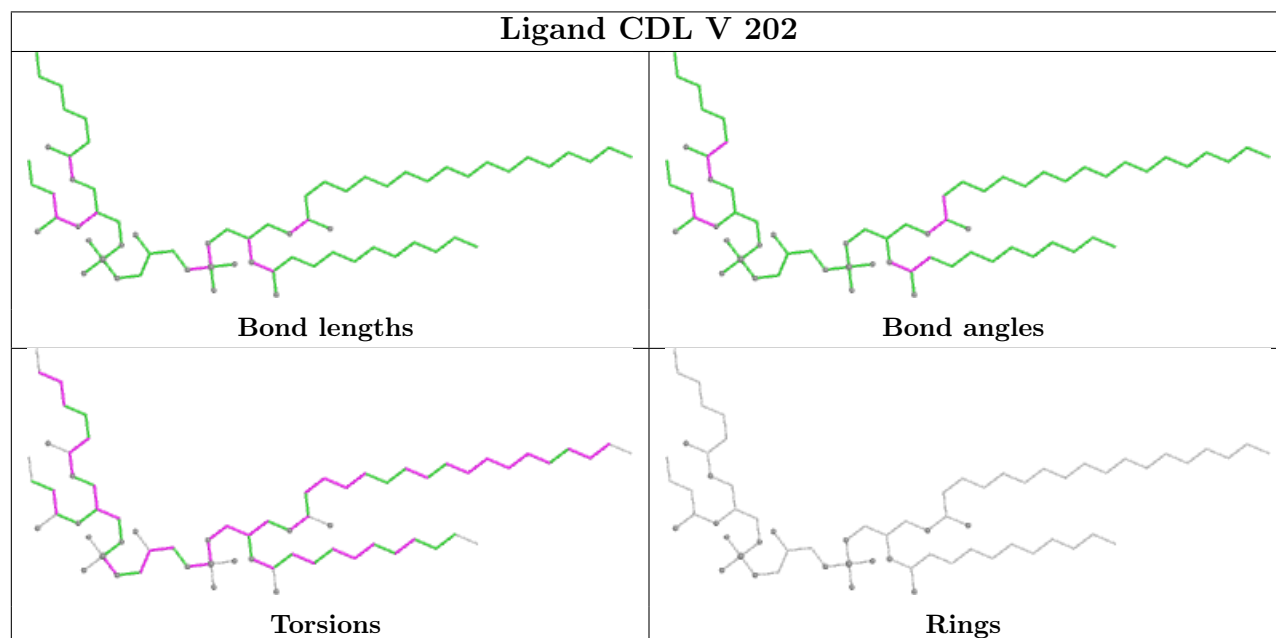
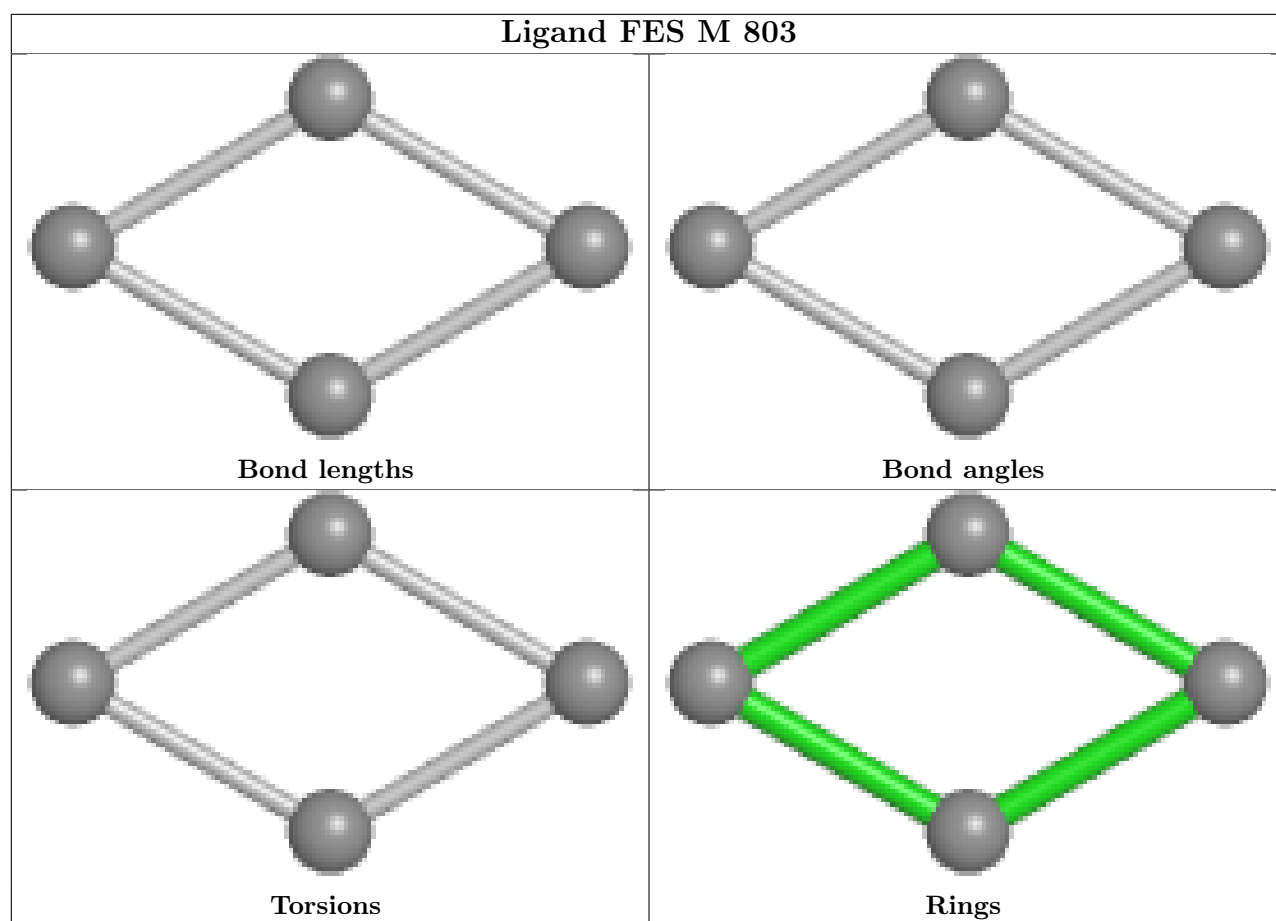
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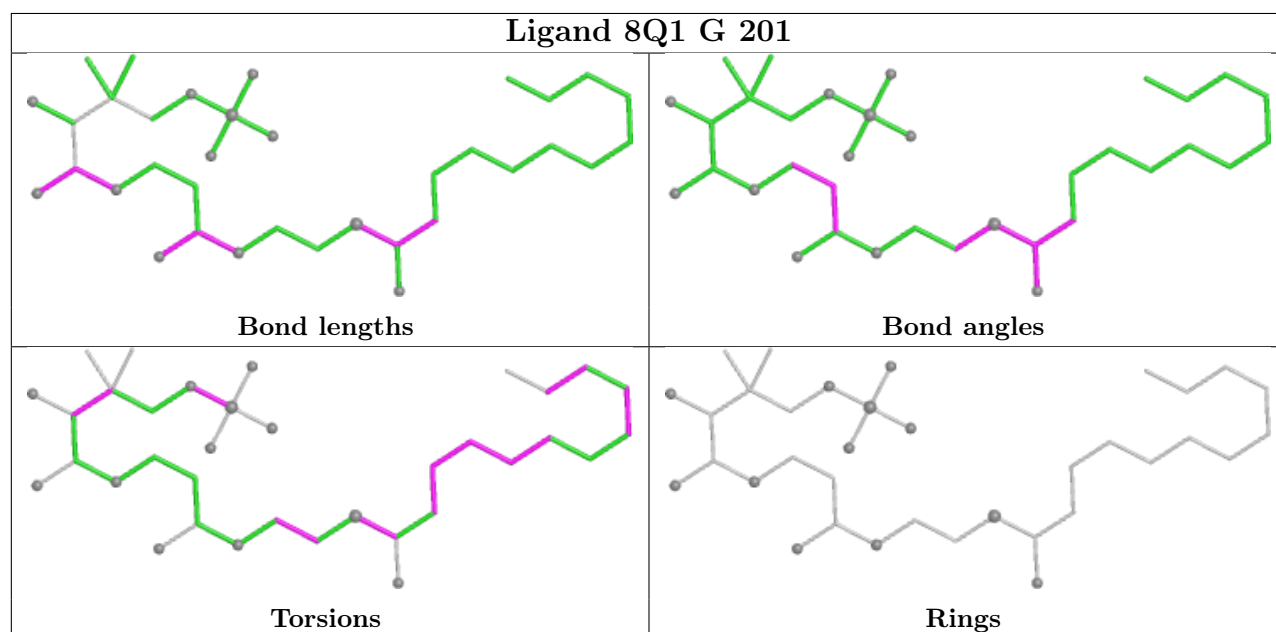
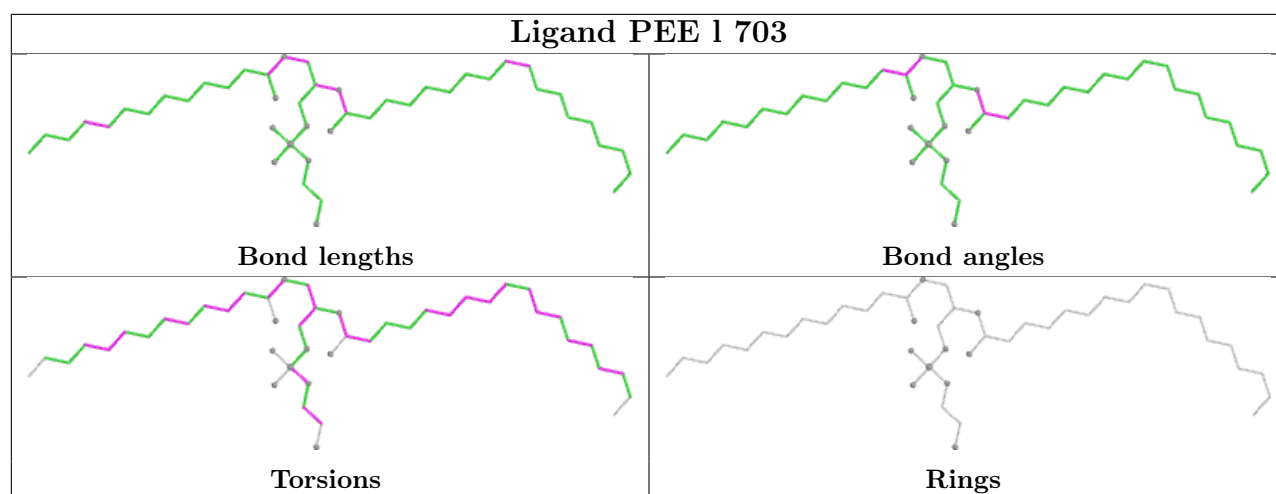


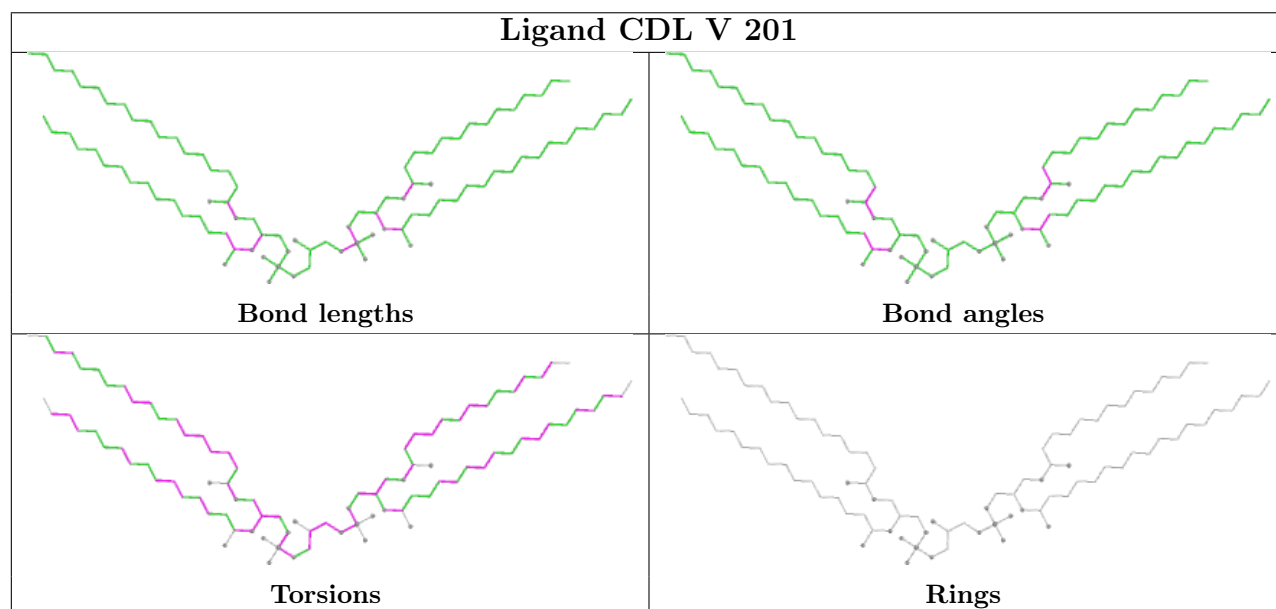
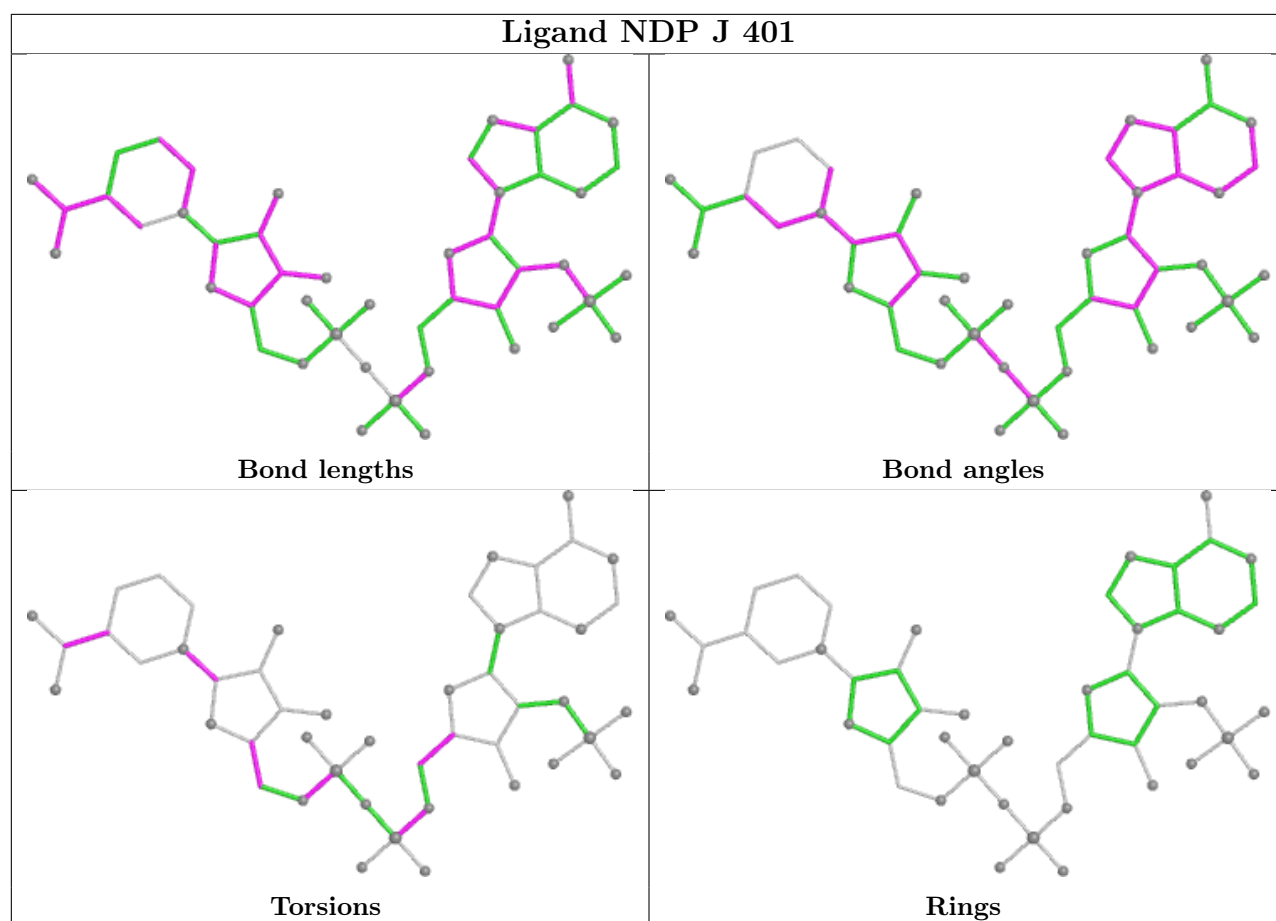
Ligand CDL u 201

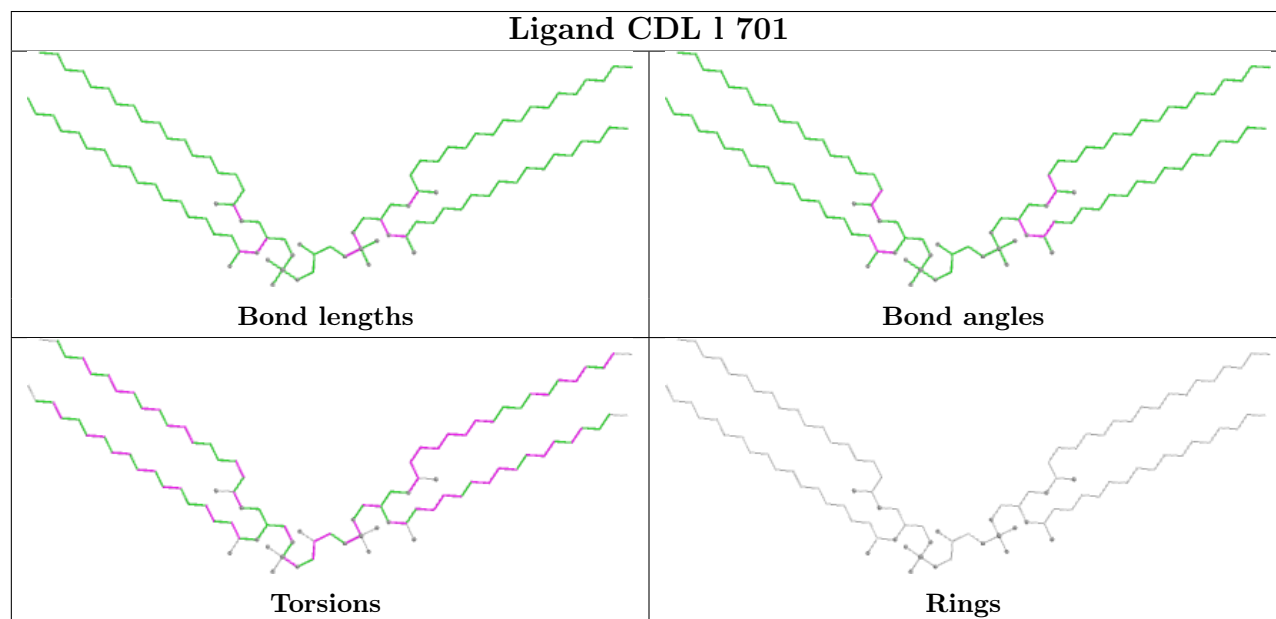
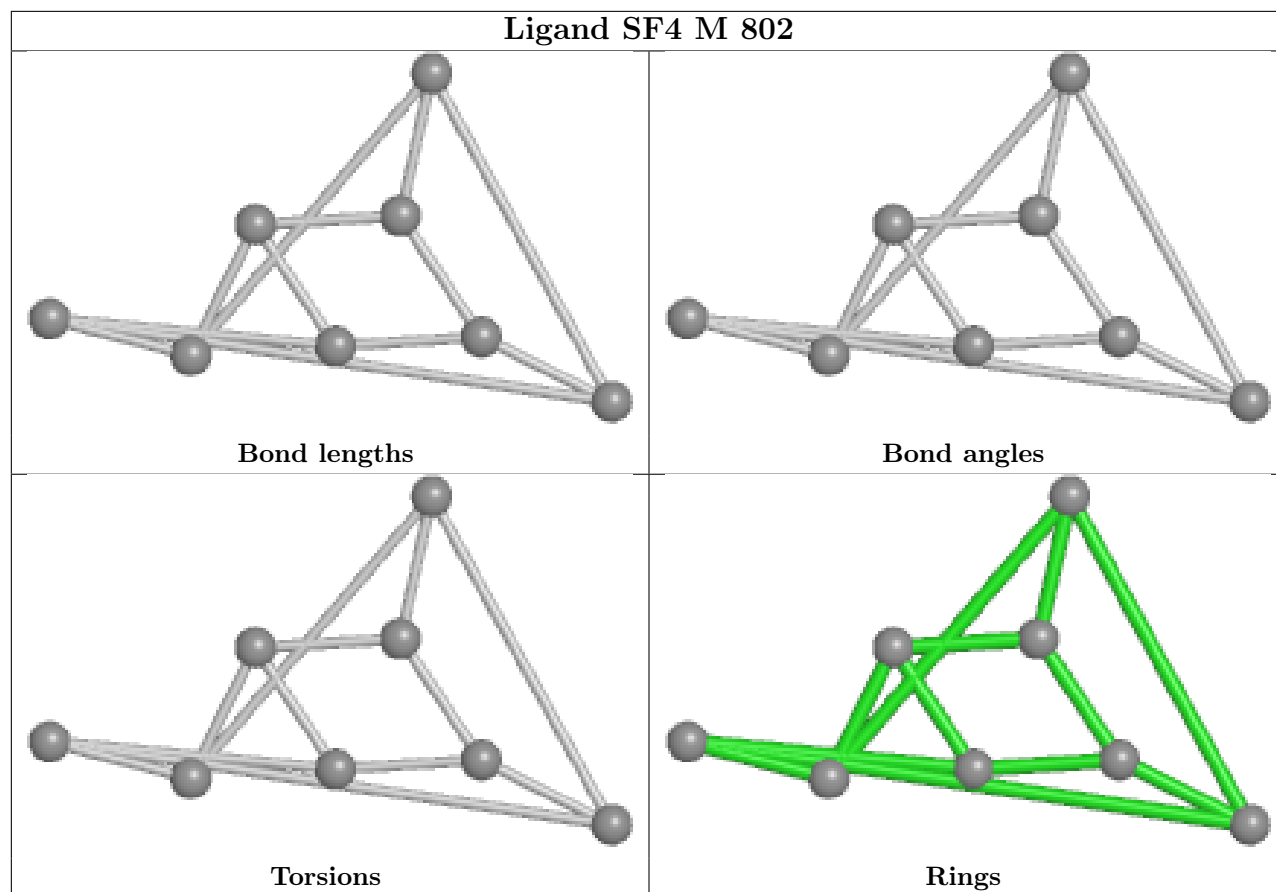


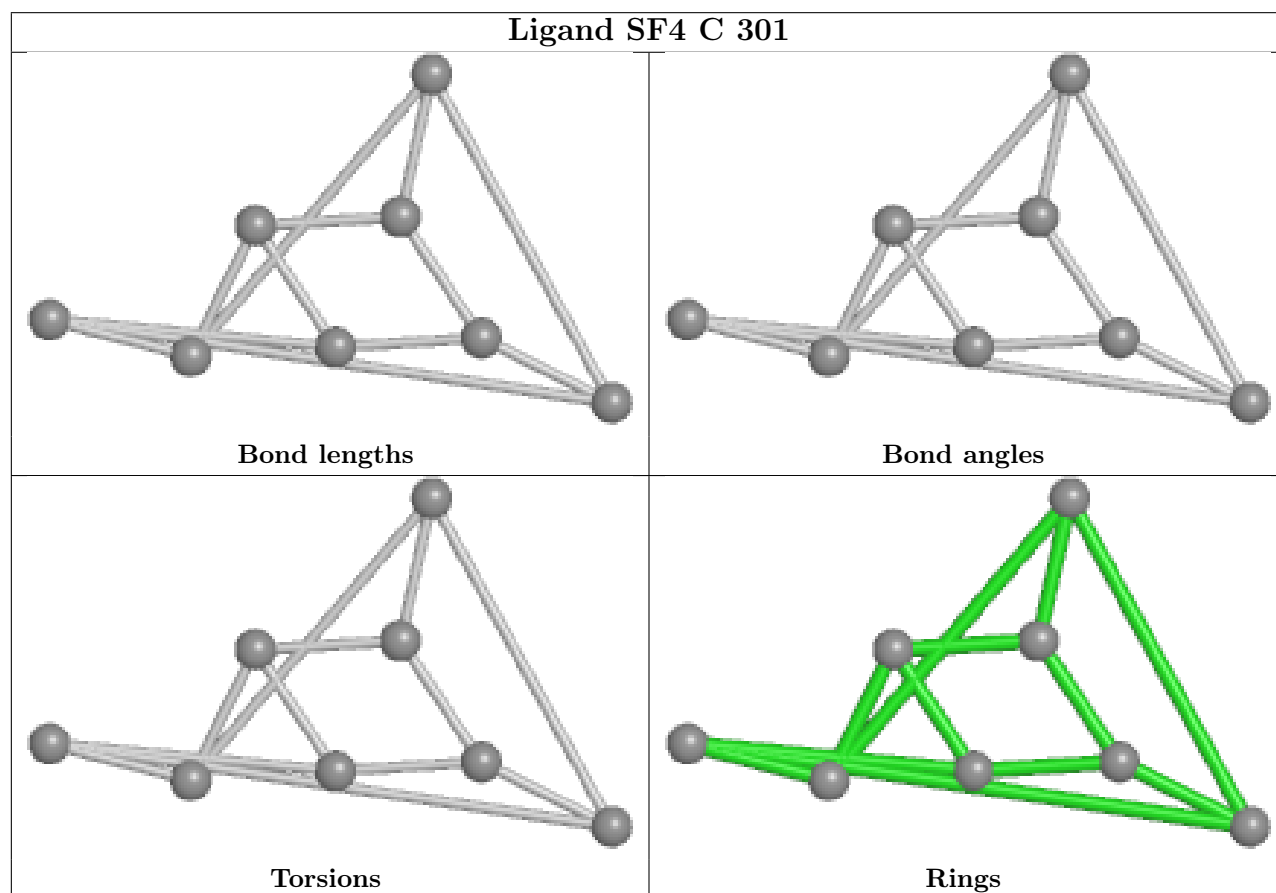
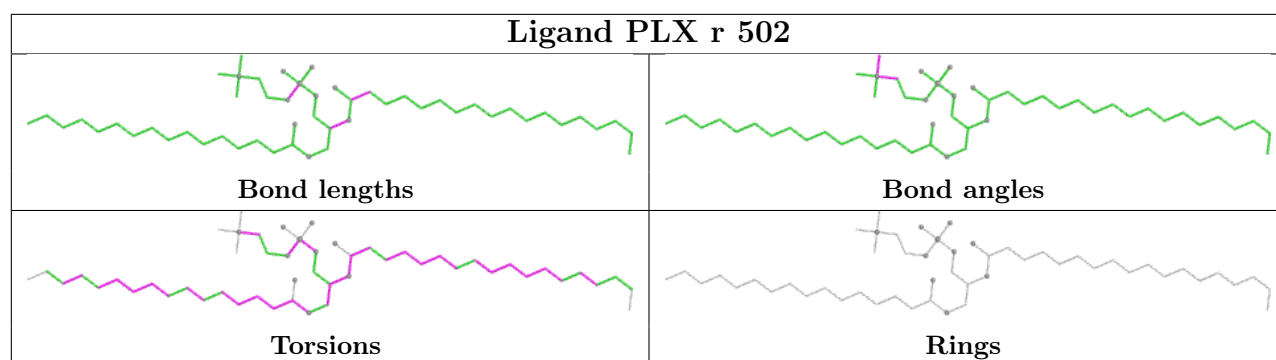


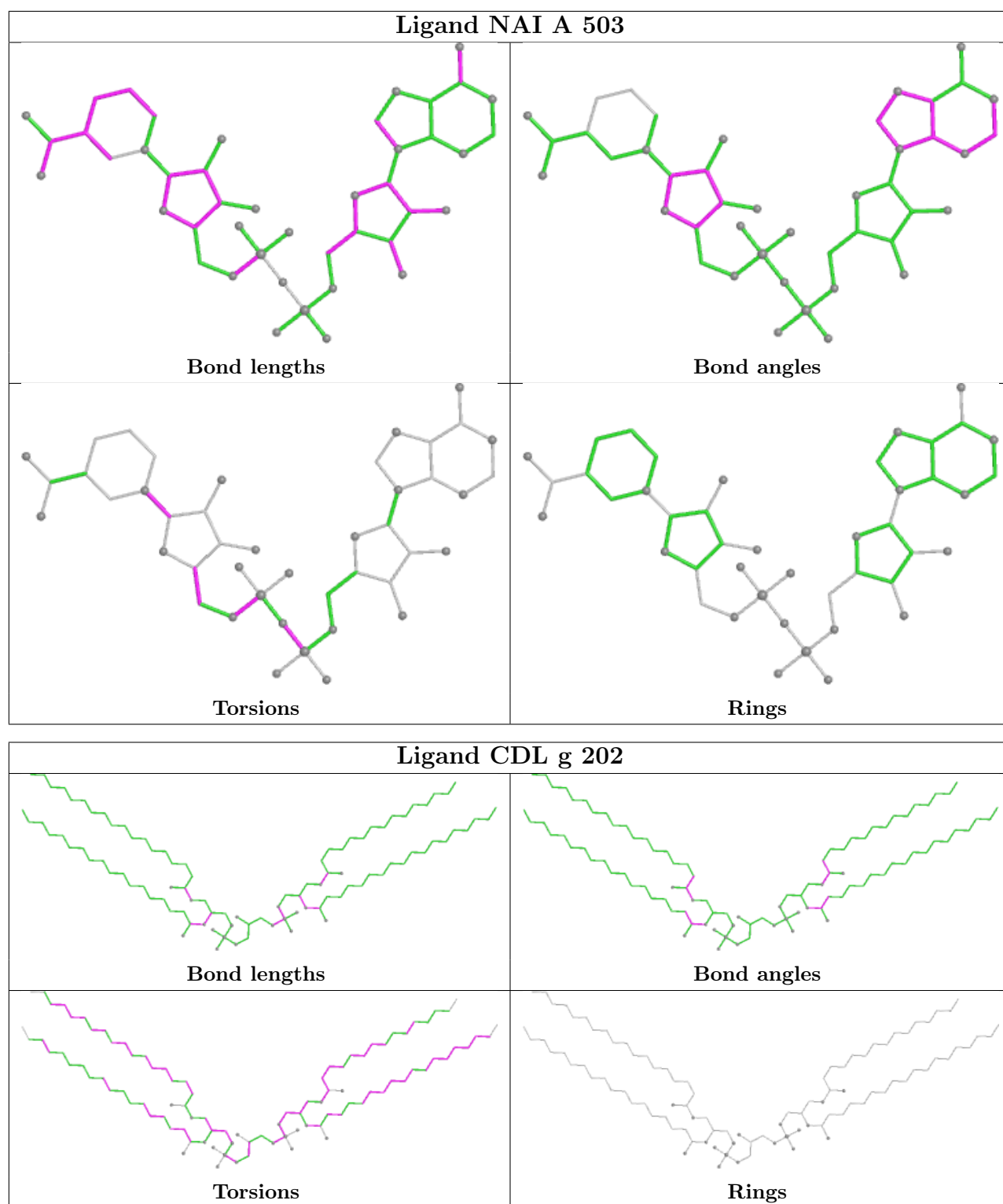


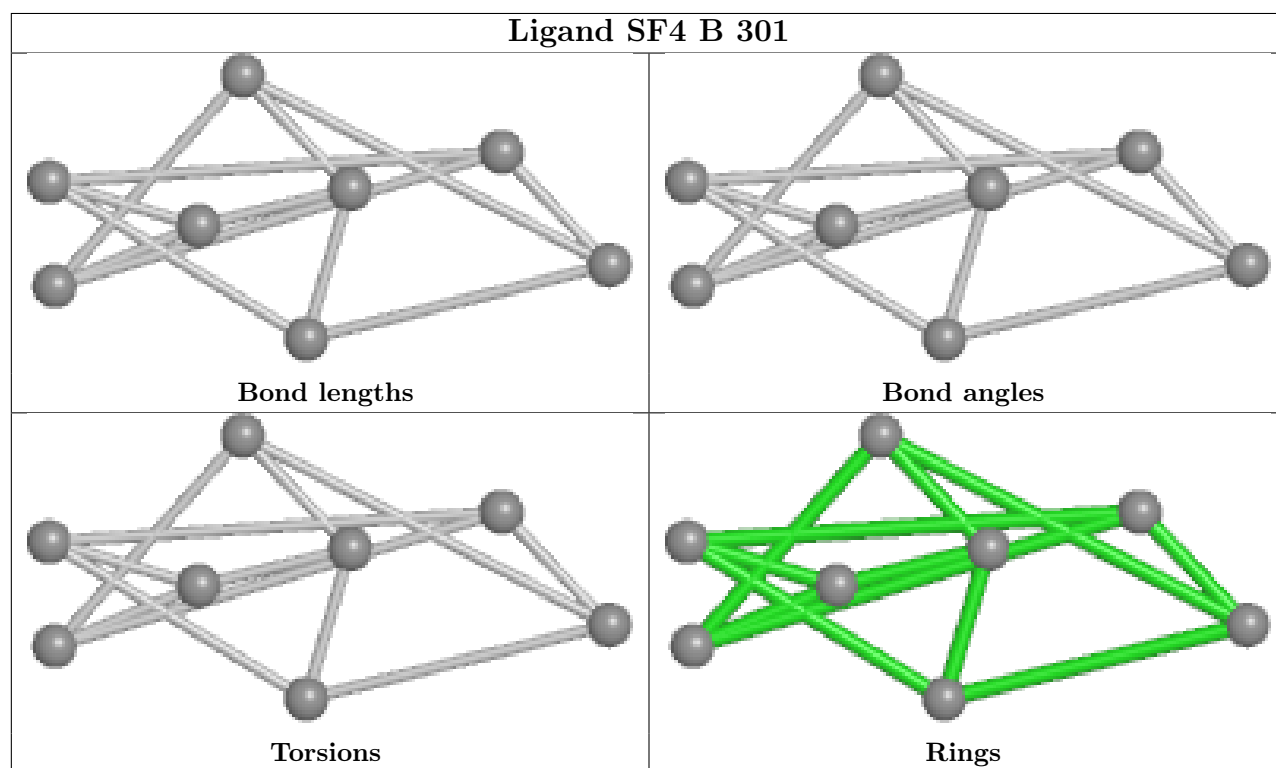
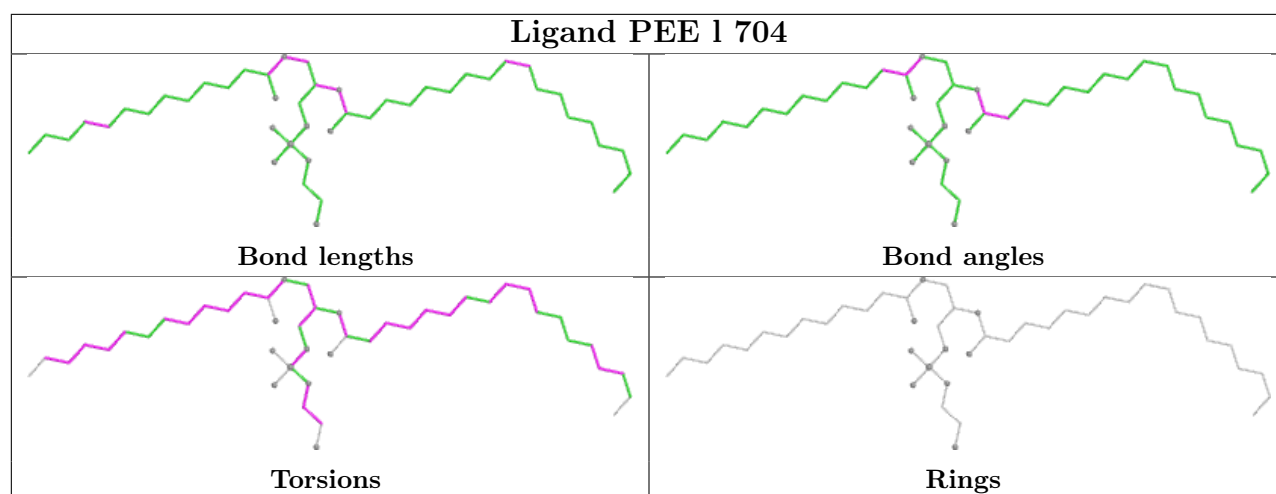


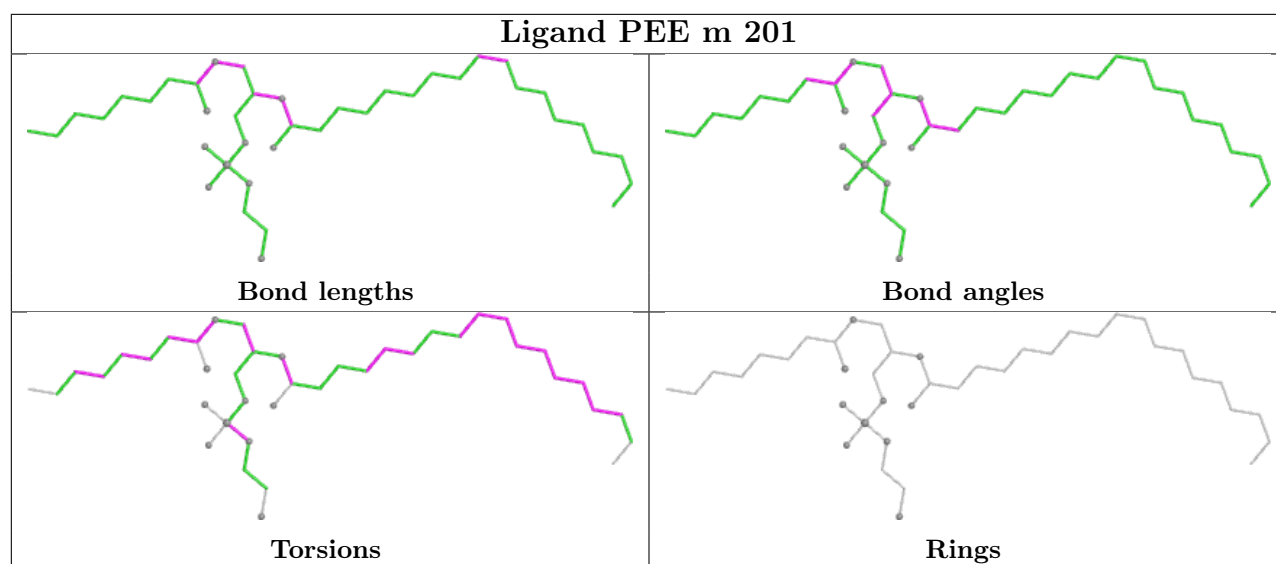












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

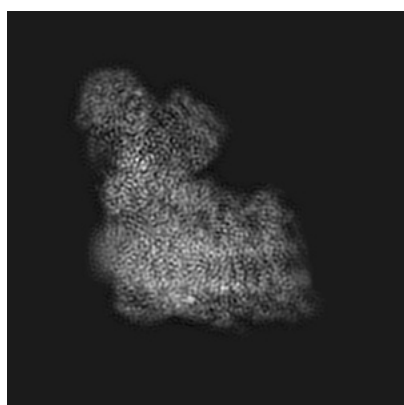
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32253. These allow visual inspection of the internal detail of the map and identification of artifacts.

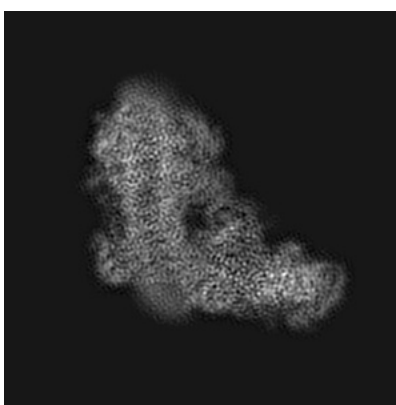
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

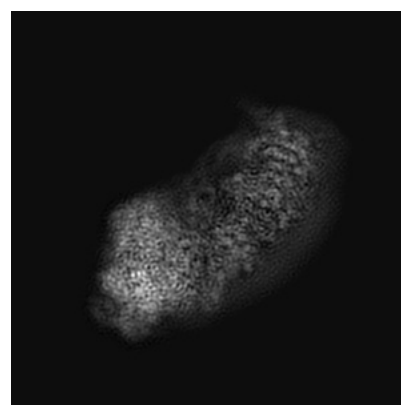
6.1.1 Primary map



X



Y

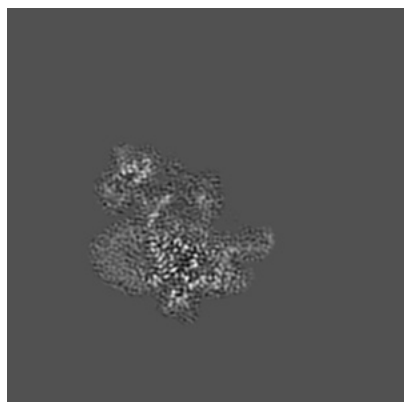


Z

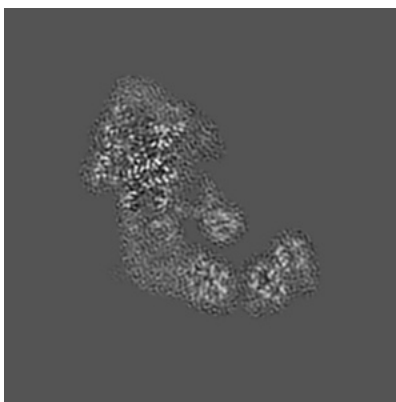
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

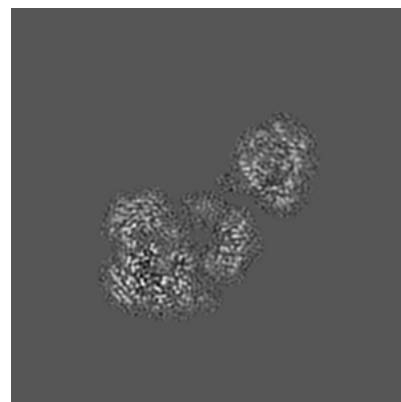
6.2.1 Primary map



X Index: 155



Y Index: 155

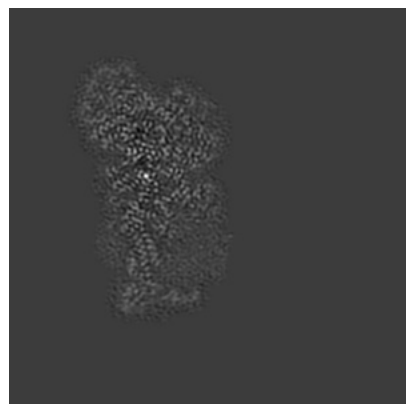


Z Index: 155

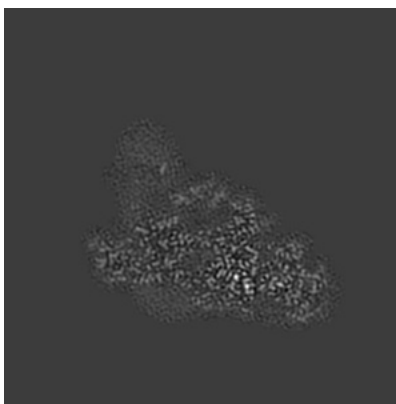
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

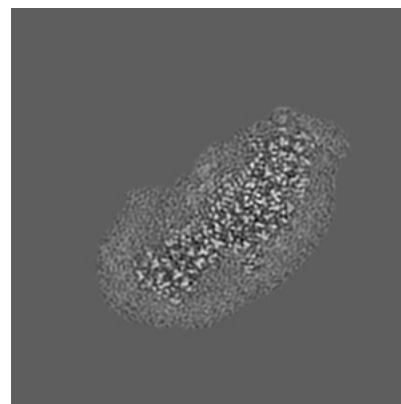
6.3.1 Primary map



X Index: 101



Y Index: 105

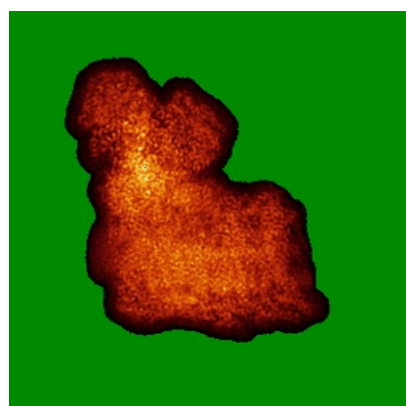


Z Index: 121

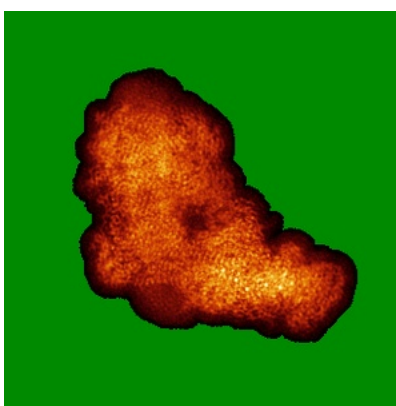
The images above show the largest variance slices of the map in three orthogonal directions.

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

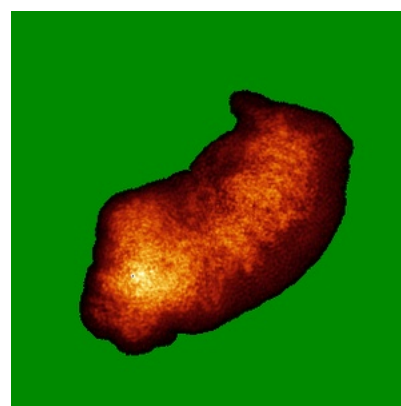
6.4.1 Primary map



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 0.0267. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

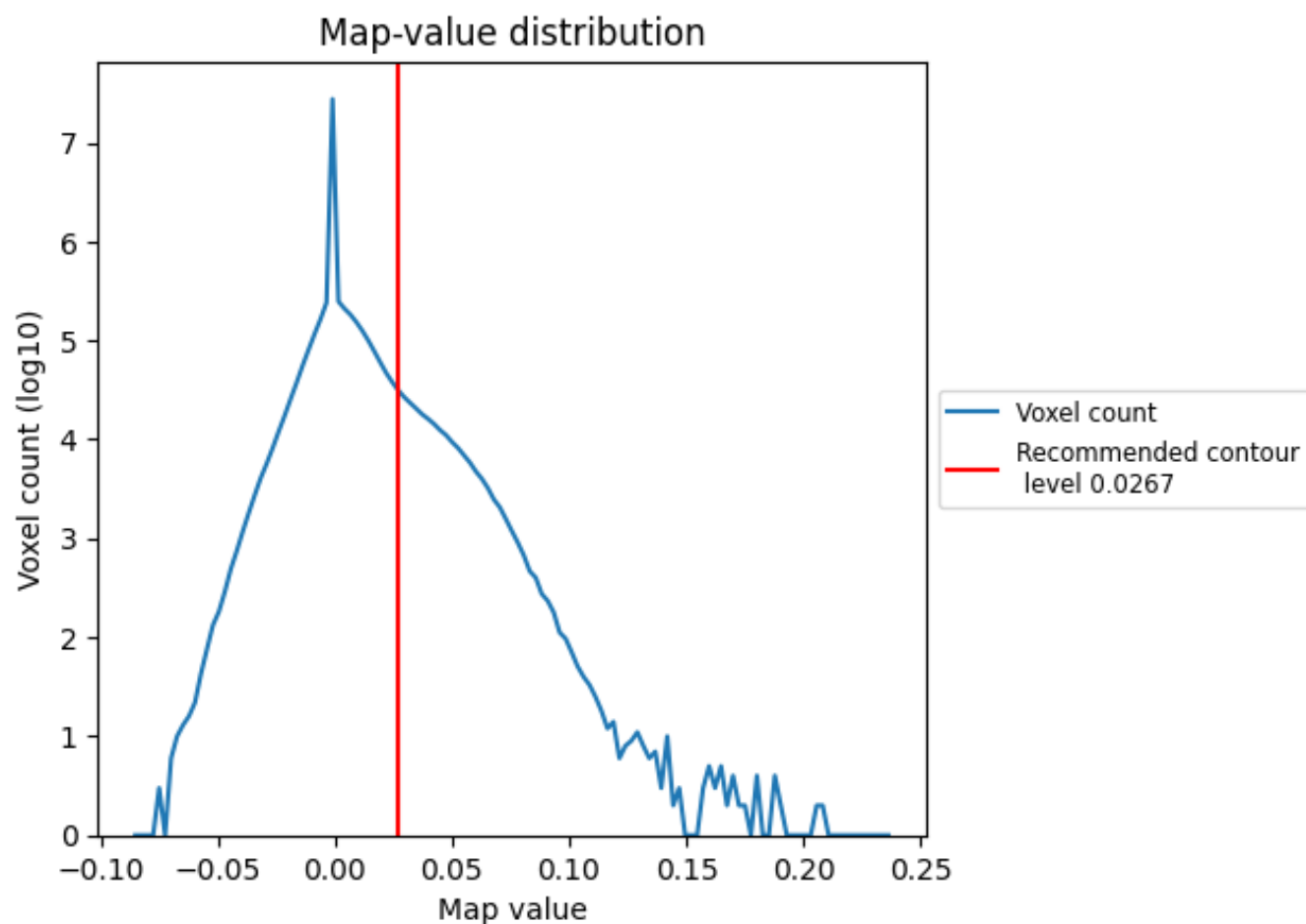
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

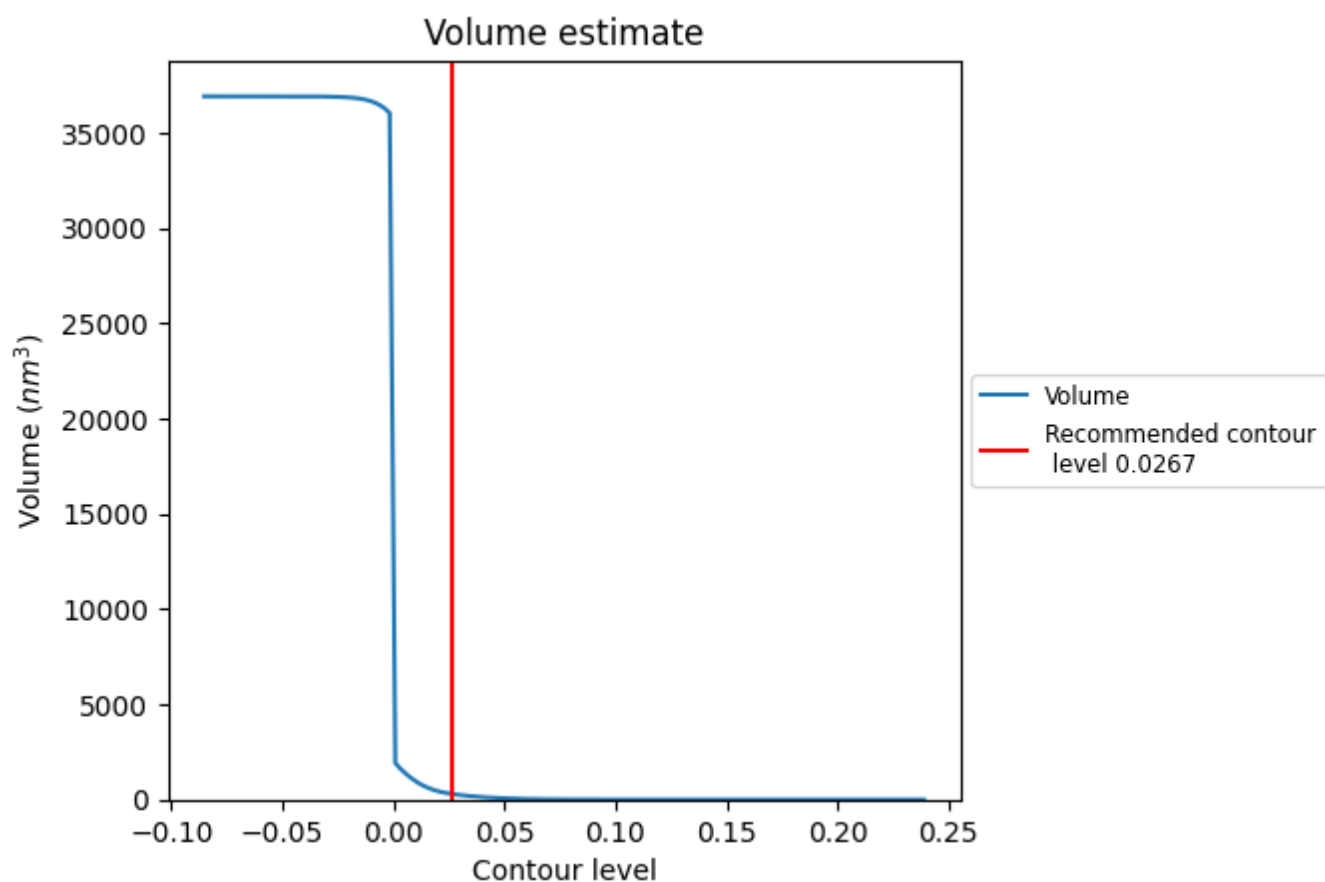
This section contains the results of statistical analysis of the map.

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.

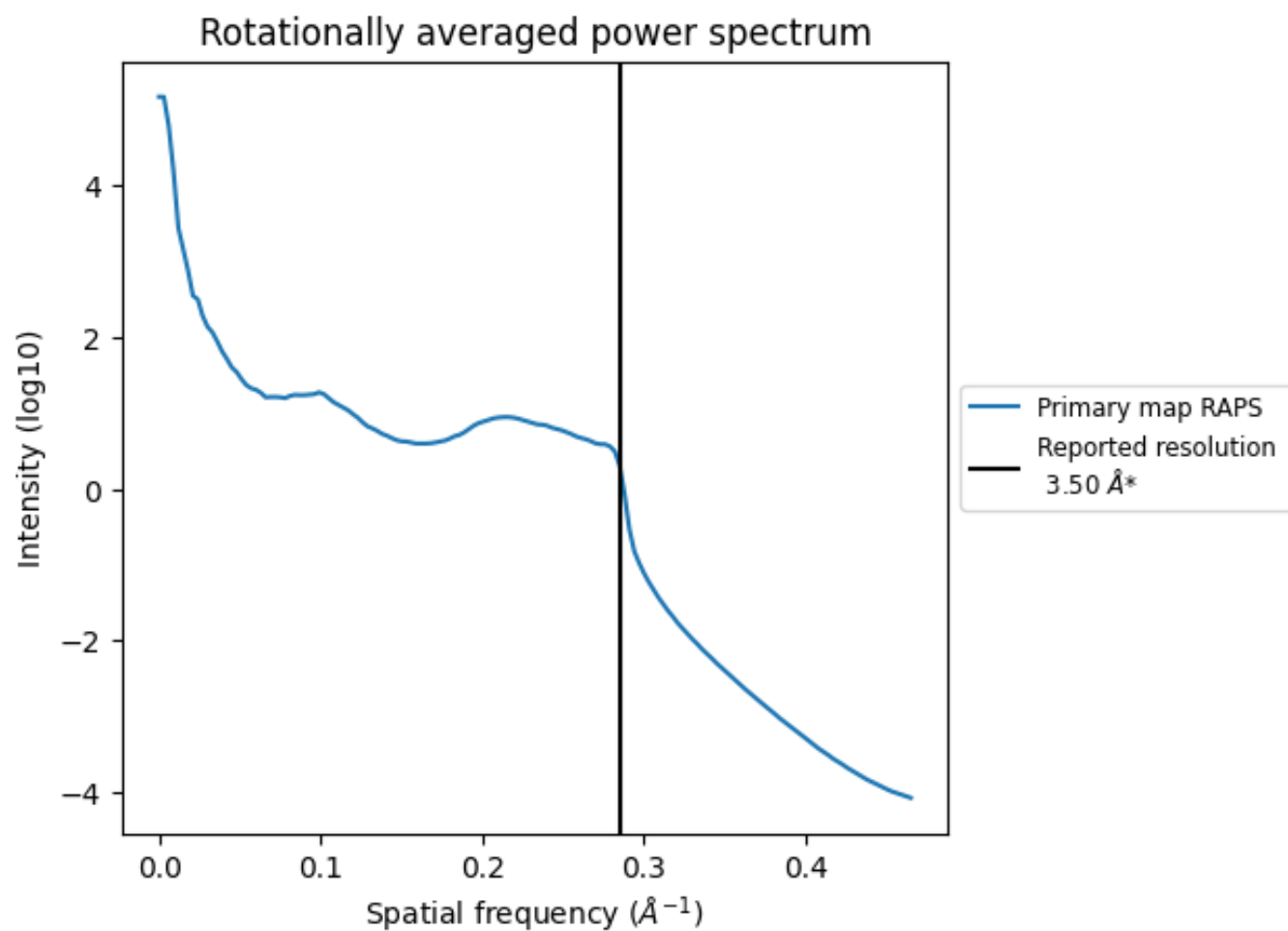
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 289 nm³; this corresponds to an approximate mass of 261 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 0.286 Å⁻¹

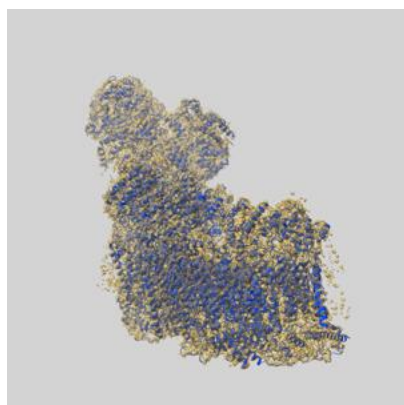
8 Fourier-Shell correlation ⓘ

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

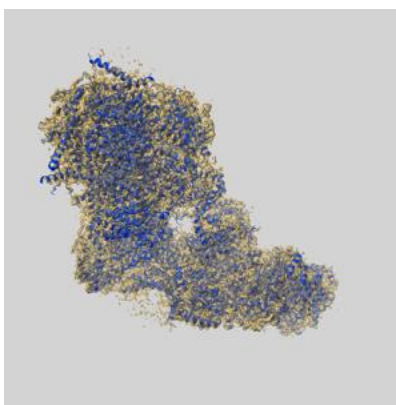
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32253 and PDB model 7W1O. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

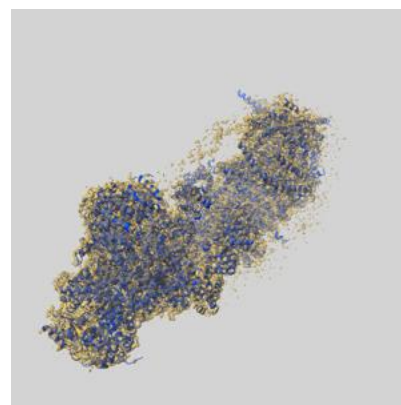
9.1 Map-model overlay [i](#)



X



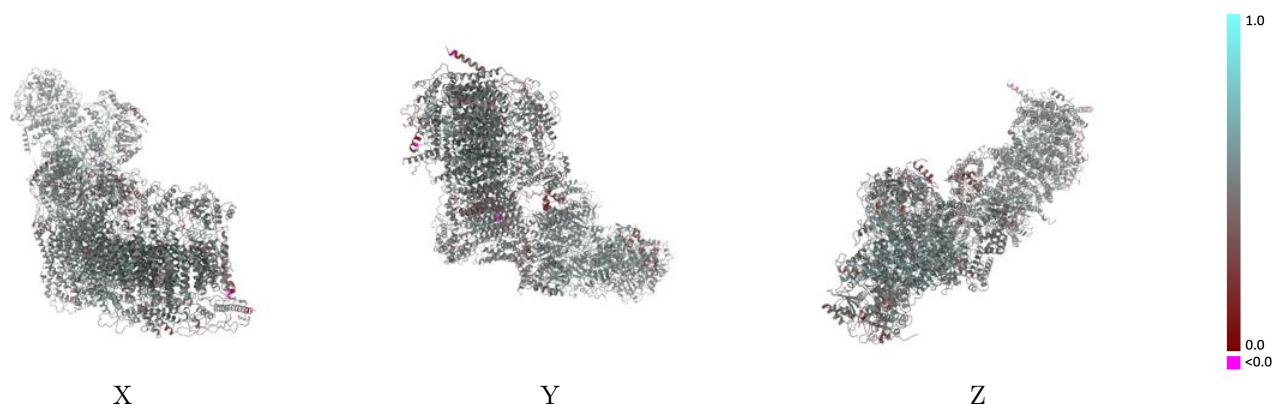
Y



Z

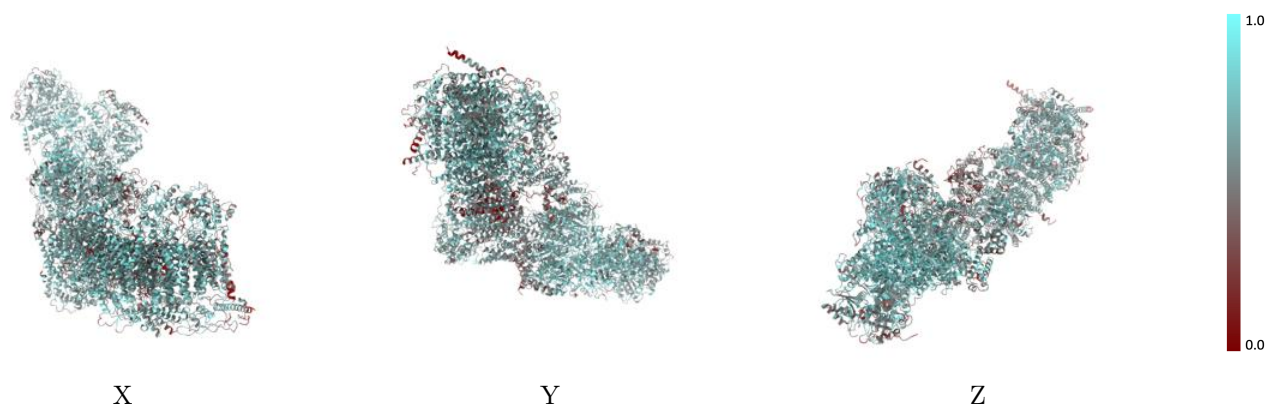
The images above show the 3D surface view of the map at the recommended contour level 0.0267 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



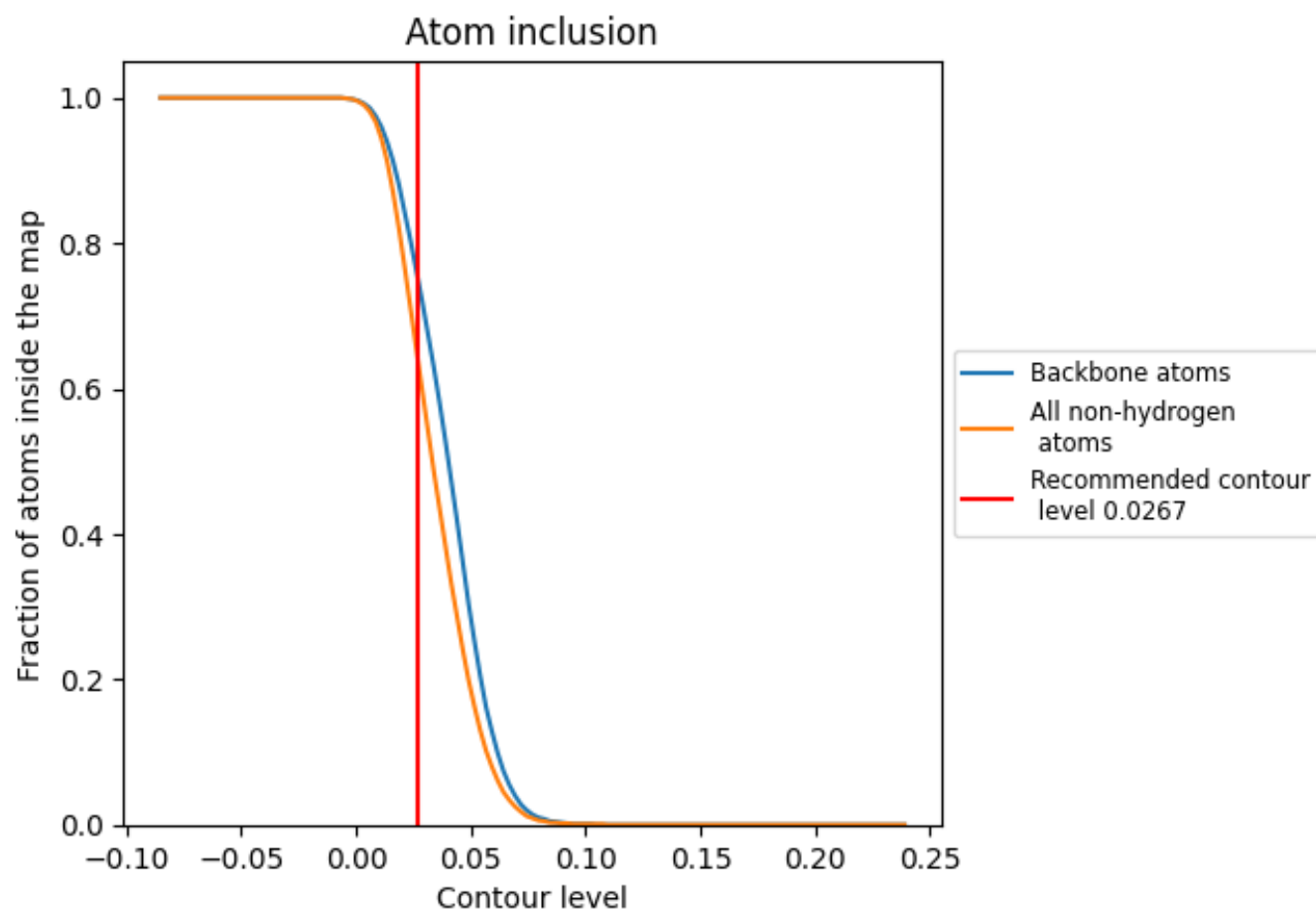
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0267).

9.4 Atom inclusion ⓘ



At the recommended contour level, 76% of all backbone atoms, 64% 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 (0.0267) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6440	 0.5020
A	 0.6230	 0.4850
B	 0.7710	 0.5530
C	 0.7660	 0.5350
E	 0.6670	 0.5000
F	 0.5370	 0.4390
G	 0.3860	 0.3860
H	 0.6160	 0.4880
I	 0.6390	 0.5110
J	 0.6210	 0.4870
K	 0.6160	 0.4970
L	 0.6980	 0.5360
M	 0.7020	 0.5200
N	 0.6460	 0.5080
O	 0.6160	 0.4840
P	 0.7670	 0.5420
Q	 0.7420	 0.5390
S	 0.7030	 0.5140
T	 0.6870	 0.5260
U	 0.6250	 0.4820
V	 0.3520	 0.4240
W	 0.6730	 0.5070
X	 0.5500	 0.4730
Y	 0.4960	 0.4390
Z	 0.4620	 0.3890
a	 0.6520	 0.5090
b	 0.5710	 0.4670
c	 0.6520	 0.5010
d	 0.6270	 0.4840
e	 0.5990	 0.4880
f	 0.5810	 0.4700
g	 0.6470	 0.5170
h	 0.6430	 0.4920
i	 0.7130	 0.5320
j	 0.5140	 0.4740



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Chain	Atom inclusion	Q-score
k	 0.5460	 0.4780
l	 0.6250	 0.5070
m	 0.5370	 0.4710
n	 0.5520	 0.4760
o	 0.6400	 0.5010
p	 0.6410	 0.4980
r	 0.7070	 0.5340
s	 0.6800	 0.5120
u	 0.6440	 0.5040
v	 0.5440	 0.4520
w	 0.6140	 0.4850