Full wwPDB EM Validation Report ⓘ

Sep 7, 2026 – 11:46 pm BST

PDB ID	:	8B9Z / pdb_00008b9z
EMDB ID	:	EMD-15936
Title	:	Drosophila melanogaster complex I in the Active state (Dm1)
Authors	:	Agip, A.A.; Chung, I.; Sanchez-Martinez, A.; Whitworth, A.J.; Hirst, J.
Deposited on	:	2022-10-10
Resolution	:	3.28 Å(reported)
Based on initial model	:	6ZR2

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:

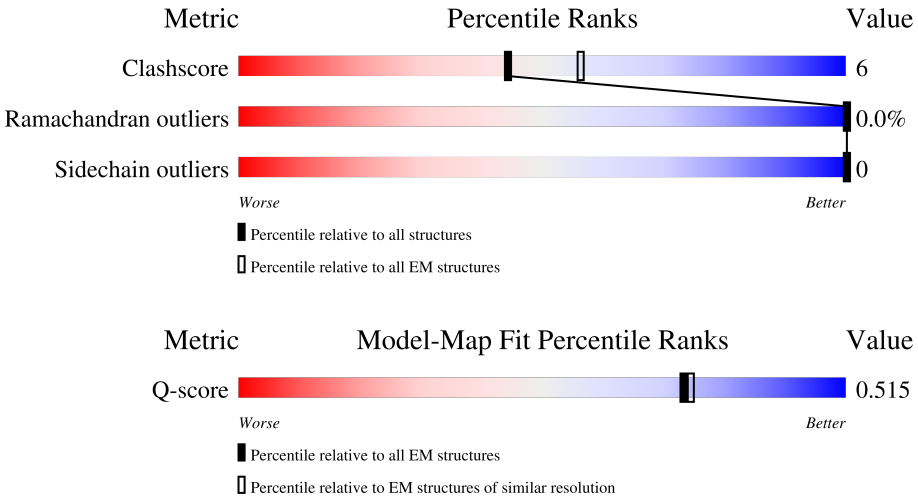
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 3.28 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	14492 (2.78 - 3.78)

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	117	78% 22%
2	B	182	81% 18%
3	C	209	83% 17%
4	D	430	84% 16%

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Mol	Chain	Length	Quality of chain
5	E	214	78% 22%
6	F	441	82% 18%
7	G	731	82% 10% 7%
8	H	315	85% 14%
9	I	186	83% 17%
10	J	173	5% 74% 25%
11	K	96	5% 72% 28%
12	L	577	84% 16%
13	M	446	79% 21%
14	N	341	82% 18%
15	O	368	5% 85% 15%
16	P	377	88% 12%
17	Q	151	9% 86% 14%
18	R	89	89% 11%
19	T	85	33% 72% 19% 9%
19	U	85	12% 80% 20%
20	V	118	80% 20%
21	W	114	88% 12%
22	X	174	7% 89% 11%
23	Y	167	10% 87% 13%
24	Z	146	90% 10%
25	a	73	12% 82% 18%
26	b	66	6% 77% 23%
27	d	115	88% 12%
28	e	100	5% 84% 16%

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Mol	Chain	Length	Quality of chain
29	f	55	16% 87% 13%
30	g	108	12% 81% 19%
31	h	145	86% 14%
32	i	161	6% 83% 17%
33	j	66	8% 91% 9%
34	k	84	10% 92% 8%
35	l	146	10% 90% 10%
36	m	108	5% 89% 11%
37	n	134	9% 82% 18%
38	o	112	87% 13%
39	p	151	81% 19%
40	q	133	11% 92% 8%
41	r	103	7% 74% 13% 14%
42	s	62	24% 82% 18%

2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 66970 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-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	117	956	652	141	156	7	0	0

- Molecule 2 is a protein called LD31474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	182	1435	920	251	250	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	209	1726	1103	303	315	5	0	0

- Molecule 4 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	430	3434	2202	579	630	23	0	0

- Molecule 5 is a protein called NADH dehydrogenase (Ubiquinone) 24 kDa subunit, isoform A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	214	1679	1062	285	320	12	0	0

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	441	Total	C	N	O	S	0	0
			3381	2136	602	617	26		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	677	Total	C	N	O	S	0	0
			5146	3225	912	980	29		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	315	Total	C	N	O	S	0	0
			2571	1764	367	418	22		

- Molecule 9 is a protein called NADH dehydrogenase (ubiquinone) 23 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	186	Total	C	N	O	S	0	0
			1485	935	251	287	12		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	173	Total	C	N	O	S	0	0
			1397	946	201	233	17		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	96	Total	C	N	O	S	0	0
			793	540	113	127	13		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	577	Total	C	N	O	S	0	0
			4606	3092	680	774	60		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	446	Total 3617	C 2459	N 533	O 583	S 42	0	0

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	341	Total 2796	C 1893	N 411	O 458	S 34	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	368	Total 3007	C 1927	N 504	O 560	S 16	0	0

- Molecule 16 is a protein called NADH dehydrogenase (Ubiquinone) 39 kDa subunit, isoform A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	377	Total 3032	C 1934	N 546	O 542	S 10	0	0

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	151	Total 1214	C 756	N 227	O 227	S 4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	89	Total 716	C 453	N 130	O 129	S 4	0	0

- Molecule 19 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	77	Total 615	C 398	N 94	O 121	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	85	Total	C	N	O	S	0	0
			684	442	103	137	2		

- Molecule 20 is a protein called NADH dehydrogenase (Ubiquinone) 13 kDa B subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	118	Total	C	N	O	S	0	0
			922	588	162	168	4		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	114	Total	C	N	O	S	0	0
			968	620	172	170	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	174	Total	C	N	O	S	0	0
			1383	867	240	266	10		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	167	Total	C	N	O	S	0	0
			1277	829	212	230	6		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	146	Total	C	N	O	S	0	0
			1201	787	203	209	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	73	Total	C	N	O	S	0	0
			601	386	101	108	6		

- Molecule 26 is a protein called RH45008p.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	66	Total	C	N	O	S	0	0
			519	327	95	96	1		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	115	Total	C	N	O	S	0	0
			907	590	159	157	1		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	100	Total	C	N	O	S	0	0
			828	523	145	149	11		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	55	Total	C	N	O	S	0	0
			429	278	76	73	2		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	108	Total	C	N	O	S	0	0
			883	567	142	173	1		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	145	Total	C	N	O	S	0	0
			1234	795	213	223	3		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	161	Total	C	N	O	S	0	0
			1302	829	242	226	5		

- Molecule 33 is a protein called GEO11417p1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	66	Total	C	N	O	S	0	0
			541	352	96	92	1		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	84	Total	C	N	O	S	0	0
			671	437	117	116	1		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	146	Total	C	N	O	S	0	0
			1215	792	194	225	4		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	108	Total	C	N	O	S	0	0
			892	571	163	157	1		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	134	Total	C	N	O	S	0	0
			1152	735	218	196	3		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	112	Total	C	N	O	S	0	0
			937	596	163	169	9		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	151	Total	C	N	O	S	0	0
			1266	795	233	228	10		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	q	133	Total	C	N	O	S	0	0
			1118	727	187	199	5		

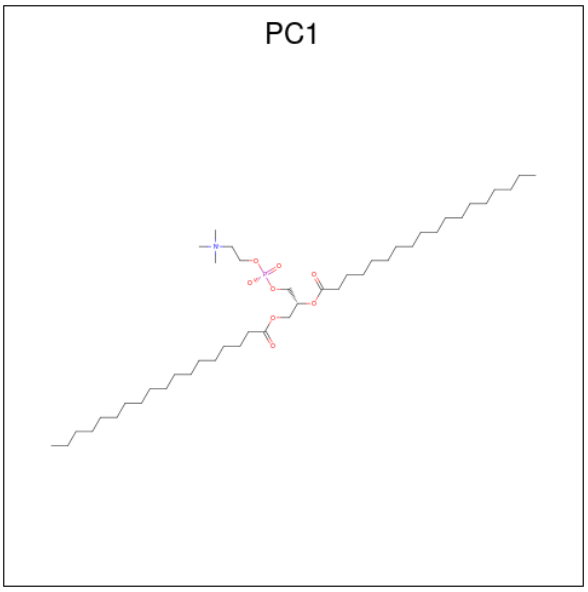
- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	r	89	Total	C	N	O	S	0	0
			724	457	136	130	1		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

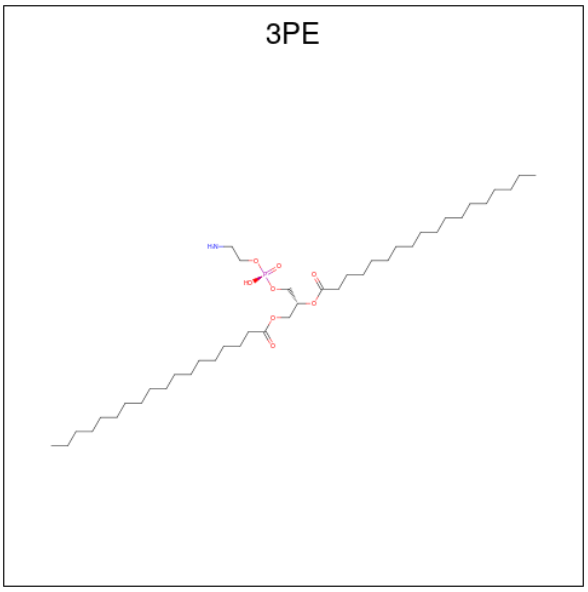
Mol	Chain	Residues	Atoms					AltConf	Trace
42	s	62	Total	C	N	O	S	0	0
			456	288	75	90	3		

- Molecule 43 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



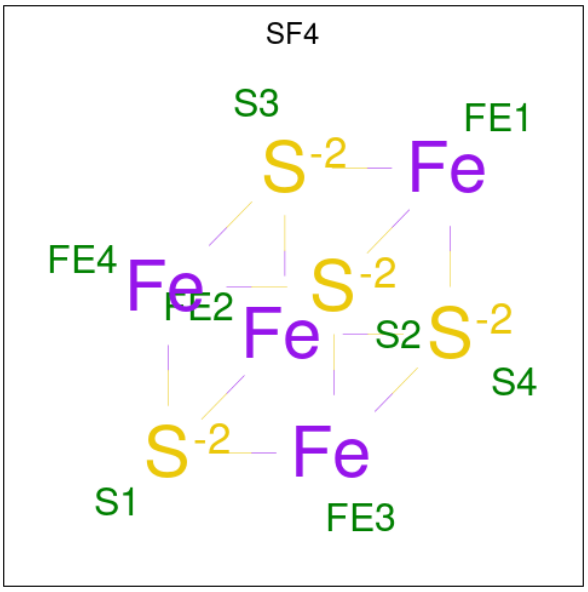
Mol	Chain	Residues	Atoms					AltConf
43	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
43	J	1	Total	C	N	O	P	0
			44	34	1	8	1	
43	i	1	Total	C	N	O	P	0
			34	24	1	8	1	

- Molecule 44 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



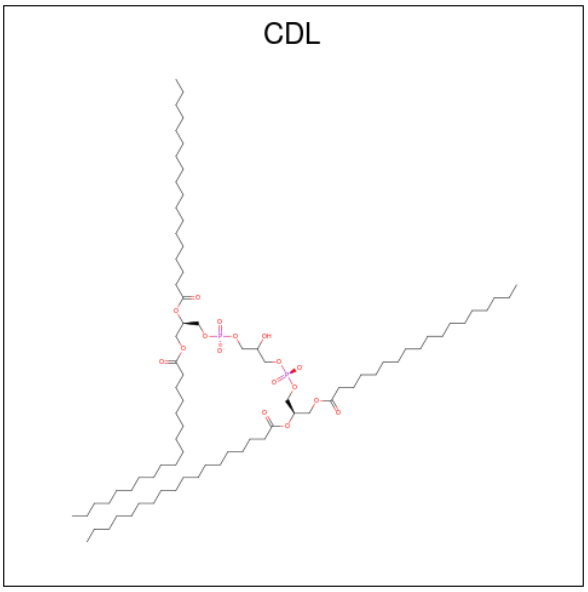
Mol	Chain	Residues	Atoms					AltConf
44	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
44	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
44	B	1	Total	C	N	O	P	0
			37	27	1	8	1	
44	H	1	Total	C	N	O	P	0
			47	37	1	8	1	
44	J	1	Total	C	N	O	P	0
			40	30	1	8	1	
44	J	1	Total	C	N	O	P	0
			24	14	1	8	1	
44	L	1	Total	C	N	O	P	0
			39	29	1	8	1	
44	L	1	Total	C	N	O	P	0
			44	34	1	8	1	
44	L	1	Total	C	N	O	P	0
			25	15	1	8	1	
44	M	1	Total	C	N	O	P	0
			35	25	1	8	1	
44	N	1	Total	C	N	O	P	0
			44	34	1	8	1	
44	X	1	Total	C	N	O	P	0
			30	20	1	8	1	
44	Y	1	Total	C	N	O	P	0
			44	34	1	8	1	
44	Y	1	Total	C	N	O	P	0
			30	20	1	8	1	
44	Y	1	Total	C	N	O	P	0
			33	23	1	8	1	
44	d	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



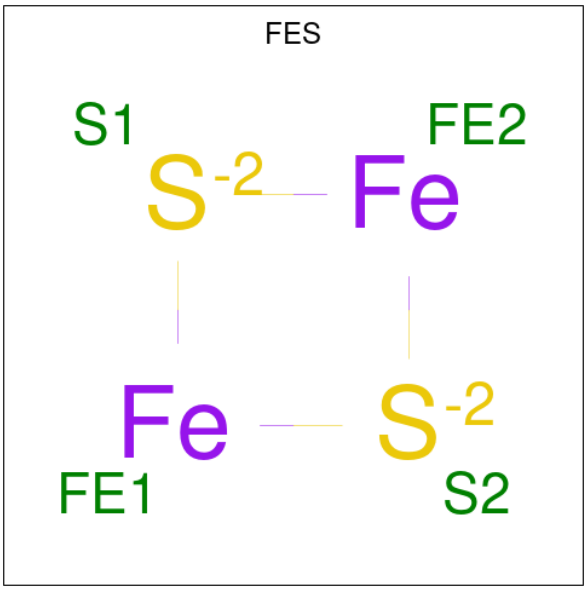
Mol	Chain	Residues	Atoms	AltConf
45	B	1	Total Fe S 8 4 4	0
45	F	1	Total Fe S 8 4 4	0
45	G	1	Total Fe S 8 4 4	0
45	G	1	Total Fe S 8 4 4	0
45	I	1	Total Fe S 8 4 4	0
45	I	1	Total Fe S 8 4 4	0

- Molecule 46 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



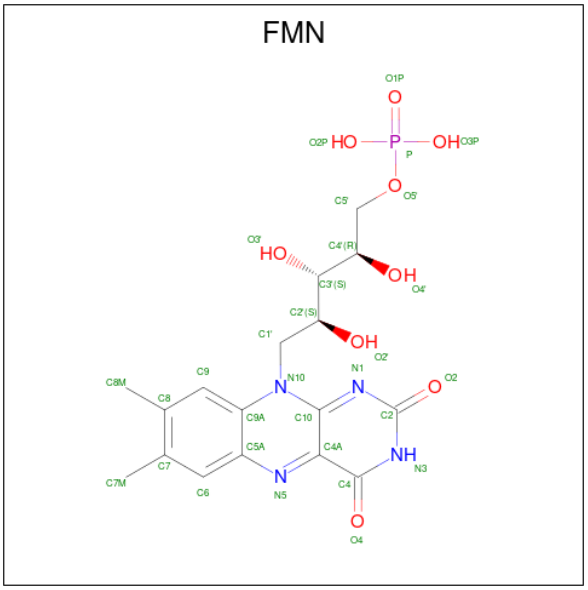
Mol	Chain	Residues	Atoms				AltConf
46	B	1	Total	C	O	P	0
			67	48	17	2	
46	P	1	Total	C	O	P	0
			54	35	17	2	
46	h	1	Total	C	O	P	0
			69	50	17	2	
46	h	1	Total	C	O	P	0
			60	41	17	2	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	AltConf
47	E	1	Total Fe S 4 2 2	0
47	G	1	Total Fe S 4 2 2	0

- Molecule 48 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

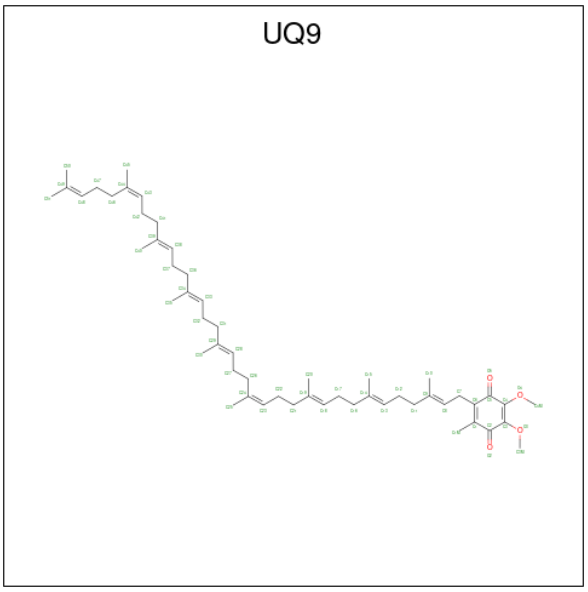


Mol	Chain	Residues	Atoms	AltConf
48	F	1	Total C N O P 31 17 4 9 1	0

- Molecule 49 is SODIUM ION (CCD ID: NA) (formula: Na).

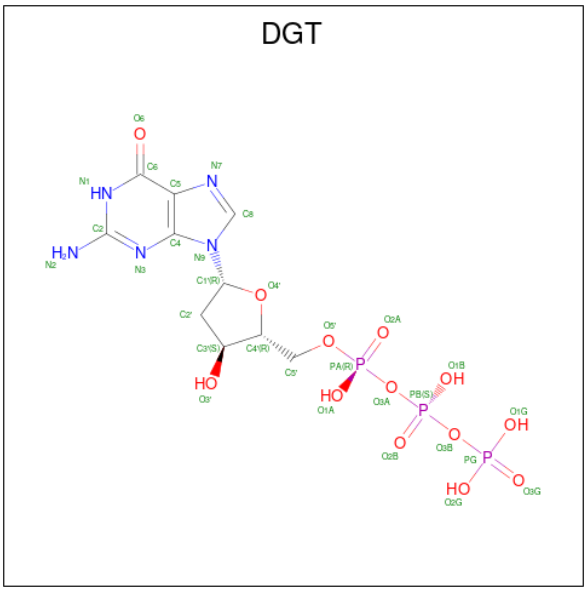
Mol	Chain	Residues	Atoms	AltConf
49	G	1	Total Na 1 1	0

- Molecule 50 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).



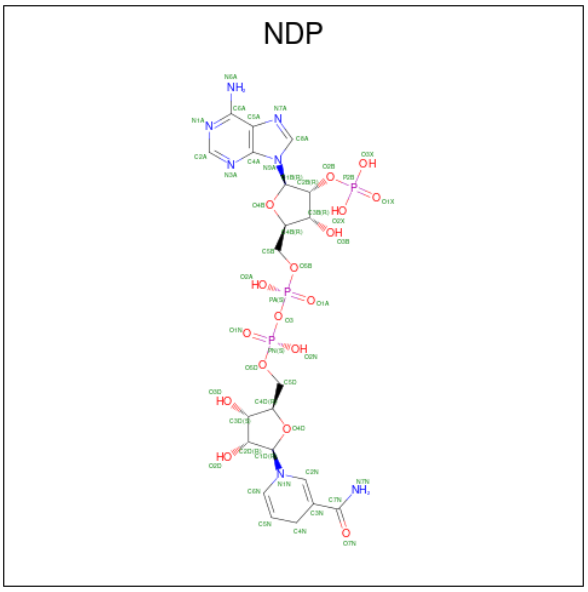
Mol	Chain	Residues	Atoms			AltConf
50	H	1	Total	C	O	0
			58	54	4	

- Molecule 51 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
51	O	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

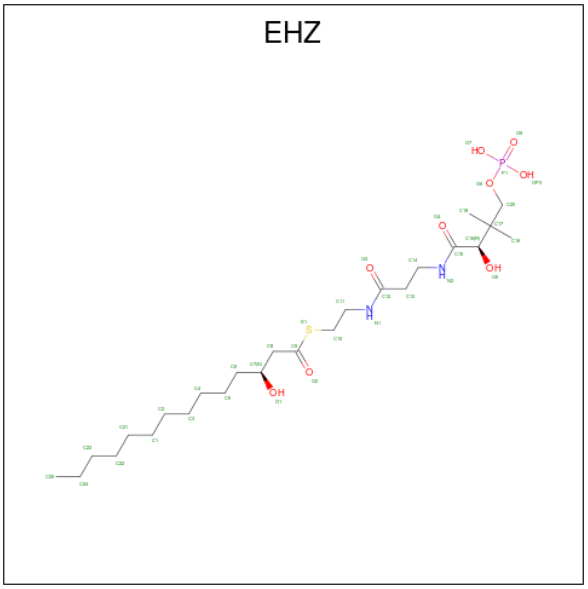


Mol	Chain	Residues	Atoms					AltConf
52	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 54 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



Mol	Chain	Residues	Atoms						AltConf
54	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
54	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

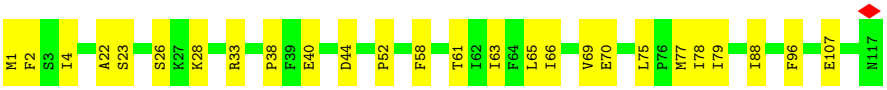
3 Residue-property plots (i)

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-ubiquinone oxidoreductase chain 3

Chain A:





• Molecule 2: LD31474p

Chain B:

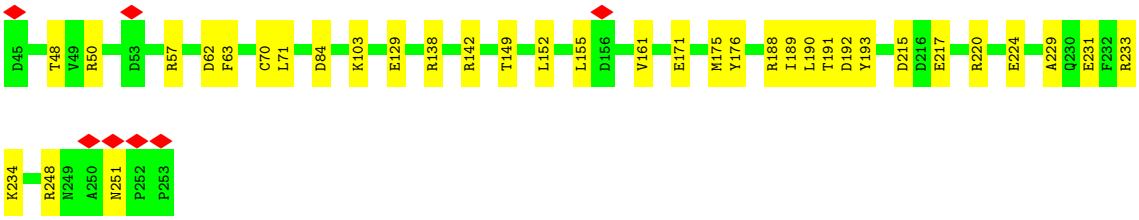




• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:

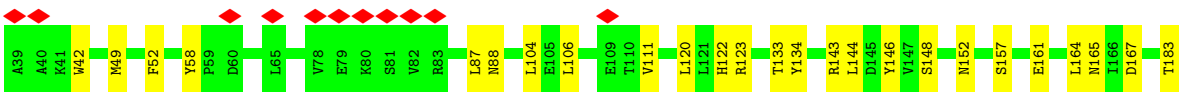


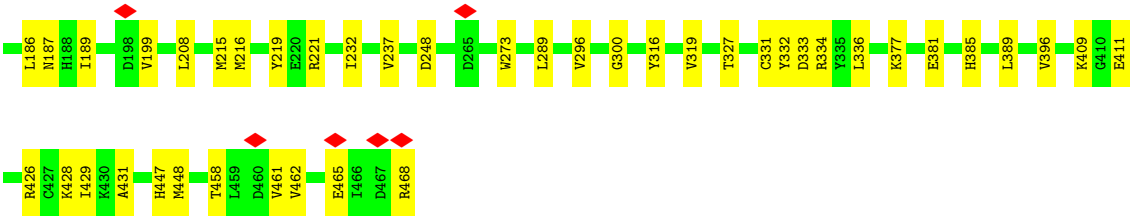


• Molecule 4: Complex I-49kD

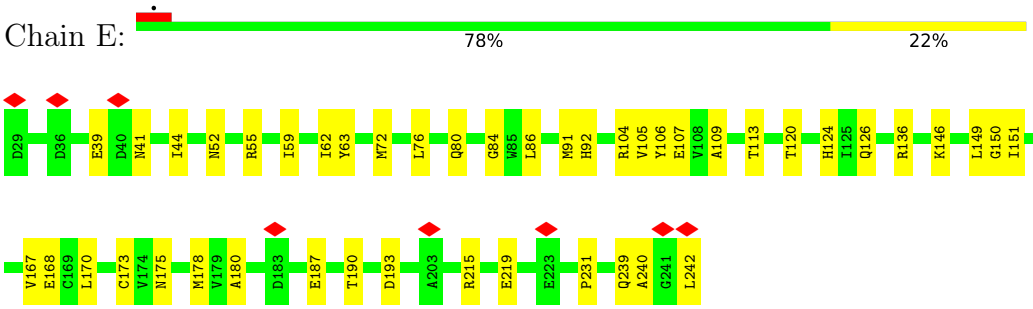
Chain D:



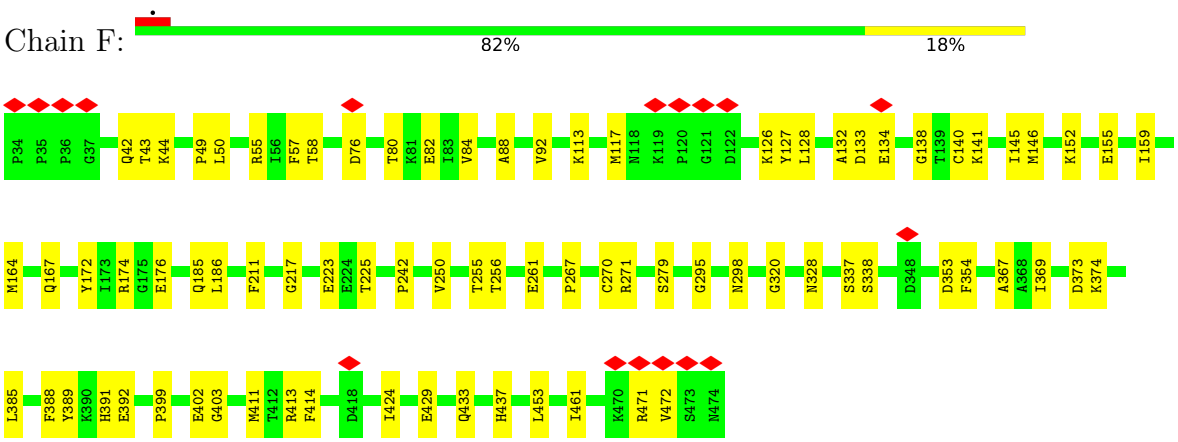




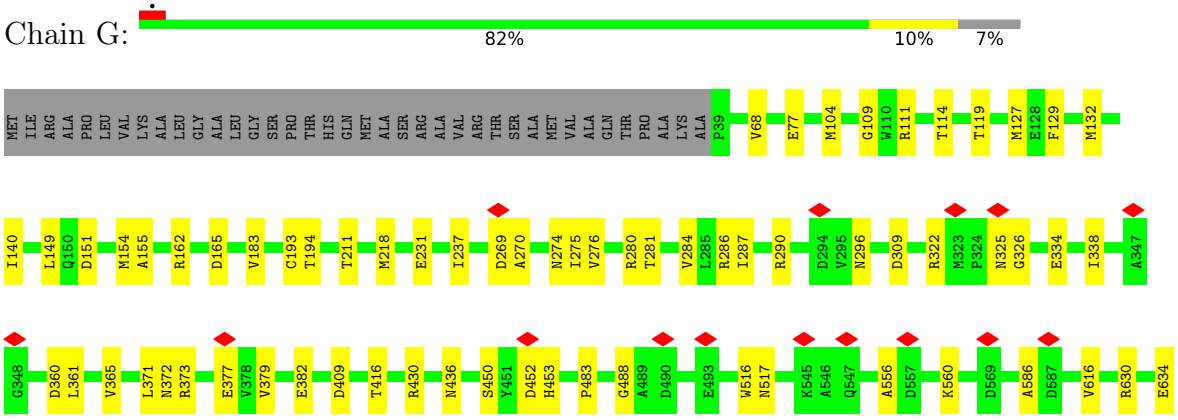
• Molecule 5: NADH dehydrogenase (Ubiquinone) 24 kDa subunit, isoform A

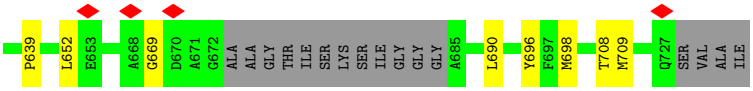


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

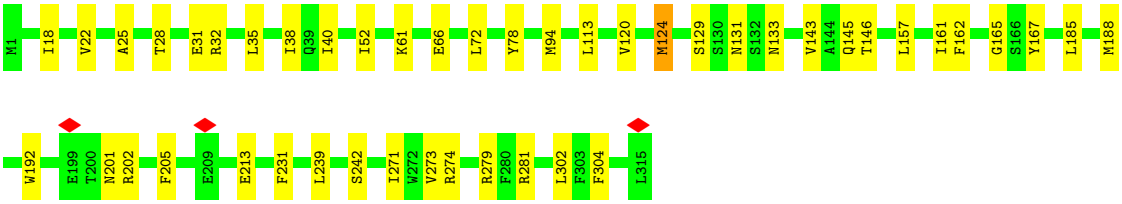




• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:

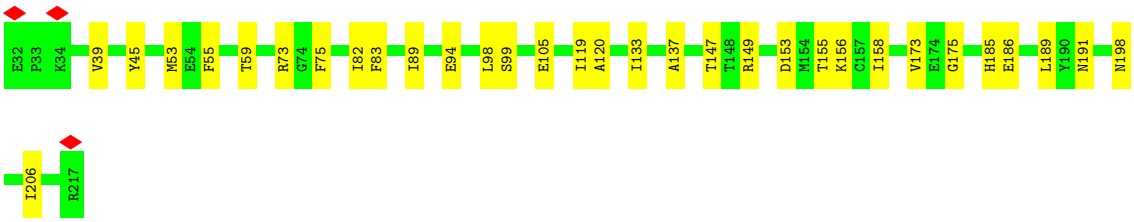




• Molecule 9: NADH dehydrogenase (ubiquinone) 23 kDa subunit

Chain I:

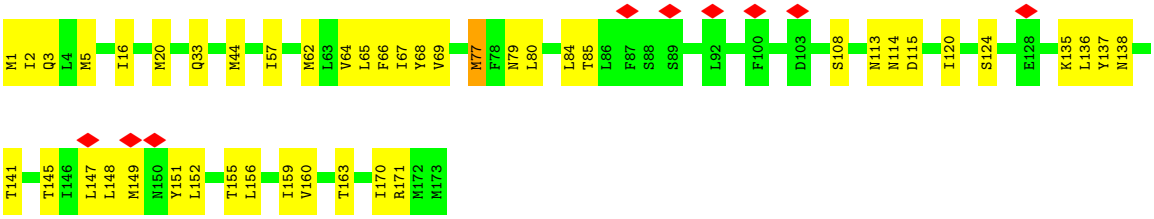




• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:

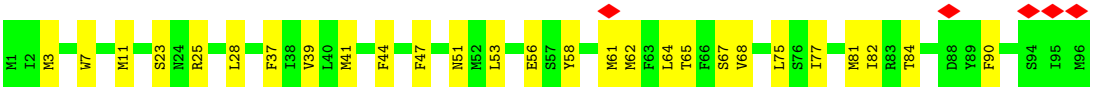




• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:

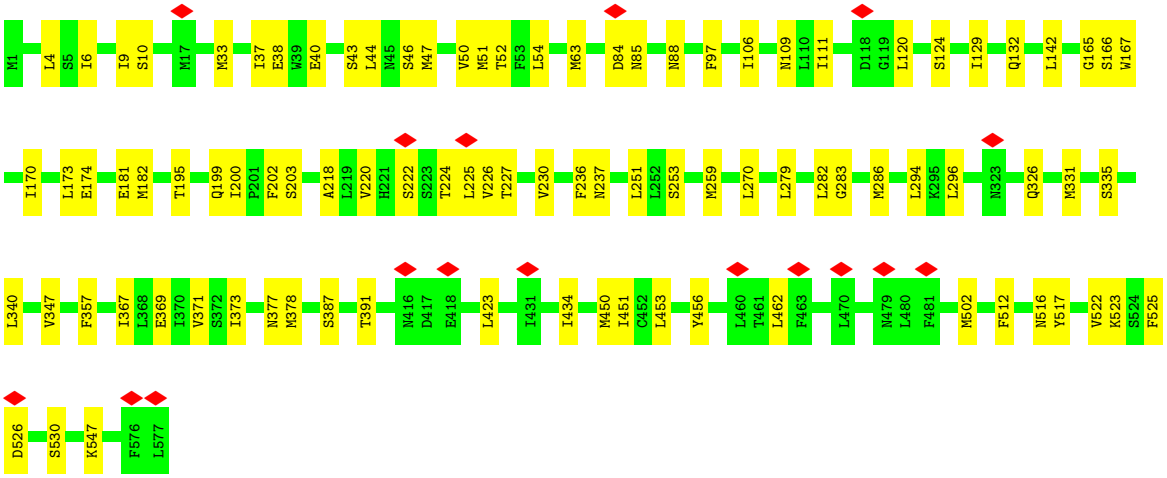




• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:

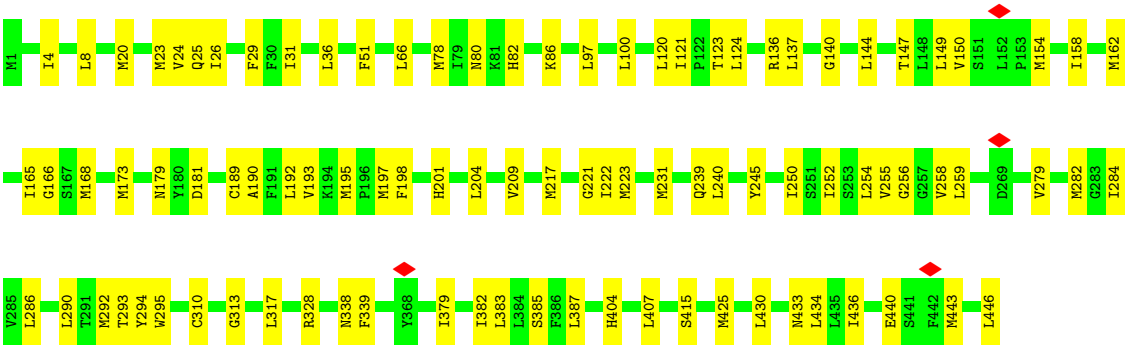




• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:

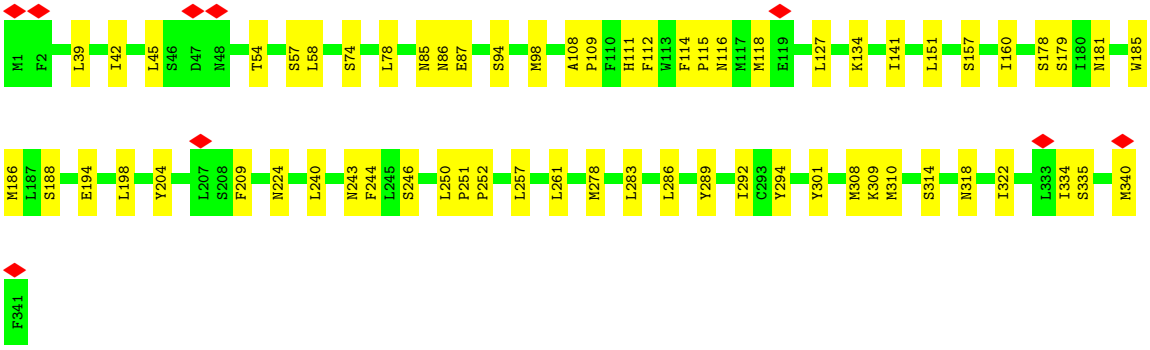




• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:

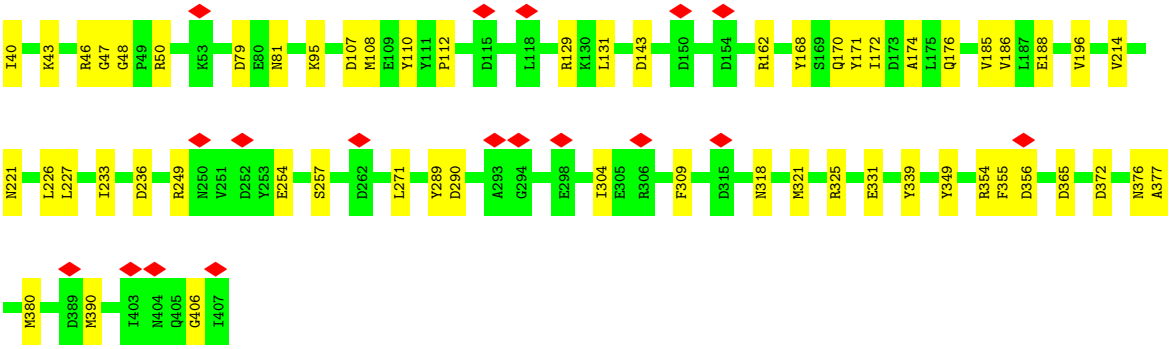




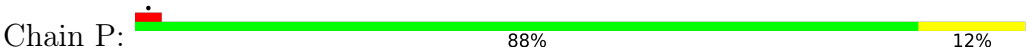
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

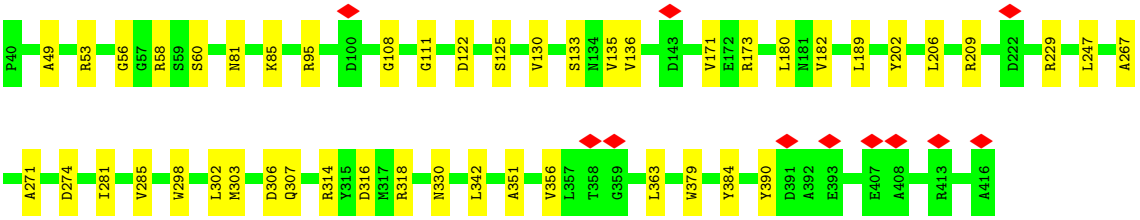
Chain O:



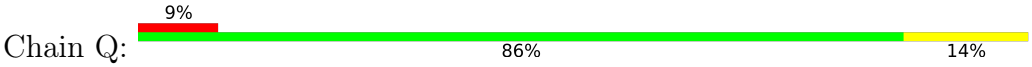


• Molecule 16: NADH dehydrogenase (Ubiquinone) 39 kDa subunit, isoform A



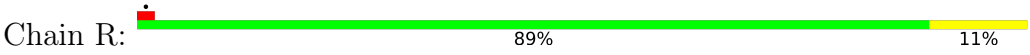


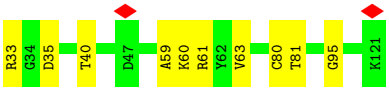
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial





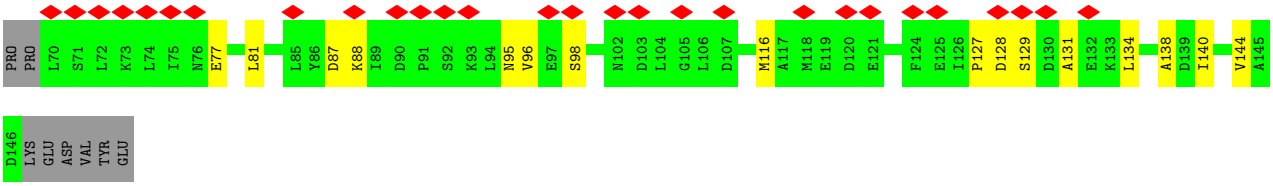
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial





• Molecule 19: Acyl carrier protein, mitochondrial

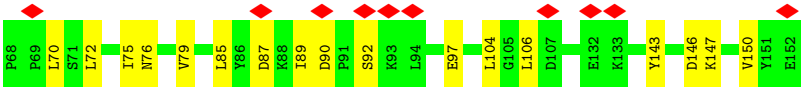




• Molecule 19: Acyl carrier protein, mitochondrial

Chain U:

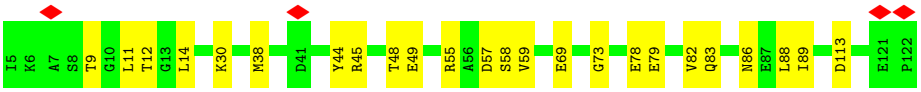




• Molecule 20: NADH dehydrogenase (Ubiquinone) 13 kDa B subunit

Chain V:

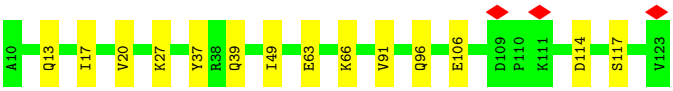




• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

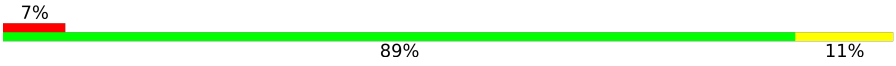
Chain W:

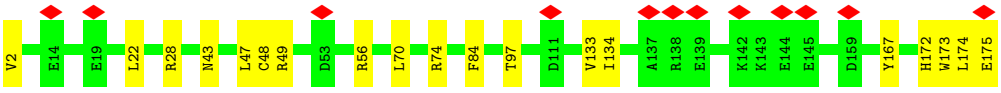




• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:

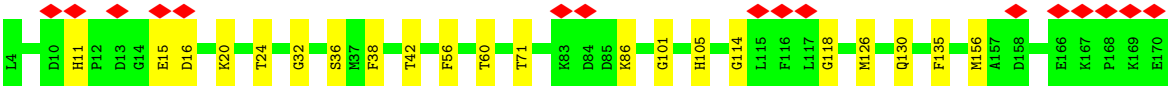




• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:

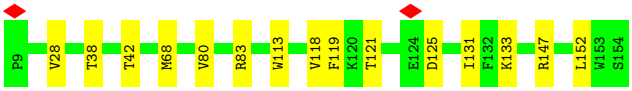




• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:

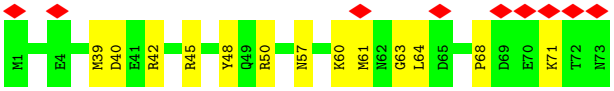




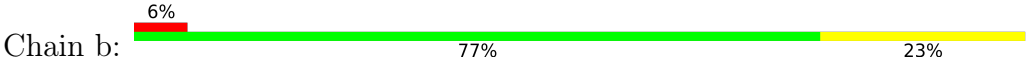
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

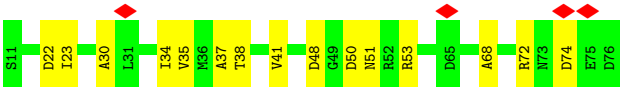
Chain a:



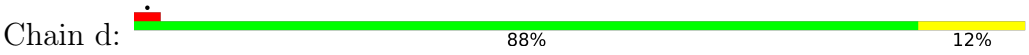


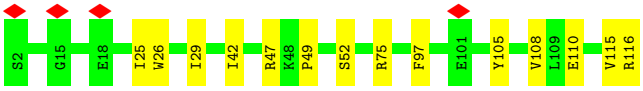
• Molecule 26: RH45008p



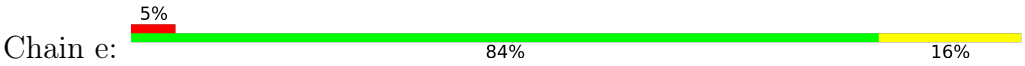


• Molecule 27: NADH dehydrogenase [ubiquinone] 1 subunit C2



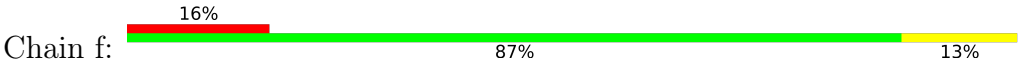


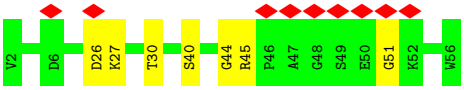
• Molecule 28: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



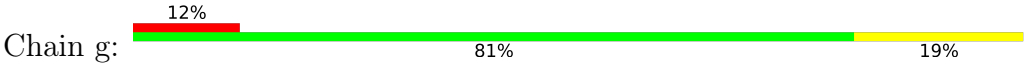


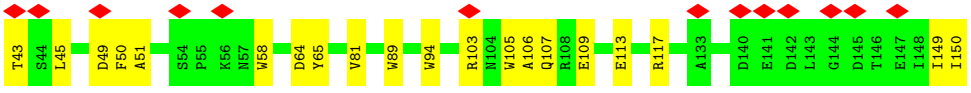
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



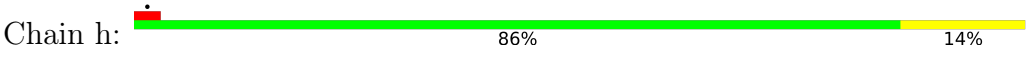


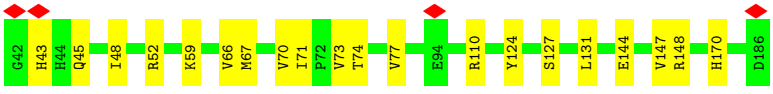
• Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial





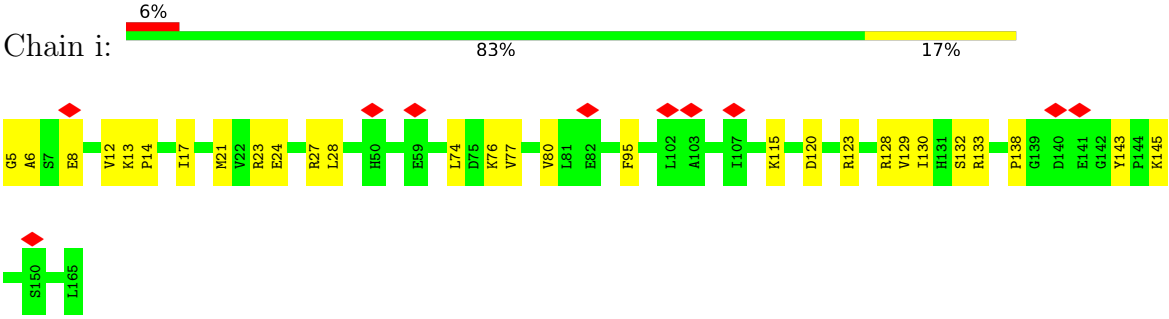
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial





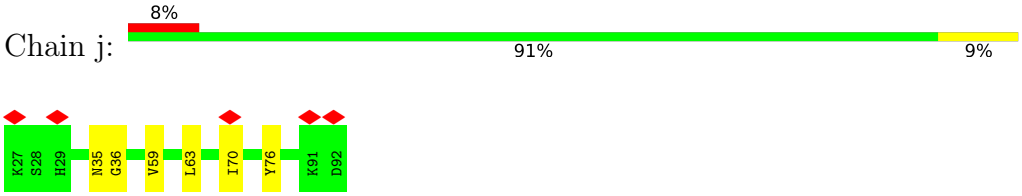
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



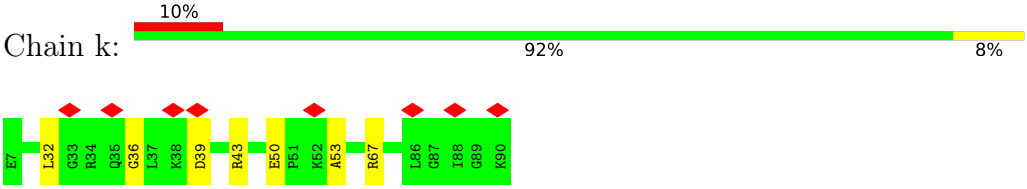
• Molecule 33: GEO11417p1

Chain j:



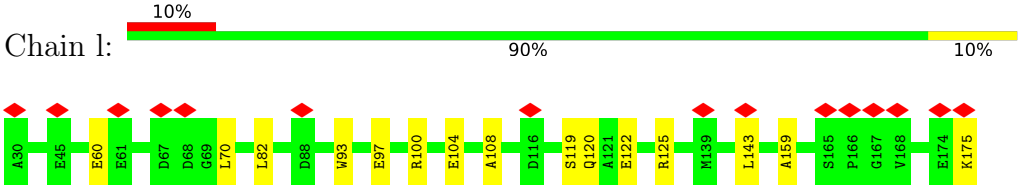
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



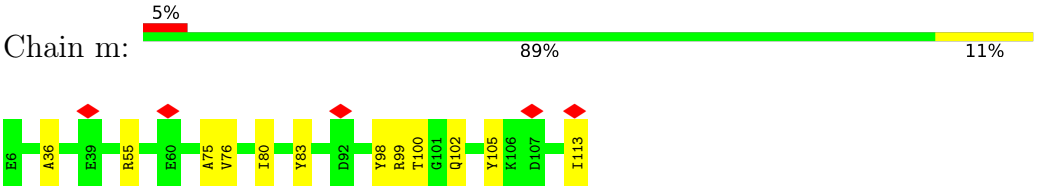
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l:



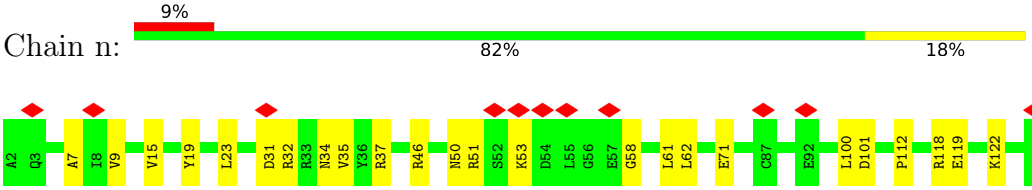
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain m:



• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n:



• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:

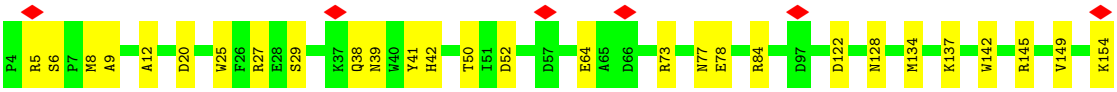




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

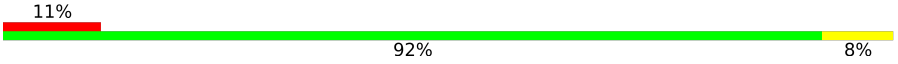
Chain p:

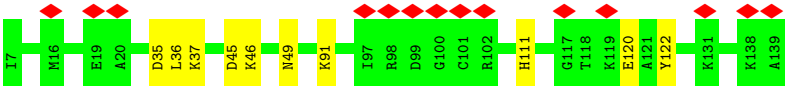




• Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:

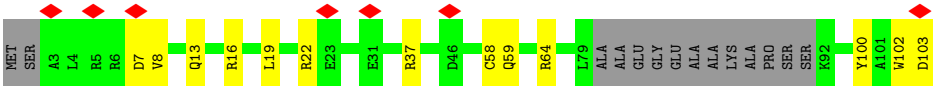




• Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:

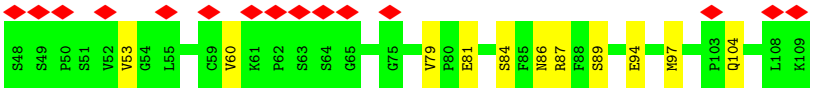




• Molecule 42: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	37608	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 ($e^-/Å^2$)	41.88	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.103	Depositor
Minimum map value	-0.018	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	471.59998, 471.59998, 471.59998	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	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: ZN, NA, DGT, 3PE, UQ9, PC1, EHZ, 2MR, FES, FMN, CDL, SF4, NDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.30	0/979	0.46	0/1325
2	B	0.34	0/1473	0.42	1/1997 (0.1%)
3	C	0.31	0/1774	0.39	0/2412
4	D	0.30	0/3505	0.36	0/4751
5	E	0.27	0/1718	0.41	0/2328
6	F	0.27	0/3461	0.36	0/4678
7	G	0.27	0/5229	0.35	0/7088
8	H	0.30	0/2651	0.43	1/3593 (0.0%)
9	I	0.35	0/1518	0.39	0/2050
10	J	0.29	0/1424	0.44	1/1925 (0.1%)
11	K	0.28	0/814	0.39	0/1095
12	L	0.26	0/4726	0.34	0/6396
13	M	0.30	0/3723	0.35	0/5045
14	N	0.30	0/2875	0.39	0/3890
15	O	0.26	0/3082	0.35	0/4168
16	P	0.27	0/3108	0.37	0/4205
17	Q	0.28	0/1245	0.39	0/1687
18	R	0.28	0/733	0.34	0/987
19	T	0.16	0/624	0.31	0/843
19	U	0.21	0/696	0.30	0/940
20	V	0.24	0/942	0.34	0/1278
21	W	0.29	0/988	0.43	0/1329
22	X	0.23	0/1416	0.38	0/1911
23	Y	0.20	0/1314	0.32	0/1784
24	Z	0.25	0/1239	0.34	0/1682
25	a	0.25	0/614	0.37	0/827
26	b	0.22	0/528	0.34	0/714
27	d	0.24	0/935	0.33	0/1271
28	e	0.31	0/846	0.45	0/1128
29	f	0.23	0/440	0.34	0/590
30	g	0.28	0/908	0.35	0/1240
31	h	0.28	0/1269	0.36	0/1714

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	i	0.25	0/1338	0.39	0/1808
33	j	0.20	0/566	0.28	0/776
34	k	0.20	0/690	0.33	0/936
35	l	0.26	0/1264	0.36	0/1719
36	m	0.25	0/913	0.36	0/1222
37	n	0.25	0/1185	0.31	0/1597
38	o	0.22	0/960	0.39	0/1290
39	p	0.29	0/1299	0.34	0/1752
40	q	0.28	0/1157	0.38	0/1569
41	r	0.22	0/740	0.38	0/1003
42	s	0.21	0/469	0.41	0/637
All	All	0.27	0/67378	0.37	3/91180 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	124	MET	CB-CG-SD	-5.77	95.40	112.70
2	B	96	CYS	CA-CB-SG	5.46	126.95	114.40
10	J	77	MET	N-CA-C	5.12	117.59	109.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	956	0	1030	30	0
2	B	1435	0	1446	30	0
3	C	1726	0	1673	28	0
4	D	3434	0	3406	56	0
5	E	1679	0	1657	36	0
6	F	3381	0	3361	61	0
7	G	5146	0	5189	50	0
8	H	2571	0	2628	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	1485	0	1422	27	0
10	J	1397	0	1513	52	0
11	K	793	0	818	24	0
12	L	4606	0	4742	74	0
13	M	3617	0	3750	71	0
14	N	2796	0	2879	51	0
15	O	3007	0	2945	40	0
16	P	3032	0	3030	32	0
17	Q	1214	0	1186	17	0
18	R	716	0	700	6	0
19	T	615	0	625	10	0
19	U	684	0	687	12	0
20	V	922	0	946	15	0
21	W	968	0	991	14	0
22	X	1383	0	1328	15	0
23	Y	1277	0	1258	14	0
24	Z	1201	0	1211	14	0
25	a	601	0	603	9	0
26	b	519	0	517	11	0
27	d	907	0	896	14	0
28	e	828	0	809	14	0
29	f	429	0	436	4	0
30	g	883	0	834	25	0
31	h	1234	0	1198	17	0
32	i	1302	0	1295	28	0
33	j	541	0	508	7	0
34	k	671	0	671	6	0
35	l	1215	0	1125	14	0
36	m	892	0	885	16	0
37	n	1152	0	1124	19	0
38	o	937	0	922	12	0
39	p	1266	0	1217	27	0
40	q	1118	0	1071	8	0
41	r	724	0	727	11	0
42	s	456	0	440	12	0
43	A	39	0	52	0	0
43	J	44	0	62	0	0
43	i	34	0	42	1	0
44	A	79	0	106	1	0
44	B	37	0	48	0	0
44	H	47	0	71	0	0
44	J	64	0	76	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	L	108	0	144	1	0
44	M	35	0	44	0	0
44	N	44	0	62	0	0
44	X	30	0	34	0	0
44	Y	107	0	139	0	0
44	d	36	0	46	0	0
45	B	8	0	0	0	0
45	F	8	0	0	0	0
45	G	16	0	0	0	0
45	I	16	0	0	0	0
46	B	67	0	78	0	0
46	P	54	0	52	0	0
46	h	129	0	146	3	0
47	E	4	0	0	0	0
47	G	4	0	0	0	0
48	F	31	0	19	1	0
49	G	1	0	0	0	0
50	H	58	0	82	15	0
51	O	31	0	12	2	0
52	P	48	0	24	2	0
53	R	1	0	0	0	0
54	T	37	0	0	3	0
54	U	37	0	0	3	0
All	All	66970	0	67038	851	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 6.

All (851) 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:F:113:LYS:NZ	48:F:501:FMN:O1P	2.06	0.88
12:L:517:TYR:OH	36:m:75:ALA:O	1.93	0.87
4:D:448:MET:SD	8:H:281:ARG:NH2	2.49	0.86
54:U:201:EHZ:O5	37:n:51:ARG:NH1	2.10	0.84
31:h:124:TYR:OH	39:p:64:GLU:OE2	1.93	0.84
7:G:430:ARG:NH1	7:G:450:SER:O	2.11	0.82
30:g:107:GLN:NE2	32:i:123:ARG:O	2.13	0.82
13:M:293:THR:HG21	36:m:113:ILE:HG21	1.62	0.81
19:U:147:LYS:NZ	32:i:24:GLU:OE2	2.14	0.81
9:I:191:ASN:OD1	40:q:122:TYR:OH	2.00	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:h:52:ARG:NH1	46:h:202:CDL:OA3	2.15	0.79
9:I:149:ARG:NH2	17:Q:119:MET:O	2.15	0.79
13:M:284:ILE:HD11	13:M:387:LEU:HD23	1.63	0.79
3:C:220:ARG:NH2	21:W:106:GLU:OE2	2.16	0.78
28:e:35:MET:HE1	31:h:170:HIS:CG	2.17	0.78
3:C:231:GLU:OE2	17:Q:124:SER:N	2.16	0.78
13:M:150:VAL:HG11	13:M:193:VAL:HG21	1.63	0.78
4:D:144:LEU:O	4:D:152:ASN:ND2	2.16	0.78
12:L:38:GLU:OE1	32:i:128:ARG:NH2	2.16	0.78
15:O:372:ASP:O	15:O:376:ASN:ND2	2.16	0.78
9:I:73:ARG:NH1	41:r:19:LEU:O	2.16	0.78
32:i:115:LYS:NZ	39:p:20:ASP:OD1	2.17	0.77
12:L:132:GLN:NE2	13:M:404:HIS:O	2.17	0.77
14:N:178:SER:OG	14:N:289:TYR:OH	1.98	0.77
6:F:76:ASP:O	6:F:271:ARG:NH2	2.17	0.77
35:l:159:ALA:O	38:o:96:ARG:NH1	2.17	0.77
23:Y:32:GLY:O	23:Y:36:SER:OG	2.02	0.76
18:R:80:CYS:SG	18:R:81:THR:N	2.58	0.76
12:L:43:SER:OG	30:g:103:ARG:NH2	2.19	0.75
6:F:353:ASP:OD1	6:F:354:PHE:N	2.20	0.75
30:g:45:LEU:HD12	30:g:49:ASP:CB	2.16	0.75
13:M:120:LEU:O	13:M:123:THR:OG1	2.04	0.74
10:J:77:MET:HE3	16:P:390:TYR:HB2	1.70	0.74
15:O:171:TYR:OH	15:O:227:LEU:O	2.06	0.74
12:L:512:PHE:O	12:L:516:ASN:ND2	2.21	0.74
26:b:48:ASP:O	26:b:72:ARG:NH1	2.21	0.74
7:G:382:GLU:O	7:G:560:LYS:NZ	2.18	0.73
12:L:251:LEU:HD21	35:l:143:LEU:HD23	1.70	0.73
2:B:133:THR:OG1	2:B:161:CYS:SG	2.45	0.73
2:B:151:GLU:N	8:H:66:GLU:OE1	2.20	0.73
32:i:13:LYS:NZ	36:m:36:ALA:O	2.19	0.73
18:R:60:LYS:NZ	40:q:120:GLU:OE1	2.21	0.73
30:g:109:GLU:OE1	39:p:42:HIS:NE2	2.22	0.72
30:g:45:LEU:HD12	30:g:49:ASP:HB3	1.72	0.72
14:N:309:LYS:HZ1	15:O:406:GLY:CA	2.02	0.72
35:l:122:GLU:N	35:l:122:GLU:OE1	2.22	0.72
41:r:8:VAL:O	41:r:13:GLN:NE2	2.22	0.72
5:E:52:ASN:OD1	5:E:55:ARG:NH1	2.23	0.72
9:I:98:LEU:O	41:r:37:ARG:NH2	2.23	0.72
13:M:198:PHE:O	13:M:201:HIS:ND1	2.22	0.72
27:d:108:VAL:O	39:p:137:LYS:NZ	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:217:GLU:OE1	16:P:81:ASN:ND2	2.22	0.72
7:G:309:ASP:OD2	7:G:708:THR:OG1	2.04	0.72
50:H:501:UQ9:H36A	50:H:501:UQ9:H40	1.72	0.72
31:h:110:ARG:NH1	39:p:38:GLN:OE1	2.23	0.72
35:l:125:ARG:NH1	37:n:71:GLU:O	2.22	0.72
8:H:32:ARG:NE	50:H:501:UQ9:H20B	2.05	0.72
9:I:105:GLU:OE1	9:I:198:ASN:ND2	2.23	0.72
23:Y:11:HIS:ND1	23:Y:16:ASP:OD2	2.23	0.72
12:L:253:SER:OG	12:L:283:GLY:O	2.07	0.71
3:C:215:ASP:OD2	16:P:81:ASN:ND2	2.24	0.71
31:h:43:HIS:O	31:h:45:GLN:NE2	2.23	0.71
6:F:429:GLU:OE2	7:G:162:ARG:NH1	2.23	0.71
4:D:42:TRP:O	13:M:136:ARG:NH2	2.24	0.71
1:A:66:ILE:O	1:A:69:VAL:HG12	1.90	0.70
12:L:326:GLN:N	12:L:326:GLN:OE1	2.24	0.70
26:b:53:ARG:NE	26:b:74:ASP:OD2	2.24	0.70
16:P:173:ARG:NH1	16:P:274:ASP:O	2.24	0.70
54:U:201:EHZ:O2	54:U:201:EHZ:O1	2.05	0.70
9:I:153:ASP:OD1	9:I:189:LEU:HD22	1.91	0.70
7:G:409:ASP:OD1	7:G:436:ASN:ND2	2.24	0.70
13:M:162:MET:HG3	13:M:168:MET:HE2	1.74	0.70
15:O:110:TYR:OH	15:O:188:GLU:OE2	2.05	0.69
13:M:293:THR:HG21	36:m:113:ILE:CG2	2.22	0.69
42:s:60:VAL:HG23	42:s:84:SER:HB2	1.74	0.69
1:A:107:GLU:OE1	10:J:160:VAL:HG11	1.92	0.69
6:F:50:LEU:HD21	6:F:55:ARG:HG2	1.75	0.68
30:g:45:LEU:N	37:n:119:GLU:OE2	2.27	0.68
4:D:327:THR:O	20:V:12:THR:OG1	2.11	0.68
22:X:2:VAL:HG22	24:Z:118:VAL:HG21	1.76	0.68
37:n:15:VAL:HG22	37:n:62:LEU:HD21	1.75	0.68
1:A:2:PHE:CE1	10:J:2:ILE:HD11	2.29	0.68
6:F:76:ASP:OD1	6:F:152:LYS:NZ	2.27	0.68
7:G:77:GLU:N	7:G:77:GLU:OE1	2.27	0.68
6:F:185:GLN:NE2	42:s:94:GLU:OE2	2.27	0.67
7:G:284:VAL:HG23	7:G:616:VAL:HG21	1.74	0.67
12:L:525:PHE:O	12:L:530:SER:OG	2.06	0.67
1:A:78:ILE:HD12	8:H:162:PHE:HA	1.76	0.67
3:C:192:ASP:OD2	3:C:193:TYR:N	2.27	0.67
12:L:47:MET:HE2	12:L:165:GLY:HA2	1.77	0.67
10:J:16:ILE:HG22	10:J:84:LEU:HD11	1.76	0.67
26:b:35:VAL:O	26:b:38:THR:OG1	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:108:ALA:O	14:N:111:HIS:ND1	2.28	0.67
30:g:58:TRP:CZ2	32:i:6:ALA:HB2	2.30	0.66
50:H:501:UQ9:C41	50:H:501:UQ9:H45	2.26	0.66
30:g:58:TRP:NE1	32:i:5:GLY:O	2.29	0.66
35:l:175:LYS:NZ	38:o:31:SER:OG	2.23	0.66
6:F:50:LEU:HD23	6:F:50:LEU:O	1.95	0.66
38:o:66:ALA:O	39:p:5:ARG:NH2	2.28	0.66
7:G:365:VAL:HG21	7:G:652:LEU:CD2	2.25	0.66
13:M:294:TYR:OH	13:M:446:LEU:O	2.13	0.66
10:J:20:MET:HE1	44:J:203:3PE:O22	1.96	0.66
35:l:60:GLU:N	35:l:60:GLU:OE1	2.29	0.66
5:E:62:ILE:HD11	6:F:211:PHE:CD1	2.31	0.65
35:l:108:ALA:O	36:m:55:ARG:NH2	2.29	0.65
12:L:63:MET:SD	12:L:106:ILE:HD11	2.37	0.65
12:L:109:ASN:OD1	12:L:111:ILE:N	2.30	0.65
39:p:50:THR:OG1	39:p:52:ASP:OD1	2.14	0.65
7:G:365:VAL:HG21	7:G:652:LEU:HD22	1.77	0.65
15:O:331:GLU:N	15:O:331:GLU:OE1	2.30	0.65
12:L:226:VAL:HB	12:L:282:LEU:HD11	1.78	0.65
7:G:109:GLY:O	7:G:111:ARG:NH2	2.30	0.65
16:P:189:LEU:HD23	16:P:351:ALA:HB1	1.78	0.65
3:C:57:ARG:NE	3:C:84:ASP:OD1	2.30	0.65
50:H:501:UQ9:H45	50:H:501:UQ9:H41	1.78	0.65
6:F:337:SER:O	6:F:338:SER:OG	2.14	0.64
32:i:23:ARG:NH2	35:l:93:TRP:O	2.31	0.64
50:H:501:UQ9:H13	50:H:501:UQ9:H20	1.78	0.64
8:H:231:PHE:CE1	50:H:501:UQ9:H15B	2.32	0.64
37:n:46:ARG:O	37:n:50:ASN:ND2	2.30	0.64
6:F:250:VAL:HG22	6:F:255:THR:HG21	1.80	0.64
8:H:120:VAL:HG21	8:H:146:THR:OG1	1.98	0.63
7:G:517:ASN:ND2	7:G:669:GLY:O	2.31	0.63
12:L:462:LEU:HD11	33:j:70:ILE:HG23	1.80	0.63
22:X:84:PHE:CD2	25:a:64:LEU:HD11	2.34	0.63
7:G:372:ASN:ND2	7:G:377:GLU:OE2	2.31	0.63
7:G:231:GLU:OE2	7:G:231:GLU:N	2.31	0.63
5:E:63:TYR:O	42:s:104:GLN:NE2	2.32	0.62
44:A:203:3PE:C2F	50:H:501:UQ9:H45A	2.29	0.62
14:N:112:PHE:O	14:N:116:ASN:ND2	2.32	0.62
15:O:46:ARG:NH1	15:O:48:GLY:O	2.31	0.62
3:C:229:ALA:O	17:Q:123:SER:OG	2.09	0.62
10:J:148:LEU:HD13	11:K:65:THR:HG21	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:h:144:GLU:OE2	31:h:148:ARG:NE	2.29	0.62
4:D:144:LEU:HD13	4:D:429:ILE:HD13	1.81	0.62
8:H:38:ILE:HG13	9:I:82:ILE:HD11	1.81	0.62
4:D:111:VAL:HG12	4:D:447:HIS:O	2.00	0.62
4:D:122:HIS:ND1	4:D:468:ARG:OXT	2.33	0.61
2:B:111:MET:HE1	2:B:118:PHE:CD1	2.35	0.61
5:E:124:HIS:ND1	5:E:126:GLN:OE1	2.33	0.61
13:M:379:ILE:O	36:m:83:TYR:OH	2.17	0.61
4:D:164:LEU:HD21	4:D:396:VAL:HG22	1.83	0.61
35:l:119:SER:O	35:l:120:GLN:NE2	2.34	0.61
11:K:53:LEU:HD13	11:K:56:GLU:HG3	1.82	0.61
13:M:338:ASN:HB2	13:M:407:LEU:HD21	1.82	0.61
30:g:113:GLU:OE2	30:g:117:ARG:NH2	2.33	0.61
20:V:45:ARG:NH2	20:V:49:GLU:OE1	2.34	0.61
14:N:108:ALA:HB2	14:N:157:SER:HA	1.81	0.61
42:s:86:ASN:OD1	42:s:87:ARG:N	2.34	0.61
12:L:173:LEU:HD23	12:L:182:MET:HE2	1.83	0.61
19:U:143:TYR:OH	32:i:28:LEU:HD23	1.99	0.61
5:E:104:ARG:NH1	5:E:107:GLU:OE2	2.34	0.60
19:U:70:LEU:O	19:U:150:VAL:HG11	2.00	0.60
1:A:52:PRO:O	10:J:171:ARG:NH2	2.34	0.60
13:M:149:LEU:HA	14:N:283:LEU:HD11	1.82	0.60
38:o:69:SER:O	39:p:6:SER:OG	2.17	0.60
4:D:183:THR:OG1	4:D:219:TYR:OH	2.18	0.60
10:J:155:THR:O	10:J:159:ILE:HD12	2.02	0.60
46:h:201:CDL:OA3	39:p:27:ARG:NH1	2.34	0.60
10:J:124:SER:OG	25:a:42:ARG:NH1	2.35	0.60
39:p:145:ARG:O	39:p:154:LYS:NZ	2.29	0.60
7:G:127:MET:HE3	7:G:127:MET:HA	1.83	0.60
7:G:269:ASP:OD1	7:G:270:ALA:N	2.35	0.60
13:M:339:PHE:CE2	13:M:407:LEU:HD22	2.36	0.60
15:O:318:ASN:O	15:O:325:ARG:NH2	2.35	0.60
14:N:294:TYR:O	14:N:301:TYR:OH	2.09	0.59
16:P:136:VAL:HG23	16:P:171:VAL:HG11	1.83	0.59
14:N:322:ILE:HG13	27:d:42:ILE:HD11	1.84	0.59
3:C:176:TYR:OH	4:D:426:ARG:NE	2.34	0.59
4:D:144:LEU:CD1	4:D:429:ILE:HD13	2.31	0.59
12:L:181:GLU:N	12:L:181:GLU:OE1	2.35	0.59
12:L:224:THR:HG22	12:L:225:LEU:H	1.67	0.59
12:L:340:LEU:HD23	12:L:423:LEU:HD13	1.84	0.59
6:F:186:LEU:HD13	42:s:53:VAL:HG22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:430:LEU:HD11	13:M:434:LEU:HD11	1.84	0.59
14:N:85:ASN:HB2	28:e:2:SER:HA	1.84	0.59
54:U:201:EHZ:O6	37:n:51:ARG:NH1	2.35	0.59
12:L:97:PHE:CZ	12:L:224:THR:HG21	2.38	0.59
33:j:35:ASN:OD1	33:j:36:GLY:N	2.36	0.59
5:E:167:VAL:HG12	5:E:168:GLU:H	1.67	0.59
40:q:35:ASP:OD1	40:q:36:LEU:N	2.36	0.59
2:B:46:ALA:O	2:B:50:GLN:N	2.35	0.59
10:J:113:ASN:OD1	10:J:114:ASN:N	2.35	0.59
12:L:9:ILE:HD12	32:i:95:PHE:CE2	2.38	0.59
13:M:440:GLU:OE2	30:g:103:ARG:NH1	2.35	0.59
23:Y:114:GLY:O	23:Y:118:GLY:N	2.34	0.59
2:B:108:ARG:HD2	9:I:89:ILE:HD12	1.85	0.59
27:d:49:PRO:O	27:d:52:SER:OG	2.21	0.59
12:L:203:SER:OG	12:L:502:MET:SD	2.61	0.58
15:O:129:ARG:NH1	15:O:143:ASP:OD2	2.35	0.58
10:J:68:TYR:CE1	11:K:75:LEU:HD21	2.38	0.58
16:P:247:LEU:HD12	16:P:314:ARG:HD2	1.84	0.58
12:L:97:PHE:CE1	12:L:224:THR:HG21	2.38	0.58
20:V:57:ASP:OD1	20:V:58:SER:N	2.35	0.58
29:f:45:ARG:NH1	29:f:51:GLY:O	2.36	0.58
42:s:86:ASN:N	42:s:89:SER:OG	2.36	0.58
10:J:115:ASP:O	24:Z:147:ARG:NH1	2.36	0.58
10:J:135:LYS:O	10:J:141:THR:OG1	2.20	0.58
16:P:209:ARG:HH12	16:P:281:ILE:HD11	1.69	0.58
12:L:456:TYR:HH	38:o:2:GLY:N	2.01	0.58
15:O:254:GLU:O	15:O:257:SER:OG	2.20	0.58
22:X:56:ARG:NH2	24:Z:125:ASP:O	2.36	0.58
34:k:32:LEU:O	34:k:36:GLY:N	2.36	0.58
6:F:373:ASP:OD2	6:F:374:LYS:N	2.37	0.57
11:K:61:MET:O	11:K:65:THR:HG23	2.04	0.57
1:A:44:ASP:OD1	21:W:96:GLN:NE2	2.36	0.57
4:D:409:LYS:NZ	4:D:462:VAL:HG23	2.20	0.57
12:L:367:ILE:O	12:L:371:VAL:HG23	2.04	0.57
37:n:58:GLY:HA2	37:n:61:LEU:HD12	1.86	0.57
5:E:80:GLN:O	5:E:84:GLY:N	2.36	0.57
10:J:65:LEU:O	10:J:69:VAL:HG23	2.05	0.57
14:N:309:LYS:HZ1	15:O:406:GLY:HA3	1.68	0.57
30:g:150:ILE:HD11	39:p:142:TRP:CG	2.40	0.57
3:C:62:ASP:OD1	3:C:63:PHE:N	2.36	0.57
13:M:192:LEU:HD22	13:M:197:MET:HE3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:n:31:ASP:OD1	37:n:32:ARG:NH1	2.38	0.57
30:g:149:ILE:HG22	36:m:99:ARG:HD2	1.85	0.57
12:L:230:VAL:HG22	12:L:286:MET:HE2	1.86	0.57
2:B:191:CYS:SG	4:D:143:ARG:NH2	2.75	0.57
6:F:399:PRO:O	6:F:403:GLY:N	2.35	0.57
9:I:105:GLU:O	9:I:175:GLY:N	2.36	0.57
23:Y:38:PHE:O	23:Y:42:THR:OG1	2.20	0.57
12:L:523:LYS:HG3	35:l:70:LEU:HD22	1.87	0.56
14:N:108:ALA:HB2	14:N:157:SER:CA	2.34	0.56
14:N:257:LEU:HD13	14:N:334:ILE:HD12	1.87	0.56
30:g:64:ASP:OD1	30:g:65:TYR:N	2.38	0.56
38:o:67:CYS:SG	38:o:68:ARG:N	2.79	0.56
10:J:151:TYR:O	10:J:155:THR:OG1	2.20	0.56
12:L:224:THR:HG22	12:L:225:LEU:N	2.20	0.56
26:b:37:ALA:O	26:b:41:VAL:HG12	2.05	0.56
42:s:81:GLU:OE2	42:s:81:GLU:N	2.38	0.56
7:G:140:ILE:HG23	9:I:119:ILE:HD12	1.86	0.56
17:Q:34:ASP:OD1	17:Q:35:GLY:N	2.37	0.56
26:b:30:ALA:O	26:b:34:ILE:HD12	2.06	0.56
29:f:40:SER:O	29:f:44:GLY:N	2.38	0.56
12:L:174:GLU:OE2	12:L:174:GLU:N	2.38	0.56
13:M:317:LEU:HD23	13:M:425:MET:HE3	1.88	0.56
15:O:174:ALA:HB1	15:O:185:VAL:HG21	1.86	0.56
5:E:146:LYS:O	5:E:150:GLY:N	2.38	0.56
37:n:34:ASN:OD1	37:n:35:VAL:N	2.39	0.56
13:M:154:MET:HE2	13:M:190:ALA:HB1	1.87	0.56
20:V:11:LEU:HD11	41:r:103:ASP:C	2.31	0.56
1:A:33:ARG:NH1	16:P:379:TRP:O	2.39	0.55
1:A:70:GLU:OE2	10:J:152:LEU:HD13	2.05	0.55
10:J:79:ASN:N	44:J:203:3PE:O12	2.39	0.55
19:U:87:ASP:OD2	34:k:43:ARG:NH1	2.35	0.55
5:E:39:GLU:N	5:E:39:GLU:OE1	2.38	0.55
12:L:200:ILE:CD1	12:L:502:MET:HE1	2.37	0.55
8:H:231:PHE:HE1	50:H:501:UQ9:H15B	1.72	0.55
1:A:40:GLU:OE1	4:D:88:ASN:N	2.36	0.55
2:B:90:LEU:O	2:B:91:THR:OG1	2.21	0.55
3:C:129:GLU:N	3:C:129:GLU:OE1	2.40	0.55
33:j:76:TYR:CZ	38:o:97:MET:HE1	2.42	0.55
7:G:630:ARG:O	7:G:630:ARG:NH1	2.38	0.55
11:K:23:SER:OG	11:K:25:ARG:NH2	2.40	0.55
19:T:128:ASP:OD1	21:W:27:LYS:NZ	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:8:MET:SD	39:p:9:ALA:N	2.80	0.55
6:F:185:GLN:OE1	42:s:97:MET:HE1	2.05	0.55
11:K:41:MET:HE3	11:K:41:MET:HA	1.87	0.55
13:M:179:ASN:OD1	13:M:240:LEU:HD23	2.07	0.55
15:O:390:MET:HA	15:O:390:MET:HE2	1.89	0.55
17:Q:86:ILE:CD1	17:Q:106:ILE:HG22	2.36	0.55
5:E:72:MET:HE2	5:E:105:VAL:HG22	1.89	0.55
4:D:157:SER:OG	4:D:161:GLU:OE2	2.23	0.54
6:F:242:PRO:HD2	7:G:104:MET:HE1	1.89	0.54
7:G:193:CYS:O	7:G:194:THR:OG1	2.23	0.54
7:G:275:ILE:HG23	7:G:287:ILE:HG23	1.89	0.54
10:J:151:TYR:CE1	14:N:39:LEU:HD21	2.41	0.54
13:M:25:GLN:O	13:M:29:PHE:N	2.33	0.54
13:M:100:LEU:HD13	13:M:222:ILE:HG21	1.88	0.54
13:M:124:LEU:CD2	13:M:144:LEU:HD22	2.36	0.54
1:A:22:ALA:O	1:A:26:SER:OG	2.07	0.54
6:F:250:VAL:HG22	6:F:255:THR:CG2	2.37	0.54
13:M:189:CYS:O	13:M:193:VAL:HG23	2.08	0.54
5:E:175:ASN:ND2	5:E:187:GLU:OE1	2.40	0.54
5:E:215:ARG:NH2	5:E:219:GLU:O	2.40	0.54
24:Z:28:VAL:O	41:r:22:ARG:NH1	2.40	0.54
25:a:68:PRO:O	25:a:71:LYS:NZ	2.36	0.54
4:D:385:HIS:ND1	7:G:154:MET:SD	2.80	0.54
16:P:58:ARG:NH1	16:P:108:GLY:O	2.40	0.54
17:Q:98:THR:O	17:Q:101:VAL:HG22	2.07	0.54
19:U:97:GLU:OE2	19:U:97:GLU:N	2.41	0.54
3:C:175:MET:HE2	3:C:175:MET:HA	1.89	0.53
3:C:188:ARG:NH1	3:C:191:THR:OG1	2.40	0.53
4:D:333:ASP:HA	4:D:336:LEU:HD12	1.90	0.53
6:F:132:ALA:HB3	6:F:172:TYR:O	2.08	0.53
32:i:17:ILE:HD11	37:n:122:LYS:HG3	1.89	0.53
30:g:45:LEU:HB2	37:n:119:GLU:OE1	2.09	0.53
2:B:86:SER:O	8:H:61:LYS:NZ	2.41	0.53
11:K:47:PHE:O	11:K:51:ASN:ND2	2.37	0.53
20:V:69:GLU:O	20:V:73:GLY:N	2.39	0.53
22:X:133:VAL:HG21	26:b:68:ALA:HB1	1.91	0.53
30:g:58:TRP:CH2	32:i:6:ALA:HB2	2.43	0.53
11:K:62:MET:HE2	11:K:62:MET:N	2.23	0.53
4:D:148:SER:OG	4:D:187:ASN:ND2	2.36	0.53
7:G:276:VAL:HG23	7:G:290:ARG:HB2	1.90	0.53
8:H:274:ARG:NH2	50:H:501:UQ9:H10B	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:76:LYS:O	32:i:80:VAL:HG23	2.09	0.53
4:D:199:VAL:HG21	4:D:273:TRP:CZ3	2.44	0.53
12:L:224:THR:O	12:L:227:THR:N	2.35	0.53
13:M:192:LEU:HD22	13:M:197:MET:CE	2.39	0.53
14:N:45:LEU:HD22	14:N:57:SER:HA	1.91	0.53
1:A:78:ILE:HD11	8:H:165:GLY:CA	2.39	0.53
5:E:173:CYS:N	6:F:140:CYS:SG	2.82	0.53
13:M:162:MET:CG	13:M:168:MET:HE2	2.39	0.53
6:F:391:HIS:ND1	6:F:392:GLU:OE2	2.31	0.53
28:e:19:ILE:O	28:e:20:ASN:ND2	2.41	0.52
1:A:69:VAL:HG21	11:K:65:THR:HA	1.90	0.52
4:D:296:VAL:O	4:D:300:GLY:N	2.40	0.52
16:P:202:TYR:CE1	16:P:206:LEU:HD11	2.44	0.52
1:A:63:ILE:HD12	10:J:156:LEU:CD1	2.39	0.52
8:H:31:GLU:HG2	8:H:271:ILE:HD12	1.90	0.52
16:P:316:ASP:OD2	16:P:318:ARG:NH2	2.43	0.52
36:m:105:TYR:CE2	39:p:149:VAL:HG21	2.45	0.52
4:D:183:THR:HG1	4:D:219:TYR:HH	1.46	0.52
15:O:108:MET:HB3	15:O:186:VAL:HG23	1.91	0.52
16:P:298:TRP:CE2	16:P:302:LEU:HD11	2.45	0.52
27:d:110:GLU:CD	39:p:134:MET:HE3	2.35	0.52
6:F:42:GLN:OE1	6:F:44:LYS:N	2.42	0.52
13:M:286:LEU:HD11	13:M:290:LEU:HD11	1.92	0.52
4:D:333:ASP:OD1	4:D:334:ARG:N	2.43	0.52
15:O:112:PRO:O	15:O:170:GLN:NE2	2.42	0.52
20:V:44:TYR:CZ	20:V:48:THR:HG21	2.45	0.52
7:G:155:ALA:O	41:r:64:ARG:NH2	2.43	0.52
12:L:51:MET:HE2	43:i:201:PC1:H362	1.92	0.52
16:P:303:MET:HE3	16:P:384:TYR:HB3	1.91	0.52
17:Q:77:GLU:OE2	17:Q:77:GLU:N	2.43	0.52
4:D:385:HIS:O	4:D:389:LEU:HD23	2.10	0.52
8:H:32:ARG:HE	50:H:501:UQ9:H20B	1.75	0.51
10:J:57:ILE:HG21	11:K:64:LEU:HD12	1.91	0.51
4:D:58:TYR:O	12:L:547:LYS:NZ	2.42	0.51
5:E:92:HIS:NE2	5:E:106:TYR:OH	2.40	0.51
26:b:50:ASP:OD1	26:b:51:ASN:N	2.43	0.51
2:B:91:THR:HG22	2:B:118:PHE:CD2	2.45	0.51
6:F:424:ILE:HD11	6:F:461:ILE:HG21	1.92	0.51
12:L:38:GLU:HB2	12:L:52:THR:HG22	1.91	0.51
16:P:130:VAL:HG12	16:P:130:VAL:O	2.11	0.51
22:X:22:LEU:O	25:a:50:ARG:NH1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:PRO:O	2:B:148:GLN:NE2	2.43	0.51
10:J:155:THR:HG22	10:J:159:ILE:HD11	1.92	0.51
15:O:221:ASN:ND2	15:O:349:TYR:O	2.44	0.51
5:E:126:GLN:HB2	5:E:180:ALA:HB3	1.92	0.51
6:F:57:PHE:CD1	6:F:145:ILE:HD12	2.44	0.51
13:M:23:MET:HE3	13:M:23:MET:HA	1.91	0.51
21:W:63:GLU:HA	21:W:66:LYS:HG2	1.93	0.51
10:J:120:ILE:HD12	24:Z:80:VAL:HG13	1.91	0.51
15:O:249:ARG:NH1	51:O:501:DGT:O3A	2.40	0.51
17:Q:109:ASP:OD1	17:Q:110:ASN:N	2.42	0.51
2:B:96:CYS:HB3	4:D:146:TYR:CG	2.46	0.51
6:F:126:LYS:N	6:F:167:GLN:OE1	2.44	0.51
15:O:176:GLN:NE2	15:O:339:TYR:O	2.40	0.51
37:n:53:LYS:HD3	37:n:61:LEU:HD11	1.93	0.51
5:E:136:ARG:NH1	6:F:295:GLY:O	2.44	0.51
12:L:251:LEU:CD2	35:l:143:LEU:HD23	2.39	0.51
22:X:173:TRP:NE1	22:X:175:GLU:HG3	2.26	0.51
31:h:70:VAL:O	31:h:74:THR:HG23	2.11	0.51
20:V:78:GLU:O	20:V:82:VAL:HG23	2.11	0.50
5:E:170:LEU:HD12	5:E:178:MET:HE1	1.93	0.50
19:T:96:VAL:HG12	19:T:138:ALA:HB2	1.92	0.50
5:E:151:ILE:HD12	5:E:164:ILE:HG22	1.93	0.50
8:H:202:ARG:O	8:H:205:PHE:N	2.43	0.50
14:N:134:LYS:NZ	14:N:179:SER:OG	2.39	0.50
14:N:151:LEU:HD21	23:Y:135:PHE:CD1	2.47	0.50
32:i:143:TYR:O	32:i:145:LYS:N	2.44	0.50
4:D:52:PHE:O	14:N:224:ASN:ND2	2.41	0.50
17:Q:61:THR:HG22	21:W:13:GLN:NE2	2.26	0.50
3:C:224:GLU:OE2	16:P:85:LYS:NZ	2.45	0.50
6:F:223:GLU:OE1	6:F:225:THR:N	2.45	0.50
7:G:360:ASP:OD1	7:G:361:LEU:N	2.45	0.50
8:H:188:MET:HE1	8:H:304:PHE:HE2	1.77	0.50
8:H:273:VAL:HG22	9:I:75:PHE:CZ	2.46	0.50
50:H:501:UQ9:H40	50:H:501:UQ9:C36	2.39	0.50
13:M:382:ILE:O	13:M:385:SER:OG	2.26	0.50
3:C:142:ARG:NH2	4:D:411:GLU:OE2	2.44	0.50
4:D:331:CYS:SG	4:D:458:THR:HG21	2.52	0.50
12:L:46:SER:O	39:p:84:ARG:NH1	2.44	0.50
19:U:90:ASP:OD2	19:U:92:SER:OG	2.29	0.50
8:H:72:LEU:O	8:H:131:ASN:ND2	2.42	0.50
9:I:94:GLU:OE1	40:q:37:LYS:NZ	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:84:THR:HG21	14:N:54:THR:HG21	1.93	0.50
2:B:114:TYR:CE2	2:B:199:MET:HE2	2.46	0.50
3:C:189:ILE:HG23	3:C:190:LEU:HG	1.93	0.50
7:G:140:ILE:CG2	9:I:119:ILE:HD12	2.41	0.50
12:L:124:SER:CB	12:L:225:LEU:HD11	2.42	0.50
16:P:49:ALA:O	16:P:53:ARG:NH2	2.44	0.50
19:T:116:MET:HE1	21:W:37:TYR:CD2	2.47	0.50
32:i:13:LYS:HD2	32:i:14:PRO:HD2	1.93	0.49
2:B:128:ILE:CG2	2:B:155:VAL:HG22	2.42	0.49
6:F:338:SER:N	6:F:389:TYR:OH	2.45	0.49
13:M:26:ILE:HG23	30:g:81:VAL:HG21	1.92	0.49
15:O:131:LEU:HD11	15:O:377:ALA:HB2	1.95	0.49
17:Q:86:ILE:HB	17:Q:154:VAL:HG22	1.94	0.49
1:A:96:PHE:CG	10:J:149:MET:HE1	2.47	0.49
5:E:76:LEU:HD22	5:E:86:LEU:HD21	1.94	0.49
10:J:20:MET:HA	10:J:20:MET:HE2	1.94	0.49
16:P:173:ARG:NH2	16:P:271:ALA:O	2.42	0.49
1:A:78:ILE:HD11	8:H:165:GLY:HA2	1.95	0.49
10:J:1:MET:SD	10:J:2:ILE:N	2.86	0.49
10:J:62:MET:HE3	10:J:62:MET:HA	1.95	0.49
25:a:57:ASN:OD1	25:a:60:LYS:N	2.46	0.49
3:C:103:LYS:NZ	3:C:161:VAL:O	2.35	0.49
10:J:77:MET:CE	16:P:390:TYR:HB2	2.40	0.49
4:D:186:LEU:HG	4:D:215:MET:HE2	1.94	0.49
10:J:145:THR:O	10:J:149:MET:HG2	2.13	0.49
11:K:28:LEU:HD12	11:K:90:PHE:CE2	2.47	0.49
11:K:58:TYR:OH	28:e:18:LEU:O	2.27	0.49
14:N:114:PHE:CE1	14:N:118:MET:HE1	2.48	0.49
32:i:21:MET:SD	32:i:21:MET:N	2.86	0.49
6:F:42:GLN:NE2	6:F:279:SER:O	2.43	0.49
12:L:387:SER:O	12:L:391:THR:N	2.37	0.49
13:M:100:LEU:HD21	13:M:223:MET:HE1	1.95	0.49
2:B:103:HIS:CE1	4:D:216:MET:HE2	2.48	0.48
3:C:138:ARG:O	41:r:100:TYR:N	2.42	0.48
8:H:302:LEU:HD23	26:b:34:ILE:HD11	1.95	0.48
39:p:8:MET:O	39:p:12:ALA:N	2.41	0.48
2:B:179:ASP:N	2:B:179:ASP:OD1	2.42	0.48
6:F:159:ILE:HD13	6:F:267:PRO:HB3	1.95	0.48
8:H:185:LEU:HD22	8:H:188:MET:SD	2.53	0.48
8:H:302:LEU:CD2	26:b:34:ILE:HD11	2.42	0.48
14:N:309:LYS:HZ1	15:O:406:GLY:HA2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:140:ILE:O	19:T:144:VAL:HG23	2.12	0.48
42:s:60:VAL:HG23	42:s:84:SER:CB	2.41	0.48
6:F:411:MET:HE1	6:F:453:LEU:CD2	2.43	0.48
13:M:181:ASP:OD2	13:M:245:TYR:OH	2.26	0.48
37:n:101:ASP:OD1	37:n:118:ARG:NH1	2.47	0.48
4:D:332:TYR:CE2	4:D:336:LEU:HD11	2.49	0.48
25:a:40:ASP:OD1	25:a:40:ASP:N	2.45	0.48
28:e:35:MET:HE1	31:h:170:HIS:CB	2.44	0.48
5:E:173:CYS:SG	6:F:138:GLY:N	2.85	0.48
9:I:83:PHE:O	41:r:16:ARG:NH1	2.46	0.48
16:P:267:ALA:CB	16:P:363:LEU:HD22	2.44	0.48
54:T:201:EHZ:C4	21:W:63:GLU:OE2	2.61	0.48
22:X:167:TYR:O	22:X:174:LEU:HD13	2.13	0.48
23:Y:156:MET:HE2	28:e:13:ASP:HB3	1.96	0.48
3:C:70:CYS:C	3:C:71:LEU:HD22	2.39	0.48
6:F:471:ARG:HE	6:F:472:VAL:HG23	1.79	0.48
13:M:137:LEU:HD22	14:N:294:TYR:CZ	2.48	0.48
18:R:40:THR:HG22	18:R:63:VAL:HG13	1.96	0.48
3:C:171:GLU:OE1	4:D:428:LYS:NZ	2.47	0.48
15:O:236:ASP:N	15:O:289:TYR:O	2.42	0.48
28:e:21:HIS:ND1	28:e:27:CYS:SG	2.86	0.48
12:L:44:LEU:HD11	13:M:295:TRP:CE2	2.48	0.48
12:L:129:ILE:HG22	12:L:129:ILE:O	2.14	0.48
14:N:309:LYS:HG2	14:N:310:MET:N	2.29	0.48
30:g:150:ILE:HD11	39:p:142:TRP:CB	2.44	0.48
10:J:170:ILE:HG23	11:K:82:ILE:HG21	1.95	0.48
30:g:89:TRP:CZ3	31:h:73:VAL:HG12	2.48	0.48
41:r:58:CYS:SG	41:r:59:GLN:NE2	2.87	0.48
6:F:117:MET:SD	6:F:256:THR:OG1	2.66	0.47
13:M:258:VAL:HG21	13:M:383:LEU:HB3	1.96	0.47
1:A:1:MET:O	1:A:4:ILE:N	2.47	0.47
12:L:218:ALA:O	12:L:222:SER:OG	2.18	0.47
24:Z:118:VAL:HG23	24:Z:119:PHE:CD2	2.50	0.47
32:i:130:ILE:HG13	32:i:130:ILE:O	2.14	0.47
37:n:19:TYR:CZ	37:n:23:LEU:HD11	2.48	0.47
4:D:409:LYS:HZ3	4:D:462:VAL:HG23	1.79	0.47
6:F:174:ARG:NE	6:F:176:GLU:OE1	2.47	0.47
13:M:252:ILE:O	13:M:256:GLY:N	2.44	0.47
16:P:229:ARG:NH1	52:P:501:NDP:O1A	2.47	0.47
19:T:87:ASP:OD2	19:T:88:LYS:N	2.40	0.47
19:U:72:LEU:O	19:U:76:ASN:ND2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:316:TYR:HA	4:D:319:VAL:HG22	1.95	0.47
9:I:186:GLU:OE1	16:P:111:GLY:N	2.44	0.47
13:M:284:ILE:HD11	13:M:387:LEU:CD2	2.41	0.47
15:O:309:PHE:HD1	15:O:321:MET:HE1	1.79	0.47
32:i:13:LYS:HE3	36:m:36:ALA:HB1	1.97	0.47
6:F:250:VAL:H	6:F:255:THR:HG21	1.78	0.47
7:G:690:LEU:HD11	7:G:696:TYR:HA	1.96	0.47
8:H:94:MET:HE2	8:H:94:MET:N	2.29	0.47
12:L:37:ILE:HG22	32:i:129:VAL:HG22	1.96	0.47
12:L:142:LEU:HD13	44:L:602:3PE:O32	2.15	0.47
12:L:357:PHE:CE1	33:j:63:LEU:HD22	2.49	0.47
23:Y:101:GLY:O	23:Y:105:HIS:N	2.48	0.47
6:F:433:GLN:O	6:F:437:HIS:ND1	2.47	0.47
7:G:274:ASN:O	7:G:296:ASN:ND2	2.48	0.47
7:G:373:ARG:NH2	7:G:639:PRO:O	2.42	0.47
14:N:250:LEU:HD21	14:N:286:LEU:HD11	1.96	0.47
28:e:4:THR:HG23	28:e:4:THR:O	2.14	0.47
7:G:483:PRO:O	7:G:516:TRP:NE1	2.40	0.47
38:o:15:PRO:HB3	38:o:19:VAL:HG21	1.97	0.47
6:F:413:ARG:NH1	7:G:165:ASP:OD1	2.43	0.47
9:I:120:ALA:HB1	9:I:137:ALA:HB2	1.96	0.47
14:N:194:GLU:O	14:N:198:LEU:N	2.38	0.47
22:X:43:ASN:HB3	22:X:134:ILE:HG21	1.97	0.47
24:Z:121:THR:OG1	28:e:56:ASP:OD1	2.09	0.47
25:a:39:MET:HE1	25:a:48:TYR:CG	2.50	0.47
5:E:59:ILE:O	5:E:62:ILE:HG22	2.14	0.47
12:L:456:TYR:OH	38:o:2:GLY:N	2.48	0.47
13:M:78:MET:SD	13:M:82:HIS:ND1	2.88	0.47
24:Z:131:ILE:HD12	24:Z:131:ILE:H	1.79	0.47
39:p:25:TRP:CD1	39:p:29:SER:HG	2.32	0.47
3:C:48:THR:O	4:D:167:ASP:N	2.47	0.46
14:N:261:LEU:HD13	14:N:340:MET:CG	2.44	0.46
28:e:9:LEU:O	28:e:12:THR:HG22	2.15	0.46
8:H:161:ILE:HD13	8:H:167:TYR:CE1	2.50	0.46
13:M:20:MET:O	13:M:24:VAL:HG23	2.15	0.46
14:N:185:TRP:O	14:N:188:SER:OG	2.31	0.46
24:Z:113:TRP:CE2	28:e:68:MET:HE3	2.50	0.46
4:D:164:LEU:CD2	4:D:396:VAL:HG22	2.44	0.46
5:E:239:GLN:NE2	6:F:270:CYS:O	2.49	0.46
9:I:39:VAL:HG12	9:I:45:TYR:CD2	2.51	0.46
10:J:114:ASN:OD1	25:a:45:ARG:NH2	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:81:MET:HE1	14:N:58:LEU:HD22	1.96	0.46
14:N:181:ASN:C	14:N:181:ASN:HD22	2.23	0.46
23:Y:15:GLU:O	23:Y:20:LYS:NZ	2.44	0.46
31:h:48:ILE:HG22	37:n:100:LEU:HD21	1.96	0.46
2:B:42:THR:OG1	40:q:111:HIS:O	2.28	0.46
10:J:147:LEU:HD22	28:e:14:LEU:HD21	1.97	0.46
14:N:114:PHE:HB3	14:N:115:PRO:HD3	1.97	0.46
15:O:356:ASP:OD2	15:O:356:ASP:N	2.47	0.46
13:M:66:LEU:HD23	13:M:97:LEU:HD21	1.96	0.46
3:C:248:ARG:NE	7:G:68:VAL:HG22	2.31	0.46
3:C:251:ASN:ND2	20:V:113:ASP:OD1	2.43	0.46
4:D:148:SER:O	4:D:152:ASN:ND2	2.49	0.46
7:G:416:THR:OG1	7:G:488:GLY:N	2.49	0.46
32:i:74:LEU:O	32:i:77:VAL:HG12	2.15	0.46
12:L:33:MET:HE3	12:L:33:MET:HA	1.98	0.46
13:M:192:LEU:HD23	13:M:231:MET:HE1	1.97	0.46
14:N:188:SER:OG	14:N:278:MET:HE1	2.16	0.46
3:C:138:ARG:NH1	20:V:79:GLU:OE1	2.49	0.46
8:H:31:GLU:OE1	8:H:35:LEU:HD22	2.16	0.46
18:R:33:ARG:NH2	18:R:59:ALA:O	2.49	0.46
27:d:105:TYR:HA	27:d:108:VAL:HG12	1.97	0.46
12:L:224:THR:O	12:L:226:VAL:N	2.49	0.46
14:N:309:LYS:NZ	15:O:406:GLY:HA3	2.31	0.46
19:U:104:LEU:HB2	19:U:106:LEU:HD23	1.97	0.46
25:a:61:MET:SD	25:a:63:GLY:N	2.89	0.46
30:g:106:ALA:O	30:g:109:GLU:N	2.49	0.46
31:h:67:MET:O	31:h:71:ILE:HD12	2.16	0.46
4:D:161:GLU:O	4:D:165:ASN:N	2.48	0.46
5:E:126:GLN:HB3	5:E:167:VAL:HG21	1.98	0.46
13:M:137:LEU:HD22	14:N:294:TYR:CE1	2.51	0.46
14:N:244:PHE:CZ	14:N:292:ILE:HG21	2.50	0.46
8:H:213:GLU:OE2	8:H:279:ARG:NH1	2.49	0.45
10:J:33:GLN:NE2	11:K:37:PHE:HE1	2.14	0.45
13:M:293:THR:HG22	13:M:294:TYR:N	2.30	0.45
15:O:40:ILE:HD12	15:O:309:PHE:CE2	2.50	0.45
12:L:522:VAL:HG23	12:L:526:ASP:HB2	1.97	0.45
7:G:698:MET:HE2	7:G:709:MET:HB3	1.99	0.45
8:H:25:ALA:O	8:H:28:THR:OG1	2.30	0.45
10:J:108:SER:O	24:Z:133:LYS:NZ	2.44	0.45
12:L:373:ILE:CD1	12:L:451:ILE:HG22	2.45	0.45
15:O:380:MET:O	27:d:47:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:95:ARG:NE	52:P:501:NDP:O1X	2.43	0.45
31:h:127:SER:O	31:h:131:LEU:HD23	2.17	0.45
7:G:151:ASP:OD1	17:Q:95:GLN:NE2	2.50	0.45
7:G:286:ARG:NH2	17:Q:94:MET:SD	2.89	0.45
15:O:95:LYS:N	51:O:501:DGT:O1G	2.49	0.45
27:d:25:ILE:O	27:d:29:ILE:HG22	2.16	0.45
1:A:69:VAL:HG11	11:K:68:VAL:HG21	1.97	0.45
6:F:367:ALA:O	6:F:369:ILE:HD12	2.16	0.45
9:I:173:VAL:HG21	9:I:206:ILE:HG21	1.98	0.45
2:B:96:CYS:HB3	4:D:146:TYR:CB	2.47	0.45
5:E:193:ASP:N	5:E:193:ASP:OD1	2.48	0.45
5:E:242:LEU:HD23	6:F:82:GLU:OE1	2.16	0.45
13:M:239:GLN:HA	13:M:292:MET:HE1	1.98	0.45
19:U:75:ILE:O	19:U:79:VAL:HG23	2.16	0.45
38:o:83:HIS:O	38:o:87:THR:OG1	2.11	0.45
5:E:120:THR:O	5:E:163:THR:OG1	2.23	0.45
9:I:53:MET:HE3	9:I:53:MET:HA	1.98	0.45
14:N:240:LEU:O	14:N:243:ASN:ND2	2.44	0.45
1:A:23:SER:O	1:A:28:LYS:NZ	2.35	0.45
8:H:273:VAL:HG22	9:I:75:PHE:CE2	2.52	0.45
12:L:6:ILE:O	12:L:10:SER:OG	2.31	0.45
13:M:4:ILE:HD13	13:M:31:ILE:HD11	1.99	0.45
19:U:146:ASP:O	32:i:27:ARG:NH1	2.50	0.45
4:D:381:GLU:OE2	4:D:381:GLU:N	2.43	0.45
8:H:231:PHE:CZ	50:H:501:UQ9:H15B	2.52	0.45
13:M:121:ILE:HD12	13:M:121:ILE:H	1.82	0.45
18:R:35:ASP:O	18:R:61:ARG:NH2	2.49	0.45
19:T:127:PRO:O	19:T:131:ALA:N	2.47	0.45
21:W:39:GLN:CD	21:W:91:VAL:HG22	2.42	0.45
27:d:115:VAL:HG23	27:d:116:ARG:N	2.32	0.45
28:e:21:HIS:CE1	28:e:61:VAL:HG21	2.52	0.45
37:n:7:ALA:O	37:n:9:VAL:HG23	2.16	0.45
4:D:377:LYS:NZ	18:R:95:GLY:O	2.46	0.45
4:D:431:ALA:HB1	4:D:465:GLU:HB3	1.99	0.45
7:G:280:ARG:O	7:G:281:THR:OG1	2.33	0.45
14:N:111:HIS:CE1	14:N:160:ILE:HG21	2.52	0.45
16:P:330:ASN:ND2	16:P:342:LEU:O	2.50	0.45
13:M:433:ASN:O	13:M:436:ILE:HG22	2.16	0.44
16:P:56:GLY:N	16:P:60:SER:OG	2.49	0.44
35:l:100:ARG:NH2	35:l:104:GLU:O	2.50	0.44
2:B:91:THR:HG23	2:B:119:ARG:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:183:VAL:HG22	7:G:237:ILE:HD11	1.98	0.44
9:I:155:THR:HG21	9:I:185:HIS:CD2	2.53	0.44
10:J:80:LEU:HD11	10:J:85:THR:HG21	1.98	0.44
22:X:70:LEU:HD23	22:X:74:ARG:NH2	2.32	0.44
32:i:138:PRO:O	39:p:5:ARG:NH1	2.42	0.44
7:G:630:ARG:NH2	7:G:634:GLU:OE2	2.46	0.44
8:H:143:VAL:HG11	10:J:67:ILE:HD11	2.00	0.44
13:M:162:MET:O	13:M:166:GLY:N	2.48	0.44
23:Y:24:THR:HG21	23:Y:71:THR:CG2	2.48	0.44
5:E:239:GLN:O	5:E:240:ALA:HB3	2.16	0.44
6:F:402:GLU:OE2	7:G:129:PHE:HB3	2.18	0.44
6:F:402:GLU:OE1	7:G:132:MET:HE2	2.17	0.44
14:N:108:ALA:HB2	14:N:157:SER:N	2.33	0.44
23:Y:56:PHE:O	23:Y:60:THR:OG1	2.17	0.44
27:d:97:PHE:CE1	31:h:147:VAL:HG22	2.52	0.44
38:o:13:VAL:HG22	38:o:108:GLU:OE2	2.18	0.44
42:s:87:ARG:HD2	42:s:87:ARG:O	2.16	0.44
8:H:239:LEU:O	8:H:242:SER:OG	2.30	0.44
20:V:9:THR:HG21	20:V:14:LEU:HD23	1.99	0.44
30:g:105:TRP:NE1	30:g:109:GLU:OE1	2.50	0.44
8:H:18:ILE:O	8:H:22:VAL:HG23	2.17	0.44
10:J:44:MET:HE1	11:K:44:PHE:CE2	2.52	0.44
11:K:39:VAL:HG11	11:K:67:SER:OG	2.17	0.44
15:O:365:ASP:OD2	15:O:365:ASP:N	2.47	0.44
19:U:89:ILE:HD11	19:U:104:LEU:HD13	1.99	0.44
12:L:40:GLU:HA	12:L:50:VAL:HG12	1.99	0.44
14:N:87:GLU:OE1	14:N:94:SER:OG	2.33	0.44
15:O:40:ILE:N	15:O:81:ASN:OD1	2.50	0.44
16:P:133:SER:OG	16:P:135:VAL:O	2.36	0.44
28:e:52:ASP:OD1	28:e:52:ASP:N	2.51	0.44
39:p:25:TRP:O	39:p:29:SER:N	2.48	0.44
42:s:86:ASN:H	42:s:89:SER:HG	1.66	0.44
4:D:87:LEU:HD12	4:D:106:LEU:HD11	1.99	0.44
4:D:87:LEU:HD21	8:H:133:ASN:HB3	1.99	0.44
4:D:461:VAL:HG23	4:D:461:VAL:O	2.18	0.44
11:K:7:TRP:O	11:K:11:MET:HE2	2.17	0.44
12:L:166:SER:OG	12:L:167:TRP:N	2.50	0.44
27:d:116:ARG:HD3	36:m:98:TYR:CD1	2.53	0.44
32:i:17:ILE:HD11	37:n:122:LYS:CG	2.46	0.44
39:p:39:ASN:ND2	39:p:41:TYR:OH	2.51	0.44
3:C:152:LEU:O	21:W:17:ILE:HD11	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:377:ASN:OD1	12:L:378:MET:N	2.51	0.44
17:Q:55:LYS:HB2	21:W:20:VAL:HG21	1.99	0.44
17:Q:86:ILE:HD12	17:Q:106:ILE:HG22	1.98	0.44
22:X:97:THR:O	22:X:97:THR:HG22	2.18	0.44
5:E:190:THR:N	5:E:193:ASP:OD1	2.47	0.43
12:L:38:GLU:CB	12:L:52:THR:HG22	2.48	0.43
12:L:173:LEU:HD21	12:L:236:PHE:CD1	2.53	0.43
13:M:259:LEU:HD13	36:m:76:VAL:HG12	2.00	0.43
14:N:186:MET:HE1	14:N:204:TYR:CD2	2.53	0.43
16:P:306:ASP:OD1	16:P:307:GLN:N	2.51	0.43
26:b:34:ILE:HD12	26:b:34:ILE:H	1.83	0.43
13:M:36:LEU:HD11	30:g:94:TRP:HE1	1.82	0.43
34:k:39:ASP:OD1	37:n:37:ARG:NH2	2.51	0.43
1:A:77:MET:HE1	10:J:137:TYR:CD2	2.53	0.43
4:D:289:LEU:HD11	41:r:102:TRP:CH2	2.53	0.43
6:F:42:GLN:OE1	6:F:43:THR:N	2.50	0.43
6:F:337:SER:OG	6:F:385:LEU:HD22	2.17	0.43
7:G:371:LEU:HD12	7:G:379:VAL:HG22	2.00	0.43
11:K:77:ILE:HD11	14:N:42:ILE:HD13	2.00	0.43
30:g:107:GLN:HA	39:p:78:GLU:OE1	2.17	0.43
1:A:65:LEU:HD21	10:J:64:VAL:CG2	2.49	0.43
13:M:255:VAL:HG11	36:m:80:ILE:HG13	2.01	0.43
19:T:134:LEU:HD22	19:T:140:ILE:HA	1.99	0.43
54:T:201:EHZ:C25	21:W:49:ILE:HD11	2.47	0.43
5:E:91:MET:HE2	5:E:109:ALA:CB	2.48	0.43
13:M:158:ILE:HG22	13:M:168:MET:HE1	2.00	0.43
16:P:356:VAL:O	16:P:356:VAL:HG13	2.18	0.43
22:X:43:ASN:CB	22:X:134:ILE:HG21	2.49	0.43
32:i:120:ASP:OD2	32:i:120:ASP:N	2.48	0.43
1:A:65:LEU:HD21	10:J:64:VAL:HG21	2.01	0.43
7:G:127:MET:HE1	7:G:149:LEU:HD12	2.00	0.43
8:H:113:LEU:HD21	8:H:157:LEU:HD12	2.00	0.43
16:P:180:LEU:HD22	16:P:285:VAL:HG12	1.99	0.43
22:X:48:CYS:SG	22:X:49:ARG:N	2.92	0.43
32:i:132:SER:OG	32:i:133:ARG:N	2.52	0.43
3:C:149:THR:HB	3:C:155:LEU:HD13	2.01	0.43
5:E:91:MET:HE2	5:E:109:ALA:HB3	2.01	0.43
12:L:6:ILE:HD12	12:L:88:ASN:CG	2.44	0.43
16:P:267:ALA:HB1	16:P:363:LEU:HD22	1.99	0.43
20:V:38:MET:HE1	20:V:44:TYR:CD1	2.53	0.43
21:W:114:ASP:OD2	21:W:117:SER:OG	2.23	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:133:THR:HG22	4:D:134:TYR:N	2.33	0.43
6:F:127:TYR:HB2	6:F:255:THR:HG22	2.01	0.43
6:F:424:ILE:HD11	6:F:461:ILE:CG2	2.48	0.43
13:M:8:LEU:HD11	13:M:97:LEU:HD23	2.01	0.43
13:M:383:LEU:HD11	36:m:83:TYR:CE1	2.54	0.43
14:N:86:ASN:OD1	14:N:87:GLU:N	2.52	0.43
14:N:243:ASN:O	14:N:246:SER:OG	2.35	0.43
14:N:308:MET:HE2	15:O:162:ARG:HH12	1.83	0.43
1:A:78:ILE:HG23	1:A:79:ILE:N	2.34	0.43
6:F:133:ASP:OD2	6:F:134:GLU:N	2.52	0.43
6:F:414:PHE:CE2	6:F:424:ILE:HD13	2.53	0.43
19:T:95:ASN:OD1	19:T:98:SER:N	2.52	0.43
26:b:22:ASP:OD1	26:b:23:ILE:N	2.51	0.43
8:H:52:ILE:HD12	8:H:52:ILE:H	1.84	0.43
30:g:43:THR:OG1	30:g:45:LEU:HD22	2.19	0.43
4:D:221:ARG:NH1	4:D:248:ASP:OD2	2.50	0.42
8:H:188:MET:O	8:H:192:TRP:N	2.37	0.42
13:M:339:PHE:CD2	13:M:407:LEU:HD22	2.54	0.42
13:M:407:LEU:O	35:l:97:GLU:OE1	2.37	0.42
20:V:55:ARG:O	20:V:59:VAL:HG23	2.19	0.42
31:h:59:LYS:NZ	46:h:202:CDL:OB3	2.39	0.42
40:q:45:ASP:OD1	40:q:49:ASN:N	2.52	0.42
11:K:3:MET:HE3	11:K:11:MET:HE1	2.00	0.42
13:M:181:ASP:OD1	23:Y:130:GLN:NE2	2.52	0.42
15:O:196:VAL:HG13	15:O:271:LEU:HB2	2.01	0.42
1:A:61:THR:HG22	10:J:64:VAL:HG13	2.00	0.42
2:B:151:GLU:OE1	2:B:153:ARG:NE	2.53	0.42
2:B:167:TYR:HB2	9:I:158:ILE:HG21	2.02	0.42
50:H:501:UQ9:H12	50:H:501:UQ9:H15	1.87	0.42
10:J:120:ILE:HD11	24:Z:83:ARG:HE	1.85	0.42
1:A:88:ILE:HG21	10:J:138:ASN:HA	2.00	0.42
6:F:132:ALA:HB1	6:F:146:MET:CE	2.50	0.42
8:H:124:MET:HE3	10:J:66:PHE:CG	2.54	0.42
11:K:81:MET:CE	14:N:58:LEU:HD22	2.50	0.42
13:M:80:ASN:OD1	13:M:86:LYS:NZ	2.27	0.42
13:M:204:LEU:HD23	13:M:279:VAL:HG23	2.01	0.42
14:N:127:LEU:HD21	14:N:209:PHE:CD1	2.55	0.42
15:O:233:ILE:HD11	15:O:304:ILE:HD11	2.02	0.42
30:g:50:PHE:HE1	32:i:12:VAL:HG21	1.84	0.42
39:p:25:TRP:NE1	39:p:29:SER:HG	2.17	0.42
5:E:167:VAL:HG12	5:E:168:GLU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:128:ASP:OD2	19:T:129:SER:N	2.50	0.42
14:N:251:PRO:N	14:N:252:PRO:HD2	2.35	0.42
39:p:128:ASN:OD1	39:p:128:ASN:N	2.52	0.42
1:A:96:PHE:CD1	10:J:149:MET:SD	3.12	0.42
4:D:232:ILE:CD1	4:D:237:VAL:HG12	2.50	0.42
17:Q:154:VAL:HG12	17:Q:155:ASP:O	2.19	0.42
22:X:47:LEU:CD2	22:X:134:ILE:HD11	2.50	0.42
2:B:128:ILE:HG22	2:B:155:VAL:HG22	2.01	0.42
14:N:335:SER:O	27:d:75:ARG:NH1	2.53	0.42
15:O:50:ARG:NH1	15:O:79:ASP:OD2	2.46	0.42
15:O:290:ASP:OD2	15:O:290:ASP:N	2.49	0.42
20:V:55:ARG:NH1	20:V:83:GLN:OE1	2.53	0.42
30:g:51:ALA:HB2	37:n:112:PRO:HB3	2.00	0.42
33:j:70:ILE:H	33:j:70:ILE:HD12	1.84	0.42
4:D:87:LEU:HD12	4:D:106:LEU:CD1	2.50	0.42
4:D:199:VAL:HG21	4:D:273:TRP:HZ3	1.85	0.42
6:F:159:ILE:HD12	6:F:159:ILE:H	1.84	0.42
7:G:322:ARG:NH1	7:G:586:ALA:O	2.53	0.42
7:G:325:ASN:OD1	7:G:326:GLY:N	2.53	0.42
9:I:120:ALA:HB2	9:I:147:THR:CG2	2.50	0.42
12:L:195:THR:HG22	12:L:202:PHE:CD2	2.55	0.42
13:M:415:SER:OG	32:i:8:GLU:OE1	2.35	0.42
20:V:86:ASN:O	20:V:89:ILE:N	2.52	0.42
23:Y:32:GLY:HA3	23:Y:60:THR:HG22	2.02	0.42
2:B:104:ILE:HD12	2:B:198:LEU:HD23	2.02	0.42
5:E:113:THR:HG22	6:F:217:GLY:O	2.19	0.42
9:I:55:PHE:O	9:I:59:THR:HG22	2.19	0.42
10:J:2:ILE:HA	10:J:5:MET:HE2	2.02	0.42
13:M:217:MET:O	13:M:221:GLY:N	2.53	0.42
24:Z:38:THR:O	24:Z:42:THR:HG23	2.20	0.42
36:m:105:TYR:CD2	39:p:149:VAL:HG21	2.55	0.42
41:r:7:ASP:OD1	41:r:8:VAL:N	2.52	0.42
1:A:75:LEU:O	8:H:167:TYR:OH	2.29	0.41
7:G:334:GLU:O	7:G:338:ILE:HD12	2.20	0.41
12:L:44:LEU:CD2	13:M:443:MET:HE2	2.50	0.41
15:O:171:TYR:HD1	15:O:226:LEU:HD22	1.85	0.41
31:h:66:VAL:HG13	31:h:67:MET:HE2	2.02	0.41
39:p:73:ARG:O	39:p:77:ASN:N	2.45	0.41
2:B:104:ILE:HD11	2:B:199:MET:SD	2.60	0.41
2:B:169:HIS:O	2:B:176:ARG:NH1	2.48	0.41
12:L:369:GLU:OE1	12:L:453:LEU:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:120:LEU:HD12	13:M:147:THR:HG21	2.03	0.41
15:O:214:VAL:HG22	15:O:354:ARG:HD3	2.02	0.41
2:B:46:ALA:HB2	40:q:46:LYS:O	2.20	0.41
12:L:220:VAL:HG13	12:L:225:LEU:HD12	2.02	0.41
12:L:237:ASN:CB	12:L:294:LEU:HD21	2.50	0.41
12:L:279:LEU:C	12:L:279:LEU:HD23	2.45	0.41
23:Y:86:LYS:HE2	23:Y:126:MET:HE3	2.01	0.41
5:E:41:ASN:H	5:E:44:ILE:HD12	1.86	0.41
5:E:231:PRO:HB3	6:F:58:THR:HG21	2.01	0.41
6:F:128:LEU:HD12	6:F:164:MET:HE2	2.02	0.41
12:L:347:VAL:CG2	12:L:434:ILE:HD11	2.51	0.41
29:f:26:ASP:OD1	29:f:27:LYS:N	2.53	0.41
36:m:100:THR:HG21	36:m:102:GLN:NE2	2.34	0.41
42:s:79:VAL:O	42:s:79:VAL:HG22	2.20	0.41
12:L:120:LEU:O	12:L:124:SER:OG	2.33	0.41
15:O:43:LYS:O	15:O:47:GLY:N	2.54	0.41
29:f:26:ASP:O	29:f:30:THR:HG23	2.20	0.41
2:B:101:MET:HE3	2:B:118:PHE:CZ	2.56	0.41
3:C:234:LYS:NZ	17:Q:130:ASN:O	2.53	0.41
5:E:149:LEU:HD22	5:E:162:PHE:CD2	2.55	0.41
8:H:145:GLN:OE1	8:H:201:ASN:ND2	2.53	0.41
12:L:259:MET:HE2	12:L:502:MET:HE1	2.02	0.41
12:L:357:PHE:CE1	33:j:70:ILE:HD11	2.56	0.41
14:N:74:SER:O	14:N:78:LEU:N	2.48	0.41
16:P:182:VAL:HG22	16:P:202:TYR:HB2	2.03	0.41
32:i:13:LYS:HE3	36:m:36:ALA:CB	2.50	0.41
1:A:63:ILE:HD12	10:J:156:LEU:HD13	2.02	0.41
6:F:80:THR:O	6:F:84:VAL:HG23	2.21	0.41
7:G:211:THR:HG21	7:G:218:MET:HE2	2.03	0.41
10:J:155:THR:HG22	10:J:159:ILE:CD1	2.50	0.41
11:K:81:MET:HE1	14:N:58:LEU:HB2	2.03	0.41
12:L:54:LEU:HD22	12:L:170:ILE:CD1	2.51	0.41
12:L:450:MET:SD	12:L:451:ILE:N	2.94	0.41
13:M:165:ILE:HD13	13:M:173:MET:CE	2.51	0.41
13:M:209:VAL:O	13:M:328:ARG:NH1	2.53	0.41
31:h:71:ILE:HD12	31:h:71:ILE:H	1.86	0.41
4:D:49:MET:SD	15:O:355:PHE:CE2	3.14	0.41
6:F:328:ASN:O	6:F:374:LYS:N	2.54	0.41
7:G:452:ASP:OD2	7:G:453:HIS:N	2.54	0.41
8:H:25:ALA:CB	50:H:501:UQ9:H30A	2.50	0.41
12:L:226:VAL:HG23	12:L:227:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:162:MET:HE1	22:X:172:HIS:CE1	2.56	0.41
15:O:46:ARG:NH2	15:O:107:ASP:OD1	2.52	0.41
21:W:39:GLN:NE2	21:W:91:VAL:HG22	2.35	0.41
38:o:81:GLN:OE1	38:o:81:GLN:N	2.48	0.41
2:B:95:ALA:O	2:B:98:ALA:N	2.40	0.41
4:D:104:LEU:HD22	4:D:111:VAL:HG21	2.02	0.41
7:G:114:THR:O	7:G:119:THR:HG21	2.21	0.41
12:L:199:GLN:O	12:L:203:SER:N	2.54	0.41
14:N:98:MET:SD	14:N:141:ILE:HG23	2.60	0.41
14:N:314:SER:O	14:N:318:ASN:N	2.41	0.41
27:d:116:ARG:N	39:p:122:ASP:OD1	2.48	0.41
35:l:82:LEU:HD21	35:l:122:GLU:C	2.46	0.41
2:B:164:GLY:O	2:B:169:HIS:ND1	2.50	0.41
6:F:88:ALA:O	6:F:92:VAL:HG23	2.21	0.41
12:L:84:ASP:O	12:L:85:ASN:CG	2.64	0.41
13:M:136:ARG:O	13:M:140:GLY:N	2.54	0.41
15:O:171:TYR:CD1	15:O:226:LEU:HD22	2.56	0.41
31:h:74:THR:HA	31:h:77:VAL:HG12	2.03	0.41
2:B:107:PRO:HB3	8:H:40:ILE:HG23	2.04	0.40
6:F:141:LYS:NZ	6:F:261:GLU:OE2	2.43	0.40
6:F:298:ASN:ND2	6:F:320:GLY:O	2.42	0.40
10:J:159:ILE:HD12	10:J:159:ILE:H	1.86	0.40
16:P:122:ASP:O	16:P:125:SER:OG	2.37	0.40
17:Q:167:ASN:OD1	17:Q:168:TYR:N	2.53	0.40
20:V:30:LYS:CB	20:V:88:LEU:HD21	2.51	0.40
23:Y:24:THR:HG21	23:Y:71:THR:HG22	2.04	0.40
27:d:110:GLU:OE1	27:d:110:GLU:N	2.48	0.40
3:C:233:ARG:NH2	9:I:133:ILE:O	2.54	0.40
6:F:57:PHE:CE1	6:F:145:ILE:HD12	2.56	0.40
7:G:104:MET:HA	7:G:104:MET:HE2	2.03	0.40
7:G:382:GLU:OE1	7:G:556:ALA:HB1	2.21	0.40
50:H:501:UQ9:H35A	50:H:501:UQ9:C38	2.51	0.40
10:J:136:LEU:O	10:J:145:THR:HG21	2.21	0.40
10:J:159:ILE:O	10:J:163:THR:OG1	2.36	0.40
12:L:270:LEU:HD22	12:L:331:MET:HE1	2.02	0.40
12:L:296:LEU:HD12	12:L:367:ILE:HG13	2.03	0.40
13:M:195:MET:HE3	13:M:282:MET:SD	2.61	0.40
13:M:250:ILE:HG22	13:M:254:LEU:HD12	2.03	0.40
1:A:2:PHE:CZ	24:Z:152:LEU:HD22	2.57	0.40
13:M:310:CYS:O	13:M:313:GLY:N	2.55	0.40
14:N:108:ALA:HB3	14:N:109:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:26:TRP:HA	27:d:29:ILE:HG22	2.03	0.40
1:A:58:PHE:CG	10:J:170:ILE:HD13	2.56	0.40
3:C:50:ARG:NH2	4:D:165:ASN:OD1	2.53	0.40
4:D:189:ILE:HG23	4:D:208:LEU:HB3	2.03	0.40
8:H:78:TYR:N	8:H:129:SER:OG	2.54	0.40
9:I:153:ASP:OD2	9:I:156:LYS:HB2	2.22	0.40
10:J:1:MET:HE1	10:J:3:GLN:HB2	2.04	0.40
12:L:4:LEU:CB	12:L:9:ILE:HD11	2.52	0.40
19:T:77:GLU:OE1	19:T:81:LEU:HD12	2.21	0.40
19:U:85:LEU:HD23	34:k:43:ARG:HD2	2.04	0.40
22:X:28:ARG:HH22	24:Z:68:MET:HE1	1.86	0.40
34:k:50:GLU:OE1	34:k:53:ALA:N	2.47	0.40
2:B:138:MET:SD	4:D:120:LEU:HD22	2.62	0.40
5:E:168:GLU:HG3	6:F:388:PHE:HD2	1.87	0.40
6:F:155:GLU:OE1	6:F:271:ARG:NH2	2.54	0.40
9:I:99:SER:O	40:q:91:LYS:NZ	2.55	0.40
12:L:335:SER:O	34:k:67:ARG:NH2	2.54	0.40
13:M:165:ILE:HD13	13:M:173:MET:HE3	2.03	0.40
15:O:168:TYR:CE1	15:O:172:ILE:HD11	2.56	0.40
54:T:201:EHZ:C24	21:W:49:ILE:HD11	2.52	0.40
33:j:59:VAL:O	33:j:63:LEU:HD23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
2	B	180/182 (99%)	172 (96%)	8 (4%)	0	100	100
3	C	207/209 (99%)	194 (94%)	13 (6%)	0	100	100
4	D	427/430 (99%)	410 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	212/214 (99%)	198 (93%)	14 (7%)	0	100	100
6	F	439/441 (100%)	422 (96%)	16 (4%)	1 (0%)	43	71
7	G	673/731 (92%)	649 (96%)	24 (4%)	0	100	100
8	H	313/315 (99%)	301 (96%)	12 (4%)	0	100	100
9	I	184/186 (99%)	177 (96%)	7 (4%)	0	100	100
10	J	171/173 (99%)	164 (96%)	7 (4%)	0	100	100
11	K	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
12	L	575/577 (100%)	553 (96%)	22 (4%)	0	100	100
13	M	444/446 (100%)	428 (96%)	15 (3%)	1 (0%)	43	71
14	N	339/341 (99%)	328 (97%)	11 (3%)	0	100	100
15	O	366/368 (100%)	358 (98%)	8 (2%)	0	100	100
16	P	375/377 (100%)	361 (96%)	14 (4%)	0	100	100
17	Q	149/151 (99%)	139 (93%)	10 (7%)	0	100	100
18	R	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
19	T	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
19	U	83/85 (98%)	80 (96%)	3 (4%)	0	100	100
20	V	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
21	W	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
22	X	172/174 (99%)	162 (94%)	10 (6%)	0	100	100
23	Y	165/167 (99%)	159 (96%)	6 (4%)	0	100	100
24	Z	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
25	a	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
26	b	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
27	d	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
28	e	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
29	f	53/55 (96%)	48 (91%)	5 (9%)	0	100	100
30	g	106/108 (98%)	101 (95%)	5 (5%)	0	100	100
31	h	143/145 (99%)	133 (93%)	10 (7%)	0	100	100
32	i	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
33	j	64/66 (97%)	64 (100%)	0	0	100	100
34	k	82/84 (98%)	80 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	l	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
36	m	106/108 (98%)	102 (96%)	4 (4%)	0	100	100
37	n	132/134 (98%)	131 (99%)	1 (1%)	0	100	100
38	o	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
39	p	149/151 (99%)	146 (98%)	3 (2%)	0	100	100
40	q	131/133 (98%)	125 (95%)	6 (5%)	0	100	100
41	r	85/103 (82%)	82 (96%)	3 (4%)	0	100	100
42	s	60/62 (97%)	54 (90%)	6 (10%)	0	100	100
All	All	8087/8254 (98%)	7778 (96%)	307 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	M	51	PHE
6	F	49	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	110/110 (100%)	110 (100%)	0	100	100
2	B	152/152 (100%)	152 (100%)	0	100	100
3	C	187/187 (100%)	187 (100%)	0	100	100
4	D	367/367 (100%)	367 (100%)	0	100	100
5	E	185/185 (100%)	185 (100%)	0	100	100
6	F	353/353 (100%)	353 (100%)	0	100	100
7	G	546/582 (94%)	546 (100%)	0	100	100
8	H	282/282 (100%)	282 (100%)	0	100	100
9	I	159/159 (100%)	159 (100%)	0	100	100
10	J	166/166 (100%)	166 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	91/91 (100%)	91 (100%)	0	100	100
12	L	518/518 (100%)	518 (100%)	0	100	100
13	M	404/404 (100%)	404 (100%)	0	100	100
14	N	317/317 (100%)	317 (100%)	0	100	100
15	O	324/324 (100%)	324 (100%)	0	100	100
16	P	319/319 (100%)	319 (100%)	0	100	100
17	Q	131/131 (100%)	131 (100%)	0	100	100
18	R	77/77 (100%)	77 (100%)	0	100	100
19	T	71/79 (90%)	71 (100%)	0	100	100
19	U	79/79 (100%)	79 (100%)	0	100	100
20	V	97/97 (100%)	97 (100%)	0	100	100
21	W	107/107 (100%)	107 (100%)	0	100	100
22	X	150/150 (100%)	150 (100%)	0	100	100
23	Y	128/128 (100%)	128 (100%)	0	100	100
24	Z	128/128 (100%)	128 (100%)	0	100	100
25	a	65/65 (100%)	65 (100%)	0	100	100
26	b	52/52 (100%)	52 (100%)	0	100	100
27	d	93/93 (100%)	93 (100%)	0	100	100
28	e	88/88 (100%)	88 (100%)	0	100	100
29	f	42/42 (100%)	42 (100%)	0	100	100
30	g	97/97 (100%)	97 (100%)	0	100	100
31	h	130/130 (100%)	130 (100%)	0	100	100
32	i	133/133 (100%)	133 (100%)	0	100	100
33	j	57/57 (100%)	57 (100%)	0	100	100
34	k	69/69 (100%)	69 (100%)	0	100	100
35	l	122/122 (100%)	122 (100%)	0	100	100
36	m	89/89 (100%)	89 (100%)	0	100	100
37	n	117/117 (100%)	117 (100%)	0	100	100
38	o	101/101 (100%)	101 (100%)	0	100	100
39	p	135/135 (100%)	135 (100%)	0	100	100
40	q	115/115 (100%)	115 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	r	78/86 (91%)	78 (100%)	0	100	100
42	s	50/50 (100%)	50 (100%)	0	100	100
All	All	7081/7133 (99%)	7081 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	136	ASN
2	B	204	GLN
3	C	59	HIS
4	D	152	ASN
4	D	310	GLN
4	D	354	ASN
4	D	436	HIS
6	F	64	HIS
6	F	296	HIS
7	G	65	GLN
7	G	350	GLN
7	G	372	ASN
7	G	399	ASN
7	G	436	ASN
7	G	610	GLN
7	G	658	HIS
8	H	201	ASN
10	J	19	ASN
10	J	117	GLN
12	L	132	GLN
12	L	321	ASN
12	L	323	ASN
14	N	133	GLN
14	N	265	GLN
14	N	318	ASN
15	O	153	HIS
15	O	274	GLN
15	O	376	ASN
16	P	116	HIS
16	P	266	GLN
16	P	343	HIS
17	Q	105	GLN

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Mol	Chain	Res	Type
17	Q	116	ASN
18	R	58	ASN
20	V	86	ASN
21	W	13	GLN
22	X	18	GLN
22	X	107	GLN
23	Y	142	GLN
24	Z	12	GLN
28	e	20	ASN
28	e	71	HIS
30	g	52	ASN
30	g	128	ASN
32	i	46	GLN
32	i	131	HIS
33	j	40	HIS
33	j	65	HIS
33	j	69	HIS
36	m	28	GLN
36	m	61	HIS
37	n	66	GLN
37	n	79	ASN
38	o	65	GLN
40	q	70	HIS
41	r	59	GLN

5.3.3 RNA (i)

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	$\#\|Z\|>2$
4	2MR	D	123	4	10,12,13	2.52	3 (30%)	5,13,15	3.08	1 (20%)

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
4	2MR	D	123	4	-	1/10/13/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	123	2MR	CZ-NE	5.43	1.45	1.34
4	D	123	2MR	CZ-NH2	5.36	1.45	1.33
4	D	123	2MR	O-C	2.02	1.28	1.19

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	123	2MR	NE-CZ-NH2	-6.55	113.48	119.48

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	123	2MR	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 39 ligands modelled in this entry, 2 are monoatomic - leaving 37 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	$\#\|Z\| > 2$
44	3PE	Y	301	-	43,43,50	0.92	4 (9%)	46,48,55	1.30	3 (6%)
50	UQ9	H	501	-	58,58,58	2.26	19 (32%)	70,73,73	1.55	11 (15%)
44	3PE	J	202	-	39,39,50	0.96	4 (10%)	42,44,55	1.17	2 (4%)
43	PC1	A	201	-	38,38,53	1.47	6 (15%)	44,46,61	1.04	2 (4%)
44	3PE	X	201	-	29,29,50	1.14	4 (13%)	32,34,55	1.23	3 (9%)
45	SF4	I	302	9	0,12,12	-	-	-		
47	FES	G	803	7	0,4,4	-	-	-		
45	SF4	B	301	2	0,12,12	-	-	-		
52	NDP	P	501	-	49,52,52	3.97	23 (46%)	66,80,80	2.07	15 (22%)
54	EHZ	T	201	19	29,36,37	1.68	6 (20%)	35,44,47	1.63	5 (14%)
46	CDL	B	303	-	66,66,99	1.10	6 (9%)	72,78,111	1.03	3 (4%)
44	3PE	N	401	-	43,43,50	0.93	2 (4%)	46,48,55	1.00	2 (4%)
46	CDL	h	201	-	68,68,99	1.07	7 (10%)	74,80,111	1.11	4 (5%)
45	SF4	I	301	9	0,12,12	-	-	-		
44	3PE	J	203	-	23,23,50	1.19	4 (17%)	26,28,55	1.23	2 (7%)
44	3PE	Y	303	-	32,32,50	1.06	4 (12%)	35,37,55	1.03	2 (5%)
44	3PE	d	201	-	35,35,50	1.01	4 (11%)	38,40,55	1.05	2 (5%)
44	3PE	B	302	-	36,36,50	1.02	3 (8%)	39,41,55	1.14	3 (7%)
46	CDL	P	502	-	53,53,99	1.21	7 (13%)	59,65,111	1.24	4 (6%)
45	SF4	F	502	6	0,12,12	-	-	-		
44	3PE	M	501	-	34,34,50	1.03	4 (11%)	37,39,55	1.10	2 (5%)
44	3PE	L	601	-	38,38,50	0.97	4 (10%)	41,43,55	1.04	2 (4%)
45	SF4	G	802	7	0,12,12	-	-	-		
44	3PE	L	603	-	24,24,50	1.18	4 (16%)	27,29,55	1.38	2 (7%)
44	3PE	A	202	-	34,34,50	1.02	4 (11%)	37,39,55	1.28	2 (5%)
44	3PE	L	602	-	43,43,50	0.92	4 (9%)	46,48,55	1.07	2 (4%)
47	FES	E	301	5	0,4,4	-	-	-		
45	SF4	G	801	7	0,12,12	-	-	-		
51	DGT	O	501	-	29,33,33	3.21	13 (44%)	44,52,52	2.02	12 (27%)
54	EHZ	U	201	19	29,36,37	1.70	6 (20%)	35,44,47	1.73	7 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	3PE	Y	302	-	29,29,50	1.10	4 (13%)	32,34,55	1.21	2 (6%)
44	3PE	A	203	-	43,43,50	0.91	4 (9%)	46,48,55	1.17	3 (6%)
43	PC1	i	201	-	33,33,53	1.53	6 (18%)	39,41,61	1.07	2 (5%)
44	3PE	H	502	-	46,46,50	0.88	4 (8%)	49,51,55	1.14	2 (4%)
46	CDL	h	202	-	59,59,99	1.13	7 (11%)	65,71,111	1.22	5 (7%)
48	FMN	F	501	-	33,33,33	2.63	10 (30%)	48,50,50	1.74	15 (31%)
43	PC1	J	201	-	43,43,53	1.38	6 (13%)	49,51,61	1.05	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
44	3PE	Y	301	-	-	13/47/47/54	-
50	UQ9	H	501	-	-	14/57/81/81	0/1/1/1
44	3PE	J	202	-	-	19/43/43/54	-
43	PC1	A	201	-	-	15/42/42/57	-
44	3PE	X	201	-	-	21/33/33/54	-
45	SF4	I	302	9	-	-	0/6/5/5
47	FES	G	803	7	-	-	0/1/1/1
45	SF4	B	301	2	-	-	0/6/5/5
52	NDP	P	501	-	-	4/34/77/77	0/5/5/5
54	EHZ	T	201	19	-	13/42/44/45	-
46	CDL	B	303	-	-	44/77/77/110	-
44	3PE	N	401	-	-	19/47/47/54	-
46	CDL	h	201	-	-	40/79/79/110	-
45	SF4	I	301	9	-	-	0/6/5/5
44	3PE	J	203	-	-	13/27/27/54	-
44	3PE	Y	303	-	-	14/36/36/54	-
44	3PE	d	201	-	-	19/39/39/54	-
44	3PE	B	302	-	-	17/40/40/54	-
46	CDL	P	502	-	-	33/64/64/110	-
45	SF4	F	502	6	-	-	0/6/5/5
44	3PE	M	501	-	-	20/38/38/54	-
44	3PE	L	601	-	-	23/42/42/54	-
45	SF4	G	802	7	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	3PE	L	603	-	-	8/27/27/54	-
44	3PE	A	202	-	-	16/38/38/54	-
44	3PE	L	602	-	-	19/47/47/54	-
47	FES	E	301	5	-	-	0/1/1/1
45	SF4	G	801	7	-	-	0/6/5/5
51	DGT	O	501	-	-	4/22/34/34	0/3/3/3
54	EHZ	U	201	19	-	12/42/44/45	-
44	3PE	Y	302	-	-	12/33/33/54	-
44	3PE	A	203	-	-	15/47/47/54	-
43	PC1	i	201	-	-	17/37/37/57	-
44	3PE	H	502	-	-	16/50/50/54	-
46	CDL	h	202	-	-	34/70/70/110	-
48	FMN	F	501	-	-	8/18/18/18	0/3/3/3
43	PC1	J	201	-	-	14/47/47/57	-

All (183) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	P	501	NDP	C6N-C5N	12.12	1.55	1.33
50	H	501	UQ9	C6-C1	10.61	1.54	1.35
52	P	501	NDP	C2B-C1B	-8.71	1.30	1.53
52	P	501	NDP	C7N-N7N	8.24	1.55	1.33
51	O	501	DGT	C3'-C4'	-8.15	1.30	1.53
52	P	501	NDP	O4B-C1B	8.05	1.61	1.42
52	P	501	NDP	O4D-C1D	7.86	1.60	1.42
51	O	501	DGT	O4'-C4'	7.59	1.62	1.45
52	P	501	NDP	C2D-C1D	-7.42	1.29	1.53
48	F	501	FMN	C4A-N5	6.82	1.44	1.30
52	P	501	NDP	O4D-C4D	-6.59	1.30	1.45
51	O	501	DGT	C4-N3	6.19	1.49	1.34
48	F	501	FMN	C10-N1	6.08	1.45	1.33
52	P	501	NDP	O4B-C4B	-5.46	1.32	1.45
54	U	201	EHZ	C15-N2	5.45	1.45	1.33
52	P	501	NDP	C6A-N6A	5.45	1.47	1.34
51	O	501	DGT	C2-N3	5.38	1.46	1.33
54	T	201	EHZ	C15-N2	5.27	1.45	1.33
52	P	501	NDP	P2B-O2B	5.24	1.69	1.59
54	T	201	EHZ	C12-N1	5.23	1.45	1.33
51	O	501	DGT	O4'-C1'	-5.22	1.30	1.42
54	U	201	EHZ	C12-N1	5.21	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	F	501	FMN	C5A-N5	4.82	1.48	1.39
48	F	501	FMN	C9A-N10	4.74	1.49	1.41
51	O	501	DGT	C2-N2	4.71	1.45	1.34
52	P	501	NDP	C2N-C3N	4.53	1.47	1.34
50	H	501	UQ9	C7-C8	4.52	1.57	1.50
48	F	501	FMN	C2-N1	4.46	1.47	1.36
52	P	501	NDP	C5A-C4A	-4.32	1.30	1.39
52	P	501	NDP	O7N-C7N	-4.12	1.14	1.24
50	H	501	UQ9	C4-C3	4.10	1.53	1.36
48	F	501	FMN	C2-N3	4.01	1.48	1.39
43	A	201	PC1	O31-C31	3.88	1.44	1.33
52	P	501	NDP	C8A-N9A	-3.86	1.30	1.37
43	i	201	PC1	O31-C31	3.81	1.44	1.33
52	P	501	NDP	O2D-C2D	3.75	1.51	1.43
43	J	201	PC1	O31-C31	3.74	1.44	1.33
43	A	201	PC1	O21-C21	3.74	1.44	1.34
43	i	201	PC1	O21-C21	3.60	1.44	1.34
48	F	501	FMN	C10-N10	3.51	1.45	1.37
48	F	501	FMN	O2-C2	-3.41	1.18	1.24
48	F	501	FMN	C4-N3	3.34	1.45	1.38
43	J	201	PC1	O21-C21	3.31	1.43	1.34
50	H	501	UQ9	C16-C14	3.26	1.58	1.51
51	O	501	DGT	C5-N7	-3.23	1.32	1.39
50	H	501	UQ9	C11-C9	3.05	1.57	1.51
52	P	501	NDP	C4N-C3N	3.01	1.55	1.49
51	O	501	DGT	O3'-C3'	2.87	1.49	1.43
52	P	501	NDP	C5A-N7A	-2.87	1.33	1.39
46	B	303	CDL	OB8-CB7	2.82	1.41	1.33
44	B	302	3PE	O21-C2	-2.81	1.39	1.46
52	P	501	NDP	C4N-C5N	2.80	1.56	1.48
46	h	201	CDL	OB8-CB7	2.76	1.41	1.33
46	P	502	CDL	OB8-CB7	2.73	1.41	1.33
46	B	303	CDL	OA6-CA4	-2.72	1.39	1.46
48	F	501	FMN	O4-C4	-2.69	1.18	1.23
52	P	501	NDP	O3B-C3B	-2.69	1.36	1.43
46	h	202	CDL	OB8-CB7	2.69	1.41	1.33
52	P	501	NDP	O3D-C3D	-2.69	1.36	1.43
43	J	201	PC1	O21-C2	-2.66	1.39	1.46
51	O	501	DGT	O6-C6	-2.65	1.18	1.23
46	P	502	CDL	OB6-CB5	2.64	1.41	1.34
44	L	602	3PE	O21-C2	-2.64	1.40	1.46
44	L	601	3PE	O21-C2	-2.62	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	Y	303	3PE	O21-C2	-2.62	1.40	1.46
46	P	502	CDL	OA6-CA4	-2.62	1.40	1.46
44	N	401	3PE	O21-C2	-2.61	1.40	1.46
44	J	203	3PE	O21-C2	-2.56	1.40	1.46
46	h	201	CDL	OB6-CB4	-2.56	1.40	1.46
44	X	201	3PE	O31-C31	2.52	1.40	1.33
50	H	501	UQ9	C21-C19	2.52	1.56	1.51
51	O	501	DGT	C2-N1	2.52	1.43	1.37
44	H	502	3PE	O21-C2	-2.51	1.40	1.46
44	J	202	3PE	O31-C3	-2.50	1.39	1.45
44	L	603	3PE	O21-C2	-2.49	1.40	1.46
50	H	501	UQ9	C46-C44	2.49	1.56	1.51
44	X	201	3PE	O21-C2	-2.49	1.40	1.46
44	N	401	3PE	O31-C31	2.48	1.40	1.33
43	i	201	PC1	O21-C2	-2.48	1.40	1.46
46	h	201	CDL	OA8-CA7	2.47	1.40	1.33
46	h	202	CDL	OA6-CA4	-2.47	1.40	1.46
46	B	303	CDL	OA8-CA7	2.46	1.40	1.33
44	A	203	3PE	O21-C2	-2.44	1.40	1.46
54	T	201	EHZ	O3-C12	-2.42	1.18	1.23
44	M	501	3PE	O21-C2	-2.42	1.40	1.46
44	B	302	3PE	O31-C31	2.42	1.40	1.33
46	h	202	CDL	OB6-CB5	2.41	1.41	1.34
46	B	303	CDL	OB6-CB5	2.41	1.41	1.34
50	H	501	UQ9	C36-C34	2.40	1.56	1.51
50	H	501	UQ9	C7-C6	2.40	1.55	1.51
44	Y	301	3PE	O21-C2	-2.39	1.40	1.46
44	J	202	3PE	O21-C21	2.39	1.41	1.34
46	P	502	CDL	OB6-CB4	-2.38	1.40	1.46
46	h	202	CDL	OA8-CA7	2.38	1.40	1.33
54	U	201	EHZ	O3-C12	-2.37	1.18	1.23
44	Y	303	3PE	O31-C31	2.36	1.40	1.33
44	M	501	3PE	O31-C31	2.35	1.40	1.33
44	J	202	3PE	O21-C2	-2.35	1.40	1.46
44	d	201	3PE	O21-C2	-2.34	1.40	1.46
44	A	203	3PE	O31-C31	2.34	1.40	1.33
44	Y	301	3PE	O31-C3	-2.33	1.39	1.45
44	Y	302	3PE	O31-C31	2.33	1.40	1.33
54	U	201	EHZ	O4-C15	-2.33	1.18	1.23
44	Y	301	3PE	O31-C31	2.32	1.40	1.33
46	P	502	CDL	OA8-CA7	2.32	1.40	1.33
44	H	502	3PE	O31-C31	2.32	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	h	202	CDL	OB6-CB4	-2.32	1.40	1.46
54	T	201	EHZ	O4-C15	-2.32	1.18	1.23
44	L	603	3PE	O31-C31	2.32	1.40	1.33
50	H	501	UQ9	C37-C38	2.32	1.58	1.50
44	A	202	3PE	O31-C31	2.31	1.40	1.33
44	Y	303	3PE	O31-C3	-2.30	1.39	1.45
46	h	201	CDL	OB6-CB5	2.30	1.40	1.34
43	A	201	PC1	C22-C21	2.29	1.57	1.50
44	d	201	3PE	O31-C3	-2.29	1.39	1.45
44	L	601	3PE	O31-C3	-2.29	1.39	1.45
46	h	201	CDL	OA6-CA5	2.28	1.40	1.34
50	H	501	UQ9	O4-C4M	-2.28	1.39	1.45
50	H	501	UQ9	C17-C18	2.28	1.57	1.50
51	O	501	DGT	C5-C6	2.28	1.52	1.44
43	A	201	PC1	P-O11	2.27	1.68	1.59
50	H	501	UQ9	C41-C39	2.27	1.56	1.51
44	L	602	3PE	O31-C3	-2.27	1.40	1.45
46	P	502	CDL	OA8-CA6	-2.26	1.40	1.45
54	T	201	EHZ	O6-C20	-2.25	1.39	1.44
44	A	202	3PE	O21-C21	2.24	1.40	1.34
44	L	602	3PE	O31-C31	2.24	1.39	1.33
44	L	601	3PE	O31-C31	2.24	1.39	1.33
44	Y	302	3PE	O21-C2	-2.23	1.41	1.46
44	M	501	3PE	O21-C21	2.23	1.40	1.34
50	H	501	UQ9	O2-C2	-2.23	1.18	1.23
50	H	501	UQ9	C42-C43	2.23	1.57	1.50
44	X	201	3PE	O21-C21	2.23	1.40	1.34
54	U	201	EHZ	C9-S1	2.23	1.81	1.76
46	B	303	CDL	OB6-CB4	-2.22	1.41	1.46
44	J	203	3PE	O31-C31	2.22	1.39	1.33
46	h	201	CDL	OA6-CA4	-2.22	1.41	1.46
50	H	501	UQ9	O5-C5	-2.22	1.18	1.23
44	J	203	3PE	O31-C3	-2.21	1.40	1.45
44	d	201	3PE	O31-C31	2.20	1.39	1.33
44	A	203	3PE	O31-C3	-2.19	1.40	1.45
46	h	201	CDL	OA8-CA6	-2.19	1.40	1.45
43	A	201	PC1	O21-C2	-2.19	1.41	1.46
43	i	201	PC1	C22-C21	2.19	1.57	1.50
44	A	202	3PE	O31-C3	-2.18	1.40	1.45
54	T	201	EHZ	C9-S1	2.17	1.81	1.76
44	Y	302	3PE	O31-C3	-2.17	1.40	1.45
46	B	303	CDL	OA8-CA6	-2.17	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	A	202	3PE	O21-C2	-2.16	1.41	1.46
52	P	501	NDP	C6N-N1N	2.16	1.42	1.37
46	h	202	CDL	OA6-CA5	2.16	1.40	1.34
43	J	201	PC1	P-O11	2.16	1.68	1.59
51	O	501	DGT	C4-N9	-2.14	1.32	1.38
44	Y	301	3PE	O21-C21	2.14	1.40	1.34
43	J	201	PC1	C22-C21	2.14	1.57	1.50
52	P	501	NDP	C7N-C3N	2.13	1.53	1.48
46	P	502	CDL	OA6-CA5	2.13	1.40	1.34
44	L	603	3PE	O21-C21	2.11	1.40	1.35
50	H	501	UQ9	O3-C3M	-2.11	1.40	1.45
44	B	302	3PE	O31-C3	-2.11	1.40	1.45
44	M	501	3PE	O31-C3	-2.11	1.40	1.45
50	H	501	UQ9	C32-C33	2.09	1.57	1.50
44	H	502	3PE	O31-C3	-2.08	1.40	1.45
44	L	602	3PE	O21-C21	2.08	1.40	1.34
44	H	502	3PE	O21-C21	2.08	1.40	1.34
52	P	501	NDP	P2B-O1X	2.08	1.57	1.50
44	J	202	3PE	O31-C31	2.08	1.39	1.33
44	d	201	3PE	O21-C21	2.07	1.40	1.34
44	A	203	3PE	O21-C21	2.07	1.40	1.34
43	i	201	PC1	P-O11	2.06	1.67	1.59
51	O	501	DGT	C6-N1	2.06	1.42	1.38
44	X	201	3PE	O31-C3	-2.06	1.40	1.45
44	J	203	3PE	O21-C21	2.06	1.40	1.34
54	U	201	EHZ	O6-C20	-2.05	1.39	1.44
44	L	603	3PE	O31-C3	-2.04	1.40	1.45
44	L	601	3PE	O21-C21	2.04	1.40	1.34
50	H	501	UQ9	C6-C5	2.04	1.52	1.46
43	J	201	PC1	P-O13	2.04	1.67	1.59
44	Y	302	3PE	O21-C21	2.03	1.40	1.34
43	A	201	PC1	P-O13	2.03	1.67	1.59
43	i	201	PC1	P-O13	2.02	1.67	1.59
44	Y	303	3PE	O21-C21	2.01	1.40	1.34
46	h	202	CDL	OA8-CA6	-2.01	1.40	1.45

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	P	501	NDP	N6A-C6A-N1A	-5.64	106.00	118.35
52	P	501	NDP	C5A-C4A-N3A	-5.41	119.69	126.75
50	H	501	UQ9	C7-C6-C5	-5.30	112.09	118.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	T	201	EHZ	C8-C9-S1	5.29	120.17	113.63
52	P	501	NDP	N3A-C2A-N1A	-5.25	120.39	128.60
44	A	202	3PE	O21-C21-C22	5.22	122.76	111.50
44	Y	301	3PE	O21-C21-C22	5.20	122.71	111.50
52	P	501	NDP	C4A-N9A-C1B	-5.08	114.49	126.59
44	L	603	3PE	O21-C21-C22	5.06	120.41	111.09
51	O	501	DGT	C5-C4-N3	-4.92	120.47	128.46
46	P	502	CDL	OB6-CB5-C51	4.91	122.09	111.50
54	U	201	EHZ	C8-C9-S1	4.89	119.68	113.63
51	O	501	DGT	C1'-N9-C8	4.87	138.75	127.85
51	O	501	DGT	C1'-N9-C4	-4.85	112.05	125.48
48	F	501	FMN	C9-C8-C7	4.68	126.38	119.67
44	X	201	3PE	O21-C21-C22	4.62	121.45	111.50
46	h	202	CDL	OA6-CA5-C11	4.58	121.38	111.50
52	P	501	NDP	C5A-C6A-N6A	4.55	133.34	123.43
52	P	501	NDP	C1B-N9A-C8A	4.53	137.36	127.14
44	J	202	3PE	O21-C21-C22	4.49	121.19	111.50
44	Y	302	3PE	O21-C21-C22	4.48	121.16	111.50
54	T	201	EHZ	C13-C14-N2	-4.44	102.94	111.90
50	H	501	UQ9	C10-C9-C11	4.24	122.41	115.27
52	P	501	NDP	N9A-C8A-N7A	-4.23	108.13	113.91
44	H	502	3PE	O21-C21-C22	4.20	120.56	111.50
54	U	201	EHZ	C14-C13-C12	-4.20	105.36	112.36
51	O	501	DGT	C2-N3-C4	4.15	119.70	112.30
46	P	502	CDL	OA6-CA5-C11	4.14	120.42	111.50
44	L	602	3PE	O21-C21-C22	4.07	120.28	111.50
48	F	501	FMN	C7M-C7-C6	4.05	126.97	119.49
43	A	201	PC1	O21-C21-C22	4.00	120.12	111.50
44	A	203	3PE	O21-C21-C22	4.00	120.11	111.50
50	H	501	UQ9	C7-C8-C9	-3.89	120.31	126.79
46	h	202	CDL	OB6-CB5-C51	3.87	119.84	111.50
44	J	203	3PE	O21-C21-C22	3.85	119.80	111.50
46	h	201	CDL	OB6-CB5-C51	3.79	119.67	111.50
46	B	303	CDL	OA6-CA5-C11	3.79	119.67	111.50
44	M	501	3PE	O21-C21-C22	3.78	119.64	111.50
44	B	302	3PE	O21-C21-C22	3.70	119.48	111.50
44	Y	303	3PE	O21-C21-C22	3.68	119.44	111.50
43	J	201	PC1	O21-C21-C22	3.68	119.42	111.50
51	O	501	DGT	PB-O3B-PG	-3.60	120.48	132.83
46	B	303	CDL	OB6-CB5-C51	3.60	119.25	111.50
52	P	501	NDP	C2A-N3A-C4A	3.59	120.24	111.75
43	i	201	PC1	O21-C21-C22	3.56	119.17	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	h	201	CDL	OB8-CB7-C71	3.54	123.00	111.91
52	P	501	NDP	PN-O3-PA	-3.49	120.85	132.83
48	F	501	FMN	C4-N3-C2	-3.49	119.20	125.64
44	N	401	3PE	O21-C21-C22	3.42	118.88	111.50
44	J	203	3PE	O31-C31-C32	3.39	120.26	111.38
44	L	601	3PE	O21-C21-C22	3.35	118.73	111.50
52	P	501	NDP	N3A-C4A-N9A	3.33	132.58	127.08
46	h	202	CDL	OB8-CB7-C71	3.30	120.03	111.38
51	O	501	DGT	N9-C4-N3	3.28	132.52	125.94
43	i	201	PC1	O31-C31-C32	3.27	122.18	111.91
54	U	201	EHZ	C13-C12-N1	3.21	121.83	116.42
46	h	201	CDL	OA6-CA5-C11	3.21	118.41	111.50
50	H	501	UQ9	C20-C19-C21	3.18	120.63	115.27
51	O	501	DGT	N9-C8-N7	-3.15	107.45	113.39
46	B	303	CDL	OB8-CB7-C71	3.08	121.59	111.91
51	O	501	DGT	C2-N1-C6	-3.08	119.48	125.10
44	N	401	3PE	O31-C31-C32	3.03	121.42	111.91
44	B	302	3PE	C2-O21-C21	-2.99	110.42	117.79
44	Y	301	3PE	C23-C22-C21	2.98	124.46	113.62
52	P	501	NDP	C5A-N7A-C8A	2.95	107.70	103.51
48	F	501	FMN	C6-C7-C8	-2.85	115.58	119.67
44	M	501	3PE	O31-C31-C32	2.85	120.87	111.91
44	B	302	3PE	O31-C31-C32	2.84	120.82	111.91
43	A	201	PC1	O31-C31-C32	2.83	120.79	111.91
48	F	501	FMN	C4A-C10-N10	2.83	120.61	116.48
46	h	201	CDL	OA8-CA7-C31	2.83	120.78	111.91
44	d	201	3PE	O21-C21-C22	2.82	117.57	111.50
44	Y	301	3PE	O31-C31-C32	2.81	120.72	111.91
51	O	501	DGT	PA-O3A-PB	-2.80	123.20	132.83
50	H	501	UQ9	C35-C34-C36	2.80	119.98	115.27
44	L	603	3PE	O31-C31-C32	2.79	120.67	111.91
43	J	201	PC1	O31-C31-C32	2.79	120.66	111.91
48	F	501	FMN	C8M-C8-C7	-2.78	115.03	120.74
51	O	501	DGT	C5-C6-N1	2.76	120.19	113.19
46	h	202	CDL	OA8-CA7-C31	2.71	120.41	111.91
44	H	502	3PE	O31-C31-C32	2.68	120.33	111.91
44	A	203	3PE	O31-C31-C32	2.67	120.29	111.91
44	d	201	3PE	O31-C31-C32	2.65	120.24	111.91
52	P	501	NDP	C2B-C1B-N9A	-2.64	109.08	113.53
44	L	601	3PE	O31-C31-C32	2.64	120.20	111.91
54	U	201	EHZ	C11-N1-C12	-2.64	117.94	122.84
54	U	201	EHZ	C13-C14-N2	-2.60	106.64	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	O	501	DGT	O6-C6-C5	-2.60	119.70	126.60
48	F	501	FMN	C5'-C4'-C3'	-2.58	107.22	112.20
52	P	501	NDP	C3N-C2N-N1N	-2.57	119.43	123.10
48	F	501	FMN	C4-C4A-C10	2.56	121.09	116.79
48	F	501	FMN	C6-C5A-C9A	2.53	122.52	118.94
44	X	201	3PE	O31-C31-C32	2.49	119.72	111.91
48	F	501	FMN	O4-C4-C4A	-2.47	120.06	126.60
46	P	502	CDL	OA8-CA7-C31	2.47	119.64	111.91
54	T	201	EHZ	C18-C17-C16	2.41	113.00	108.82
50	H	501	UQ9	C41-C39-C38	-2.41	116.24	121.12
54	T	201	EHZ	O2-C9-S1	-2.40	119.49	122.61
48	F	501	FMN	C4A-C4-N3	2.40	119.28	113.19
44	L	602	3PE	O31-C31-C32	2.35	119.30	111.91
50	H	501	UQ9	C27-C28-C29	-2.33	122.05	127.66
44	Y	302	3PE	O31-C31-C32	2.30	119.14	111.91
44	Y	303	3PE	O31-C31-C32	2.30	119.14	111.91
50	H	501	UQ9	C35-C34-C33	-2.30	117.77	123.68
44	J	202	3PE	O31-C31-C32	2.26	119.01	111.91
48	F	501	FMN	C5A-C9A-N10	2.26	120.29	117.95
44	A	202	3PE	O31-C31-C32	2.26	119.00	111.91
46	P	502	CDL	OB8-CB7-C71	2.25	118.97	111.91
52	P	501	NDP	C4A-N9A-C8A	2.24	108.15	105.73
48	F	501	FMN	C4A-C10-N1	-2.23	119.55	124.73
50	H	501	UQ9	C8-C7-C6	2.21	118.01	112.05
54	T	201	EHZ	C10-S1-C9	2.16	108.59	101.87
46	h	202	CDL	OA6-CA5-OA7	-2.15	118.51	123.70
54	U	201	EHZ	C5-C6-C7	-2.10	108.81	114.85
44	X	201	3PE	O31-C3-C2	2.08	114.49	108.43
48	F	501	FMN	C10-C4A-N5	-2.08	120.45	124.86
44	A	203	3PE	C3A-C39-C38	-2.08	103.88	114.42
52	P	501	NDP	C6A-C5A-C4A	2.07	119.96	117.18
50	H	501	UQ9	C22-C23-C24	-2.06	122.69	127.66
50	H	501	UQ9	C30-C29-C31	2.03	118.68	115.27
48	F	501	FMN	C9A-C5A-N5	-2.02	120.23	122.43
51	O	501	DGT	C8-N7-C5	2.00	107.87	104.24
54	U	201	EHZ	C7-C8-C9	-2.00	109.32	113.89

There are no chirality outliers.

All (516) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	A	201	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
43	A	201	PC1	C1-O11-P-O14
43	J	201	PC1	O22-C21-O21-C2
43	i	201	PC1	C11-O13-P-O12
43	i	201	PC1	C11-O13-P-O14
43	i	201	PC1	C2-C1-O11-P
44	A	202	3PE	C1-O11-P-O12
44	A	202	3PE	C1-O11-P-O13
44	A	202	3PE	C1-O11-P-O14
44	A	202	3PE	O11-C1-C2-O21
44	A	203	3PE	C1-O11-P-O12
44	A	203	3PE	C1-O11-P-O13
44	A	203	3PE	C1-O11-P-O14
44	A	203	3PE	C11-O13-P-O14
44	B	302	3PE	C1-O11-P-O12
44	B	302	3PE	C1-O11-P-O13
44	B	302	3PE	C1-O11-P-O14
44	B	302	3PE	C22-C21-O21-C2
44	H	502	3PE	C1-O11-P-O12
44	H	502	3PE	C1-O11-P-O14
44	H	502	3PE	C11-O13-P-O11
44	H	502	3PE	C12-C11-O13-P
44	H	502	3PE	O22-C21-O21-C2
44	J	203	3PE	C1-O11-P-O12
44	J	203	3PE	C1-O11-P-O14
44	J	203	3PE	O13-C11-C12-N
44	J	203	3PE	O32-C31-O31-C3
44	L	601	3PE	C1-O11-P-O12
44	L	601	3PE	C1-O11-P-O14
44	L	601	3PE	O22-C21-O21-C2
44	L	601	3PE	C22-C21-O21-C2
44	L	602	3PE	C12-C11-O13-P
44	L	603	3PE	C1-O11-P-O12
44	M	501	3PE	C1-O11-P-O14
44	M	501	3PE	C11-O13-P-O11
44	M	501	3PE	C11-O13-P-O12
44	M	501	3PE	C11-O13-P-O14
44	N	401	3PE	C1-O11-P-O12
44	N	401	3PE	C1-O11-P-O13
44	N	401	3PE	C1-O11-P-O14
44	X	201	3PE	C2-C1-O11-P
44	X	201	3PE	O13-C11-C12-N
44	Y	301	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
44	Y	301	3PE	C1-O11-P-O14
44	Y	302	3PE	C1-O11-P-O12
44	Y	302	3PE	C1-O11-P-O14
44	Y	302	3PE	C22-C21-O21-C2
44	Y	303	3PE	C1-O11-P-O14
44	Y	303	3PE	C12-C11-O13-P
44	d	201	3PE	C11-O13-P-O14
44	d	201	3PE	O13-C11-C12-N
46	B	303	CDL	CA2-OA2-PA1-OA3
46	B	303	CDL	CA2-OA2-PA1-OA4
46	B	303	CDL	CA2-OA2-PA1-OA5
46	B	303	CDL	CA3-OA5-PA1-OA2
46	B	303	CDL	CA3-OA5-PA1-OA4
46	B	303	CDL	CB2-OB2-PB2-OB3
46	B	303	CDL	CB2-OB2-PB2-OB4
46	B	303	CDL	C51-CB5-OB6-CB4
46	P	502	CDL	CA2-C1-CB2-OB2
46	h	201	CDL	O1-C1-CB2-OB2
46	h	201	CDL	CA2-OA2-PA1-OA3
46	h	201	CDL	CA2-OA2-PA1-OA4
46	h	201	CDL	CA2-OA2-PA1-OA5
46	h	201	CDL	CA3-OA5-PA1-OA2
46	h	201	CDL	CA3-OA5-PA1-OA4
46	h	201	CDL	CB2-OB2-PB2-OB3
46	h	201	CDL	OB7-CB5-OB6-CB4
46	h	201	CDL	OB9-CB7-OB8-CB6
46	h	201	CDL	C71-CB7-OB8-CB6
46	h	202	CDL	CA2-OA2-PA1-OA3
46	h	202	CDL	CA2-OA2-PA1-OA4
46	h	202	CDL	CA2-OA2-PA1-OA5
46	h	202	CDL	OA7-CA5-OA6-CA4
46	h	202	CDL	C11-CA5-OA6-CA4
46	h	202	CDL	CB2-OB2-PB2-OB3
46	h	202	CDL	CB2-OB2-PB2-OB4
46	h	202	CDL	C51-CB5-OB6-CB4
48	F	501	FMN	N10-C1'-C2'-O2'
48	F	501	FMN	C5'-O5'-P-O1P
48	F	501	FMN	C5'-O5'-P-O2P
50	H	501	UQ9	C41-C42-C43-C44
50	H	501	UQ9	C36-C37-C38-C39
50	H	501	UQ9	C35-C34-C36-C37
50	H	501	UQ9	C33-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
50	H	501	UQ9	C14-C16-C17-C18
50	H	501	UQ9	C12-C11-C9-C10
50	H	501	UQ9	C12-C11-C9-C8
50	H	501	UQ9	C1-C6-C7-C8
50	H	501	UQ9	C5-C6-C7-C8
51	O	501	DGT	C5'-O5'-PA-O1A
51	O	501	DGT	C5'-O5'-PA-O2A
52	P	501	NDP	O4D-C1D-N1N-C6N
54	T	201	EHZ	C6-C7-C8-C9
54	T	201	EHZ	S1-C10-C11-N1
54	T	201	EHZ	C16-C17-C20-O6
54	T	201	EHZ	O2-C9-S1-C10
54	T	201	EHZ	C8-C9-S1-C10
54	U	201	EHZ	C6-C7-C8-C9
54	U	201	EHZ	S1-C10-C11-N1
54	U	201	EHZ	C11-C10-S1-C9
44	X	201	3PE	O32-C31-O31-C3
44	J	203	3PE	C32-C31-O31-C3
44	L	601	3PE	C32-C31-O31-C3
44	X	201	3PE	C32-C31-O31-C3
44	L	601	3PE	O32-C31-O31-C3
44	M	501	3PE	O32-C31-O31-C3
44	Y	301	3PE	O32-C31-O31-C3
44	B	302	3PE	O22-C21-O21-C2
44	Y	302	3PE	O22-C21-O21-C2
46	h	202	CDL	OB7-CB5-OB6-CB4
44	M	501	3PE	C32-C31-O31-C3
44	Y	301	3PE	C32-C31-O31-C3
43	J	201	PC1	C22-C21-O21-C2
44	H	502	3PE	C22-C21-O21-C2
46	h	201	CDL	C51-CB5-OB6-CB4
46	B	303	CDL	C76-C77-C78-C79
44	L	602	3PE	C32-C31-O31-C3
46	B	303	CDL	OB7-CB5-OB6-CB4
43	A	201	PC1	O32-C31-O31-C3
46	P	502	CDL	O1-C1-CB2-OB2
43	A	201	PC1	C32-C31-O31-C3
44	d	201	3PE	C32-C31-O31-C3
44	L	602	3PE	O32-C31-O31-C3
44	d	201	3PE	O32-C31-O31-C3
46	P	502	CDL	CA4-CA3-OA5-PA1
50	H	501	UQ9	C19-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
44	L	602	3PE	C32-C33-C34-C35
46	h	201	CDL	CA2-C1-CB2-OB2
43	i	201	PC1	C32-C31-O31-C3
46	B	303	CDL	C71-CB7-OB8-CB6
44	A	202	3PE	C32-C33-C34-C35
44	N	401	3PE	C32-C33-C34-C35
46	B	303	CDL	O1-C1-CB2-OB2
46	P	502	CDL	CB5-C51-C52-C53
43	i	201	PC1	C32-C33-C34-C35
43	i	201	PC1	O32-C31-O31-C3
44	L	601	3PE	C24-C25-C26-C27
46	B	303	CDL	CB5-C51-C52-C53
46	P	502	CDL	CA7-C31-C32-C33
46	h	201	CDL	CA5-C11-C12-C13
46	P	502	CDL	CA5-C11-C12-C13
46	h	201	CDL	CB5-C51-C52-C53
46	h	202	CDL	CA5-C11-C12-C13
46	h	202	CDL	CB4-CB3-OB5-PB2
44	d	201	3PE	C22-C21-O21-C2
46	B	303	CDL	OB9-CB7-OB8-CB6
44	N	401	3PE	C22-C21-O21-C2
43	i	201	PC1	C11-O13-P-O11
43	i	201	PC1	C1-O11-P-O13
44	A	203	3PE	C11-O13-P-O11
44	H	502	3PE	C1-O11-P-O13
44	J	202	3PE	C1-O11-P-O13
44	L	601	3PE	C11-O13-P-O11
44	L	602	3PE	C1-O11-P-O13
44	X	201	3PE	C1-O11-P-O13
44	Y	301	3PE	C1-O11-P-O13
44	Y	302	3PE	C1-O11-P-O13
44	d	201	3PE	C1-O11-P-O13
46	B	303	CDL	CB2-OB2-PB2-OB5
46	h	202	CDL	CB2-OB2-PB2-OB5
44	Y	303	3PE	C36-C37-C38-C39
46	B	303	CDL	CA2-C1-CB2-OB2
44	N	401	3PE	O22-C21-O21-C2
44	d	201	3PE	O22-C21-O21-C2
46	h	201	CDL	C31-CA7-OA8-CA6
46	B	303	CDL	C11-CA5-OA6-CA4
44	J	202	3PE	C39-C3A-C3B-C3C
46	B	303	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
46	B	303	CDL	C51-C52-C53-C54
44	L	602	3PE	C2D-C2E-C2F-C2G
44	B	302	3PE	C33-C34-C35-C36
44	B	302	3PE	C25-C26-C27-C28
46	h	201	CDL	OA9-CA7-OA8-CA6
44	N	401	3PE	C21-C22-C23-C24
44	X	201	3PE	C32-C33-C34-C35
44	L	602	3PE	C2A-C2B-C2C-C2D
44	H	502	3PE	C2B-C2C-C2D-C2E
46	B	303	CDL	CA5-C11-C12-C13
44	H	502	3PE	C33-C34-C35-C36
44	L	601	3PE	C2A-C2B-C2C-C2D
46	h	201	CDL	C33-C34-C35-C36
54	T	201	EHZ	C1-C21-C22-C23
46	h	201	CDL	C51-C52-C53-C54
54	T	201	EHZ	C3-C4-C5-C6
44	M	501	3PE	C35-C36-C37-C38
44	A	202	3PE	C32-C31-O31-C3
46	B	303	CDL	O1-C1-CA2-OA2
54	U	201	EHZ	C21-C1-C2-C3
44	N	401	3PE	C26-C27-C28-C29
44	A	202	3PE	C22-C21-O21-C2
46	B	303	CDL	C31-C32-C33-C34
44	L	601	3PE	C21-C22-C23-C24
44	M	501	3PE	C32-C33-C34-C35
46	B	303	CDL	C75-C76-C77-C78
46	P	502	CDL	C31-CA7-OA8-CA6
44	B	302	3PE	C27-C28-C29-C2A
44	L	601	3PE	C26-C27-C28-C29
46	P	502	CDL	C51-CB5-OB6-CB4
54	U	201	EHZ	C2-C3-C4-C5
44	A	202	3PE	O32-C31-O31-C3
46	P	502	CDL	OB7-CB5-OB6-CB4
43	i	201	PC1	O21-C2-C3-O31
44	L	601	3PE	O21-C2-C3-O31
46	B	303	CDL	OA6-CA4-CA6-OA8
44	A	203	3PE	C34-C35-C36-C37
44	A	203	3PE	C35-C36-C37-C38
46	h	202	CDL	CB5-C51-C52-C53
46	h	201	CDL	C53-C54-C55-C56
43	A	201	PC1	C35-C36-C37-C38
43	A	201	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
44	J	203	3PE	C1-O11-P-O13
44	L	601	3PE	C1-O11-P-O13
44	L	603	3PE	C1-O11-P-O13
44	M	501	3PE	C1-O11-P-O13
44	Y	303	3PE	C1-O11-P-O13
46	h	201	CDL	CB2-OB2-PB2-OB5
46	h	202	CDL	CA3-OA5-PA1-OA2
44	B	302	3PE	C2-C1-O11-P
44	A	202	3PE	O11-C1-C2-C3
44	X	201	3PE	O11-C1-C2-C3
44	A	202	3PE	O22-C21-O21-C2
46	P	502	CDL	OA9-CA7-OA8-CA6
43	i	201	PC1	C1-C2-C3-O31
44	B	302	3PE	C1-C2-C3-O31
46	h	202	CDL	CA3-CA4-CA6-OA8
54	U	201	EHZ	C2-C1-C21-C22
46	B	303	CDL	C53-C54-C55-C56
46	P	502	CDL	C52-C51-CB5-OB6
44	L	602	3PE	C24-C25-C26-C27
43	J	201	PC1	C35-C36-C37-C38
44	M	501	3PE	C24-C25-C26-C27
46	h	201	CDL	C17-C18-C19-C20
46	h	202	CDL	CB6-CB4-OB6-CB5
46	h	202	CDL	C15-C16-C17-C18
43	J	201	PC1	C32-C31-O31-C3
43	i	201	PC1	O11-C1-C2-O21
44	N	401	3PE	O11-C1-C2-O21
46	h	202	CDL	OB5-CB3-CB4-OB6
46	h	201	CDL	C55-C56-C57-C58
44	B	302	3PE	C22-C23-C24-C25
44	A	202	3PE	C2-C3-O31-C31
46	h	202	CDL	C17-C18-C19-C20
46	B	303	CDL	C73-C74-C75-C76
46	h	202	CDL	C37-C38-C39-C40
46	h	201	CDL	CA7-C31-C32-C33
46	h	202	CDL	C51-C52-C53-C54
44	J	202	3PE	O11-C1-C2-C3
44	J	203	3PE	O11-C1-C2-C3
44	Y	303	3PE	O11-C1-C2-C3
44	d	201	3PE	O11-C1-C2-C3
46	B	303	CDL	OB5-CB3-CB4-CB6
46	h	202	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
44	L	603	3PE	O13-C11-C12-N
44	L	601	3PE	C22-C23-C24-C25
54	U	201	EHZ	C21-C22-C23-C24
44	d	201	3PE	C2-C1-O11-P
46	B	303	CDL	C17-C18-C19-C20
54	T	201	EHZ	C10-C11-N1-C12
46	h	201	CDL	C75-C76-C77-C78
43	J	201	PC1	C1-C2-C3-O31
46	B	303	CDL	CA3-CA4-CA6-OA8
46	P	502	CDL	C51-C52-C53-C54
46	B	303	CDL	C33-C34-C35-C36
43	A	201	PC1	C11-O13-P-O11
44	X	201	3PE	C11-O13-P-O11
44	d	201	3PE	C11-O13-P-O11
44	X	201	3PE	C31-C32-C33-C34
44	Y	302	3PE	C21-C22-C23-C24
44	L	601	3PE	O11-C1-C2-O21
44	X	201	3PE	O11-C1-C2-O21
44	Y	303	3PE	O11-C1-C2-O21
44	J	202	3PE	C25-C26-C27-C28
43	J	201	PC1	O32-C31-O31-C3
44	L	602	3PE	C25-C26-C27-C28
46	h	201	CDL	C71-C72-C73-C74
43	i	201	PC1	C34-C35-C36-C37
46	h	202	CDL	C12-C13-C14-C15
43	J	201	PC1	O21-C2-C3-O31
46	P	502	CDL	OB6-CB4-CB6-OB8
46	B	303	CDL	CA4-CA3-OA5-PA1
46	h	201	CDL	CA4-CA3-OA5-PA1
46	h	202	CDL	C1-CA2-OA2-PA1
48	F	501	FMN	C4'-C5'-O5'-P
54	U	201	EHZ	O2-C9-S1-C10
44	N	401	3PE	C37-C38-C39-C3A
46	h	201	CDL	C11-CA5-OA6-CA4
46	B	303	CDL	C78-C79-C80-C81
44	Y	302	3PE	C31-C32-C33-C34
44	L	601	3PE	O11-C1-C2-C3
46	h	201	CDL	OA5-CA3-CA4-CA6
44	M	501	3PE	C33-C34-C35-C36
54	T	201	EHZ	C18-C17-C20-O6
46	B	303	CDL	C11-C12-C13-C14
46	h	201	CDL	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
43	A	201	PC1	C3-C2-O21-C21
44	N	401	3PE	C3-C2-O21-C21
44	Y	302	3PE	C1-C2-O21-C21
46	B	303	CDL	CB6-CB4-OB6-CB5
54	U	201	EHZ	C8-C9-S1-C10
44	d	201	3PE	C22-C23-C24-C25
44	L	601	3PE	C1-C2-C3-O31
44	N	401	3PE	C1-C2-C3-O31
46	B	303	CDL	CB4-CB3-OB5-PB2
44	H	502	3PE	O11-C1-C2-O21
44	J	202	3PE	O11-C1-C2-O21
44	J	203	3PE	O11-C1-C2-O21
46	h	201	CDL	OA5-CA3-CA4-OA6
44	A	202	3PE	C34-C35-C36-C37
44	J	202	3PE	C35-C36-C37-C38
44	X	201	3PE	O22-C21-O21-C2
46	h	201	CDL	OA7-CA5-OA6-CA4
51	O	501	DGT	PB-O3B-PG-O1G
54	T	201	EHZ	O1-C7-C8-C9
43	A	201	PC1	O21-C2-C3-O31
44	J	202	3PE	O21-C2-C3-O31
46	h	201	CDL	OB6-CB4-CB6-OB8
46	h	202	CDL	OA6-CA4-CA6-OA8
46	B	303	CDL	C12-C13-C14-C15
46	h	202	CDL	C31-C32-C33-C34
44	X	201	3PE	C22-C21-O21-C2
43	J	201	PC1	C25-C26-C27-C28
46	B	303	CDL	C35-C36-C37-C38
44	L	602	3PE	C2-C3-O31-C31
44	N	401	3PE	C11-O13-P-O11
46	P	502	CDL	CA2-OA2-PA1-OA5
46	P	502	CDL	C1-CA2-OA2-PA1
43	i	201	PC1	C1-O11-P-O12
44	B	302	3PE	C11-O13-P-O14
44	J	202	3PE	C1-O11-P-O12
44	J	202	3PE	C1-O11-P-O14
44	L	601	3PE	C11-O13-P-O14
44	L	602	3PE	C1-O11-P-O12
44	L	602	3PE	C1-O11-P-O14
44	L	603	3PE	C1-O11-P-O14
44	M	501	3PE	C1-O11-P-O12
44	X	201	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
44	X	201	3PE	C11-O13-P-O12
44	d	201	3PE	C1-O11-P-O12
44	d	201	3PE	C1-O11-P-O14
46	B	303	CDL	CA3-OA5-PA1-OA3
46	P	502	CDL	CA2-OA2-PA1-OA3
46	P	502	CDL	CB2-OB2-PB2-OB4
46	h	201	CDL	CA3-OA5-PA1-OA3
46	h	201	CDL	CB2-OB2-PB2-OB4
44	H	502	3PE	O11-C1-C2-C3
44	L	602	3PE	O11-C1-C2-C3
44	N	401	3PE	O11-C1-C2-C3
46	B	303	CDL	OA5-CA3-CA4-CA6
46	P	502	CDL	OA5-CA3-CA4-CA6
44	Y	303	3PE	C33-C34-C35-C36
44	L	601	3PE	C33-C34-C35-C36
44	A	202	3PE	C12-C11-O13-P
44	B	302	3PE	C12-C11-O13-P
44	L	601	3PE	C12-C11-O13-P
44	L	603	3PE	C12-C11-O13-P
44	M	501	3PE	C12-C11-O13-P
44	N	401	3PE	C12-C11-O13-P
44	X	201	3PE	C12-C11-O13-P
44	Y	303	3PE	C32-C33-C34-C35
44	B	302	3PE	O11-C1-C2-O21
44	L	602	3PE	O11-C1-C2-O21
44	Y	301	3PE	O11-C1-C2-O21
44	d	201	3PE	O11-C1-C2-O21
46	B	303	CDL	OA5-CA3-CA4-OA6
44	J	203	3PE	O31-C31-C32-C33
44	J	202	3PE	C33-C34-C35-C36
43	A	201	PC1	O13-C11-C12-N
43	J	201	PC1	O13-C11-C12-N
46	h	201	CDL	CB3-CB4-CB6-OB8
44	Y	302	3PE	C22-C23-C24-C25
43	A	201	PC1	C36-C37-C38-C39
44	Y	303	3PE	O31-C31-C32-C33
44	Y	301	3PE	C3B-C3C-C3D-C3E
44	L	602	3PE	C2B-C2C-C2D-C2E
44	M	501	3PE	C21-C22-C23-C24
44	A	202	3PE	C35-C36-C37-C38
44	X	201	3PE	C3-C2-O21-C21
44	d	201	3PE	C1-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
46	h	201	CDL	CA3-CA4-OA6-CA5
43	i	201	PC1	O11-C1-C2-C3
44	Y	301	3PE	O11-C1-C2-C3
44	X	201	3PE	C22-C23-C24-C25
46	h	202	CDL	C32-C33-C34-C35
54	T	201	EHZ	C1-C2-C3-C4
44	d	201	3PE	O21-C21-C22-C23
44	B	302	3PE	O21-C2-C3-O31
44	N	401	3PE	O21-C2-C3-O31
43	J	201	PC1	C11-O13-P-O11
44	L	603	3PE	C11-O13-P-O11
46	P	502	CDL	CB3-OB5-PB2-OB2
44	N	401	3PE	C34-C35-C36-C37
44	J	202	3PE	C38-C39-C3A-C3B
44	J	202	3PE	C36-C37-C38-C39
46	P	502	CDL	C12-C13-C14-C15
44	X	201	3PE	C33-C34-C35-C36
44	M	501	3PE	C36-C37-C38-C39
44	Y	303	3PE	O22-C21-O21-C2
54	U	201	EHZ	C1-C2-C3-C4
44	J	203	3PE	O32-C31-C32-C33
44	Y	302	3PE	O21-C2-C3-O31
44	A	202	3PE	O21-C21-C22-C23
50	H	501	UQ9	C21-C22-C23-C24
46	h	202	CDL	C19-C20-C21-C22
44	M	501	3PE	C25-C26-C27-C28
54	T	201	EHZ	C19-C17-C20-O6
44	L	602	3PE	C34-C35-C36-C37
44	J	202	3PE	C32-C33-C34-C35
46	h	201	CDL	C78-C79-C80-C81
43	i	201	PC1	C1-C2-O21-C21
44	Y	301	3PE	O22-C21-O21-C2
44	A	203	3PE	C23-C24-C25-C26
46	h	202	CDL	C72-C71-CB7-OB8
46	P	502	CDL	C14-C15-C16-C17
44	H	502	3PE	C2-C1-O11-P
44	L	603	3PE	O11-C1-C2-O21
43	A	201	PC1	O21-C21-C22-C23
44	A	203	3PE	O21-C21-C22-C23
50	H	501	UQ9	C25-C24-C26-C27
46	P	502	CDL	C52-C51-CB5-OB7
44	d	201	3PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
43	J	201	PC1	C26-C27-C28-C29
46	P	502	CDL	C15-C16-C17-C18
50	H	501	UQ9	C9-C11-C12-C13
44	d	201	3PE	C33-C34-C35-C36
44	Y	301	3PE	C22-C21-O21-C2
46	P	502	CDL	O1-C1-CA2-OA2
44	Y	303	3PE	C34-C35-C36-C37
44	A	202	3PE	O31-C31-C32-C33
44	Y	303	3PE	C22-C21-O21-C2
44	H	502	3PE	C2A-C2B-C2C-C2D
44	J	202	3PE	C34-C35-C36-C37
48	F	501	FMN	O3'-C3'-C4'-C5'
48	F	501	FMN	C2'-C3'-C4'-O4'
46	h	201	CDL	C32-C33-C34-C35
46	h	202	CDL	C31-CA7-OA8-CA6
44	X	201	3PE	C34-C35-C36-C37
48	F	501	FMN	C5'-O5'-P-O3P
54	T	201	EHZ	N2-C15-C16-O5
44	H	502	3PE	C28-C29-C2A-C2B
43	i	201	PC1	O21-C21-C22-C23
46	B	303	CDL	C72-C71-CB7-OB8
44	X	201	3PE	C23-C24-C25-C26
44	J	202	3PE	C3-C2-O21-C21
44	X	201	3PE	C1-C2-O21-C21
46	P	502	CDL	OA7-CA5-OA6-CA4
44	H	502	3PE	O31-C31-C32-C33
50	H	501	UQ9	C23-C24-C26-C27
44	L	601	3PE	O31-C31-C32-C33
46	P	502	CDL	C12-C11-CA5-OA6
46	h	201	CDL	C72-C71-CB7-OB8
43	A	201	PC1	C1-C2-C3-O31
44	J	202	3PE	C1-C2-C3-O31
46	P	502	CDL	CB3-CB4-CB6-OB8
46	h	202	CDL	OA9-CA7-OA8-CA6
44	L	602	3PE	C2C-C2D-C2E-C2F
44	M	501	3PE	O21-C21-C22-C23
54	U	201	EHZ	O1-C7-C8-C9
44	M	501	3PE	O31-C31-C32-C33
44	B	302	3PE	O11-C1-C2-C3
44	L	603	3PE	O11-C1-C2-C3
44	L	601	3PE	C31-C32-C33-C34
46	h	202	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
44	A	203	3PE	O31-C31-C32-C33
51	O	501	DGT	C5'-O5'-PA-O3A
52	P	501	NDP	C2B-O2B-P2B-O3X
46	h	202	CDL	C71-CB7-OB8-CB6
44	L	602	3PE	O21-C21-C22-C23
44	Y	302	3PE	O21-C21-C22-C23
44	N	401	3PE	C2B-C2C-C2D-C2E
43	J	201	PC1	C24-C25-C26-C27
52	P	501	NDP	O4B-C4B-C5B-O5B
52	P	501	NDP	PN-O3-PA-O2A
54	U	201	EHZ	C3-C4-C5-C6
44	A	203	3PE	C32-C31-O31-C3
44	A	203	3PE	C22-C23-C24-C25
43	i	201	PC1	O22-C21-C22-C23
44	H	502	3PE	O32-C31-C32-C33
44	M	501	3PE	O22-C21-C22-C23
46	B	303	CDL	C72-C71-CB7-OB9
48	F	501	FMN	O3'-C3'-C4'-O4'
46	B	303	CDL	CB7-C71-C72-C73
46	P	502	CDL	C12-C11-CA5-OA7
44	Y	302	3PE	O22-C21-C22-C23
46	P	502	CDL	CA2-OA2-PA1-OA4
46	P	502	CDL	CB3-OB5-PB2-OB3
46	h	202	CDL	CA3-OA5-PA1-OA4
46	P	502	CDL	C71-C72-C73-C74
44	L	601	3PE	O32-C31-C32-C33
44	M	501	3PE	O32-C31-C32-C33
46	h	201	CDL	C72-C71-CB7-OB9
43	A	201	PC1	O31-C31-C32-C33
44	Y	303	3PE	O21-C21-C22-C23
44	B	302	3PE	C26-C27-C28-C29
43	J	201	PC1	C12-C11-O13-P
44	J	202	3PE	C1-C2-O21-C21
44	Y	301	3PE	C12-C11-O13-P
44	A	203	3PE	O32-C31-O31-C3
44	Y	301	3PE	O31-C31-C32-C33
44	L	602	3PE	O22-C21-C22-C23
44	J	203	3PE	O21-C21-C22-C23
44	J	202	3PE	C31-C32-C33-C34
44	A	203	3PE	O32-C31-C32-C33
43	A	201	PC1	O22-C21-O21-C2
44	J	203	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
46	P	502	CDL	OA5-CA3-CA4-OA6
44	J	202	3PE	O21-C21-C22-C23
44	A	203	3PE	C33-C34-C35-C36
46	B	303	CDL	C12-C11-CA5-OA6
46	P	502	CDL	C16-C17-C18-C19
44	Y	301	3PE	O32-C31-C32-C33
44	Y	303	3PE	O22-C21-C22-C23
43	J	201	PC1	O31-C31-C32-C33
44	N	401	3PE	O31-C31-C32-C33
44	d	201	3PE	O31-C31-C32-C33
44	J	203	3PE	O22-C21-C22-C23

There are no ring outliers.

12 monomers are involved in 33 short contacts:

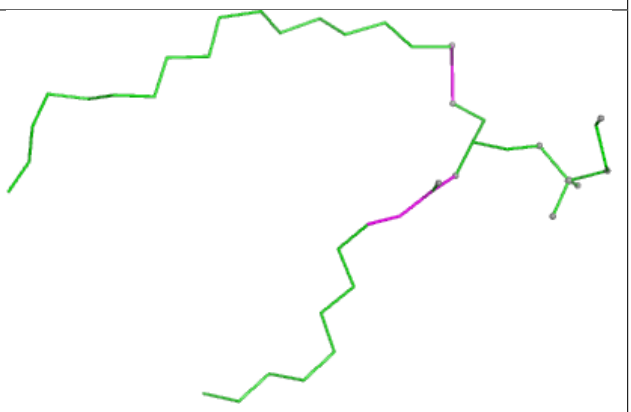
Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	H	501	UQ9	15	0
52	P	501	NDP	2	0
54	T	201	EHZ	3	0
46	h	201	CDL	1	0
44	J	203	3PE	2	0
44	L	602	3PE	1	0
51	O	501	DGT	2	0
54	U	201	EHZ	3	0
44	A	203	3PE	1	0
43	i	201	PC1	1	0
46	h	202	CDL	2	0
48	F	501	FMN	1	0

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 3PE Y 301



Bond lengths



Bond angles

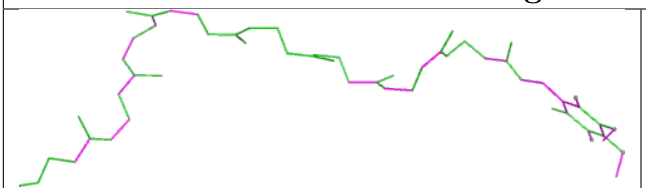


Torsions

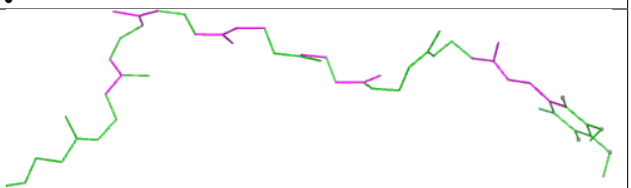


Rings

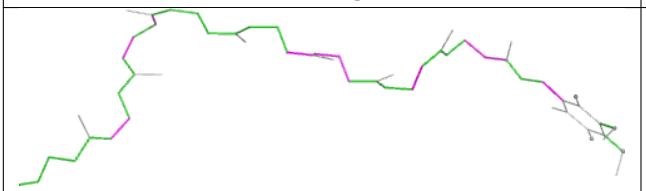
Ligand UQ9 H 501



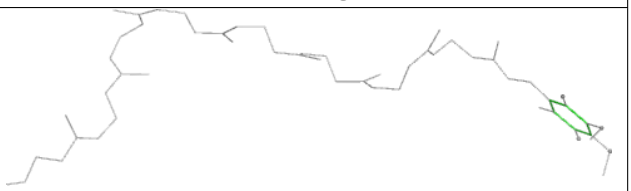
Bond lengths



Bond angles

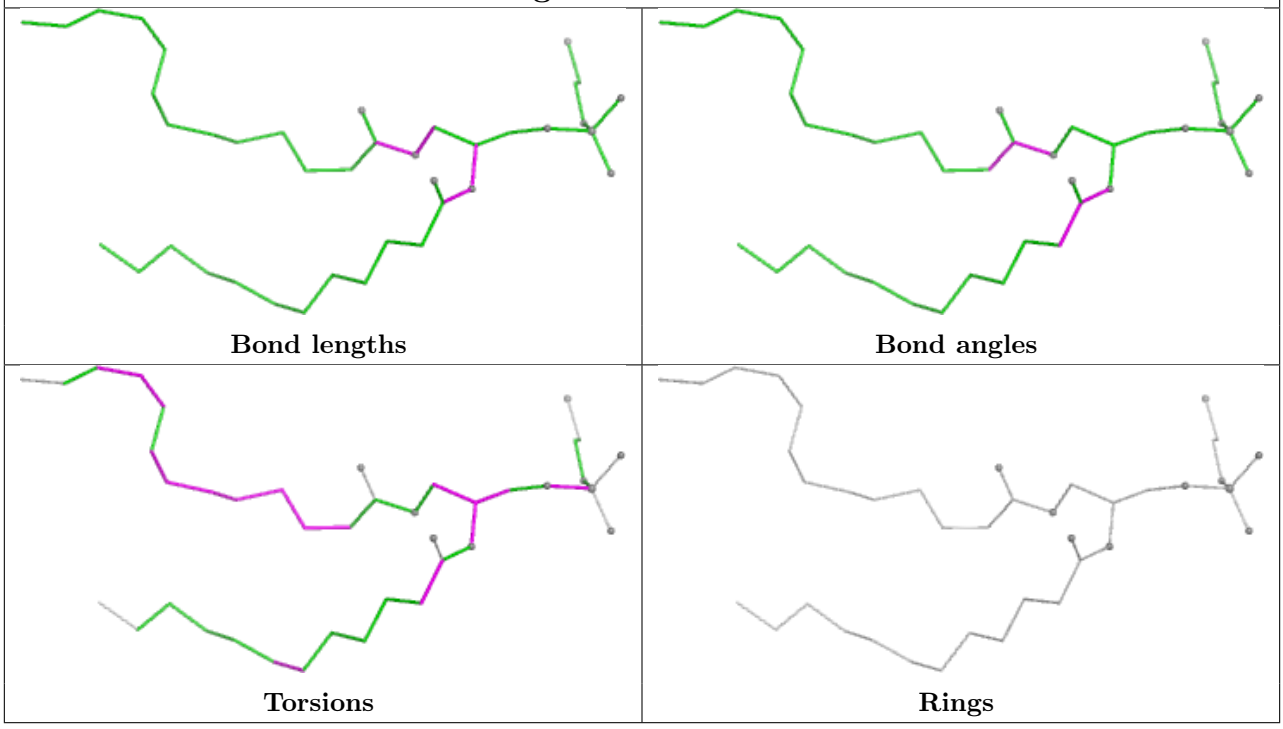


Torsions

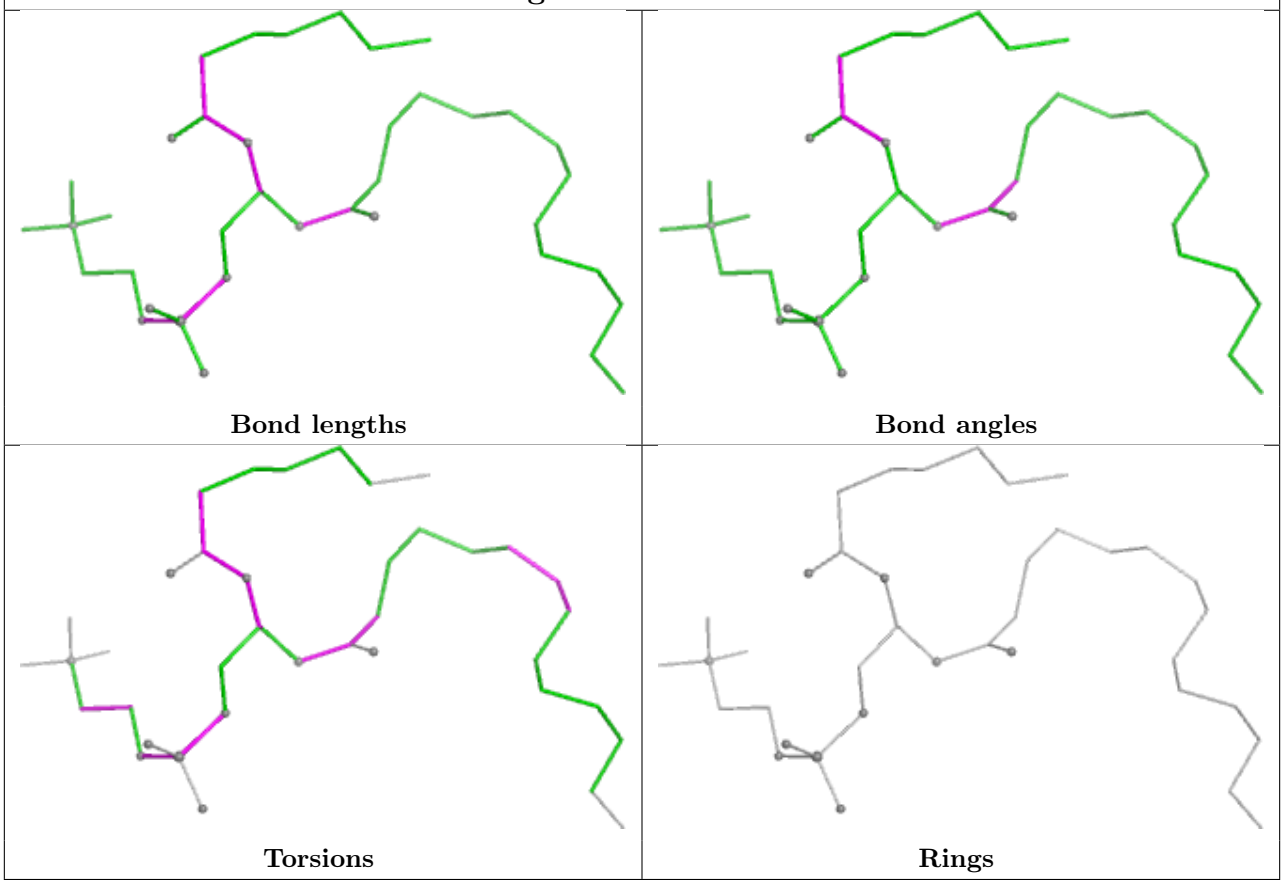


Rings

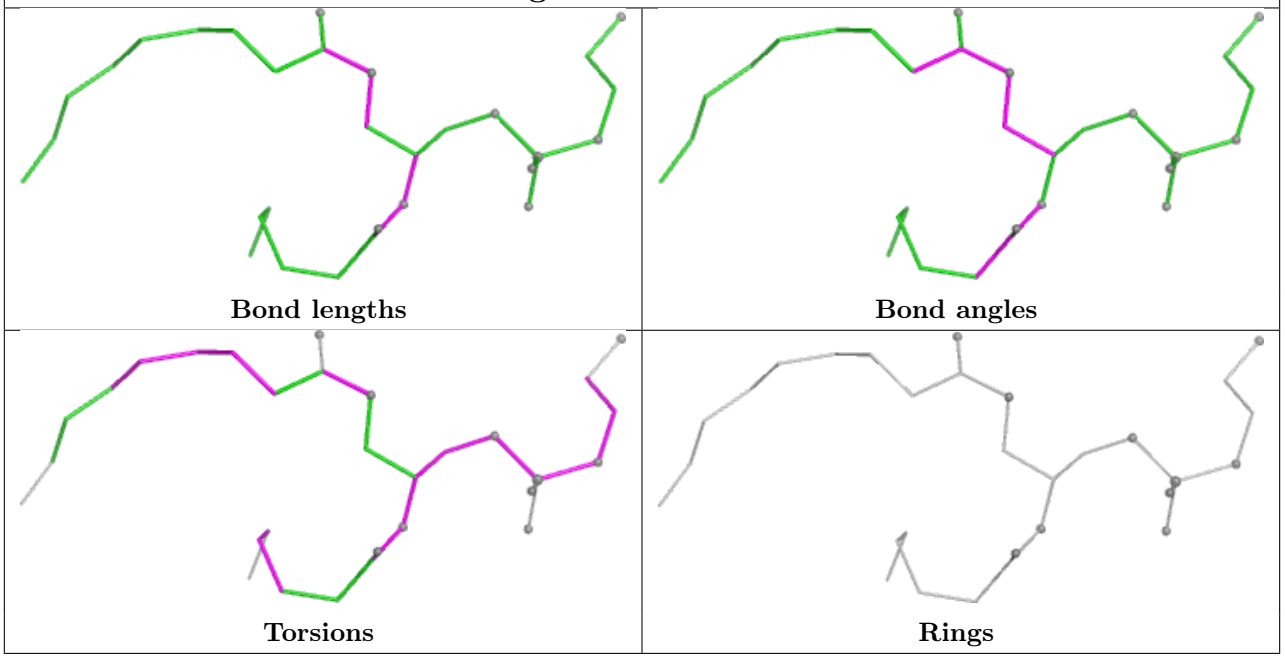
Ligand 3PE J 202



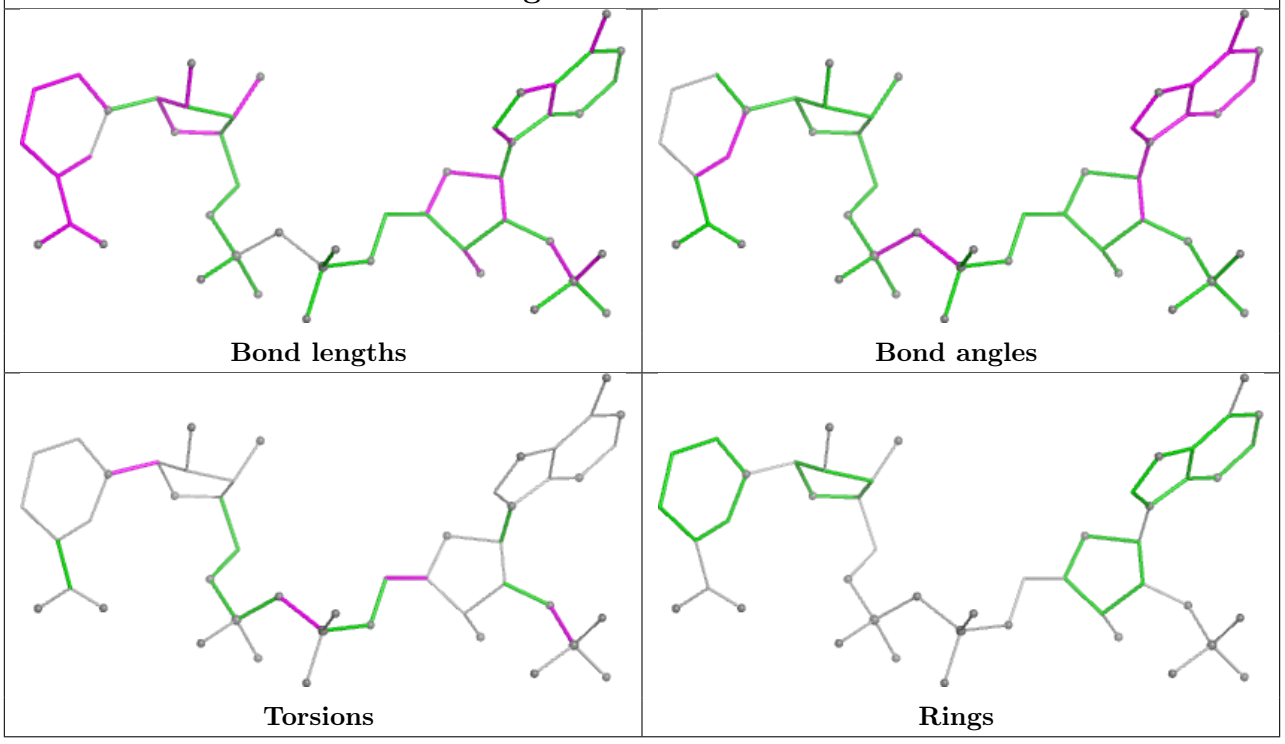
Ligand PC1 A 201



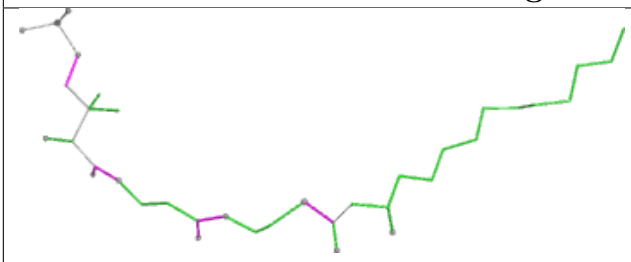
Ligand 3PE X 201



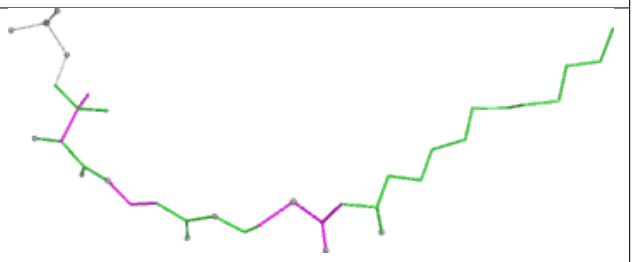
Ligand NDP P 501



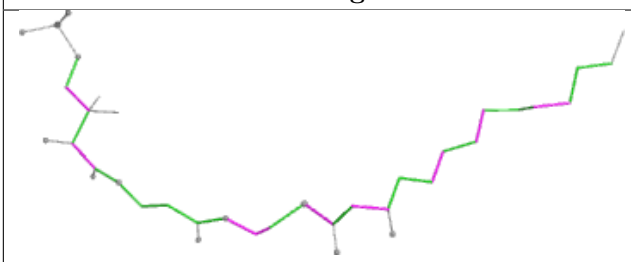
Ligand EHZ T 201



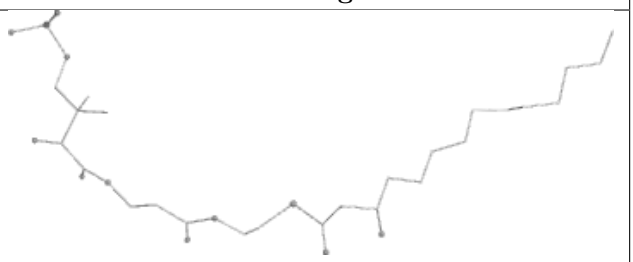
Bond lengths



Bond angles



Torsions

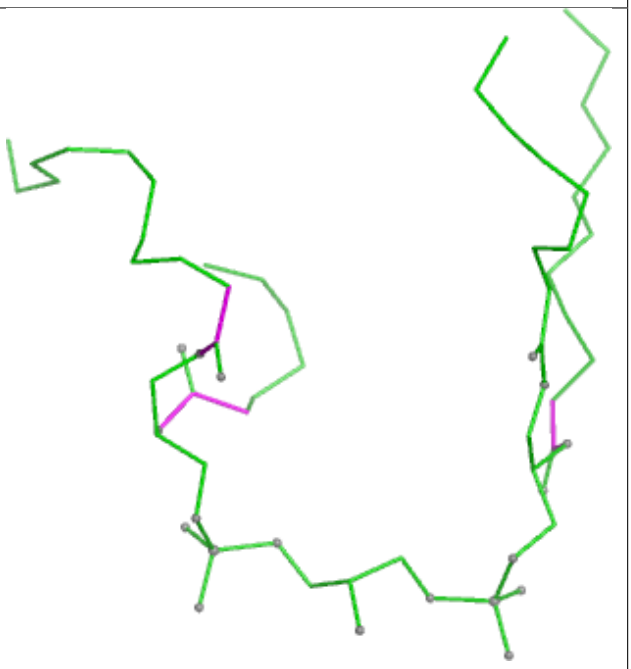


Rings

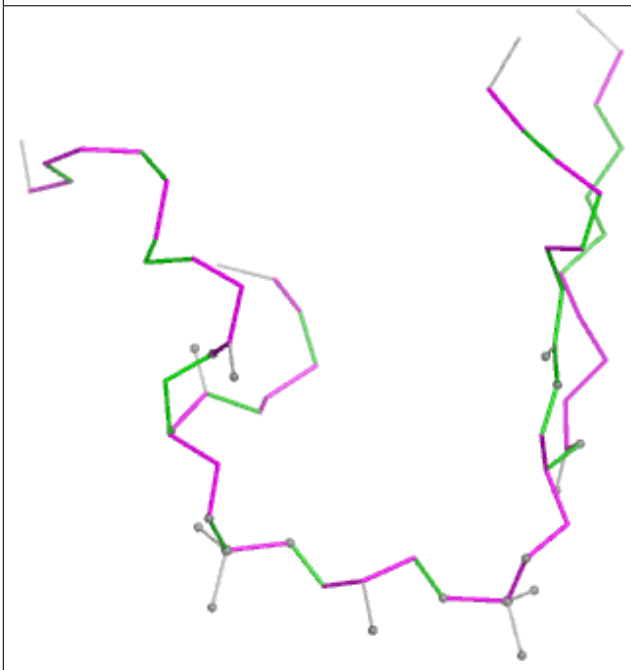
Ligand CDL B 303



Bond lengths



Bond angles

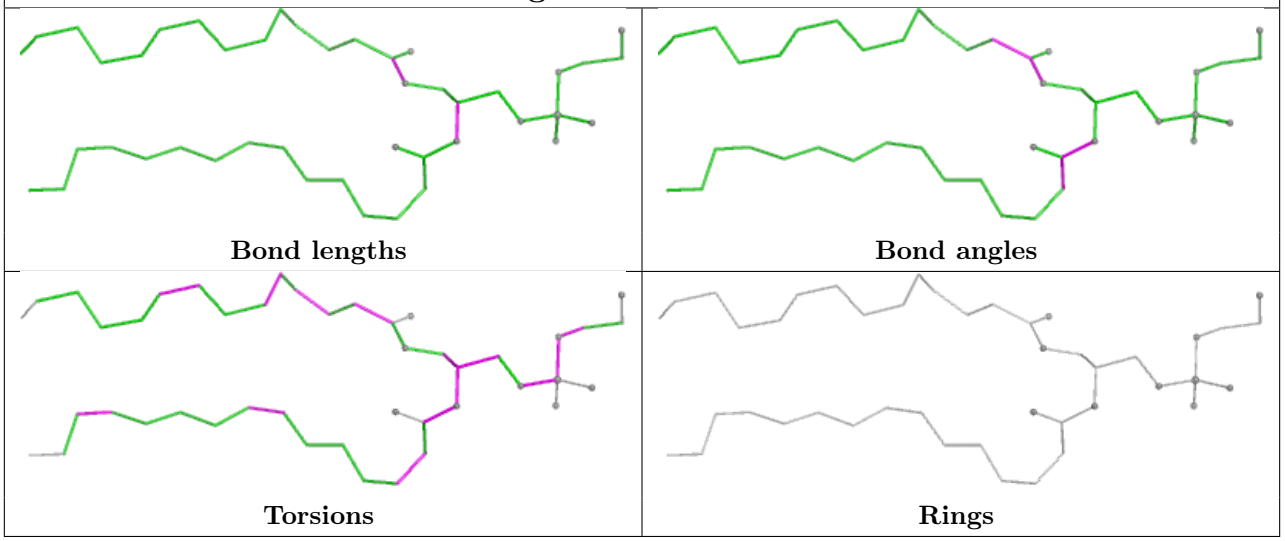


Torsions

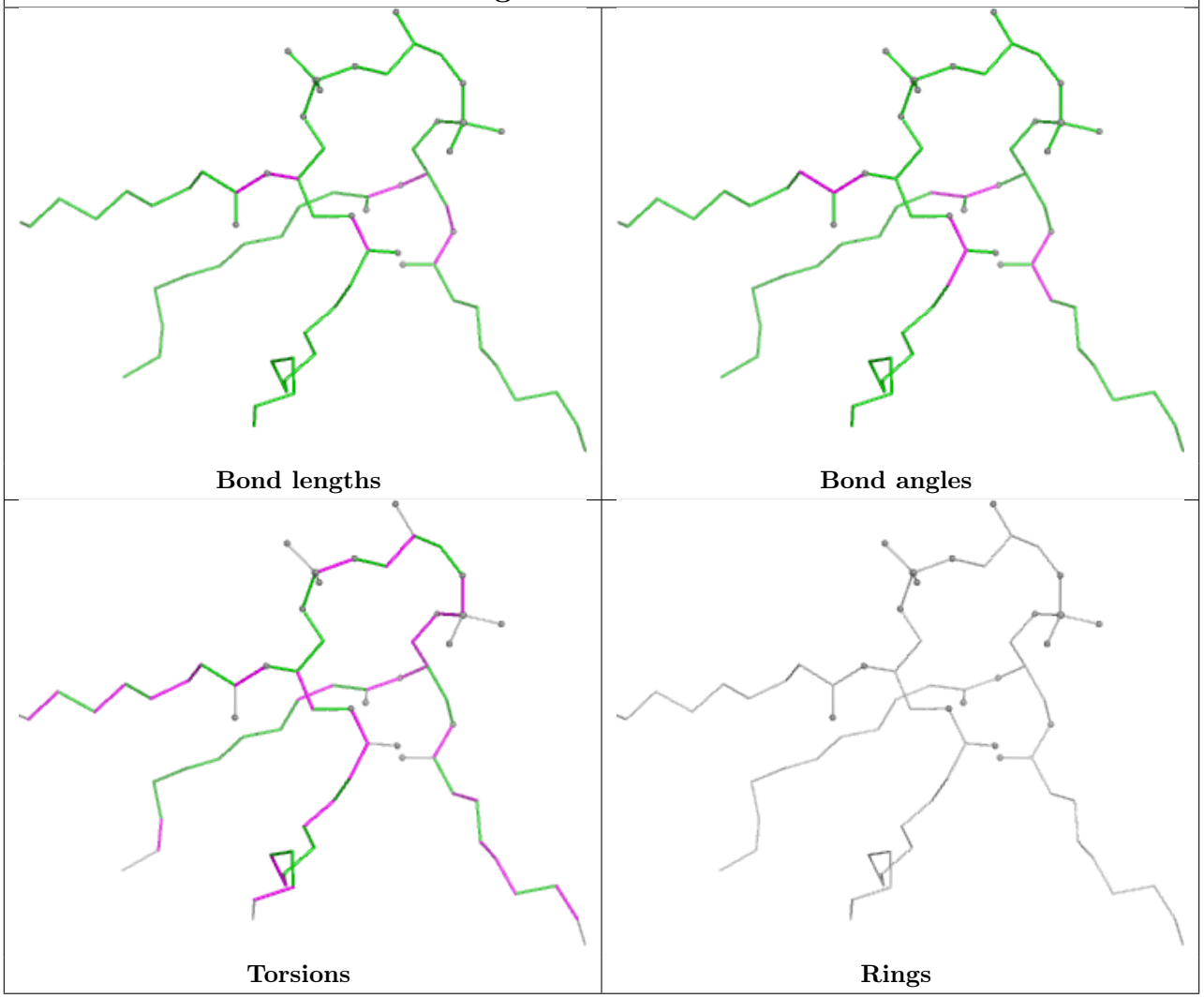


Rings

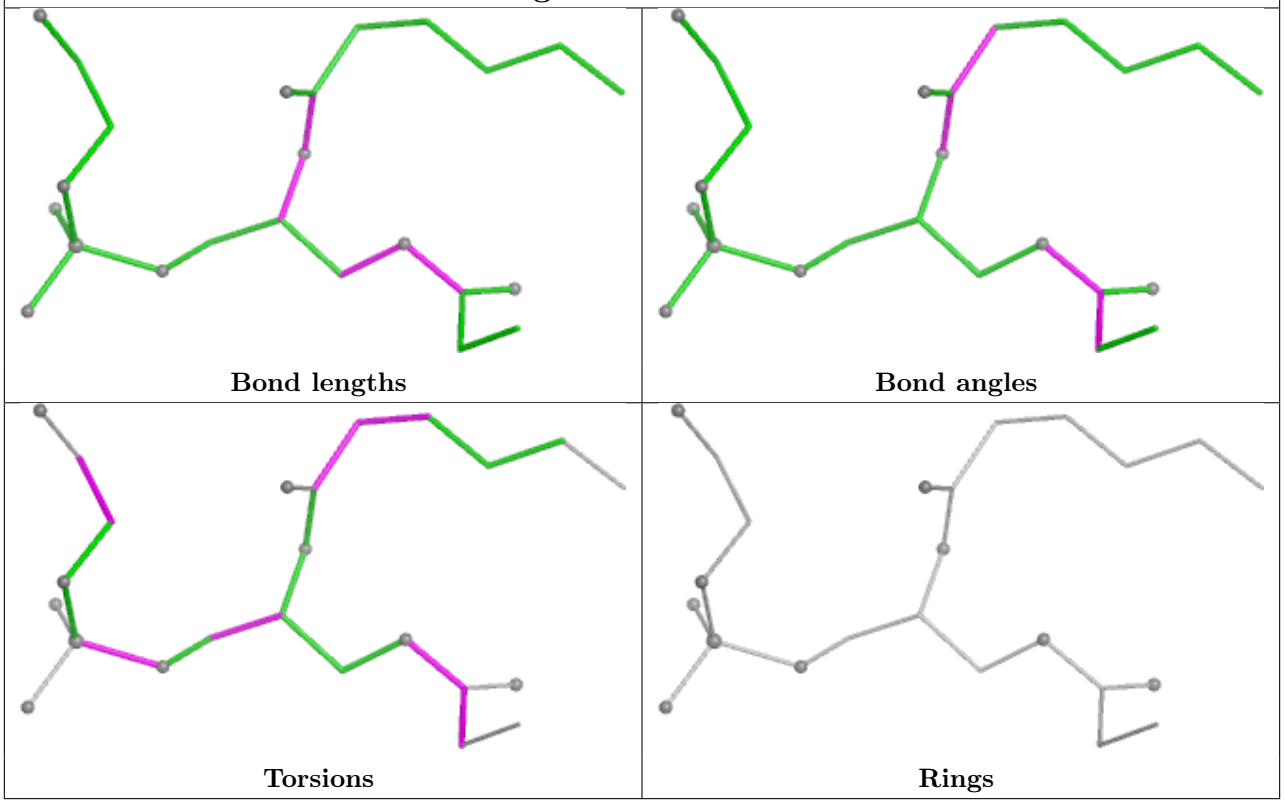
Ligand 3PE N 401



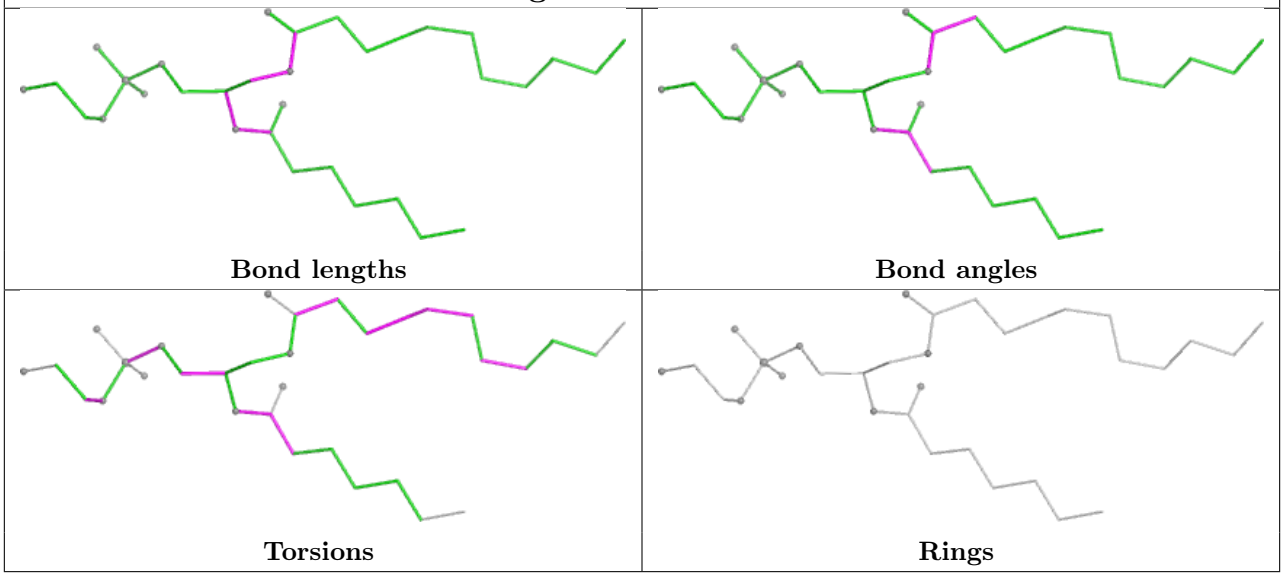
Ligand CDL h 201



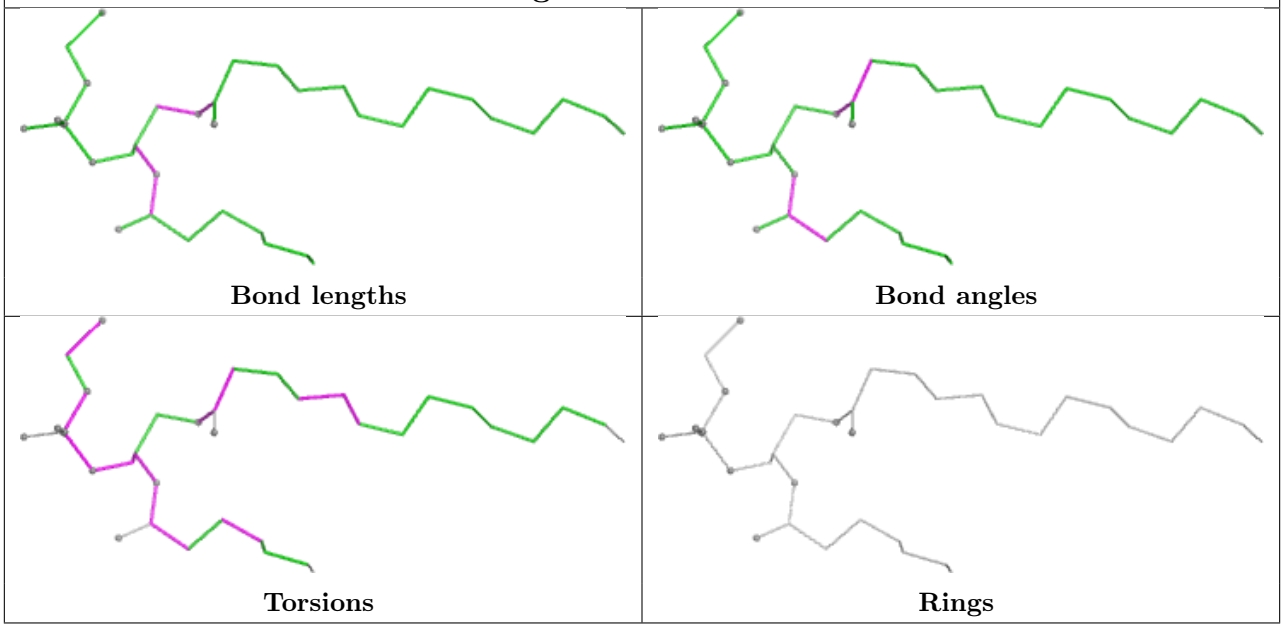
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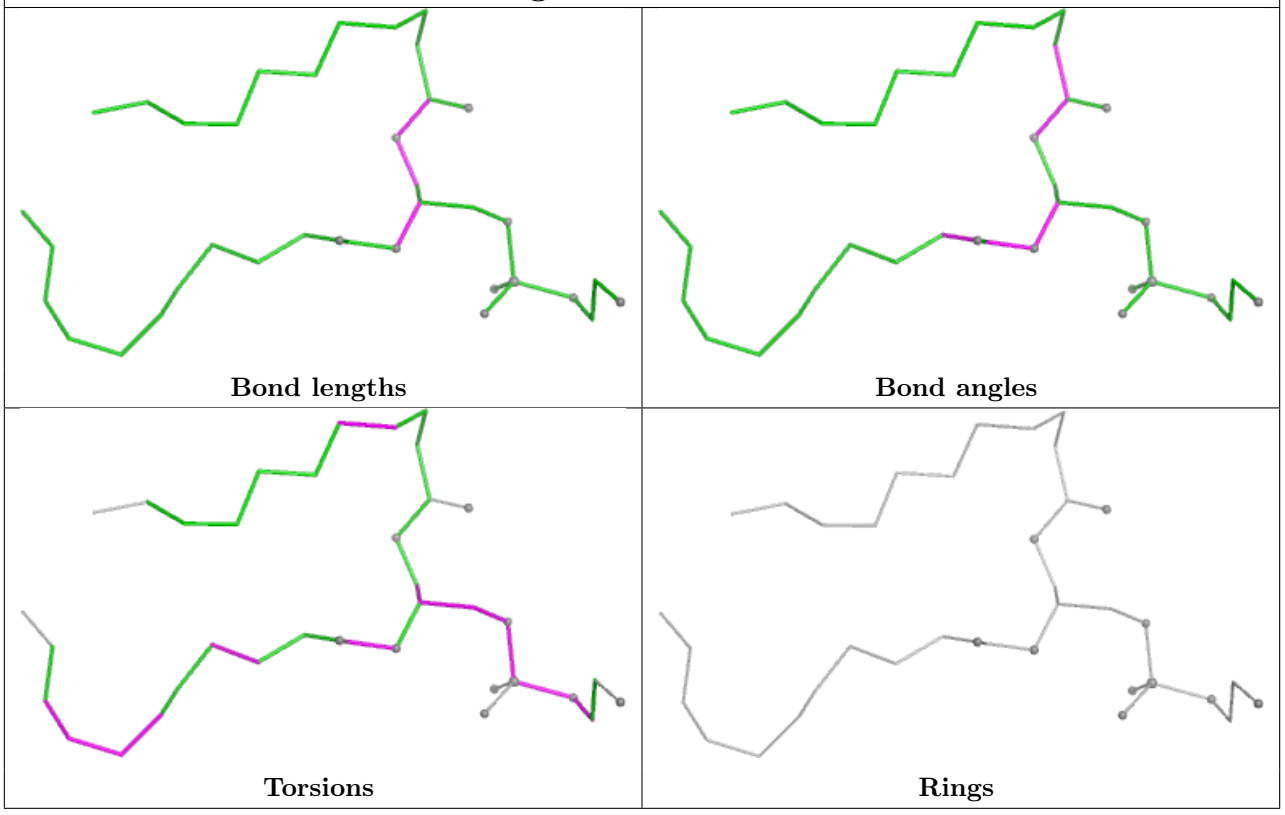
Ligand 3PE Y 303



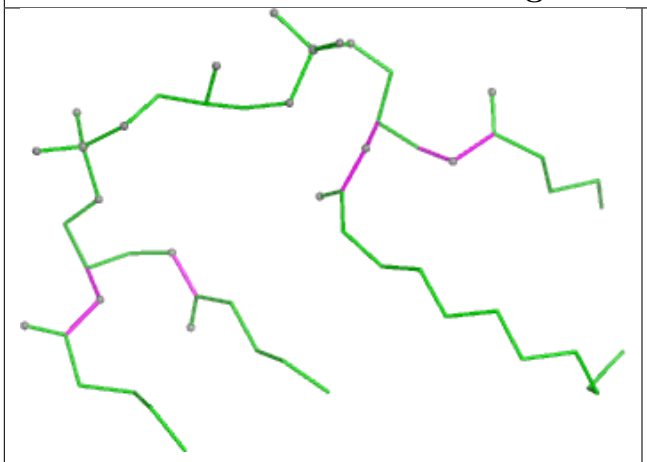
Ligand 3PE d 201



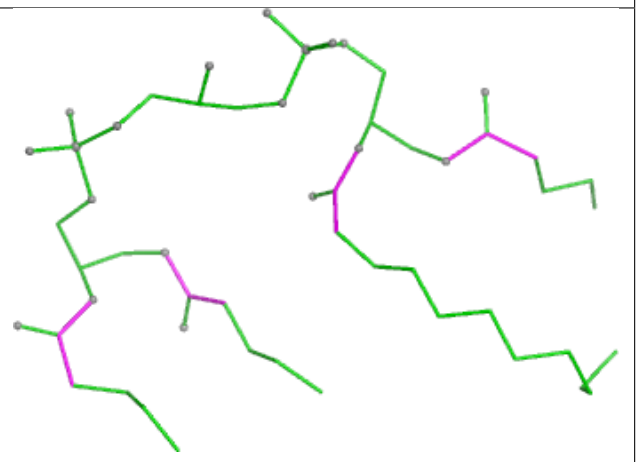
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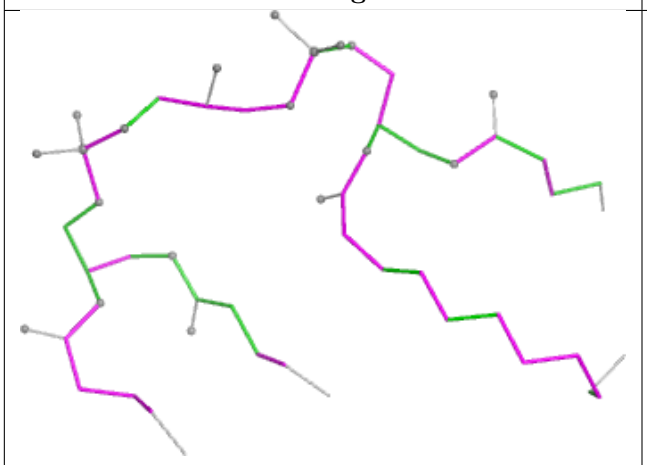
Ligand CDL P 502



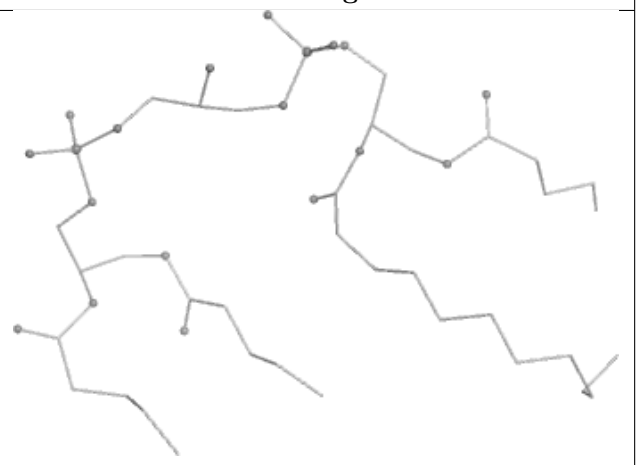
Bond lengths



Bond angles

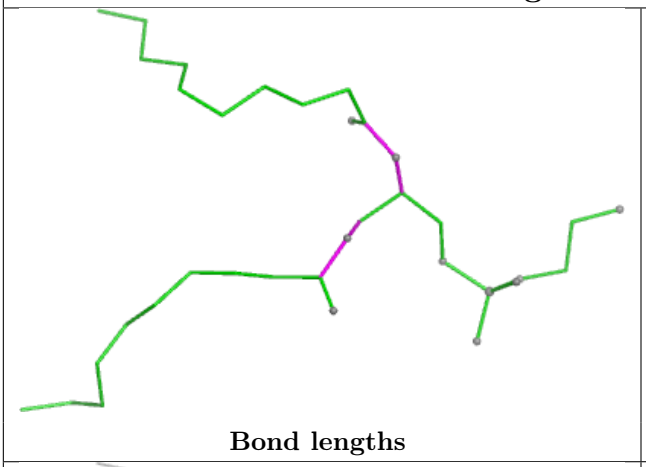


Torsions

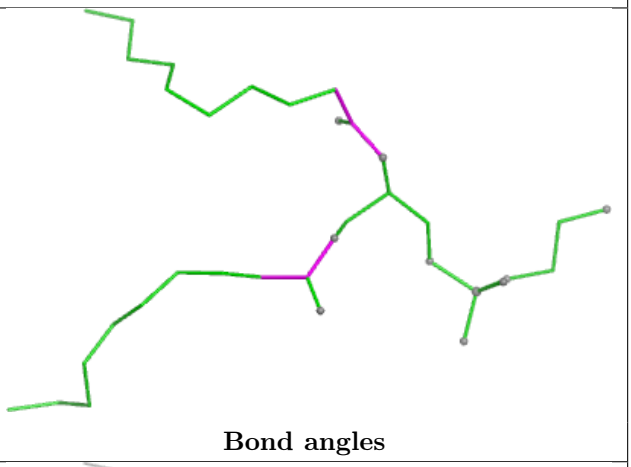


Rings

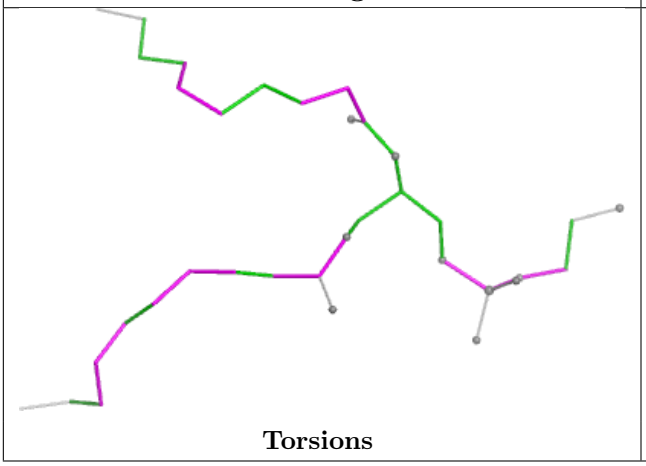
Ligand 3PE M 501



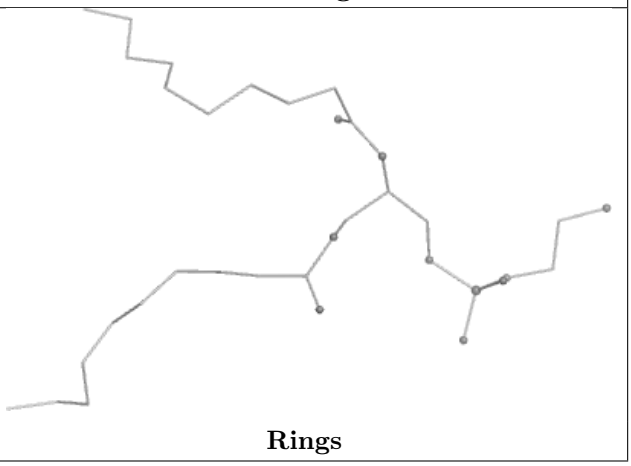
Bond lengths



Bond angles

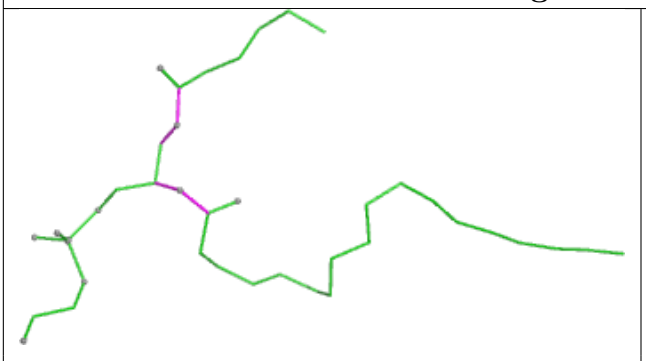


Torsions

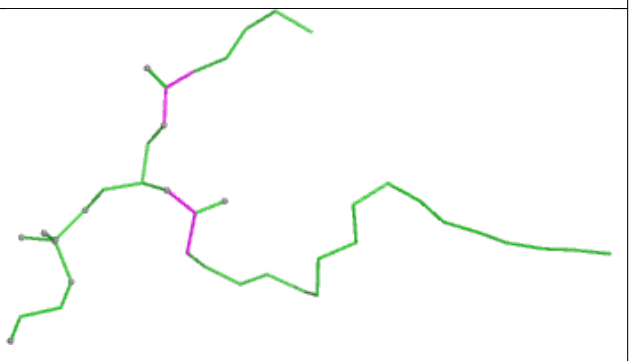


Rings

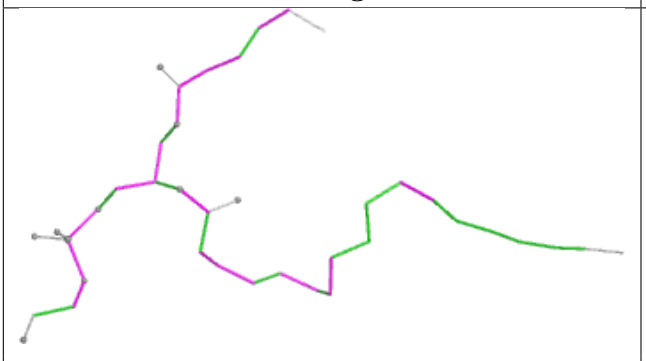
Ligand 3PE L 601



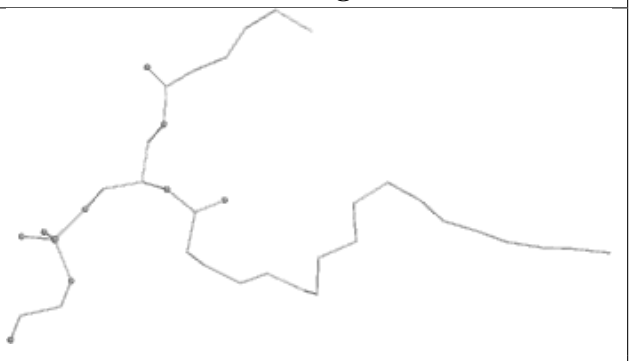
Bond lengths



Bond angles

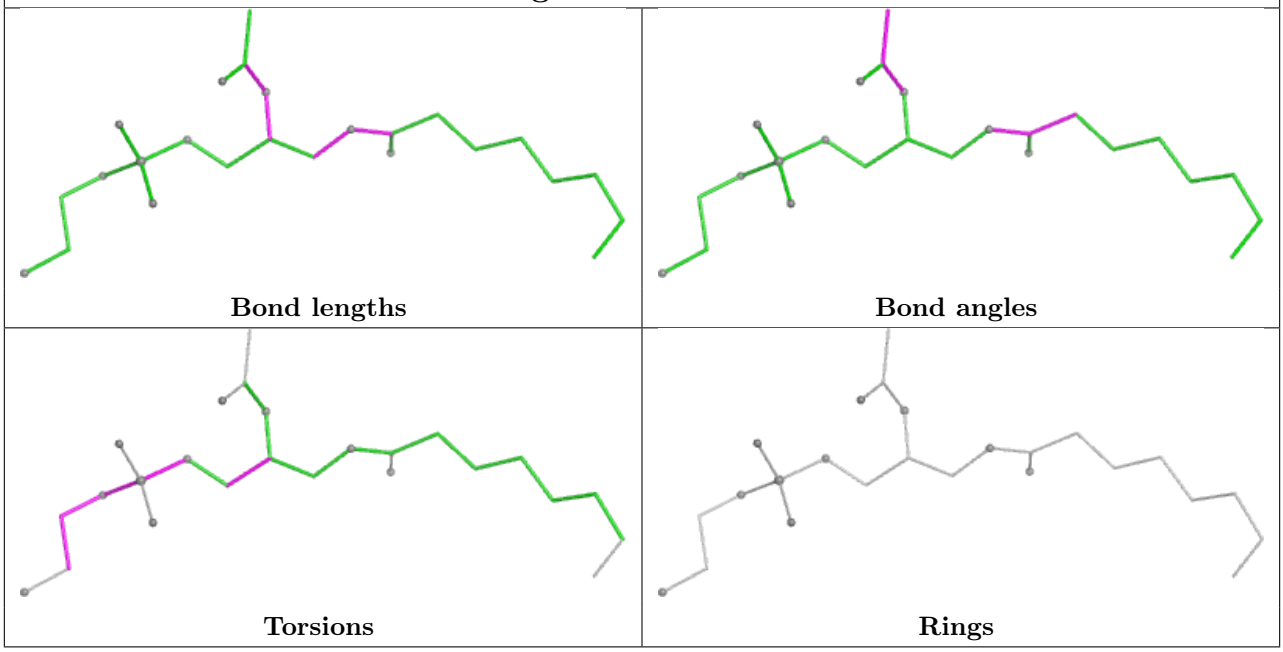


Torsions

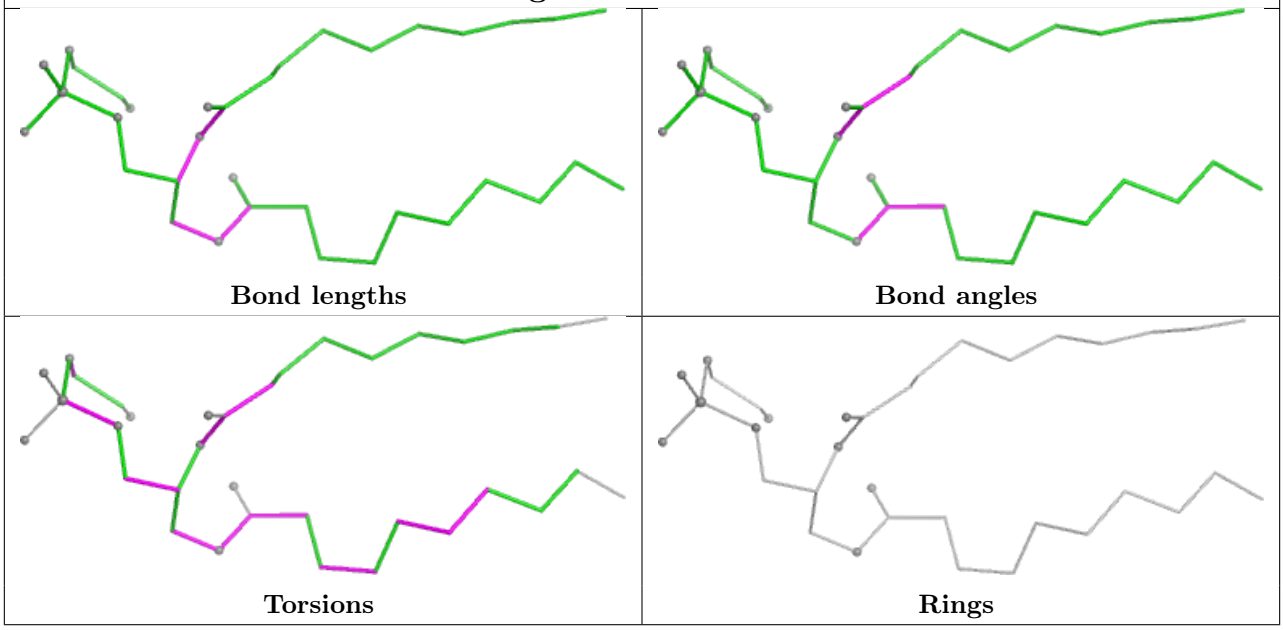


Rings

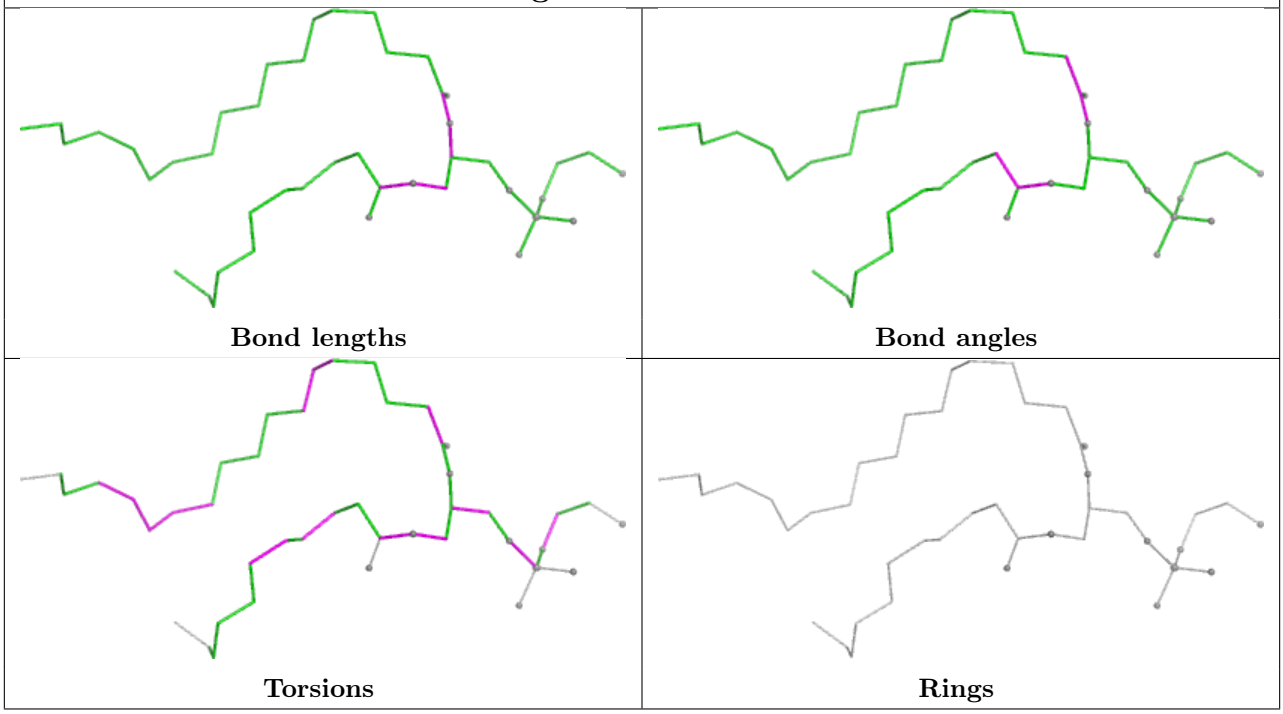
Ligand 3PE L 603



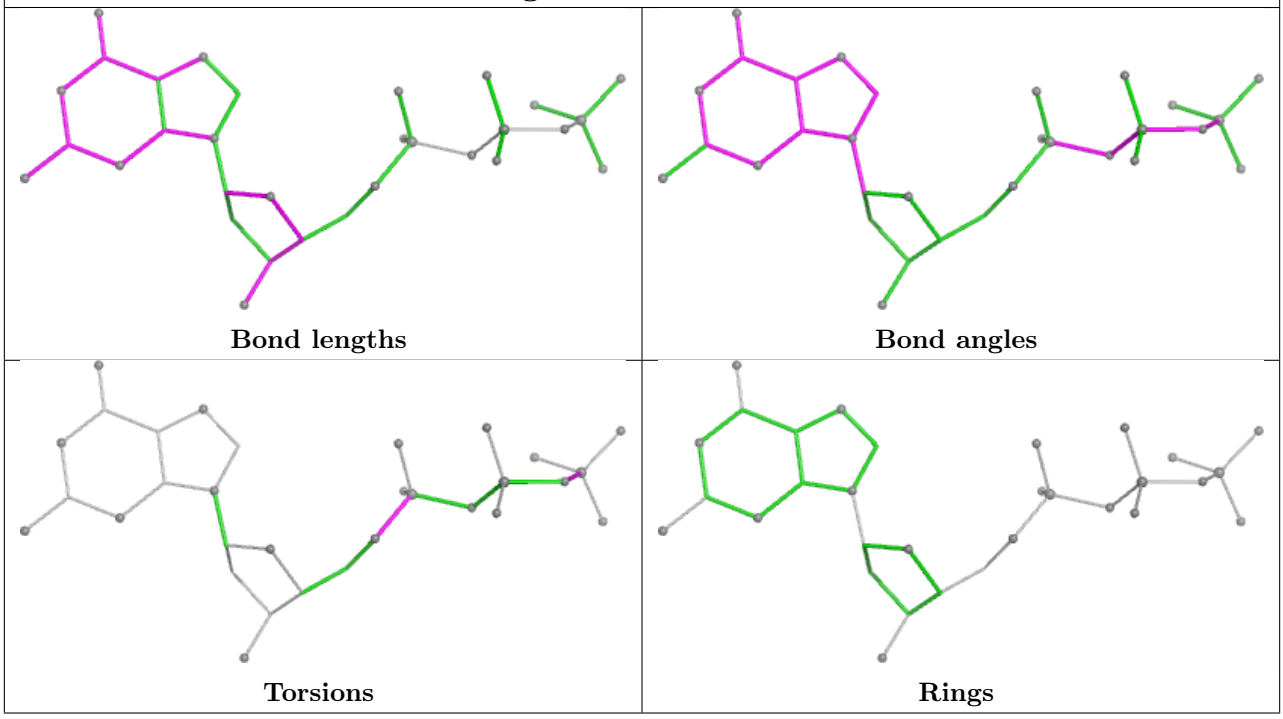
Ligand 3PE A 202



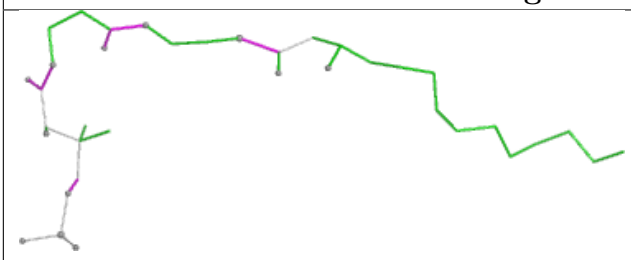
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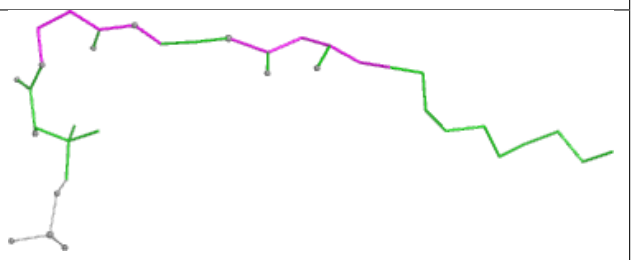
Ligand DGT O 501



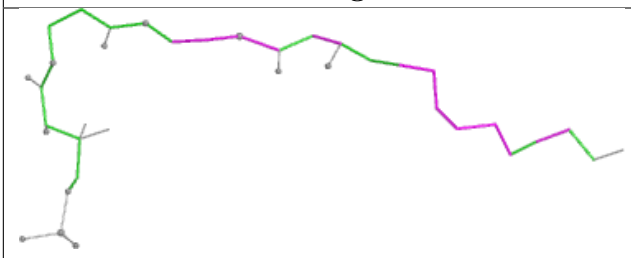
Ligand EHZ U 201



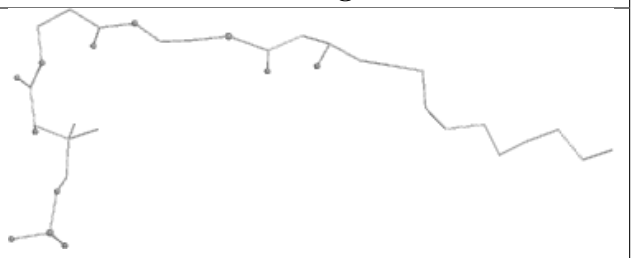
Bond lengths



Bond angles

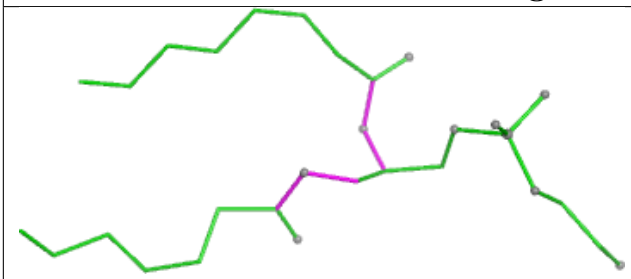


Torsions

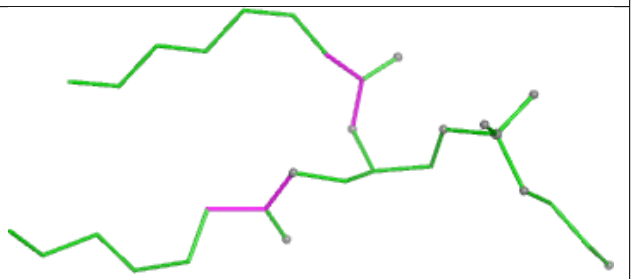


Rings

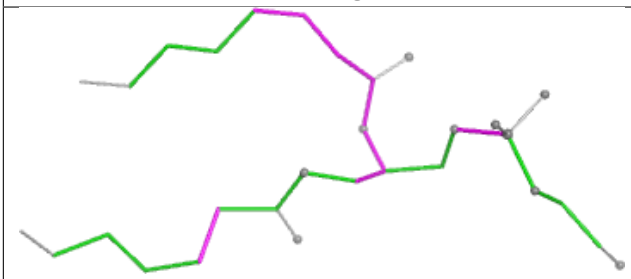
Ligand 3PE Y 302



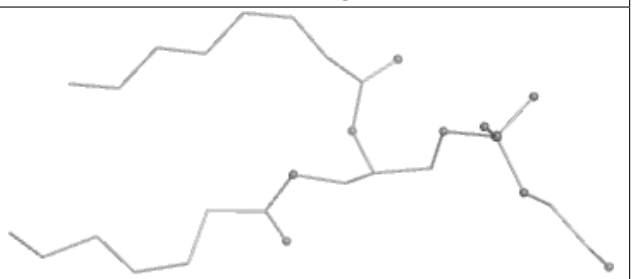
Bond lengths



Bond angles

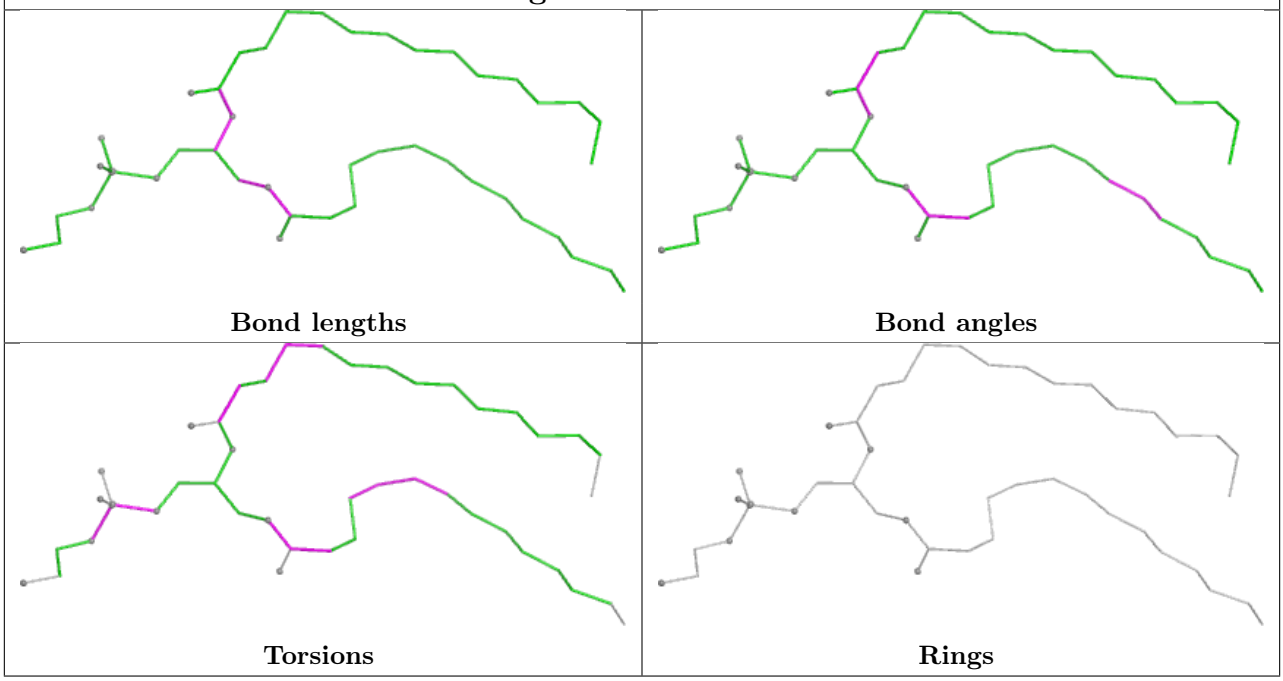


Torsions

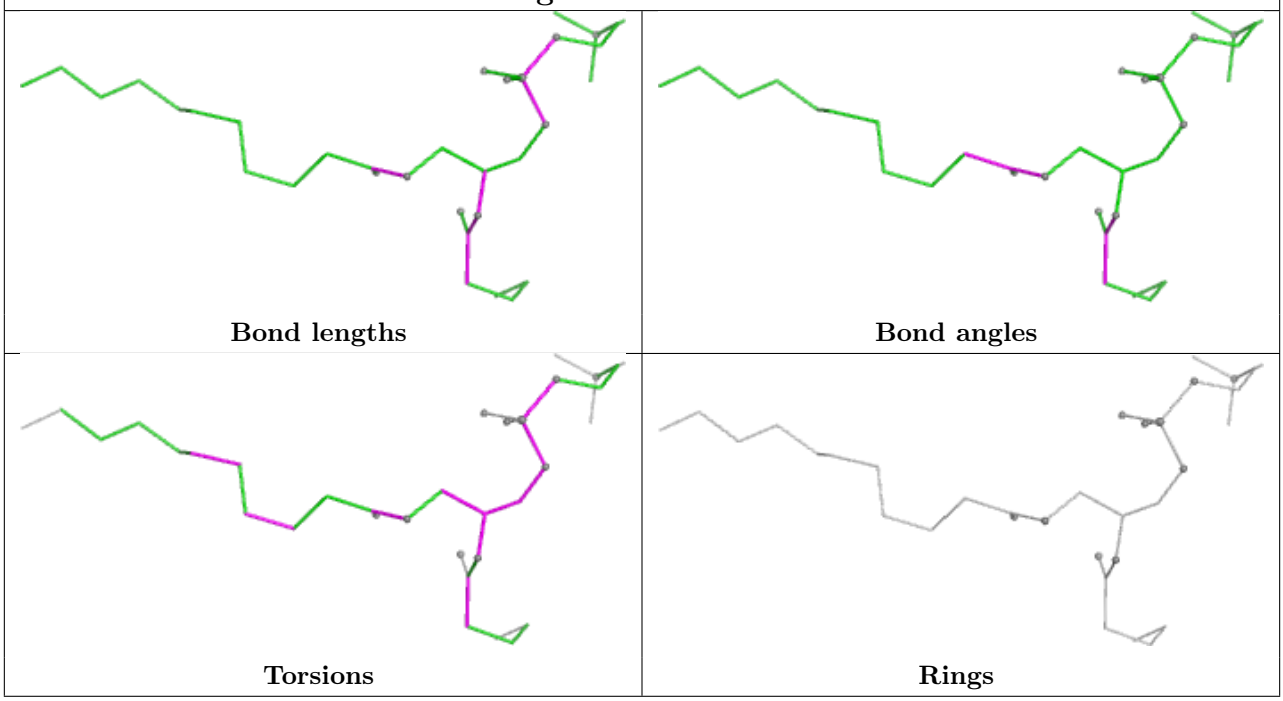


Rings

Ligand 3PE A 203



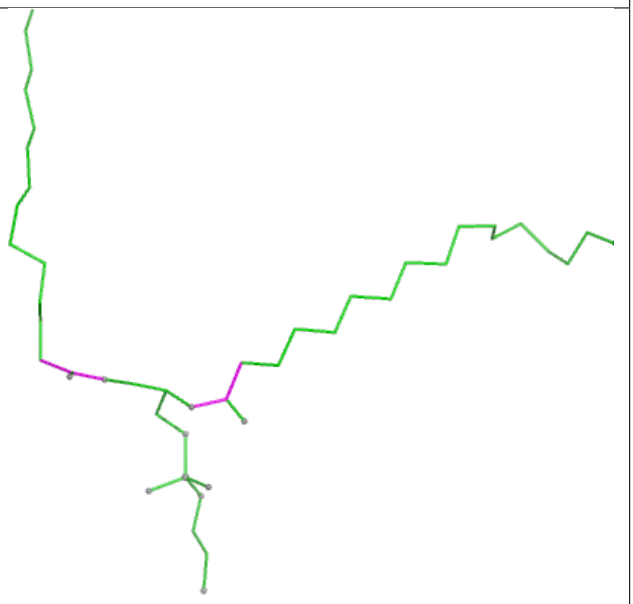
Ligand PC1 i 201



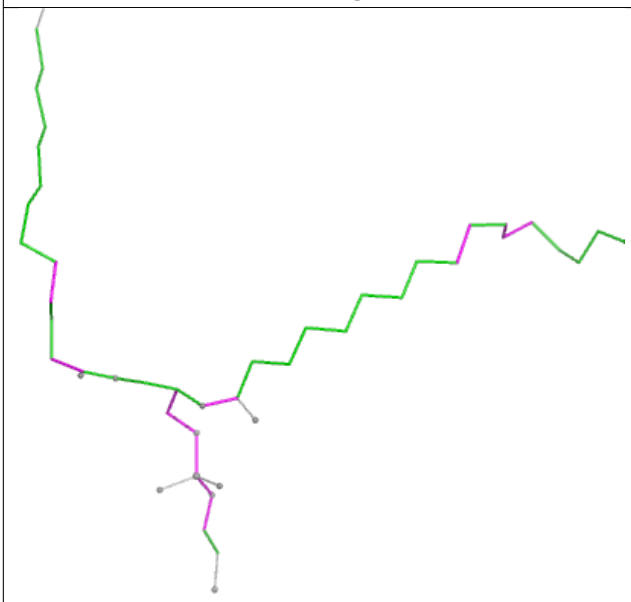
Ligand 3PE H 502



Bond lengths



Bond angles

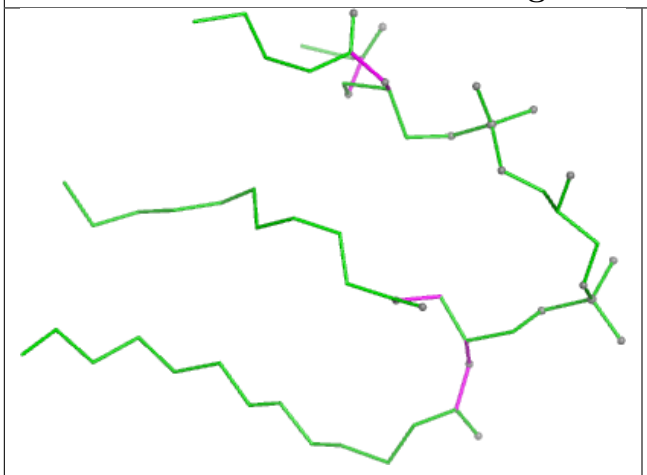


Torsions

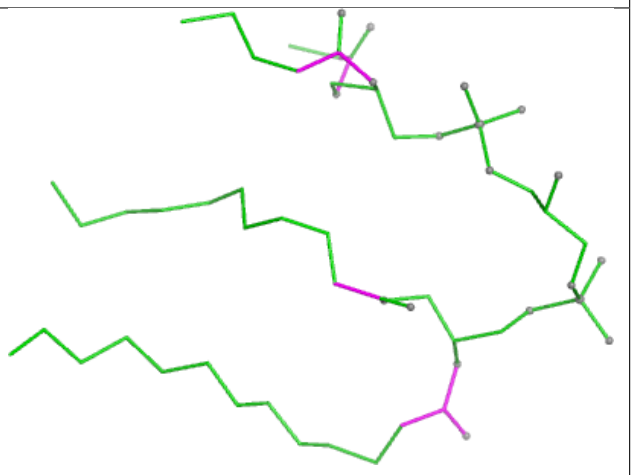


Rings

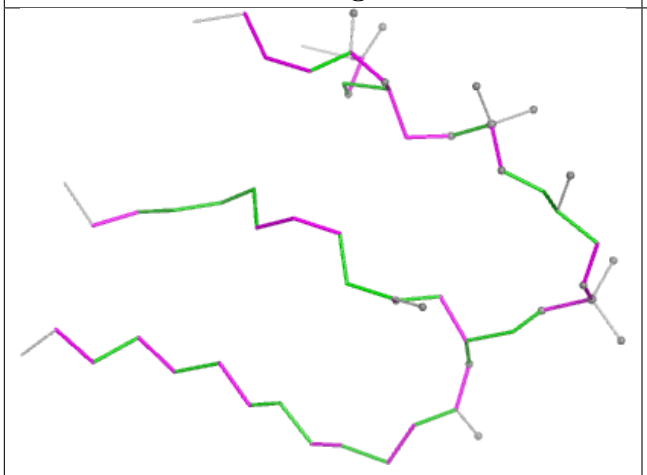
Ligand CDL h 202



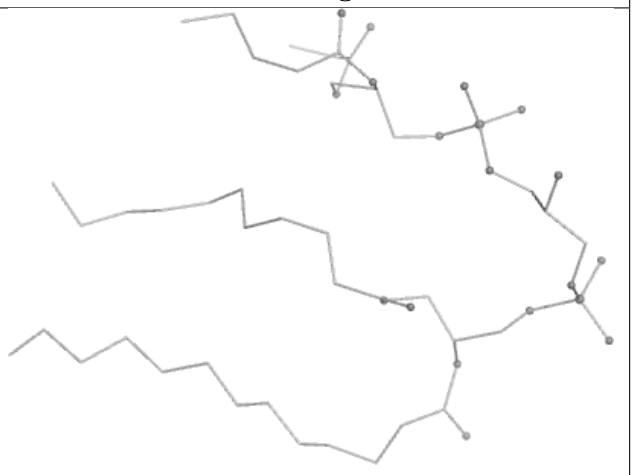
Bond lengths



Bond angles

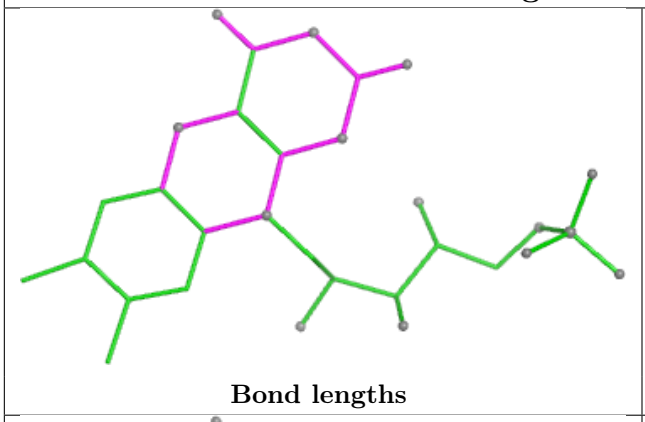


Torsions

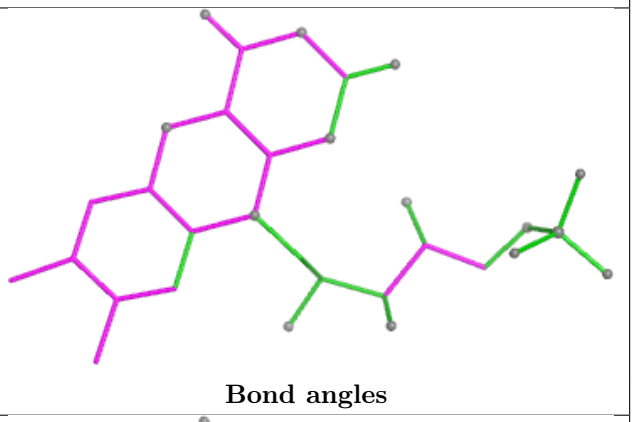


Rings

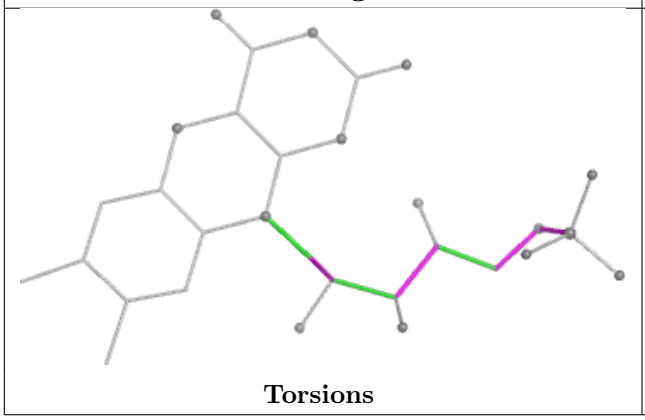
Ligand FMN F 501



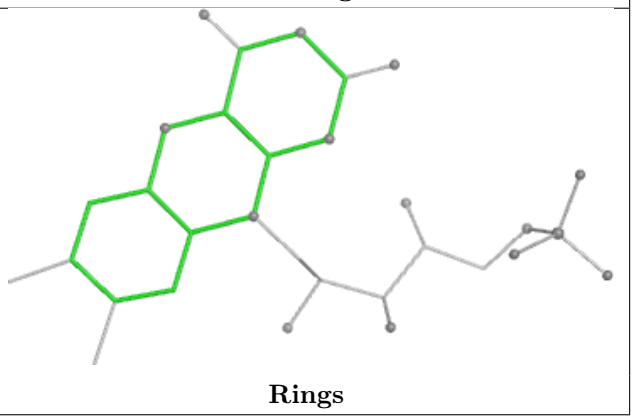
Bond lengths



Bond angles

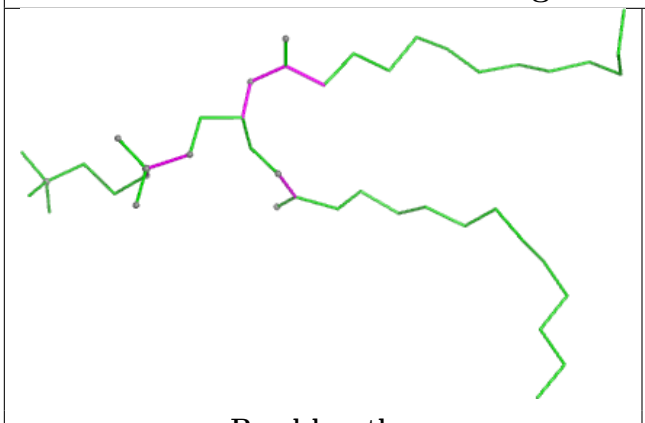


Torsions

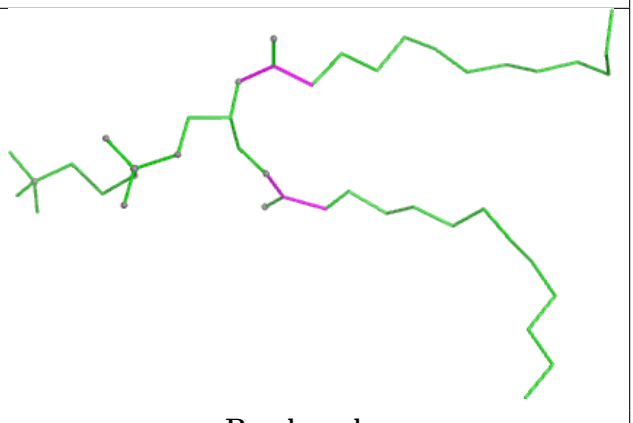


Rings

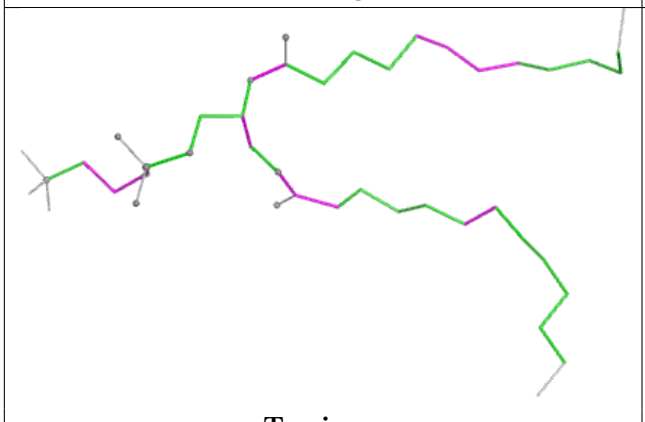
Ligand PC1 J 201



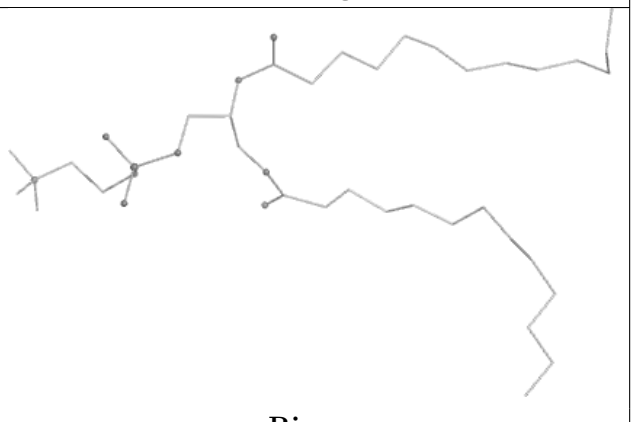
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

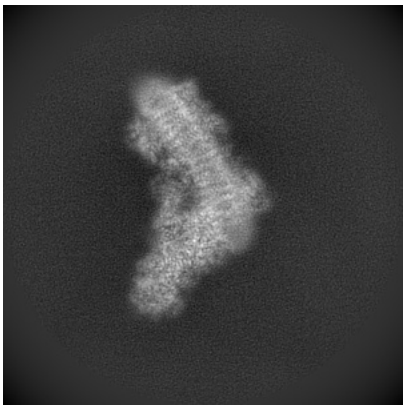
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15936. These allow visual inspection of the internal detail of the map and identification of artifacts.

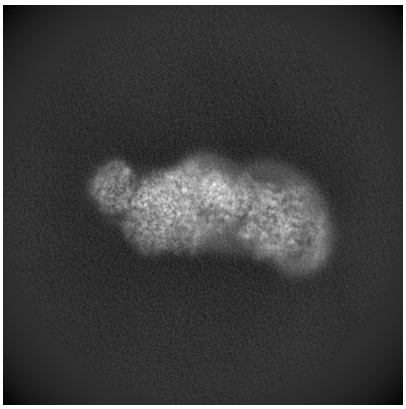
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

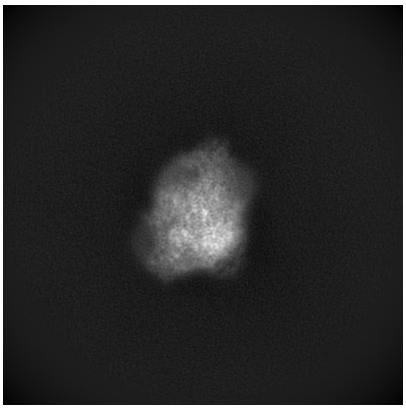
6.1.1 Primary map



X

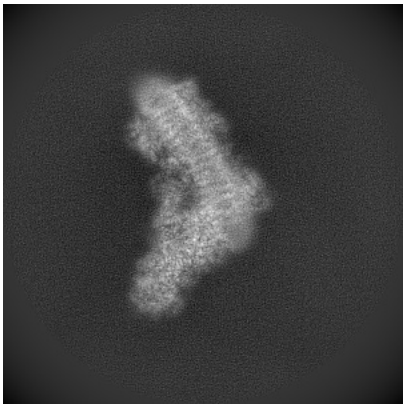


Y

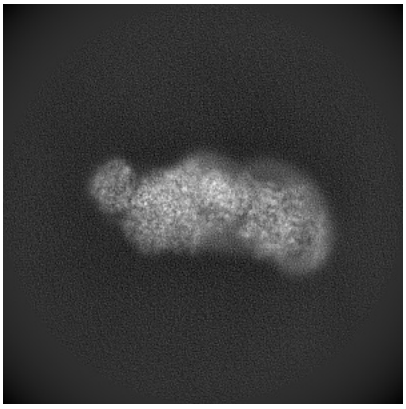


Z

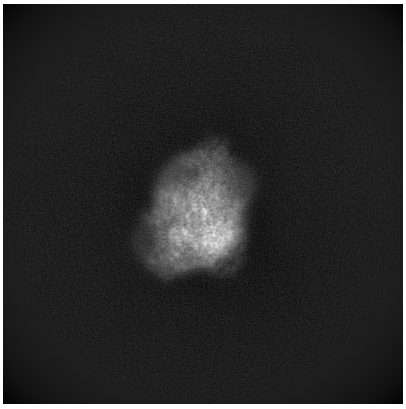
6.1.2 Raw map



X



Y

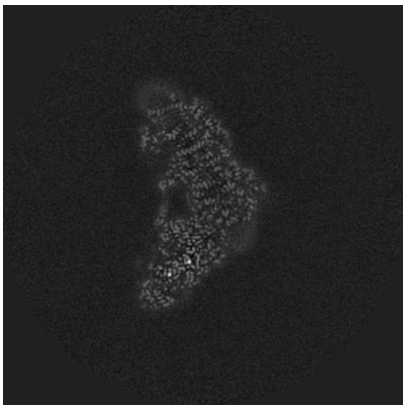


Z

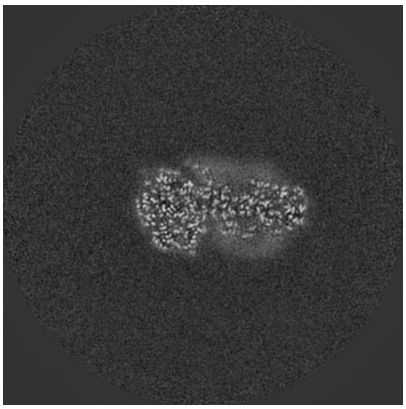
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

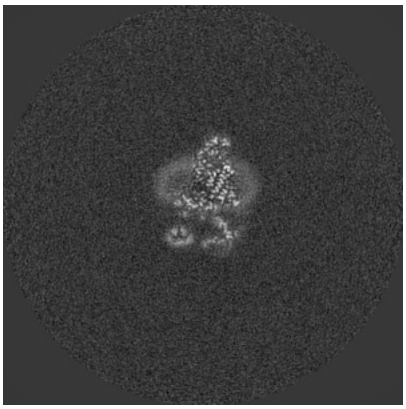
6.2.1 Primary map



X Index: 225

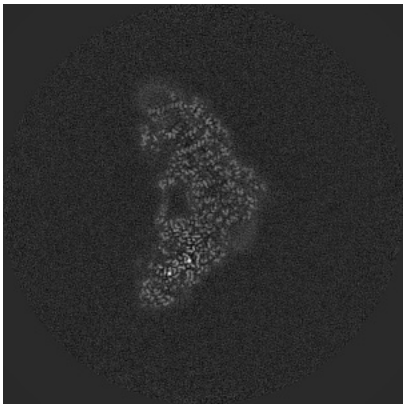


Y Index: 225

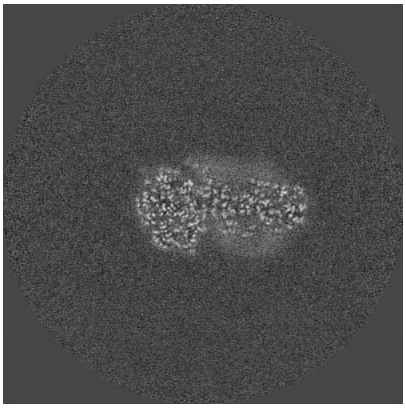


Z Index: 225

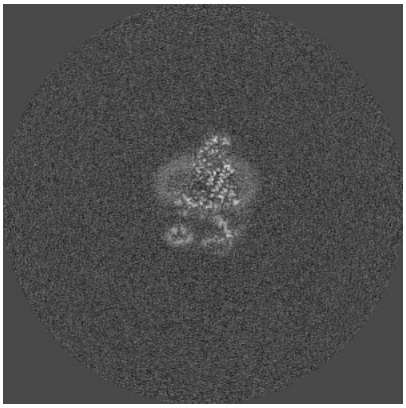
6.2.2 Raw map



X Index: 225



Y Index: 225

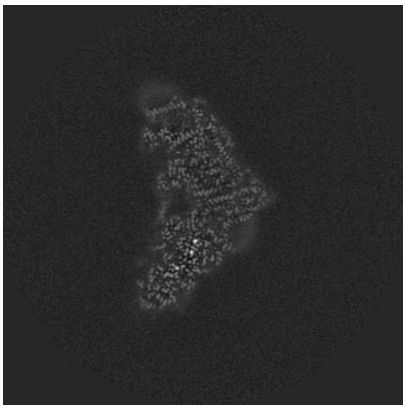


Z Index: 225

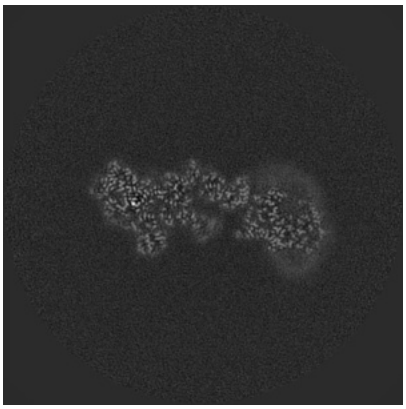
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

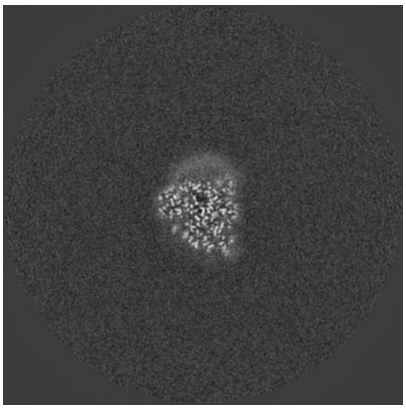
6.3.1 Primary map



X Index: 228

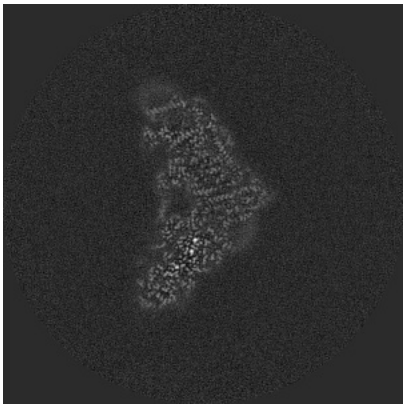


Y Index: 188

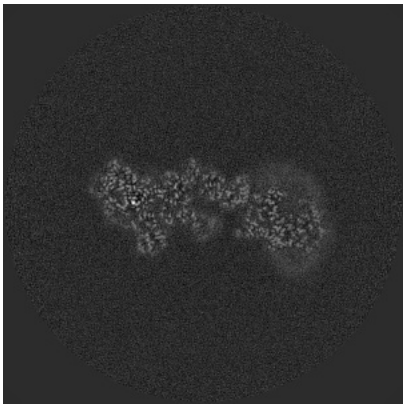


Z Index: 188

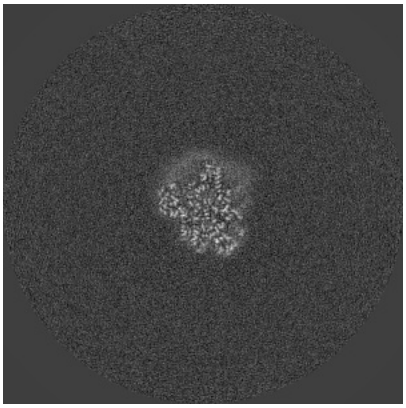
6.3.2 Raw map



X Index: 228



Y Index: 188

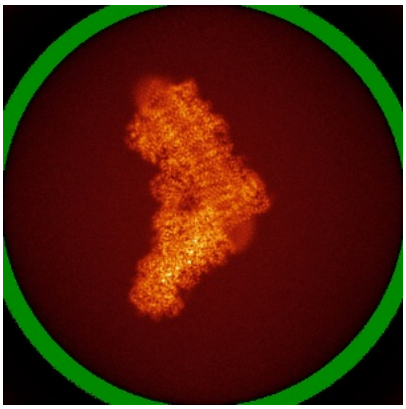


Z Index: 206

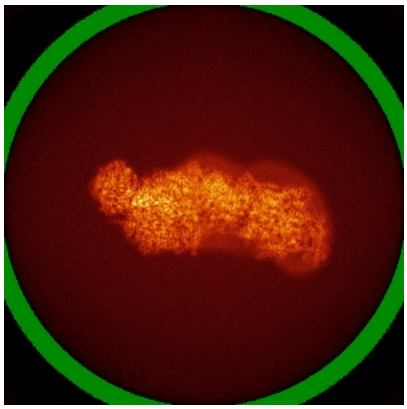
The images above show the largest variance slices of the map in three orthogonal directions.

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

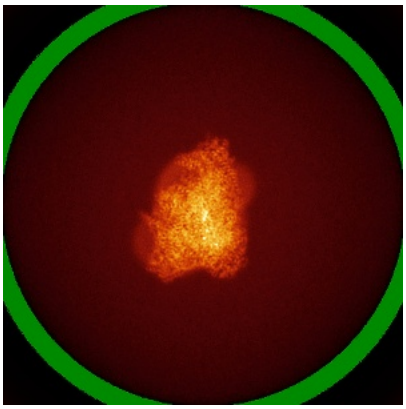
6.4.1 Primary map



X

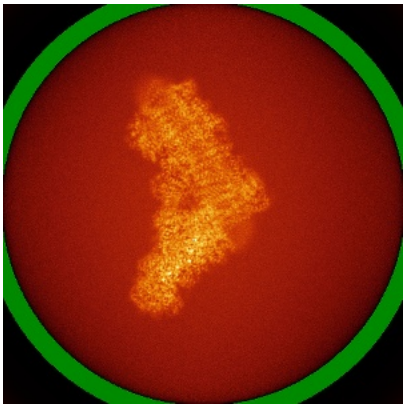


Y

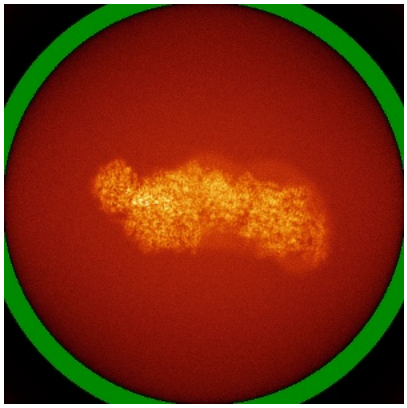


Z

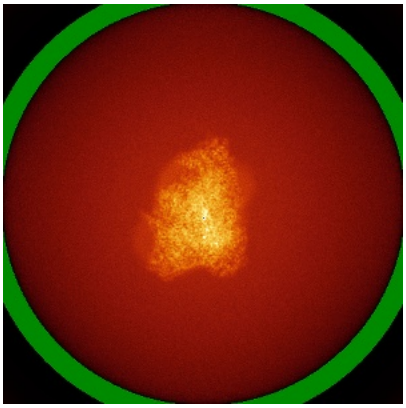
6.4.2 Raw map



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

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

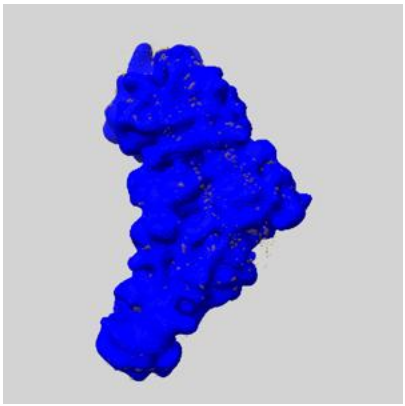
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

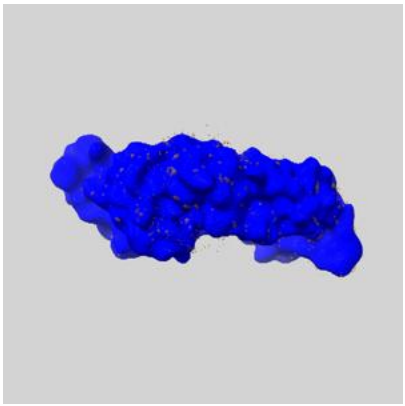
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

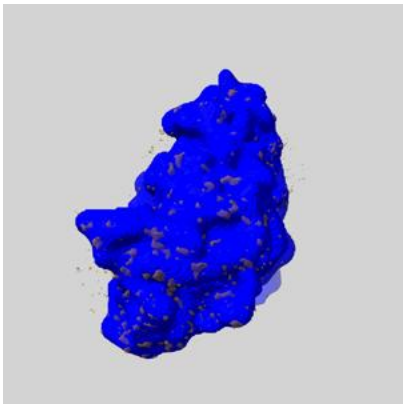
6.6.1 emd_15936_msk_1.map (i)



X



Y

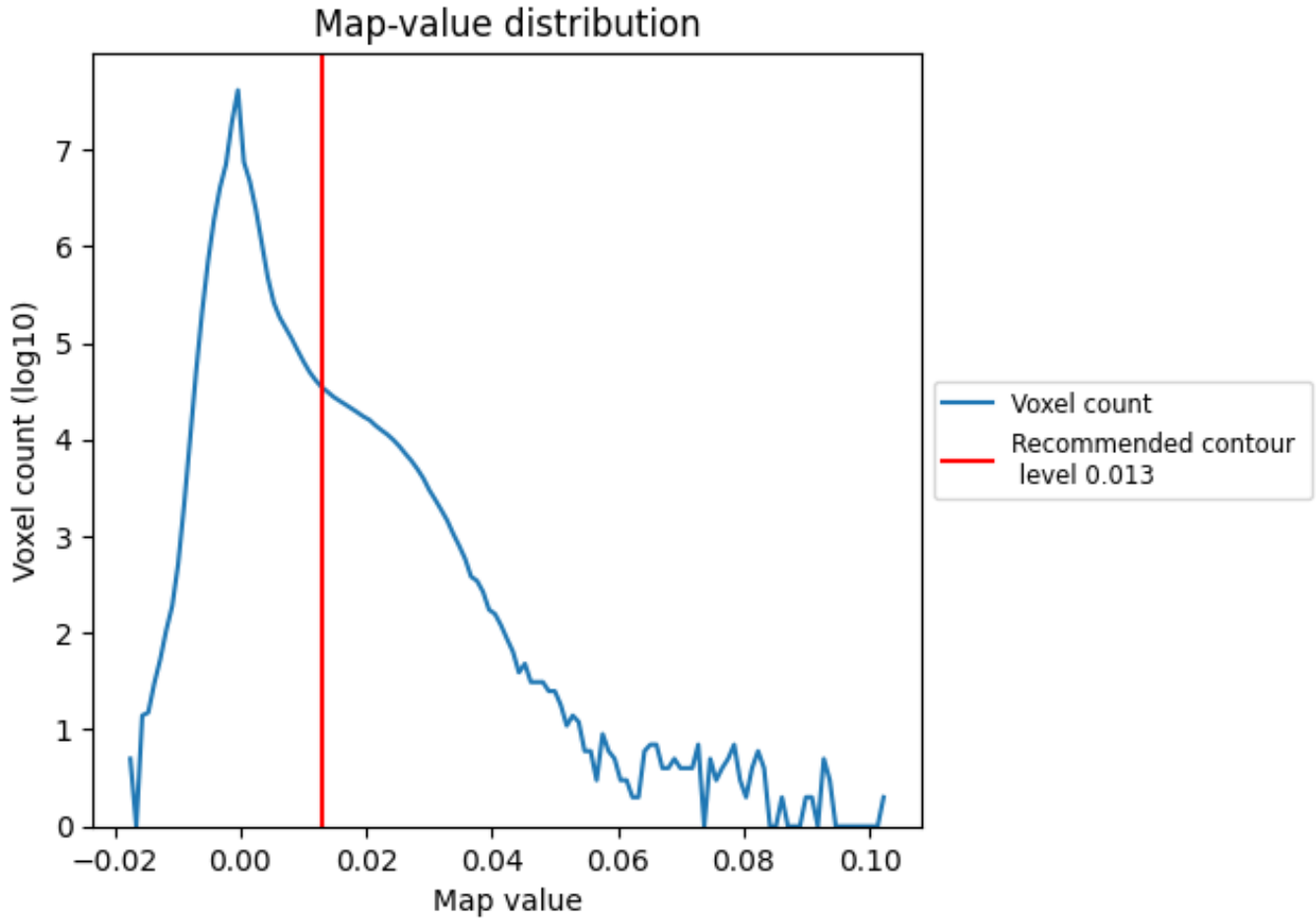


Z

7 Map analysis

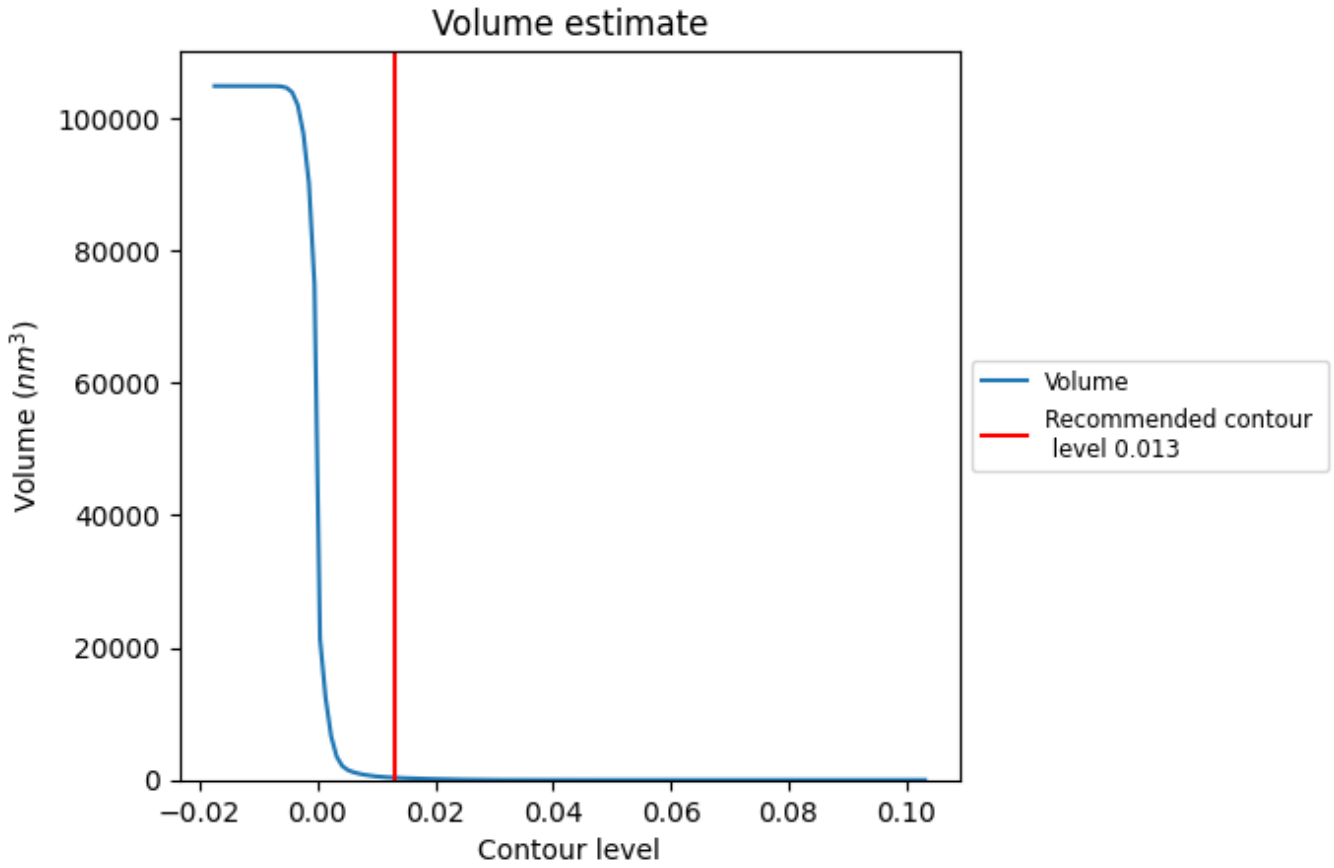
This section contains the results of statistical analysis of the map.

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.

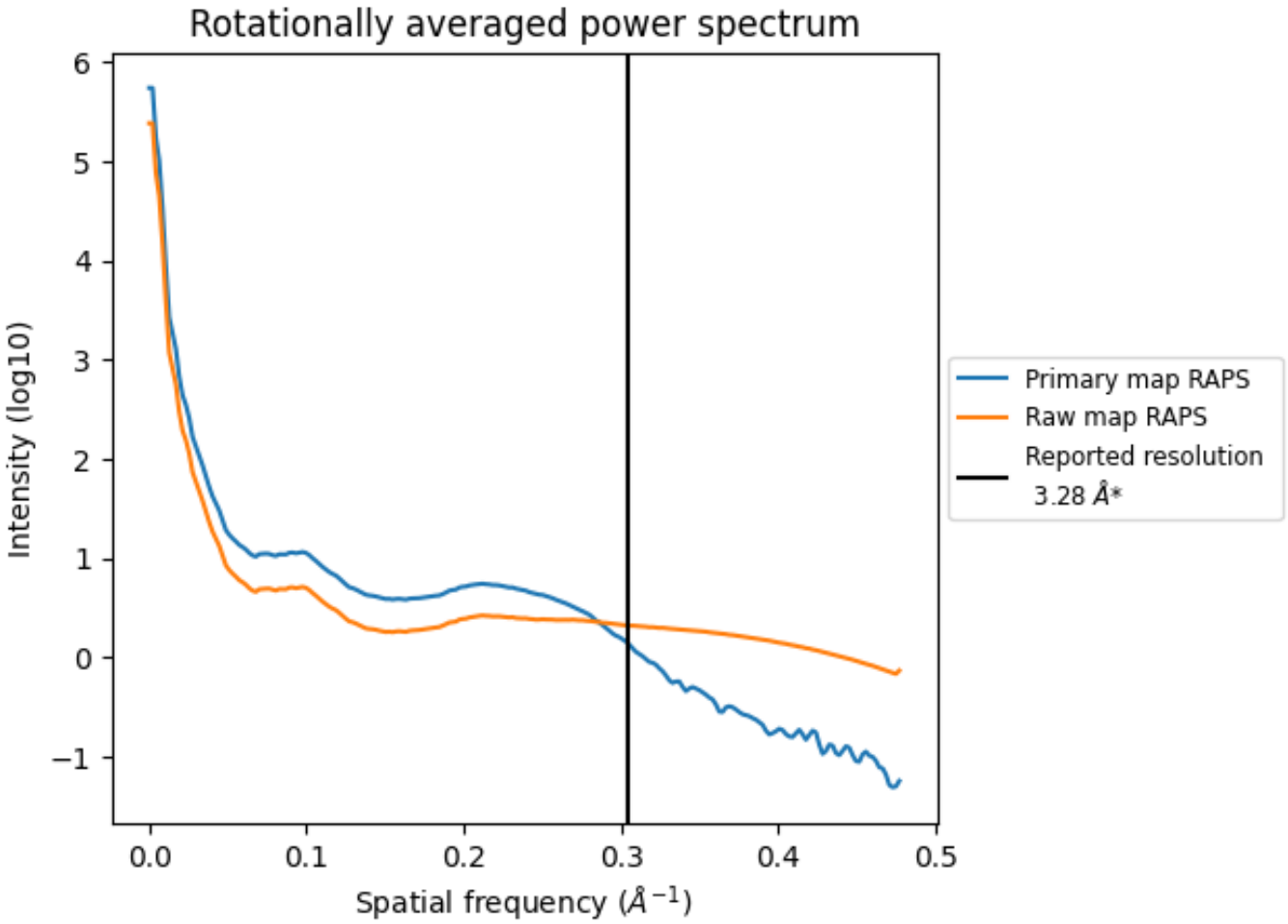
7.2 Volume estimate



The volume at the recommended contour level is 349 nm^3; this corresponds to an approximate mass of 315 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)

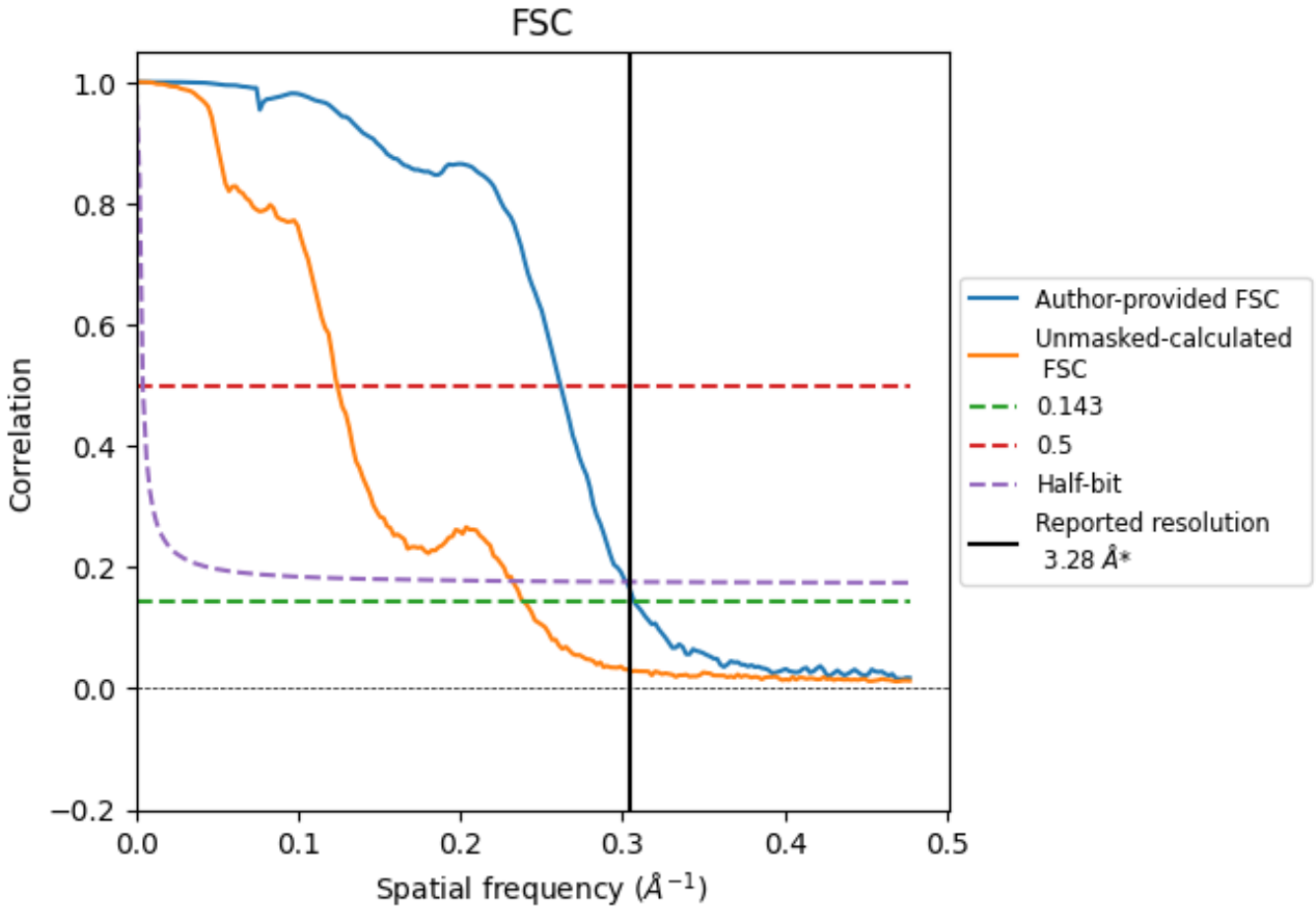


*Reported resolution corresponds to spatial frequency of 0.305 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.305 Å^{-1}

8.2 Resolution estimates (i)

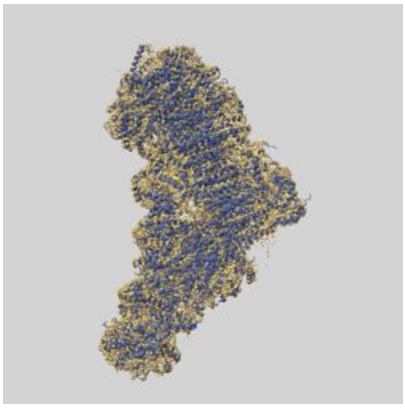
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	3.26	3.82	3.31
Unmasked-calculated*	4.18	8.06	4.30

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.18 differs from the reported value 3.28 by more than 10 %

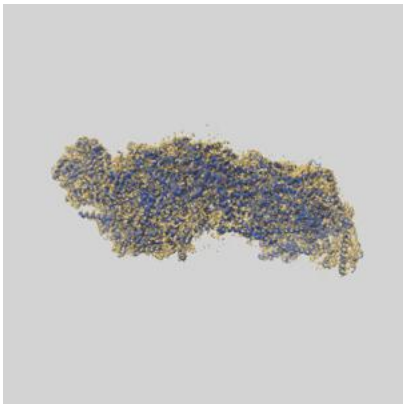
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15936 and PDB model 8B9Z. Per-residue inclusion information can be found in section 3 on page 20.

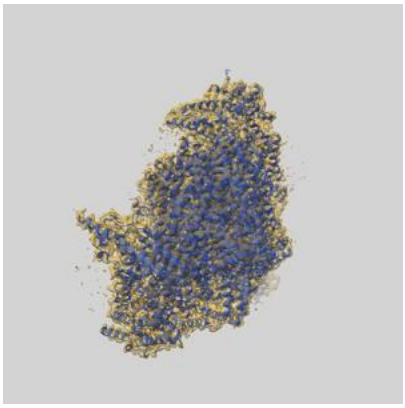
9.1 Map-model overlay



X



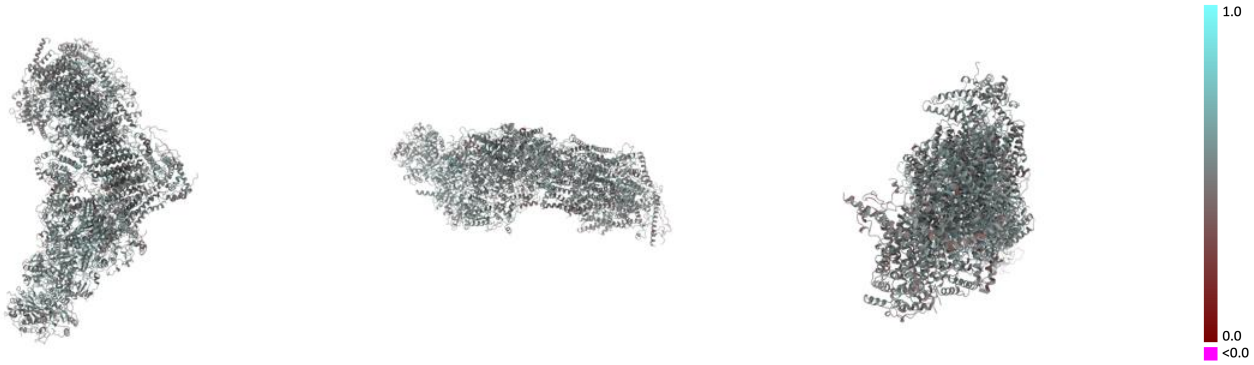
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013 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.

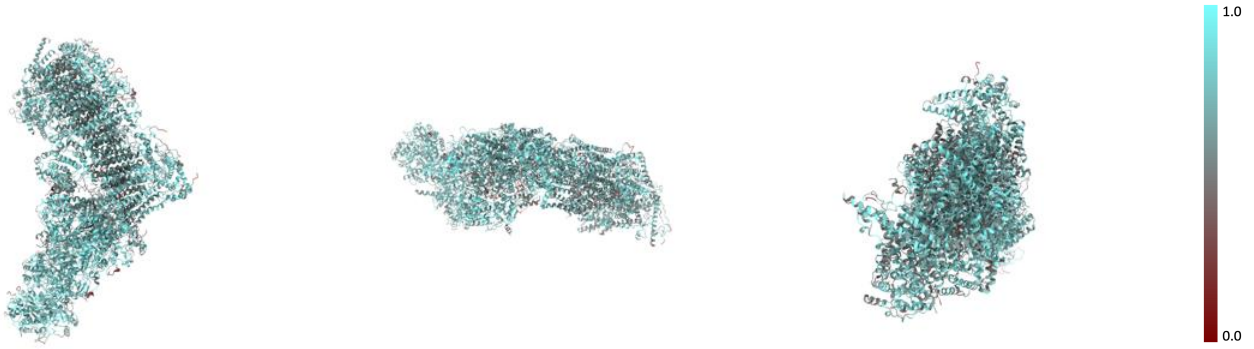
9.2 Q-score mapped to coordinate model (i)



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.

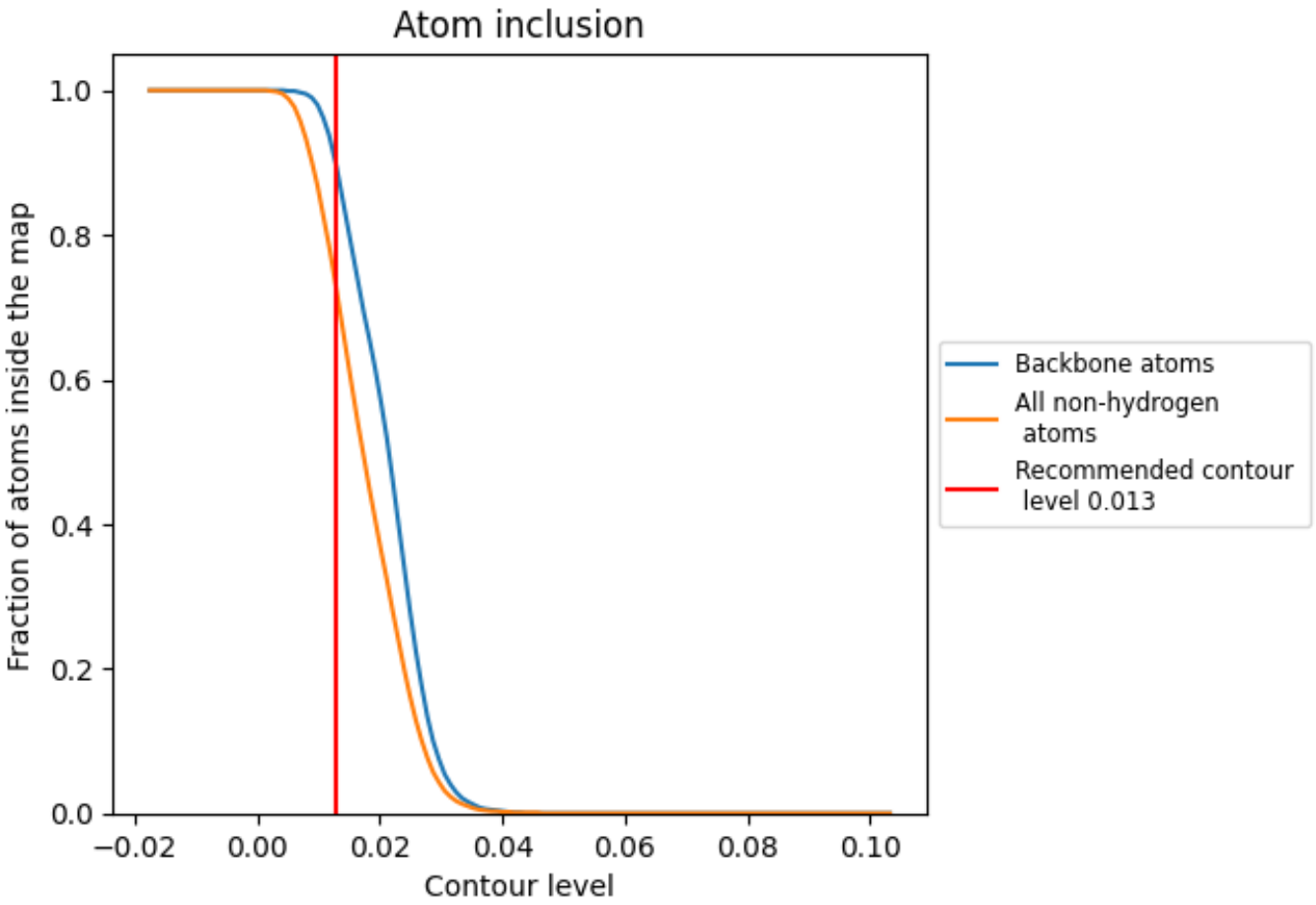
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.013).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 72% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7210	0.5150
A	0.6370	0.5070
B	0.7580	0.5360
C	0.7910	0.5430
D	0.7580	0.5340
E	0.7410	0.5090
F	0.7750	0.5210
G	0.7620	0.5290
H	0.6990	0.5190
I	0.8060	0.5410
J	0.6320	0.5060
K	0.6500	0.5100
L	0.6770	0.5060
M	0.7080	0.5290
N	0.6920	0.5220
O	0.7460	0.5180
P	0.7660	0.5250
Q	0.7360	0.5250
R	0.8060	0.5420
T	0.4810	0.4040
U	0.5990	0.4740
V	0.7170	0.5110
W	0.7360	0.5150
X	0.7160	0.5070
Y	0.6030	0.4900
Z	0.7700	0.5180
a	0.7060	0.5020
b	0.7210	0.4920
d	0.7070	0.5110
e	0.7370	0.5140
f	0.6240	0.4940
g	0.6810	0.5110
h	0.7140	0.5220
i	0.7060	0.4950
j	0.6630	0.4720



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Chain	Atom inclusion	Q-score
k	0.6540	0.4750
l	0.7290	0.5140
m	0.7390	0.5050
n	0.7270	0.5010
o	0.6990	0.4750
p	0.7620	0.5100
q	0.7580	0.5210
r	0.7170	0.5220
s	0.6090	0.4830