Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 01:31 PM JST

PDB ID	:	7W4M / pdb_00007w4m
EMDB ID	:	EMD-32308
Title	:	Deactive state CI from Q1-NADH dataset, Subclass 4
Authors	:	Gu, J.; Yang, M.
Deposited on	:	2021-11-28
Resolution	:	3.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

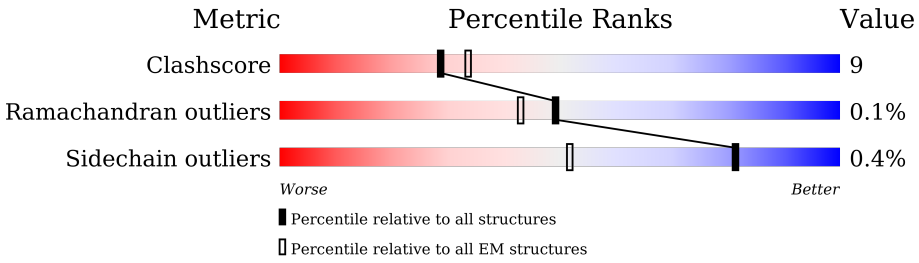
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

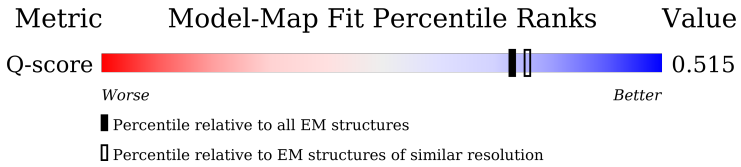
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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





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

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

Mol	Chain	Length	Quality of chain
1	A	433	21% 76% 24%
2	B	176	80% 20%
3	C	156	87% 13%
4	E	115	17% 70% 30%

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Mol	Chain	Length	Quality of chain
5	F	86	29% 80% 20%
6	G	88	70% 68% 32%
6	X	88	49% 72% 28%
7	H	112	21% 78% 21%
8	I	112	5% 77% 10% 13%
9	J	341	18% 69% 17% 13%
10	K	43	33% 74% 23%
11	L	125	6% 86% 14%
12	M	690	6% 84% 16%
13	N	144	5% 81% 19%
14	O	217	29% 79% 21%
15	P	208	83% 17%
16	Q	430	8% 78% 18%
17	S	70	73% 27%
18	T	96	12% 89% 10%
19	U	83	10% 84% 16%
20	V	140	74% 81% 18%
21	W	142	7% 85% 15%
22	Y	70	46% 67% 30%
23	Z	84	51% 85% 15%
24	a	140	8% 86% 14%
25	b	126	28% 63% 19% 18%
26	c	156	28% 79% 20%
27	d	175	17% 78% 21%
28	e	107	21% 79% 21%

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Mol	Chain	Length	Quality of chain
29	f	49	24% 71% 14% 14%
30	g	122	5% 85% 14%
31	h	105	10% 80% 19%
32	i	347	75% 25%
33	j	113	22% 59% 27% 12%
34	k	98	23% 83% 17%
35	l	603	12% 71% 29%
36	m	175	17% 57% 17% 26%
37	n	56	30% 84% 16%
38	o	128	25% 84% 16%
39	p	178	28% 80% 20%
40	r	459	78% 22%
41	s	318	6% 69% 26% 5%
42	u	171	9% 80% 20%
43	v	124	48% 75% 25%
44	w	320	39% 79% 21%

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

There are 57 unique types of molecules in this entry. The entry contains 66210 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
			Total	C	N	O	S		
1	A	431	3314	2092	590	612	20	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	156	1244	792	227	211	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	115	968	618	179	166	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	86	683	431	127	123	2	0	0

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total 690	C 446	N 102	O 137	S 5	0	0
6	X	88	Total 693	C 448	N 103	O 137	S 5	0	0

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

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

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

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

- 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 2339	C 1503	N 417	O 411	S 8	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	42	Total 344	C 214	N 67	O 63	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	125	Total 1002	C 634	N 180	O 185	S 3	0	0

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

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

- 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
			1193	761	217	211	4		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	419	Total	C	N	O	S	0	0
			3366	2156	577	609	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
			563	362	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
			1017	648	174	189	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
			597	392	98	106	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
			875	571	158	145	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
			1312	852	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
			1445	908	259	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
			890	568	145	173	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	42	Total	C	N	O	0	0
			338	223	57	58		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	99	Total	C	N	O	S	0	0
			793	539	118	131	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
			4764	3159	737	817	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
			948	636	138	166	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
			460	301	81	77	1		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	303	Total	C	N	O	S	0	0
			2387	1602	369	395	21		

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

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

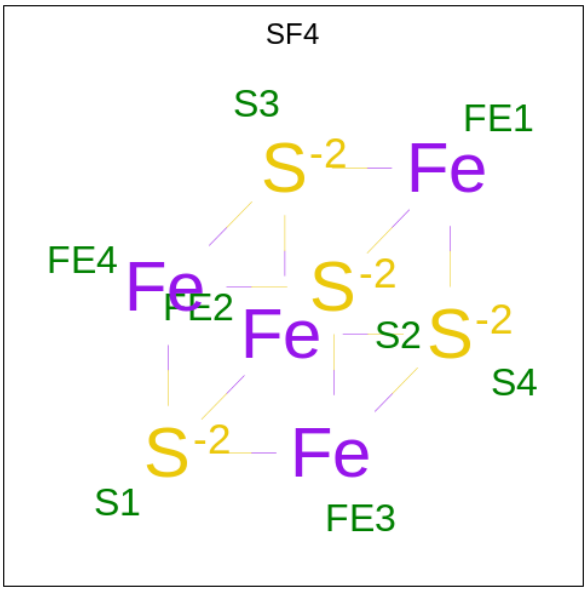
- Molecule 43 is a protein called Complex I-B18.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			1022	639	192	182	9		

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

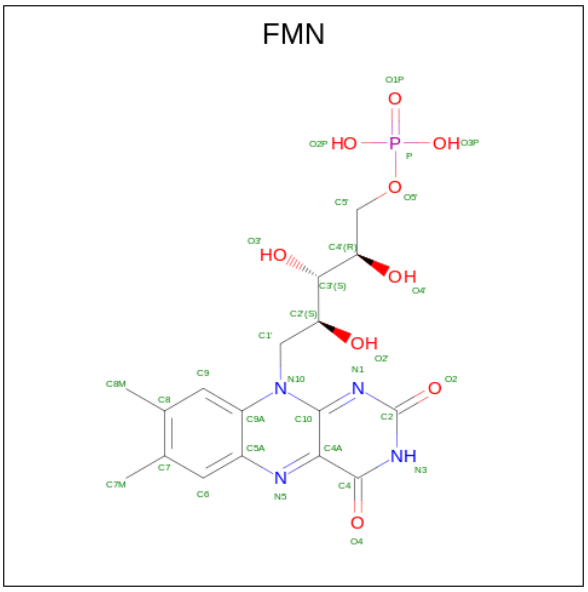
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2562	1629	435	488	10		

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



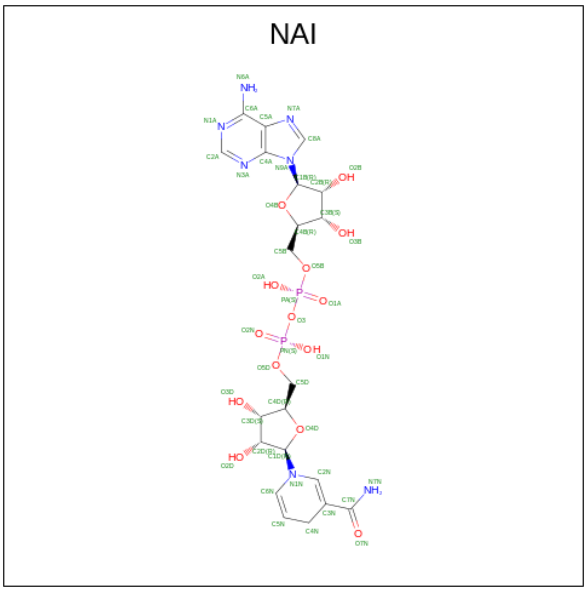
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total 8	Fe 4	S 4	0
45	B	1	Total 8	Fe 4	S 4	0
45	B	1	Total 8	Fe 4	S 4	0
45	C	1	Total 8	Fe 4	S 4	0
45	M	1	Total 8	Fe 4	S 4	0
45	M	1	Total 8	Fe 4	S 4	0

- 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	

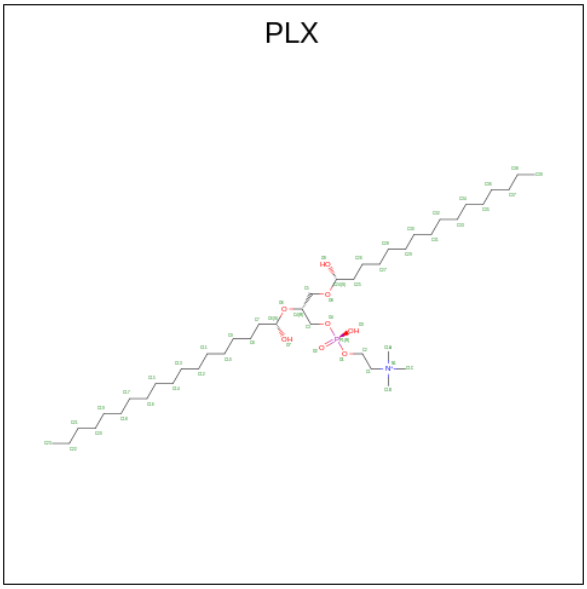
- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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

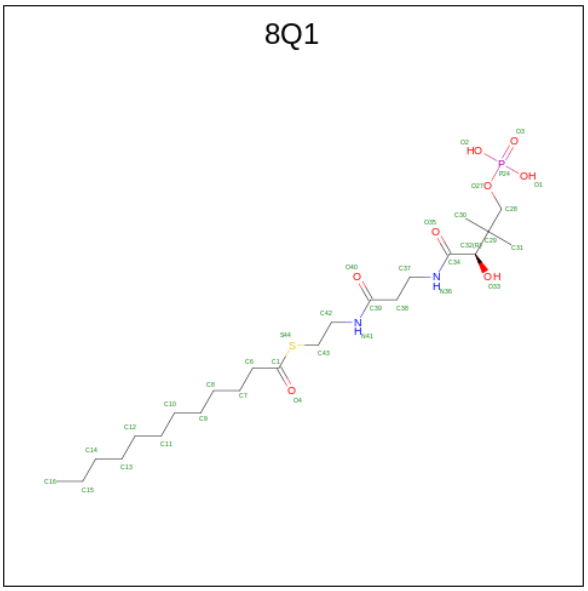
- Molecule 48 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-

6,6,11-TRIOL (CCD ID: PLX) (formula: $C_{42}H_{89}NO_8P$) (labeled as "Ligand of Interest" by depositor).



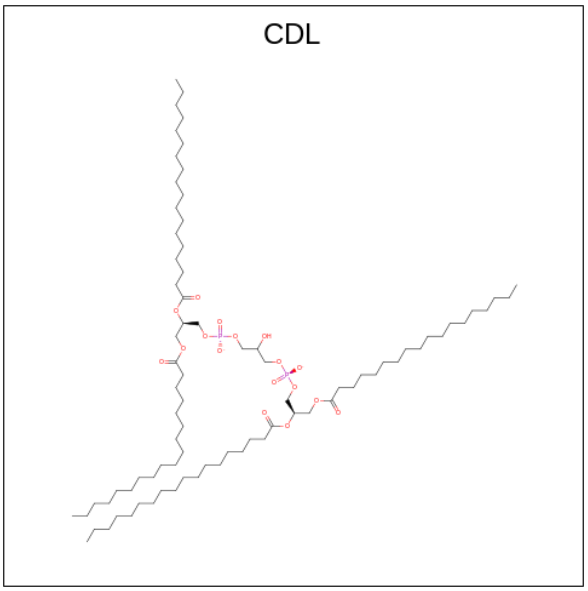
Mol	Chain	Residues	Atoms					AltConf
48	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 49 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (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 CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



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

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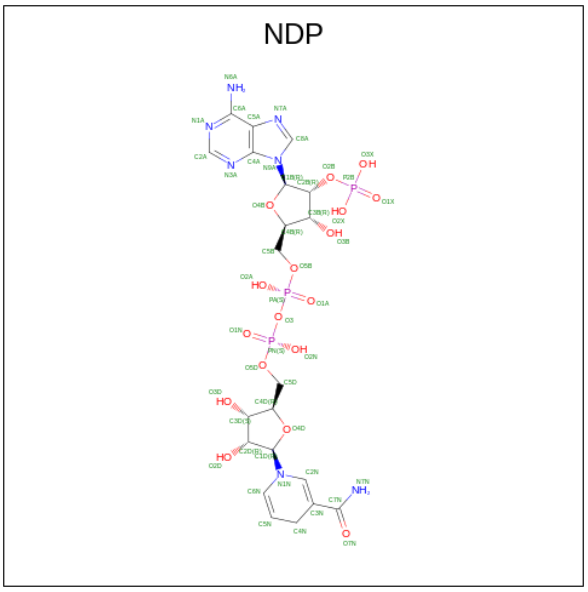
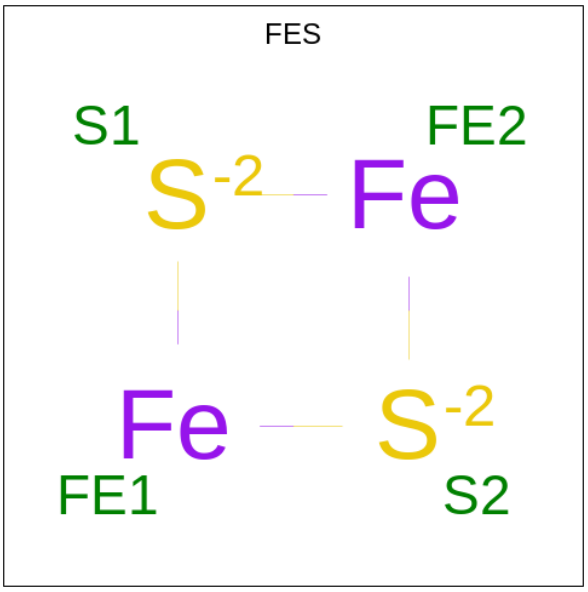
Mol	Chain	Residues	Atoms				AltConf
50	a	1	Total	C	O	P	0
			91	72	17	2	
50	g	1	Total	C	O	P	0
			100	81	17	2	
50	i	1	Total	C	O	P	0
			66	47	17	2	

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



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

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

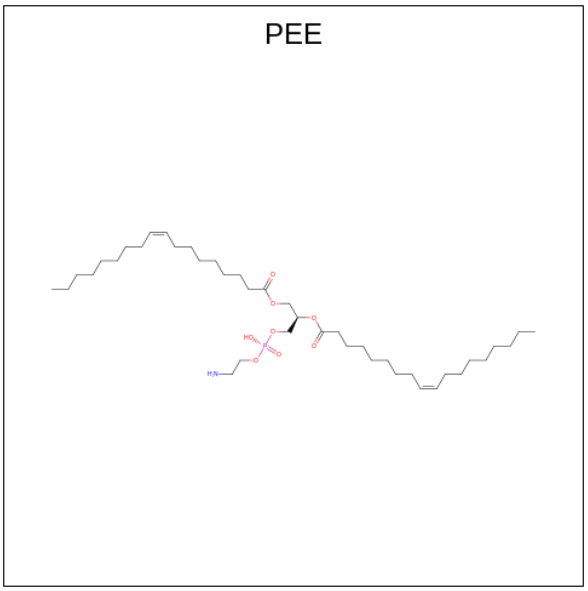


Mol	Chain	Residues	Atoms			AltConf
52	M	1	Total	Fe	S	0
			4	2	2	
52	O	1	Total	Fe	S	0
			4	2	2	

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

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

- Molecule 54 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).

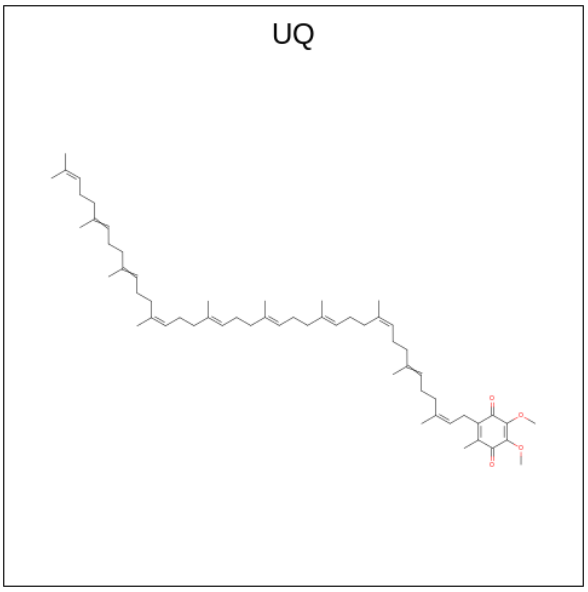


Mol	Chain	Residues	Atoms					AltConf
54	Q	1	Total	C	N	O	P	0
			51	41	1	8	1	
54	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
54	b	1	Total	C	N	O	P	0
			46	36	1	8	1	
54	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
54	j	1	Total	C	N	O	P	0
			47	37	1	8	1	
54	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
54	m	1	Total	C	N	O	P	0
			41	31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

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

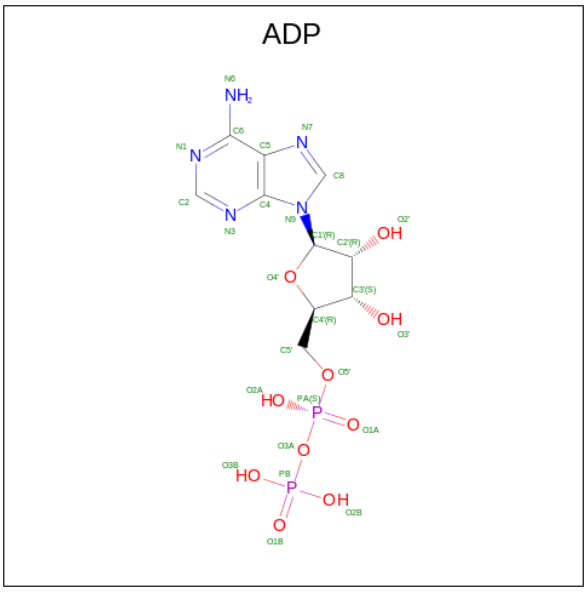
Mol	Chain	Residues	Atoms		AltConf
55	T	1	Total	Zn	0
			1	1	

- Molecule 56 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



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

- 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
			Total	C	N	O	P	
57	w	1	27	10	5	10	2	0

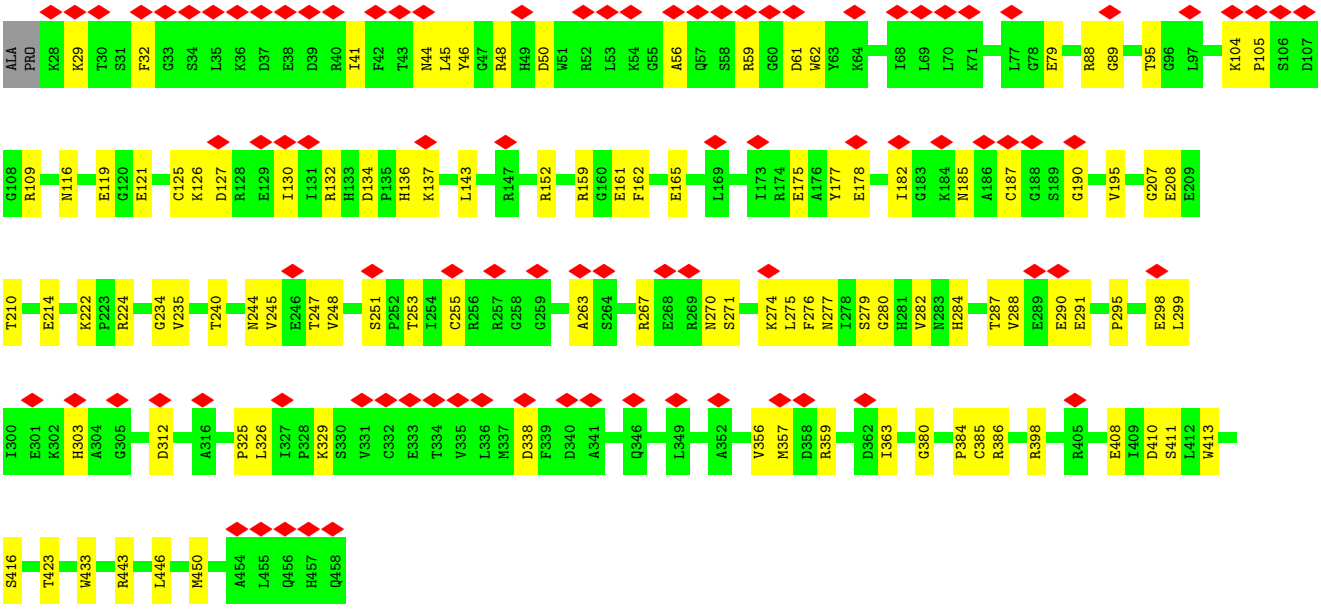
3 Residue-property plots (i)

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

Chain A:

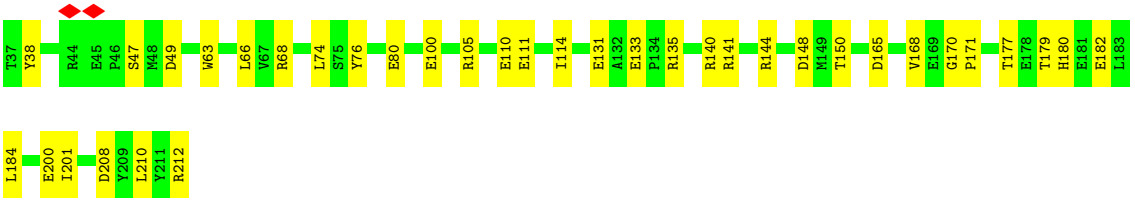




• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain B:

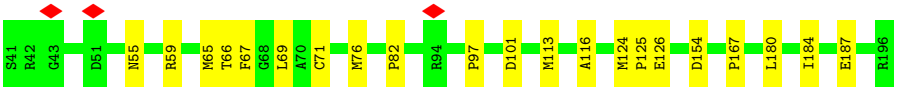




• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain C:

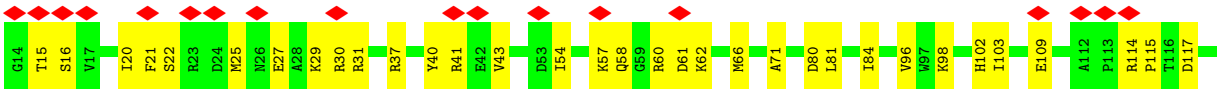




• Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain E:



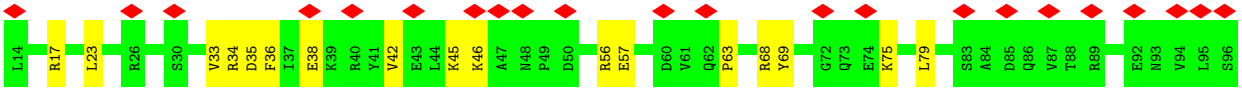




• Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain F:



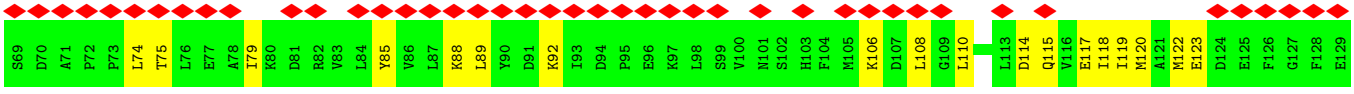


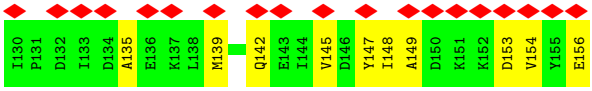


• Molecule 6: Acyl carrier protein

Chain G:



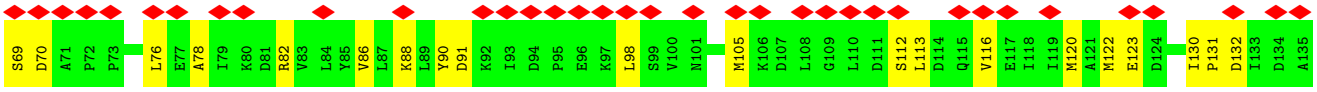


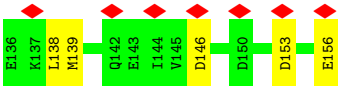


• Molecule 6: Acyl carrier protein

Chain X:

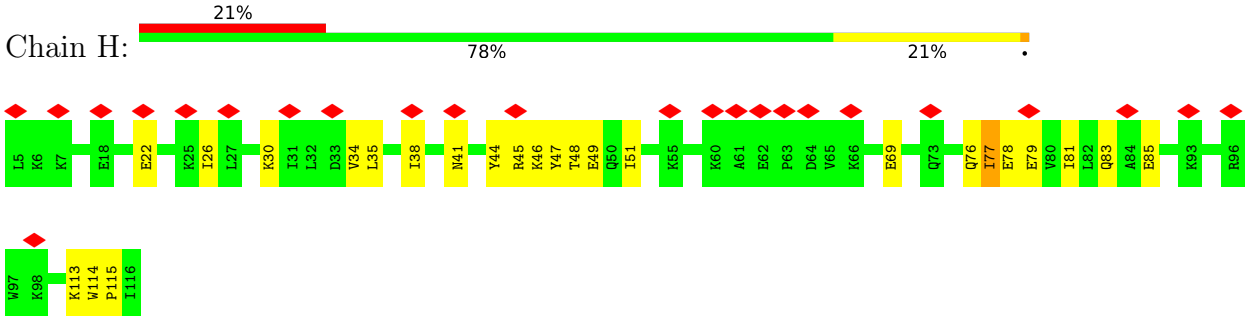






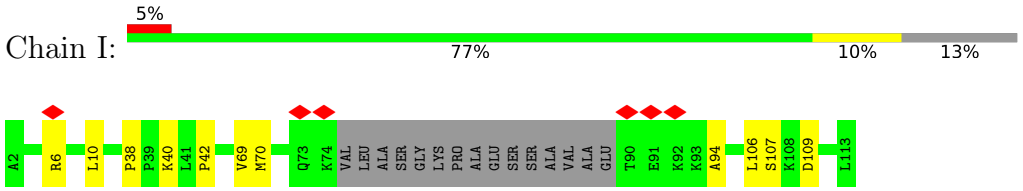
• Molecule 7: Complex I subunit B13

Chain H:



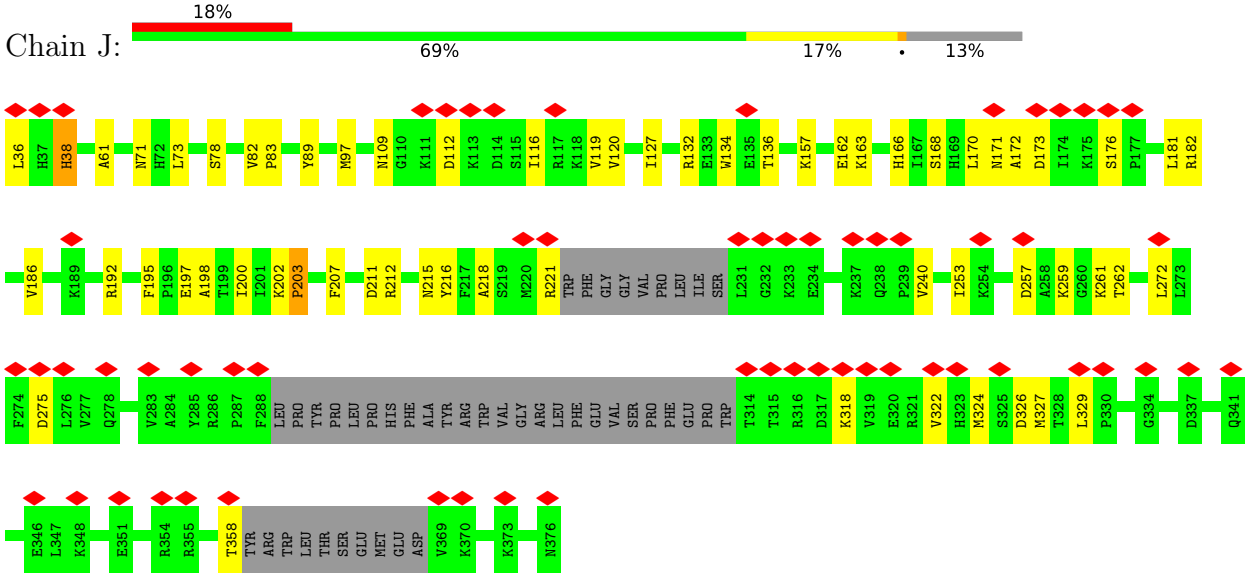
• Molecule 8: Complex I-B14.5a

Chain I:



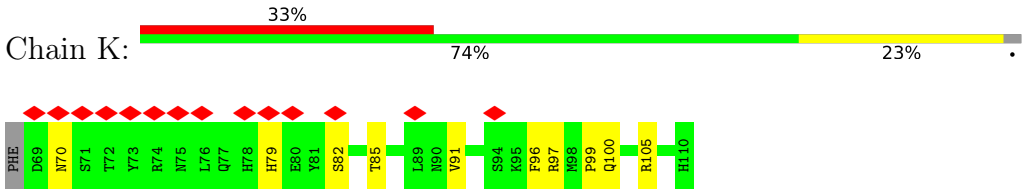
• Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

Chain J:



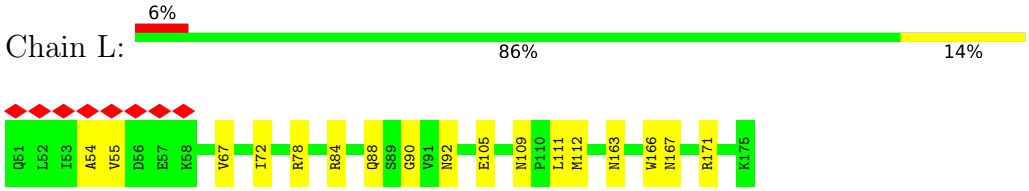
• Molecule 10: Complex I-9kD

Chain K:



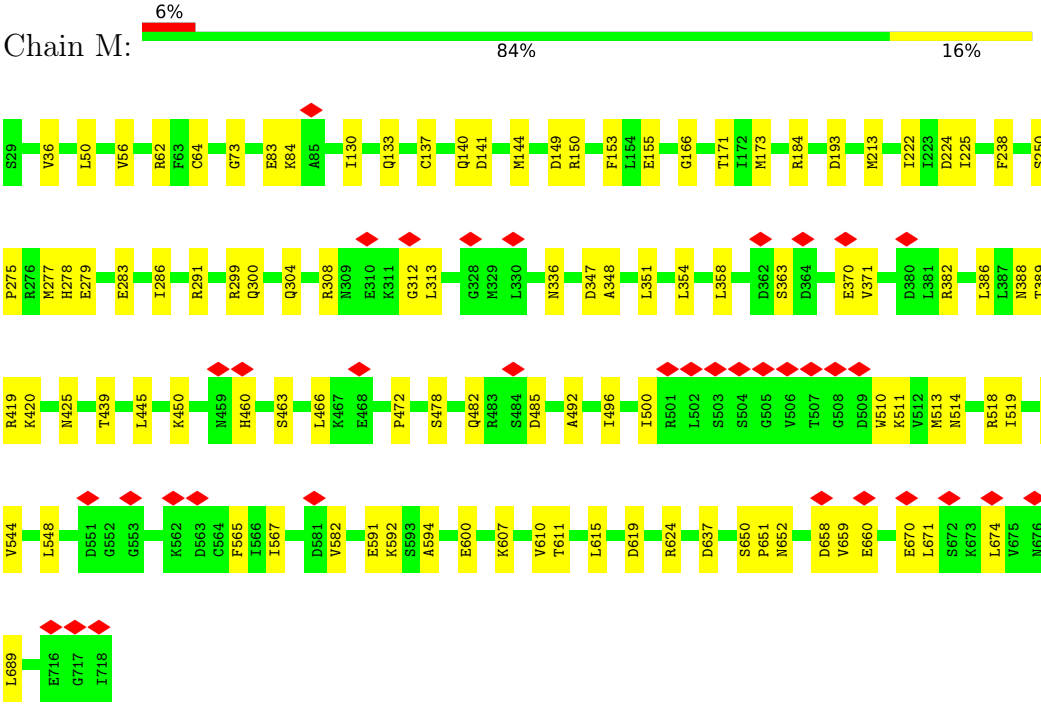
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain L:



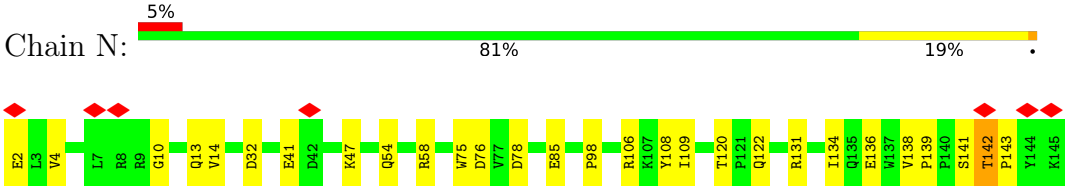
• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain M:



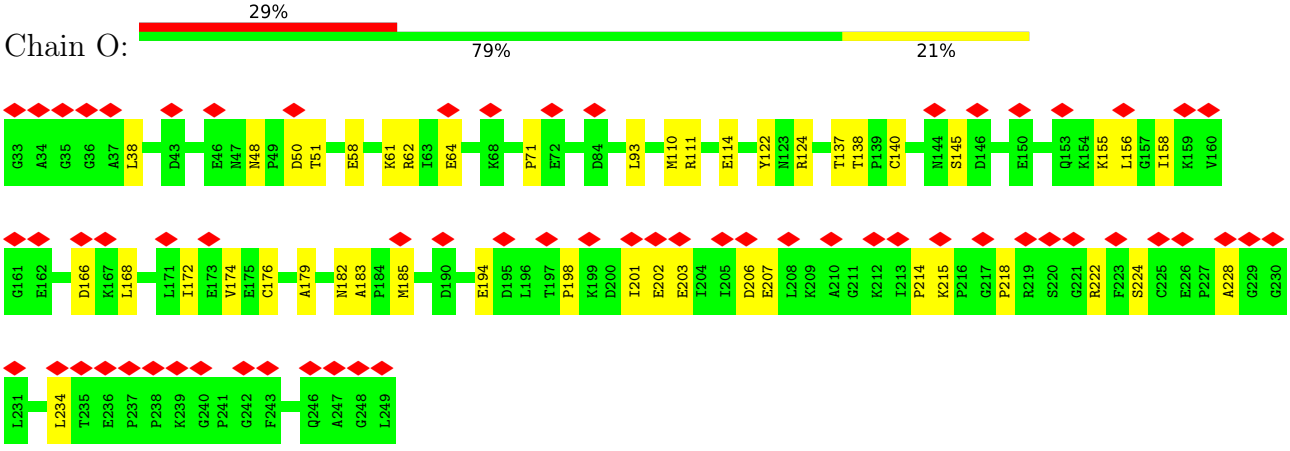
• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain N:



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

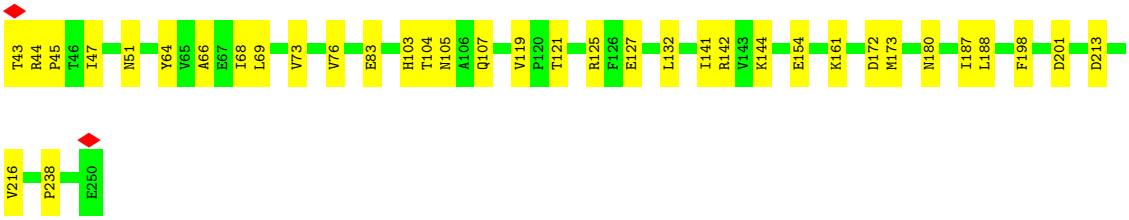
Chain O:



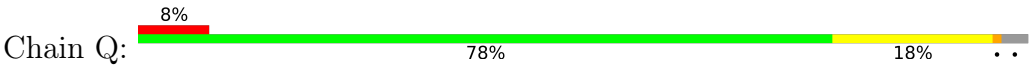
• Molecule 15: Complex I-30kD

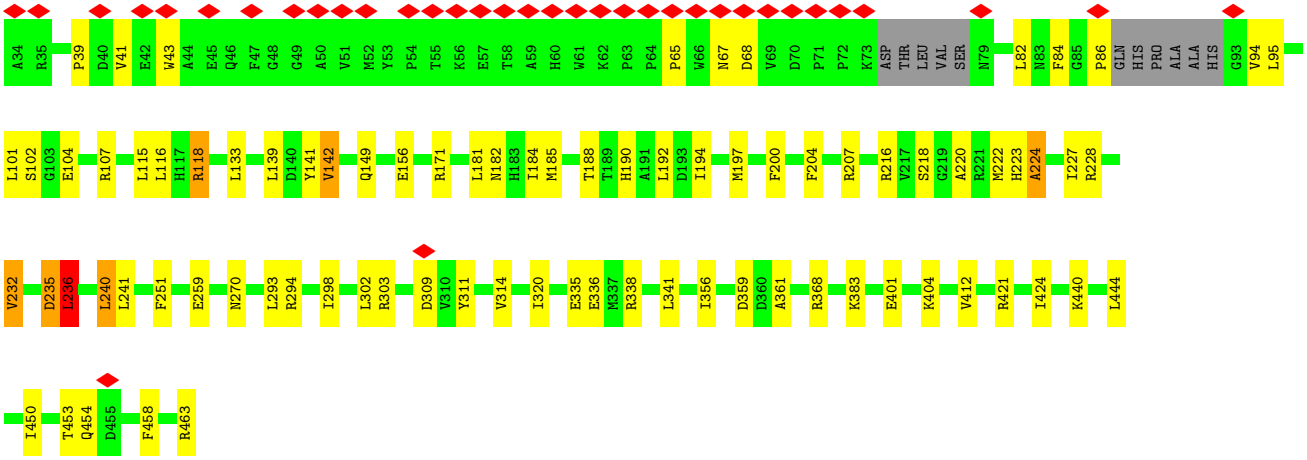
Chain P:





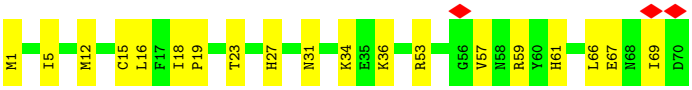
• Molecule 16: Complex I-49kD



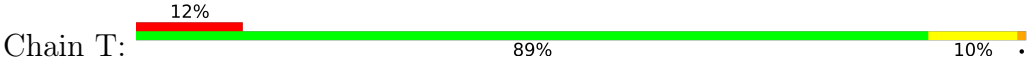


• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



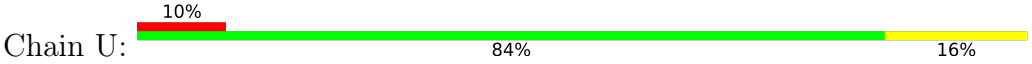


• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial





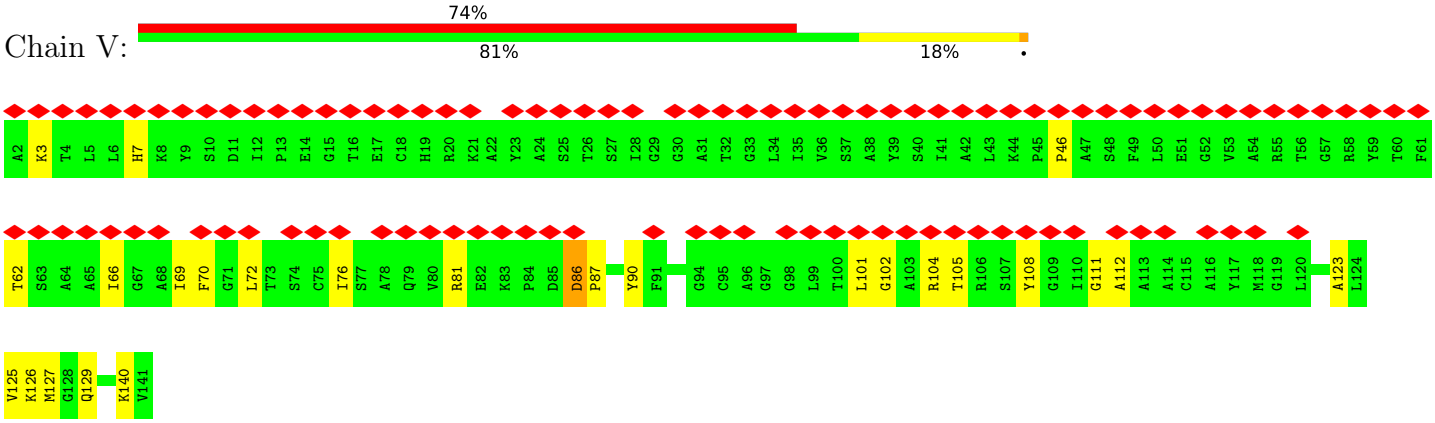
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3





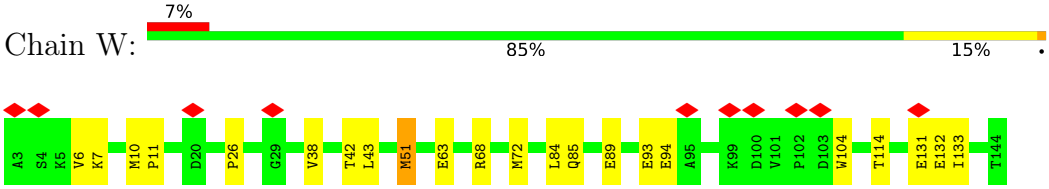
• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:



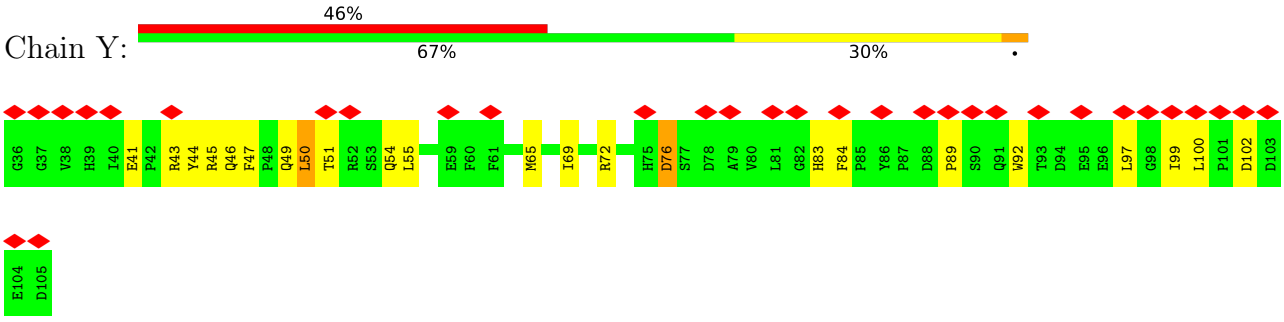
• Molecule 21: Complex I-B16.6

Chain W:



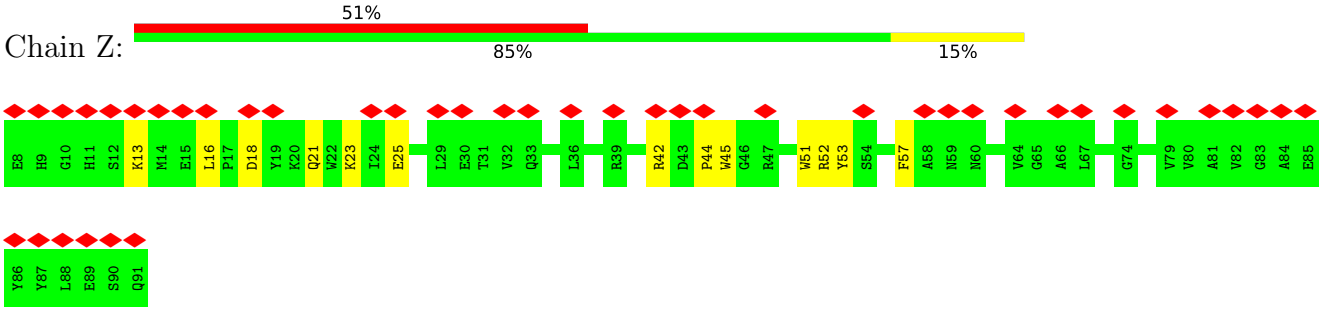
• Molecule 22: Complex I-AGGG

Chain Y:



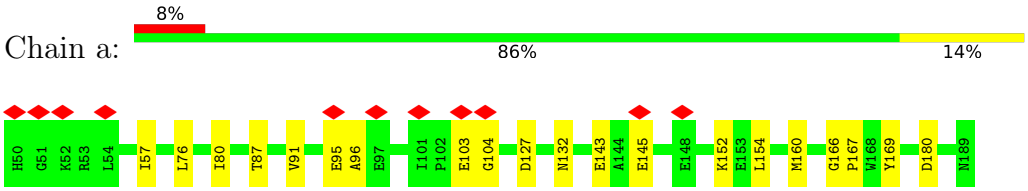
• Molecule 23: Complex I-B12

Chain Z:



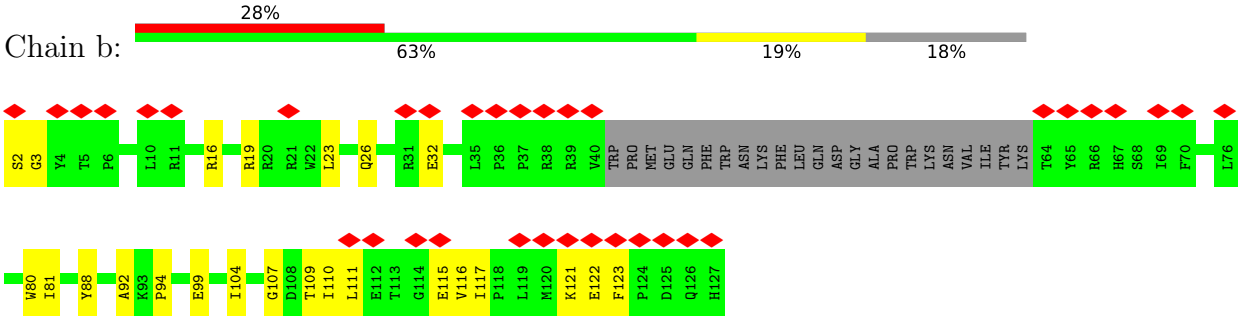
• Molecule 24: Complex I-SGDH

Chain a:



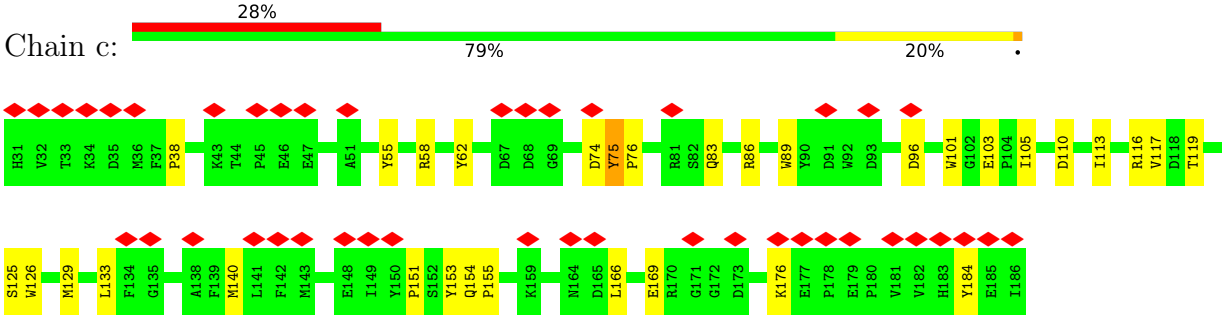
• Molecule 25: Complex I-B17

Chain b:



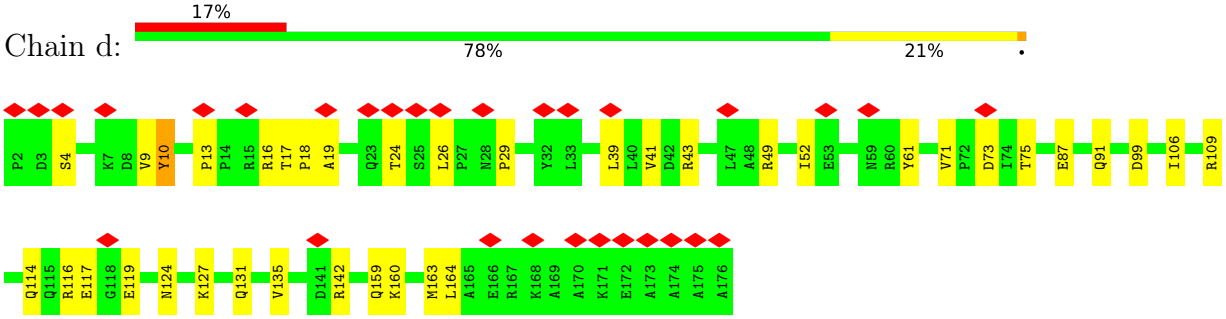
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c:



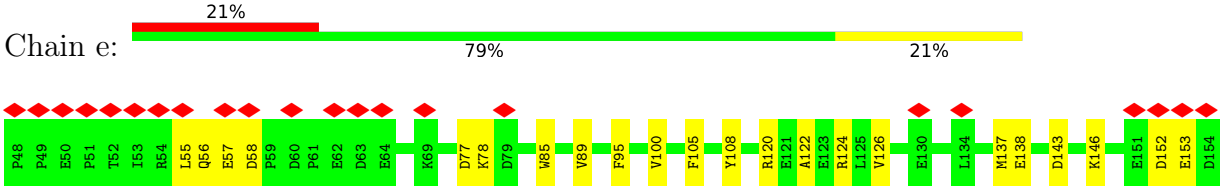
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d:



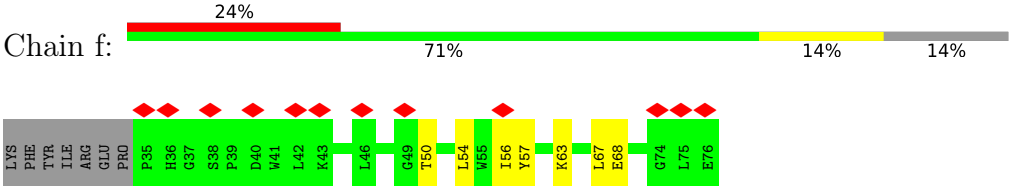
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e:



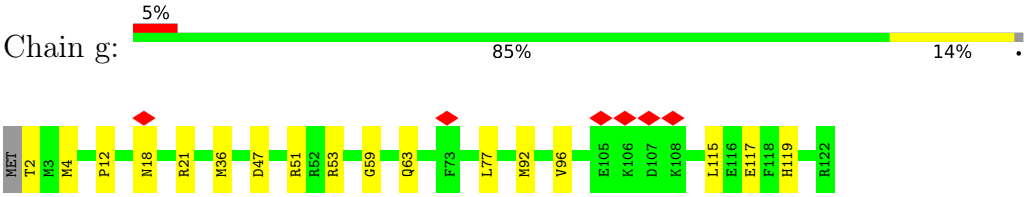
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f:



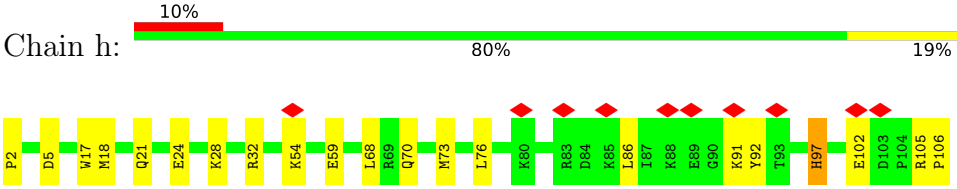
• Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g:



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

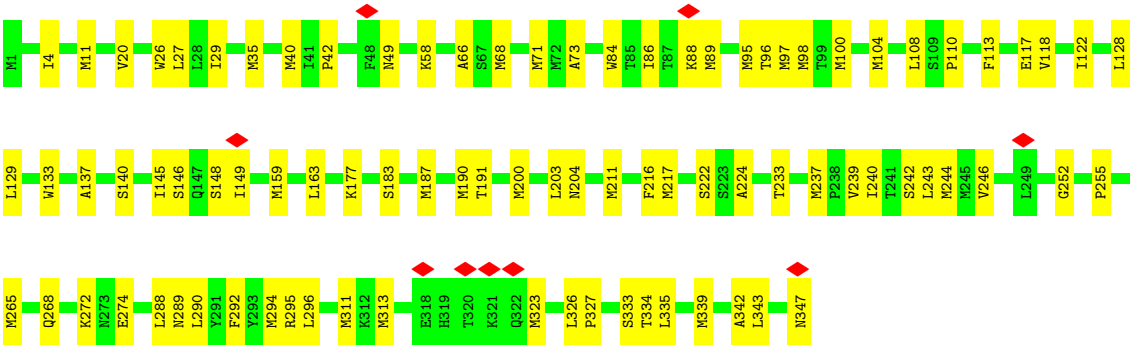
Chain h:



• Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain i:

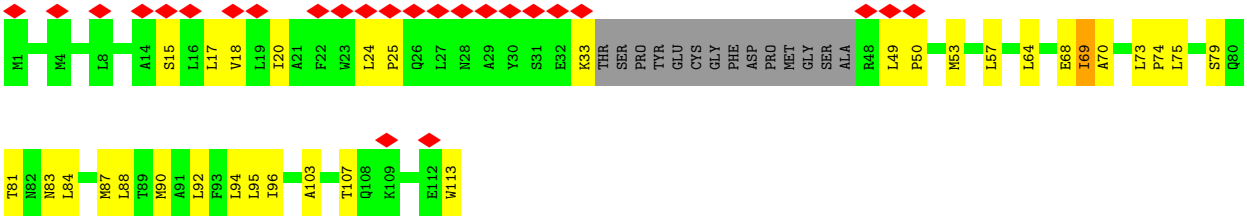




• Molecule 33: NADH-ubiquinone oxidoreductase chain 3

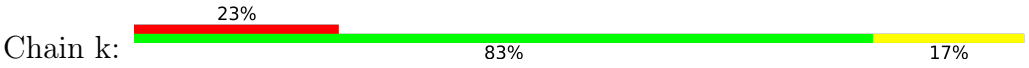
Chain j:

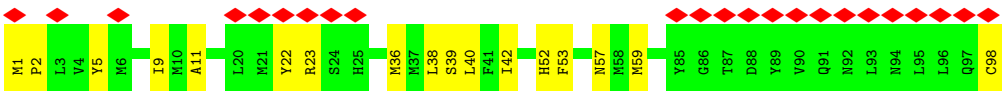




• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain k:

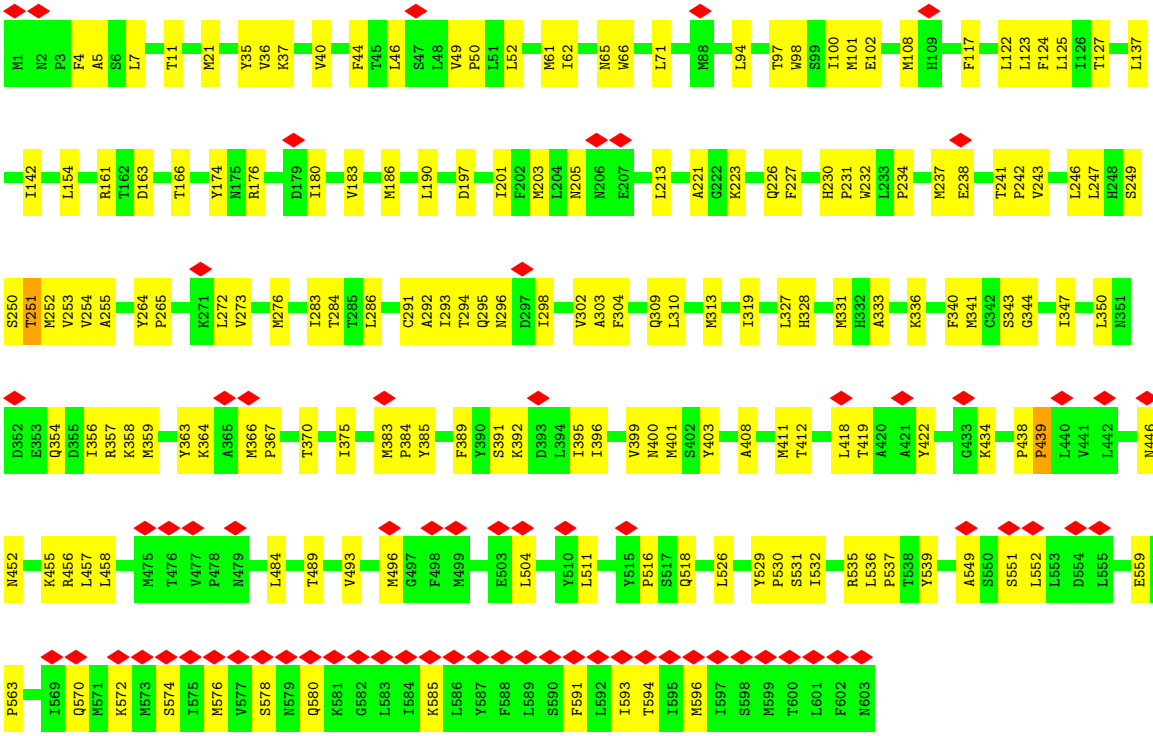




• Molecule 35: NADH-ubiquinone oxidoreductase chain 5

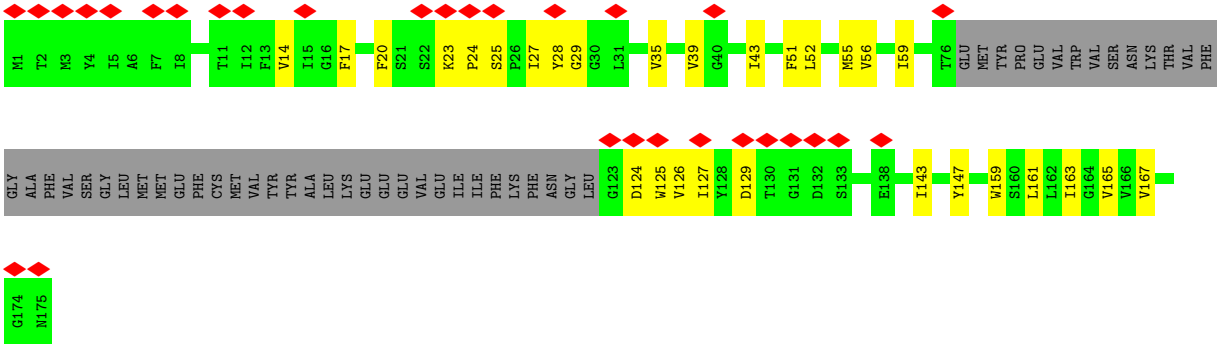
Chain l:



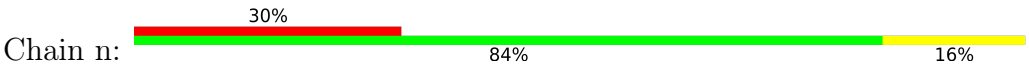


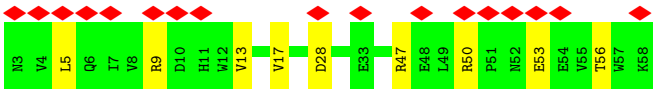
• Molecule 36: NADH-ubiquinone oxidoreductase chain 6



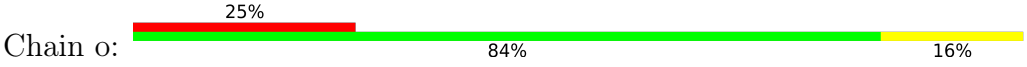


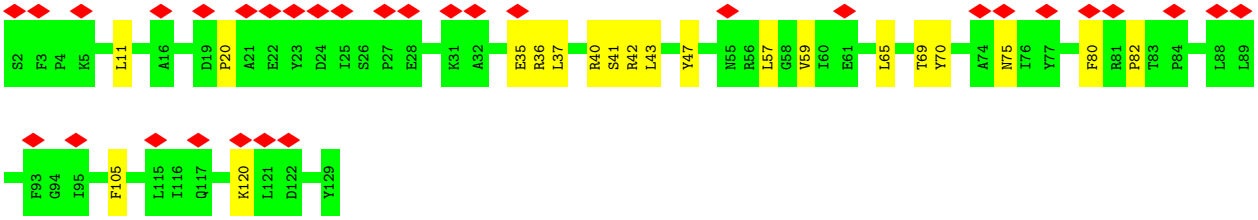
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1





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

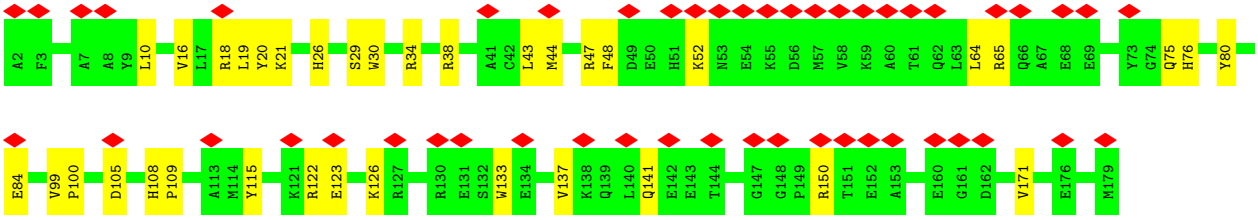




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p:

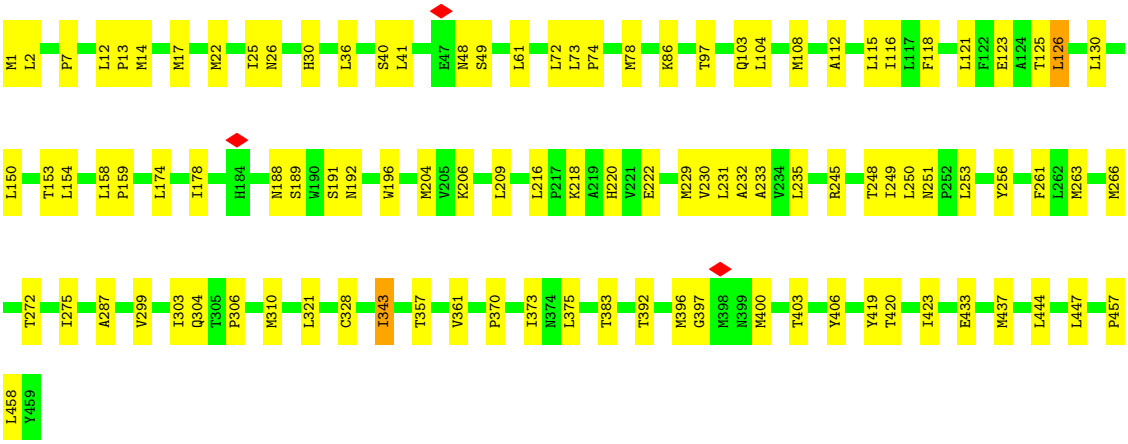




• Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r:

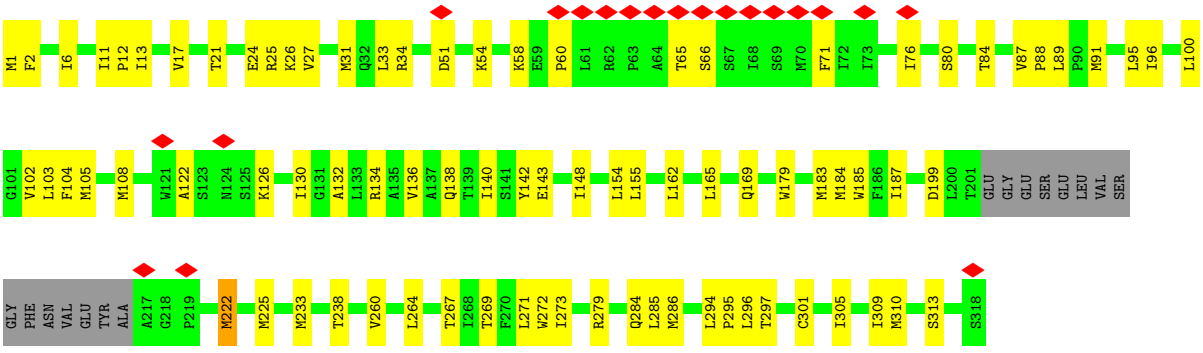




• Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s:

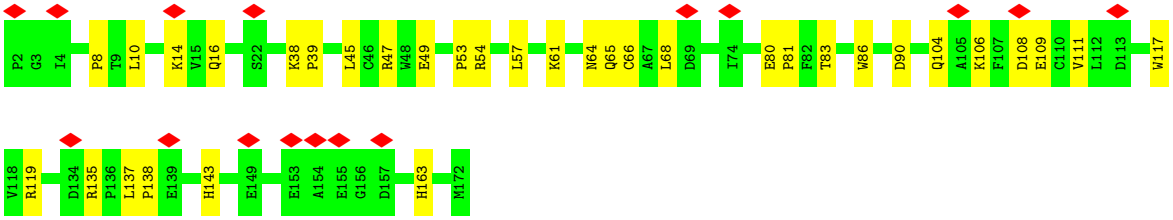




• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:

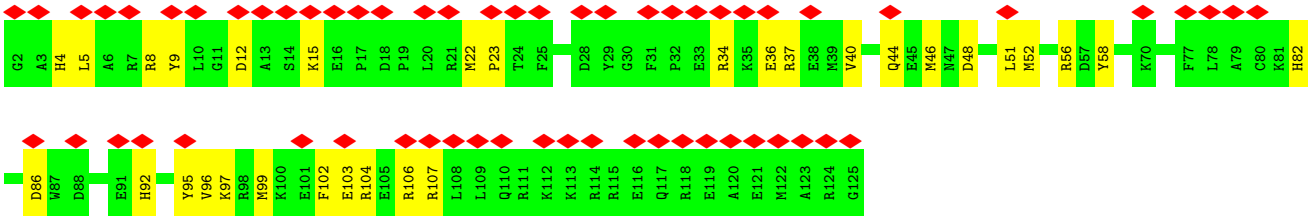




• Molecule 43: Complex I-B18

Chain v:

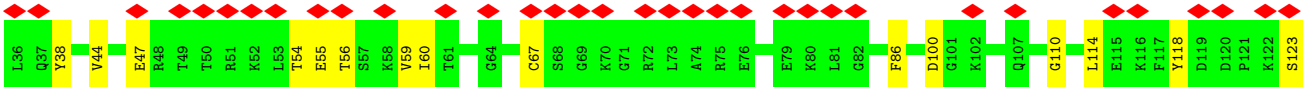


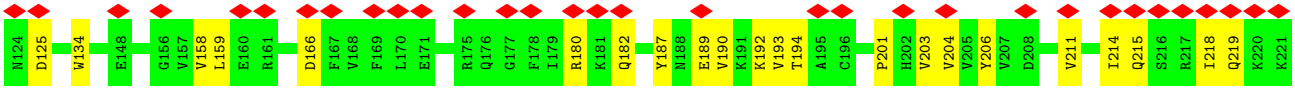


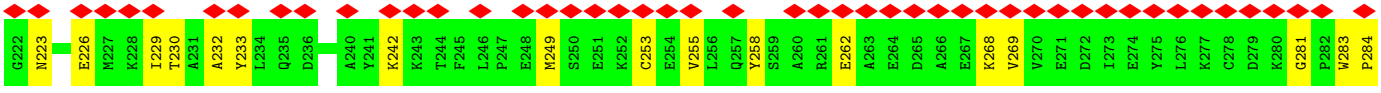
• Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

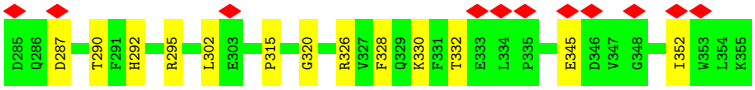
Chain w:











4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25219	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 ($e^-/Å^2$)	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	0.231	Depositor
Minimum map value	-0.102	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0299	Depositor
Map size (Å)	333.7616, 333.7616, 333.7616	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.14	0/3389	0.32	0/4580
2	B	0.20	0/1443	0.33	0/1952
3	C	0.19	0/1275	0.42	2/1725 (0.1%)
4	E	0.14	0/992	0.35	0/1336
5	F	0.14	0/694	0.35	0/935
6	G	0.17	0/702	0.49	0/952
6	X	0.15	0/705	0.41	0/955
7	H	0.14	0/929	0.33	0/1258
8	I	0.17	0/798	0.40	0/1079
9	J	0.15	0/2391	0.37	0/3230
10	K	0.22	0/354	0.58	0/480
11	L	0.16	0/1025	0.29	0/1386
12	M	0.15	0/5384	0.30	0/7295
13	N	0.17	0/1233	0.46	2/1679 (0.1%)
14	O	0.14	0/1711	0.36	0/2328
15	P	0.18	0/1789	0.36	0/2436
16	Q	0.22	0/3440	0.46	4/4659 (0.1%)
17	S	0.21	0/578	0.46	0/778
18	T	0.16	0/755	0.33	0/1018
19	U	0.13	0/664	0.33	0/912
20	V	0.20	0/1038	0.52	2/1406 (0.1%)
21	W	0.16	0/1198	0.32	0/1617
22	Y	0.17	0/623	0.43	0/853
23	Z	0.13	0/695	0.31	0/939
24	a	0.15	0/1199	0.33	0/1623
25	b	0.15	0/902	0.37	0/1227
26	c	0.16	0/1368	0.50	2/1871 (0.1%)
27	d	0.16	0/1478	0.44	0/1996
28	e	0.14	0/916	0.35	0/1246
29	f	0.15	0/346	0.36	0/468
30	g	0.15	0/1031	0.28	0/1394
31	h	0.15	0/889	0.34	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	i	0.18	0/2773	0.35	0/3768
33	j	0.19	0/811	0.40	0/1106
34	k	0.19	0/759	0.38	0/1029
35	l	0.19	0/4892	0.43	2/6657 (0.0%)
36	m	0.19	0/970	0.41	0/1316
37	n	0.21	0/472	0.49	0/641
38	o	0.16	0/1092	0.38	0/1481
39	p	0.16	0/1590	0.35	0/2155
40	r	0.18	0/3723	0.35	0/5078
41	s	0.21	0/2457	0.40	0/3360
42	u	0.15	0/1436	0.35	0/1938
43	v	0.15	0/1046	0.41	0/1404
44	w	0.15	0/2620	0.42	2/3551 (0.1%)
All	All	0.17	0/66575	0.38	16/90287 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	c	75	TYR	CA-C-N	9.31	129.25	119.85
26	c	75	TYR	C-N-CA	9.31	129.25	119.85
16	Q	240	LEU	N-CA-C	8.63	120.69	111.28
20	V	86	ASP	CA-C-N	6.85	126.65	119.05
20	V	86	ASP	C-N-CA	6.85	126.65	119.05
44	w	281	GLY	CA-C-N	6.58	128.85	120.89
44	w	281	GLY	C-N-CA	6.58	128.85	120.89
35	l	251	THR	N-CA-C	6.50	120.83	112.12
3	C	124	MET	CA-C-N	6.12	126.03	119.85
3	C	124	MET	C-N-CA	6.12	126.03	119.85
13	N	142	THR	CA-C-N	6.00	125.91	119.85
13	N	142	THR	C-N-CA	6.00	125.91	119.85
35	l	439	PRO	CA-N-CD	-5.86	103.80	112.00
16	Q	142	VAL	N-CA-C	-5.30	107.66	112.96
16	Q	224	ALA	N-CA-C	5.10	117.96	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Q	236	LEU	N-CA-C	5.06	115.42	109.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	126	GLU	Peptide

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	3314	0	3269	76	0
2	B	1412	0	1363	28	0
3	C	1244	0	1250	17	0
4	E	968	0	973	26	0
5	F	683	0	691	15	0
6	G	690	0	669	24	0
6	X	693	0	678	25	0
7	H	910	0	950	16	0
8	I	780	0	808	11	0
9	J	2339	0	2364	48	0
10	K	344	0	313	8	0
11	L	1002	0	992	14	0
12	M	5296	0	5326	76	0
13	N	1193	0	1144	18	0
14	O	1671	0	1673	31	0
15	P	1738	0	1693	26	0
16	Q	3366	0	3301	77	0
17	S	563	0	561	17	0
18	T	741	0	702	8	0
19	U	643	0	642	11	0
20	V	1017	0	1015	23	0
21	W	1167	0	1155	18	0
22	Y	597	0	537	44	0
23	Z	674	0	643	28	0
24	a	1165	0	1174	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	b	875	0	895	29	0
26	c	1312	0	1206	31	0
27	d	1445	0	1403	36	0
28	e	890	0	837	17	0
29	f	338	0	335	4	0
30	g	1000	0	994	15	0
31	h	867	0	871	20	0
32	i	2710	0	2874	75	0
33	j	793	0	848	29	0
34	k	748	0	799	24	0
35	l	4764	0	4893	135	0
36	m	948	0	960	32	0
37	n	460	0	451	6	0
38	o	1062	0	1072	18	0
39	p	1534	0	1470	34	0
40	r	3631	0	3839	79	0
41	s	2387	0	2495	76	0
42	u	1398	0	1378	24	0
43	v	1022	0	969	32	0
44	w	2562	0	2504	42	0
45	A	8	0	0	2	0
45	B	16	0	0	0	0
45	C	8	0	0	1	0
45	M	16	0	0	0	0
46	A	31	0	19	4	0
47	A	44	0	27	5	0
48	C	52	0	88	2	0
48	a	52	0	88	14	0
48	g	52	0	88	8	0
48	j	52	0	88	2	0
48	r	52	0	88	3	0
49	G	35	0	0	1	0
49	X	35	0	0	8	0
50	I	51	0	46	0	0
50	a	91	0	132	4	0
50	g	100	0	156	8	0
50	i	66	0	76	5	0
51	J	48	0	24	5	0
52	M	4	0	0	1	0
52	O	4	0	0	0	0
53	M	1	0	0	0	0
54	Q	51	0	82	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	U	51	0	82	2	0
54	b	46	0	69	2	0
54	i	47	0	71	4	0
54	j	47	0	71	0	0
54	l	46	0	69	0	0
54	m	41	0	59	1	0
54	r	51	0	82	5	0
55	T	1	0	0	0	0
56	s	28	0	31	5	0
57	w	27	0	11	3	0
All	All	66210	0	66526	1242	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 9.

All (1242) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:112:SER:CB	49:X:201:8Q1:O1	1.67	1.40
16:Q:188:THR:CG2	16:Q:200:PHE:HA	1.49	1.39
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.20
51:J:401:NDP:O4D	51:J:401:NDP:C4D	1.68	1.19
16:Q:188:THR:CG2	16:Q:200:PHE:CA	2.29	1.10
16:Q:188:THR:HG21	16:Q:200:PHE:CA	1.84	1.05
20:V:66:ILE:HD11	20:V:101:LEU:HD13	1.06	1.03
25:b:110:ILE:HG21	27:d:16:ARG:CB	1.90	1.01
41:s:184:MET:HE1	41:s:296:LEU:HB3	1.44	1.00
20:V:90:TYR:CE1	20:V:126:LYS:CE	2.49	0.96
48:a:202:PLX:H282	48:a:202:PLX:H322	1.46	0.95
20:V:90:TYR:CE1	20:V:126:LYS:HE2	2.00	0.94
17:S:31:ASN:HD22	17:S:36:LYS:HA	1.36	0.90
6:X:112:SER:CB	49:X:201:8Q1:P24	2.59	0.90
12:M:544:VAL:HG23	12:M:565:PHE:HB3	1.55	0.88
16:Q:188:THR:HG21	16:Q:200:PHE:HA	0.89	0.86
25:b:109:THR:O	27:d:18:PRO:HA	1.77	0.84
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.62	0.82
9:J:71:ASN:HB2	9:J:97:MET:HE2	1.61	0.82
3:C:125:PRO:HG2	41:s:58:LYS:HE3	1.61	0.81
37:n:28:ASP:OD1	40:r:2:LEU:HB2	1.80	0.79
41:s:148:ILE:CG2	41:s:297:THR:HG22	2.12	0.79
17:S:31:ASN:ND2	17:S:36:LYS:HA	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:44:TYR:CE2	23:Z:16:LEU:HG	2.19	0.78
22:Y:44:TYR:CE2	23:Z:16:LEU:CG	2.67	0.78
20:V:90:TYR:CD1	20:V:126:LYS:HE2	2.19	0.77
9:J:38:HIS:HB3	13:N:136:GLU:OE2	1.82	0.77
41:s:148:ILE:HG21	41:s:297:THR:HG22	1.67	0.77
22:Y:45:ARG:HD3	23:Z:51:TRP:CD1	2.20	0.76
42:u:80:GLU:HG3	42:u:81:PRO:HD3	1.68	0.76
31:h:97:HIS:HA	31:h:102:GLU:HB3	1.68	0.75
35:l:383:MET:HE3	35:l:384:PRO:HD2	1.66	0.75
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.67	0.75
1:A:95:THR:HG21	1:A:247:THR:HG21	1.69	0.75
48:a:202:PLX:O4	48:a:202:PLX:O7	2.05	0.74
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.21	0.74
16:Q:188:THR:HG23	16:Q:200:PHE:HA	1.65	0.74
16:Q:235:ASP:HB2	16:Q:356:ILE:HD13	1.68	0.73
40:r:22:MET:O	40:r:26:ASN:ND2	2.22	0.73
27:d:13:PRO:HG3	27:d:116:ARG:HD3	1.69	0.73
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.70	0.72
16:Q:188:THR:HG23	16:Q:200:PHE:CA	2.18	0.72
48:a:202:PLX:H1A2	48:a:202:PLX:O3	1.90	0.71
35:l:190:LEU:HD23	40:r:383:THR:HG21	1.72	0.71
1:A:185:ASN:OD1	1:A:190:GLY:N	2.20	0.71
48:a:202:PLX:H282	48:a:202:PLX:C32	2.19	0.71
2:B:171:PRO:HG3	2:B:200:GLU:HG2	1.71	0.71
20:V:66:ILE:CD1	20:V:101:LEU:HD13	2.03	0.71
35:l:161:ARG:NH1	35:l:238:GLU:OE2	2.22	0.71
1:A:41:ILE:O	1:A:137:LYS:NZ	2.24	0.71
25:b:110:ILE:CG2	27:d:16:ARG:CB	2.67	0.70
24:a:169:TYR:HH	30:g:2:THR:N	1.89	0.70
22:Y:44:TYR:CE2	23:Z:16:LEU:HD21	2.26	0.70
33:j:69:ILE:HD11	41:s:148:ILE:HG12	1.73	0.70
41:s:184:MET:HE1	41:s:296:LEU:CB	2.19	0.70
26:c:83:GLN:OE1	26:c:86:ARG:NH1	2.25	0.70
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.71	0.70
40:r:220:HIS:HE1	40:r:232:ALA:HB2	1.57	0.70
35:l:341:MET:HE2	35:l:457:LEU:HD12	1.73	0.69
35:l:391:SER:O	35:l:395:ILE:HG12	1.92	0.69
25:b:109:THR:HG22	25:b:116:VAL:HG12	1.73	0.69
22:Y:45:ARG:HD3	23:Z:51:TRP:CG	2.27	0.69
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.28	0.69
26:c:140:MET:HG2	35:l:283:ILE:HD13	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:44:TYR:CE2	23:Z:16:LEU:HD11	2.27	0.69
41:s:148:ILE:CG2	41:s:297:THR:CG2	2.70	0.69
17:S:57:VAL:HG23	17:S:59:ARG:HG3	1.75	0.68
20:V:90:TYR:CE1	20:V:126:LYS:HE3	2.28	0.68
26:c:155:PRO:HG3	43:v:4:HIS:CE1	2.28	0.68
9:J:166:HIS:HB3	9:J:200:ILE:HD13	1.76	0.68
33:j:90:MET:HE1	48:j:202:PLX:H281	1.76	0.68
15:P:154:GLU:OE2	15:P:180:ASN:ND2	2.25	0.68
25:b:32:GLU:HG3	39:p:115:TYR:HA	1.76	0.68
39:p:10:LEU:HD21	39:p:18:ARG:HH21	1.59	0.68
2:B:68:ARG:NH2	21:W:26:PRO:O	2.27	0.67
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.27	0.67
1:A:50:ASP:O	1:A:59:ARG:NH2	2.26	0.67
32:i:295:ARG:NH2	54:i:402:PEE:O2P	2.27	0.67
41:s:148:ILE:HG22	41:s:297:THR:CG2	2.25	0.67
27:d:71:VAL:O	27:d:91:GLN:NE2	2.26	0.67
9:J:83:PRO:HG3	9:J:119:VAL:HG11	1.77	0.67
22:Y:44:TYR:CD2	23:Z:16:LEU:HG	2.29	0.67
50:g:202:CDL:H612	50:g:202:CDL:H662	1.76	0.67
22:Y:43:ARG:HB3	22:Y:46:GLN:HB2	1.77	0.67
2:B:131:GLU:HG3	2:B:144:ARG:HD2	1.77	0.66
6:G:85:TYR:HA	6:G:88:LYS:HZ2	1.60	0.66
19:U:74:GLN:N	19:U:74:GLN:OE1	2.27	0.66
11:L:109:ASN:ND2	11:L:111:LEU:O	2.27	0.66
22:Y:44:TYR:CD2	23:Z:16:LEU:CD1	2.79	0.66
44:w:283:TRP:N	44:w:284:PRO:HD2	2.11	0.66
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.36	0.66
40:r:420:THR:HB	40:r:423:ILE:HD12	1.78	0.66
20:V:126:LYS:NZ	20:V:129:GLN:OE1	2.28	0.66
7:H:78:GLU:HA	7:H:81:ILE:HD12	1.78	0.66
35:l:7:LEU:HD22	35:l:46:LEU:HD11	1.78	0.66
9:J:207:PHE:CE1	9:J:240:VAL:C	2.74	0.66
16:Q:184:ILE:HD11	16:Q:251:PHE:HZ	1.60	0.66
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.78	0.66
22:Y:47:PHE:HE2	22:Y:50:LEU:HD11	1.59	0.65
27:d:24:THR:HG23	27:d:26:LEU:H	1.61	0.65
43:v:37:ARG:HH12	43:v:97:LYS:HD3	1.62	0.65
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.79	0.65
21:W:94:GLU:OE2	21:W:104:TRP:NE1	2.26	0.65
9:J:171:ASN:HD21	9:J:326:ASP:HA	1.62	0.65
1:A:143:LEU:HB2	1:A:182:ILE:HD11	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:50:LEU:HD12	22:Y:50:LEU:N	2.12	0.65
12:M:171:THR:HG23	12:M:173:MET:HE2	1.77	0.65
12:M:283:GLU:OE2	12:M:420:LYS:NZ	2.28	0.65
36:m:55:MET:HA	36:m:55:MET:HE2	1.79	0.65
1:A:398:ARG:NH1	12:M:155:GLU:OE1	2.30	0.64
9:J:176:SER:O	9:J:182:ARG:NH1	2.30	0.64
32:i:110:PRO:HG2	35:l:594:THR:HG21	1.78	0.64
5:F:42:VAL:HG23	12:M:671:LEU:HG	1.78	0.64
6:G:85:TYR:HA	6:G:88:LYS:NZ	2.11	0.64
35:l:343:SER:O	35:l:347:ILE:HG13	1.96	0.64
7:H:69:GLU:HG2	7:H:77:ILE:HG12	1.78	0.64
22:Y:41:GLU:OE2	22:Y:41:GLU:N	2.30	0.64
35:l:227:PHE:O	35:l:230:HIS:ND1	2.30	0.64
16:Q:142:VAL:HG11	16:Q:185:MET:HG2	1.80	0.64
34:k:5:TYR:O	34:k:9:ILE:HG13	1.97	0.64
24:a:154:LEU:HD21	32:i:272:LYS:HD3	1.80	0.64
35:l:518:GLN:OE1	35:l:518:GLN:HA	1.97	0.64
35:l:593:ILE:HA	35:l:596:MET:HE3	1.78	0.64
34:k:23:ARG:HG2	36:m:23:LYS:HE2	1.80	0.64
1:A:185:ASN:ND2	1:A:187:CYS:O	2.31	0.64
16:Q:294:ARG:NH1	16:Q:336:GLU:OE2	2.31	0.64
6:X:105:MET:HE3	6:X:139:MET:HE1	1.80	0.64
41:s:102:VAL:HG11	41:s:154:LEU:HD11	1.80	0.64
6:G:74:LEU:HD12	6:G:79:ILE:HD11	1.80	0.63
11:L:88:GLN:NE2	12:M:141:ASP:OD2	2.31	0.63
27:d:119:GLU:N	27:d:119:GLU:OE2	2.30	0.63
35:l:100:ILE:HG13	35:l:246:LEU:HB2	1.79	0.63
19:U:45:ILE:HD11	19:U:81:LEU:HD13	1.81	0.63
15:P:68:ILE:HG22	15:P:69:LEU:HG	1.80	0.63
14:O:182:ASN:ND2	14:O:194:GLU:OE1	2.32	0.63
26:c:184:TYR:HA	43:v:34:ARG:HH12	1.64	0.63
43:v:22:MET:HE1	43:v:102:PHE:HA	1.81	0.63
44:w:47:GLU:OE2	44:w:295:ARG:NH1	2.26	0.63
2:B:76:TYR:HE1	41:s:33:LEU:HB2	1.64	0.63
20:V:69:ILE:HD12	20:V:72:LEU:HD21	1.81	0.63
3:C:59:ARG:NH1	48:C:302:PLX:O3	2.27	0.63
16:Q:188:THR:CG2	16:Q:200:PHE:CB	2.77	0.63
25:b:115:GLU:OE1	25:b:115:GLU:N	2.31	0.63
37:n:5:LEU:O	37:n:9:ARG:NH2	2.32	0.63
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.33	0.62
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:84:GLU:N	39:p:84:GLU:OE1	2.32	0.62
16:Q:236:LEU:HB3	16:Q:240:LEU:HD23	1.82	0.62
27:d:29:PRO:HG2	35:l:52:LEU:HD21	1.81	0.62
33:j:73:LEU:HD12	36:m:55:MET:HE1	1.82	0.62
24:a:76:LEU:O	24:a:80:ILE:HG13	2.00	0.62
10:K:105:ARG:NH1	11:L:167:ASN:O	2.33	0.62
21:W:10:MET:HE3	21:W:11:PRO:HD2	1.80	0.61
9:J:127:ILE:HD11	9:J:253:ILE:HD11	1.81	0.61
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.82	0.61
16:Q:68:ASP:O	32:i:49:ASN:ND2	2.33	0.61
22:Y:44:TYR:CD2	23:Z:16:LEU:HD11	2.35	0.61
33:j:25:PRO:HB2	41:s:60:PRO:HD3	1.82	0.61
12:M:624:ARG:NH2	12:M:637:ASP:OD1	2.29	0.61
22:Y:44:TYR:CE2	23:Z:16:LEU:CD2	2.83	0.61
32:i:159:MET:HE3	32:i:163:LEU:HD21	1.83	0.61
35:l:241:THR:HG21	35:l:344:GLY:HA3	1.82	0.61
16:Q:259:GLU:OE1	16:Q:338:ARG:NH2	2.32	0.61
9:J:182:ARG:O	9:J:186:VAL:HG23	2.01	0.61
40:r:61:LEU:HD23	40:r:245:ARG:HH21	1.64	0.61
7:H:38:ILE:O	7:H:45:ARG:NH1	2.30	0.61
9:J:218:ALA:O	9:J:221:ARG:NH1	2.34	0.61
31:h:59:GLU:N	31:h:59:GLU:OE1	2.34	0.60
33:j:92:LEU:O	33:j:96:ILE:HG12	2.01	0.60
21:W:63:GLU:OE2	42:u:119:ARG:NH2	2.34	0.60
6:G:115:GLN:HE22	6:G:119:ILE:HD11	1.66	0.60
34:k:98:CYS:HB2	35:l:580:GLN:HB2	1.83	0.60
35:l:526:LEU:HD12	35:l:530:PRO:HG2	1.83	0.60
39:p:133:TRP:O	39:p:137:VAL:HG23	2.02	0.60
41:s:269:THR:O	41:s:273:ILE:HG12	2.00	0.60
43:v:44:GLN:NE2	43:v:48:ASP:OD2	2.34	0.60
6:X:112:SER:CA	49:X:201:8Q1:O1	2.48	0.60
22:Y:44:TYR:CE2	23:Z:16:LEU:CD1	2.84	0.60
35:l:154:LEU:HD12	35:l:247:LEU:HD21	1.83	0.60
4:E:27:GLU:HA	4:E:30:ARG:HG2	1.83	0.60
40:r:370:PRO:HB3	40:r:375:LEU:HD22	1.83	0.60
34:k:11:ALA:HB1	36:m:17:PHE:CD2	2.36	0.60
2:B:177:THR:HG21	2:B:182:GLU:HB2	1.84	0.60
20:V:81:ARG:NH2	20:V:86:ASP:OD2	2.35	0.60
33:j:15:SER:HA	41:s:76:ILE:HD12	1.83	0.60
7:H:79:GLU:O	7:H:83:GLN:HG3	2.01	0.59
16:Q:227:ILE:O	16:Q:227:ILE:HG22	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:408:ALA:O	35:l:412:THR:HG23	2.02	0.59
25:b:111:LEU:HD11	27:d:19:ALA:HA	1.84	0.59
2:B:100:GLU:O	2:B:170:GLY:N	2.34	0.59
21:W:133:ILE:HD11	36:m:125:TRP:CZ3	2.37	0.59
40:r:433:GLU:O	40:r:437:MET:HG2	2.02	0.59
1:A:295:PRO:HB2	1:A:298:GLU:HG2	1.83	0.59
43:v:95:TYR:O	43:v:99:MET:HG3	2.02	0.59
28:e:56:GLN:NE2	44:w:315:PRO:O	2.36	0.59
28:e:58:ASP:OD2	44:w:326:ARG:NE	2.34	0.59
39:p:29:SER:HB3	39:p:76:HIS:HD2	1.67	0.59
12:M:395:GLU:O	12:M:425:ASN:ND2	2.36	0.59
41:s:105:MET:HE3	41:s:162:LEU:HD11	1.84	0.59
43:v:8:ARG:NH2	43:v:9:TYR:OH	2.35	0.59
9:J:109:ASN:ND2	9:J:112:ASP:OD2	2.35	0.59
12:M:382:ARG:NH1	12:M:527:ASP:OD2	2.35	0.59
16:Q:232:VAL:CG2	16:Q:356:ILE:HB	2.33	0.59
8:I:70:MET:HE1	15:P:73:VAL:HG12	1.85	0.58
16:Q:188:THR:HG22	16:Q:200:PHE:HB2	1.85	0.58
6:X:78:ALA:O	6:X:82:ARG:HG2	2.03	0.58
1:A:152:ARG:NH2	10:K:99:PRO:O	2.36	0.58
36:m:35:VAL:O	36:m:39:VAL:HG23	2.03	0.58
12:M:299:ARG:HG2	12:M:300:GLN:HG2	1.84	0.58
12:M:388:ASN:HB3	12:M:511:LYS:HE2	1.85	0.58
29:f:68:GLU:HG3	30:g:21:ARG:NH2	2.19	0.58
19:U:21:ALA:O	19:U:25:ILE:HG13	2.03	0.58
4:E:15:THR:OG1	11:L:55:VAL:O	2.20	0.58
9:J:203:PRO:HG2	51:J:401:NDP:C6N	2.33	0.58
9:J:211:ASP:O	9:J:215:ASN:ND2	2.37	0.58
9:J:172:ALA:HA	9:J:181:LEU:HB3	1.84	0.58
49:X:201:8Q1:C12	39:p:44:MET:HE1	2.34	0.58
26:c:119:THR:HG22	38:o:11:LEU:HA	1.85	0.58
48:g:201:PLX:H301	32:i:347:ASN:HB3	1.86	0.58
1:A:62:TRP:HE1	1:A:136:HIS:HB3	1.69	0.58
12:M:193:ASP:OD1	14:O:111:ARG:NH2	2.32	0.58
17:S:34:LYS:HZ1	17:S:61:HIS:HB2	1.69	0.58
44:w:118:TYR:OH	57:w:401:ADP:O2'	2.21	0.58
44:w:230:THR:HG22	44:w:232:ALA:H	1.66	0.58
17:S:66:LEU:O	17:S:69:ILE:HG22	2.02	0.58
54:i:402:PEE:H27	35:l:563:PRO:HA	1.85	0.58
1:A:380:GLY:O	1:A:386:ARG:NH1	2.37	0.58
4:E:37:ARG:HG2	6:G:120:MET:SD	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:41:ARG:NH2	6:G:123:GLU:OE1	2.37	0.58
54:r:501:PEE:H71	54:r:501:PEE:H32	1.85	0.58
8:I:6:ARG:O	8:I:10:LEU:HD12	2.03	0.58
25:b:104:ILE:HB	43:v:48:ASP:HB3	1.85	0.58
32:i:133:TRP:HE3	50:i:401:CDL:H391	1.67	0.58
35:l:221:ALA:HA	35:l:226:GLN:HG2	1.85	0.58
43:v:92:HIS:O	43:v:96:VAL:HG13	2.04	0.58
13:N:142:THR:OG1	13:N:143:PRO:HD2	2.04	0.57
6:X:82:ARG:HD2	22:Y:44:TYR:HE2	1.67	0.57
35:l:516:PRO:HG3	39:p:30:TRP:HZ2	1.69	0.57
39:p:19:LEU:HD13	39:p:64:LEU:HD12	1.86	0.57
10:K:100:GLN:HB3	14:O:71:PRO:HA	1.86	0.57
4:E:80:ASP:O	4:E:84:ILE:HG13	2.05	0.57
7:H:35:LEU:HD13	7:H:49:GLU:HG3	1.85	0.57
31:h:86:LEU:HD11	31:h:91:LYS:HB3	1.85	0.57
43:v:46:MET:HE3	43:v:56:ARG:HB3	1.87	0.57
44:w:190:VAL:O	44:w:194:THR:HG23	2.04	0.57
24:a:96:ALA:HB2	27:d:61:TYR:CE1	2.39	0.57
40:r:248:THR:HG23	40:r:249:ILE:HG23	1.86	0.57
54:m:201:PEE:H52	41:s:104:PHE:HE1	1.69	0.57
15:P:64:TYR:CE1	15:P:68:ILE:HD11	2.40	0.57
20:V:72:LEU:O	20:V:76:ILE:HG12	2.04	0.57
35:l:419:THR:HA	35:l:422:TYR:CE2	2.40	0.57
9:J:192:ARG:NH1	9:J:198:ALA:O	2.38	0.57
16:Q:133:LEU:CD2	16:Q:228:ARG:HD3	2.34	0.57
1:A:413:TRP:O	1:A:416:SER:OG	2.20	0.57
24:a:87:THR:O	24:a:91:VAL:HG23	2.05	0.57
26:c:96:ASP:N	26:c:96:ASP:OD1	2.34	0.57
44:w:229:ILE:HD11	44:w:233:TYR:HD2	1.70	0.57
7:H:30:LYS:O	7:H:34:VAL:HG23	2.05	0.56
35:l:102:GLU:OE1	35:l:456:ARG:NH2	2.31	0.56
12:M:466:LEU:HB3	12:M:500:ILE:HD11	1.86	0.56
14:O:156:LEU:HB3	14:O:158:ILE:HG12	1.85	0.56
35:l:183:VAL:HG21	40:r:400:MET:HE1	1.86	0.56
5:F:23:LEU:HD12	5:F:34:ARG:HG2	1.87	0.56
16:Q:311:TYR:O	16:Q:314:VAL:HG22	2.06	0.56
28:e:85:TRP:O	28:e:89:VAL:HG13	2.05	0.56
9:J:275:ASP:OD1	9:J:275:ASP:N	2.38	0.56
19:U:38:TYR:HB2	41:s:310:MET:O	2.04	0.56
2:B:111:GLU:O	2:B:141:ARG:NH1	2.38	0.56
12:M:358:LEU:HB3	12:M:363:SER:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:99:GLU:HG3	35:l:61:MET:HG2	1.87	0.56
1:A:130:ILE:HD11	1:A:245:VAL:HG12	1.87	0.56
4:E:96:VAL:HG12	4:E:96:VAL:O	2.06	0.56
16:Q:101:LEU:HD21	16:Q:444:LEU:HD13	1.88	0.56
30:g:117:GLU:HG3	30:g:119:HIS:CE1	2.40	0.56
35:l:250:SER:CB	35:l:333:ALA:HA	2.34	0.56
43:v:51:LEU:O	43:v:52:MET:HG2	2.06	0.56
44:w:123:SER:OG	44:w:125:ASP:OD1	2.23	0.56
54:r:501:PEE:H79	54:r:501:PEE:H41	1.88	0.56
3:C:113:MET:HE3	3:C:116:ALA:HB3	1.88	0.56
9:J:203:PRO:HG2	51:J:401:NDP:H6N	1.86	0.56
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.35	0.56
22:Y:45:ARG:HH11	23:Z:51:TRP:CD1	2.24	0.56
40:r:231:LEU:HA	40:r:235:LEU:HB2	1.87	0.56
41:s:148:ILE:HG21	41:s:297:THR:CG2	2.34	0.56
1:A:282:VAL:HG13	1:A:356:VAL:HG21	1.88	0.56
7:H:44:TYR:O	7:H:48:THR:HG23	2.05	0.56
12:M:445:LEU:HD22	12:M:460:HIS:HE1	1.71	0.56
42:u:106:LYS:O	42:u:109:GLU:HG3	2.05	0.56
1:A:274:LYS:HD2	1:A:275:LEU:H	1.71	0.56
4:E:37:ARG:O	4:E:41:ARG:HG2	2.05	0.56
36:m:129:ASP:OD1	36:m:129:ASP:N	2.39	0.56
39:p:26:HIS:ND1	39:p:75:GLN:O	2.37	0.56
4:E:22:SER:OG	4:E:31:ARG:NH1	2.39	0.55
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.39	0.55
44:w:59:VAL:HG13	44:w:201:PRO:HA	1.87	0.55
20:V:125:VAL:O	20:V:129:GLN:HG3	2.06	0.55
9:J:257:ASP:O	9:J:261:LYS:NZ	2.40	0.55
13:N:32:ASP:OD2	13:N:58:ARG:NH2	2.38	0.55
21:W:51:MET:HA	41:s:313:SER:HB2	1.87	0.55
26:c:55:TYR:CE2	26:c:76:PRO:HD3	2.41	0.55
50:g:202:CDL:H402	32:i:335:LEU:HD21	1.88	0.55
35:l:137:LEU:HD13	35:l:186:MET:HG2	1.89	0.55
50:g:202:CDL:H362	32:i:246:VAL:HG21	1.88	0.55
27:d:142:ARG:NE	28:e:138:GLU:O	2.39	0.55
27:d:10:TYR:CD1	27:d:10:TYR:N	2.75	0.55
27:d:73:ASP:OD1	27:d:75:THR:OG1	2.22	0.55
33:j:68:GLU:HG2	36:m:161:LEU:HD13	1.89	0.55
4:E:25:MET:O	4:E:29:LYS:HG3	2.07	0.55
5:F:33:VAL:O	5:F:36:PHE:HB3	2.06	0.55
9:J:173:ASP:OD1	9:J:173:ASP:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:104:GLU:OE2	41:s:134:ARG:NH1	2.40	0.55
41:s:148:ILE:HG22	41:s:297:THR:HG22	1.85	0.55
12:M:650:SER:OG	12:M:652:ASN:OD1	2.22	0.55
14:O:203:GLU:HG3	14:O:207:GLU:OE1	2.06	0.55
20:V:140:LYS:NZ	32:i:274:GLU:OE1	2.27	0.55
32:i:40:MET:HE1	32:i:129:LEU:HD23	1.89	0.55
44:w:189:GLU:O	44:w:193:VAL:HG22	2.07	0.55
14:O:61:LYS:O	14:O:64:GLU:HG3	2.07	0.55
16:Q:118:2MR:CD	16:Q:118:2MR:CQ2	2.85	0.55
30:g:12:PRO:HB3	31:h:5:ASP:HB3	1.89	0.55
40:r:447:LEU:HD21	48:r:502:PLX:H393	1.88	0.55
43:v:12:ASP:HB3	43:v:15:LYS:HB2	1.89	0.55
35:l:511:LEU:N	35:l:511:LEU:HD23	2.21	0.54
41:s:132:ALA:O	41:s:136:VAL:HG23	2.06	0.54
12:M:472:PRO:O	12:M:510:TRP:NE1	2.35	0.54
26:c:75:TYR:CG	26:c:76:PRO:HD2	2.42	0.54
37:n:50:ARG:HB2	37:n:53:GLU:HB2	1.88	0.54
38:o:57:LEU:HD23	38:o:57:LEU:O	2.07	0.54
3:C:67:PHE:HE2	3:C:113:MET:HE2	1.72	0.54
4:E:57:LYS:NZ	4:E:61:ASP:OD1	2.32	0.54
14:O:38:LEU:O	14:O:124:ARG:NH2	2.40	0.54
32:i:211:MET:HG2	32:i:333:SER:HB2	1.89	0.54
35:l:4:PHE:HD2	35:l:61:MET:HE2	1.73	0.54
3:C:66:THR:HG21	3:C:76:MET:HE2	1.88	0.54
17:S:12:MET:HE3	41:s:264:LEU:HD22	1.90	0.54
18:T:50:TYR:O	18:T:53:VAL:HG12	2.08	0.54
6:X:82:ARG:HD2	22:Y:44:TYR:CE2	2.42	0.54
44:w:67:CYS:N	57:w:401:ADP:O2A	2.37	0.54
11:L:78:ARG:HD2	12:M:607:LYS:HE3	1.89	0.54
17:S:53:ARG:HH12	31:h:106:PRO:HA	1.72	0.54
49:X:201:8Q1:N36	49:X:201:8Q1:O40	2.41	0.54
44:w:226:GLU:O	44:w:229:ILE:HG22	2.07	0.54
15:P:44:ARG:HB3	15:P:45:PRO:CD	2.37	0.54
35:l:296:ASN:HD22	35:l:357:ARG:CZ	2.19	0.54
43:v:34:ARG:HH21	43:v:36:GLU:HA	1.73	0.54
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.23	0.54
12:M:260:ASN:HD21	12:M:278:HIS:HD2	1.55	0.54
44:w:345:GLU:HG3	44:w:352:ILE:HG13	1.89	0.54
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.90	0.54
14:O:140:CYS:O	14:O:145:SER:OG	2.21	0.54
6:G:75:THR:OG1	6:G:156:GLU:OE1	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:144:MET:HG3	16:Q:383:LYS:HG3	1.89	0.54
13:N:10:GLY:O	13:N:14:VAL:HG23	2.06	0.54
37:n:13:VAL:HG22	40:r:14:MET:HG2	1.90	0.54
37:n:47:ARG:HH21	37:n:56:THR:HG23	1.72	0.54
2:B:177:THR:HG22	2:B:179:THR:H	1.72	0.54
3:C:71:CYS:HB3	16:Q:141:TYR:CG	2.43	0.54
6:X:132:ASP:HB3	39:p:18:ARG:NH1	2.22	0.54
11:L:84:ARG:NH1	11:L:88:GLN:O	2.41	0.53
13:N:2:GLU:OE1	13:N:2:GLU:N	2.41	0.53
16:Q:107:ARG:O	16:Q:440:LYS:NZ	2.36	0.53
24:a:91:VAL:HG13	27:d:52:ILE:HG12	1.88	0.53
33:j:64:LEU:HD13	36:m:165:VAL:HG22	1.89	0.53
1:A:210:THR:HB	1:A:224:ARG:HG2	1.90	0.53
22:Y:50:LEU:HD12	22:Y:50:LEU:H	1.71	0.53
22:Y:72:ARG:NH1	22:Y:76:ASP:OD2	2.40	0.53
40:r:104:LEU:O	40:r:108:MET:HG3	2.09	0.53
35:l:123:LEU:O	35:l:127:THR:HG23	2.09	0.53
35:l:366:MET:HG3	35:l:366:MET:O	2.09	0.53
41:s:13:ILE:O	41:s:17:VAL:HG13	2.08	0.53
41:s:138:GLN:HA	41:s:286:MET:HE1	1.90	0.53
7:H:22:GLU:O	7:H:26:ILE:HG13	2.07	0.53
7:H:76:GLN:O	7:H:79:GLU:HG2	2.09	0.53
20:V:62:THR:OG1	20:V:104:ARG:NH1	2.41	0.53
32:i:200:MET:HE1	32:i:343:LEU:HD13	1.91	0.53
32:i:265:MET:O	32:i:268:GLN:HG3	2.09	0.53
17:S:69:ILE:HD11	42:u:68:LEU:HD13	1.89	0.53
6:X:153:ASP:HB3	25:b:23:LEU:HD21	1.91	0.53
23:Z:53:TYR:CE1	35:l:434:LYS:HG3	2.44	0.53
27:d:159:GLN:HG2	27:d:163:MET:HE2	1.90	0.53
32:i:255:PRO:HG2	40:r:123:GLU:HB3	1.90	0.53
35:l:535:ARG:HB3	38:o:11:LEU:HD22	1.89	0.53
40:r:188:ASN:OD1	40:r:256:TYR:OH	2.22	0.53
5:F:42:VAL:HG21	12:M:670:GLU:HG3	1.90	0.53
12:M:348:ALA:HA	12:M:351:LEU:HD12	1.91	0.53
15:P:43:THR:HA	15:P:47:ILE:HD12	1.90	0.53
25:b:94:PRO:HG3	27:d:10:TYR:CE2	2.43	0.53
35:l:347:ILE:HD13	35:l:354:GLN:HG2	1.90	0.53
41:s:162:LEU:HD23	41:s:165:LEU:HD12	1.90	0.53
1:A:446:LEU:O	1:A:450:MET:HG3	2.09	0.53
2:B:47:SER:OG	2:B:49:ASP:OD1	2.27	0.53
14:O:58:GLU:O	14:O:62:ARG:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:104:THR:O	15:P:107:GLN:NE2	2.42	0.53
19:U:33:PRO:HD3	41:s:310:MET:HE3	1.91	0.53
27:d:99:ASP:HB3	28:e:137:MET:SD	2.49	0.53
41:s:76:ILE:O	41:s:80:SER:OG	2.25	0.53
12:M:166:GLY:HA2	12:M:213:MET:HE3	1.91	0.53
22:Y:69:ILE:HD13	35:l:383:MET:HE2	1.91	0.53
35:l:250:SER:HB3	35:l:333:ALA:HA	1.91	0.53
43:v:103:GLU:O	43:v:107:ARG:HG2	2.09	0.53
42:u:80:GLU:HG3	42:u:81:PRO:CD	2.39	0.52
1:A:159:ARG:NH2	14:O:176:CYS:O	2.41	0.52
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.44	0.52
9:J:212:ARG:O	9:J:216:TYR:HB3	2.09	0.52
13:N:122:GLN:HA	18:T:59:GLN:HG2	1.91	0.52
15:P:172:ASP:OD2	15:P:187:ILE:N	2.35	0.52
48:a:202:PLX:HO7	48:a:202:PLX:P1	2.30	0.52
26:c:184:TYR:HA	43:v:34:ARG:NH1	2.24	0.52
28:e:122:ALA:O	28:e:126:VAL:HG12	2.09	0.52
32:i:96:THR:O	32:i:100:MET:HG2	2.09	0.52
34:k:23:ARG:HD3	36:m:23:LYS:HB2	1.90	0.52
38:o:37:LEU:O	38:o:41:SER:OG	2.23	0.52
56:s:401:UQ:H152	56:s:401:UQ:H101	1.91	0.52
20:V:90:TYR:CZ	20:V:126:LYS:CE	2.93	0.52
21:W:89:GLU:O	21:W:93:GLU:HG2	2.10	0.52
22:Y:100:LEU:O	22:Y:102:ASP:N	2.40	0.52
30:g:2:THR:HG22	30:g:4:MET:HG3	1.91	0.52
34:k:11:ALA:HB1	36:m:17:PHE:HD2	1.72	0.52
40:r:72:LEU:HD11	40:r:233:ALA:HB3	1.89	0.52
41:s:100:LEU:HD23	41:s:103:LEU:HD12	1.91	0.52
41:s:185:TRP:NE1	41:s:238:THR:OG1	2.35	0.52
6:G:74:LEU:H	6:G:74:LEU:HD23	1.73	0.52
9:J:163:LYS:HG2	9:J:259:LYS:HZ3	1.73	0.52
11:L:92:ASN:HB3	15:P:238:PRO:HA	1.92	0.52
35:l:574:SER:O	35:l:578:SER:OG	2.24	0.52
17:S:23:THR:O	17:S:27:HIS:HD2	1.93	0.52
17:S:34:LYS:CD	42:u:90:ASP:OD2	2.58	0.52
35:l:71:LEU:HD22	40:r:310:MET:HE1	1.90	0.52
8:I:70:MET:HE3	15:P:76:VAL:HG23	1.91	0.52
23:Z:23:LYS:NZ	23:Z:25:GLU:HB2	2.24	0.52
1:A:410:ASP:OD1	1:A:443:ARG:NH2	2.40	0.52
35:l:395:ILE:O	35:l:399:VAL:HG13	2.10	0.52
9:J:168:SER:O	9:J:203:PRO:CD	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:86:VAL:HB	6:X:122:MET:HE1	1.92	0.52
27:d:13:PRO:CG	27:d:116:ARG:HD3	2.36	0.52
35:l:272:LEU:O	35:l:276:MET:HG3	2.09	0.52
1:A:177:TYR:CD1	10:K:96:PHE:HB3	2.45	0.52
35:l:5:ALA:HB2	35:l:61:MET:HE1	1.92	0.52
35:l:197:ASP:O	35:l:201:ILE:HG13	2.10	0.52
1:A:325:PRO:HG3	1:A:433:TRP:HB3	1.92	0.52
9:J:168:SER:O	9:J:202:LYS:HA	2.10	0.52
14:O:166:ASP:OD1	14:O:168:LEU:HB2	2.10	0.52
40:r:74:PRO:O	40:r:78:MET:HG3	2.09	0.52
42:u:83:THR:HA	42:u:86:TRP:CD1	2.45	0.52
1:A:234:GLY:HA3	1:A:240:THR:HB	1.92	0.51
13:N:85:GLU:HB2	13:N:98:PRO:HB3	1.92	0.51
35:l:559:GLU:O	35:l:563:PRO:HD2	2.10	0.51
38:o:42:ARG:HG3	38:o:43:LEU:N	2.25	0.51
40:r:112:ALA:HB1	40:r:118:PHE:HB2	1.92	0.51
1:A:125:CYS:H	1:A:277:ASN:ND2	2.07	0.51
6:G:85:TYR:CE1	6:G:89:LEU:HD21	2.46	0.51
31:h:21:GLN:HA	34:k:53:PHE:CE1	2.45	0.51
3:C:82:PRO:HA	41:s:34:ARG:HB3	1.92	0.51
16:Q:220:ALA:HB3	16:Q:224:ALA:HA	1.91	0.51
18:T:65:ASN:HB3	18:T:70:LEU:HD11	1.93	0.51
22:Y:54:GLN:OE1	35:l:446:ASN:ND2	2.41	0.51
4:E:114:ARG:HD3	4:E:115:PRO:HD2	1.93	0.51
17:S:5:ILE:HG12	41:s:26:LYS:HG2	1.93	0.51
27:d:13:PRO:HG3	27:d:116:ARG:CD	2.40	0.51
32:i:84:TRP:HH2	34:k:59:MET:HE2	1.76	0.51
35:l:227:PHE:N	35:l:284:THR:OG1	2.43	0.51
39:p:137:VAL:O	39:p:141:GLN:HG2	2.11	0.51
40:r:306:PRO:O	40:r:310:MET:HG3	2.10	0.51
12:M:153:PHE:CZ	12:M:155:GLU:HB2	2.45	0.51
12:M:460:HIS:O	12:M:463:SER:OG	2.23	0.51
39:p:20:TYR:HB2	39:p:48:PHE:CZ	2.44	0.51
9:J:171:ASN:HD22	9:J:324:MET:HE1	1.75	0.51
16:Q:218:SER:OG	16:Q:224:ALA:HB1	2.10	0.51
17:S:67:GLU:OE2	17:S:67:GLU:N	2.38	0.51
26:c:133:LEU:HD22	35:l:532:ILE:HD11	1.93	0.51
34:k:57:ASN:HB3	36:m:143:ILE:HG13	1.92	0.51
6:G:119:ILE:HD13	6:G:135:ALA:HB1	1.93	0.51
9:J:171:ASN:HA	9:J:327:MET:HE2	1.93	0.51
32:i:295:ARG:HH12	54:i:402:PEE:H9	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:366:MET:O	35:l:370:THR:HG23	2.10	0.51
40:r:1:MET:HE1	40:r:41:LEU:HD21	1.91	0.51
1:A:88:ARG:HG3	1:A:274:LYS:NZ	2.25	0.51
35:l:251:THR:O	35:l:254:VAL:HG22	2.11	0.51
1:A:326:LEU:HD11	1:A:363:ILE:HD11	1.91	0.51
3:C:55:ASN:ND2	3:C:187:GLU:O	2.44	0.51
3:C:101:ASP:OD2	41:s:54:LYS:HD2	2.10	0.51
22:Y:44:TYR:CZ	23:Z:16:LEU:CD2	2.94	0.51
23:Z:45:TRP:HB2	39:p:38:ARG:HH21	1.76	0.51
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.91	0.51
35:l:286:LEU:HD22	35:l:411:MET:SD	2.51	0.51
35:l:319:ILE:HD13	35:l:399:VAL:HG12	1.92	0.51
40:r:150:LEU:HG	40:r:154:LEU:HD12	1.93	0.51
44:w:166:ASP:OD1	44:w:187:TYR:OH	2.23	0.51
8:I:69:VAL:HG23	15:P:76:VAL:HB	1.93	0.51
16:Q:116:LEU:O	16:Q:116:LEU:HG	2.10	0.51
16:Q:182:ASN:OD1	16:Q:404:LYS:NZ	2.43	0.51
20:V:123:ALA:O	20:V:127:MET:HG3	2.10	0.51
24:a:57:ILE:HG22	39:p:99:VAL:HG12	1.93	0.51
48:a:202:PLX:C32	48:a:202:PLX:C28	2.89	0.51
11:L:90:GLY:HA3	15:P:238:PRO:HB2	1.91	0.50
12:M:224:ASP:OD2	12:M:291:ARG:NH2	2.37	0.50
19:U:56:PRO:HG2	42:u:45:LEU:HB2	1.93	0.50
27:d:160:LYS:HE3	30:g:115:LEU:HA	1.93	0.50
32:i:26:TRP:CZ2	32:i:86:ILE:HG13	2.46	0.50
35:l:291:CYS:O	35:l:295:GLN:HG2	2.11	0.50
40:r:12:LEU:HB2	40:r:13:PRO:HD3	1.94	0.50
17:S:16:LEU:HB3	41:s:260:VAL:HG22	1.93	0.50
26:c:62:TYR:OH	26:c:74:ASP:O	2.25	0.50
27:d:127:LYS:O	27:d:131:GLN:HG3	2.11	0.50
32:i:190:MET:HG2	32:i:204:ASN:HB3	1.92	0.50
44:w:328:PHE:O	44:w:332:THR:HG23	2.11	0.50
9:J:162:GLU:HG2	9:J:163:LYS:HG3	1.93	0.50
32:i:11:MET:HE1	50:i:401:CDL:H771	1.92	0.50
34:k:38:LEU:O	34:k:42:ILE:HG12	2.11	0.50
36:m:125:TRP:CZ3	36:m:126:VAL:HG22	2.46	0.50
43:v:34:ARG:O	43:v:34:ARG:HG3	2.09	0.50
2:B:74:LEU:HB2	41:s:272:TRP:CZ2	2.46	0.50
12:M:492:ALA:O	12:M:496:ILE:HG13	2.11	0.50
12:M:658:ASP:OD1	12:M:660:GLU:HG3	2.12	0.50
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:69:SER:OG	6:X:70:ASP:N	2.45	0.50
38:o:105:PHE:CD2	40:r:263:MET:HE1	2.47	0.50
42:u:57:LEU:O	42:u:61:LYS:HG2	2.11	0.50
6:G:142:GLN:O	6:G:145:VAL:HG12	2.12	0.50
27:d:114:GLN:HG3	35:l:203:MET:HG2	1.93	0.50
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.93	0.50
48:g:201:PLX:H312	48:g:201:PLX:H211	1.92	0.50
32:i:71:MET:HG3	34:k:40:LEU:HD13	1.93	0.50
12:M:388:ASN:ND2	12:M:513:MET:O	2.38	0.50
16:Q:188:THR:HG23	16:Q:200:PHE:N	2.25	0.50
50:g:202:CDL:H791	50:g:202:CDL:H251	1.91	0.50
34:k:2:PRO:HD2	34:k:5:TYR:CD2	2.46	0.50
34:k:11:ALA:HB2	36:m:14:VAL:HG22	1.92	0.50
35:l:65:ASN:OD1	35:l:66:TRP:N	2.42	0.50
33:j:88:LEU:HD13	41:s:309:ILE:HD12	1.93	0.50
33:j:103:ALA:O	33:j:107:THR:HG23	2.11	0.50
36:m:17:PHE:CD1	36:m:20:PHE:HE2	2.29	0.50
41:s:294:LEU:HB3	41:s:295:PRO:HD3	1.94	0.50
42:u:16:GLN:CD	42:u:16:GLN:H	2.18	0.50
20:V:108:TYR:O	20:V:112:ALA:N	2.35	0.50
35:l:117:PHE:CZ	35:l:243:VAL:HG23	2.46	0.50
1:A:125:CYS:H	1:A:277:ASN:HD22	1.60	0.50
11:L:67:VAL:HG13	11:L:72:ILE:HD11	1.93	0.50
13:N:2:GLU:HG2	13:N:4:VAL:HG22	1.94	0.50
32:i:118:VAL:O	32:i:122:ILE:HG12	2.12	0.50
32:i:239:VAL:O	32:i:243:LEU:HG	2.12	0.50
39:p:100:PRO:HG3	40:r:419:TYR:CE1	2.47	0.50
40:r:220:HIS:CE1	40:r:232:ALA:HB2	2.42	0.50
22:Y:44:TYR:CZ	23:Z:16:LEU:HD21	2.47	0.49
22:Y:99:ILE:HD11	43:v:107:ARG:HG3	1.93	0.49
25:b:94:PRO:CG	27:d:10:TYR:CE2	2.95	0.49
33:j:79:SER:HA	33:j:87:MET:HE3	1.94	0.49
34:k:22:TYR:HB3	35:l:585:LYS:HG2	1.94	0.49
40:r:403:THR:HA	40:r:406:TYR:CE2	2.46	0.49
41:s:2:PHE:HZ	41:s:96:ILE:HD11	1.77	0.49
45:C:301:SF4:S4	16:Q:223:HIS:CD2	3.05	0.49
30:g:92:MET:O	30:g:96:VAL:HG13	2.12	0.49
6:G:149:ALA:O	6:G:153:ASP:N	2.44	0.49
16:Q:82:LEU:HD13	16:Q:84:PHE:CZ	2.47	0.49
28:e:108:TYR:CE1	48:r:502:PLX:H1B2	2.47	0.49
38:o:80:PHE:CZ	38:o:82:PRO:HD3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:21:THR:O	41:s:25:ARG:HG2	2.11	0.49
9:J:327:MET:HE3	9:J:329:LEU:HD11	1.94	0.49
13:N:120:THR:HG22	13:N:122:GLN:H	1.77	0.49
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.47	0.49
8:I:70:MET:HE2	15:P:66:ALA:HB1	1.93	0.49
30:g:36:MET:HE1	48:g:201:PLX:H382	1.95	0.49
31:h:32:ARG:HD3	34:k:52:HIS:HD2	1.77	0.49
32:i:187:MET:HA	32:i:190:MET:HE2	1.94	0.49
34:k:39:SER:OG	36:m:17:PHE:HE2	1.95	0.49
41:s:88:PRO:HG2	41:s:105:MET:HE2	1.94	0.49
9:J:272:LEU:HB2	9:J:275:ASP:OD1	2.12	0.49
32:i:334:THR:HG22	32:i:335:LEU:HG	1.95	0.49
35:l:384:PRO:HA	35:l:389:PHE:CG	2.47	0.49
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.94	0.49
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.95	0.49
16:Q:293:LEU:HD22	16:Q:298:ILE:HD12	1.95	0.49
22:Y:43:ARG:HH12	22:Y:49:GLN:HB2	1.76	0.49
25:b:123:PHE:HB3	43:v:40:VAL:HG21	1.94	0.49
40:r:189:SER:HB3	40:r:192:ASN:HD22	1.78	0.49
14:O:218:PRO:HG3	14:O:224:SER:H	1.77	0.49
41:s:225:MET:HE1	56:s:401:UQ:H161	1.95	0.49
8:I:40:LYS:HB3	21:W:7:LYS:H	1.78	0.49
16:Q:188:THR:HG22	16:Q:200:PHE:CB	2.42	0.49
19:U:32:LEU:HD23	41:s:310:MET:HE1	1.95	0.49
26:c:126:TRP:CH2	35:l:532:ILE:HG22	2.48	0.49
31:h:68:LEU:HD22	34:k:1:MET:N	2.28	0.49
32:i:128:LEU:HD12	32:i:216:PHE:HB3	1.94	0.49
32:i:347:ASN:N	32:i:347:ASN:OD1	2.45	0.49
35:l:37:LYS:HD3	35:l:98:TRP:HE1	1.78	0.49
12:M:250:SER:OG	12:M:251:ILE:N	2.46	0.49
12:M:370:GLU:OE2	12:M:518:ARG:NH2	2.46	0.49
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.78	0.49
21:W:114:THR:HG1	42:u:143:HIS:HD1	1.60	0.49
33:j:64:LEU:O	33:j:68:GLU:HG3	2.13	0.49
44:w:218:ILE:HD12	44:w:226:GLU:HG2	1.95	0.49
11:L:105:GLU:HA	12:M:611:THR:HG21	1.95	0.48
12:M:275:PRO:HB3	12:M:286:ILE:HG23	1.95	0.48
16:Q:232:VAL:HG23	16:Q:356:ILE:HB	1.94	0.48
6:X:123:GLU:OE2	6:X:130:ILE:N	2.44	0.48
24:a:160:MET:HE2	24:a:167:PRO:HD2	1.95	0.48
26:c:58:ARG:NE	38:o:35:GLU:OE2	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.48	0.48
35:l:142:ILE:HG12	40:r:370:PRO:HB2	1.94	0.48
35:l:356:ILE:HA	35:l:359:MET:HG2	1.94	0.48
22:Y:50:LEU:HD21	35:l:364:LYS:O	2.13	0.48
26:c:151:PRO:HD2	43:v:9:TYR:OH	2.13	0.48
32:i:68:MET:HG2	34:k:36:MET:HE3	1.96	0.48
21:W:38:VAL:O	21:W:42:THR:HG23	2.12	0.48
27:d:71:VAL:HG11	27:d:87:GLU:HB3	1.95	0.48
1:A:270:ASN:HD22	1:A:338:ASP:HB2	1.77	0.48
9:J:318:LYS:O	9:J:322:VAL:HG12	2.12	0.48
12:M:83:GLU:HG2	12:M:84:LYS:HG3	1.95	0.48
12:M:398:ASP:OD1	12:M:398:ASP:N	2.47	0.48
1:A:116:ASN:ND2	1:A:207:GLY:O	2.46	0.48
4:E:98:LYS:HB3	4:E:102:HIS:HB2	1.95	0.48
24:a:95:GLU:OE2	50:a:201:CDL:O1	2.31	0.48
28:e:57:GLU:OE1	44:w:320:GLY:HA3	2.14	0.48
29:f:63:LYS:O	29:f:67:LEU:HD23	2.13	0.48
2:B:150:THR:HG21	2:B:180:HIS:CD2	2.49	0.48
5:F:45:LYS:HB3	12:M:671:LEU:HD21	1.95	0.48
12:M:36:VAL:HB	12:M:56:VAL:HG21	1.95	0.48
12:M:308:ARG:NH1	12:M:312:GLY:O	2.43	0.48
24:a:180:ASP:OD2	31:h:28:LYS:NZ	2.44	0.48
35:l:163:ASP:HA	35:l:166:THR:HG22	1.95	0.48
35:l:363:TYR:HA	35:l:370:THR:HG21	1.95	0.48
40:r:373:ILE:HD11	40:r:444:LEU:HD23	1.95	0.48
1:A:195:VAL:O	10:K:97:ARG:NH1	2.45	0.48
3:C:69:LEU:HD23	16:Q:94:VAL:HG11	1.94	0.48
48:a:202:PLX:H1A2	48:a:202:PLX:P1	2.54	0.48
35:l:292:ALA:HB2	35:l:304:PHE:HB3	1.95	0.48
44:w:287:ASP:OD1	44:w:290:THR:HG23	2.14	0.48
12:M:304:GLN:HG2	12:M:615:LEU:HD12	1.95	0.48
12:M:313:LEU:CD2	13:N:141:SER:O	2.61	0.48
14:O:50:ASP:N	14:O:50:ASP:OD1	2.47	0.48
20:V:102:GLY:HA3	20:V:111:GLY:HA2	1.96	0.48
41:s:27:VAL:O	41:s:31:MET:HG2	2.12	0.48
43:v:37:ARG:HD3	43:v:58:TYR:CE2	2.49	0.48
43:v:103:GLU:OE1	43:v:106:ARG:NE	2.47	0.48
44:w:180:ARG:NH2	44:w:182:GLN:OE1	2.45	0.48
30:g:59:GLY:O	30:g:63:GLN:HG3	2.14	0.48
35:l:250:SER:HB2	35:l:333:ALA:HA	1.96	0.48
39:p:43:LEU:O	39:p:47:ARG:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LEU:HD21	1:A:287:THR:HG23	1.96	0.48
6:G:139:MET:HE3	6:G:139:MET:O	2.14	0.48
9:J:132:ARG:HD2	9:J:134:TRP:CE2	2.49	0.48
27:d:117:GLU:OE2	27:d:124:ASN:HB3	2.14	0.48
32:i:290:LEU:O	32:i:294:MET:HG2	2.14	0.48
36:m:51:PHE:CD2	36:m:143:ILE:HD13	2.48	0.48
41:s:104:PHE:O	41:s:108:MET:HG2	2.14	0.48
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.49	0.47
35:l:293:ILE:HG13	35:l:418:LEU:HD22	1.96	0.47
39:p:105:ASP:OD1	39:p:122:ARG:NH2	2.33	0.47
41:s:142:TYR:CE2	41:s:285:LEU:HD11	2.49	0.47
42:u:38:LYS:HB3	42:u:39:PRO:HD3	1.96	0.47
44:w:114:LEU:HD21	57:w:401:ADP:H1'	1.96	0.47
23:Z:45:TRP:HB2	39:p:38:ARG:NH2	2.30	0.47
35:l:237:MET:HE2	35:l:303:ALA:HB2	1.96	0.47
7:H:81:ILE:O	7:H:85:GLU:HG3	2.14	0.47
12:M:478:SER:O	12:M:482:GLN:HG2	2.13	0.47
39:p:108:HIS:CD2	39:p:109:PRO:HD2	2.49	0.47
40:r:61:LEU:HB2	40:r:457:PRO:HD3	1.96	0.47
40:r:204:MET:HG3	40:r:209:LEU:HB2	1.95	0.47
41:s:142:TYR:HE2	41:s:285:LEU:HD11	1.79	0.47
1:A:104:LYS:HD3	1:A:105:PRO:N	2.30	0.47
9:J:73:LEU:O	9:J:78:SER:OG	2.24	0.47
12:M:347:ASP:OD1	12:M:347:ASP:N	2.45	0.47
6:X:146:ASP:HB3	25:b:16:ARG:CZ	2.45	0.47
22:Y:44:TYR:CD2	23:Z:16:LEU:CG	2.93	0.47
35:l:298:ILE:O	35:l:302:VAL:HG23	2.15	0.47
5:F:17:ARG:HB2	5:F:68:ARG:HE	1.79	0.47
22:Y:55:LEU:HD23	35:l:367:PRO:HG3	1.96	0.47
27:d:159:GLN:O	27:d:163:MET:HG3	2.15	0.47
33:j:17:LEU:HA	33:j:20:ILE:HG12	1.97	0.47
33:j:75:LEU:HA	33:j:75:LEU:HD23	1.77	0.47
44:w:223:ASN:OD1	44:w:226:GLU:N	2.38	0.47
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.96	0.47
9:J:203:PRO:HG2	51:J:401:NDP:C5N	2.45	0.47
9:J:358:THR:O	41:s:65:THR:OG1	2.30	0.47
12:M:64:CYS:O	12:M:184:ARG:NH2	2.38	0.47
35:l:327:LEU:O	35:l:331:MET:HG2	2.13	0.47
6:G:118:ILE:HG23	6:G:122:MET:HE2	1.96	0.47
9:J:168:SER:O	9:J:203:PRO:HD2	2.14	0.47
22:Y:47:PHE:CE2	22:Y:50:LEU:HD11	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:51:ASP:HB3	56:s:401:UQ:H8	1.96	0.47
9:J:157:LYS:NZ	9:J:197:GLU:OE2	2.43	0.47
9:J:192:ARG:NH2	9:J:262:THR:OG1	2.48	0.47
48:a:202:PLX:H81	40:r:40:SER:CB	2.44	0.47
36:m:23:LYS:N	36:m:24:PRO:HD3	2.30	0.47
38:o:59:VAL:HG22	40:r:423:ILE:HG23	1.95	0.47
39:p:16:VAL:HG23	39:p:64:LEU:HD13	1.96	0.47
40:r:14:MET:HE2	40:r:30:HIS:ND1	2.30	0.47
40:r:22:MET:HE3	40:r:22:MET:HB3	1.80	0.47
40:r:115:LEU:HD12	40:r:174:LEU:HD22	1.96	0.47
41:s:84:THR:O	41:s:87:VAL:HG12	2.15	0.47
3:C:65:MET:HE2	3:C:65:MET:HB2	1.82	0.47
9:J:207:PHE:CD1	9:J:240:VAL:O	2.68	0.47
25:b:107:GLY:H	25:b:117:ILE:HB	1.80	0.47
30:g:77:LEU:HD11	48:g:201:PLX:H291	1.97	0.47
42:u:16:GLN:NE2	42:u:65:GLN:OE1	2.47	0.47
7:H:46:LYS:HG3	7:H:47:TYR:N	2.30	0.47
10:K:79:HIS:CE1	14:O:215:LYS:HB2	2.49	0.47
26:c:38:PRO:HB2	38:o:75:ASN:ND2	2.29	0.47
32:i:294:MET:HE1	40:r:130:LEU:HD21	1.97	0.47
40:r:73:LEU:HD22	40:r:103:GLN:OE1	2.15	0.47
6:G:85:TYR:O	6:G:89:LEU:HG	2.15	0.46
11:L:163:ASN:O	11:L:171:ARG:HA	2.15	0.46
50:g:202:CDL:H742	50:g:202:CDL:H271	1.97	0.46
35:l:243:VAL:HG13	35:l:247:LEU:HD22	1.97	0.46
35:l:400:ASN:ND2	35:l:489:THR:HG21	2.30	0.46
39:p:29:SER:HB3	39:p:76:HIS:CD2	2.48	0.46
15:P:173:MET:HB3	15:P:198:PHE:HB2	1.97	0.46
16:Q:188:THR:CG2	16:Q:200:PHE:HB2	2.42	0.46
21:W:84:LEU:HD22	42:u:8:PRO:HD2	1.97	0.46
43:v:37:ARG:NH1	43:v:97:LYS:HD3	2.27	0.46
1:A:284:HIS:CE1	14:O:228:ALA:HB3	2.50	0.46
4:E:62:LYS:HD2	4:E:66:MET:HE2	1.97	0.46
12:M:313:LEU:HD21	13:N:141:SER:O	2.16	0.46
21:W:85:GLN:HG3	42:u:10:LEU:HD21	1.98	0.46
22:Y:44:TYR:CZ	23:Z:16:LEU:HG	2.49	0.46
26:c:55:TYR:CD2	26:c:76:PRO:HD3	2.51	0.46
32:i:88:LYS:HD2	32:i:148:SER:OG	2.15	0.46
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.51	0.46
56:s:401:UQ:HM53	56:s:401:UQ:H72	1.74	0.46
35:l:36:VAL:HG13	35:l:122:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:516:PRO:HG3	39:p:30:TRP:CZ2	2.49	0.46
44:w:55:GLU:OE2	44:w:55:GLU:N	2.49	0.46
1:A:270:ASN:ND2	1:A:338:ASP:OD2	2.48	0.46
15:P:127:GLU:OE1	15:P:144:LYS:HD3	2.16	0.46
21:W:84:LEU:HD21	42:u:54:ARG:HG2	1.97	0.46
21:W:131:GLU:HG2	21:W:132:GLU:N	2.29	0.46
48:g:201:PLX:H351	32:i:339:MET:HB2	1.98	0.46
40:r:457:PRO:HG2	40:r:458:LEU:HD12	1.96	0.46
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.96	0.46
3:C:71:CYS:HB3	16:Q:141:TYR:CB	2.45	0.46
29:f:50:THR:O	29:f:54:LEU:HG	2.15	0.46
35:l:213:LEU:HB3	35:l:273:VAL:HG11	1.97	0.46
44:w:249:MET:HG3	44:w:253:CYS:HB2	1.98	0.46
1:A:29:LYS:HE3	1:A:32:PHE:HE1	1.81	0.46
4:E:80:ASP:OD1	4:E:81:LEU:N	2.49	0.46
6:X:76:LEU:HG	6:X:156:GLU:C	2.41	0.46
32:i:113:PHE:HD2	35:l:591:PHE:HE1	1.64	0.46
56:s:401:UQ:H101	56:s:401:UQ:H121	1.60	0.46
12:M:390:THR:HA	12:M:600:GLU:HG2	1.98	0.46
6:X:82:ARG:CD	22:Y:44:TYR:HE2	2.29	0.46
28:e:77:ASP:OD1	28:e:78:LYS:N	2.49	0.46
31:h:86:LEU:HG	31:h:92:TYR:HB3	1.98	0.46
32:i:27:LEU:HD22	34:k:59:MET:HG2	1.96	0.46
32:i:159:MET:O	32:i:163:LEU:HG	2.15	0.46
32:i:326:LEU:HB3	32:i:327:PRO:HD3	1.98	0.46
35:l:7:LEU:O	35:l:11:THR:HG23	2.15	0.46
44:w:110:GLY:HA2	44:w:134:TRP:CD2	2.51	0.46
2:B:80:GLU:HG3	17:S:1:MET:SD	2.56	0.46
16:Q:294:ARG:HG2	16:Q:320:ILE:HD13	1.98	0.46
6:X:90:TYR:HE1	23:Z:44:PRO:HB2	1.81	0.46
6:X:112:SER:CB	49:X:201:8Q1:O3	2.64	0.46
27:d:39:LEU:HD23	27:d:39:LEU:HA	1.84	0.46
31:h:54:LYS:HB3	31:h:54:LYS:HE3	1.56	0.46
12:M:389:THR:O	12:M:390:THR:OG1	2.28	0.46
48:g:201:PLX:H332	32:i:342:ALA:HB3	1.98	0.46
40:r:266:MET:HE3	40:r:396:MET:HE2	1.98	0.46
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.98	0.45
54:Q:501:PEE:H60	54:Q:501:PEE:H51	1.98	0.45
22:Y:51:THR:O	22:Y:54:GLN:HG2	2.16	0.45
26:c:110:ASP:OD1	26:c:110:ASP:N	2.49	0.45
32:i:339:MET:HE3	32:i:339:MET:HB3	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:484:LEU:HD23	35:l:484:LEU:HA	1.75	0.45
40:r:17:MET:HA	40:r:17:MET:HE2	1.97	0.45
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.98	0.45
15:P:125:ARG:HH22	15:P:201:ASP:CG	2.24	0.45
16:Q:194:ILE:O	41:s:279:ARG:HG2	2.16	0.45
18:T:66:PHE:O	18:T:70:LEU:HG	2.16	0.45
31:h:70:GLN:HE21	34:k:1:MET:H1	1.65	0.45
44:w:38:TYR:OH	44:w:292:HIS:ND1	2.33	0.45
2:B:133:GLU:OE1	13:N:131:ARG:NH2	2.50	0.45
3:C:167:PRO:HG3	16:Q:222:MET:SD	2.56	0.45
9:J:171:ASN:ND2	9:J:326:ASP:HA	2.29	0.45
12:M:370:GLU:HG3	12:M:519:ILE:HG12	1.99	0.45
26:c:113:ILE:HD11	26:c:116:ARG:HD2	1.98	0.45
32:i:58:LYS:HD3	32:i:117:GLU:OE1	2.16	0.45
33:j:84:LEU:HD23	33:j:84:LEU:HA	1.79	0.45
36:m:124:ASP:O	36:m:126:VAL:HG23	2.15	0.45
40:r:86:LYS:HB2	40:r:86:LYS:HE3	1.62	0.45
1:A:210:THR:O	1:A:214:GLU:HG2	2.16	0.45
9:J:203:PRO:CG	51:J:401:NDP:H6N	2.47	0.45
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.99	0.45
20:V:90:TYR:CZ	20:V:126:LYS:NZ	2.83	0.45
25:b:19:ARG:HA	39:p:171:VAL:HG13	1.97	0.45
36:m:25:SER:O	36:m:28:TYR:N	2.48	0.45
40:r:108:MET:HB2	40:r:121:LEU:HD13	1.97	0.45
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.99	0.45
1:A:41:ILE:HG23	1:A:253:THR:HG21	1.98	0.45
1:A:125:CYS:HB2	1:A:277:ASN:HD21	1.82	0.45
1:A:214:GLU:OE2	1:A:224:ARG:NE	2.40	0.45
12:M:336:ASN:OD1	12:M:540:ASN:ND2	2.50	0.45
15:P:161:LYS:HD3	15:P:161:LYS:HA	1.63	0.45
22:Y:76:ASP:O	35:l:385:TYR:OH	2.30	0.45
50:a:201:CDL:H472	27:d:43:ARG:HH21	1.82	0.45
31:h:70:GLN:HE21	34:k:1:MET:N	2.14	0.45
33:j:18:VAL:HG22	41:s:222:MET:HG3	1.98	0.45
39:p:10:LEU:HD23	39:p:10:LEU:HA	1.74	0.45
48:r:502:PLX:H121	48:r:502:PLX:H152	1.58	0.45
41:s:267:THR:O	41:s:271:LEU:HG	2.16	0.45
1:A:312:ASP:OD1	1:A:329:LYS:NZ	2.49	0.45
4:E:20:ILE:HB	4:E:80:ASP:OD2	2.16	0.45
27:d:119:GLU:H	27:d:119:GLU:CD	2.24	0.45
35:l:375:ILE:HD12	35:l:458:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:199:ASP:CG	41:s:279:ARG:HH21	2.25	0.45
5:F:35:ASP:HA	5:F:38:GLU:HG3	1.98	0.45
25:b:23:LEU:O	25:b:26:GLN:HB2	2.17	0.45
32:i:237:MET:O	32:i:240:ILE:HG22	2.16	0.45
44:w:54:THR:O	44:w:56:THR:HG23	2.16	0.45
4:E:117:ASP:O	4:E:121:LYS:HG3	2.17	0.45
15:P:103:HIS:CD2	15:P:105:ASN:HB2	2.52	0.45
17:S:53:ARG:NH1	31:h:105:ARG:O	2.49	0.45
20:V:3:LYS:O	20:V:7:HIS:ND1	2.49	0.45
48:a:202:PLX:H291	40:r:36:LEU:HD21	1.99	0.45
25:b:80:TRP:HD1	27:d:41:VAL:HG13	1.82	0.45
32:i:4:ILE:HD11	44:w:44:VAL:HG13	1.98	0.45
40:r:159:PRO:HG2	54:r:501:PEE:H38	1.97	0.45
14:O:137:THR:HG22	14:O:138:THR:H	1.82	0.45
20:V:86:ASP:OD1	20:V:87:PRO:HD2	2.17	0.45
22:Y:100:LEU:C	22:Y:102:ASP:H	2.24	0.45
24:a:160:MET:HE2	24:a:166:GLY:HA3	1.99	0.45
26:c:103:GLU:OE2	38:o:40:ARG:HD3	2.17	0.45
40:r:321:LEU:HD13	40:r:444:LEU:HG	1.98	0.45
1:A:48:ARG:HD2	10:K:70:ASN:O	2.17	0.45
12:M:50:LEU:HD21	12:M:62:ARG:NH2	2.32	0.45
12:M:354:LEU:HD22	12:M:548:LEU:HD22	1.99	0.45
24:a:76:LEU:HB3	24:a:80:ILE:HD11	1.99	0.45
24:a:145:GLU:OE2	42:u:163:HIS:NE2	2.44	0.45
26:c:153:TYR:HB3	35:l:403:TYR:HD1	1.81	0.45
48:j:202:PLX:H342	48:j:202:PLX:H372	1.76	0.45
35:l:40:VAL:HG21	35:l:101:MET:SD	2.56	0.45
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.98	0.45
44:w:283:TRP:N	44:w:284:PRO:CD	2.79	0.45
2:B:76:TYR:CE1	41:s:33:LEU:HB2	2.47	0.44
2:B:208:ASP:OD2	2:B:212:ARG:NH2	2.51	0.44
9:J:61:ALA:HB3	9:J:82:VAL:HG13	1.98	0.44
6:X:131:PRO:HB3	26:c:89:TRP:CD2	2.52	0.44
23:Z:18:ASP:OD1	23:Z:21:GLN:HB2	2.18	0.44
24:a:103:GLU:OE2	24:a:104:GLY:N	2.50	0.44
48:a:202:PLX:H102	40:r:40:SER:HB3	1.98	0.44
32:i:203:LEU:HB2	32:i:347:ASN:HD21	1.82	0.44
43:v:22:MET:HG2	43:v:23:PRO:HA	1.97	0.44
1:A:126:LYS:O	1:A:130:ILE:HG23	2.17	0.44
6:G:147:TYR:CD1	6:G:147:TYR:C	2.95	0.44
16:Q:335:GLU:OE1	16:Q:335:GLU:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:91:ASP:OD2	23:Z:42:ARG:NH2	2.37	0.44
32:i:183:SER:O	32:i:187:MET:HG2	2.17	0.44
32:i:244:MET:HB2	32:i:244:MET:HE2	1.71	0.44
1:A:357:MET:HE3	1:A:357:MET:HB2	1.90	0.44
4:E:21:PHE:HB3	4:E:31:ARG:HH22	1.82	0.44
5:F:46:LYS:HE2	12:M:674:LEU:HD21	1.99	0.44
13:N:41:GLU:OE1	13:N:47:LYS:NZ	2.50	0.44
17:S:15:CYS:O	17:S:19:PRO:HD3	2.18	0.44
32:i:73:ALA:HB2	32:i:97:MET:HG2	1.99	0.44
33:j:49:LEU:N	33:j:50:PRO:HD2	2.32	0.44
35:l:309:GLN:O	35:l:313:MET:HG3	2.17	0.44
35:l:358:LYS:HG3	39:p:80:TYR:CZ	2.53	0.44
36:m:25:SER:O	36:m:27:ILE:N	2.49	0.44
38:o:120:LYS:HB3	38:o:120:LYS:HE2	1.80	0.44
2:B:114:ILE:HD12	12:M:130:ILE:HG23	1.97	0.44
48:C:302:PLX:H31	13:N:75:TRP:CD2	2.53	0.44
9:J:168:SER:O	9:J:203:PRO:HD3	2.17	0.44
16:Q:133:LEU:HD22	16:Q:228:ARG:HD3	2.00	0.44
54:Q:501:PEE:H16	54:Q:501:PEE:H21	1.68	0.44
20:V:90:TYR:CZ	20:V:126:LYS:HE2	2.48	0.44
25:b:121:LYS:C	25:b:122:GLU:HG3	2.42	0.44
29:f:56:ILE:HG13	29:f:57:TYR:N	2.32	0.44
35:l:293:ILE:HD13	35:l:293:ILE:HA	1.86	0.44
42:u:39:PRO:HG2	42:u:66:CYS:SG	2.58	0.44
4:E:16:SER:HA	11:L:54:ALA:HA	2.00	0.44
7:H:48:THR:HG22	15:P:103:HIS:HE1	1.82	0.44
9:J:89:TYR:C	9:J:89:TYR:CD1	2.95	0.44
12:M:277:MET:HE3	12:M:279:GLU:HG2	1.99	0.44
14:O:48:ASN:OD1	14:O:51:THR:OG1	2.32	0.44
25:b:2:SER:OG	25:b:3:GLY:N	2.45	0.44
26:c:125:SER:O	26:c:129:MET:HG3	2.18	0.44
32:i:89:MET:HG3	32:i:95:MET:SD	2.57	0.44
32:i:323:MET:H	32:i:323:MET:HG2	1.56	0.44
35:l:44:PHE:HB2	35:l:94:LEU:HB3	2.00	0.44
36:m:51:PHE:HD1	41:s:100:LEU:HD21	1.83	0.44
40:r:266:MET:HE1	40:r:392:THR:HB	1.98	0.44
50:i:401:CDL:H312	50:i:401:CDL:H342	1.54	0.44
35:l:4:PHE:CD2	35:l:61:MET:HE2	2.52	0.44
35:l:21:MET:SD	35:l:35:TYR:OH	2.67	0.44
41:s:140:ILE:HA	41:s:143:GLU:HG2	2.00	0.44
41:s:260:VAL:O	41:s:264:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:v:46:MET:HG2	43:v:56:ARG:HG2	1.99	0.44
1:A:88:ARG:HG3	1:A:274:LYS:HZ3	1.82	0.44
9:J:173:ASP:OD1	9:J:176:SER:HB2	2.17	0.44
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.47	0.44
32:i:35:MET:HE3	36:m:159:TRP:HD1	1.83	0.44
40:r:229:MET:HE3	40:r:328:CYS:SG	2.58	0.44
46:A:502:FMN:O4'	46:A:502:FMN:O2'	2.29	0.44
3:C:113:MET:SD	16:Q:115:LEU:HD23	2.57	0.44
16:Q:65:PRO:HB2	16:Q:67:ASN:O	2.18	0.44
19:U:78:LEU:HD23	19:U:78:LEU:HA	1.85	0.44
26:c:75:TYR:OH	26:c:105:ILE:O	2.34	0.44
26:c:176:LYS:HA	26:c:176:LYS:HD2	1.74	0.44
27:d:9:VAL:HB	27:d:10:TYR:CD1	2.52	0.44
35:l:180:ILE:HG23	40:r:397:GLY:HA3	2.00	0.44
42:u:104:GLN:NE2	42:u:108:ASP:OD2	2.50	0.44
12:M:658:ASP:OD1	12:M:659:VAL:N	2.51	0.44
14:O:198:PRO:O	14:O:201:ILE:HG22	2.17	0.44
32:i:95:MET:HE1	32:i:145:ILE:HD12	1.99	0.44
33:j:24:LEU:HB3	33:j:25:PRO:HD3	2.00	0.44
40:r:126:LEU:HD11	40:r:153:THR:HG21	2.00	0.44
40:r:253:LEU:HD12	40:r:256:TYR:CE1	2.52	0.44
4:E:80:ASP:OD1	4:E:80:ASP:C	2.62	0.43
12:M:73:GLY:HA2	52:M:803:FES:S2	2.58	0.43
16:Q:41:VAL:HG23	28:e:55:LEU:HD23	2.00	0.43
6:X:132:ASP:HB3	39:p:18:ARG:HH11	1.80	0.43
48:a:202:PLX:H81	40:r:40:SER:HB3	1.99	0.43
32:i:252:GLY:HA3	32:i:290:LEU:HD13	2.00	0.43
50:i:401:CDL:H151	50:i:401:CDL:H122	1.84	0.43
38:o:105:PHE:HD2	40:r:263:MET:HE1	1.83	0.43
3:C:65:MET:HE3	3:C:97:PRO:HG3	1.99	0.43
6:G:108:LEU:HB3	6:G:110:LEU:HD13	2.00	0.43
25:b:88:TYR:CE1	27:d:49:ARG:HG2	2.53	0.43
32:i:84:TRP:HE1	34:k:53:PHE:HE2	1.66	0.43
32:i:242:SER:O	32:i:246:VAL:HG23	2.18	0.43
33:j:113:TRP:CH2	41:s:286:MET:HB3	2.53	0.43
35:l:61:MET:C	35:l:62:ILE:HD13	2.43	0.43
35:l:438:PRO:HA	35:l:439:PRO:HD2	1.89	0.43
35:l:572:LYS:O	35:l:576:MET:HG3	2.19	0.43
41:s:165:LEU:O	41:s:169:GLN:HG3	2.17	0.43
43:v:5:LEU:HD12	43:v:9:TYR:HE2	1.83	0.43
5:F:69:TYR:HE2	5:F:75:LYS:HD3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:g:77:LEU:HD21	32:i:342:ALA:HB1	2.00	0.43
32:i:177:LYS:NZ	34:k:98:CYS:O	2.51	0.43
36:m:39:VAL:O	36:m:43:ILE:HG13	2.19	0.43
41:s:199:ASP:OD1	41:s:199:ASP:N	2.43	0.43
22:Y:65:MET:HE2	35:l:375:ILE:HG12	2.01	0.43
24:a:152:LYS:HE3	30:g:96:VAL:HG11	1.99	0.43
50:g:202:CDL:H832	50:g:202:CDL:H861	1.69	0.43
32:i:313:MET:HE2	32:i:313:MET:HB3	1.96	0.43
36:m:20:PHE:HB2	36:m:29:GLY:HA2	1.99	0.43
41:s:1:MET:HE2	41:s:1:MET:HB3	1.80	0.43
42:u:111:VAL:HG12	42:u:117:TRP:HB2	2.01	0.43
1:A:185:ASN:C	1:A:187:CYS:H	2.27	0.43
5:F:63:PRO:HB2	5:F:79:LEU:HB2	1.99	0.43
9:J:116:ILE:O	9:J:120:VAL:HG22	2.18	0.43
13:N:78:ASP:OD1	13:N:78:ASP:C	2.61	0.43
41:s:155:LEU:HD12	41:s:155:LEU:HA	1.85	0.43
42:u:47:ARG:NH2	42:u:53:PRO:HG3	2.34	0.43
43:v:34:ARG:NH2	43:v:36:GLU:HA	2.33	0.43
1:A:274:LYS:HB3	1:A:276:PHE:CE1	2.53	0.43
46:A:502:FMN:N5	47:A:503:NAI:H4N	2.34	0.43
14:O:172:ILE:HG22	14:O:174:VAL:HG13	2.01	0.43
16:Q:102:SER:O	16:Q:102:SER:OG	2.33	0.43
26:c:101:TRP:CE3	38:o:47:TYR:HB2	2.54	0.43
31:h:2:PRO:HA	32:i:140:SER:HB2	2.01	0.43
31:h:73:MET:CE	36:m:127:ILE:HG23	2.49	0.43
33:j:94:LEU:HD12	36:m:147:TYR:HE1	1.83	0.43
35:l:292:ALA:HB2	35:l:304:PHE:CB	2.49	0.43
14:O:198:PRO:HA	14:O:201:ILE:HG22	2.00	0.43
19:U:19:LEU:HD23	19:U:19:LEU:HA	1.86	0.43
23:Z:13:LYS:HD2	23:Z:13:LYS:HA	1.75	0.43
35:l:49:VAL:HB	35:l:50:PRO:HD3	2.01	0.43
41:s:71:PHE:C	41:s:71:PHE:CD1	2.97	0.43
41:s:296:LEU:HD23	41:s:296:LEU:HA	1.87	0.43
43:v:37:ARG:HH12	43:v:97:LYS:NZ	2.17	0.43
1:A:248:VAL:O	1:A:251:SER:OG	2.36	0.43
14:O:140:CYS:HA	14:O:183:ALA:HB1	2.01	0.43
22:Y:72:ARG:HB3	35:l:385:TYR:CD1	2.54	0.43
30:g:18:ASN:O	30:g:21:ARG:HG3	2.18	0.43
40:r:121:LEU:O	40:r:125:THR:HG23	2.19	0.43
40:r:272:THR:HA	40:r:275:ILE:HD12	2.00	0.43
41:s:11:ILE:HB	41:s:12:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:14:LYS:HE3	42:u:14:LYS:HB3	1.87	0.43
43:v:82:HIS:CE1	43:v:86:ASP:OD1	2.72	0.43
1:A:134:ASP:OD2	1:A:137:LYS:HD2	2.19	0.43
1:A:279:SER:OG	1:A:280:GLY:N	2.52	0.43
1:A:288:VAL:HG21	1:A:303:HIS:ND1	2.34	0.43
4:E:71:ALA:HA	49:G:201:8Q1:O40	2.18	0.43
12:M:445:LEU:HD22	12:M:460:HIS:CE1	2.52	0.43
12:M:592:LYS:NZ	12:M:619:ASP:OD2	2.49	0.43
16:Q:190:HIS:O	16:Q:194:ILE:HG12	2.18	0.43
16:Q:270:ASN:HB3	41:s:284:GLN:NE2	2.34	0.43
25:b:92:ALA:O	27:d:4:SER:OG	2.30	0.43
25:b:123:PHE:HD2	43:v:40:VAL:HG11	1.83	0.43
54:i:402:PEE:H37	54:i:402:PEE:H60	2.01	0.43
33:j:95:LEU:HD23	33:j:95:LEU:HA	1.90	0.43
41:s:301:CYS:O	41:s:305:ILE:HG13	2.19	0.43
8:I:42:PRO:HD3	21:W:6:VAL:HG13	2.01	0.43
12:M:382:ARG:HG2	12:M:386:LEU:HD11	2.00	0.43
14:O:206:ASP:OD1	14:O:207:GLU:N	2.52	0.43
15:P:119:VAL:HG12	15:P:121:THR:HG22	1.99	0.43
16:Q:463:ARG:HE	16:Q:463:ARG:HB2	1.50	0.43
18:T:47:ASP:HA	18:T:52:ARG:HH12	1.84	0.43
20:V:101:LEU:O	20:V:105:THR:HG23	2.18	0.43
6:X:113:LEU:O	6:X:116:VAL:HG12	2.19	0.43
47:A:503:NAI:H6N	47:A:503:NAI:H2D	1.73	0.42
6:G:92:LYS:NZ	6:G:114:ASP:OD1	2.33	0.42
9:J:170:LEU:HD11	9:J:329:LEU:HD13	2.02	0.42
12:M:389:THR:OG1	12:M:514:ASN:ND2	2.46	0.42
23:Z:23:LYS:HZ2	23:Z:25:GLU:HB2	1.84	0.42
25:b:99:GLU:HG3	35:l:61:MET:CG	2.48	0.42
48:g:201:PLX:H22	48:g:201:PLX:H1C3	1.76	0.42
50:g:202:CDL:H242	40:r:97:THR:HG21	2.00	0.42
35:l:174:TYR:CD2	35:l:232:TRP:HB3	2.54	0.42
35:l:223:LYS:NZ	35:l:252:MET:HE3	2.34	0.42
40:r:263:MET:N	40:r:263:MET:SD	2.92	0.42
40:r:357:THR:O	40:r:361:VAL:HG23	2.19	0.42
44:w:86:PHE:HB2	44:w:159:LEU:HD23	2.00	0.42
2:B:105:ARG:HD2	13:N:108:TYR:CG	2.54	0.42
6:G:106:LYS:H	6:G:106:LYS:HG2	1.70	0.42
12:M:371:VAL:HG22	12:M:533:GLY:HA2	2.00	0.42
13:N:138:VAL:HA	13:N:139:PRO:HD3	1.87	0.42
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	2.00	0.42
32:i:311:MET:HE2	32:i:311:MET:HB2	1.85	0.42
35:l:253:VAL:C	35:l:255:ALA:H	2.26	0.42
39:p:123:GLU:HA	39:p:126:LYS:HD2	2.00	0.42
44:w:262:GLU:OE2	44:w:268:LYS:NZ	2.41	0.42
4:E:54:ILE:HB	4:E:58:GLN:HG3	2.01	0.42
7:H:41:ASN:OD1	7:H:41:ASN:N	2.49	0.42
14:O:155:LYS:HD2	14:O:202:GLU:HG3	2.01	0.42
15:P:44:ARG:HE	15:P:45:PRO:HD3	1.84	0.42
16:Q:251:PHE:HB3	16:Q:341:LEU:HD11	2.00	0.42
18:T:122:HIS:ND1	18:T:122:HIS:C	2.77	0.42
22:Y:84:PHE:HB3	43:v:92:HIS:CD2	2.55	0.42
31:h:18:MET:O	31:h:18:MET:HG3	2.19	0.42
35:l:452:ASN:HA	35:l:455:LYS:HG2	2.00	0.42
41:s:89:LEU:HD11	41:s:233:MET:SD	2.60	0.42
1:A:109:ARG:HG2	11:L:166:TRP:CD1	2.54	0.42
2:B:184:LEU:HD23	11:L:112:MET:HG3	2.01	0.42
4:E:109:GLU:H	4:E:109:GLU:HG2	1.69	0.42
12:M:133:GLN:O	12:M:137:CYS:HB2	2.20	0.42
16:Q:450:ILE:O	16:Q:454:GLN:HG3	2.19	0.42
32:i:217:MET:HB2	32:i:326:LEU:HD13	2.00	0.42
35:l:176:ARG:O	35:l:180:ILE:HG13	2.19	0.42
35:l:596:MET:HE2	35:l:596:MET:HB3	1.93	0.42
38:o:65:LEU:O	38:o:69:THR:HG23	2.20	0.42
39:p:10:LEU:HD21	39:p:18:ARG:NH2	2.32	0.42
40:r:158:LEU:HD23	40:r:158:LEU:HA	1.84	0.42
40:r:204:MET:HE3	40:r:261:PHE:CD1	2.55	0.42
1:A:32:PHE:CE2	1:A:267:ARG:HG2	2.54	0.42
1:A:56:ALA:HB1	1:A:61:ASP:HB2	2.00	0.42
1:A:119:GLU:OE2	1:A:127:ASP:HB2	2.19	0.42
8:I:107:SER:C	8:I:109:ASP:H	2.28	0.42
14:O:93:LEU:HD12	14:O:122:TYR:HB3	2.02	0.42
14:O:166:ASP:OD1	14:O:166:ASP:C	2.62	0.42
16:Q:235:ASP:HB2	16:Q:356:ILE:HG21	2.01	0.42
16:Q:235:ASP:CB	16:Q:356:ILE:HD13	2.46	0.42
30:g:47:ASP:OD1	30:g:51:ARG:NH1	2.52	0.42
50:g:202:CDL:H391	32:i:334:THR:HG21	2.01	0.42
36:m:52:LEU:O	36:m:56:VAL:HG23	2.19	0.42
40:r:174:LEU:HD23	40:r:174:LEU:HA	1.88	0.42
22:Y:97:LEU:HD12	43:v:104:ARG:HB2	2.01	0.42
50:a:201:CDL:H311	50:a:201:CDL:H342	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:e:95:PHE:O	28:e:100:VAL:HG23	2.19	0.42
28:e:137:MET:HE2	28:e:137:MET:HB3	1.78	0.42
28:e:143:ASP:OD1	28:e:146:LYS:NZ	2.44	0.42
32:i:296:LEU:HD12	32:i:296:LEU:HA	1.87	0.42
33:j:53:MET:HG3	33:j:57:LEU:HD23	2.00	0.42
35:l:336:LYS:HD3	35:l:336:LYS:HA	1.79	0.42
1:A:385:CYS:HB3	45:A:501:SF4:S2	2.59	0.42
14:O:110:MET:O	14:O:114:GLU:HG3	2.19	0.42
16:Q:139:LEU:HD23	16:Q:139:LEU:HA	1.73	0.42
1:A:408:GLU:O	1:A:411:SER:HB3	2.19	0.42
4:E:43:VAL:HG11	4:E:60:ARG:HG3	2.02	0.42
5:F:56:ARG:HB3	12:M:651:PRO:HD2	2.02	0.42
9:J:195:PHE:HB3	9:J:198:ALA:HB2	2.01	0.42
12:M:689:LEU:HD12	12:M:689:LEU:HA	1.89	0.42
16:Q:67:ASN:OD1	16:Q:67:ASN:N	2.53	0.42
23:Z:52:ARG:HD2	39:p:34:ARG:HG3	2.02	0.42
50:a:201:CDL:H792	50:a:201:CDL:H762	1.90	0.42
50:i:401:CDL:H142	50:i:401:CDL:H171	1.72	0.42
35:l:313:MET:HG2	35:l:328:HIS:HD2	1.84	0.42
36:m:163:ILE:HD13	36:m:163:ILE:HA	1.91	0.42
40:r:191:SER:HB3	54:r:501:PEE:H3	2.01	0.42
40:r:218:LYS:O	40:r:222:GLU:HG2	2.19	0.42
44:w:211:VAL:O	44:w:214:ILE:HG22	2.19	0.42
4:E:40:TYR:CZ	6:G:117:GLU:HG2	2.55	0.42
14:O:207:GLU:OE2	14:O:214:PRO:HB3	2.20	0.42
15:P:51:ASN:OD1	15:P:51:ASN:C	2.63	0.42
15:P:213:ASP:HB3	15:P:216:VAL:HG22	2.01	0.42
54:U:101:PEE:H59	54:U:101:PEE:H64	1.75	0.42
25:b:109:THR:O	27:d:19:ALA:N	2.45	0.42
31:h:17:TRP:CZ3	31:h:18:MET:HB2	2.54	0.42
37:n:17:VAL:HG13	40:r:7:PRO:HB3	2.02	0.42
1:A:161:GLU:N	1:A:161:GLU:OE1	2.52	0.42
1:A:290:GLU:OE2	1:A:291:GLU:N	2.53	0.42
6:G:149:ALA:HB1	6:G:154:VAL:HG22	2.02	0.42
12:M:144:MET:HE3	12:M:144:MET:HB3	1.85	0.42
16:Q:156:GLU:OE2	16:Q:171:ARG:NH2	2.52	0.42
48:a:202:PLX:H162	28:e:105:PHE:HB2	2.02	0.42
27:d:9:VAL:O	27:d:109:ARG:NH2	2.52	0.42
44:w:206:TYR:HE2	44:w:242:LYS:HE3	1.85	0.42
1:A:89:GLY:O	47:A:503:NAI:H2N	2.20	0.41
7:H:113:LYS:HE3	7:H:113:LYS:HB3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:591:GLU:HG2	12:M:610:VAL:HG23	2.01	0.41
23:Z:57:PHE:O	35:l:434:LYS:NZ	2.42	0.41
24:a:143:GLU:HB3	40:r:178:ILE:HG13	2.00	0.41
28:e:120:ARG:O	28:e:124:ARG:HG3	2.20	0.41
30:g:51:ARG:HB2	30:g:53:ARG:HG3	2.02	0.41
33:j:88:LEU:O	33:j:92:LEU:HG	2.20	0.41
35:l:201:ILE:O	35:l:205:ASN:ND2	2.48	0.41
35:l:241:THR:N	35:l:242:PRO:CD	2.83	0.41
35:l:356:ILE:HA	35:l:359:MET:CG	2.50	0.41
35:l:531:SER:O	35:l:535:ARG:HG3	2.20	0.41
35:l:549:ALA:HB1	40:r:275:ILE:HG13	2.02	0.41
44:w:215:GLN:O	44:w:219:GLN:HG2	2.20	0.41
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.53	0.41
5:F:23:LEU:O	5:F:57:GLU:HA	2.20	0.41
16:Q:139:LEU:HD13	16:Q:424:ILE:HG21	2.01	0.41
6:X:112:SER:N	49:X:201:8Q1:O1	2.53	0.41
6:X:138:LEU:HA	6:X:138:LEU:HD12	1.81	0.41
49:X:201:8Q1:C31	39:p:52:LYS:HG3	2.50	0.41
22:Y:83:HIS:HD1	22:Y:83:HIS:C	2.27	0.41
25:b:19:ARG:NH1	39:p:171:VAL:O	2.50	0.41
25:b:121:LYS:O	25:b:122:GLU:HG3	2.20	0.41
40:r:216:LEU:HD23	40:r:287:ALA:HB1	2.01	0.41
44:w:302:LEU:HD23	44:w:302:LEU:HA	1.89	0.41
2:B:210:LEU:HA	2:B:210:LEU:HD23	1.84	0.41
4:E:40:TYR:HD2	6:G:120:MET:CE	2.32	0.41
5:F:35:ASP:O	5:F:36:PHE:C	2.62	0.41
5:F:36:PHE:C	5:F:36:PHE:CD1	2.95	0.41
12:M:419:ARG:NH1	12:M:439:THR:O	2.53	0.41
32:i:89:MET:HE3	32:i:89:MET:HB3	1.92	0.41
35:l:493:VAL:HA	35:l:496:MET:HE2	2.01	0.41
40:r:230:VAL:HG22	40:r:235:LEU:HD13	2.02	0.41
40:r:251:ASN:HD21	40:r:304:GLN:NE2	2.18	0.41
41:s:126:LYS:O	41:s:130:ILE:HG12	2.18	0.41
44:w:204:VAL:HG13	44:w:255:VAL:HG13	2.02	0.41
1:A:46:TYR:CD2	14:O:234:LEU:HD12	2.55	0.41
1:A:214:GLU:HG3	1:A:222:LYS:O	2.20	0.41
2:B:110:GLU:HG3	18:T:67:ALA:HB1	2.03	0.41
2:B:210:LEU:HD12	8:I:38:PRO:HB3	2.02	0.41
9:J:36:LEU:HB3	12:M:304:GLN:NE2	2.36	0.41
16:Q:303:ARG:HG3	16:Q:401:GLU:HB3	2.03	0.41
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:88:LYS:HG2	6:X:98:LEU:HD21	2.02	0.41
31:h:76:LEU:HD12	31:h:76:LEU:HA	1.80	0.41
32:i:288:LEU:HD21	35:l:570:GLN:HG3	2.01	0.41
41:s:2:PHE:CE2	41:s:6:ILE:HD11	2.56	0.41
1:A:182:ILE:HD13	1:A:182:ILE:HA	1.83	0.41
2:B:38:TYR:CZ	8:I:106:LEU:HD13	2.56	0.41
2:B:135:ARG:HD3	2:B:141:ARG:HG3	2.03	0.41
4:E:58:GLN:HA	4:E:61:ASP:OD2	2.19	0.41
10:K:82:SER:N	10:K:85:THR:OG1	2.53	0.41
24:a:132:ASN:ND2	40:r:49:SER:O	2.48	0.41
26:c:166:LEU:HD22	26:c:169:GLU:OE1	2.21	0.41
27:d:106:ILE:HG13	27:d:135:VAL:HG21	2.02	0.41
28:e:152:ASP:OD1	28:e:153:GLU:N	2.51	0.41
32:i:66:ALA:HB2	32:i:104:MET:HG2	2.01	0.41
33:j:81:THR:C	33:j:83:ASN:H	2.29	0.41
35:l:230:HIS:O	35:l:234:PRO:HD2	2.19	0.41
35:l:230:HIS:N	35:l:231:PRO:HD3	2.35	0.41
44:w:100:ASP:OD1	44:w:100:ASP:N	2.53	0.41
1:A:299:LEU:HD12	1:A:303:HIS:CD2	2.55	0.41
7:H:51:ILE:HD11	8:I:94:ALA:HB3	2.03	0.41
14:O:222:ARG:HE	14:O:222:ARG:HB2	1.68	0.41
16:Q:192:LEU:HD12	16:Q:197:MET:HB2	2.01	0.41
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	2.01	0.41
54:U:101:PEE:H35	54:U:101:PEE:H30	1.84	0.41
26:c:55:TYR:HD2	26:c:62:TYR:HE1	1.68	0.41
35:l:529:TYR:HB3	35:l:530:PRO:HD3	2.00	0.41
44:w:258:TYR:CE2	44:w:269:VAL:HG22	2.55	0.41
12:M:347:ASP:HB3	12:M:594:ALA:HB1	2.02	0.41
21:W:68:ARG:O	21:W:72:MET:HG3	2.20	0.41
32:i:20:VAL:HG13	32:i:29:ILE:HG23	2.02	0.41
33:j:94:LEU:HD23	33:j:94:LEU:HA	1.94	0.41
35:l:108:MET:HE3	35:l:108:MET:HB3	1.87	0.41
39:p:150:ARG:HE	39:p:150:ARG:HB3	1.75	0.41
1:A:235:VAL:HG12	1:A:240:THR:OG1	2.21	0.41
1:A:244:ASN:N	46:A:502:FMN:O1P	2.51	0.41
16:Q:241:LEU:HD23	16:Q:241:LEU:HA	1.83	0.41
6:X:120:MET:HE2	39:p:21:LYS:HD3	2.02	0.41
25:b:81:ILE:HG23	54:b:201:PEE:H58	2.02	0.41
35:l:286:LEU:HA	35:l:286:LEU:HD12	1.71	0.41
40:r:206:LYS:HE3	40:r:206:LYS:HB3	1.94	0.41
1:A:79:GLU:OE1	1:A:255:CYS:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:ASP:OD1	2:B:150:THR:OG1	2.37	0.41
6:G:106:LYS:HE2	6:G:106:LYS:HB3	1.94	0.41
14:O:179:ALA:HB3	14:O:185:MET:HE3	2.02	0.41
54:Q:501:PEE:H20	41:s:183:MET:HE3	2.03	0.41
18:T:84:ILE:HD12	18:T:84:ILE:HA	1.98	0.41
24:a:180:ASP:HB2	31:h:24:GLU:H	1.86	0.41
25:b:23:LEU:HD12	25:b:23:LEU:HA	1.96	0.41
26:c:58:ARG:HD2	38:o:36:ARG:HG3	2.02	0.41
32:i:20:VAL:HG11	32:i:137:ALA:HB1	2.03	0.41
32:i:222:SER:O	32:i:224:ALA:N	2.54	0.41
32:i:323:MET:HE2	32:i:323:MET:HB3	2.00	0.41
33:j:33:LYS:HD2	33:j:33:LYS:HA	1.87	0.41
35:l:551:SER:OG	35:l:552:LEU:N	2.54	0.41
40:r:343:ILE:O	40:r:343:ILE:HG13	2.21	0.41
41:s:66:SER:HB2	41:s:122:ALA:O	2.20	0.41
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.55	0.41
3:C:180:LEU:O	3:C:184:ILE:HG13	2.21	0.41
9:J:207:PHE:CD1	9:J:240:VAL:C	2.98	0.41
12:M:485:ASP:OD2	12:M:680:LEU:HG	2.21	0.41
16:Q:450:ILE:O	16:Q:453:THR:HG22	2.21	0.41
20:V:102:GLY:HA3	20:V:111:GLY:CA	2.51	0.41
22:Y:45:ARG:HH11	23:Z:51:TRP:HD1	1.69	0.41
22:Y:89:PRO:HA	22:Y:92:TRP:CE3	2.56	0.41
33:j:84:LEU:HD13	41:s:309:ILE:HG23	2.03	0.41
3:C:113:MET:HE1	16:Q:86:PRO:HB2	2.03	0.40
6:G:75:THR:O	6:G:79:ILE:HG13	2.22	0.40
12:M:567:ILE:HG23	12:M:582:VAL:HG13	2.03	0.40
17:S:18:ILE:HD13	17:S:18:ILE:HA	1.85	0.40
19:U:53:TYR:HB2	21:W:72:MET:SD	2.61	0.40
22:Y:89:PRO:HB2	43:v:103:GLU:OE2	2.21	0.40
32:i:86:ILE:O	32:i:86:ILE:HG23	2.21	0.40
32:i:113:PHE:HD2	35:l:591:PHE:CE1	2.38	0.40
33:j:70:ALA:HB2	36:m:59:ILE:HG13	2.02	0.40
35:l:97:THR:HG21	35:l:125:LEU:HD22	2.02	0.40
35:l:124:PHE:CE1	35:l:252:MET:HB2	2.56	0.40
35:l:310:LEU:HD23	35:l:313:MET:HE3	2.04	0.40
35:l:392:LYS:O	35:l:396:ILE:HG12	2.21	0.40
41:s:183:MET:O	41:s:187:ILE:HG12	2.21	0.40
1:A:263:ALA:HA	1:A:271:SER:OG	2.21	0.40
26:c:38:PRO:HD2	38:o:70:TYR:CD2	2.57	0.40
26:c:154:GLN:HG3	35:l:401:MET:SD	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:g:201:PLX:H72	48:g:201:PLX:H101	1.77	0.40
35:l:293:ILE:HG22	35:l:294:THR:HG22	2.03	0.40
35:l:504:LEU:HD23	35:l:504:LEU:HA	1.89	0.40
38:o:20:PRO:HG3	39:p:65:ARG:HH21	1.86	0.40
1:A:175:GLU:O	1:A:178:GLU:HG2	2.21	0.40
26:c:117:VAL:HG21	35:l:539:TYR:HB2	2.03	0.40
33:j:74:PRO:HB3	36:m:143:ILE:HG22	2.04	0.40
35:l:411:MET:HE2	35:l:411:MET:HA	2.03	0.40
54:r:501:PEE:H21	54:r:501:PEE:H28	1.92	0.40
2:B:168:VAL:HG21	2:B:201:ILE:HG21	2.04	0.40
5:F:69:TYR:CE2	5:F:75:LYS:HD3	2.56	0.40
16:Q:216:ARG:NH2	16:Q:240:LEU:HA	2.37	0.40
19:U:84:LEU:HA	19:U:84:LEU:HD23	1.86	0.40
32:i:233:THR:HG23	32:i:237:MET:HG3	2.04	0.40
40:r:299:VAL:O	40:r:303:ILE:HG12	2.22	0.40
41:s:87:VAL:HG23	41:s:95:LEU:HD23	2.04	0.40
44:w:192:LYS:HB2	44:w:192:LYS:HE2	1.84	0.40
1:A:312:ASP:O	1:A:359:ARG:NH1	2.51	0.40
16:Q:311:TYR:O	16:Q:314:VAL:CG2	2.69	0.40
24:a:127:ASP:OD1	48:a:202:PLX:H1B3	2.21	0.40
48:a:202:PLX:O7	48:a:202:PLX:P1	2.79	0.40
54:b:201:PEE:H60	54:b:201:PEE:H55	1.87	0.40
32:i:146:SER:O	32:i:149:ILE:HG12	2.22	0.40
34:k:57:ASN:HD22	34:k:57:ASN:N	2.19	0.40
35:l:249:SER:CB	35:l:340:PHE:CD2	3.05	0.40
35:l:350:LEU:HD12	35:l:359:MET:HE2	2.03	0.40
40:r:48:ASN:OD1	40:r:48:ASN:N	2.52	0.40
44:w:60:ILE:HG12	44:w:203:VAL:HB	2.02	0.40
44:w:60:ILE:HB	44:w:158:VAL:HG22	2.04	0.40
44:w:330:LYS:HE3	44:w:330:LYS:HB3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/433 (99%)	409 (95%)	20 (5%)	0	100	100
2	B	174/176 (99%)	170 (98%)	4 (2%)	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%)	81 (96%)	3 (4%)	0	100	100
6	G	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	101 (92%)	9 (8%)	0	100	100
8	I	93/112 (83%)	79 (85%)	14 (15%)	0	100	100
9	J	289/341 (85%)	275 (95%)	12 (4%)	2 (1%)	18	49
10	K	40/43 (93%)	39 (98%)	1 (2%)	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	665 (97%)	23 (3%)	0	100	100
13	N	142/144 (99%)	133 (94%)	9 (6%)	0	100	100
14	O	215/217 (99%)	208 (97%)	7 (3%)	0	100	100
15	P	206/208 (99%)	194 (94%)	12 (6%)	0	100	100
16	Q	412/430 (96%)	393 (95%)	17 (4%)	2 (0%)	24	55
17	S	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
18	T	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
19	U	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
20	V	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	18	49
21	W	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
22	Y	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
23	Z	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
24	a	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
25	b	99/126 (79%)	91 (92%)	8 (8%)	0	100	100
26	c	154/156 (99%)	145 (94%)	9 (6%)	0	100	100
27	d	173/175 (99%)	172 (99%)	1 (1%)	0	100	100
28	e	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
29	f	40/49 (82%)	38 (95%)	2 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	g	119/122 (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%)	334 (97%)	11 (3%)	0	100	100
33	j	95/113 (84%)	88 (93%)	7 (7%)	0	100	100
34	k	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
35	l	601/603 (100%)	571 (95%)	30 (5%)	0	100	100
36	m	125/175 (71%)	115 (92%)	10 (8%)	0	100	100
37	n	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
38	o	126/128 (98%)	117 (93%)	9 (7%)	0	100	100
39	p	176/178 (99%)	163 (93%)	13 (7%)	0	100	100
40	r	457/459 (100%)	444 (97%)	13 (3%)	0	100	100
41	s	299/318 (94%)	283 (95%)	16 (5%)	0	100	100
42	u	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
43	v	122/124 (98%)	113 (93%)	9 (7%)	0	100	100
44	w	318/320 (99%)	305 (96%)	13 (4%)	0	100	100
All	All	8029/8319 (96%)	7672 (96%)	352 (4%)	5 (0%)	49	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	203	PRO
16	Q	235	ASP
9	J	38	HIS
16	Q	232	VAL
20	V	46	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	344/346 (99%)	343 (100%)	1 (0%)	86 86
2	B	151/151 (100%)	151 (100%)	0	100 100
3	C	131/132 (99%)	130 (99%)	1 (1%)	73 79
4	E	106/107 (99%)	105 (99%)	1 (1%)	70 78
5	F	73/76 (96%)	73 (100%)	0	100 100
6	G	75/81 (93%)	74 (99%)	1 (1%)	61 74
6	X	76/81 (94%)	76 (100%)	0	100 100
7	H	99/99 (100%)	98 (99%)	1 (1%)	68 76
8	I	87/97 (90%)	87 (100%)	0	100 100
9	J	249/295 (84%)	248 (100%)	1 (0%)	84 84
10	K	37/42 (88%)	36 (97%)	1 (3%)	39 63
11	L	109/113 (96%)	109 (100%)	0	100 100
12	M	580/580 (100%)	579 (100%)	1 (0%)	87 88
13	N	128/130 (98%)	124 (97%)	4 (3%)	35 60
14	O	183/183 (100%)	183 (100%)	0	100 100
15	P	190/190 (100%)	190 (100%)	0	100 100
16	Q	358/370 (97%)	357 (100%)	1 (0%)	86 86
17	S	57/58 (98%)	57 (100%)	0	100 100
18	T	79/79 (100%)	78 (99%)	1 (1%)	61 74
19	U	69/69 (100%)	69 (100%)	0	100 100
20	V	99/101 (98%)	98 (99%)	1 (1%)	68 76
21	W	122/123 (99%)	121 (99%)	1 (1%)	73 79
22	Y	62/63 (98%)	60 (97%)	2 (3%)	34 60
23	Z	65/65 (100%)	65 (100%)	0	100 100
24	a	122/122 (100%)	122 (100%)	0	100 100
25	b	97/119 (82%)	97 (100%)	0	100 100
26	c	140/141 (99%)	140 (100%)	0	100 100
27	d	152/155 (98%)	149 (98%)	3 (2%)	48 68
28	e	99/99 (100%)	99 (100%)	0	100 100
29	f	34/45 (76%)	34 (100%)	0	100 100
30	g	108/109 (99%)	108 (100%)	0	100 100
31	h	93/93 (100%)	92 (99%)	1 (1%)	65 76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
32	i	311/311 (100%)	310 (100%)	1 (0%)	86 86
33	j	87/99 (88%)	86 (99%)	1 (1%)	65 76
34	k	85/85 (100%)	85 (100%)	0	100 100
35	l	531/537 (99%)	531 (100%)	0	100 100
36	m	98/141 (70%)	98 (100%)	0	100 100
37	n	49/53 (92%)	49 (100%)	0	100 100
38	o	113/113 (100%)	113 (100%)	0	100 100
39	p	159/159 (100%)	159 (100%)	0	100 100
40	r	410/410 (100%)	407 (99%)	3 (1%)	76 80
41	s	261/275 (95%)	259 (99%)	2 (1%)	73 79
42	u	153/153 (100%)	152 (99%)	1 (1%)	76 80
43	v	103/111 (93%)	103 (100%)	0	100 100
44	w	277/283 (98%)	277 (100%)	0	100 100
All	All	7011/7244 (97%)	6981 (100%)	30 (0%)	81 84

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
3	C	154	ASP
4	E	103	ILE
6	G	148	ILE
7	H	77	ILE
9	J	136	THR
10	K	91	VAL
12	M	450	LYS
13	N	13	GLN
13	N	54	GLN
13	N	76	ASP
13	N	134	ILE
16	Q	236	LEU
18	T	122	HIS
20	V	70	PHE
21	W	51	MET
22	Y	50	LEU
22	Y	76	ASP
27	d	10	TYR

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Mol	Chain	Res	Type
27	d	17	THR
27	d	164	LEU
31	h	97	HIS
32	i	98	MET
33	j	69	ILE
40	r	116	ILE
40	r	126	LEU
40	r	343	ILE
41	s	91	MET
41	s	222	MET
42	u	64	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	277	ASN
1	A	422	HIS
5	F	31	GLN
7	H	76	GLN
8	I	25	GLN
9	J	122	HIS
9	J	128	ASN
9	J	166	HIS
9	J	171	ASN
9	J	238	GLN
9	J	323	HIS
12	M	278	HIS
12	M	336	ASN
12	M	464	GLN
12	M	540	ASN
12	M	569	GLN
15	P	75	GLN
15	P	77	GLN
15	P	124	ASN
15	P	196	HIS
16	Q	160	ASN
16	Q	190	HIS
16	Q	285	ASN
17	S	31	ASN
18	T	63	ASN
20	V	89	ASN

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Mol	Chain	Res	Type
22	Y	46	GLN
22	Y	54	GLN
23	Z	48	ASN
24	a	50	HIS
24	a	170	GLN
25	b	89	HIS
25	b	127	HIS
30	g	90	HIS
30	g	119	HIS
31	h	70	GLN
32	i	83	GLN
32	i	174	GLN
32	i	268	GLN
32	i	310	ASN
34	k	50	ASN
34	k	57	ASN
35	l	2	ASN
35	l	270	ASN
35	l	295	GLN
35	l	323	HIS
35	l	348	HIS
35	l	354	GLN
35	l	446	ASN
37	n	3	ASN
37	n	14	HIS
39	p	78	GLN
40	r	26	ASN
40	r	175	ASN
40	r	192	ASN
40	r	251	ASN
41	s	47	GLN
41	s	138	GLN
41	s	171	HIS
41	s	317	GLN
42	u	16	GLN
42	u	151	ASN
44	w	306	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	1.12	1 (10%)	5,13,15	1.68	2 (40%)

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	-	5/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NH2	-3.05	1.26	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Q	118	2MR	NE-CZ-NH2	2.91	122.15	119.48
16	Q	118	2MR	CQ2-NH2-CZ	2.25	128.83	123.86

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	Q	118	2MR	NH1-CZ-NE-CD
16	Q	118	2MR	NH2-CZ-NE-CD
16	Q	118	2MR	CA-CB-CG-CD
16	Q	118	2MR	NE-CD-CG-CB
16	Q	118	2MR	N-CA-CB-CG

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 34 ligands modelled in this entry, 2 are monoatomic - leaving 32 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	$\#\|Z\| > 2$
48	PLX	j	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.60	1 (1%)
46	FMN	A	502	-	33,33,33	1.10	2 (6%)	48,50,50	1.22	8 (16%)
54	PEE	r	501	-	50,50,50	1.15	6 (12%)	53,55,55	0.98	2 (3%)
54	PEE	b	201	-	45,45,50	1.21	6 (13%)	48,50,55	0.95	2 (4%)
57	ADP	w	401	-	27,29,29	2.97	8 (29%)	42,45,45	2.02	10 (23%)
48	PLX	a	202	-	51,51,51	0.61	0	55,59,59	0.66	0
52	FES	M	803	12	0,4,4	-	-	-		
45	SF4	A	501	1	0,12,12	-	-	-		
50	CDL	I	201	-	50,50,99	1.40	8 (16%)	56,62,111	1.14	4 (7%)
51	NDP	J	401	-	49,52,52	4.40	23 (46%)	66,80,80	2.23	15 (22%)
48	PLX	C	302	-	51,51,51	1.14	3 (5%)	55,59,59	0.64	1 (1%)
54	PEE	i	402	-	46,46,50	1.21	6 (13%)	49,51,55	1.02	2 (4%)
45	SF4	M	802	12	0,12,12	-	-	-		
49	8Q1	G	201	-	31,34,34	1.69	5 (16%)	40,43,43	1.57	6 (15%)
54	PEE	Q	501	-	50,50,50	1.15	6 (12%)	53,55,55	1.00	3 (5%)
49	8Q1	X	201	-	31,34,34	1.72	6 (19%)	40,43,43	1.53	6 (15%)
52	FES	O	301	14	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	SF4	B	302	2	0,12,12	-	-	-		
48	PLX	r	502	-	51,51,51	1.13	3 (5%)	55,59,59	0.61	1 (1%)
54	PEE	l	701	-	45,45,50	1.22	6 (13%)	48,50,55	0.99	2 (4%)
56	UQ	s	401	-	28,28,63	3.29	7 (25%)	34,37,79	2.71	10 (29%)
45	SF4	B	301	2	0,12,12	-	-	-		
45	SF4	C	301	3,16	0,12,12	-	-	-		
50	CDL	a	201	-	90,90,99	1.12	8 (8%)	96,102,111	0.93	4 (4%)
50	CDL	i	401	-	65,65,99	1.28	8 (12%)	71,77,111	1.03	4 (5%)
50	CDL	g	202	-	99,99,99	1.08	8 (8%)	105,111,111	0.86	4 (3%)
54	PEE	U	101	-	50,50,50	1.14	6 (12%)	53,55,55	0.98	2 (3%)
54	PEE	j	201	-	46,46,50	1.21	6 (13%)	49,51,55	0.95	2 (4%)
48	PLX	g	201	-	51,51,51	1.13	3 (5%)	55,59,59	0.62	1 (1%)
45	SF4	M	801	12	0,12,12	-	-	-		
47	NAI	A	503	-	45,48,48	3.91	21 (46%)	60,73,73	1.78	12 (20%)
54	PEE	m	201	-	40,40,50	1.14	4 (10%)	43,45,55	1.04	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PLX	j	202	-	-	31/55/55/55	-
46	FMN	A	502	-	-	2/18/18/18	0/3/3/3
54	PEE	r	501	-	-	26/54/54/54	-
54	PEE	b	201	-	-	26/49/49/54	-
57	ADP	w	401	-	-	4/16/32/32	0/3/3/3
48	PLX	a	202	-	-	13/55/55/55	-
52	FES	M	803	12	-	-	0/1/1/1
45	SF4	A	501	1	-	-	0/6/5/5
50	CDL	I	201	-	-	40/61/61/110	-
51	NDP	J	401	-	-	11/34/77/77	0/4/5/5
48	PLX	C	302	-	-	28/55/55/55	-
54	PEE	i	402	-	-	25/50/50/54	-
49	8Q1	G	201	-	-	20/41/41/41	-
45	SF4	M	802	12	-	-	0/6/5/5
54	PEE	Q	501	-	-	21/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	8Q1	X	201	-	-	20/41/41/41	-
52	FES	O	301	14	-	-	0/1/1/1
45	SF4	B	302	2	-	-	0/6/5/5
48	PLX	r	502	-	-	36/55/55/55	-
54	PEE	l	701	-	-	25/49/49/54	-
56	UQ	s	401	-	-	9/21/45/87	0/1/1/1
45	SF4	B	301	2	-	-	0/6/5/5
45	SF4	C	301	3,16	-	-	0/6/5/5
50	CDL	a	201	-	-	36/101/101/110	-
50	CDL	i	401	-	-	36/76/76/110	-
50	CDL	g	202	-	-	64/110/110/110	-
54	PEE	U	101	-	-	30/54/54/54	-
54	PEE	j	201	-	-	22/50/50/54	-
48	PLX	g	201	-	-	25/55/55/55	-
45	SF4	M	801	12	-	-	0/6/5/5
47	NAI	A	503	-	-	6/29/72/72	0/5/5/5
54	PEE	m	201	-	-	18/44/44/54	-

All (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	J	401	NDP	C3B-C2B	-12.79	1.24	1.52
51	J	401	NDP	C6N-C5N	12.45	1.55	1.33
51	J	401	NDP	O4D-C4D	10.69	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.28	1.26	1.53
51	J	401	NDP	C3D-C4D	-9.84	1.27	1.53
56	s	401	UQ	C13-C14	9.34	1.55	1.33
47	A	503	NAI	O4B-C1B	9.13	1.63	1.42
56	s	401	UQ	C8-C9	8.94	1.54	1.33
57	w	401	ADP	C3'-C4'	-8.81	1.30	1.53
47	A	503	NAI	O4B-C4B	-8.27	1.26	1.45
56	s	401	UQ	C18-C19	8.27	1.56	1.32
51	J	401	NDP	O4B-C4B	-8.07	1.27	1.45
57	w	401	ADP	O4'-C4'	7.78	1.62	1.45
47	A	503	NAI	C2D-C1D	-7.61	1.29	1.53
51	J	401	NDP	C2N-C3N	7.39	1.55	1.34
47	A	503	NAI	C2B-C1B	-7.28	1.30	1.53
47	A	503	NAI	O4D-C4D	6.89	1.60	1.45
47	A	503	NAI	C2D-C3D	5.93	1.69	1.53
51	J	401	NDP	C6A-N6A	5.92	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	C7N-N7N	5.77	1.48	1.33
51	J	401	NDP	P2B-O2B	5.65	1.70	1.59
57	w	401	ADP	C6-N6	5.57	1.48	1.34
49	X	201	8Q1	C39-N41	5.52	1.45	1.33
49	X	201	8Q1	C34-N36	5.45	1.45	1.33
49	G	201	8Q1	C34-N36	5.39	1.45	1.33
47	A	503	NAI	O4D-C1D	5.35	1.54	1.42
49	G	201	8Q1	C39-N41	5.35	1.45	1.33
51	J	401	NDP	C3B-C4B	5.33	1.66	1.53
47	A	503	NAI	C6A-N6A	5.17	1.47	1.34
47	A	503	NAI	C4N-C3N	-5.12	1.39	1.49
51	J	401	NDP	C6N-N1N	4.94	1.49	1.37
51	J	401	NDP	O4D-C1D	-4.92	1.30	1.42
51	J	401	NDP	C1B-N9A	-4.54	1.33	1.46
47	A	503	NAI	O2B-C2B	4.50	1.53	1.43
57	w	401	ADP	O4'-C1'	-4.48	1.31	1.42
51	J	401	NDP	O4B-C1B	4.44	1.52	1.42
51	J	401	NDP	O2D-C2D	-4.22	1.33	1.43
51	J	401	NDP	C7N-N7N	4.19	1.44	1.33
47	A	503	NAI	C6N-C5N	3.96	1.40	1.33
46	A	502	FMN	C4A-N5	3.82	1.38	1.30
54	j	201	PEE	C18-C19	3.75	1.53	1.31
54	m	201	PEE	C18-C19	3.74	1.53	1.31
54	i	402	PEE	C18-C19	3.73	1.53	1.31
54	r	501	PEE	C18-C19	3.72	1.53	1.31
54	Q	501	PEE	C18-C19	3.72	1.53	1.31
54	b	201	PEE	C18-C19	3.70	1.53	1.31
54	l	701	PEE	C18-C19	3.69	1.53	1.31
54	U	101	PEE	C18-C19	3.68	1.53	1.31
54	j	201	PEE	C39-C38	3.66	1.53	1.31
54	i	402	PEE	C39-C38	3.65	1.52	1.31
54	r	501	PEE	C39-C38	3.65	1.52	1.31
54	b	201	PEE	C39-C38	3.65	1.52	1.31
54	l	701	PEE	C39-C38	3.63	1.52	1.31
54	U	101	PEE	C39-C38	3.63	1.52	1.31
54	Q	501	PEE	C39-C38	3.62	1.52	1.31
47	A	503	NAI	C7N-C3N	3.56	1.56	1.48
50	i	401	CDL	OA8-CA7	3.50	1.43	1.33
50	I	201	CDL	OA8-CA7	3.45	1.43	1.33
50	g	202	CDL	OA8-CA7	3.41	1.43	1.33
47	A	503	NAI	C4N-C5N	-3.40	1.40	1.48
50	a	201	CDL	OA8-CA7	3.37	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	w	401	ADP	O2'-C2'	-3.35	1.35	1.43
57	w	401	ADP	C8-N9	-3.19	1.31	1.37
57	w	401	ADP	O3'-C3'	3.15	1.50	1.43
51	J	401	NDP	C8A-N9A	-3.10	1.32	1.37
50	a	201	CDL	OB6-CB5	3.08	1.43	1.34
51	J	401	NDP	O3D-C3D	3.07	1.50	1.43
50	i	401	CDL	OB6-CB5	3.04	1.42	1.34
51	J	401	NDP	C7N-C3N	3.03	1.55	1.48
50	I	201	CDL	OB8-CB7	3.02	1.42	1.33
51	J	401	NDP	C5A-N7A	-3.01	1.33	1.39
50	g	202	CDL	OB6-CB5	3.00	1.42	1.34
50	I	201	CDL	OB6-CB5	3.00	1.42	1.34
50	i	401	CDL	OA6-CA5	2.99	1.42	1.34
50	i	401	CDL	OB8-CB7	2.98	1.42	1.33
50	g	202	CDL	OB8-CB7	2.97	1.42	1.33
50	a	201	CDL	OA6-CA5	2.94	1.42	1.34
50	I	201	CDL	OA6-CA5	2.93	1.42	1.34
50	a	201	CDL	OB8-CB7	2.92	1.41	1.33
50	g	202	CDL	OA6-CA5	2.89	1.42	1.34
48	C	302	PLX	O6-C4	-2.87	1.40	1.44
48	r	502	PLX	O6-C4	-2.86	1.40	1.44
48	g	201	PLX	O6-C4	-2.84	1.40	1.44
56	s	401	UQ	C6-C1	2.68	1.54	1.46
54	Q	501	PEE	O2-C2	-2.62	1.40	1.46
47	A	503	NAI	C8A-N9A	-2.54	1.33	1.37
48	j	202	PLX	O6-C4	-2.53	1.41	1.44
54	l	701	PEE	O3-C30	2.51	1.40	1.33
54	j	201	PEE	O3-C30	2.49	1.40	1.33
54	l	701	PEE	O2-C2	-2.49	1.40	1.46
47	A	503	NAI	O3B-C3B	-2.48	1.37	1.43
54	U	101	PEE	O2-C2	-2.48	1.40	1.46
54	i	402	PEE	O3-C30	2.47	1.40	1.33
50	g	202	CDL	OA6-CA4	-2.46	1.40	1.46
54	b	201	PEE	O3-C30	2.44	1.40	1.33
54	b	201	PEE	O2-C2	-2.44	1.40	1.46
49	X	201	8Q1	C1-S44	2.43	1.82	1.76
54	r	501	PEE	O2-C2	-2.43	1.40	1.46
54	m	201	PEE	O3-C30	2.43	1.40	1.33
47	A	503	NAI	PN-O5D	2.42	1.69	1.59
51	J	401	NDP	O2B-C2B	2.42	1.52	1.44
54	U	101	PEE	O3-C30	2.42	1.40	1.33
54	Q	501	PEE	O3-C30	2.41	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	a	201	CDL	OA6-CA4	-2.40	1.40	1.46
50	I	201	CDL	OA6-CA4	-2.39	1.40	1.46
54	m	201	PEE	O2-C10	2.38	1.41	1.34
49	X	201	8Q1	C6-C1	2.37	1.53	1.50
46	A	502	FMN	C10-N1	2.37	1.38	1.33
48	j	202	PLX	C7-C6	2.37	1.55	1.50
54	j	201	PEE	O2-C2	-2.37	1.40	1.46
49	G	201	8Q1	C1-S44	2.36	1.81	1.76
54	r	501	PEE	O3-C30	2.35	1.40	1.33
54	i	402	PEE	O2-C10	2.34	1.40	1.34
49	G	201	8Q1	O35-C34	-2.32	1.18	1.23
51	J	401	NDP	C2D-C3D	2.32	1.59	1.53
54	j	201	PEE	O2-C10	2.31	1.40	1.34
50	i	401	CDL	OA6-CA4	-2.30	1.40	1.46
48	g	201	PLX	C7-C6	2.30	1.55	1.50
54	i	402	PEE	O2-C2	-2.29	1.40	1.46
48	r	502	PLX	C7-C6	2.28	1.55	1.50
57	w	401	ADP	C5-N7	-2.26	1.34	1.39
54	b	201	PEE	O2-C10	2.26	1.40	1.34
50	i	401	CDL	PB2-OB2	2.25	1.68	1.59
49	G	201	8Q1	O40-C39	-2.25	1.18	1.23
56	s	401	UQ	O4-C4	-2.25	1.18	1.23
48	C	302	PLX	C7-C6	2.24	1.55	1.50
50	i	401	CDL	PB2-OB5	2.23	1.68	1.59
49	X	201	8Q1	O35-C34	-2.22	1.19	1.23
54	m	201	PEE	O2-C2	-2.22	1.41	1.46
56	s	401	UQ	C7-C8	2.21	1.53	1.50
54	l	701	PEE	O2-C10	2.20	1.40	1.34
50	g	202	CDL	PB2-OB2	2.20	1.68	1.59
48	j	202	PLX	P1-O4	2.20	1.68	1.59
54	U	101	PEE	O2-C10	2.19	1.40	1.34
54	r	501	PEE	O2-C10	2.19	1.40	1.34
50	i	401	CDL	OB6-CB4	-2.17	1.41	1.46
49	X	201	8Q1	O40-C39	-2.17	1.18	1.23
47	A	503	NAI	C5B-C4B	2.17	1.58	1.51
50	I	201	CDL	PB2-OB5	2.17	1.68	1.59
50	I	201	CDL	OB6-CB4	-2.16	1.41	1.46
54	U	101	PEE	O3-C3	-2.15	1.40	1.45
51	J	401	NDP	O7N-C7N	-2.15	1.19	1.24
54	l	701	PEE	O3-C3	-2.15	1.40	1.45
54	r	501	PEE	O3-C3	-2.15	1.40	1.45
50	g	202	CDL	PB2-OB5	2.15	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	g	202	CDL	OB6-CB4	-2.14	1.41	1.46
50	a	201	CDL	PB2-OB5	2.13	1.67	1.59
50	I	201	CDL	PB2-OB2	2.13	1.67	1.59
50	a	201	CDL	PB2-OB2	2.12	1.67	1.59
54	Q	501	PEE	O2-C10	2.10	1.40	1.34
50	a	201	CDL	OB6-CB4	-2.09	1.41	1.46
54	b	201	PEE	O3-C3	-2.08	1.40	1.45
48	g	201	PLX	P1-O4	2.08	1.67	1.59
54	Q	501	PEE	O3-C3	-2.07	1.40	1.45
54	i	402	PEE	O3-C3	-2.07	1.40	1.45
48	j	202	PLX	P1-O1	2.06	1.67	1.59
47	A	503	NAI	C2N-C3N	2.05	1.40	1.34
48	r	502	PLX	P1-O4	2.04	1.67	1.59
51	J	401	NDP	PA-O5B	2.03	1.67	1.59
56	s	401	UQ	O1-C1	-2.01	1.19	1.23
47	A	503	NAI	C5A-N7A	-2.01	1.35	1.39
54	j	201	PEE	O3-C3	-2.00	1.40	1.45
48	C	302	PLX	P1-O1	2.00	1.67	1.59

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	s	401	UQ	C7-C8-C9	-9.26	111.38	126.79
51	J	401	NDP	C3N-C2N-N1N	-8.48	111.00	123.10
51	J	401	NDP	C1D-N1N-C2N	-6.65	110.04	121.11
49	G	201	8Q1	C6-C1-S44	6.05	120.50	113.46
49	X	201	8Q1	C6-C1-S44	5.97	120.41	113.46
51	J	401	NDP	C5A-C4A-N3A	-5.88	119.08	126.75
56	s	401	UQ	C12-C13-C14	-5.85	113.58	127.66
57	w	401	ADP	C5-C4-N3	-5.80	119.18	126.75
47	A	503	NAI	C5A-C4A-N3A	-5.77	119.22	126.75
51	J	401	NDP	C1D-N1N-C6N	-5.27	109.48	120.83
56	s	401	UQ	C11-C9-C8	-4.54	111.92	121.12
57	w	401	ADP	N3-C2-N1	-4.49	121.58	128.60
56	s	401	UQ	C10-C9-C8	-4.48	112.19	123.68
57	w	401	ADP	N3-C4-N9	4.46	134.43	127.08
54	m	201	PEE	O2-C10-C11	4.31	120.78	111.50
50	a	201	CDL	OA6-CA5-C11	4.23	120.63	111.50
47	A	503	NAI	N3A-C2A-N1A	-4.21	122.02	128.60
54	i	402	PEE	O2-C10-C11	4.16	120.46	111.50
50	i	401	CDL	OA6-CA5-C11	4.14	120.43	111.50
51	J	401	NDP	N3A-C4A-N9A	4.12	133.86	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	a	201	CDL	OB6-CB5-C51	4.10	120.34	111.50
51	J	401	NDP	N3A-C2A-N1A	-4.08	122.23	128.60
54	Q	501	PEE	O2-C10-C11	4.07	120.26	111.50
54	r	501	PEE	O2-C10-C11	4.05	120.23	111.50
50	g	202	CDL	OB6-CB5-C51	4.00	120.13	111.50
50	I	201	CDL	OA6-CA5-C11	4.00	120.12	111.50
50	i	401	CDL	OB6-CB5-C51	3.99	120.10	111.50
47	A	503	NAI	N3A-C4A-N9A	3.98	133.65	127.08
50	I	201	CDL	OB6-CB5-C51	3.97	120.06	111.50
56	s	401	UQ	C17-C18-C19	-3.97	114.19	127.75
54	l	701	PEE	O2-C10-C11	3.91	119.94	111.50
56	s	401	UQ	C15-C14-C13	-3.84	113.83	123.68
50	g	202	CDL	OA6-CA5-C11	3.83	119.76	111.50
54	j	201	PEE	O2-C10-C11	3.82	119.73	111.50
54	U	101	PEE	O2-C10-C11	3.81	119.71	111.50
47	A	503	NAI	C2A-N3A-C4A	3.80	120.73	111.75
56	s	401	UQ	C16-C14-C13	-3.80	113.43	121.12
57	w	401	ADP	C2-N3-C4	3.78	120.69	111.75
51	J	401	NDP	C2A-N3A-C4A	3.76	120.63	111.75
47	A	503	NAI	C5A-N7A-C8A	3.72	108.80	103.51
57	w	401	ADP	N9-C8-N7	-3.71	108.84	113.91
54	b	201	PEE	O2-C10-C11	3.60	119.25	111.50
49	G	201	8Q1	O4-C1-C6	-3.60	119.74	123.99
57	w	401	ADP	C5-N7-C8	3.57	108.58	103.51
47	A	503	NAI	N9A-C8A-N7A	-3.45	109.19	113.91
49	X	201	8Q1	O4-C1-C6	-3.43	119.94	123.99
56	s	401	UQ	C21-C19-C18	-3.34	113.00	122.65
47	A	503	NAI	C4A-C5A-N7A	-3.29	106.61	110.62
51	J	401	NDP	C5A-N7A-C8A	3.27	108.16	103.51
51	J	401	NDP	N9A-C8A-N7A	-3.22	109.52	113.91
49	G	201	8Q1	C37-C38-C39	3.16	117.61	112.36
47	A	503	NAI	C4D-O4D-C1D	-3.15	102.53	109.47
57	w	401	ADP	C4-N9-C8	3.14	109.14	105.73
46	A	502	FMN	C4-N3-C2	-3.12	119.88	125.64
56	s	401	UQ	C20-C19-C18	-3.00	113.96	122.65
51	J	401	NDP	C4A-C5A-N7A	-3.00	106.97	110.62
57	w	401	ADP	C4-C5-N7	-2.94	107.04	110.62
56	s	401	UQ	CM5-C5-C6	-2.91	119.65	124.40
47	A	503	NAI	C3D-C2D-C1D	2.79	106.73	101.43
47	A	503	NAI	PN-O3-PA	-2.77	123.32	132.83
51	J	401	NDP	C2B-C3B-C4B	2.76	107.98	101.99
54	l	701	PEE	O3-C30-C31	2.73	120.49	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	I	201	CDL	OB8-CB7-C71	2.72	120.45	111.91
54	r	501	PEE	O3-C30-C31	2.72	120.43	111.91
50	i	401	CDL	OB8-CB7-C71	2.70	120.39	111.91
54	m	201	PEE	O3-C30-C31	2.70	120.37	111.91
50	i	401	CDL	OA8-CA7-C31	2.69	120.36	111.91
50	I	201	CDL	OA8-CA7-C31	2.67	120.30	111.91
54	Q	501	PEE	O3-C30-C31	2.67	120.30	111.91
46	A	502	FMN	C4A-C4-N3	2.66	119.95	113.19
50	a	201	CDL	OB8-CB7-C71	2.66	120.25	111.91
51	J	401	NDP	PN-O3-PA	-2.61	123.86	132.83
50	g	202	CDL	OB8-CB7-C71	2.61	120.10	111.91
47	A	503	NAI	C2D-C3D-C4D	2.60	107.69	102.64
54	U	101	PEE	O3-C30-C31	2.60	120.06	111.91
54	i	402	PEE	O3-C30-C31	2.56	119.95	111.91
48	g	201	PLX	C1A-N1-C1	2.55	120.33	109.92
54	j	201	PEE	O3-C30-C31	2.55	119.90	111.91
54	b	201	PEE	O3-C30-C31	2.54	119.88	111.91
49	X	201	8Q1	C37-C38-C39	2.54	116.58	112.36
50	g	202	CDL	OA8-CA7-C31	2.50	119.76	111.91
46	A	502	FMN	C4A-C10-N10	2.48	120.10	116.48
48	r	502	PLX	C1A-N1-C1	2.48	120.05	109.92
46	A	502	FMN	O4-C4-C4A	-2.47	120.06	126.60
50	a	201	CDL	OA8-CA7-C31	2.46	119.62	111.91
48	j	202	PLX	C1A-N1-C1	2.43	119.84	109.92
51	J	401	NDP	C4A-N9A-C8A	2.38	108.30	105.73
57	w	401	ADP	PA-O3A-PB	-2.37	124.68	132.83
47	A	503	NAI	C4A-N9A-C8A	2.35	108.27	105.73
57	w	401	ADP	C4'-O4'-C1'	-2.30	104.40	109.47
49	X	201	8Q1	C43-S44-C1	2.28	108.97	101.87
49	X	201	8Q1	O4-C1-S44	-2.28	119.65	122.61
48	C	302	PLX	C1A-N1-C1	2.26	119.17	109.92
49	X	201	8Q1	C38-C39-N41	2.25	120.21	116.42
46	A	502	FMN	C10-C4A-N5	-2.24	120.10	124.86
54	Q	501	PEE	C2-O2-C10	-2.22	112.31	117.79
51	J	401	NDP	C2B-C1B-N9A	-2.22	109.80	113.53
49	G	201	8Q1	O4-C1-S44	-2.20	119.75	122.61
49	G	201	8Q1	C43-S44-C1	2.16	108.60	101.87
46	A	502	FMN	C9A-C5A-N5	-2.16	120.08	122.43
49	G	201	8Q1	C38-C39-N41	2.13	120.00	116.42
46	A	502	FMN	C4A-C10-N1	-2.10	119.86	124.73
46	A	502	FMN	C5A-C9A-N10	2.09	120.11	117.95
51	J	401	NDP	C4B-O4B-C1B	-2.03	105.00	109.47

There are no chirality outliers.

All (574) 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	C5B-O5B-PA-O1A
48	C	302	PLX	C3-C4-O6-C6
48	C	302	PLX	N1-C1-C2-O1
48	g	201	PLX	O7-C6-O6-C4
48	g	201	PLX	C3-O4-P1-O2
48	g	201	PLX	O9-C24-O8-C5
48	j	202	PLX	O7-C6-C7-C8
48	j	202	PLX	C7-C6-O6-C4
48	j	202	PLX	O7-C6-O6-C4
48	j	202	PLX	C3-O4-P1-O3
48	r	502	PLX	O7-C6-O6-C4
48	r	502	PLX	C3-O4-P1-O2
48	r	502	PLX	C2-O1-P1-O4
48	r	502	PLX	C2-O1-P1-O2
48	r	502	PLX	C2-O1-P1-O3
48	r	502	PLX	O9-C24-O8-C5
48	r	502	PLX	O9-C24-C25-C26
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-C34
49	G	201	8Q1	C31-C29-C32-O33
49	G	201	8Q1	N41-C42-C43-S44
49	G	201	8Q1	C28-O27-P24-O3
49	G	201	8Q1	C28-O27-P24-O2
49	G	201	8Q1	C28-O27-P24-O1
49	X	201	8Q1	O4-C1-S44-C43
49	X	201	8Q1	C6-C1-S44-C43
49	X	201	8Q1	O27-C28-C29-C32
49	X	201	8Q1	C28-C29-C32-C34
49	X	201	8Q1	C28-C29-C32-O33
49	X	201	8Q1	C30-C29-C32-C34
49	X	201	8Q1	C30-C29-C32-O33
49	X	201	8Q1	C31-C29-C32-C34
49	X	201	8Q1	C31-C29-C32-O33
49	X	201	8Q1	N36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
49	X	201	8Q1	C42-C43-S44-C1
49	X	201	8Q1	C28-O27-P24-O3
49	X	201	8Q1	C28-O27-P24-O2
49	X	201	8Q1	C28-O27-P24-O1
50	I	201	CDL	O1-C1-CA2-OA2
50	I	201	CDL	O1-C1-CB2-OB2
50	I	201	CDL	CA2-OA2-PA1-OA4
50	I	201	CDL	OA5-CA3-CA4-OA6
50	I	201	CDL	CB2-OB2-PB2-OB3
50	I	201	CDL	CB2-OB2-PB2-OB4
50	I	201	CDL	CB2-OB2-PB2-OB5
50	I	201	CDL	CB3-OB5-PB2-OB3
50	a	201	CDL	CA2-OA2-PA1-OA3
50	a	201	CDL	CA2-OA2-PA1-OA4
50	a	201	CDL	CA2-OA2-PA1-OA5
50	a	201	CDL	CB3-OB5-PB2-OB3
50	g	202	CDL	CA2-OA2-PA1-OA3
50	g	202	CDL	CA2-OA2-PA1-OA4
50	g	202	CDL	CA3-OA5-PA1-OA3
50	g	202	CDL	CA3-OA5-PA1-OA4
50	g	202	CDL	OA6-CA4-CA6-OA8
50	g	202	CDL	CB3-OB5-PB2-OB3
50	i	401	CDL	CA2-OA2-PA1-OA4
50	i	401	CDL	CB2-OB2-PB2-OB3
50	i	401	CDL	CB2-OB2-PB2-OB4
51	J	401	NDP	C5B-O5B-PA-O3
51	J	401	NDP	C2N-C3N-C7N-N7N
54	U	101	PEE	C1-O3P-P-O2P
54	U	101	PEE	C1-O3P-P-O1P
54	b	201	PEE	C1-O3P-P-O1P
54	i	402	PEE	C1-O3P-P-O2P
54	i	402	PEE	C1-O3P-P-O1P
54	i	402	PEE	C4-O4P-P-O2P
54	j	201	PEE	C11-C10-O2-C2
54	j	201	PEE	C1-O3P-P-O2P
54	j	201	PEE	C1-O3P-P-O1P
54	l	701	PEE	C11-C10-O2-C2
54	l	701	PEE	C4-O4P-P-O3P
54	l	701	PEE	C4-O4P-P-O2P
54	l	701	PEE	C4-O4P-P-O1P
54	m	201	PEE	C11-C10-O2-C2
54	m	201	PEE	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
54	r	501	PEE	C1-O3P-P-O2P
54	r	501	PEE	C1-O3P-P-O1P
54	r	501	PEE	C1-O3P-P-O4P
54	r	501	PEE	C4-O4P-P-O3P
54	r	501	PEE	C4-O4P-P-O2P
54	r	501	PEE	C4-O4P-P-O1P
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-C11-C9-C10
56	s	401	UQ	C9-C11-C12-C13
56	s	401	UQ	C12-C13-C14-C16
56	s	401	UQ	C14-C16-C17-C18
57	w	401	ADP	C5'-O5'-PA-O3A
50	i	401	CDL	OA9-CA7-OA8-CA6
50	i	401	CDL	C31-CA7-OA8-CA6
56	s	401	UQ	C17-C18-C19-C21
54	b	201	PEE	O5-C30-O3-C3
54	i	402	PEE	O4-C10-O2-C2
54	j	201	PEE	O4-C10-O2-C2
54	l	701	PEE	O4-C10-O2-C2
54	m	201	PEE	O4-C10-O2-C2
54	i	402	PEE	C11-C10-O2-C2
50	g	202	CDL	OB9-CB7-OB8-CB6
48	C	302	PLX	C28-C29-C30-C31
54	b	201	PEE	C31-C30-O3-C3
54	l	701	PEE	C31-C30-O3-C3
54	Q	501	PEE	C17-C18-C19-C20
54	Q	501	PEE	C37-C38-C39-C40
54	U	101	PEE	C17-C18-C19-C20
54	b	201	PEE	C37-C38-C39-C40
54	r	501	PEE	C17-C18-C19-C20
54	m	201	PEE	O5-C30-O3-C3
50	g	202	CDL	O1-C1-CA2-OA2
50	g	202	CDL	C71-CB7-OB8-CB6
54	l	701	PEE	O5-C30-O3-C3
51	J	401	NDP	C2D-C1D-N1N-C6N
48	j	202	PLX	C28-C29-C30-C31
48	r	502	PLX	C12-C13-C14-C15
50	i	401	CDL	C31-C32-C33-C34
51	J	401	NDP	O4B-C4B-C5B-O5B
54	m	201	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
56	s	401	UQ	C13-C14-C16-C17
48	g	201	PLX	C7-C8-C9-C10
50	I	201	CDL	CB2-C1-CA2-OA2
50	I	201	CDL	CA2-C1-CB2-OB2
50	g	202	CDL	CB2-C1-CA2-OA2
50	i	401	CDL	C71-CB7-OB8-CB6
50	g	202	CDL	C74-C75-C76-C77
50	i	401	CDL	OB9-CB7-OB8-CB6
48	j	202	PLX	C15-C16-C17-C18
54	U	101	PEE	C31-C30-O3-C3
50	I	201	CDL	CA7-C31-C32-C33
50	g	202	CDL	C83-C84-C85-C86
50	g	202	CDL	CB5-C51-C52-C53
50	g	202	CDL	CB7-C71-C72-C73
50	i	401	CDL	CA7-C31-C32-C33
50	i	401	CDL	CB7-C71-C72-C73
51	J	401	NDP	C3B-C4B-C5B-O5B
50	a	201	CDL	C31-C32-C33-C34
50	I	201	CDL	CB7-C71-C72-C73
54	r	501	PEE	C10-C11-C12-C13
54	Q	501	PEE	C12-C13-C14-C15
50	i	401	CDL	O1-C1-CA2-OA2
50	g	202	CDL	CA7-C31-C32-C33
54	i	402	PEE	C17-C18-C19-C20
54	U	101	PEE	O5-C30-O3-C3
50	g	202	CDL	C51-CB5-OB6-CB4
54	U	101	PEE	C11-C10-O2-C2
48	C	302	PLX	C3-O4-P1-O1
48	a	202	PLX	C3-O4-P1-O1
48	j	202	PLX	C3-O4-P1-O1
48	r	502	PLX	C3-O4-P1-O1
50	I	201	CDL	CA2-OA2-PA1-OA5
50	I	201	CDL	CB3-OB5-PB2-OB2
50	a	201	CDL	CA3-OA5-PA1-OA2
50	g	202	CDL	CA2-OA2-PA1-OA5
50	g	202	CDL	CA3-OA5-PA1-OA2
50	g	202	CDL	CB2-OB2-PB2-OB5
50	g	202	CDL	CB3-OB5-PB2-OB2
50	i	401	CDL	CA2-OA2-PA1-OA5
50	i	401	CDL	CA3-OA5-PA1-OA2
50	i	401	CDL	CB2-OB2-PB2-OB5
54	U	101	PEE	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
54	i	402	PEE	C1-O3P-P-O4P
54	i	402	PEE	C4-O4P-P-O3P
54	j	201	PEE	C1-O3P-P-O4P
54	m	201	PEE	C4-O4P-P-O3P
50	a	201	CDL	C71-CB7-OB8-CB6
50	g	202	CDL	C78-C79-C80-C81
50	g	202	CDL	CA5-C11-C12-C13
50	i	401	CDL	CB2-C1-CA2-OA2
54	U	101	PEE	O4-C10-O2-C2
48	C	302	PLX	O8-C24-C25-C26
54	l	701	PEE	C30-C31-C32-C33
48	g	201	PLX	C33-C34-C35-C36
48	g	201	PLX	C32-C33-C34-C35
50	i	401	CDL	C52-C53-C54-C55
49	X	201	8Q1	O27-C28-C29-C30
49	X	201	8Q1	O27-C28-C29-C31
48	C	302	PLX	C17-C18-C19-C20
48	j	202	PLX	C25-C26-C27-C28
50	a	201	CDL	C75-C76-C77-C78
50	g	202	CDL	C56-C57-C58-C59
50	i	401	CDL	C11-C12-C13-C14
54	Q	501	PEE	C22-C23-C24-C25
54	Q	501	PEE	C33-C34-C35-C36
54	m	201	PEE	C11-C12-C13-C14
50	g	202	CDL	OB7-CB5-OB6-CB4
50	I	201	CDL	CB5-C51-C52-C53
48	g	201	PLX	C9-C10-C11-C12
50	a	201	CDL	C11-C12-C13-C14
54	j	201	PEE	C37-C38-C39-C40
50	a	201	CDL	C37-C38-C39-C40
50	g	202	CDL	C71-C72-C73-C74
48	g	201	PLX	C10-C11-C12-C13
48	r	502	PLX	C13-C14-C15-C16
48	j	202	PLX	C12-C13-C14-C15
54	Q	501	PEE	C34-C35-C36-C37
50	a	201	CDL	OB9-CB7-OB8-CB6
48	g	201	PLX	C11-C10-C9-C8
50	g	202	CDL	C55-C56-C57-C58
50	i	401	CDL	C71-C72-C73-C74
50	a	201	CDL	CA7-C31-C32-C33
48	C	302	PLX	C25-C26-C27-C28
48	j	202	PLX	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
48	r	502	PLX	C14-C15-C16-C17
50	a	201	CDL	C73-C74-C75-C76
50	g	202	CDL	C17-C18-C19-C20
50	g	202	CDL	C73-C74-C75-C76
50	g	202	CDL	C75-C76-C77-C78
50	g	202	CDL	C82-C83-C84-C85
54	l	701	PEE	C23-C24-C25-C26
54	r	501	PEE	C31-C32-C33-C34
54	U	101	PEE	C43-C44-C45-C46
50	I	201	CDL	OB7-CB5-OB6-CB4
50	I	201	CDL	C51-CB5-OB6-CB4
48	C	302	PLX	C13-C14-C15-C16
48	r	502	PLX	C27-C28-C29-C30
49	G	201	8Q1	C11-C12-C13-C14
48	C	302	PLX	C33-C34-C35-C36
48	g	201	PLX	C27-C28-C29-C30
48	j	202	PLX	C10-C11-C12-C13
50	a	201	CDL	C17-C18-C19-C20
50	a	201	CDL	C32-C33-C34-C35
50	g	202	CDL	C81-C82-C83-C84
54	b	201	PEE	C12-C13-C14-C15
54	l	701	PEE	C31-C32-C33-C34
48	r	502	PLX	C2-C1-N1-C1A
48	g	201	PLX	C30-C31-C32-C33
50	I	201	CDL	C11-C12-C13-C14
50	g	202	CDL	C32-C33-C34-C35
54	j	201	PEE	C42-C43-C44-C45
48	C	302	PLX	C30-C31-C32-C33
48	j	202	PLX	C14-C15-C16-C17
50	i	401	CDL	C35-C36-C37-C38
48	a	202	PLX	C10-C11-C12-C13
49	G	201	8Q1	C7-C8-C9-C10
50	a	201	CDL	C21-C22-C23-C24
48	j	202	PLX	C13-C14-C15-C16
48	r	502	PLX	C25-C26-C27-C28
54	j	201	PEE	C13-C14-C15-C16
54	r	501	PEE	C12-C13-C14-C15
54	b	201	PEE	C17-C18-C19-C20
48	g	201	PLX	C28-C29-C30-C31
49	G	201	8Q1	C12-C13-C14-C15
54	j	201	PEE	C10-C11-C12-C13
48	j	202	PLX	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
54	r	501	PEE	C11-C10-O2-C2
48	C	302	PLX	O9-C24-C25-C26
48	a	202	PLX	O7-C6-C7-C8
50	g	202	CDL	C62-C63-C64-C65
54	U	101	PEE	C23-C24-C25-C26
54	b	201	PEE	C33-C34-C35-C36
48	C	302	PLX	C16-C17-C18-C19
50	i	401	CDL	C14-C15-C16-C17
48	g	201	PLX	C25-C26-C27-C28
48	r	502	PLX	C28-C29-C30-C31
54	r	501	PEE	O4-C10-O2-C2
54	i	402	PEE	C2-C1-O3P-P
50	g	202	CDL	C41-C42-C43-C44
50	i	401	CDL	C36-C37-C38-C39
54	i	402	PEE	C32-C33-C34-C35
48	r	502	PLX	C2-C1-N1-C1C
50	a	201	CDL	C71-C72-C73-C74
50	g	202	CDL	C43-C44-C45-C46
48	a	202	PLX	C7-C8-C9-C10
48	C	302	PLX	C15-C16-C17-C18
54	m	201	PEE	C33-C34-C35-C36
48	C	302	PLX	C14-C15-C16-C17
50	g	202	CDL	C59-C60-C61-C62
50	g	202	CDL	C20-C21-C22-C23
48	C	302	PLX	C7-C8-C9-C10
54	b	201	PEE	C31-C32-C33-C34
49	G	201	8Q1	N36-C37-C38-C39
48	j	202	PLX	C9-C10-C11-C12
54	Q	501	PEE	C11-C10-O2-C2
50	a	201	CDL	OA5-CA3-CA4-OA6
54	l	701	PEE	O3P-C1-C2-O2
48	j	202	PLX	C26-C27-C28-C29
50	a	201	CDL	C54-C55-C56-C57
50	g	202	CDL	C52-C53-C54-C55
50	g	202	CDL	OB6-CB4-CB6-OB8
48	g	201	PLX	C14-C15-C16-C17
54	i	402	PEE	C19-C20-C21-C22
54	i	402	PEE	C35-C36-C37-C38
54	m	201	PEE	C13-C14-C15-C16
54	i	402	PEE	C22-C23-C24-C25
50	g	202	CDL	C14-C15-C16-C17
54	Q	501	PEE	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
48	r	502	PLX	C10-C11-C12-C13
54	U	101	PEE	C36-C37-C38-C39
54	i	402	PEE	C18-C19-C20-C21
48	j	202	PLX	O4-C3-C4-C5
50	I	201	CDL	OA5-CA3-CA4-CA6
50	a	201	CDL	C52-C53-C54-C55
50	g	202	CDL	C11-C12-C13-C14
50	i	401	CDL	C32-C33-C34-C35
54	U	101	PEE	C34-C35-C36-C37
49	X	201	8Q1	C9-C10-C11-C12
48	r	502	PLX	C15-C16-C17-C18
48	C	302	PLX	C27-C28-C29-C30
48	r	502	PLX	C3-C4-C5-O8
50	g	202	CDL	CA3-CA4-CA6-OA8
50	g	202	CDL	C42-C43-C44-C45
50	g	202	CDL	CB3-CB4-CB6-OB8
54	b	201	PEE	C1-C2-C3-O3
54	i	402	PEE	C1-C2-C3-O3
54	j	201	PEE	C1-C2-C3-O3
54	j	201	PEE	C32-C33-C34-C35
48	r	502	PLX	C31-C32-C33-C34
50	g	202	CDL	C35-C36-C37-C38
54	U	101	PEE	C21-C22-C23-C24
48	C	302	PLX	C9-C10-C11-C12
48	r	502	PLX	C29-C30-C31-C32
54	i	402	PEE	C23-C24-C25-C26
54	r	501	PEE	C41-C42-C43-C44
48	C	302	PLX	O6-C6-C7-C8
48	r	502	PLX	O8-C24-C25-C26
48	r	502	PLX	C36-C37-C38-C39
54	Q	501	PEE	C10-C11-C12-C13
48	r	502	PLX	C9-C10-C11-C12
50	I	201	CDL	C52-C53-C54-C55
54	r	501	PEE	C40-C41-C42-C43
50	a	201	CDL	C35-C36-C37-C38
48	C	302	PLX	C31-C32-C33-C34
50	I	201	CDL	C31-CA7-OA8-CA6
48	r	502	PLX	C2-C1-N1-C1B
50	g	202	CDL	C60-C61-C62-C63
50	g	202	CDL	C64-C65-C66-C67
50	i	401	CDL	C74-C75-C76-C77
48	j	202	PLX	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
48	r	502	PLX	C30-C31-C32-C33
54	r	501	PEE	C11-C12-C13-C14
49	G	201	8Q1	C30-C29-C32-O33
49	X	201	8Q1	C7-C8-C9-C10
54	b	201	PEE	C11-C10-O2-C2
50	i	401	CDL	C73-C74-C75-C76
54	i	402	PEE	C24-C25-C26-C27
54	l	701	PEE	C24-C25-C26-C27
54	r	501	PEE	C36-C37-C38-C39
50	I	201	CDL	OB5-CB3-CB4-CB6
50	a	201	CDL	OA5-CA3-CA4-CA6
54	l	701	PEE	O3P-C1-C2-C3
49	G	201	8Q1	C11-C10-C9-C8
54	U	101	PEE	C32-C33-C34-C35
48	r	502	PLX	C7-C8-C9-C10
54	j	201	PEE	C31-C30-O3-C3
48	r	502	PLX	C33-C34-C35-C36
50	I	201	CDL	C71-CB7-OB8-CB6
54	r	501	PEE	C1-C2-C3-O3
48	r	502	PLX	C26-C27-C28-C29
48	a	202	PLX	C11-C12-C13-C14
48	j	202	PLX	C34-C35-C36-C37
48	r	502	PLX	C11-C12-C13-C14
48	C	302	PLX	O7-C6-C7-C8
48	C	302	PLX	O4-C3-C4-O6
48	j	202	PLX	O4-C3-C4-O6
50	I	201	CDL	OB5-CB3-CB4-OB6
54	Q	501	PEE	O3P-C1-C2-O2
50	I	201	CDL	OA9-CA7-OA8-CA6
48	j	202	PLX	O6-C4-C5-O8
48	r	502	PLX	O6-C4-C5-O8
50	i	401	CDL	OB6-CB4-CB6-OB8
54	U	101	PEE	O2-C2-C3-O3
54	b	201	PEE	O2-C2-C3-O3
54	i	402	PEE	O2-C2-C3-O3
50	I	201	CDL	C11-CA5-OA6-CA4
54	b	201	PEE	C22-C23-C24-C25
54	b	201	PEE	O4-C10-O2-C2
48	j	202	PLX	C30-C31-C32-C33
50	g	202	CDL	C72-C73-C74-C75
54	U	101	PEE	C38-C39-C40-C41
54	m	201	PEE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
47	A	503	NAI	C2D-C1D-N1N-C2N
54	U	101	PEE	C41-C42-C43-C44
48	C	302	PLX	O4-C3-C4-C5
54	Q	501	PEE	O3P-C1-C2-C3
50	a	201	CDL	C60-C61-C62-C63
54	l	701	PEE	C33-C34-C35-C36
51	J	401	NDP	O4D-C4D-C5D-O5D
48	g	201	PLX	C12-C13-C14-C15
54	Q	501	PEE	C15-C16-C17-C18
48	j	202	PLX	C3-C4-C5-O8
50	I	201	CDL	CA3-CA4-CA6-OA8
54	U	101	PEE	C1-C2-C3-O3
54	b	201	PEE	C32-C33-C34-C35
48	g	201	PLX	C36-C37-C38-C39
50	I	201	CDL	OA7-CA5-OA6-CA4
49	G	201	8Q1	C30-C29-C32-C34
50	I	201	CDL	OB9-CB7-OB8-CB6
50	i	401	CDL	C15-C16-C17-C18
50	I	201	CDL	OA6-CA4-CA6-OA8
54	j	201	PEE	O2-C2-C3-O3
54	j	201	PEE	O5-C30-O3-C3
49	X	201	8Q1	C12-C13-C14-C15
50	i	401	CDL	C75-C76-C77-C78
54	Q	501	PEE	C19-C20-C21-C22
54	b	201	PEE	C13-C14-C15-C16
48	a	202	PLX	C11-C10-C9-C8
48	g	201	PLX	C3-O4-P1-O1
50	a	201	CDL	CB3-OB5-PB2-OB2
54	l	701	PEE	C14-C15-C16-C17
48	C	302	PLX	C3-O4-P1-O3
48	a	202	PLX	C3-O4-P1-O2
48	j	202	PLX	C3-O4-P1-O2
48	j	202	PLX	C2-O1-P1-O3
50	I	201	CDL	CB3-OB5-PB2-OB4
50	a	201	CDL	CA3-OA5-PA1-OA4
50	a	201	CDL	CB2-OB2-PB2-OB4
50	g	202	CDL	CB2-OB2-PB2-OB3
50	g	202	CDL	CB2-OB2-PB2-OB4
50	i	401	CDL	CA3-OA5-PA1-OA4
51	J	401	NDP	C5B-O5B-PA-O1A
51	J	401	NDP	C5B-O5B-PA-O2A
54	U	101	PEE	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
54	U	101	PEE	C4-O4P-P-O1P
54	m	201	PEE	C4-O4P-P-O2P
54	m	201	PEE	C4-O4P-P-O1P
57	w	401	ADP	C5'-O5'-PA-O2A
48	g	201	PLX	O4-C3-C4-C5
48	j	202	PLX	C25-C24-O8-C5
54	r	501	PEE	C31-C30-O3-C3
47	A	503	NAI	C3D-C4D-C5D-O5D
48	g	201	PLX	O4-C3-C4-O6
50	g	202	CDL	OB5-CB3-CB4-OB6
50	a	201	CDL	CB5-C51-C52-C53
54	b	201	PEE	C30-C31-C32-C33
54	i	402	PEE	C30-C31-C32-C33
51	J	401	NDP	C2N-C3N-C7N-O7N
54	l	701	PEE	C1-C2-C3-O3
50	i	401	CDL	OA6-CA4-CA6-OA8
54	l	701	PEE	O2-C2-C3-O3
54	r	501	PEE	O2-C2-C3-O3
50	I	201	CDL	C72-C73-C74-C75
54	i	402	PEE	C31-C30-O3-C3
54	r	501	PEE	C38-C39-C40-C41
50	g	202	CDL	CB4-CB3-OB5-PB2
48	g	201	PLX	O8-C24-C25-C26
54	i	402	PEE	O5-C30-O3-C3
54	r	501	PEE	O5-C30-O3-C3
48	g	201	PLX	O7-C6-C7-C8
48	g	201	PLX	O9-C24-C25-C26
48	j	202	PLX	O9-C24-C25-C26
54	U	101	PEE	C44-C45-C46-C47
54	b	201	PEE	C11-C12-C13-C14
48	r	502	PLX	C19-C20-C21-C22
54	m	201	PEE	C3-C2-O2-C10
50	g	202	CDL	C31-C32-C33-C34
48	a	202	PLX	O4-C3-C4-O6
47	A	503	NAI	O4D-C1D-N1N-C2N
54	Q	501	PEE	C30-C31-C32-C33
54	Q	501	PEE	C14-C15-C16-C17
50	g	202	CDL	C76-C77-C78-C79
54	r	501	PEE	C33-C34-C35-C36
54	j	201	PEE	C38-C39-C40-C41
54	U	101	PEE	C40-C41-C42-C43
48	a	202	PLX	C2-O1-P1-O4

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Mol	Chain	Res	Type	Atoms
50	i	401	CDL	CB3-OB5-PB2-OB2
54	U	101	PEE	C4-O4P-P-O3P
50	a	201	CDL	C55-C56-C57-C58
50	g	202	CDL	C23-C24-C25-C26
48	j	202	PLX	C31-C32-C33-C34
51	J	401	NDP	PN-O3-PA-O1A
54	i	402	PEE	C11-C12-C13-C14
54	l	701	PEE	C35-C36-C37-C38
54	l	701	PEE	C37-C38-C39-C40
54	b	201	PEE	C18-C19-C20-C21
48	C	302	PLX	C11-C10-C9-C8
50	i	401	CDL	C12-C13-C14-C15
54	Q	501	PEE	C38-C39-C40-C41
48	r	502	PLX	C16-C17-C18-C19
50	g	202	CDL	C80-C81-C82-C83
48	a	202	PLX	C34-C35-C36-C37
54	b	201	PEE	C39-C40-C41-C42
48	j	202	PLX	O6-C6-C7-C8
54	j	201	PEE	C20-C21-C22-C23
54	m	201	PEE	C16-C17-C18-C19
47	A	503	NAI	C2D-C1D-N1N-C6N
54	U	101	PEE	C22-C23-C24-C25
54	Q	501	PEE	C13-C14-C15-C16
50	a	201	CDL	C36-C37-C38-C39
54	l	701	PEE	C34-C35-C36-C37
54	b	201	PEE	C38-C39-C40-C41
54	l	701	PEE	C32-C33-C34-C35
48	C	302	PLX	C26-C27-C28-C29
54	l	701	PEE	C13-C14-C15-C16
54	l	701	PEE	C19-C20-C21-C22
50	g	202	CDL	OB5-CB3-CB4-CB6
50	i	401	CDL	O1-C1-CB2-OB2
49	G	201	8Q1	C42-C43-S44-C1
50	i	401	CDL	C72-C73-C74-C75
54	U	101	PEE	C37-C38-C39-C40
54	j	201	PEE	C17-C18-C19-C20
48	r	502	PLX	C18-C19-C20-C21
54	m	201	PEE	O3-C30-C31-C32
54	Q	501	PEE	O5-C30-O3-C3
48	j	202	PLX	C18-C19-C20-C21
48	g	201	PLX	C13-C14-C15-C16
54	Q	501	PEE	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
54	m	201	PEE	C18-C19-C20-C21
48	r	502	PLX	C24-C25-C26-C27
48	a	202	PLX	O6-C6-C7-C8
48	a	202	PLX	O4-C3-C4-C5
54	Q	501	PEE	C31-C30-O3-C3
54	b	201	PEE	O4P-C4-C5-N
54	j	201	PEE	O4P-C4-C5-N
54	j	201	PEE	C18-C19-C20-C21
50	a	201	CDL	C32-C31-CA7-OA8
50	a	201	CDL	CA2-C1-CB2-OB2
54	b	201	PEE	C34-C35-C36-C37
50	g	202	CDL	C52-C51-CB5-OB6
51	J	401	NDP	C3D-C4D-C5D-O5D
54	U	101	PEE	C16-C17-C18-C19
49	X	201	8Q1	O33-C32-C34-N36
50	I	201	CDL	C52-C51-CB5-OB6
48	g	201	PLX	C16-C17-C18-C19
54	b	201	PEE	C1-O3P-P-O4P
49	G	201	8Q1	O27-C28-C29-C30
50	a	201	CDL	C76-C77-C78-C79
54	U	101	PEE	O3-C30-C31-C32
54	j	201	PEE	O3-C30-C31-C32
54	i	402	PEE	C36-C37-C38-C39
54	i	402	PEE	C38-C39-C40-C41
54	l	701	PEE	C16-C17-C18-C19
47	A	503	NAI	O4D-C1D-N1N-C6N
54	l	701	PEE	C36-C37-C38-C39
50	i	401	CDL	CA3-CA4-CA6-OA8
50	i	401	CDL	CB3-CB4-CB6-OB8
48	C	302	PLX	C11-C12-C13-C14
48	r	502	PLX	O4-C3-C4-O6
50	g	202	CDL	C44-C45-C46-C47
54	b	201	PEE	C16-C17-C18-C19
50	I	201	CDL	C12-C11-CA5-OA6
54	r	501	PEE	C43-C44-C45-C46
50	a	201	CDL	OB6-CB4-CB6-OB8
50	g	202	CDL	C54-C55-C56-C57
54	Q	501	PEE	C18-C19-C20-C21
54	U	101	PEE	O2-C10-C11-C12
50	a	201	CDL	C18-C19-C20-C21
54	b	201	PEE	C23-C24-C25-C26
57	w	401	ADP	PB-O3A-PA-O2A

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Mol	Chain	Res	Type	Atoms
54	r	501	PEE	C24-C25-C26-C27
50	g	202	CDL	C31-CA7-OA8-CA6
48	C	302	PLX	C18-C19-C20-C21
54	U	101	PEE	O5-C30-C31-C32
50	g	202	CDL	C52-C51-CB5-OB7
54	m	201	PEE	C31-C32-C33-C34
50	a	201	CDL	CB3-CB4-CB6-OB8
54	j	201	PEE	C11-C12-C13-C14
48	C	302	PLX	C36-C37-C38-C39
50	I	201	CDL	C72-C71-CB7-OB8
54	r	501	PEE	C34-C35-C36-C37
50	I	201	CDL	C12-C11-CA5-OA7
54	r	501	PEE	C20-C21-C22-C23
50	I	201	CDL	C31-C32-C33-C34
50	g	202	CDL	C36-C37-C38-C39
48	a	202	PLX	C2-O1-P1-O2
50	I	201	CDL	CA3-OA5-PA1-OA3
50	i	401	CDL	CB3-OB5-PB2-OB3
54	m	201	PEE	C1-O3P-P-O1P
57	w	401	ADP	C5'-O5'-PA-O1A
50	I	201	CDL	C52-C51-CB5-OB7
54	j	201	PEE	O5-C30-C31-C32
54	i	402	PEE	C31-C32-C33-C34
54	U	101	PEE	O4-C10-C11-C12
48	g	201	PLX	C25-C24-O8-C5
54	b	201	PEE	C5-C4-O4P-P
50	a	201	CDL	OA9-CA7-OA8-CA6
50	g	202	CDL	OA9-CA7-OA8-CA6
48	j	202	PLX	C32-C33-C34-C35
50	I	201	CDL	C72-C71-CB7-OB9

There are no ring outliers.

24 monomers are involved in 97 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	j	202	PLX	2	0
46	A	502	FMN	4	0
54	r	501	PEE	5	0
54	b	201	PEE	2	0
57	w	401	ADP	3	0
48	a	202	PLX	14	0
52	M	803	FES	1	0

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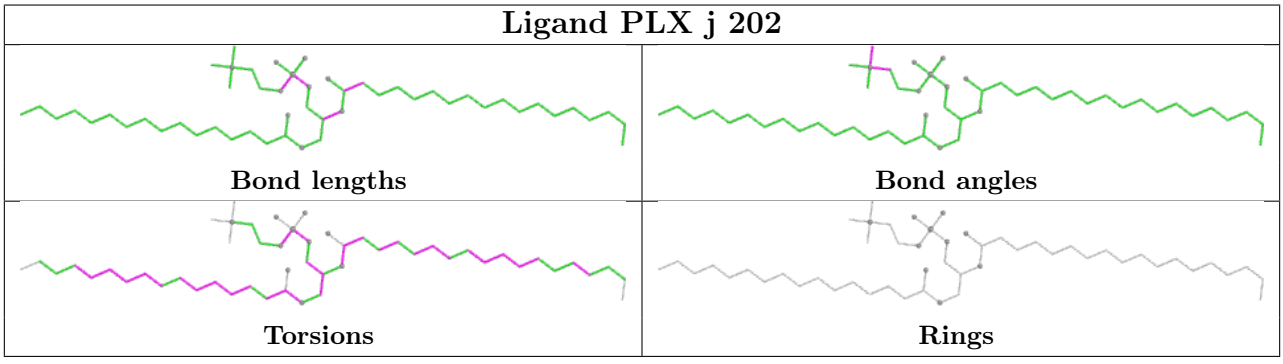
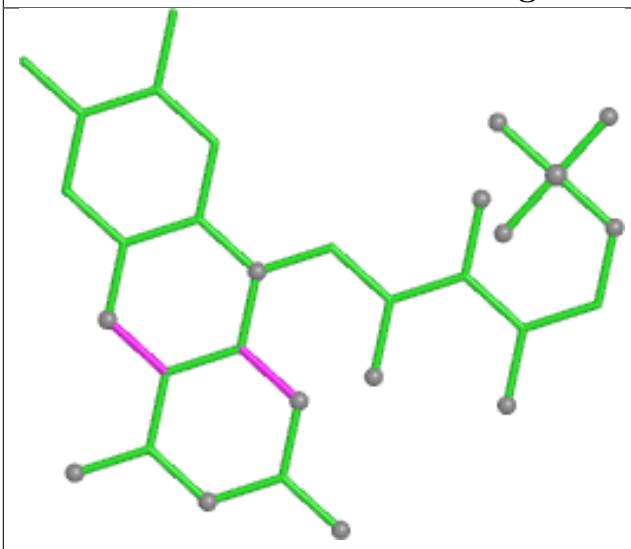
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	A	501	SF4	2	0
51	J	401	NDP	5	0
48	C	302	PLX	2	0
54	i	402	PEE	4	0
49	G	201	8Q1	1	0
54	Q	501	PEE	3	0
49	X	201	8Q1	8	0
48	r	502	PLX	3	0
56	s	401	UQ	5	0
45	C	301	SF4	1	0
50	a	201	CDL	4	0
50	i	401	CDL	5	0
50	g	202	CDL	8	0
54	U	101	PEE	2	0
48	g	201	PLX	8	0
47	A	503	NAI	5	0
54	m	201	PEE	1	0

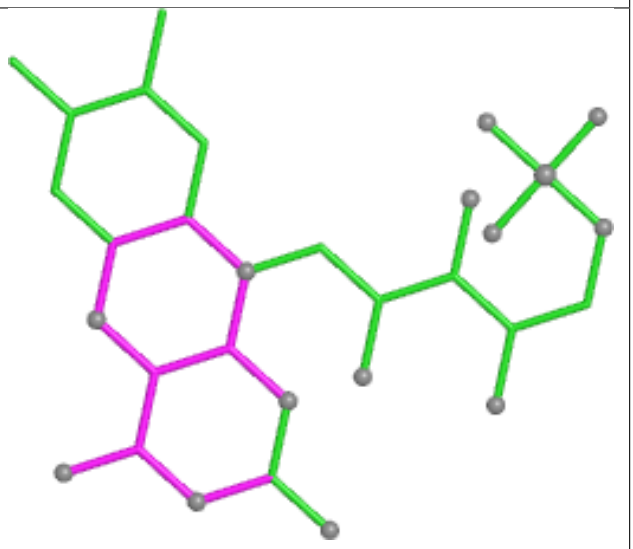
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.



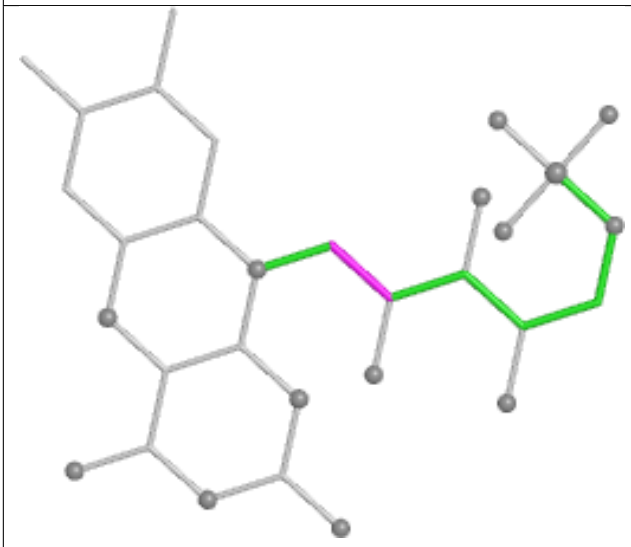
Ligand FMN A 502



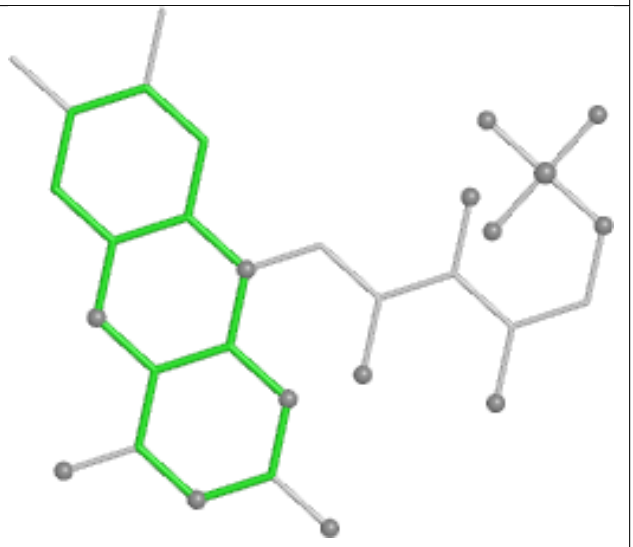
Bond lengths



Bond angles

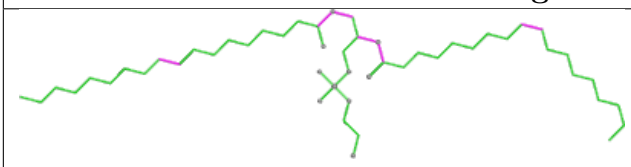


Torsions

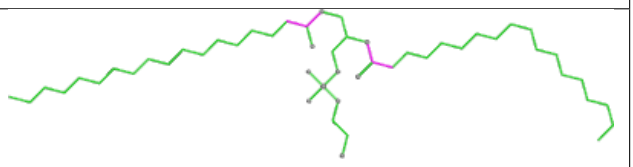


Rings

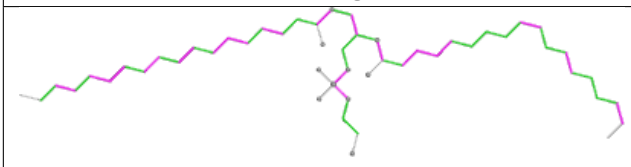
Ligand PEE r 501



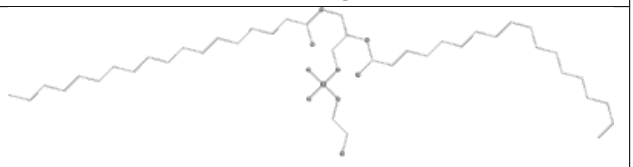
Bond lengths



Bond angles

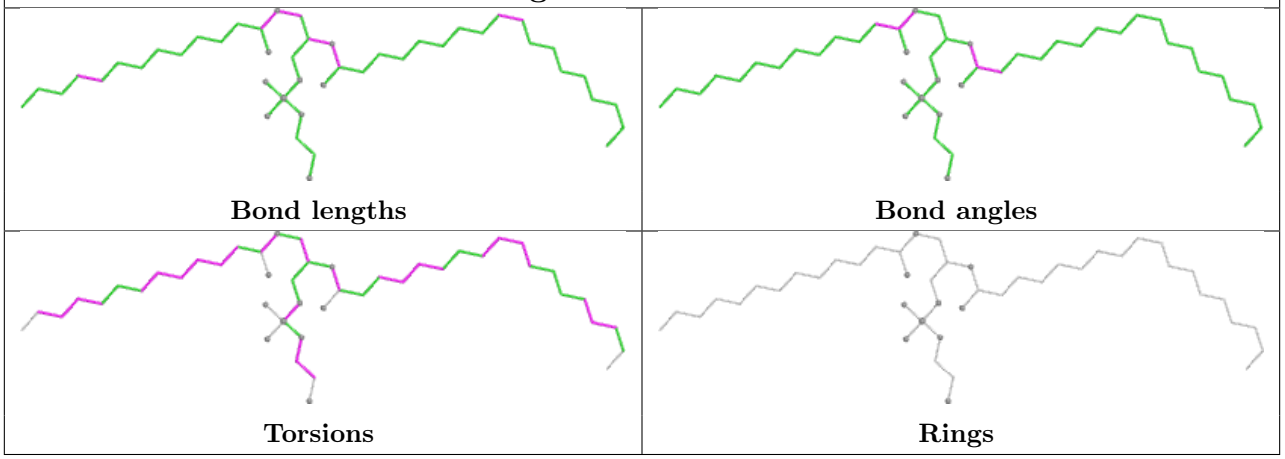


Torsions



Rings

Ligand PEE b 201



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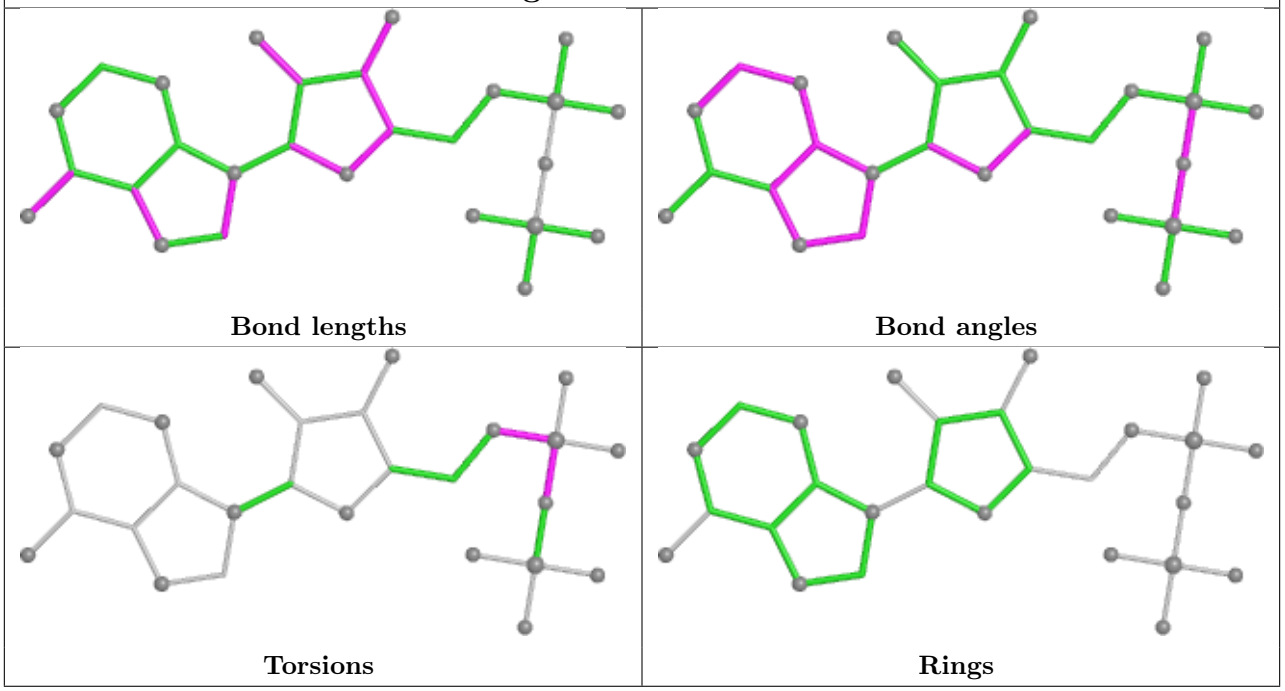
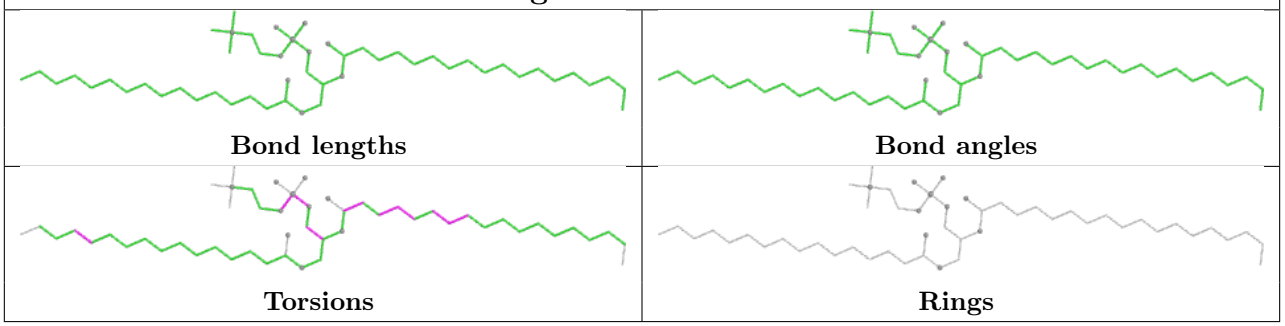
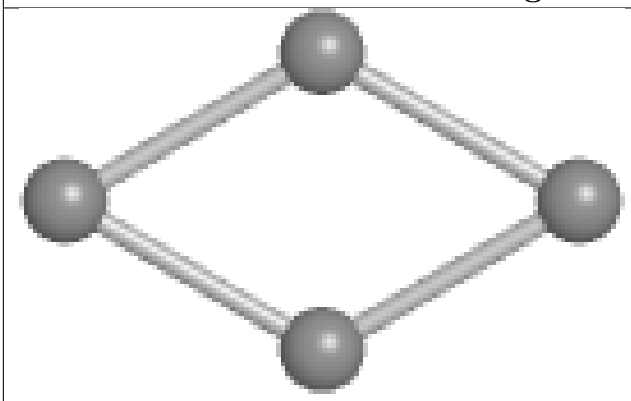


Ligand PLX a 202



Ligand FES M 803



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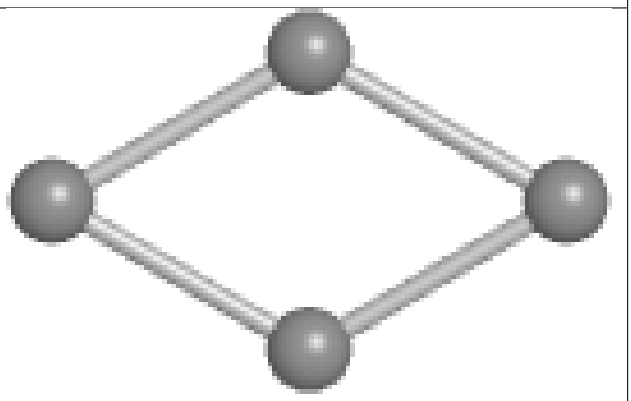
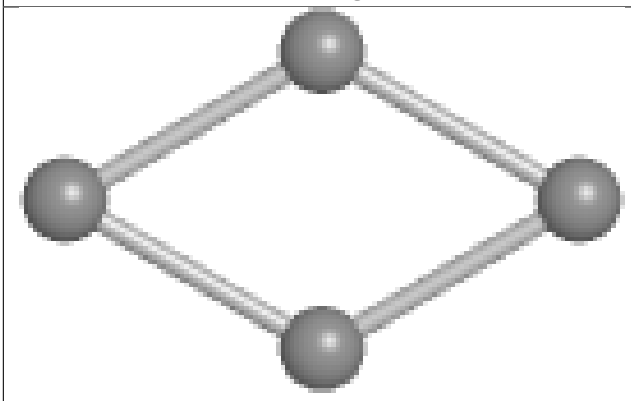
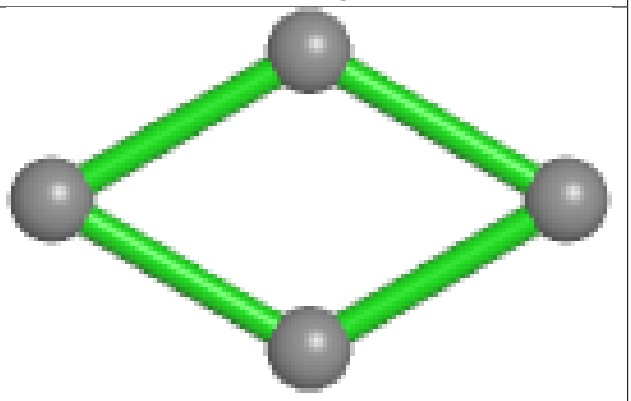


Bond angles

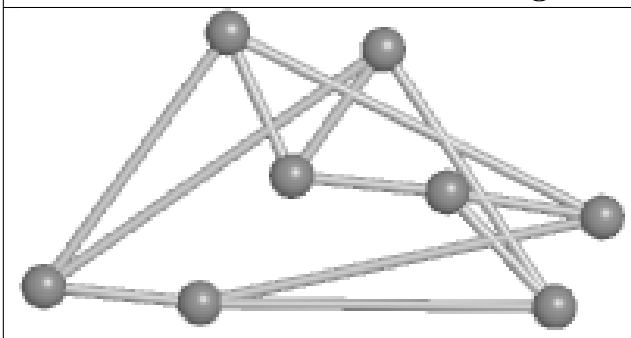


Torsions

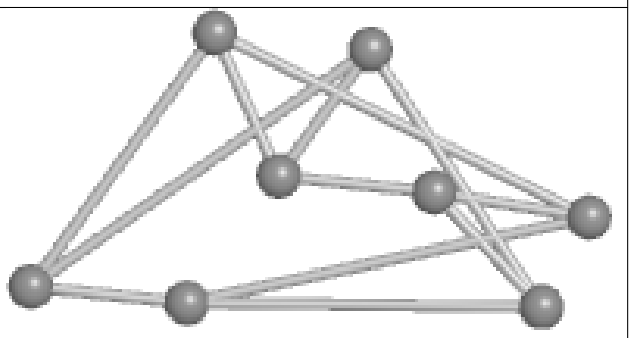


Rings

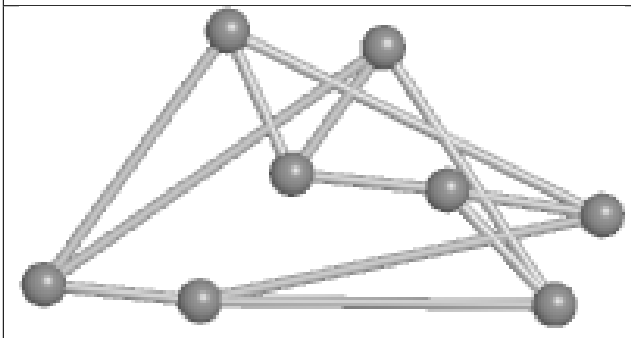
Ligand SF4 A 501



Bond lengths



Bond angles



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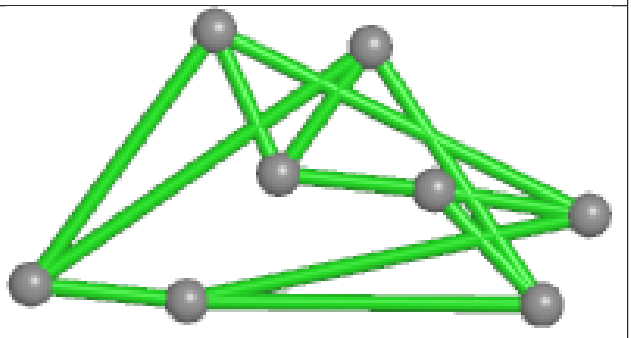
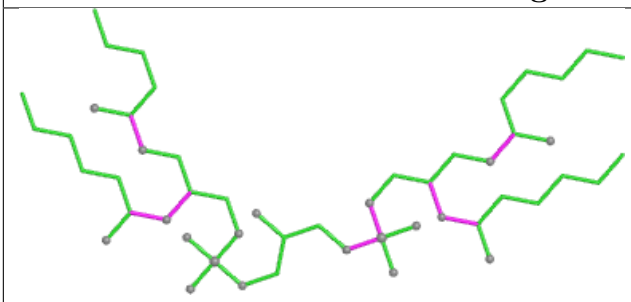


Rings

Ligand CDL I 201



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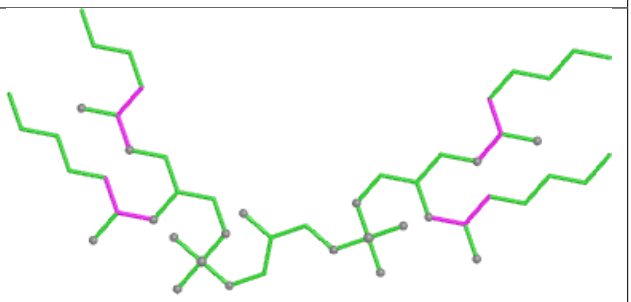

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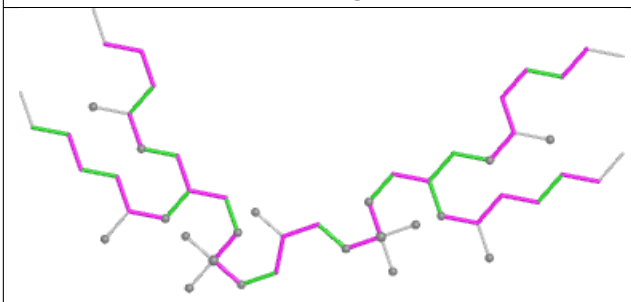

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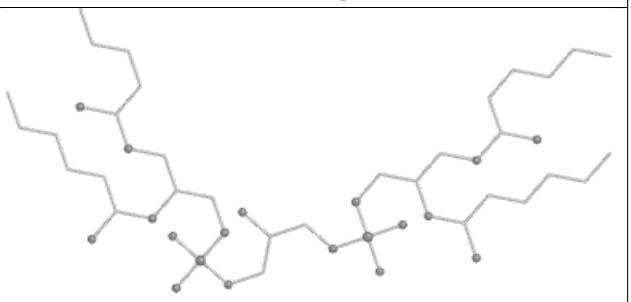
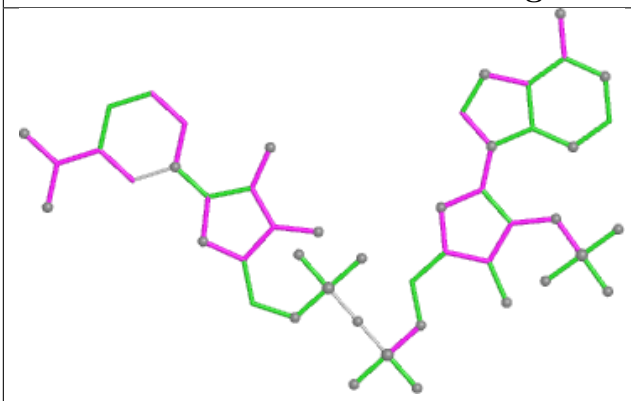


Rings

Ligand NDP J 401



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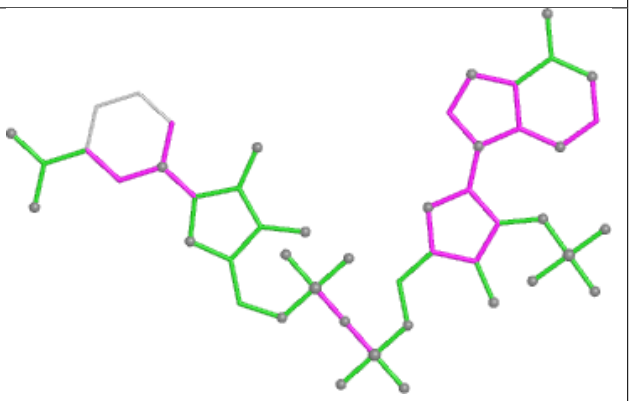

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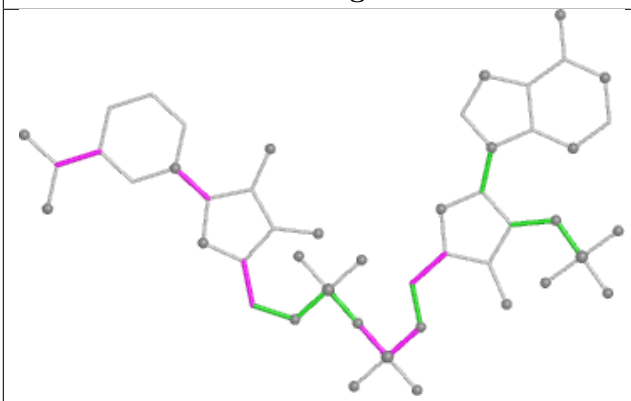

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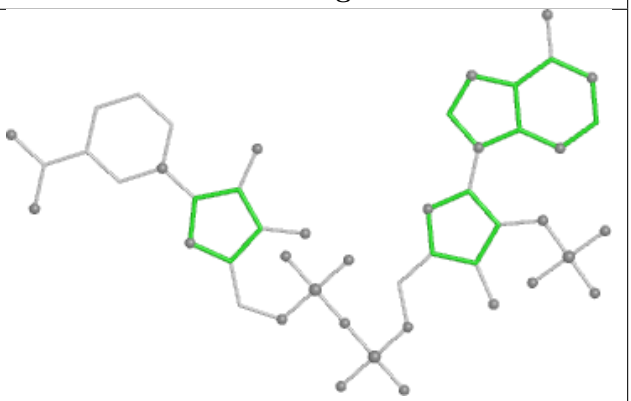
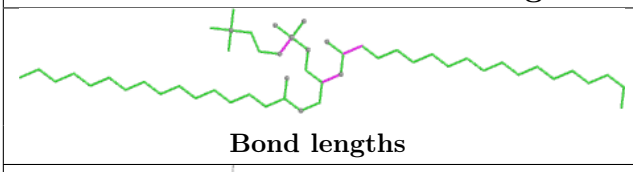


Rings

Ligand PLX C 302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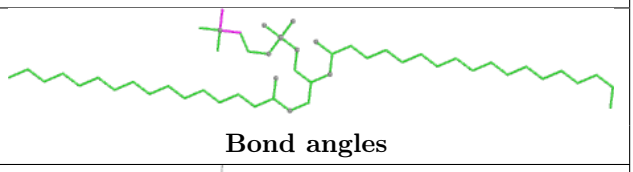
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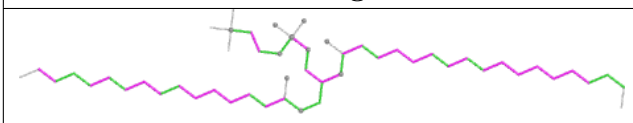
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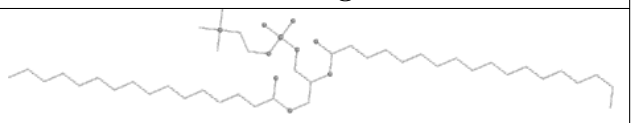
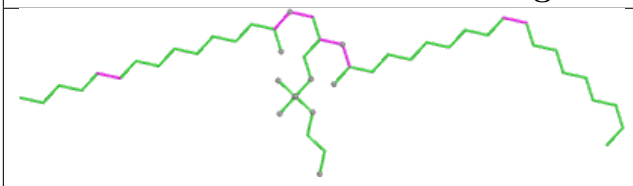

Rings

Ligand PEE i 402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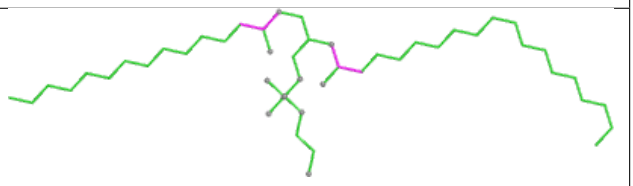
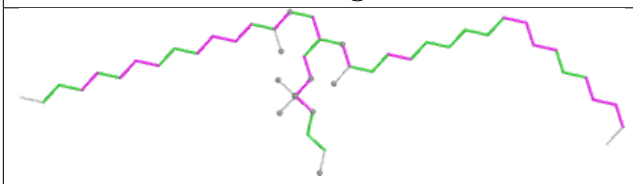
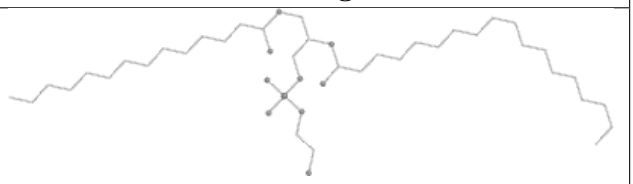
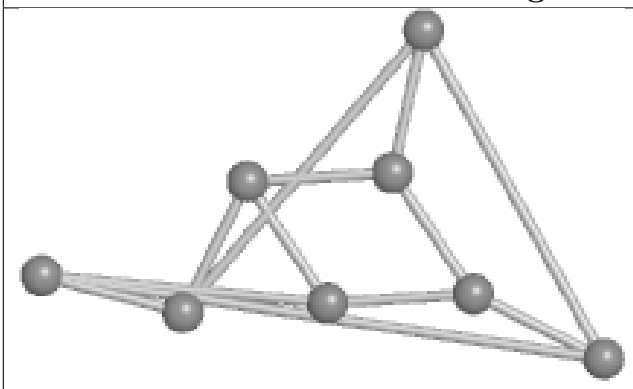
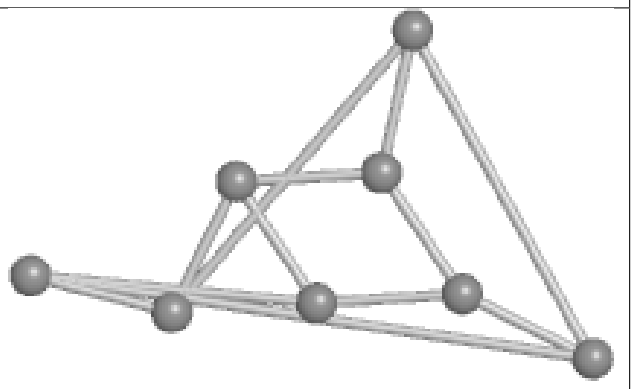

Bond angles

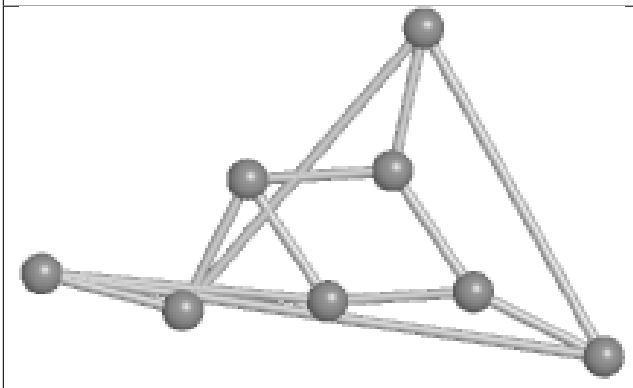

Torsions


Rings

Ligand SF4 M 802


Bond lengths


Bond angles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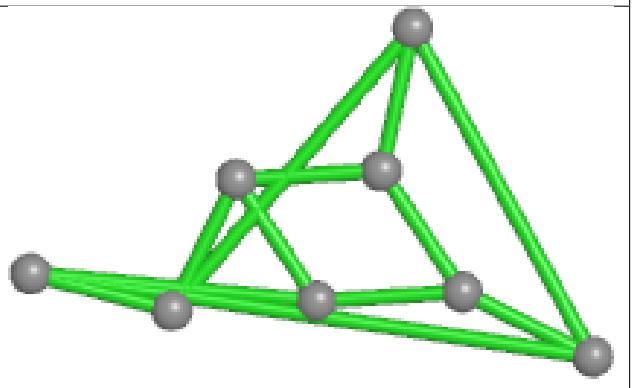
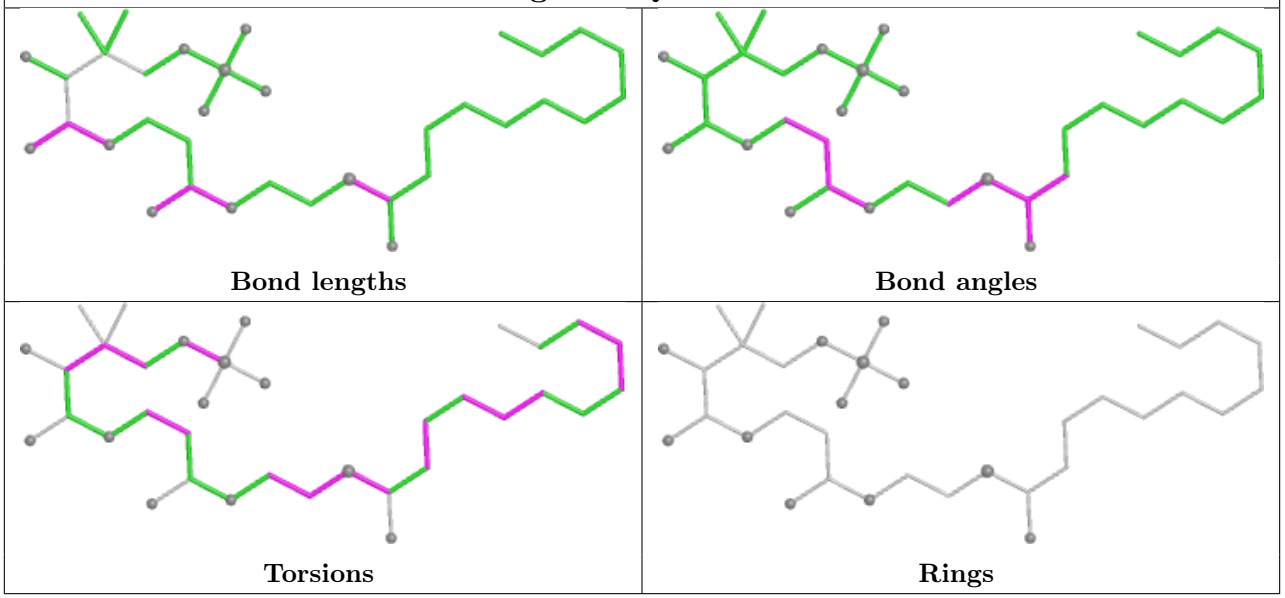

Rings

Ligand 8Q1 G 201



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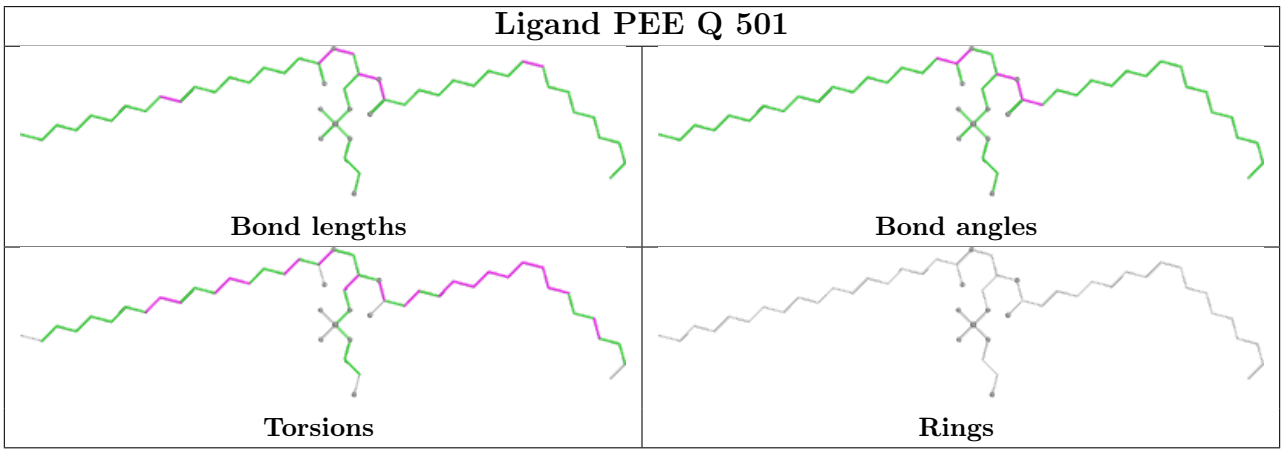

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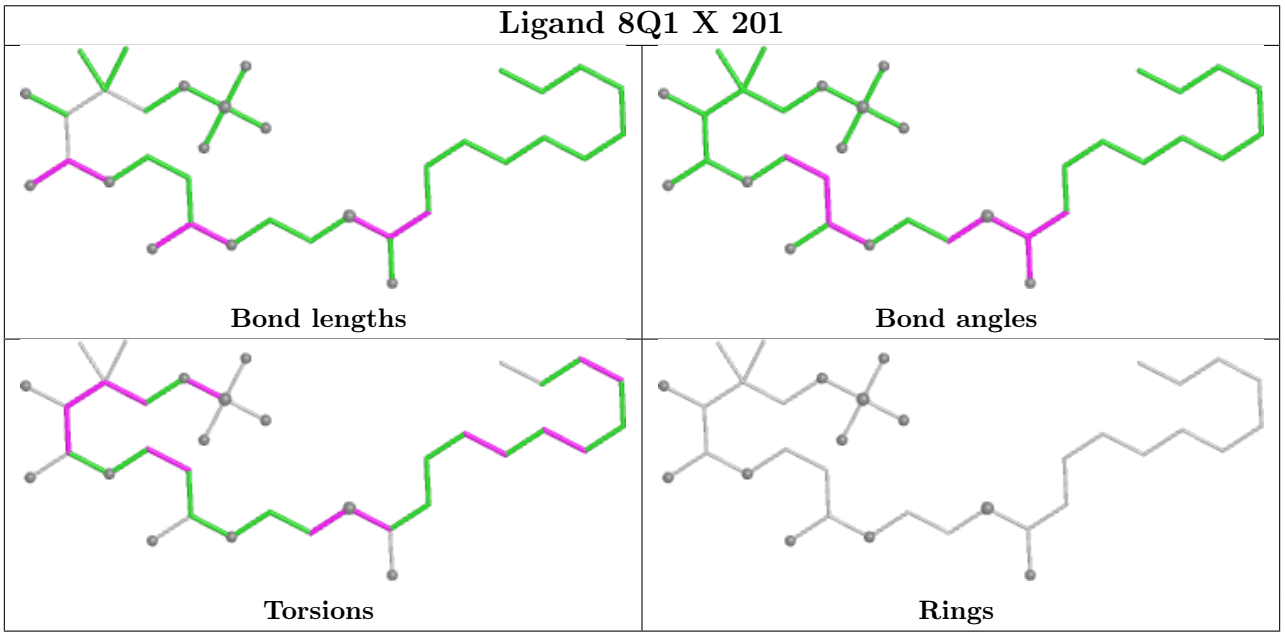
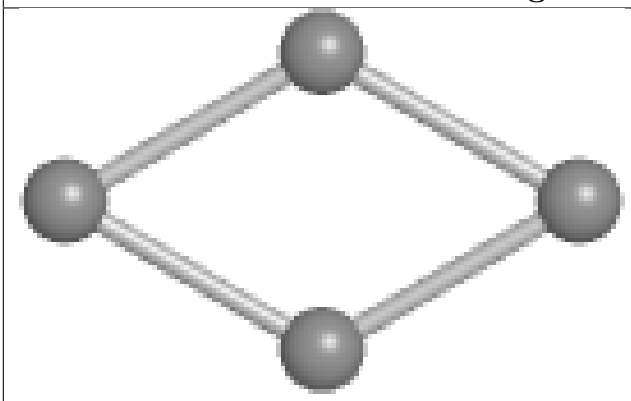
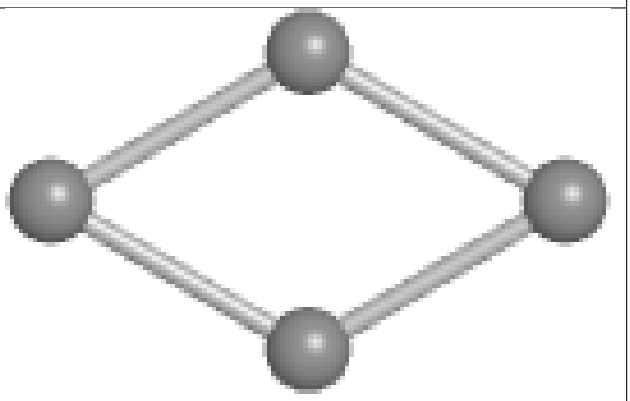


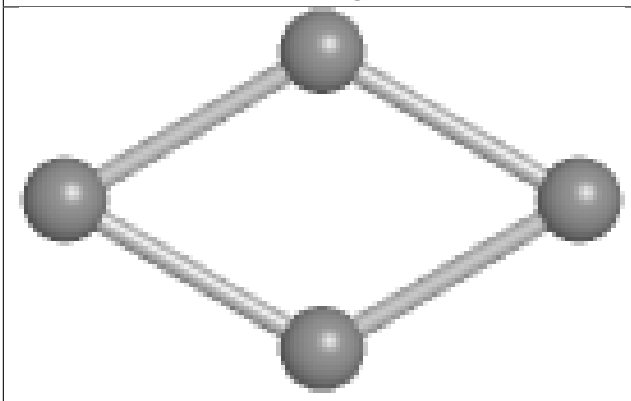
Ligand FES O 301



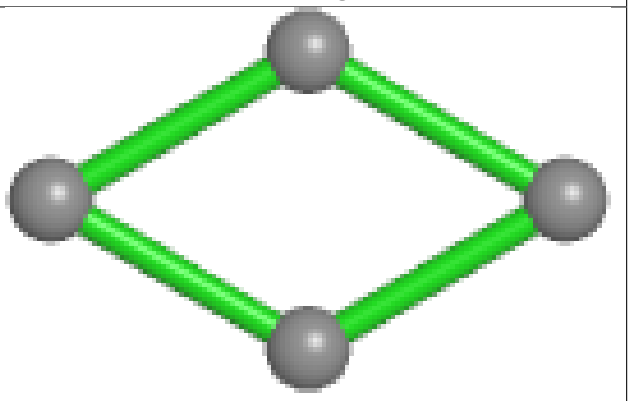
Bond lengths



Bond angles

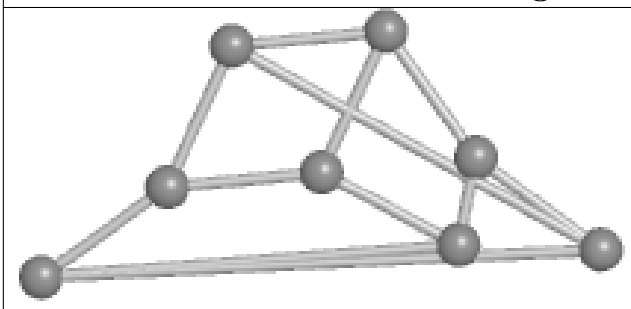


Torsions

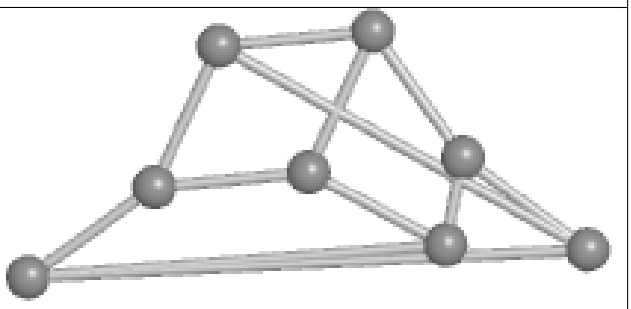


Rings

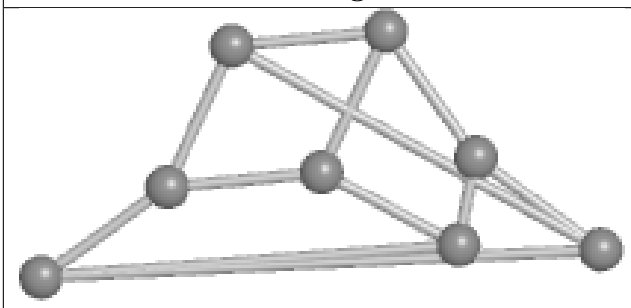
Ligand SF4 B 302



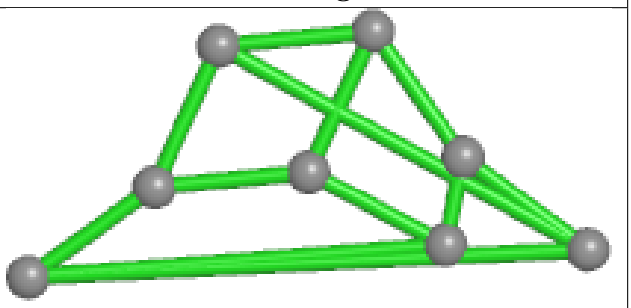
Bond lengths



Bond angles

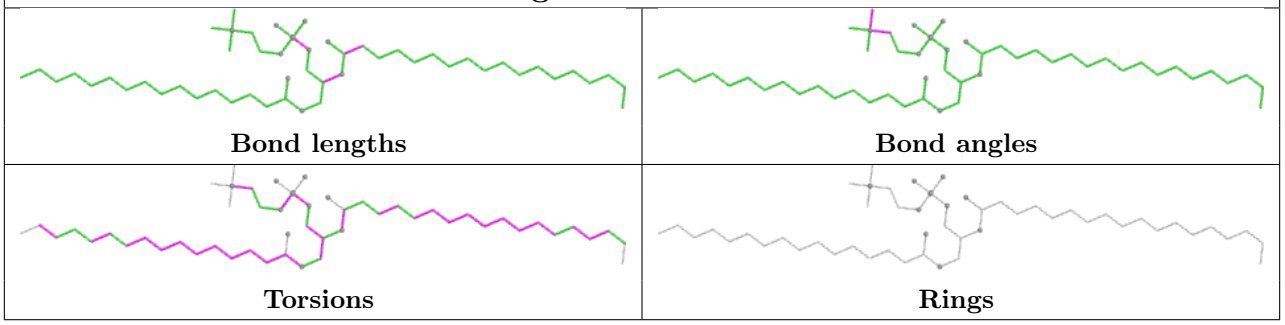


Torsions

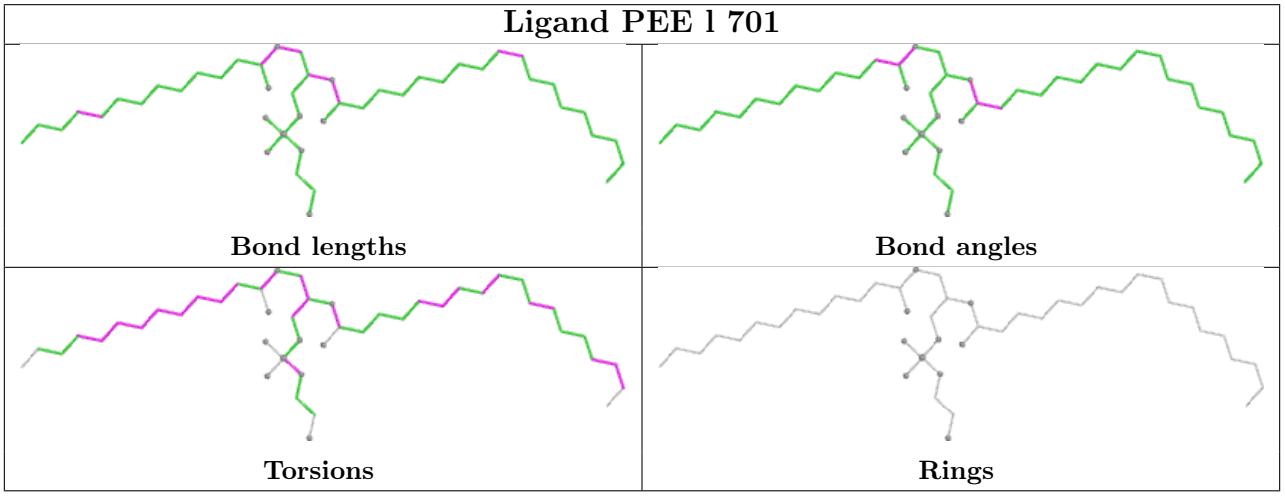


Rings

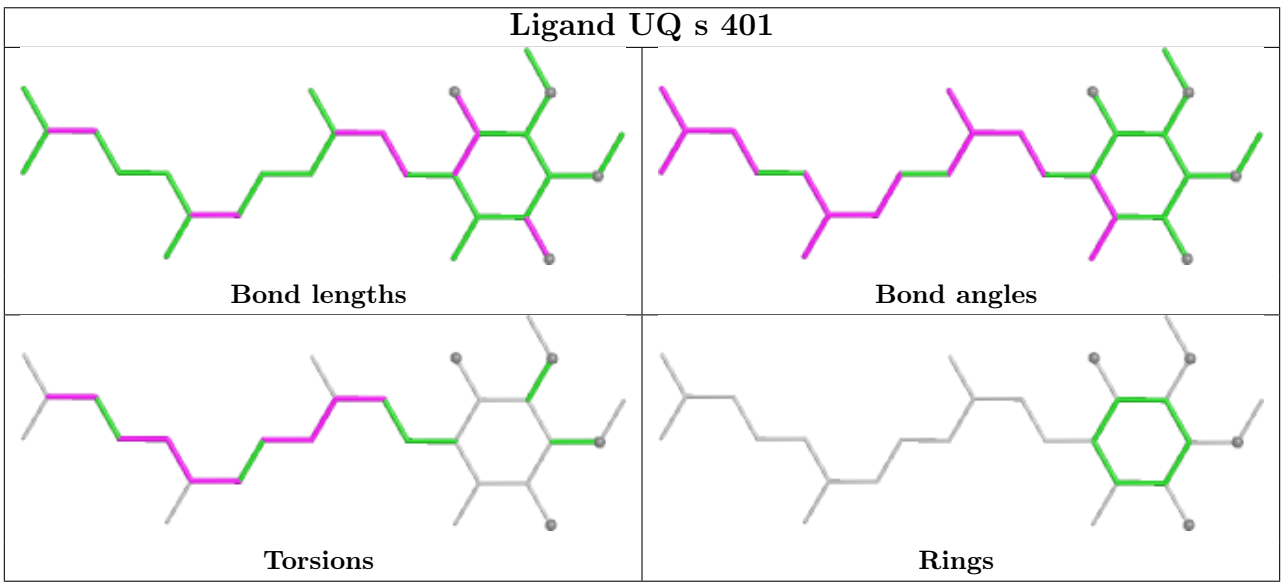
Ligand PLX r 502



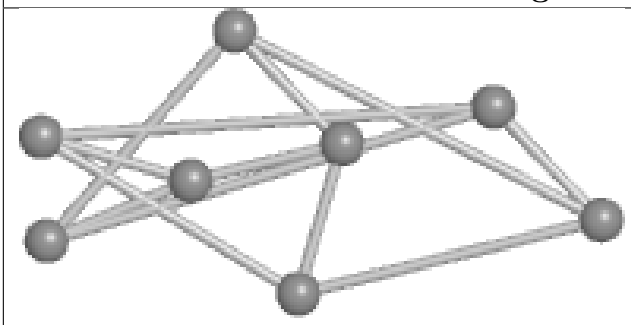
Ligand PEE l 701



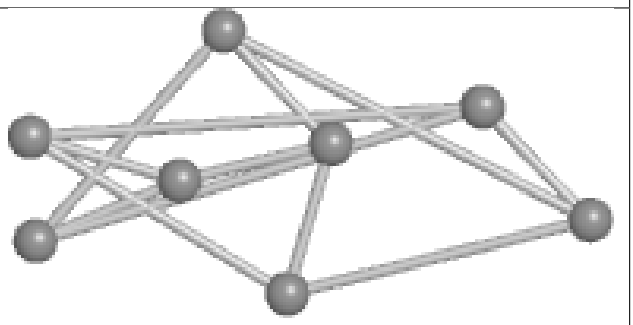
Ligand UQ s 401



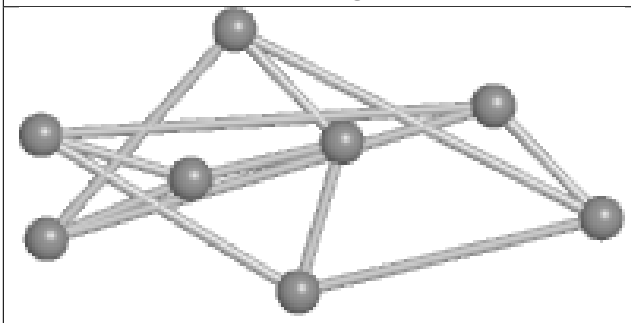
Ligand SF4 B 301



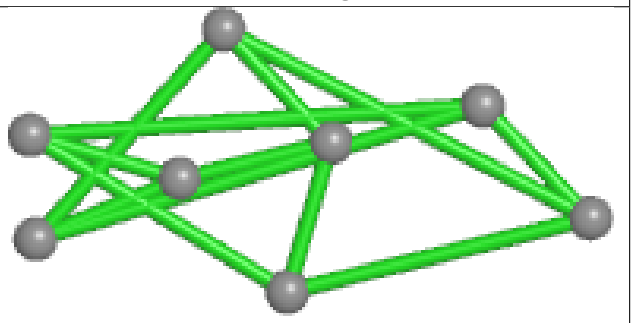
Bond lengths



Bond angles

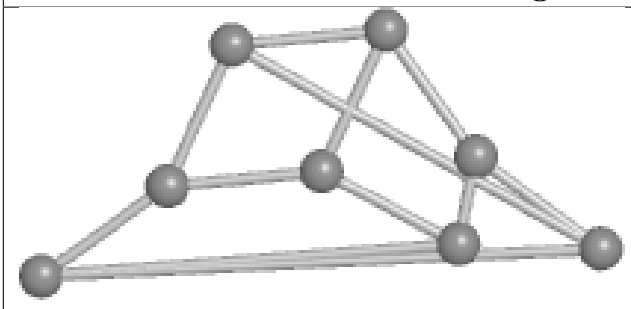


Torsions

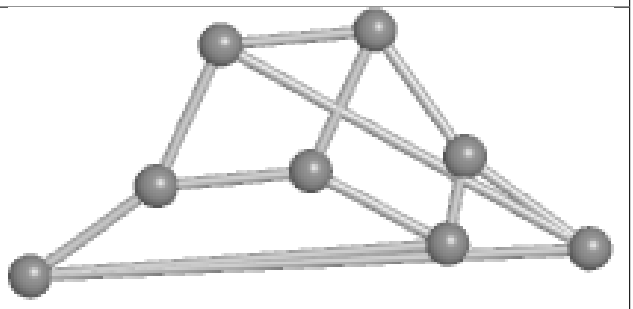


Rings

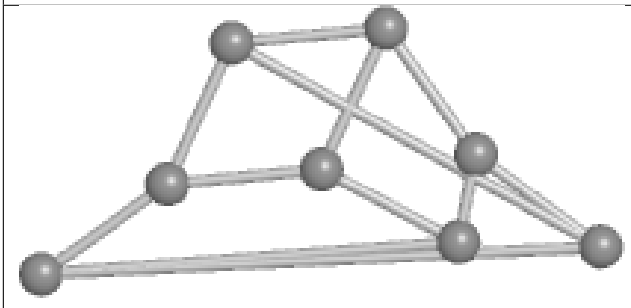
Ligand SF4 C 301



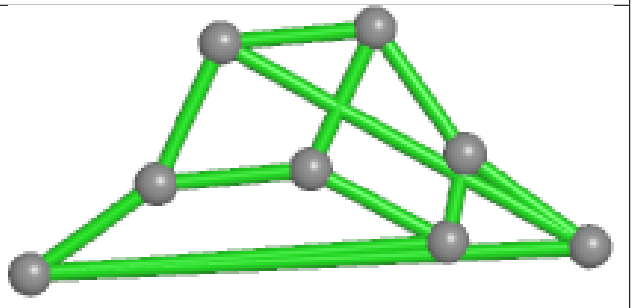
Bond lengths



Bond angles

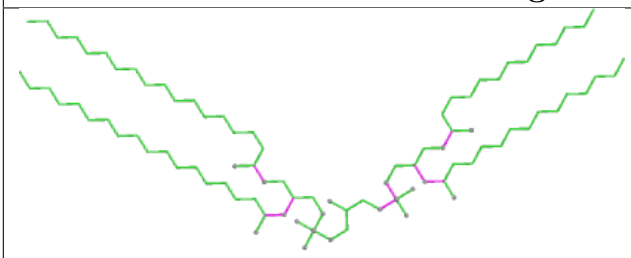


Torsions

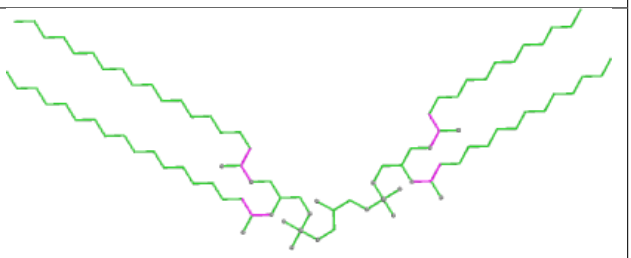


Rings

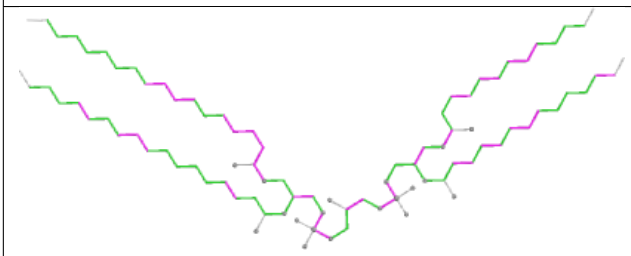
Ligand CDL a 201



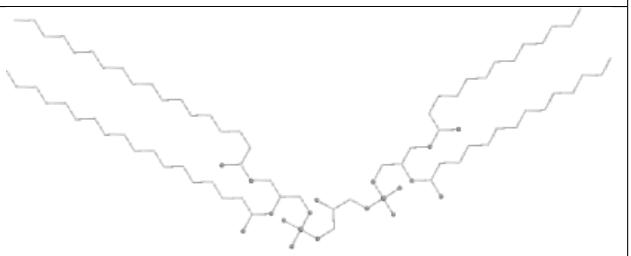
Bond lengths



Bond angles

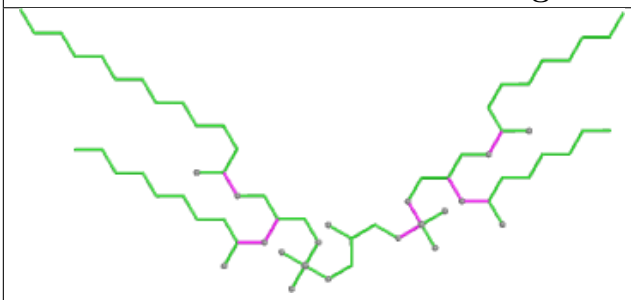


Torsions

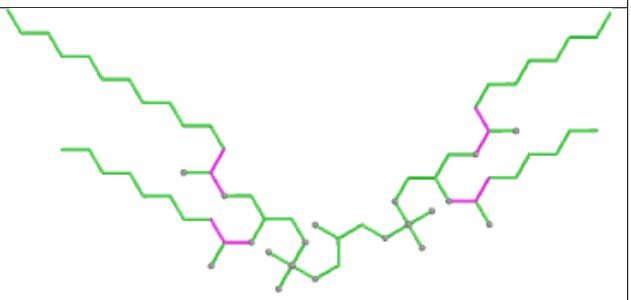


Rings

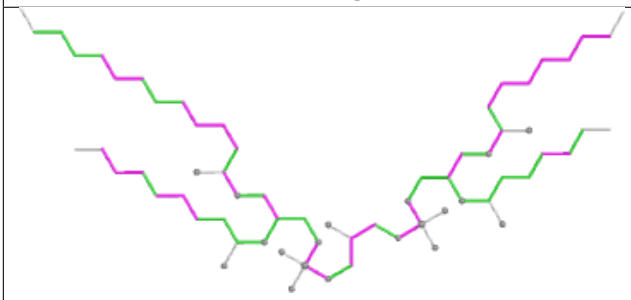
Ligand CDL i 401



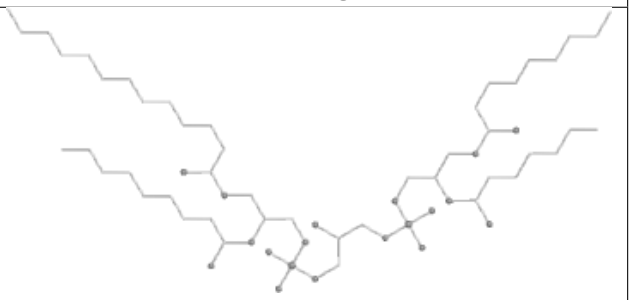
Bond lengths



Bond angles

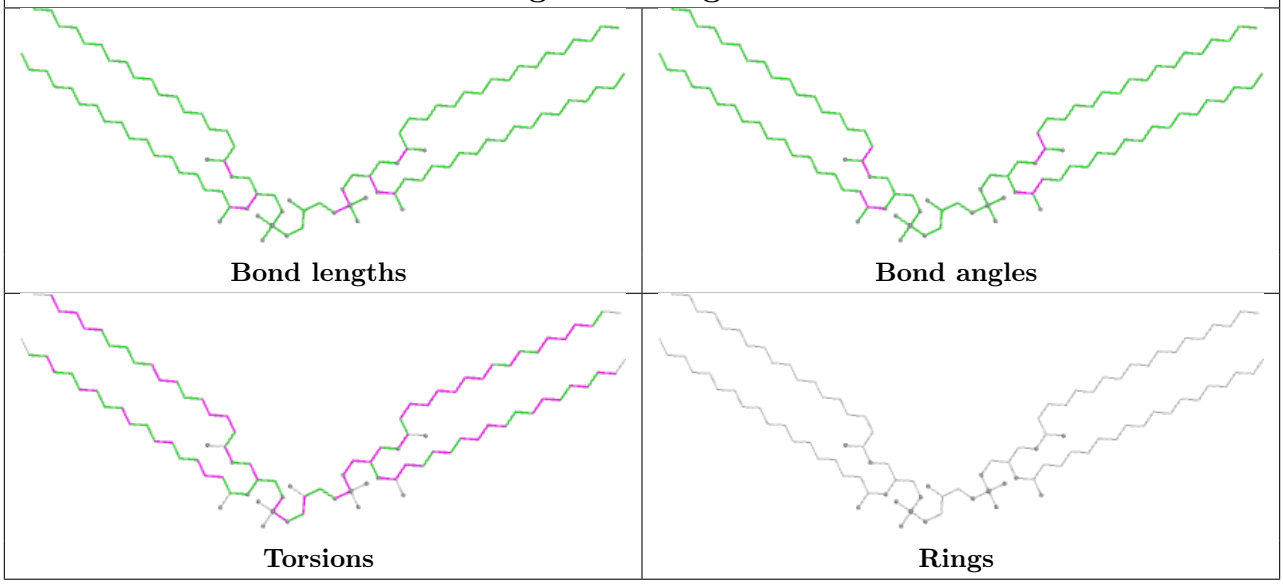


Torsions

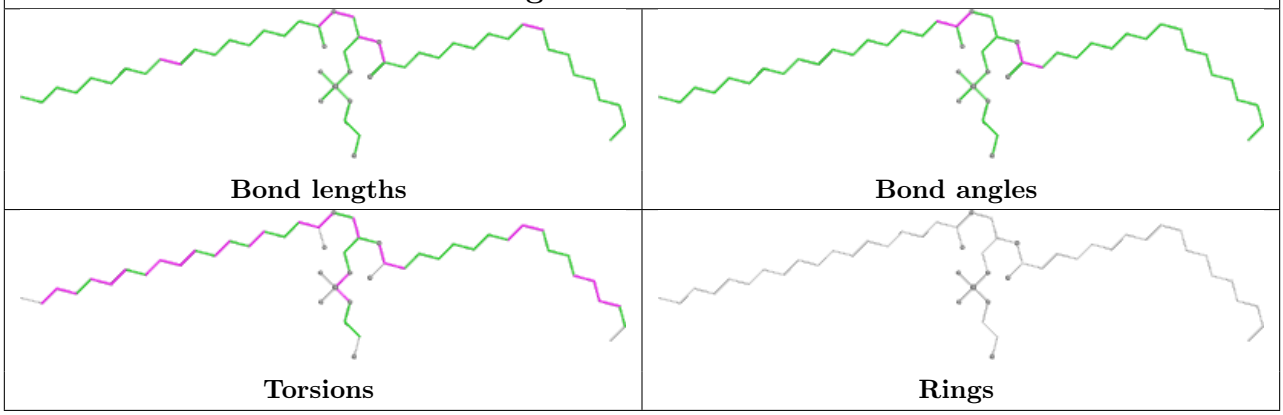


Rings

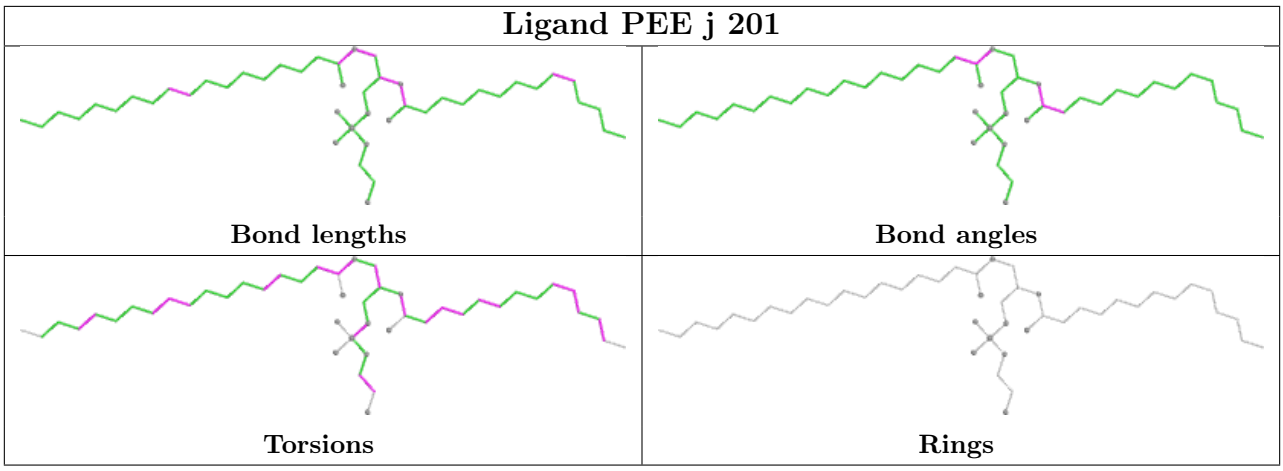
Ligand CDL g 202



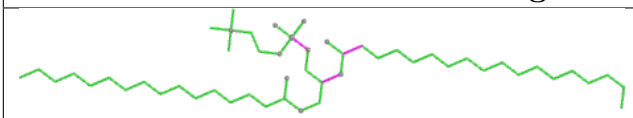
Ligand PEE U 101



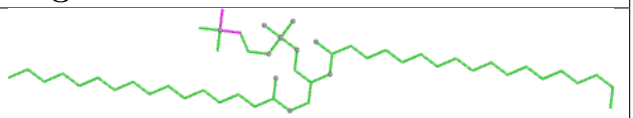
Ligand PEE j 201



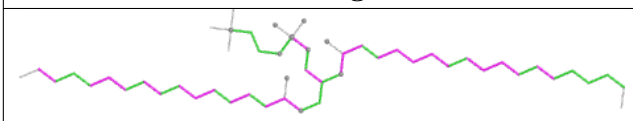
Ligand PLX g 201



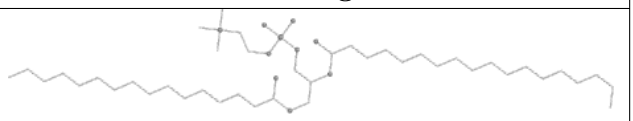
Bond lengths



Bond angles

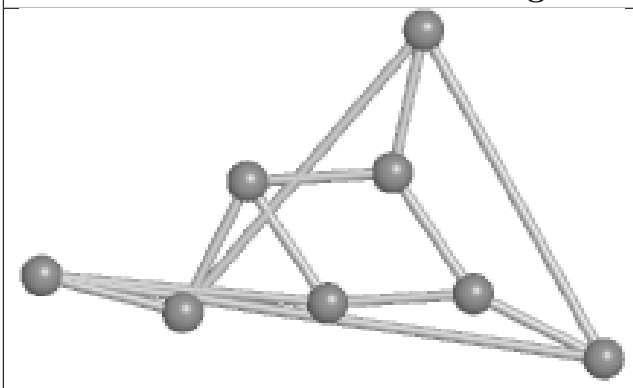


Torsions

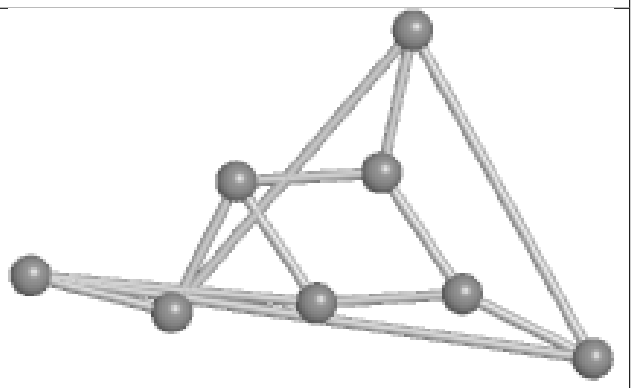


Rings

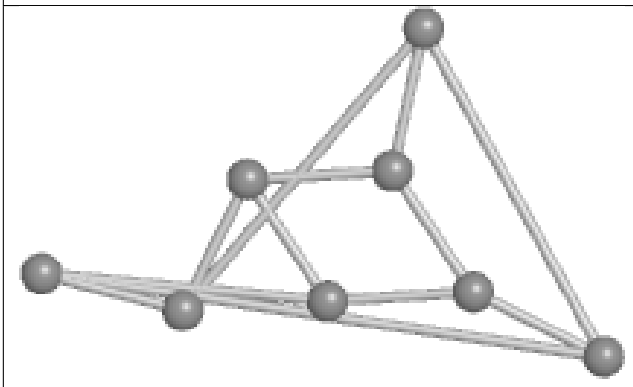
Ligand SF4 M 801



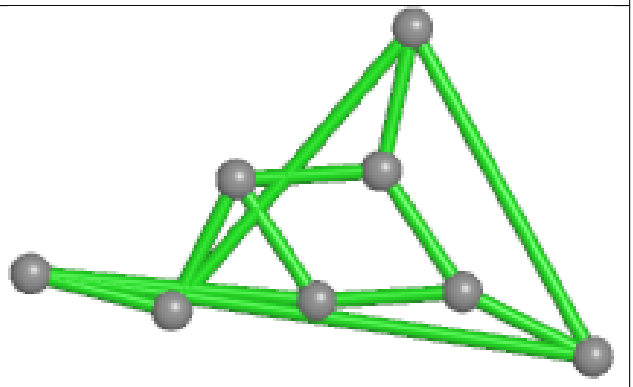
Bond lengths



Bond angles

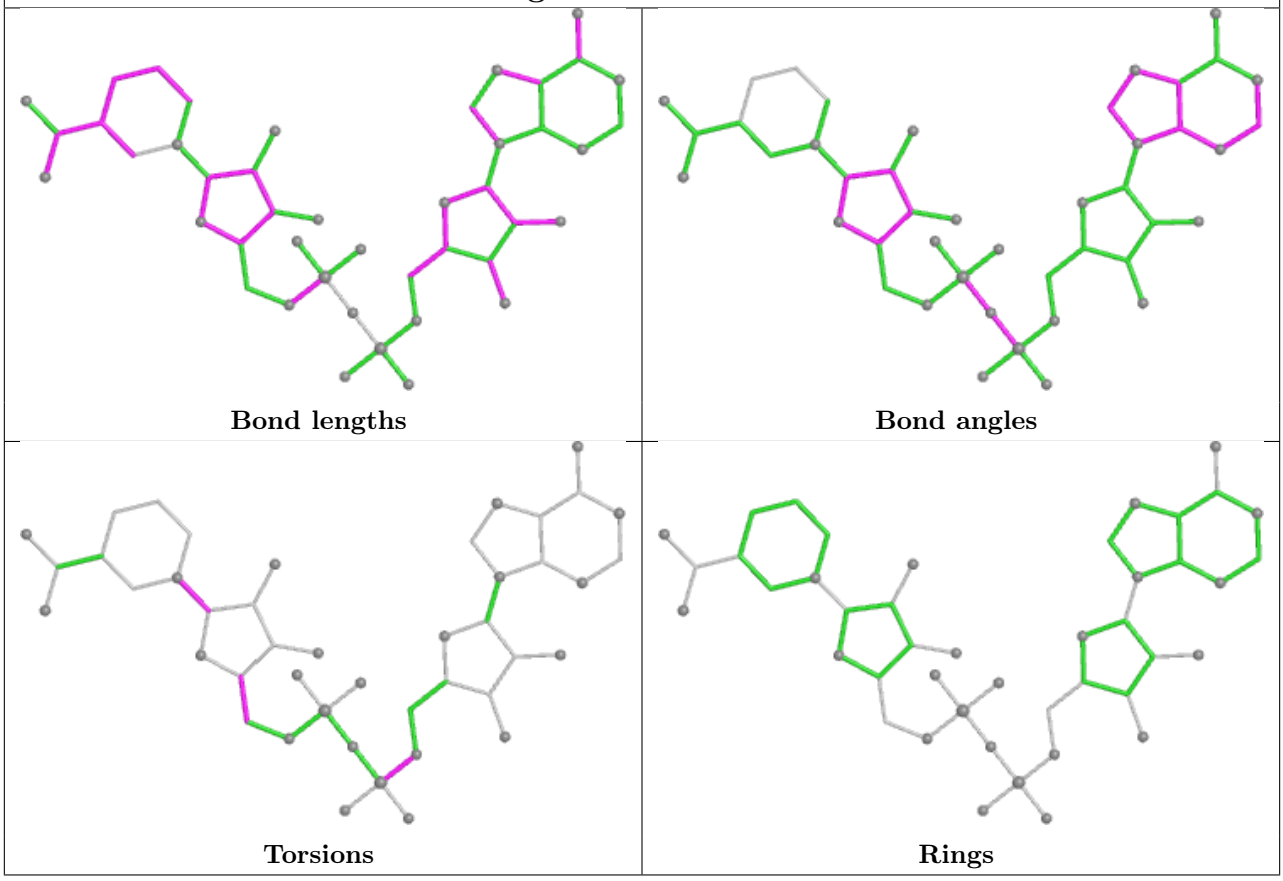


Torsions

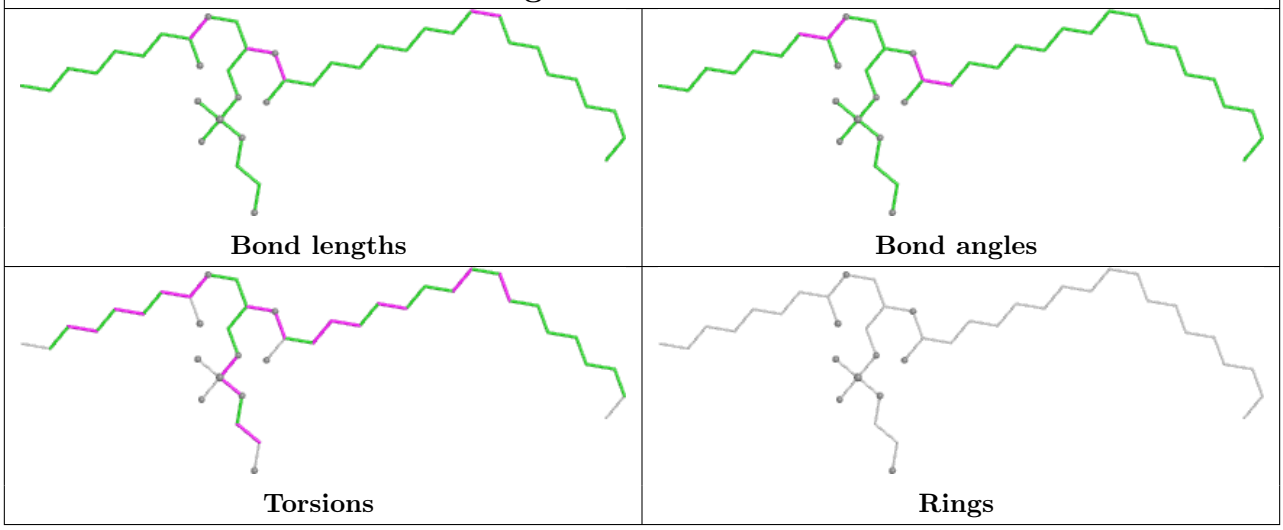


Rings

Ligand NAI A 503



Ligand PEE m 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.

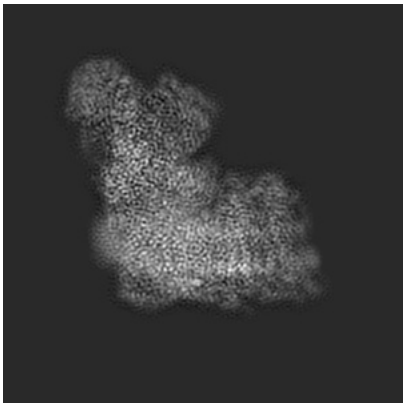
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32308. These allow visual inspection of the internal detail of the map and identification of artifacts.

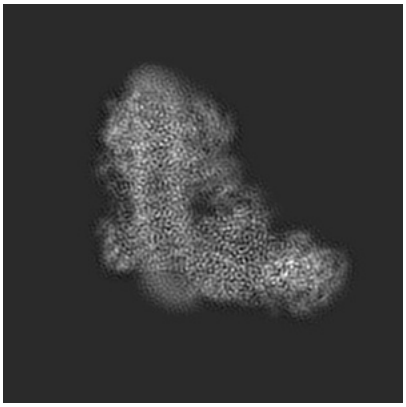
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

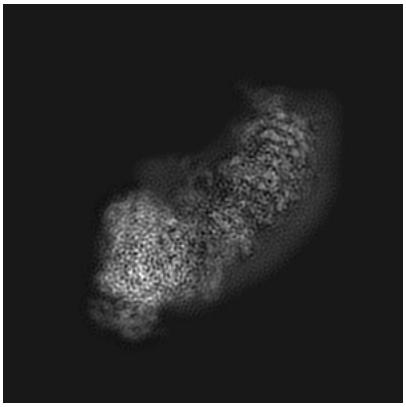
6.1.1 Primary map



X



Y

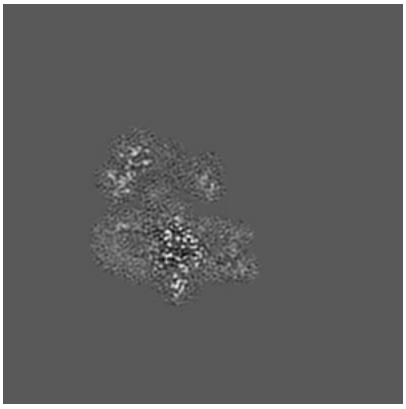


Z

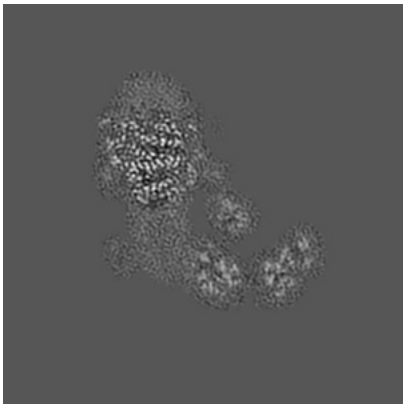
The images above show the map projected in three orthogonal directions.

6.2 Central slices

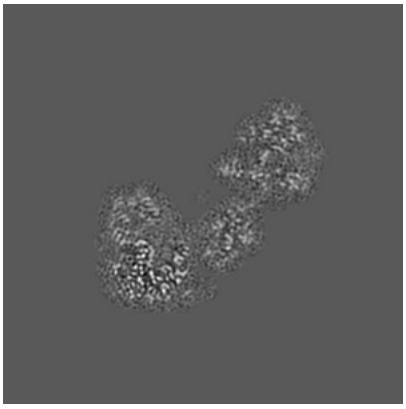
6.2.1 Primary map



X Index: 152



Y Index: 152

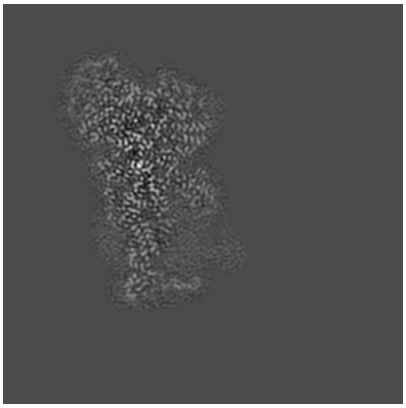


Z Index: 152

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

6.3 Largest variance slices (i)

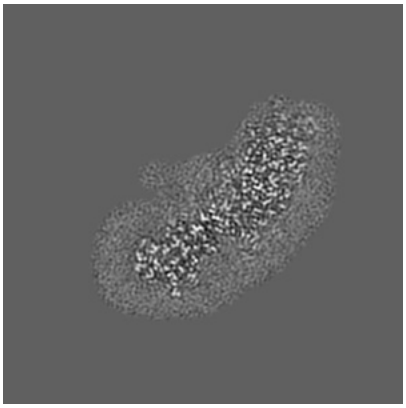
6.3.1 Primary map



X Index: 104



Y Index: 98

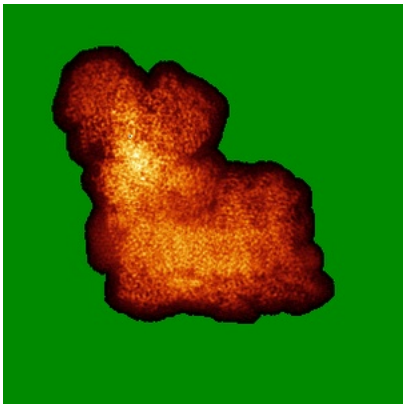


Z Index: 127

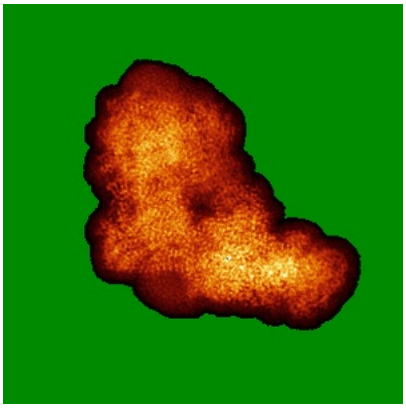
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

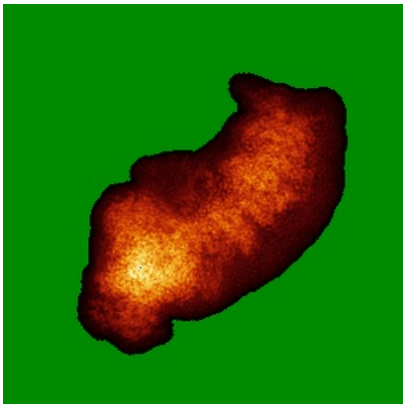
6.4.1 Primary map



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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0299. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

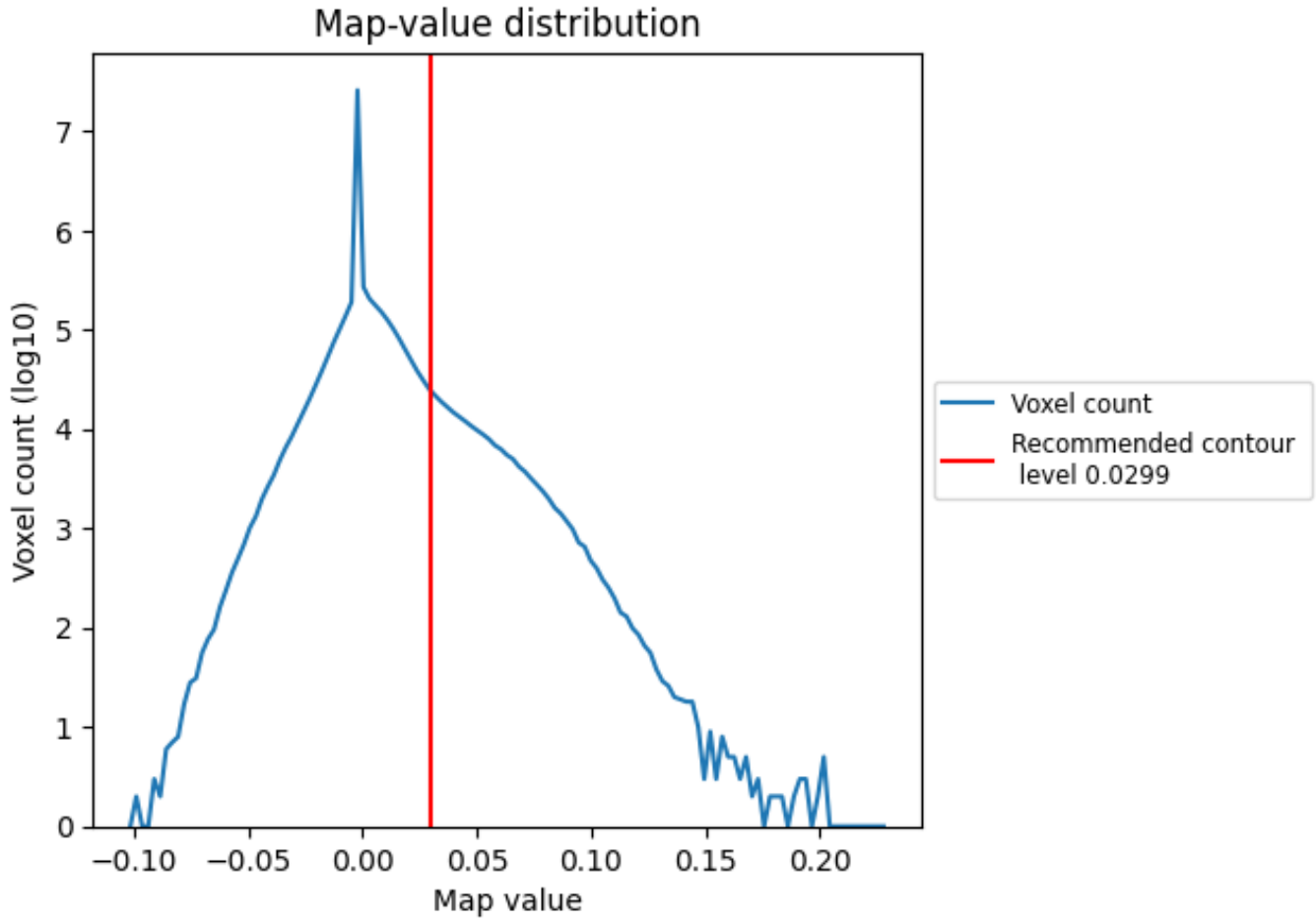
6.6 Mask visualisation (i)

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

7 Map analysis

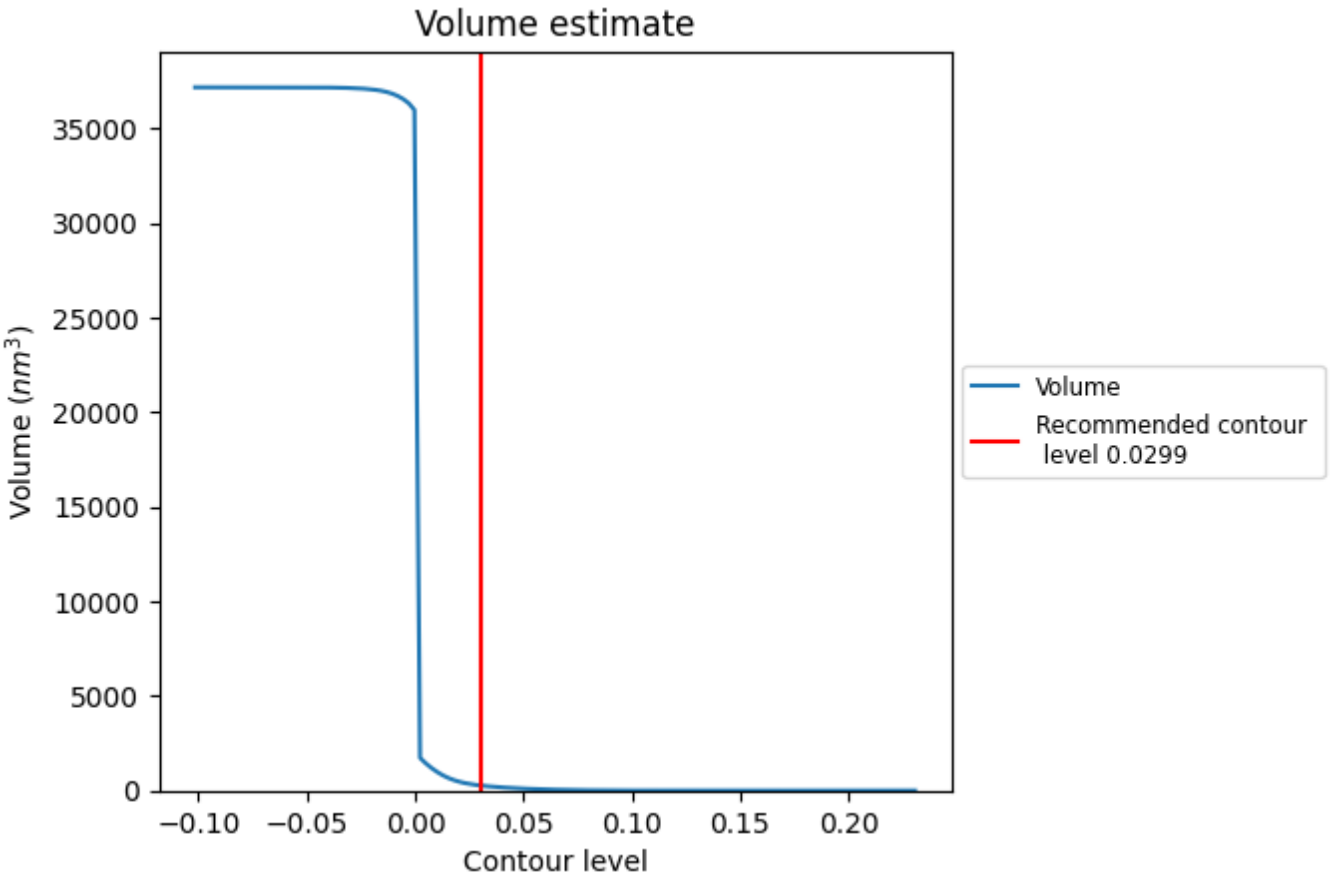
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

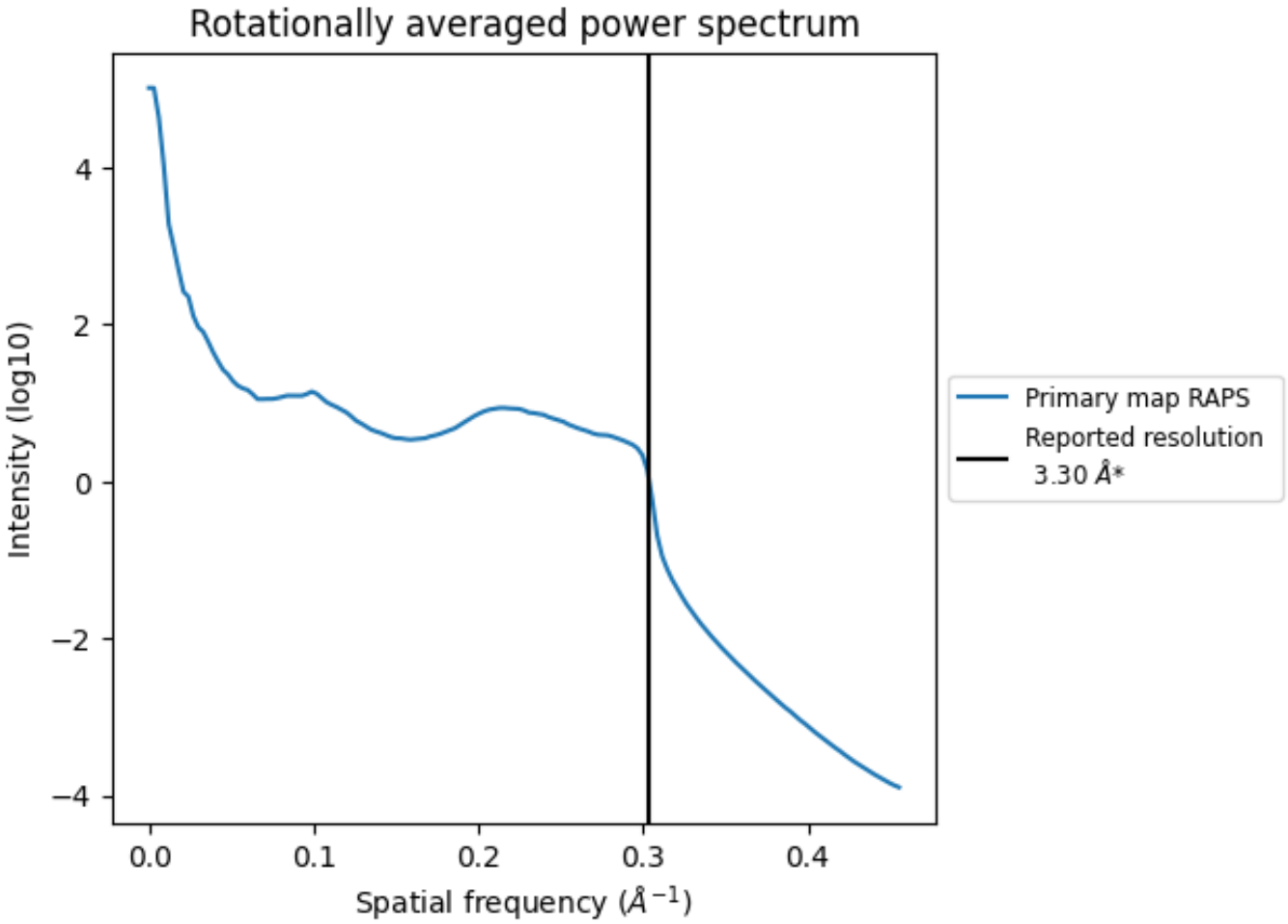
7.2 Volume estimate



The volume at the recommended contour level is 271 nm^3; this corresponds to an approximate mass of 245 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 (i)



*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

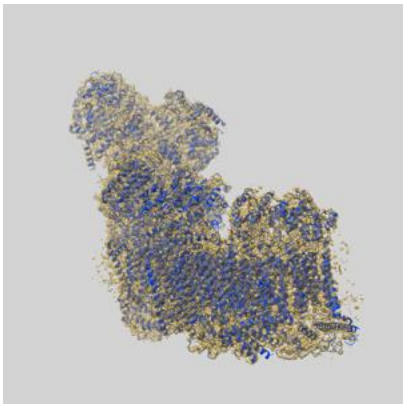
8 Fourier-Shell correlation

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

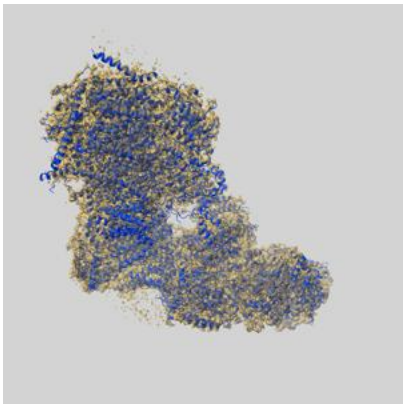
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32308 and PDB model 7W4M. Per-residue inclusion information can be found in section 3 on page 20.

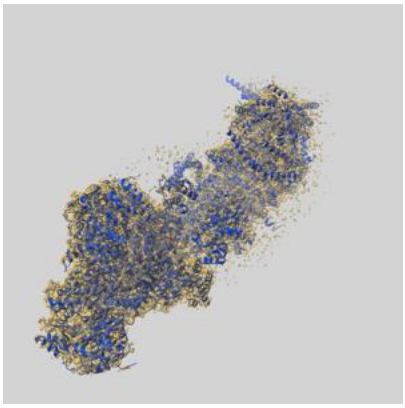
9.1 Map-model overlay



X



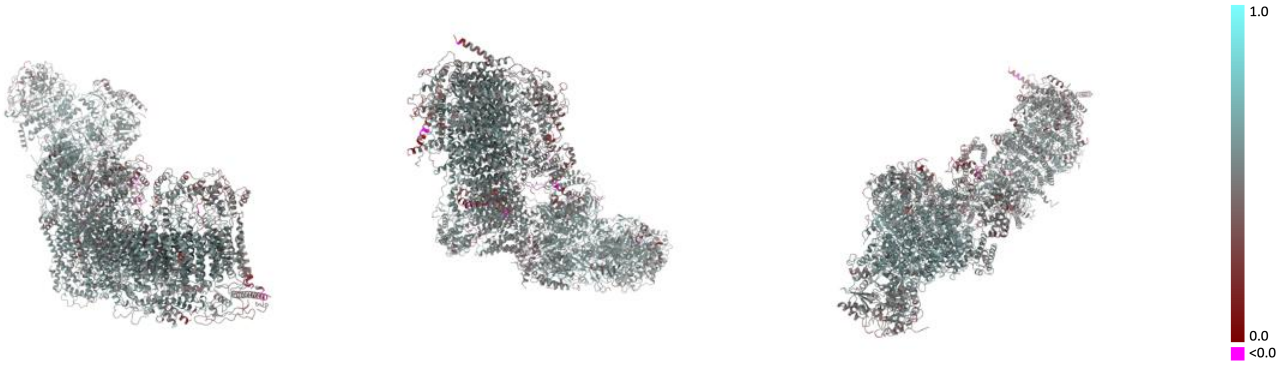
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0299 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.

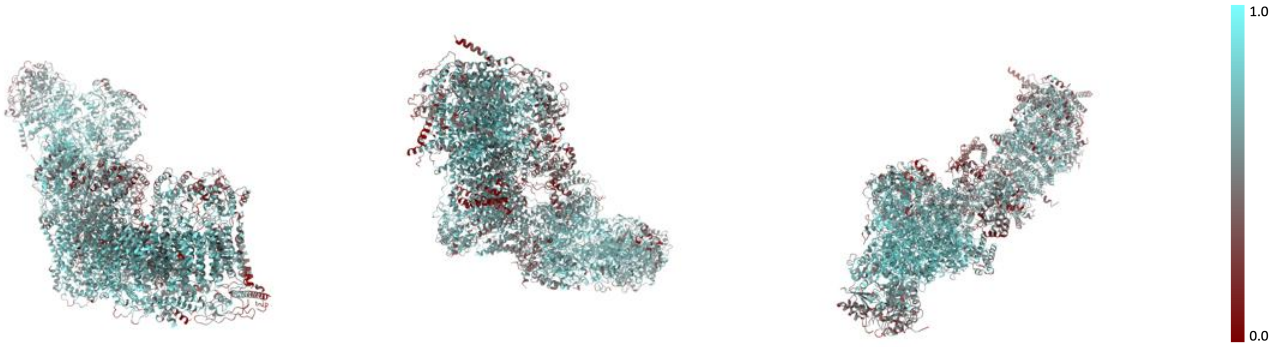
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

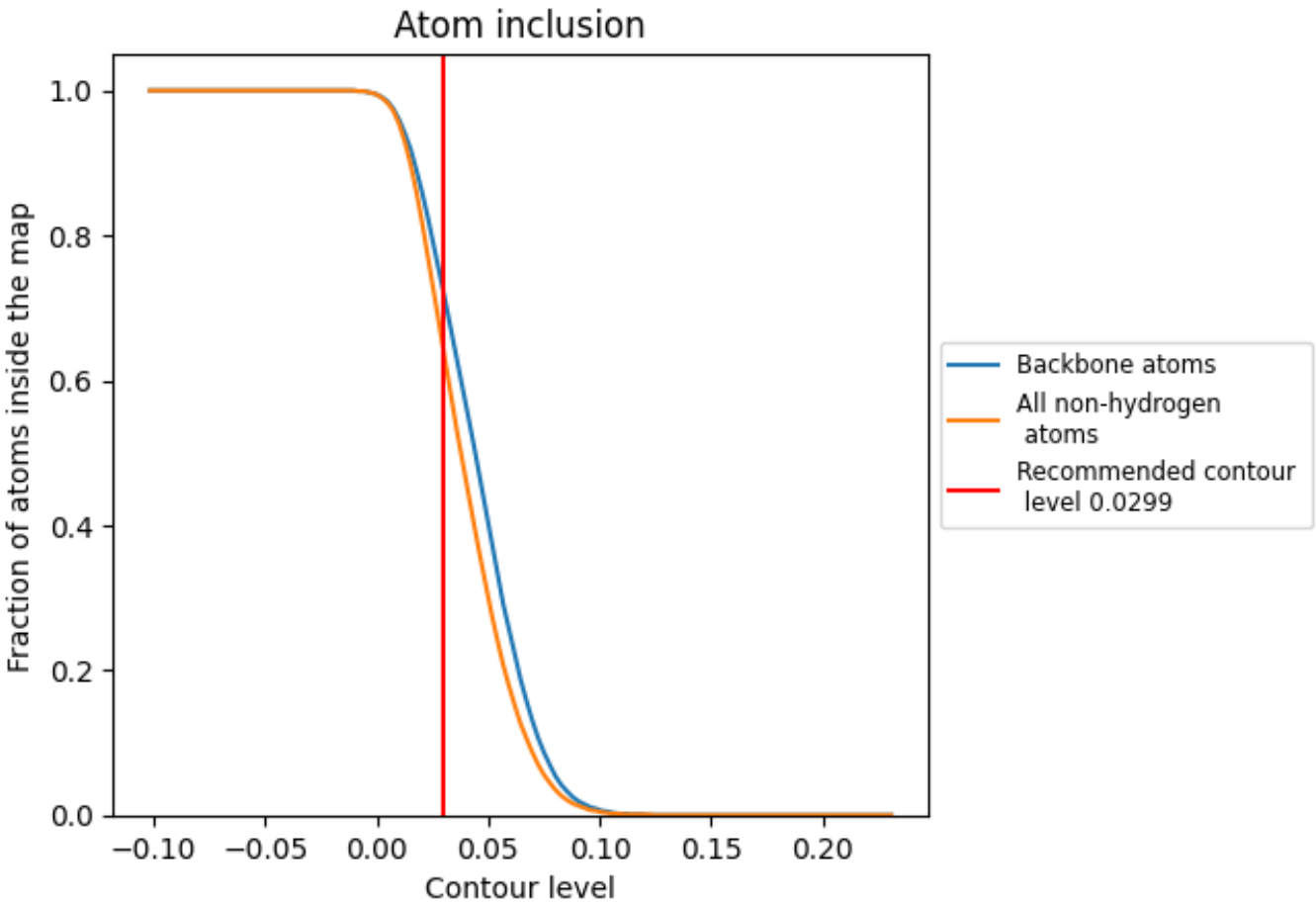
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0299).

9.4 Atom inclusion (i)



At the recommended contour level, 72% 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 (0.0299) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6420	0.5150
A	0.5840	0.4970
B	0.8400	0.5800
C	0.7950	0.5700
E	0.6550	0.5200
F	0.5240	0.4690
G	0.3160	0.3480
H	0.5930	0.5050
I	0.6770	0.5380
J	0.5940	0.5010
K	0.5530	0.4790
L	0.7390	0.5540
M	0.7190	0.5460
N	0.7340	0.5540
O	0.5440	0.4790
P	0.7980	0.5740
Q	0.7580	0.5620
S	0.7520	0.5450
T	0.6860	0.5470
U	0.6660	0.5260
V	0.2580	0.3720
W	0.7160	0.5360
X	0.4490	0.4380
Y	0.4380	0.4350
Z	0.3510	0.3720
a	0.6730	0.5400
b	0.4850	0.4470
c	0.5850	0.4900
d	0.6370	0.5030
e	0.5710	0.4840
f	0.5330	0.4640
g	0.6620	0.5350
h	0.6800	0.5350
i	0.7320	0.5530
j	0.5500	0.4810



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Chain	Atom inclusion	Q-score
k	0.5970	0.4950
l	0.6500	0.5290
m	0.5810	0.5000
n	0.5500	0.4840
o	0.5910	0.4970
p	0.5710	0.4760
r	0.7600	0.5620
s	0.7310	0.5320
u	0.6650	0.5260
v	0.4280	0.4120
w	0.4680	0.4640